EuropaCat XII

SCIENTIFIC PROGRAM

KAZAN, RUSSIA
30 AUGUST – 4 SEPTEMBER, 2015

EUROPACAT XII

CATALYSIS: BALANCING THE USE OF FOSSIL AND RENEWABLE RESOURCES

EUROPACAT XII

ORGANIZERS

Российская Академия Наук

Russian Academy of Sciences

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Tatarstan Regional Government

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of Organic Chemistry RAS

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Mendeleev Chemical Society
of Republic of Tatarstan

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XII European Congress on Catalysis “Catalysis: Balancing the use of fossil and renewable resources”

Kazan, Russia
30th August - 4th September, 2015

SCIENTIFIC PROGRAM

SHORT ABSTRACTS

Novosibirsk - 2015

Welcome to EuropaCat-XII!

Dear Colleagues,
On behalf of the International Scientific and Local Committees I congratulate you as participants in the XII European Congress on Catalysis ”Catalysis: Balancing the use of fossil and renewable resources” which is held in Kazan (Russia) from 30th August to 4th September, 2015.

For more than two decades, the EuropaCat Congress has appeared the leading European catalytic event which since 1993 successfully served as a focal point for scientists in the front lines of innovative catalysis. EuropaCat XII is held in Kazan, which, together with Moscow and St. Petersburg, is one of the major historical centers of Russian chemistry. The Kazan University was renowned for organic chemists as long ago as in XIX century: Nikolay Zinin, Alexander Butlerov, Vladimir Markovnikov, Alexander Zaytsev and others. The Tatarstan Region is rich in traditional fossil raw materials, such as oil and associated petroleum gas; nowadays there is advanced chemical industry in Kazan with surroundings, which in many respects holds leading positions in Russia.

The catalysis expert community knows that the catalysis research has entered a new phase, marking the end of the era driven primarily by trial and error. Scientists have found a common molecular basis for the chemical processes for which catalysis is used. Catalysis research is now unified into a general scientific framework to allow heterogeneous, homogeneous and bio-catalysis to be studied using similar approaches. Another field of unification is the development of novel catalytic technologies for the conversion of both fossil resources, including heavy oil fractions, methane, ethane and C_{3+} components in natural gas, and alternative resources such as biomass, carbon dioxide, and water. Hope that EuropaCat XII will focus particularly on balancing the production of energy and chemicals from fossil and renewable resources.

EuropaCat XII has attracted a huge global interest: 1200 delegates from 64 countries were registered and 1100 abstracts submitted. All submitted abstracts were peer-reviewed and, based on the evaluation, the oral and poster presentations were selected.

We approached prominent scientists to give plenary and keynote lectures. Plenary lectures are given by Dr. G. Bellussi, Prof. J.T. Hupp, Prof. G. Hutchings**,** Prof. Dr. R. Schlögl, and Prof. M. Skoglundh. We are also pleased to announce the Butlerov Honorary Lecture by Prof. V. Ananikov, the Michel Boudart Award Lecture lecture by Prof. Dr. H.-J. Freund, and the François Gault Award Lecture by Prof. Dr. J. Lercher. The selection of the plenary and keynote speakers reflect the broad scope of catalysis – from theory to industrial practice.

The Congress program includes 8 plenary and 23 keynote lectures, 244 oral presentations, about 800 poster presentations and 126 short oral presentations within 12 microsymposia.

We expect that this meeting will provide a versatile platform for formal and informal discussions with colleagues both from academia and industry, and foster new collaborations and partnerships.

Welcome to Kazan and good luck in all the events of the EuropaCat XII!

Professor Valentin PARMON
Chairman of International Scientific Committee,
President of the National Catalysis Society

Professor Valerii BUKHTIYAROV
Chairman of Organizing Committee,
Vice-President of EFCATS

Professor Oleg SINYASHIN
Vice-Chairman of Organizing Committee

Professor Alexander STAKHEEV
Vice-Chairman of Organizing Committee

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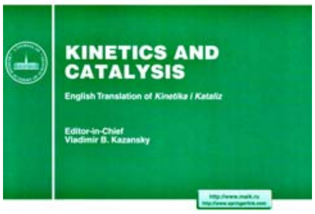

KINETICS AND CATALYSIS

English Translation of *Kinetika i Kataliz*

Editor-in-Chief
Vladimir B. Kazansky

Journal "Kinetics and catalysis"

Journal "Supercritical fluids: theory and practice"

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SCIENTIFIC PROGRAM

Congress program includes 8 plenary and 19 keynote lectures, 228 oral presentations, about 770 poster presentations and 115 short oral presentations (5-7 min) within 11 microsymposia.
Program of the XI European Workshop on Innovation in Selective Oxidation (ISO '15) "Selectivity in Oxidation: Key to new resources valorization" includes 2 keynote lectures, 16 oral (20 min) presentations and 30 posters. Program of the Symposium "Education in the Field of Catalysis: State of the Art and Possible Improvements" includes 11 oral presentations.
Four parallel Congress sessions are addressed 5 topics covering the following aspects of catalysis:

I. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

- Processing of crude oil including heavy oil fractions
- Natural gas conversion including ethane and C3+ hydrocarbons
- Catalytic processes for coal utilization
- Renewables and alternative fossils for fuels
- Reactors design for efficiency improvement

II. Catalyst Preparation and Characterization

- Bridging the gap between model and real catalysts
- Methods for characterization of catalysts, including in-situ and operando techniques
- Design and synthesis of heterogeneous, homogeneous, heterogenized and immobilized, and hybrid catalysts
- Theoretical calculation and molecular simulation
- High-throughput and combinatorial experimentation

III. Energy-related Catalysis

- Clean fuel production
- Hydrogen production and storage
- Fuel cell technologies and electrocatalysis
- Energy storage and conversion
- Electrocatalysis

IV. Catalysis and Chemicals

- Petrochemicals, including production of monomers, and polymerization processes
- Conversion of synthesis gas to chemicals
- Development of new platforms for chemicals from renewables
- Catalysis for fine chemistry and pharmaceuticals
- Catalysis in new reaction media
- Selective catalytic oxidation (including stereoselective oxidation)

V. Catalysis and Environmental Protection

- Catalysis and green chemistry
- Biomimetic/bioinspired catalysts and approaches
- CO_2 capture and utilization
- New catalysts and approaches for pollution control
- Automotive exhaust cleanup
- Treatment, valorization and utilization of industrial gases and waste water

Time-table

Saturday, August 29

KORSTON, 1st floor hall	
18:00-22:00	Registration

Sunday, August 30

KORSTON, 1st floor hall	
10:00-18:00	Registration
KORSTON Napoleon hall	
09:00-13:00; **17:00-18:00**	EFCATS meeting
KORSTON, Ball-hall	
	Chairmen: V. Parmon, J. Lercher, V. Bukhtiyarov, O. Sinyashin
14:00-15:00	Opening Ceremony
15:00-16.00	**Butlerov Honorary Plenary Lecture, V. Ananikov, PL-1**
16:00-17:00	**François Gault Lectureship Award (2013), J. Lercher, PL-2**
17:00-19:00	***Break to prepare Ball-hall for Welcome reception***
19:00	**Welcome reception**

PL – Plenary Lecture

KN – Keynote Lecture

OP – Oral Presentation

PP – Poster Presentation

Monday, August 31

TIME				
8.30-13.00	Registration			
	Chairmen: J. Lercher, A. Stakheev			
08:30-09:30	**G.Bellussi, PL-3** *(KORSTON Ball hall)*			
09:30-10:30	**G. J. Hutchings, PL-4** *(KORSTON Ball hall)*			
	KORSTON Ball hall-1	***KORSTON Ball hall-2***	***KORSTON Pushkin hall***	***KORSTON Tolstoy hall***
10:30-11:00	***(Break to separate Ball hall) Coffee break***			
	Chairmen: *V. Yakovlev,* *Y. Kamiya*	*Chairmen:* *G. Rupprechter,* *G. Landi*	*Chairmen:* *V. Ananikov,* *B. Koenig*	*Chairmen:* *S. Ordonez,* *M. Sinev*
11:00-11:20	V-KN1 C. Descorme	II-OP01 J. Ruiz-Martínez	IV-OP01 N. Perret	I-OP01 G.W. Wang
11:20-11:40		II-OP02 I. Ivanova	IV-OP02 V. Likholobov	I-OP02 A. Astafan
11:40-12:00	V-OP01 D. Cani	II-KN2 V. Parvulescu	IV-OP03 F.Cárdenas-Lizana	I-OP03 A. Simakov
12:00-12:20	V-OP02 D. Kozlov		IV-OP04 E. Nowicka	I-OP04 A. Gervasini
12:20-12:40	V-OP03 J. Hirayama	II-OP03 W. Huang	IV-OP05 O. Beswick	I-OP05 S. Kegnæs
12:40-13:00	V-OP04 E. Parhomchuk	II-OP04 A. Stepanov	IV-OP06 K. Koltunov	I-OP06 R. Henry
13:00-14:30	***Lunch***			
	Chairmen: *M. Tsodikov,* *P. Mortensen*	*Chairmen:* *I. Ivanova,* *J. Ruiz-Martínez.*	*Chairmen:* *J.S. McIndoe,* *N. Perret*	*Chairmen:* *A. Simakov,* *D. Teschner*
14:30-14:50	V-OP05 G. Garbarino	II-OP05 A. Stakheev	IV-KN3 C.W. Jones	I-OP07 P. Pandis
14:50-15:10	V-OP06 L. Falbo	II-OP06 C. Sprung		I-OP08 J. Horáček
15:10-15:30	V-OP07 Z. Bukina	II-OP07 K. Kovtunov	IV-OP07 K. Bryliakov	I-OP09 M. Peroni
15:30-16:00	***Coffee break***			
	Chairmen: *C. Li ,* *A. Karasik*	*Chairmen:* *J. Hargreaves,* *K. Kovtunov*	*Chairmen:* *K. Koltunov,* *V. Hulea*	*Chairmen:* *V.I. Parvulescu,* *A. Lemonidou*
16:00-16:20	III-KN4 G. Centi	II-OP08 Yu. Gulyaeva	IV-OP08 Z.-G. Zhang	I-OP10 Z. Ismagilov
16:20-16:40		II-OP09 V. Ermolaev	IV-OP09 H.J. Venvik	I-OP11 V. Yakovlev
16:40-17:00	III-OP01 M. Muhler	II-OP10 E. Talsi	IV-OP10 J.K. Erickson	I-OP12 S. Ordonez
17:30-20:00	**Excursion «Millennial Kazan»**			

Tuesday, September 1

TIME	*Chairmen: V. Bukhtiyarov, H.-J. Freund*			
08:30-09:30	**J.T. Hupp, PL-5** *(KORSTON Ball hall)*			
09:30-10:30	**R. Schloegl, PL-6** *(KORSTON Ball hall)*			
	KORSTON Ball hall-1	***KORSTON Ball hall-2***	***KORSTON Pushkin hall***	***KORSTON Tolstoy hall***
10:30-11:00	***(Break to separate Ball hall)*** ***Coffee break***			
	Chairmen: C. Aprile, A. Rempel	*Chairmen: S. Penner, J.A. van Bokhoven*	*Chairmen: C. Jones, E. Talsi*	*Chairmen: K. Takanabe, T. Tatsumi*
11:00-11:20	V-KN5 W. Leitner	II-OP11 S. Mossin	IV-OP11 F. Cavani	III-OP02 L. Gao
11:20-11:40		II-OP12 D. Zemlyanov	IV-OP12 V. Nese	III-OP03 E. Kozlova
11:40-12:00	V-OP08 P.M. Mortensen	II-KN6 S. Helveg	IV-OP13 Y. Zhu	III-OP04 S. Pokrant
12:00-12:20	V-OP09 M. Bukhtiyarova		IV-OP14 N. d'Alessandro	III-OP05 P. Weide
12:20-12:40	V-OP10 M. Gaillard	II-OP13 F.J. Cadete Santos Aires	IV-KN7 B. Koenig	III-OP06 C. Marchal
12:40-13:00	V-OP11 G. Bonura	II-OP14 M. Ek		III-OP07 A.V. Puga
13:00-14:30	***Lunch***			
	Chairmen: W. Leitner, I. Nova	*Chairmen: D. Zemlyanov, S. Bordiga*	*Chairmen: A. Trifonov, Qihua Yang*	*Chairmen: M. Millan, D. Bulushev*
14:30-14:50	V-OP12 A. Suknev	II-OP15 D.Doronkin	IV-OP15 W.N.P. van der Graaff	III-OP08 J. Amouroux
14:50-15:10	V-OP13 S. Yashnik	II-OP16 M. Hävecker	IV-OP16 E.A. Pidko	III-OP09 D. Teschner
15:10-15:30	V-OP14 A. Khudorozhkov	II-OP17 V. Kaichev	IV-OP17 S. Tolborg	III-OP10 K. Villa
15:30-15:50	V-OP15 H. Stotz	II-OP18 A. Klyushin	IV-OP18 I. Delidovich	III-OP11 A. Rempel
15:50-16:10	V-OP16 A.W. Petrov	II-OP19 C. M. Schilling	IV-OP19 A. Padovani	III-OP12 J.L. Faria
16:10-16:30	V-OP17 D. Lopez-Gonzalez	II-OP20 E. Vovk	IV-OP20 S.M. Coman	III-OP13 K.E. Sanwald
16:30-17:00	***Coffee break***			
17:00-19:00	**Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155, ISO-PP1÷ISO-PP30** *(KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich, Poster set-up time 09:00 – 19:00)*			

			TIME
			08:30-09:30
			09:30-10:30
KORSTON ***Dostoevsky hall***	***KORSTON*** ***Lermontov hall***	***KORSTON*** ***Chekhov hall***	
			10:30-11:00
ISO '15 *Chairmen: J. Lercher,* *V. Cortés Corberán*	*Chairmen:* *D. Murzin,* *Yu. Román-Leshkov*	*Chairmen:* *C. Mirodatos,* *V. Sadykov*	
Opening ceremony	Discussion symposium 1 "Value-Added Chemicals from Renewables"	Discussion symposium 2 "Fuel Reforming"	**11:00-11:20**
ISO-OP01 J.M. Lopez Nieto			**11:20-11:40**
ISO-OP02 P.P. Pescarmona			**11:40-12:00**
ISO-OP03 L. Prati			**12:00-12:20**
ISO-OP04 M.N. Simonov			**12:20-12:40**
ISO-OP05 V. Cortés Corberán			**12:40-13:00**
			13:00-14:30
Chairmen: *S. Perathoner,* *V. Sadykov*	*Chairmen:* *V. Likholobov,* *N. d'Allessandro*	*Chairmen:* *E. Kozlova,* *D. Kozlov*	
ISO-KN1 O. Kholdeeva	Discussion symposium 3 "Selective Catalytic Hydrogenation"	Discussion symposium 4 "Photocatalysis: Water Splitting, CO_2 Reduction and Oxidative Processes"	**14:30-14:50**
			14:50-15:10
ISO-OP06 A. Pestryakov			**15:10-15:30**
ISO-OP07 L. Moskaleva			**15:30-15:50**
ISO-OP08 E. Khaskin			**15:50-16:10**
ISO-OP09 G.V. Mamontov			**16:10-16:30**
			16:30-17:00
			17:00-19:00

Wednesday, September 2

TIME	*Chairmen: R. Schlögl, M. Scoglundh*			
08:30-09:30	**Michel Boudart Award Lecture (2015), H.-J. Freund, PL-7** *(KORSTON Ball hall)*			
	KORSTON Ball hall-1	***KORSTON Ball hall-2***	***KORSTON Pushkin hall***	***KORSTON Tolstoy hall***
09:30-10:00	***(Break to separate Ball hall) Coffee break***			
	Chairmen: *A. Vedyagin,* *M. Bukhtiyarova*	*Chairmen:* *S. Mossin,* *M. Hävecker*	*Chairmen:* *S. Coman,* *Wang Ye*	*Chairmen:* *J.C. Conesa* *E. Pidko*
10:00-10:20	V-KN8 Yu. Román-Leshkov	II-OP21 M. Cortés-Reyes	IV-OP21 A. Terent'ev	III-OP14 P. Castaño
10:20-10:40		II-OP22 T.H. Vuong	IV-OP22 D.B. Rasmussen	III-OP15 P. Snytnikov
10:40-11:00	V-OP18 F. Calaza	II-KN9 J.S. McIndoe	IV-OP23 Yue Liu	III-OP16 G.I. Konstantinov
11:00-11:20	V-OP19 C. Aprile		IV-OP24 T. Otroshchenko	III-OP17 S.D. Angeli
11:20-11:40	V-OP20 Y. Demidova	II-OP23 K.R. Rout	IV-OP25 O. Martyanov	III-OP18 V. Sadykov
11:40-12:00	V-OP21 E. Nowicka	II-OP24 Z.D. Wang	IV-KN10 X.L. Hu	III-OP19 R. Watanabe
12:00-12:20	V-OP22 A.A. Lemonidou	II-OP25 L. Van Haandel		III-OP20 R. Mafessanti
12:20-12:40	V-OP23 M. Zacharska	II-OP26 V. Pfeifer	IV-OP26 H. Atia	III-OP21 A.A. Lytkina
12:40-13:00	V-OP24 M.V. Tsodikov	II-OP27 H. Li	IV-OP27 A.A. Zagidullin	III-OP22 C. Lucarelli
13:00-14:30	***Lunch***			
	Chairmen: *W. Grünert,* *I.-S. Nam*	*Chairmen:* *A. Auroux,* *F.J. Cadete Santos Aires*	*Chairmen:* *O. Taran,* *Yu. Román-Leshkov*	*Chairmen:* *V. Ordomsky* *P. Snytnikov*
14:30-14:50	I-KN11 U. Olsbye	II-OP28 J. Schnee	IV-OP28 E. Girard	III-OP23 D. Bulushev
14:50-15:10		II-OP29 S. Bordiga	IV-OP29 Ye Wang	III-OP24 E. Ozensoy
15:10-15:30	I-KN12 T. Tatsumi	II-OP30 J.A. van Bokhoven	IV-OP30 T. Yokoi	III-OP25 M. Millan
15:30-15:50		II-OP31 G.H. Agata	IV-OP31 O. Kasaikina	III-OP26 E. Frei
15:50-16:10	I-OP13 P. Mäki-Arvela	II-OP32 W. Karim	Award Applied Catalysis Researcher, KN20 I. Vasalos	III-OP27 L.A. Petrov
16:10-16:30	I-OP14 G.D. Yadav	II-OP33 H.O. Fredriksson		III-OP28 J. Kirchner
16:30-17:00	***Coffee break***			
17:00-19:00	**Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150** *(KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich, Poster set-up time 09:00 – 19:00)*			

			TIME
			08:30-09:30
KORSTON ***Dostoevsky hall***	***KORSTON*** ***Lermontov hall***	***KORSTON*** ***Chekhov hall***	
			09:30-10:00
ISO ‘15 *Chairmen: G. Centi,* *O. Kholdeeva*	*Chairmen:* *Søren Kegnæs,* *E. Lokteva*	*Chairmen:* *W. Grünert,* *A. Stakheev*	
ISO-OP10 S. Solmi	Discussion symposium 5 “CO_2 Capture & Valorization”	Discussion symposium 6 “Pollution Control & Oxidation Catalysis”	**10:00-10:20**
ISO-OP11 J.A. Odriozola			**10:20-10:40**
ISO-OP12 W. Shen			**10:40-11:00**
ISO-OP13 R. Ottenbacher			**11:00-11:20**
ISO-OP14 S. Perathoner			**11:20-11:40**
ISO-OP15 S. Paul			**11:40-12:00**
ISO-OP16 M. Florea			**12:00-12:20**
ISO-KN2 Kolb G.			**12:20-12:40**
			12:40-13:00
Lunch			**13:00-14:30**
Chairmen: *P. Ruiz,* *F. Cavani*	*Chairmen:* *G. Rupprechter,* *D. Teschner*	*Chairmen:* *K. Neyman,* *E. Pidko*	
ISO- Discussion symposium 7 "Selective Oxidation"	Discussion symposium 8 “In Situ Measurements for Catalytic Studies: Identification of the Structure of Catalytically Active Sites”	Discussion symposium 9 “DFT Calculation in Catalytic Studies”	**14:30-14:50**
			14:50-15:10
			15:10-15:30
			15:30-15:50
			15:50-16:10
			16:10-16:30
			16:30-17:00
			17:00-19:00

Thursday, September 3

TIME	*Chairmen: J.T. Hupp, G. Bellussi*			
08:30-09:30	**M. Skoglundh, PL-8** *(KORSTON Ball hall)*			
	KORSTON Ball hall-1	***KORSTON Ball hall-2***	***KORSTON Pushkin hall***	***KORSTON Tolstoy hall***
09:30-10:00	***(Break to separate Ball hall)*** ***Coffee break***			
	Chairmen: *A. Khodakov,* *Z. Sojka*	*Chairmen:* *W. Huang,* *M.C. Roman-Martinez*	*Chairmen:* *E. Kozlova* *S. Damyanova*	*Chairmen:* *V. Gevorgyan,* *E. Ozensoy*
10:00-10:20	V-KN13 I.-S. Nam	II-OP34 J. C. Conesa	III-OP29 N. Weidler	I-OP15 C. van der Wijst
10:20-10:40		II-OP35 W.K. Offermans	III-OP30 R. Thalinger	I-OP16 I. Simakova
10:40-11:00	V-OP25 W. Grünert	II-KN14 K. Neyman	III-OP31 C. Nervi	I-OP17 E. Heracleous
11:00-11:20	V-OP26 P.G. Moses		III-OP32 A.G.Oshchepkov	I-OP18 V. Ordomsky
			Chairmen: *X. Hu, K. Bryliakov*	
11:20-11:40	V-OP27 I. Nova	II-OP36 D. Pichugina	IV-OP34 V. Hulea	I-OP19 B.N. Kuznetsov
11:40-12:00	V-OP28 J.M. Garcia-Vargas	II-OP37 H.J. Venvik	IV-OP35 E.I. Ruppel	I-OP20 R. Tschentscher
12:00-12:20	V-OP29 P. Granger	II-OP38 I.A.W. Filot	IV-OP36 L.V. Parfenova	I-OP21 R.U. McVicker
12:20-12:40	V-OP30 M. Sridhar	II-OP39 Mohamad Saab	IV-OP37 G. Fu	I-OP22 A.V. Chistyakov
12:40-13:00	V-OP31 Z. Say	II-OP40 M. Bykova	IV-OP38 M.N. Khrizanforov	I-OP23 V.M. Kogan
13:00-14:30	***Lunch***			
	Chairmen: *V. Kaichev,* *O. Martyanov*	*Chairmen:* *L. Soler,* *S. Helveg*	*Chairmen:* *V. Likholobov,* *C. Descorme*	*Chairmen:* *Granger Pascal* *T. Tabakova*
14:30-14:50	III-KN15 G. Rupprechter	II-OP41 E. Lokteva	IV-OP39 A. Trifonov	V-OP32 A. García-García
14:50-15:10		II-OP42 W.Z. Weng	IV-OP40 M. Botavina	V-OP33 A. Porsin
15:10-15:30	III-OP33 V. Arutyunov	II-OP43 L. Piccolo	IV-KN17 V. Gevorgyan	V-OP34 J. Zheng
15:30-15:50	III-OP34 V. Simagina	II-OP44 E. Suslova		V-OP35 A. Serve
15:50-16:10	III-KN16 C. Li	II-OP45 P. Ruiz	IV-OP41 D. Murzin	V-OP36 A. Kotarba
16:10-16:30		II-OP46 S. Penner	IV-OP42 Q. Yang	V-OP37 S. Kureti
16:30-17:00	***Coffee break***			
	Chairmen: *U. Olsbye,* *C. Nervi*	*Chairmen:* *E. Shor,* *M. Smirnov*	*Chairmen:* *Zhang Zhanguo,* *F. Cardenas-Lizana*	*Chairmen:* *A. Garcia-Garcia* *S. Kureti*
17:00-17:20	III-OP35 Jayakodi Karuppiah J.	II-OP47 Youzhu Yuan	IV-OP43 V.M. Chernyshev	V-OP38 S. Heikens
17:20-17:40	III-OP36 K. Cheng	II-OP48 Wenjie Shen	IV-OP44 Á. Berenguer-Murcia	V-OP39 H. Arandiyan
17:40-18:00	III-OP37 W. Chen	II-OP49 Z. Zhao	IV-OP45 A. Auroux	V-OP40 Tang Long
19:30	**Banquet (restaurant PANORAMA)**			
19:00	**Young scientists party** *(club "Extra Lounge" at the 25th floor of "Korston Tower" hotel)*			

		TIME
		08:30-09:30
KORSTON ***Dostoevsky hall***	***KORSTON*** ***Lermontov hall***	
		09:30-10:00
Chairmen: *V. Lunin,* *D. Murzin*	*Chairmen:* *G. Kolb* *J.M. Lopez Nieto*	
Symposium “Education in the Field of Catalysis”	ISO-OP17 C. Mirodatos	**10:00-10:20**
	ISO-OP18 M. Sinev	**10:20-10:40**
	ISO-OP19 D.V. Ivanov	**10:40-11:00**
	ISO-OP20 S.I. Ishikawa	**11:00-11:20**
	ISO-OP21 O. Taran	
		11:20-11:40
	ISO-OP22 I.C .Marcu	**11:40-12:00**
	ISO-OP23 I. Pakharukov	**12:00-12:20**
	ISO-OP24 E. Starokon	**12:20-12:40**
	Closing remarks	**12:40-13:00**
		13:00-14:30
Chairmen: *M. Muhler,* *F. Cavani*	*Chairmen:* *M. Sinev,* *D. Murzin*	
Discussion symposium 10 «Design of Gold Catalysts for Selective Processes: from Science to Real Application»	Discussion symposium 11 «Feasibility of Biomass Utilization for Making Fuels and Chemicals»	**14:30-14:50**
		14:50-15:10
		15:10-15:30
		15:30-15:50
		15:50-16:10
		16:10-16:30
		16:30-17:00
		17:00-17:20
		17:20-17:40
		17:40-18:00
		19:30
		19:00

Friday, September 4

	KORSTON ***Ball hall-1***	***KORSTON*** ***Ball hall-2***	***KORSTON*** ***Pushkin hall***	***KORSTON*** ***Tolstoy hall***
TIME	*Chairmen:* *E. Gaigneaux,* *I. Vasalos*	*Chairmen:* *J. Faria,* *E. Vovk*	*Chairmen:* *Z. Zhao,* *V. Simagina*	*Chairmen:* *K. Koehler* *P. Moses*
08:30-08:50	I-KN18 A.Y. Khodakov	III-OP38 X. Huang	II-OP50 S. Vereshchagin	V-OP41 E. Tronconi
08:50-09:10		III-OP39 F. Frusteri	II-OP51 A. Nartova	V-OP42 A. Shishkin
09:10-09:30	I-OP24 L. Fratalocchi	III-KN19 K. Takanabe	II-OP52 X. Zhu	V-OP43 B. Pereda-Ayo
09:30-09:50	I-OP25 C.G. Visconti		II-OP53 N. Bion	V-OP44 J. Thøgersen
09:50-10:10	I-OP26 D. Otyuskaya	III-OP40 J. He	II-OP54 R. van den Berg	V-OP45 S. Alcove
10:10-10:30	I-OP27 P. Benito Martin	III-OP41 J.S. Martinez-Espin	II-OP55 D. Ishutenko	V-OP46 P.L. Thomassen
10:30-11:00	***Coffee break***			
	Chairmen: *E. Lokteva* *A. Nartova*	*Chairmen:* *F. Cunill,* *E. Suslova*	*Chairmen:* *P. Pescarmona* *I. Simakova*	*Chairmen:* *E. Tronconi* *L. Pinaeva*
11:00-11:20	KN21 E. Karakhanov	III-OP42 A. Beretta	II-OP56 A. Dewaele	V-OP47 Z. Sojka
11:20-11:40		III-OP43 T.E. Bell	II-OP57 B. Acosta	V-OP48 T. Franken
11:40-12:00	IV-OP46 G. Trunfio	III-OP44 J. Anton	II-OP58 A. Lavrenov	V-OP49 E. Papista
12:00-12:20	IV-OP47 B. Schaller	III-OP45 O. Gutierrez Tinoco	II-OP59 I. Ismagilov	V-OP50 M. Zabilskiy
12:20-12:40	IV-OP48 M. Rose	III-OP46 G. Landi	II-OP60 E. Redekop	V-OP51 C. Bradu
12:50-13:30	**Closing ceremony** *(KORSTON Ball hall)*			
13:30-15:00	***Lunch***			

Saturday, August 29

Korston Hotel & Mall Kazan (Ershov street, 1A)

1st floor hall

18:00-22:00 Registration

Sunday, August 30

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON, 1st floor hall

10:00-18:00 **Registration**

KORSTON Napoleon hall

09:00-13:00; **EFCATS Meeting**
17:00-18:00

14:00-15:00 **Opening Ceremony**

KORSTON, Ball-hall

Chairmen:
Prof. Parmon Valentin, *Russian Catalysis Society,*
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russian Federation
Prof. Lercher Johannes, *Technical University of Munich, Department of Chemistry, Garching, Germany; Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA*
Prof. Bukhtiyarov Valerii, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russian Federation*
Prof. Sinyashin Oleg, *Kazan Scientific Center RAS, Kazan, Russian Federation*

Welcome speech: Rustam Minnikhanov, President of the Republic of Tatarstan

Plenary Lectures

15:00-16:00 **PL-1** Butlerov Honorary Plenary Lecture, Prof. Ananikov Valentin
Catalysis in Organic Chemistry: from Butlerov to these Days
Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia

16:00-17:00 **PL-2** François Gault Lectureship Award (2013), Prof. Lercher Johannes A.[1,2]
Enhancing Catalytic Rates in Constraints – from Acid-base to Metal Catalyzed Reactions
1 - TU München, Department of Chemistry, Garching, Germany
2 - Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA

17:00-19:00 ***Break to prepare Ball-hall for Welcome reception***

19:00 **Welcome reception** (*KORSTON Ball hall*)

Monday, August 31

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Lercher Johannes, *Technical University of Munich, Department of Chemistry, Garching, Germany; Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA*
Prof. Stakheev Alexander, *Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia*

Plenary Lectures

08:30-09:30 **PL-3** Dr. Bellussi Giuseppe
Fossil and Renewable Energy: the Turning Point of the Liquid Fuels Production
Eni S.p.A, SVP Downstream R&D, San Donato Milanese — I, Italy

09:30-10:30 **PL-4** Prof. Hutchings Graham J.
Catalysis Using Supported Gold and Gold Palladium Nanoparticles
Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, UK

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-1

Section 5. Catalysis and Environmental Protection

Chairmen: Dr. Yakovlev Vadim, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Dr. Kamiya Yuichi, *Research Faculty of Environmental Earth Science, Hokkaido University, Sapporo, Japan*

Keynote Lecture

11:00-11:40 **V-KN1** Prof. Descorme Claude
Catalytic Wastewater Treatment
Institut de Recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON), UMR5256 CNRS – University of Lyon, 2 avenue Albert Einstein, 69626 Villeurbanne, France

Oral Presentations

11:40-12:00 **V-OP01** Cani Damiano
Cani D.[1], Pescarmona P.P.[1,2]
Highly Accessible TiO_2 Nanoparticles Embedded at the Surface of SiO_2 for the Photocatalytic Degradation of Pollutants under Visible and UV Radiation
1 - COK, University of Leuven, Belgium
2 - Chemical Engineering Department, University of Groningen, Groningen, The Netherlands

12:00-12:20 **V-OP02** Dr. Kozlov Denis
Filippov T.[1,2], Kolinko P.[1], Glebov E.[3], Kozlov D.[1,2]
Photocatalytic Activity of the Uranyl Modified Titania, Silica and Alumina under Visible Light Irradiation
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Research and Educational Centre for Energoefficient Catalysis (Novosibirsk State University), Novosibirsk, Russia
3 - Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia

12:20-12:40 **V-OP03** Hirayama Jun
Hirayama J.[1], Kamiya Y.[2]
Combining the Photocatalyst Pt/TiO_2 and the Non-photocatalyst SnPd/Al_2O_3 for Effective Photocatalytic Purification of Groundwater Polluted with Nitrate
1 - Graduate School of Environmental Science, Hokkaido University, Sapporo, Japan
2 - Research Faculty of Environmental Earth Science, Hokkaido University, Sapporo, Japan

12:40-13:00 **V-OP04** Dr. Parkhomchuk Ekaterina
Sashkina K.A.[1,2,3], Labko V.S.[4], Parkhomchuk E.V.[1,3,2]
Hierarchically Porous Fe-silicalites for Total Oxidation of Organic Molecules
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Research and Education Centre, NSU, Novosibirsk, Russia
4 - State Scientific Institution "The Joint Institute for Power and Nuclear Research – Sosny", Minsk, Belarus

13:00-14:30 ***Lunch***

KORSTON Ball hall-1

Evening Session

Chairmen: Prof. Tsodikov Mark, *A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia*
Dr. Mortensen Peter, *Haldor Topsoe A/S, Kgs. Lyngby, Denmark*

Oral Presentations

14:30-14:50 **V-OP05** Dr. Garbarino Gabriella
Garbarino G.[1], Bellotti D.[2], Riani P.[3], Magistri L.[2], Busca G.[1]
CO_2 Methanation on Commercial Ni/Al_2O_3 and Ru/Al_2O_3 Catalysts
1 - University of Genova, DICCA Dipartimento di Ingegneria Civile Chimica e Ambientale, Genova, Italy
2 - University of Genova, DIME Dipartimento di Ingegneria Meccanica, Energetica, Gestionale e dei Trasporti, Genova, Italy
3 - University of Genova, DCCI Dipartimento di Chimica e Chimica Industriale, Genova, Italy

14:50-15:10 **V-OP06** Falbo Leonardo
Martinelli M.[1], Falbo L.[1], Visconti C.G.[1], Lietti L.[1], Forzatti P.[1], Bassano C.[2], Deiana P.[2]
CO_x Hydrogenation on Promoted Iron Based Catalysts: the Key Role of the Potassium on the Process Selectivity
1 - Politecnico di Milano, Dipartimento di Energia, Via Lambruschini 4, 20156 Milan, Italy
2 - ENEA- Italian Agency for New Technologies, Energy and Environment, Via Anguillarese 301, 00123 S.M. Galeria, Rome, Italy

15:10-15:30 **V-OP07** Bukina Zareta
Ionin I., Bukina Z., Kolesnichenko N., Khadzhiev S.
Conversion of CO and H_2 to Liquid Hydrocarbons via Dimethyl Ether on Zeolit Catalysts
Topchiev Institute of Petrochemical Synthesis RAS (TIPS RAS), Moscow, Russia

15:30-16:00 ***Coffee break***

KORSTON Ball hall-1

Section 3. Energy-Related Catalysis

Chairmen: Prof. Li Can, *Dalian Institute of Chemical Physics, CAS, National Laboratory for Clean Energy, Dalian, China*
Prof. Karasik Andrey A*., A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, RAS, Kazan, Russia*

Keynote Lecture

16:00-16:40 **III-KN4** Prof. Centi Gabriele
Centi G., Perathoner S.
Catalysis to Produce Solar Fuels. Status and Challenges
Dept. DIECII, Section Industrial Chemistry, University of Messina, ERIC aisbl and CASPE/INSTM, V.le F. Stagno D'Alcontre 31, 98166 Messina, Italy

Oral Presentations

16:40-17:00 **III-OP01** Prof. Muhler Martin
Muhler M.[1,2], Zhao A.[1,2], Xie K.[1,2], Masa J.[1,3], Xia W.[1,2], Schuhmann W.[1,3]
Spinel Mn-Co oxide in N-doped Carbon Nanotubes as Bifunctional Electrocatalyst
1 - Ruhr-University Bochum, Bochum, Germany
2 - Laboratory of Industrial Chemistry, Ruhr-University Bochum, Bochum, Germany
3 - Analytical Chemistry and Center of Electrochemistry, Ruhr-Universität Bochum, Bochum, Germany

17:30-20:00 **Excursion «Millennial Kazan»**

Monday, August 31

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Lercher Johannes, *Technical University of Munich, Department of Chemistry, Garching, Germany; Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA*
Prof. Stakheev Alexander, *Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia*

Plenary Lectures (*KORSTON Ball hall)*

08:30-09:30 **PL-3** Dr. Bellussi Giuseppe
Fossil and Renewable Energy: the Turning Point of the Liquid Fuels Production
Eni S.p.A, SVP Downstream R&D, Via Maritano 26, 20097 San Donato Milanese — I, Italy

09:30-10:30 **PL-4** Prof. Hutchings Graham
Catalysis Using Supported Gold and Gold Palladium Nanoparticles
Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, UK

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-2

Section 2. Catalyst Preparation and Characterization

Chairmen: Prof. Rupprechter Günther, *Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria*
Dr. Landi Gianluca, *Research Institute on Combustion – CNR, Naples, Italy*

Oral Presentations

11:00-11:20 **II-OP01** Dr. Ruiz-Martínez Javier
Ruiz-Martínez J.[1], Borodina E.[1], Meirer F.[1], Lezcano-González I.[1], Mokhtar M.[2], Asiri A.M.[2,3], Al-Thabaiti S.A.[2], Basahel S.N.[2], Weckhuysen B.M.[1]
Combining Operando Spectroscopy and Chemometrics to Understand Changes in the Active and Deactivating Species During the Methanol-to-Olefins Reaction over H-SSZ-13
1 - Utrecht University, Debye Institute for Nanomaterials Science, Inorganic Chemistry and Catalysis Department, Utrecht, The Netherlands
2 - Department of Chemistry, Faculty of Science, King Abdulaziz University, Saudi Arabia
3 - Center of Excellence for Advance Materials Research, King Abdulaziz University, Saudi Arabia

11:20-11:40 **II-OP02** Prof. Ivanova Irina
Ivanova I.I.[1,2], Kolyagin Yu.G.[1,2]
Elucidation of the Mechanism of Hydrothermal Synthesis of Zeolite Catalysts Using Ex-situ and In situ Approaches
1 - M.V. Lomonosov Moscow State University, Chemistry Department, Moscow, Russia
2 - A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia

Keynote Lecture

11:40-12:20 **II-KN2** Prof. Pârvulescu Vasile
Lewis Acid-base Catalysts for the Synthesis of Fine Chemicals
University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis, B-dul Regina Elisabeta 4-12, Bucharest 030016, Romania

Oral Presentations

12:20-12:40 **II-OP03** Prof. Huang Weixin
Optimizing Catalytic Performances of Oxide Catalysts Via Morphology Engineering
Department of Chemical Physics, University of Science and Technology of China, Hefei 230026, China

12:40-13:00 **II-OP04** Prof. Stepanov Alexander
Stepanov A.G.[1,2], Gabrienko A.A.[1], Arzumanov S.S.[1], Moroz I.B.[1], Toktarev A.V.[1], Freude D.[2]
Methane Activation on In-Modified ZSM-5 Zeolite. Solid-State NMR Characterization of the Pathways of the Alkane Transformation to Surface Species
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Universität Leipzig, Fakultät für Physik und Geowissenschaften, Linnéstrasse 5, 04103 Leipzig, Germany

13:00-14:30 ***Lunch***

KORSTON Ball hall-2

Evening Session

Chairmen: Prof. Ivanova Irina, *Moscow State University, Moscow, Russia*
Dr. Ruiz-Martínez Javier, *Utrecht University, Utrecht, The Netherlands*

Oral Presentations

14:30-14:50 **II-OP05** Prof. Stakheev Alexander Yu.
Stakheev A.Yu.[1], Markov P.V.[1], Turova O.V.[1], Mashkovsky I.S.[1], Khudorozhkov A.K.[2], Bukhtiyarov V.I.[2]
Pd Size Effect in Liquid Phase Semihydrogenation of Substituted Alkynes on Supported Pd Catalysts
1 - Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

14:50-15:10 **II-OP06** Dr. Sprung Christoph
Sprung C., Weckhuysen B.M.
Dispersion and Orientation of Zeolite ZSM-5 Crystallites within a Fluid Catalytic Cracking Catalyst Particle
Utrecht University, Department of Chemistry, Inorganic Chemistry and Catalysis, Universiteitsweg 99, 3584 CG Utrecht, The Netherlands

15:10-15:30 **II-OP07** Dr. Kovtunov Kirill
Kovtunov K.[1], Barskiy D.[1,2], Salnikov O.[1,2], Burueva D.[1,2], Bukhtiyarov V.[3], Koptyug I.[1,2]
Parahydrogen-Induced Polarization in Heterogeneous Catalytic Processes
1 - International Tomography Center, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

15:30-16:00 ***Coffee break***

KORSTON Ball hall-2

Chairmen: Dr. Hargreaves Justin, *School of Chemistry, University of Glasgow, Glasgow, United Kingdom*
Dr. Kovtunov Kirill, *International Tomography Center, Novosibirsk, Russia*

Oral Presentations

16:00-16:20 **II-OP08** Dr. Gulyaeva Yuliya
Gulyaeva Yu.K.[1], Kaichev V.V.[1,2], Zaikovskii V.I.[1,2], Suknev A.P.[1], Brongersma H.H.[3,4], Bal'zhinimaev B.S.[1]
Selective Hydrogenation Processes Over Novel Fiberglass Based Catalysts
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - ION-TOF GmbH, Heisenbergstrasse 15, 48149, Munster, Germany
4 - Eindhoven University of Technology, 5612, Eindhoven, Netherlands

16:20-16:40 **II-OP09** Dr. Ermolaev Vadim
Ermolaev V.V., Arkhipova D.M., Miluykov V.A., Gaynanova G.A., Zakharova L. Ya., Sinyashin O.G.
Dependence of Catalytic Activity of Palladium Nanoparticles on Stabilization Models
A.E. Arbuzov Institute of Organic and Physical Chemistry KSC RAS, Kazan, Russia

16:40-17:00 **II-OP10** Prof. Talsi Evgenii
Soshnikov I.E.[1,2], Semikolenova N.V.[1], Bryliakov K.P.[1,2], Zakharov V.A.[1,2], Talsi E.P.[1,2]
Selective Ethylene Trimerization by Titanium Complexes Bearing Phenoxy-Imine Ligands with Pendant arm: NMR and EPR Spectroscopic Study of the Reaction Intermediates
1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

17:30-20:00 **Excursion «Millennial Kazan»**

Monday, August 31

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Lercher Johannes, *Technical University of Munich, Department of Chemistry, Garching, Germany; Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA*
Prof. Stakheev Alexander, *Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia*

Plenary Lectures (*KORSTON Ball hall)*

08:30-09:30 **PL-3** Dr. Bellussi Giuseppe
Fossil and Renewable Energy: the Turning Point of the Liquid Fuels Production
Eni S.p.A, SVP Downstream R&D, San Donato Milanese — I, Italy

09:30-10:30 **PL-4** Prof. Hutchings Graham
Catalysis Using Supported Gold and Gold Palladium Nanoparticles
Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, UK

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Pushkin hall

Section 4. Catalysis and Chemicals

Chairmen: Prof. Ananikov Valentin, *Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia*
Prof. Koenig Burkhard, *University of Regensburg, Regensburg, Germany*

Oral Presentations

11:00-11:20 **IV-OP01** Dr. Perret Noemie
Perret N., Grigoropoulos A., Manning T., Claridge J., Rosseinsky M.J.
Selectivity in the Liquid-Phase Hydrogenation of 5-Hydroxymethyl Furfural over Ni-Al Catalysts
University of Liverpool, Liverpool, United Kingdom

11:20-11:40 **IV-OP02** Prof. Likholobov Vladimir
Mironenko R.M.[1], Belskaya O.B.[1], Lavrenov A.V.[1], Likholobov V.A.[1,2]
Liquid-Phase Hydrogenation of Benzaldehyde and Furfural over Pd/C and Ru/C Catalysts
1 - Institute of Hydrocarbons Processing SB RAS, Omsk, Russia
2 - Omsk Scientific Center SB RAS, Omsk, Russia

11:40-12:00 **IV-OP03** Dr. Cárdenas-Lizana Fernando
Cárdenas-Lizana F., Li M., Keane M. A.
Sustainable "Hydrogen Free" Catalytic Hydrogenation: From Concept to Reality
Heriot-Watt University, Chemical Engineering, Edinburgh EH14 4AS, Scotland

12:00-12:20 **IV-OP04** Dr. Nowicka Ewa
Iqbal S.[1], Liu X.[1], Aldosari O.F.[1], Miedziak P.J.[1], Edwards J.K.[1], Brett G.L.[1], Akram A.[1], Davies T.E.[2], Morgan D.J.[1], Knight D.K.[1], Hutchings G.J.[1], Nowicka E.[1]
Conversion of Furfuryl Alcohol into 2-methylfuran at Room Temperature Using Pd/TiO_2 Catalyst
1 - Cardiff Catalysis Institute, School of chemistry, Cardiff, UK
2 - Stephenson Institute for Renewable Energy, Chemistry Department, the University of Liverpool, Liverpool, UK

12:20-12:40 **IV-OP05** Beswick Oliver
Beswick O.[1], Parastaev A.[1,2], Yuranov I.[1], Kiwi-Minsker L.[1]
Transition Metal Oxides Nanoparticles on Activated Carbon Fibres as Efficient Catalyst for Nitroarenes Reduction under Mild Conditions
1 - Ecole Polytechnique Fédérale de Lausanne, GGRC-ISIC-EPFL, Lausanne CH-1015, Switzlerand
2 - Lomonosov Moscow University of Fine Chemical Technology, Moscow, Russia

12:40-13:00 **IV-OP06** Prof. Koltunov Konstantin
Koltunov K.Yu.[1,2], Sobolev V.I.[1,3], Bondareva V.M.[1]
Oxidation, Oxidative Esterification and Ammoxidation of Acrolein over Metal Oxides: Do These Reactions Include Nucleophilic Acyl Substitution?
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Tomsk State University, Tomsk, Russia

13:00-14:30 ***Lunch***

KORSTON Pushkin hall

Evening Session

Chairmen: Dr. McIndoe Jason, *Department of Chemistry, University of Victoria, Victoria, Canada*
Dr. Perret Noemie, *University of Liverpool, Liverpool, United Kingdom*

Keynote Lecture

14:30-15:10 **IV-KN3** Prof. Jones Christopher
Design of Supported Molecular Catalysts for Organic Synthesis
Georgia Institute of Technology, Atlanta, USA

Oral Presentation

15:10-15:30 **IV-OP07** Prof. Bryliakov Konstantin
Talsi E.P., Bryliakov K.P.
Highly Enantioselective Oxidation of Olefins and Thioethers with H_2O_2 Mediated by Chiral Titanium(IV) Complexes
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia

15:30-16:00 ***Coffee break***

Chairmen: Prof. Koltunov Konstantin, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Hulea Vasile, *Charles Gerhardt Institut, Ecole Nationale Superieure de Chimie, Montpellier, France*

Oral Presentations

16:00-16:20 **IV-OP08** Dr. Zhang Zhanguo
Zhang Z.-G.[1], Xu Y.[1], Suzuki Y.[1], Ma H.[2], Yamamoto Y.[2]
Catalytic Performance of Fluidizable Binder-free Mo/HZSM-5 Catalyst in the Non-oxidative Methane Conversion to Benzene at Severe Conditions
1 - National Institute of Advanced Industrial Science and Technology (AIST), Onogawa 16-1, Tsukuba-shi, Ibaraki 305-8569, Japan
2 - Core Research Technology Laboratories, Meidensha Corporation, Osaki 2-8-1, Shinagawa-ku, Tokyo 141-8642, Japan

16:20-16:40 **IV-OP09** Prof. Venvik Hilde
Dadgar F.[1], Myrstad R.[2], Pfeifer P.[3], Holmen A.1, Venvik H.J.[1]
Direct Dimethyl Ether Synthesis from Synthesis Gas: the Influence of Methanol Dehydration on Methanol Synthesis Reaction
1 - Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway
2 - SINTEF Materials and Chemistry, N-7465 Trondheim, Norway
3 - Karlsruhe Institute of Technology (KIT), Institute for Micro Process Engineering (IMVT), Hermann-von-Helmholtz-Platz, DE-76344 Eggesnstein-Leopoldshafen, Germany

16:40-17:00 **IV-OP10** Erickson James K.
Erickson J.K.[1], Baucherel X.[2], Gladden L.F.[1]
Methanol to Hydrocarbons over ZSM-5: Diffusion and the External Particle Surface
1 - University of Cambridge, Department of Chemical Engineering and Biotechnology, Cambridge, CB2 3RA, United Kingdom
2 - Johnson Matthey Technology Centre, Chilton, Billingham, TS23 1LH, United Kingdom

17:30-20:00 **Excursion «Millennial Kazan»**

Monday, August 31

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Lercher Johannes, *Technical University of Munich, Department of Chemistry, Garching, Germany; Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA*
Prof. Stakheev Alexander, *Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia*

Plenary Lectures

08:30-09:30 **PL-3** Dr. Bellussi Giuseppe
Fossil and Renewable Energy: the Turning Point of the Liquid Fuels Production
Eni S.p.A, SVP Downstream R&D, Via Maritano 26, 20097 San Donato Milanese — I, Italy

09:30-10:30 **PL-4** Prof. Hutchings Graham
Catalysis Using Supported Gold and Gold Palladium Nanoparticles
Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, UK

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Tolstoy hall

Section 1. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

Chairmen: Dr. Ordonez Salvador, *University of Oviedo, Oviedo, Spain*
Dr. Sinev Mikhail, *Semenov Institute of Chemical Physics RAS, Moscow, Russia*

Oral Presentations

11:00-11:20 **I-OP01** Dr. Wang Gaowei W.
Wang G.W., Wei Y.L., Gao H.X., Yang W.M.
Layered Zeolite SRZ-21 for Cumene Production
Sinopec Shanghai Research Institute of Petrochemical Technology, Shanghai, China

11:20-11:40 **I-OP02** Astafan A.
Astafan A.[1,2], Benghalem M.A.[1], Belin T.[1], Pouilloux Y.[1], Patarin J.[2], Bats N.[3], Bouchy C.[3], Pinard L.[1], Daou T.J.[2]
Relationship between the Crystal Morphology and Acidity of the *BEA-type Zeolites and the Resistance to Coke Formation during Ethanol to Hydrocarbons Transformation
1 - Institut de Chimie des Milieux et Matériaux de Poitiers, UMR 7285 CNRS, 4 Rue Michel Brunet, 86073 Poitiers, France
2 - Université de Strasbourg, Université de Haute Alsace, Equipe Matériaux à Porosité Contrôlée (MPC), Institut Science des Matériaux de Mulhouse (IS2M), UMR CNRS 7361, ENSCMu, 68093 Mulhouse, France
3 - IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize, France

11:40-12:00 **I-OP03** Prof. SimakovAndrey
Evangelista V.[1], Acosta B.[1], Miridonov S.[2], Pestryakov A.[3], Fuentes S.[4], Simakov A.[4]
Gold-based Yolk-shell Nanoreactors. Enhancement of Catalytic Performance via Gold Cores Decoration with Ceria or Pd
1 - Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), Posgrado en Física de Materia les, Ensenada, B. C., 22860, México
2 - Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), Departamento de Óptica, Ensenada, B. C., 22860, México
3 - Tomsk Polytechnic University, Department of Technology of Organic Substance and Polymer Materials, Tomsk, Russia
4 - Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México (CNyN-UNAM), Departamento de Nanocatálisis, Ensenada, B. C., 22860, México

12:00-12:20 **I-OP04** Dr. Gervasini Antonella
Ly N.[1], Al-Shamery K.[1], Gervasini A.[2], Carniti P.[2], Chan-Thaw C.E.[2], Prati L.[2]
Tuning the Catalytic Activity of Pt and PtCo Nanoparticles by Acidic Mixed-oxide Supports
1 - Carl von Ossietzky University of Oldenburg, Institute of Chemistry, Physical Chemistry 1, Carl-von-Ossietzky-Straße 9-11, 26129 Oldenburg, Germany
2 - Università degli Studi di Milano, Dipartimento di Chimica, via Camillo Golgi 19, 20133 Milano, Italy

12:20-12:40 **I-OP05** Prof. Kegnæs Soeren
Abildstrøm J., Gallas Hulin A., Mielby J., Kegnæs S.
Selective Catalysis with Metal Nanoparticles Encapsulated in Porous Materials
Technical University of Denmark, Department of Chemistry, Lyngby, Denmark

12:40-13:00 **I-OP06** Dr. Henry Reynald
Henry R.[1], Brogaard R.Y.[1], Ganjkhanlou Y.[2], Berlier G.[2], Bleken B.T.[1], Groppo E.[2], Olsbye U.[1], Bordiga S.[1,2]
Ethene Oligomerization in Ni-based Zeolites: Experimental and Theoretical Investigations of the Reaction Mechanism
1 - Department of Chemistry, University of Oslo, Postboks 1033 – Blindern – 0315 Oslo, Norway
2 - Dipartimento di Chimica and NIS, Università di Torino, Via P.Giuria 7-9 – Torino, Italy

13:00-14:30 ***Lunch***

KORSTON Tolstoy hall

Evening Session

Chairmen: Prof. Simakov Andrey, *Centro de Nanociencias y Nanotecnologia de la UNAM, Ensenada, Mexico*
Dr. Teschner Detre, *Department of Inorganic Chemistry, Fritz-Haber Institute, Berlin, Germany*

Oral Presentations

14:30-14:50 **I-OP07** Dr. Pandis Pavlos
Pandis P.[1], Charisiou N.[2], Goula M.[2], Stathopoulos V.N.[1]
Synthesis, Characterization and Catalytic Study of Ni supported Apatite-type Lanthanum Silicates in Glycerol Steam Reforming Reaction
1 - Laboratory of Chemistry and Materials Technology, School of Technological Applications, Technological Educational Institute of Sterea Ellada, GR – 34400, Psahna, Chalkida, Greece
2 - Department of Environmental and Pollution Control Engineering, School of Technological Applications, Technological Educational Institute of Western Macedonia, GR – 50100, Koila, Kozani, Greece

14:50-15:10 **I-OP08** Horacek Jan
Horáček J., Kubička D.
Renewable Feedstocks for Refineries & Conventional Sulfided Catalysts
Research Institute of Inorganic Chemistry, RENTECH-UniCRE, Litvinov, Czech Republic

15:10-15:30 **I-OP09** Peroni Marco
Peroni M., Huang X., Lee I., Baráth E., Gutiérrez O.Y., Lercher J.A.
Towards Efficient Hydrodeoxygenation on Transition Metal Phosphides
Technische Universität München, Department of Chemistry and Catalysis Research Center, Germany

15:30-16:00 ***Coffee break***

KORSTON Tolstoy hall

Chairmen: Prof. Pârvulescu Vasile, *University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis, Bucharest, Romania*
Prof. Lemonidou Angeliki, *Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece*

Oral Presentations

16:00-16:20 **I-OP10** Prof. Ismagilov Zinfer
Ismagilov Z.R.[1,2], Kerzhentsev M.A.[1], Yashnik S.A.[1], Khairulin S.R.[1], Kuznetsov V.V.[1], Salnikov S.V.[1], Bourane A.[3], J. Yaming[3], Koseoglu O.R.[3]
Catalytic Oxidative Desulfurization of Diesel Fuel as an Alternative to and Combination with HDS Process
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia
3 - Saudi Aramco, Research and Development Center, Dhahran, Kingdom of Saudi Arabia

16:20-16:40 **I-OP11** Dr. Yakovlev Vadim
Yakovlev V.A.[1], Khromova S.A.[1], Kukushkin R.G.[1,2], Rodina VO.[1], Bykova M.V.[1,2], Venderbosch R.H.[3], Parmon V.N.[1]
Hydrotreatment Catalysts for Bio-oil and Lipids Processing into Valuable Chemicals and Biofuels
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Biomass Technology Group B.V., 7545 PN, Josink Esweg 34, Enschede, The Netherlands

16:40-17:00 **I-OP12** Dr. Ordonez Salvador
Cueto J., Faba L., Díaz E., Ordonez S.
Aldol Condensation of Biomass Derived Aldehydes: Comparison of the Reactivity of Furfural and Hydroximethylfurfural
University of Oviedo, Oviedo, Spain

17:30-20:00 **Excursion «Millennial Kazan»**

Tuesday, September 1

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Bukhtiyarov Valerii, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Freund Hans-Joachim, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Plenary Lectures

08:30-09:30 **PL5** Prof. Hupp Joseph T.
Mesoporous Metal-Organic Frameworks as Platforms for Single-site Heterogeneous Catalysts
Northwestern University, Evanston, IL 60208, USA

09:30-10:30 **PL6** Prof. Robert Schlögl
Dynamics in Heterogeneous Catalysis
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-1

Section 5. Catalysis and Environmental Protection

Chairmen: Prof. Aprile Carmela, *Unit of Nanomaterial Chemistry (CNano), University of Namur (UNAMUR), Department of Chemistry, Namur, Belgium*
Prof. Rempel Andrey A., *Institute of Solid State Chemistry, Ural Branch of the RAS, Ural Federal University, Ekaterinburg, Russia*

Keynote Lecture

11:00-11:40 **V-KN5** Prof. Leitner Walter
Carbon Dioxide as Carbon Source for the Energetic and Chemical Value Chain: Challenges and Opportunities for Catalysis
Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, Aachen, Germany

Oral Presentations

11:40-12:00 **V-OP08** Dr. Mortensen Peter M.
Mortensen P.M., Dybkjær I.
Performing Industrial Scale Steam Reforming of CO_2-rich Gas
Haldor Topsoe A/S, Nymøllevej 55, DK-2800 Kgs. Lyngby, Denmark

12:00-12:20 **V-OP09** Dr. Bukhtiyarova Marina
Bukhtiyarova M.[1], Schlögl R.[1,2]
Methanol Synthesis from Steel Mill Gases
1 - MPI for Chemical Energy Conversion, Mülheim a.d. Ruhr, Germany
2 - Fritz Haber Institute of MPG, Berlin, Germany

12:20-12:40 **V-OP10** Gaillard Marine
Gaillard M., Virginie M., Khodakov A.
Molybdenum-based Catalysts for the Biogas Dry Reforming
UCCS - Unité de Catalyse et de Chimie du solide - UMR 8181, Villeneuve d'Ascq, France

12:40-13:00 **V-OP11** Dr. Bonura Giuseppe
Frusteri F.[1], Bonura G.[1], Cannilla C.[1], Drago Ferrante G.[1], Aloise A.[2], Catizzone E.[2], Migliori M.[2], Giordano G.[2]
Stepwise Tuning of Multi-sites CuZnZr-HZSM5 Catalysts for Direct DME Synthesis from CO_2-H_2 Mixtures
1 - CNR-ITAE, Istituto di Tecnologie Avanzate per l’Energia “Nicola Giordano” Via S. Lucia sopra Contesse, 5 – 98126 Messina, Italy
2 - Università della Calabria, Dip. Ingegneria per l’Ambiente e il Territorio ed Ingegneria Chimica Via Pietro Bucci Cubo 44a – 87036 Arcavacata di Rende (CS), Italy

13:00-14:30 ***Lunch***

KORSTON Ball hall-1

Evening Session

Chairmen: Prof. Leitner Walter, *Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, Aachen, Germany*
Prof. Nova Isabella, *Dip.Energia, Politecnico di Milano, Milano, Italy*

Oral Presentations

14:30-14:50 **V-OP12** Dr. Suknev Alexey P.
Kovalyov E.V.[1], Suknev A.P.[1], Gulyaeva Yu.K.[1], Zaikovskii V.I.[1,2], Kaichev V.V.[1,2], Bal'Zhinimaev B.S.[1]
New Fiberglass Based Pt Catalyst for VOC and CVOC Removal
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

14:50-15:10 **V-OP13** Dr. Yashnik Svetlana A.
Yashnik S.A.[1], Danchenko N.M.[2], Ismagilov Z.R.[1,3]
Synergetic Effect of Pd Addition on Catalytic Behaviour of Monolithic Catalysts for Diesel Vehicle Emission Control
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Ural Electrochemical Integrated Plant, Novouralsk, Russia
3 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia

15:10-15:30 **V-OP14** Khudorozhkov Alexander K.
Khudorozhkov A.K.[1,2], Prosvirin I.P.[1,2], Chetyrin I.A.[1,2], Bukhtiyarov V.I.[1,2]
Propane Oxidation over Pd/Al_2O_3: Selectivity, Activity and Size Effect
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

15:30-15:50 **V-OP15** Stotz Henning
Stotz H.[1], Maier L.[2], Deutschmann O.[1,2]
Methane Oxidation over Palladium: On the Mechanism in Rich Methane-Oxygen Mixtures at High Temperatures
1 - Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology (KIT), Engesserstrasse 20, 76131 Karlsruhe, Germany
2 - Institute for Catalysis Research and Technology, Karlsruhe Institute of Technology (KIT), Engesserstrasse 20, 76131 Karlsruhe, Germany

15:50-16:10 **V-OP16** Petrov Andrey W.
Petrov A.W.[1,2], Ferri D.[1], van Bokhoven J.A.[1,2], Kröcher O.[1,3]
Hierarchical Pd/ZSM-5 Catalysts for Methane Oxidation in the Presence of Steam
1 - Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
2 - ETH Zürich, Department of Chemistry and Applied Biosciences, Zürich, Switzerland
3 - EPF Lausanne, Institute of Chemical Sciences and Engineering, Lausanne, Switzerland

16:10-16:30 **V-OP17** Lopez-Gonzalez Diego
Lopez-Gonzalez D.[1], Jimènez-Cadena G.[2], Tsampas M.[1], Boréave A.[1], Klotz M.[2], Tardivat C.[2], Cartoixa B.[3], Pajot K.[4], Vernoux P.[1]
Mixed Ionic-electronic Conducting Catalysts for Catalysed Gasoline Particulate Filter
1 - CNRS, UMR 5256, IRCELYON, Institut de Recherches sur la Catalyse et l'Environnement de Lyon, 2 Av. Albert Einstein, F-69626, Villeurbanne, France
2 - Laboratoire de Synthèse et Fonctionnalisation des Céramiques, UMR3080, CNRS/Saint-Gobain, 550 Av. Alphonse Jauffret 84306 Cavaillon Cedex, France
3 - CTI, Céramiques Techniques Industrielles, 382 Avenue du Moulinas 30340 Salindres, France
4 - PSA PEUGEOT CITROËN, Centre technique de Vélizy, Route de Gisy 78943 Vélizy-Villacoublay, France

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155,**

ISO-PP1÷ISO-PP30 (Poster set-up time 09:00 – 19:00)

Tuesday, September 1

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Bukhtiyarov Valerii, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Freund Hans-Joachim, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Plenary Lectures

08:30-09:30 **PL5** Prof. Hupp Joseph T.
Mesoporous Metal-Organic Frameworks as Platforms for Single-site Heterogeneous Catalysts
Northwestern University, Evanston, IL 60208, USA

09:30-10:30 **PL6** Prof. Robert Schlögl
Dynamics in Heterogeneous Catalysis
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-2

Section 2. Catalyst Preparation and Characterization

Chairmen: Dr. Penner Simon, *University of Innsbruck, Institute for Physical Chemistry, Innsbruck, Austria*
Prof. van Bokhoven Jeroen A., *Institute for Chemical and Bioengineering, ETH Zurich and Paul Scherrer Institute, Villigen, Switzerland*

Oral Presentations

11:00-11:20 **II-OP11** Prof. Mossin Susanne
Mossin S.[1], Janssens T.V.W.[2], Rasmussen S.B.[2], Vennestrøm P.N.R.[2], Lundegaard L.F.[2], Moses P.G.[2], Giordanino F.[3], Borfecchia E.[3], Lomachenko K.A.[3,4], Bordiga S.[3], Godiksen A.[1], Beato P.[2]
Chemistry of the Active Metal Center in the Selective Catalytic Reduction of NO by NH_3
1 - Department of Chemistry, Technical University of Denmark, Lyngby, Denmark
2 - Haldor Topsøe A/S, Lyngby, Denmark
3 - Department of Chemistry, NIS Centre of Excellence and INSTM Reference Center, University of Turin, Turin, Italy
4 - Southern Federal University, Rostov-on-Don, Russia

11:20-11:40 **II-OP12** Dr. Zemlyanov Dmitry
Paul R.[1,2], Gharachorlou A.[3,2], Detwiler M.D.[3,2], Delgass W.N.[3,2], Ribeiro F.H.[3,2], Reifenberger R.G.[4,2], Fisher T.S.[5,2], Zemlyanov D.Y.[1,2]
Novel Preparation of Reverse Model Catalyst for CO Oidation and H_2O Dissociation
1 - Birck Nanotechnology Center, West Lafayette, IN, USA
2 - Purdue University, West Lafayette, IN, USA
3 - School of Chemical Engineering, West Lafayette, IN, USA
4 - Department of Physics, West Lafayette, IN, USA
5 - Department of Mechanical Engineering, West Lafayette, IN, USA

Keynote Lecture

11:40-12:20 **II-KN6** Dr. Helveg Stig
Electron Microscopy Advances in Catalysis
Haldor Topsoe A/S, Nymøllevej 55, Kgs. Lyngby, Denmark

Oral Presentations

12:20-12:40 **II-OP13** Dr. Cadete Santos Aires Francisco Jose
Cadete Santos Aires F.J.[1], Aouine M.[1], Li S.[1], Tuel A.[1], Epicier T.[1,2]
Dynamic High-Resolution Study of the Structural Evolution of Ag Nanoparticles During Carbon Gasification within an Aberration-Corrected Environmental Transmission Electron Microscope
1 - Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256 CNRS/UCB Lyon 1, 2 Avenue Albert Einstein, 69626 Villeurbanne, France
2 - Laboratoire MATEIS, UMR 5510, CNRS/INSA de Lyon, 69621 Villeurbanne Cedex, France

12:40-13:00 **II-OP14** Dr. Ek Carl Martin
Ek M.[1], Zhu Y.[1], Brorson M.[1], Moses P.G.[1], Puig Molina A.M.[1], Ramasse Q.[2], Kisielowski C.[3], Helveg S.[1]
Atomic-Resolution Imaging of Environmental Catalysts
1 - Haldor Topsoe A/S, Nymøllevej 55, Kgs. Lyngby, DK-2800, Denmark
2 - SuperSTEM Laboratory, SciTech Daresbury Campus, Daresbury WA4 4AD, UK
3 - NCEM, Lawrence Berkeley National Laboratory, CA, USA

13:00-14:30 ***Lunch***

KORSTON Ball hall-2

Evening Session

Chairmen: Dr. Zemlyanov Dmitry, *Birck Nanotechnology Center, Purdue University, West Lafayette, IN, USA*
Prof. Bordiga Silvia, *Department of Chemistry, NIS and INSTM Reference Centre, University of Turin, Torino, Italy*

Oral Presentations

14:30-14:50 **II-OP15** Dr. Doronkin Dmitry E.
Doronkin D.E., Günter T., Carvalho H.W.P., Baier S., Boubnov A., Sheppard T., Casapu M., Grunwaldt J.-D.
Operando Spatially- and Time-Resolved XES Andvalence-to-Core-XES for the Characterization of Fe- and Cu-Zeolite Catalysts for NH_3-SCR of NO_x
Karlsruhe Institute of Technology, Karlsruhe, Germany

14:50-15:10 **II-OP16** Dr. Hävecker Michael
Hävecker M.[1,2], Heine C.[2], Eichelbaum M.[2,3], Rosowski F.[3], Trunschke A.[2], Pfeifer V.[2], Velasco Vélez J.J.[2,4], Lips K.[1], Reichardt G.[1], Reichardt G.[1], Knop A.[2], Schlögl R.[2,4]
Novel Research platforms ISISS and EMIL at BESSY II: In Situ Surface Characterization of Catalysts by Synchrotron Based Near Ambient Pressure X-ray Electron Spectroscopy
1 - Helmholtz-Zentrum Berlin für Materialien und Energy / BESSY II, Energy Materials, Berlin, Germany
2 - Fritz-Haber-Institut der Max-Planck-Gesellschaft, Inorganic Chemistry, Berlin, Germany
3 - TU Berlin, BasCat, UniCAT BASF JointLab, Berlin, Germany
4 - Max-Planck-Institut für Chemische Energiekonversion, Heterogeneous Reactions, Mülheim a.d. Ruhr, Germany

15:10-15:30 **II-OP17** Dr. Kaichev Vasily
Kaichev V.[1], Chesalov Y.[1], Saraev A.[1], Klyushin A.[2], Knop-Gericke A.[2], Andrushkevich T.[1], Bukhtiyarov V.[1]
Mechanism for Selective Oxidation of Ethanol over V-Ti Catalyst
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Department of Inorganic Chemistry, Fritz Haber Institute of the Max Plank Society, Berlin, Germany

15:30-15:50 **II-OP18** Klyushin Alexander Yu.
Klyushin A.Yu.[1], Rocha T.C.R.[1], Li X.[1], Huang X.[1], Lunkeinbein T.[1], Friedrich M.[1], Hävecker M.[1,2], Bukhtiyarov A.V.[3,4], Prosvirin I.P.[3,4], Bukhtiyarov V.I.[3,4], Knop-Gericke A.[1], Schlögl R.[1]
What are the Active Sites of Gold in CO Oxidation Reaction?
1 - Fritz-Haber-Institute of the Max Planck Society, Department of Inorganic Chemistry, Berlin, Germany
2 - Helmholtz-Zentrum Berlin/BESSY II, Department of Solar Energy Research, Berlin, Germany
3 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
4 - Novosibirsk State University, Novosibirsk, Russia

15:50-16:10 **II-OP19** Schilling Christian M.
Schilling C.M., Lohrenscheit M., Hess C.
Ceria Supported Gold Catalysts: Mechanistic Studies of CO Oxidation Using a Combined Operando Approach
Technische Universität Darmstadt, Darmstadt, Germany
Eduard Zintl-Institut für Anorganische und Physikalische Chemie, Darmstadt, Germany

16:10-16:30 **II-OP20** Dr. Vovk Evgeny
Vovk E.I.[1,2], Karatok M.[2], Shah S.A.A.[2], Turksoy A.[2], Bukhtiyarov V.I.[1], Ozensoy E.[3]
Reactivity of Oxygen in Methanol Partial Oxidation over Au(111) Model Catalyst Surface
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Bilkent University, Chemistry Department, Bilkent, Turkey
3 - Bilkent University, Department of Chemistry, Bilkent, Turkey

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155, ISO-PP1÷ISO-PP30** (Poster set-up time 09:00 – 19:00)

Tuesday, September 1

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Bukhtiyarov Valerii, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Freund Hans-Joachim, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Plenary Lectures

08:30-09:30 **PL5** Prof. Hupp Joseph T.
Mesoporous Metal-Organic Frameworks as Platforms for Single-site Heterogeneous Catalysts
Northwestern University, Evanston, IL, USA

09:30-10:30 **PL6** Prof. Schlögl Robert
Dynamics in Heterogeneous Catalysis
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Pushkin hall

Section 4. Catalysis and Chemicals

Chairmen: Prof. Jones Christopher W., *Georgia Institute of Technology, Atlanta, USA*
Prof. Talsi Evgenii P., *Boreskov Institute of Catalysis, Novosibirsk, Russia*

Oral Presentations

11:00-11:20 **IV-OP11** Prof. Cavani Fabrizio
Cavani F.[1], Lolli A.[1], Utili L.[1], Amadori R.[1], Lucarelli C.[1,2], Albonetti S.[1]
Insights in the Reaction Mechanism for HMF Oxidation to FDCA over Bimetallic Au/Pd Nanoparticles
1 - Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Bologna, Italy
2 - Università dell'Insubria, Via Valleggio 11, 22100 Como, Italy

11:20-11:40 **IV-OP12** Nese Valentina
Nese V., Schüth F.
Noble Metal Nanoparticles Supported on Carbon-based Materials as Catalysts for 5-HMF Oxidation to FDCA
Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany

11:40-12:00 **IV-OP13** Dr. Zhu Yinghuai
Catalytic Applications of Palladium Nanoparticles-supported Nanocomposites in Carbonylation Reactions
Institute of Chemical and Engineering Sciences, Jurong Island, Singapore

12:00-12:20 **IV-OP14** Prof. d'Alessandro Nicola
Di Pietrantonio K.[1,2], Tonucci L.[1,3], d'Alessandro N.[1,2], Bressan M.[1,2]
Hydrogenation Reactions in Aqueous Media Catalysed by Pd and Pt Green Nanoparticles
1 - 'Gabriele d'Annunzio' University of Chieti Pescara
2 - Department INGEO
3 - Department of Philosophical, Educational and Economic Science

Keynote Lecture

12:20-13:00 **IV-KN7** Prof. Koenig Burkhard
Chemical Photocatalysis Using Visible Light
Faculty of Chemistry and Pharmacy, University of Regensburg, Regensburg, Germany

13:00-14:30 ***Lunch***

KORSTON Pushkin hall

Evening Session

Chairmen: Prof. Trifonov Alexander, *Institute of Organometallic Chemistry of Russian Academy of Sciences, Nizhny Novgorod, Russian Federation*
Prof. Yang Qihua, *State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

Oral Presentation

14:30-14:50 **IV-OP15** Van Der Graaff Willem N.P.
Van Der Graaff W.N.P., Tempelman C.H.L., Pidko E.A., Hensen E.J.M.
Room Temperature Glucose Isomerization in Sn-BEA: on the Role of Diffusion under Practical Reaction Conditions
Inorganic Materials Chemistry Group, Eindhoven University of Technology, Eindhoven, The Netherlands

14:50-15:10 **IV-OP16** Prof. Pidko Evgeny A.
Pidko E.A., Hensen E.J.M.
A Theoretical Perspective on the Role of Cooperativity in Glucose Activation by Lewis Acid Zeolite and Oxide Catalysts
Eindhoven University of Technology, Eindhoven, the Netherlands
Institute for Complex Molecular Systems, Eindhoven University of Technology, Eindhoven, the Netherlands

15:10-15:30 **IV-OP17** Tolborg Søren
Tolborg S.[1,2], Sádaba I.[2], Osmundsen C.M.[2], Fristrup P.[1], Taarning E.[2]
New Insights in the Catalytic Conversion of Sugars with Sn-Beta
1 - Technical University of Denmark, Department of Chemistry, Nymøllevej 55, 2800 Kgs. Lyngby, Denmark
2 - Haldor Topsøe A/S, Nymøllevej 55, 2800 Kgs. Lyngby, Denmark

15:30-15:50 **IV-OP18** Dr. Delidovich Irina
Delidovich I., Palkovits R.
Mg-Al Hydrotalcites with Tailored Structure as Efficient Catalysts for Glucose Isomerization into Fructose
RWTH Aachen University, Aachen, Germany

15:50-16:10 **IV-OP19** Dr. Padovani Alessia
Padovani A., Schüth F.
Liquid Phase Oxidation of Glucose to Gluconic Acid over Supported Metal Catalysts
Max Planck Institut für Kohlenforschung, Mülheim an der Ruhr, Germany

16:10-16:30 **IV-OP20** Prof. Coman Simona M.
Anita F., Podolean I., Parvulescu V.I., Coman S.M.
Efficient Carbon Based Catalysts with Acid Sites and Magnetic Properties for Starch Valorization to Bio-chemicals
University of Bucharest, Faculty of Chemistry, Bucharest, Romania

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155, ISO-PP1÷ISO-PP30** (Poster set-up time 09:00 – 19:00)

Tuesday, September 1

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

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Prof. Freund Hans-Joachim, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Plenary Lectures

08:30-09:30 **PL5** Prof. Hupp Joseph T.
Mesoporous Metal-Organic Frameworks as Platforms for Single-site Heterogeneous Catalysts
Northwestern University, Evanston, IL 60208, USA

09:30-10:30 **PL6** Prof. Robert Schlögl
Dynamics in Heterogeneous Catalysis
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Tolstoy hall

Section 3. Energy-Related Catalysis

Chairmen: Dr. Takanabe Kazuhiro, *Division of Physical Sciences and Engineering, KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia*
Dr. Tatsumi Takashi, *Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8550, Japan*

Oral Presentations

11:00-11:20 **III-OP02** Gao Lu
Gao L.[1], Hofmann J.P.[1], Bakkers E.P.A.M.[2], Emiel E.J.M.[1]
Efficient Nanostructured in Photocathodes for Water Reduction through Optimization of Interface Energetics and Structure
1 - Laboratory of Inorganic Materials Chemistry, Department of Chemical Engineering and Chemistry Eindhoven University of Technology, Eindhoven, The Netherlands
2 - Photonics and Semiconductor Nanophysics, Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

11:20-11:40 **III-OP03** Dr. Kozlova Ekaterina A.
Kozlova E.A.[1,2,3], Cherepanova S.V.[1,2,3], Markovskaya D.V.[1,2], Parmon V.N.[1,2]
Novel Photocatalysts Based on $Cd_{1-x}Zn_xS/Zn(OH)_2$: Activation during the Hydrogen Evolution from Aqueous Solutions of Ethanol
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3- Educational Center for Energoefficient Catalysis in Novosibirsk State University, Novosibirsk, Russia

11:40-12:00 **III-OP04** Prof. Pokrant Simone
Landsmann S., Mägli A., Pokrant S., Trottmann M.
The Role of Co-catalysts in Photoelectrochemical Versus Photocatalytic Water Splitting: CoO_x on $LaTiO_2N$
Laboratory Materials for Energy Conversion, Empa, Dübendorf

12:00-12:20 **III-OP05** Weide Philipp
Muhler M.[1], Weide P.[1], Busser G. W.[1], Mei B.[2], Lukic S.[3], Winterer M.[3]
Photocatalytic Overall Water Splitting using Ga_2O_3 with Various Phase Compositions Loaded with Rh-free Co-catalysts
1 - Laboratory of Industrial Chemistry, Ruhr-University Bochum, Germany
2 - Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark
3 - Nanoparticle Process Technology, University of Duisburg-Essen, Duisburg, Germany

12:20-12:40 **III-OP06** Marchal Clément
Caps V., Keller N., Keller V., Marchal C.
Synthesis and Reactivity of $Au/g\text{-}C_3N_4/TiO_2$ Nanocomposites for Water-Splitting under Solar Light Illumination
ICPEES, Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé, CNRS/Université de Strasbourg, UMR 7515 (CNRS), 25 rue Becquerel 67087 Strasbourg Cedex, France

12:40-13:00 **III-OP07** Prof. Puga Alberto V.
Puga A.V., Sastre F., Liu L.C., García H., Corma A.
Efficient Solar Production of Methane from CO_2 and H_2 Using Nickel Catalysts
Instituto de Tecnología Química, Valencia, Spain

13:00-14:30 ***Lunch***

KORSTON Tolstoy hall

Evening Session

Chairmen: Prof. Millan Marcos, *Department of Chemical Engineering, Imperial College London, London, UK*
Dr. Bulushev Dmitri, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

14:30-14:50 **III-OP08** Prof. Amouroux Jacques
Amouroux J.[1,2], Siffert P.[2]
Carbon Dioxide and Circular Economy for an Industrial Revolution
1 - Ecole Nationale Superieure de Chimie de Paris, Université Pierre et Marie Curie. 11, Rue Pierre et Marie Curie – 75231 Paris Cedex 05, France
2 - The European Materials Research Society, BP. 20 F-67037 Strasbourg Cedex 2, France

14:50-15:10 **III-OP09** Dr. Teschner Detre
Nong H.N.[1], Reier T.[1], Oh H.-S.[1], Gan L.[1], Willinger E.[2], Teschner D.[2], Strasser P.[1]
IrNiO$_X$-based Oxide Thin-Films and Metal-Oxide Hybrid Core-Shell Nanoparticles as Efficient Electrocatalysts of Oxygen Evolution
1 - Technical University Berlin, Department of Chemistry, Berlin, Germany
2 - Fritz-Haber Institute, Department of Inorganic Chemistry, Berlin, Germany

15:10-15:30 **III-OP10** Dr. Villa K.
Murcia S.[1], Villa K.[1], Andreu T.[1], Morante J.R.[1,2]
Partial Oxidation of Methane to Methanol with Bismuth-Based Photocatalysts
1 - Catalonia Institute for Energy Research (IREC), Sant Adrià de Besòs, Spain
2 - University of Barcelona (UB), Department of Electronics, Barcelona, Spain

15:30-15:50 **III-OP11** Prof. Rempel Andrey A.
Rempel A.A.[1,2], Sadovnikov S.I.[1], Kozlova E.A.[2,3], Gerasimov E.Yu.[3]
Photocatalytic Hydrogen Evolution from Aqueous Solutions of Na_2S/Na_2SO_3 under Visible Light Irradiation of Nonstoichiometric Silver Sulfide Nanoparticles
1 - Institute of Solid State Chemistry, Ural Branch of the RAS, Ekaterinburg, Russia
2 - Ural Federal University, Ekaterinburg, Russia
3 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

15:50-16:10 **III-OP12** Prof. Faria Joaquim L.
Pastrana-Martínez L.M., Silva A.M.T., Fonseca N.N.C., Figueiredo J.L., Faria J.L.
CO_2 Conversion into Solar Fuels
LSRE-LCM, Departamento de Engenharia Química, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal

16:10-16:30 **III-OP13** Sanwald Kai E.
Sanwald K.E., Berto T.F., Eisenreich W., Gutiérrez O.Y., Lercher J.A.
Photocatalytic Pathways for Hydrogen Production from Biomass over UV- and Visible-Light Responsive Materials
Department of Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155, ISO-PP1÷ISO-PP30** (Poster set-up time 09:00 – 19:00)

Tuesday, September 1

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Bukhtiyarov Valerii, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Freund Hans-Joachim, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Plenary Lectures

08:30-09:30 **PL5** Prof. Hupp Joseph T.
Mesoporous Metal-Organic Frameworks as Platforms for Single-site Heterogeneous Catalysts
Northwestern University, Evanston, IL 60208, USA

09:30-10:30 **PL6** Prof. Robert Schlögl
Dynamics in Heterogeneous Catalysis
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Dostoevsky hall

XI European Workshop on Innovation in Selective Oxidation (ISO'15) "Selectivity in Oxidation: Key to new resources valorization" (1-3 September, 2015)

The Workshop is focused on selectivity improvement by: Molecular design of catalytic sites and new reactions; Synthesis of novel catalytic materials; Use of non-conventional oxidants; In situ and operando mechanistic studies; Chemical reaction and reactor engineering

Chairmen: Prof. Lercher Johannes, *Technical University of Munich, Department of Chemistry, Garching, Germany; Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA*
Dr. Cortés Corberán Vicente, *Institute of Catalysis and Petroleumchemistry (ICP), CSIC, Madrid, Spain*

11:00-11:20 Opening ceremony

Oral Presentations

11:20-11:40 **ISO-OP01** Dr. Lopez Nieto Jose M.
Soriano M.D.[1], Chieregato A.[1], Zamora S.[1], Bandinelli C.[2], Cavani F.[2], Lopez Nieto J.M.[1]
V-, Nb-, and Ti-promoted Hexagonal Tungsten Bronzes as Selective Catalysts in the Transformation of Glycerol and Methanol in Aerobic Conditions
1 - Instituto Tecnologia Quimica, UPV-CSIC, Valencia, Spain
2 - Dipartimento Chimica Industriale e di Materiali, Universitá di Bologna, Bologna, Italy

11:40-12:00 **ISO-OP02** Prof. Pescarmona Paolo P.
Lueangchaichaweng W.[1], Sheng X.[1], Vankelecom I.F.[1], Pescarmona P.P.[1,2]
Metal-free Heterogeneous Catalysts for the Epoxidation of Alkenes with H_2O_2
1 - COK, University of Leuven, Belgium
2 - Chemical Engineering Department, University of Groningen, The Netherlands

12:00-12:20 **ISO-OP03** Prof. Prati Laura
Campisi S.[1], Villa A.[1], Chan Thaw C.E.[1], Ferri D.[2], Prati L.[1]
Tuning the Selectivity in Pd Catalyzed Liquid-phase Oxidation of Benzyl Alcohol: an in situ ATR-IR Study
1 - Università degli Studi di MIlano, Dipartimento di Chimica, Milano, Italy
2 - Paul Scherrer Institute, Villigen, Switzerland

12:20-12:40 **ISO-OP04** Dr. Simonov Mikhail
Simonov M.N.[1,2], Sadykov V.A.[1,2], Rogov V.A.[1,2], Bobin A.S.[1,2], Sadovskaya E.M.[1,2], Mezentseva N.V.[1,2], Roger A.-C.[3], Van Veen A.C.[4]
Ethanol Selective Oxidation into Syngas over Pt-promoted Fluorite-like Oxide: SSITKA and Pulse Microcalorimetry Study
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - University of Strasbourg, Strasbourg, Srausbourg, France
4 - University of Warwick, Coventry CV4 7AL, UK

12:40-13:00 **ISO-OP05** Dr. Cortes Corberan Vicente
Martínez-González S.[1], Ivanova S.[2], Domínguez M.I.[2], Cortés Corberán V.[1]
Selectivity Control in Oxidation of 1-tetradecanol on Supported Nano Au Catalysts
1 - Institute of Catalysis and Petroleumchemistry (ICP), CSIC, 28049 Madrid, Spain
2 - Institute of Materials Science of Seville (ICMS), University of Seville - CSIC, 41092 Seville, Spain

13:00-14:30 ***Lunch***

KORSTON Dostoevsky hall

Evening Session

Chairmen: Prof. Perathoner Siglinda, *Department of Electronic Engineering, Industrial Chemistry and Engineering, University of Messina, Messina, Italy*
Prof. Sadykov Vladislav, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Keynote Lecture

14:30-15:10 **ISO-KN01** Dr. Kholdeeva Oxana A.
Liquid-Phase Selective Oxidation Catalysis with Metal-Organic Frameworks
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia

15:10-15:30 **ISO-OP06** Prof. Pestryakov Alexey
Kotolevich Y.[1], Kolobova E.[2], Cabrera Ortega J.E.[3], Tiznado Vazquez H.J.[1], Bogdanchikova N.[1], Cortés Corberán V.[4], Zanella R.[5], Pestryakov A.[2]
Promoted Au and Ag Catalysts for Liquid Phase Selective Oxidation of Octanol
1 - Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, 22860, México
2 - Tomsk Polytechnic University, 634050 Tomsk, Russia
3 - Universidad Autónoma de Baja California, Ensenada, 22860, México
4 - Institute of Catalysis and Petroleumchemistry (ICP), CSIC, 28049 Madrid, Spain
5 - Centro de Ciencias Aplicadas y Desarrollo Tecnológico (UNAM), México, DF, 04510, México

15:30-15:50 **ISO-OP07** Dr. Moskaleva Lyudmila V.
Selective Epoxidation of Propylene to Propylene Oxide on Gold-based Catalysts: a Theoretical Study
Institute of Applied and Physical Chemistry and Center for Environmental Research and Sustainable Technology, Universität Bremen, Bremen, Germany

15:50-16:10 **ISO-OP08** Dr. Khaskin Eugene
Khaskin E.[1,2], Milstein D.[2]
Oxidant-free Formal Oxidation of Alcohol Substrates towards Higher Value Added Products
1 - Okinawa Institute of Science and Technology Graduate School, Japan
2 - Weizmann Institute of Science, Rehovot, Israel

16:10-16:30 **ISO-OP09** Dr. Mamontov Grigory V.
Mamontov G.V.[1], Dutov V.V.[1], Grabchenko M.V.[1], Zaikovskii V.I.[2,3], Sobolev V.I.[1,2], Vodyankina O.V.[1]
Metal-Support Interaction – A Key Reason for Ag Catalyst Activity in Low-Temperature Oxidation
1 - Tomsk State University, Laboratory of Catalytic Research, Tomsk, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155,**

ISO-PP1÷ISO-PP30 (Poster set-up time 09:00 – 19:00)

Tuesday, September 1

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KORSTON Ball hall

Morning Session

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Prof. Freund Hans-Joachim, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Plenary Lectures

08:30-09:30 **PL5** Prof. Hupp Joseph T.
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Dynamics in Heterogeneous Catalysis
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Lermontov hall

Discussion symposium 1. “Value-Added Chemicals from Renewables”

Chairmen: Prof. Murzin Dmitry, *Åbo Akademi University, Turku, Finland*
Prof. Román-Leshkov Yuriy, *Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*

11:00-13:00 **DS1-1**
Gromov N.V.[1,2,3], Taran O.P.[1,4], Aymonier C.[2], Parmon V.N.[1,5]
Conversion of Cellulose into 5-Hydroxymethylfurfural over Solid Acid Catalysts Based on Sibunit Carbon Material
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institut de chimie de la matière condensée de Bordeaux, CNRS, ICMCB, UPR 9048, 87, av. du Dr Schweitzer, Pessac, 33608, France
3 - Universite Bordeaux, ICMCB UPR 9048, Pessac, 33600, France
4 - Novosibirsk State Technical University, Novosibirsk, Russia
5 - Novosibirsk State University, Novosibirsk, Russia

DS1-2
Deng W.P.[1], Zhou C.M.[1,2], Wan X.Y.[1], Zhang Q.H.[1], Yang Y.H.[2], Wang Y.[1]
Carbon Nanotube-supported Pt Nanoparticles as Efficient Catalysts for Base-free Aerobic Oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic Acid
1 - State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China
2 - School of Chemical and Biomedical Engineering, Nanyang Technological University Singapore 637459, Singapore

DS1-3
Laforge S., Mijoin J., Pouilloux Y., Dialo M.D.
Transformation of Glycerol to Acrolein over Isomorphously Substituted Iron Zeolites
Institut des Milieux et Matériaux de Poitiers (IC2MP), UMR CNRS 7285, 4 Rue Michel Brunet, Bâtiment B27, TSA 51106 86073 Poitiers Cedex 9, France

DS1-4
Kale S.[1], Armbruster U.[1], Umbarkar S.[2], Dongare M.[2,3], Eckelt R.[1], Martin A.[1]
Gas Phase Glycerol Acetylation to Fuel Additive over Solid Acid Catalysts
1 - Leibniz Institute for Catalysis, Rostock, Germany
2 - National Chemical Laboratory, Pune, India
3 - Mojj Eng. Syst. Ltd, Pune, India

DS1-5
Lombardi E., Basile F., Fornasari G., Mafessanti R., Vaccari A.
Effect of Microemulsion-synthesized Support in the Aqueous Phase Reforming Reaction of Glycerol
University of Bologna, dep. of Industrial Chemistry, Bologna, Italy

DS1-6
Liu R., Wang T., Jin Y.
Dehydration of Biodiesel-derived Crude Glycerol into Acrolein over HPW Supported on Cs-modified SBA-15
Beijing Key Laboratory of Green Reaction Engineering and Technology, Department of Chemical Engineering, Tsinghua University, Beijing, China

DS1-7
Isa Y.M.
Effects of Promotion Techniques on ZSM-5 activity in Conversion of Alcohols to Fuel Range Hydrocarbons
Durban University of Technology, Durban, South Africa

DS1-8
Phung T.K., Garbarino G., Busca G.
Ethanol Conversion to Useful Products: Ethylene, Diethyl Ether, Higher Hydrocarbons, Acetaldehyde and Acetone
University of Genova, Department of Civil, Chemical and Environmental Engineering, Genova, Italy

DS1-9
Quesada J., Faba L., Diaz E., Ordonez S.
Deactivation of Mixed Oxides as Catalysts for Ethanol Condensation: in situ DRIFT Spectroscopy Studies
University of Oviedo, Oviedo, Spain

DS1-10
Velasquez Ochoa J.[1], Chieregato A.[1], Bandinelli C.[1], Fornasari G.[1], Cavani F.[1], Mella M.[2]
Insights on the Mechanism for the Transformation of Ethanol on Basic Oxides (Lebedev and Guerbet Reactions)
1 - Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Viale del Risorgimento 4, 40136, Bologna, Italy
2 - Dipartimento di Scienze ed Alta Tecnologia, Università degli Studi dell'Insubria, Via Valleggio 11, 22100, Como, Italy

DS1-11
Suknev A.P.[1], Zaikovskii V.I.[1,2], Kaichev V.V.[1,2], Paukshtis E.A.[1,2], Sadovskaya E.M.[1,2], Bal'zhinimaev B.S.[1]
Selective Hydrogenation of Hexanoic Acid to Hexanol under Mild Conditions over Titania-based Pt-Re Catalyst
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

13:00-14:30 ***Lunch***

KORSTON Lermontov hall

Evening Session

Chairmen: Dr. Likholobov Vladimir, *Omsk Scientific Center SB RAS, Institute of Hydrocarbons Processing SB RAS, Omsk, Russia*
Prof. d'Alessandro Nicola, *'Gabriele d'Annunzio' University of Chieti Pescara, Chieti, Italy*

Discussion symposium 3. "Selective Catalytic Hydrogenation"

14:30-16:30 **DS3-1**
Rajkhowa T., Thybaut J.W., Marin G.B.
"Green" Propylene Glycol: Kinetic Determination for the Valorization of Biodiesel Side Stream
Laboratory for Chemical Technology, Ghent University, Gent, Belgium

DS3-2
Nindakova L.O.[1], Badyrova N.M.[1], Sadykov E.Kh.[2], Smirnov V.V.[1], Ushakov I.A.[1], Khatashkeev A.V.[1]
Transfer Hydrogenation of Acetophenone in the Presence Bis-imine Rhodium(I) Complexes
1 - Irkutsk State Technical University, Irkutsk, Russia
2 - A.E. Favorsky Irkutsk Institute of Chemistry SB RAS, Irkutsk, Russia

DS3-3
Maccarrone M.J.[1], Lederhos C.[1], Betti C.[1], Coloma-Pascual F.[2], Vera C.[1], Quiroga M.E.[1]
Obtaining (Z)-3-hexene with Ni Catalysts Supported on Alumina Modified with Magnesium Precursor
1 - Instituto de Investigaciones en Catálisis y Petroquímica, INCAPE, Colectora Ruta Nac. Nº 168 Km. 0 – Paraje El Pozo, Santa Fe (3000), Argentina
2 - Facultad de Ciencias, Universidad de Alicante, Apartado 99, E-03080 Alicante, Spain

DS3-4
Mashkovsky I.S.[1], Markov P.V.[1], Bragina G.O.[1], Baeva G.N.[1], Tkachenko O.P.[1], Kozitsyna N.Yu.[2], Vargaftik M.N.[2], Stakheev A.Yu.[1]
Highly Selective Pd-Cu Supported Catalyst for Liquid-Phase Semihydrogenation of Substituted Alkynes
1 - Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
2 - Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia

DS3-5
O'Driscoll Á., Leahy J.J., Curtin T.
Selective Hydrogenation of Furfural Using SiO_2 Based Catalysts: Impact of Reaction Conditions and Metals Employed
University of Limerick, Limerick, Ireland
Materials and Surface Science Institute, University of Limerick, Limerick, Ireland
Carbolea Research Group, University of Limerick, Limerick, Ireland

DS3-6
Okhlopkova L.B.[1], Matus E.V.[1], Prosvirin I.P.[1], Kerzhentsev M.A.[1], Ismagilov Z.R.[1,2]
Selective Hydrogenation of 2-methyl-3-butyne-2-ol catalyzed by Embedded Polymer-protected PdZn Nanoparticles
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia

DS3-7
Sulman E., Rakitin M., Petrova A., Doluda V., Matveeva V., Sulman M.
Research of Hydrogenation of the Nitrobenzene in Supercritical Carbon Dioxide with Use Ru/HPS Catalysts
Tver Technical University, Tver, Russia

DS3-8
de Miguel S., Rodriguez V., Scelza O., Stassi J., Vilella I., Zgolicz P.
Pt Based Bimetallic Catalysts Prepared by Conventional Impregnation and Deposition and Reduction in Liquid Phase Methods for Selective Hydrogenation of Citral
Instituto de Catálisis y Petroquímica, UNL-CONICET, Sgo del Estero 2654, Sta Fe (3000), Argentina

DS3-9
Suyunbayev U., Yergaziyeva G., Zhumagazin A.
Catalytic Hydrogenation of Dienone for Getting Vitamins and Odorous Substances
Institute of Combustion Problems, 050012, 172 Bogenbay batyr, Almaty, Kazakhstan

DS3-10
Nindakova L.O., Strakhov V.O., Chvanova K.A.
Enantioselective Hydrogenation of Prochiral Arylketones and Keto Acid Ethers Catalyzed by $Pd(acac)_2$- Chiral Base
Irkutsk State Technical University, Irkutsk, Russia

16:30-17:00 *Coffee break*

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155, ISO-PP1÷ISO-PP30 (Poster set-up time 09:00 – 19:00)

Tuesday, September 1

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Bukhtiyarov Valerii, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Freund Hans-Joachim, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Plenary Lectures

08:30-09:30 **PL5** Prof. Hupp Joseph T.
Mesoporous Metal-Organic Frameworks as Platforms for Single-site Heterogeneous Catalysts
Northwestern University, Evanston, IL 60208, USA

09:30-10:30 **PL6** Prof. Robert Schlögl
Dynamics in Heterogeneous Catalysis
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
Max Planck Institute for Chemical Energy Conversion, Mülheim a.d.Ruhr, Germany

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Chekhov hall

Discussion symposium 2. “Fuel Reforming”

Chairmen: Prof. Mirodatos Claude, *Institut de Recherches sur la Catalyse et l’Environnement de Lyon, Université Lyon 1, CNRS, Villeurbanne, France*
Prof. Sadykov Vladislav, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

11:00-13:00 **DS2-1**
Somacescu S.[1], Petrea N.[2], Sonu M.[2], Somoghi V.[3], Neatu F.[4], Neatu S.[3,5], Florea M.[4]
Synthesis of Mesoporous SnO_2 as Anode for PEMFCs
1 - ”Ilie Murgulescu” Institute of Physical Chemistry, Romanian Academy, Spl. Independentei 202, 060021, Bucharest, Romania
2 - Scientific Research Centre for CBRN Defense and Ecology, 225 Oltenitei Road, 041309 Bucharest, Romania
3 - S.C. STIMPEX S.A., 46-48 Teclu Nicolae Street, 032368 Bucharest, Romania
4 - University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis, 4 – 12 Regina Elisabeta Bvd., Bucharest 030016, Romania
5 - National Institute of Materials Physics, 105bis Atomistilor Street, 077125, Bucharest, Romania

DS2-2
Puleo F.[1], Banerjee D.[2], Pantaleo G.[1], Longo A.[1,3], Aprile C.[4], Collard X.[4], Martinez-Arias A.[5], Liotta L.F.[1]
Ni-based Catalysts for Methane dry Reforming: EXAFS, TEM and DRIFT Investigation on the Au/Pt/Pd Effects
1 - ISMN-CNR, Palermo, Via Ugo La Malfa, 90146, Palermo, Italy
2 - DUBBLE, European Synchrotron Radiation Facility (ESRF), Grenoble, France
3 - Netherlands Organization for Scientific Research (NWO) Grenoble CEDEX, France
4 - University of Namur (UNAMUR), 61 rue de Bruxelles, B-5000 Namur, Belgium
5 - CSIC, C/Marie Curie 2, Cantoblanco, 28049, Madrid, Spain

DS2-3
Mansur A.J.[1], Vallezi Paladino L.A.[2]
Catalysts (NiMg)AlO$_x$ + CeO$_2$ Derived of Hydrotalcite Type Structures Applied to Dry Reforming of Biogas
1 - Federal University of São Carlos, Chemical Engineering Department, Brazil
2 - Federal University of São Carlos, Chemical Engineering Department, Brazil

DS2-4
Mondal T.[1], Pant K.K.[1], Dalai A.K.[2]
Role of Rh as a Promoter on the Activity of Ni/CeO$_2$-ZrO$_2$ Catalyst for Oxidative Steam Reforming of Bio-ethanol
1 - Indian Institute of Technology Delhi, Department of Chemical Engineering, Hauz Khas, New Delhi 110016, India
2 - University of Saskatchewan, Department of Chemical and Biochemical Engineering, Saskatoon, SK S7N 5A9, Canada

DS2-5
Smal E.A.[1,2], Mezentseva N.V.[1,2], Sadykov V.A.[1,2], Krieger T.A.[1], Rogov V.A.[1,2], Simonov M.N.[1], Larina T.V.[1]
Ethanol Steam Reforming over Mn$_x$Cr$_{3-x}$O$_4$-based Spinel-type Oxide
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

DS2-6
Fedotov A.[1], Antonov D.[1], Tsodikov M.[1], Uvarov V.[2]
Syngas and Hydrogen Production by Dry and Steam Reforming of Methane and Fermentation Products on Porous Ceramic Membrane-Catalytic Ni-Co-containing Converters
1 - A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia
2 - Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow Region, Russia

DS2-7
Karuppiah J., Mok Y.S.
Dry Reforming of Propane over CeO$_2$/Ni-foam Catalysts
Jeju National University, Department of Chemical Engineering, Jeju 690-756, South Korea

DS2-8
Palma V., Ricca A., Miccio M., Martino M., Meloni E., Ciambelli P.
Steam Reforming of Methane on Ni-based Catalysts Characterized by Innovative Structured Carriers
University of Salerno, Department of Industrial Engineering, Fisciano (SA), Italy

DS2-9
Braga A.H.[1], Batista J.B.O.[1], Damyanova S.[2], Bueno J.M.C.[1]
Ethanol Steam Reforming to Hydrogen over CoNi-based Catalysts
1 - Universidade Federal de São Carlos, Departamento de Engenharia Química, C.P. 676, 13565-905, São Carlos, São Paulo, Brazil
2 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

DS2-10
Erdinç E., Aksoylu A.E.
A Study on Kinetics of Methane Oxidative Steam Reforming (OSR) over Pt-Ni/Al_2O_3 Bimetallic Catalysts
Bogazici University, Department of Chemical Engineering, Istanbul, Turkey

13:00-14:30 *Lunch*

KORSTON Chekhov hall

Evening Session

Chairmen: Dr. Kozlova Ekaterina, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Dr. Kozlov Denis, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Discussion symposium 4. “Photocatalysis: Water Splitting, CO_2 Reduction and Oxidative Processes”

14:30-16:30 **DS4-1**
Jiao J.Q., Wei Y.C., Zhao Z., Liu J., Li J.M., Jiang G.Y., Duan A.J.
3D Ordered Macroporous Ti-based Catalysts: Design, Synthesis and High Catalytic Activity for the Photoreduction of CO_2 with Water to Mechane
State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing, China

DS4-2
Tsyganenko A.
Advances in Catalyst Characterization by FTIR spectroscopy
V.A. Fock Institute of Physics, St.Petersburg State University, St.Petersburg, Russia

DS4-3
Keller V.[1], Pichot V.[2], Minetti Q.[1]
New Nanodiamonds/TiO_2 Composite Materials for the Solar Energy Conversion into Hydrogen by Water Splitting
1 - ICPEES, « Institut de Chimie et Procédés pour l’Energie, l’Environnement et la Santé », Université de Strasbourg, UMR 7515 (CNRS), 25 rue Becquerel 67087 Strasbourg Cedex, France
2 - NS3E, « Nanomatériaux pour les Systèmes Sous Sollicitations Extrêmes », UMR 3208 (ISL/CNRS/UdS) Institut franco-allemand de recherche de Saint-Louis, 5 rue du Général Cassagnou, BP 70034, 68301 Saint-Louis Cedex, France

DS4-4
Szíjjártó G.P., Tálas E., Pászti Z., Mihályi J., Bálint S., Tompos A., Boráth I.
Pt-SnO_x-TiO_2 Catalysts for Methanol Photocatalytic Reforming: Influence of Co-catalysts on the Hydrogen Production
Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary

DS4-5
Lisachenko A.A.
Sensitization of Wide-Bandgap Oxides ZnO and TiO_2 to the Visible Region Using Intrinsic Point Defects, Surface 2D Nanostructures and Composites ZnO/Si, TiO_2/Si
St. Petersburg State University, Department of Physics, Saint-Petersburg, Russia

DS4-6
Altunoz Erdogan D.[1], Solouki T.[2], Ozensoy E.[1]
Bio-inspired “Buckyball-shaped” Photocatalytic Architectures
1 - Bilkent University, Department of Chemistry, 06800, Ankara, Turkey
2 - Baylor University, Department of Chemistry & Biochemistry, Waco, TX, USA

DS4-7
Bellardita M., García-López E., Marcì G., Palmisano L.
Photocatalytic Conversion of Glucose in TiO_2 Aqueous Suspensions
”Schiavello-Grillone” Photocatalysis Group, Dipartimento di Energia, Ingegneria dell’informazione, e modelli Matematici (DEIM), Università degli Studi di Palermo, Viale delle Scienze Ed. 6, 90128, Palermo, Italy

DS4-8
Kolinko P.[1,2], Lyulyukin M.[1], Besov A.[1,2], Parkhomchuk E.[1,2,3], Kozlov D.[1,2,3]
Development of the Methods for Fast Catalytic Air Purification from CWAs
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Research and Educational Centre for Energoefficient Catalysis (Novosibirsk State University), Novosibirsk, Russia

DS4-9
Striegler K.[1], Richter D.[1], Benndorf G.[2], Gläser R.[3]
New Approaches for Solar Fuel from Suspended Photocatalysts
1 - Universtät Leipzig, Faculty of Chemistry and Mineralogy, Institute of Chemical Technology, Leipzig, Germany
2 - Universtät Leipzig, Faculty of Physics and Earth Science, Institute for Experimental Physics II, Leipzig, Germany
3 - Universtät Leipzig, Faculty of Chemistry and Mineralogy, Institute of Chemical Technology, Leipzig, Germany

DS4-10
Xie S., Wang Y., Zhang Q., Wang Y.
Two-dimensional $SrNb_2O_6$ as an Efficient Photocatalyst for the Preferential Reduction of Carbon Dioxide in the Presence of Water
State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, China

DS4-11
Selishchev D.S., Kozlov D.V.
Photocatalytic Oxidation of Diethyl Sulfide Vapor over TiO_2 Deposited on Porous Supports
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia
Research and Educational Centre for Energoefficient Catalysis (NSU), Novosibirsk, Russia

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-I: I-PP1÷I-PP114, III-PP1÷III-PP130, IV-PP1÷IV-PP155, ISO-PP1÷ISO-PP30** (Poster set-up time 09:00 – 19:00)

Wednesday, September 2

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Schlögl Robert, *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*
Prof. Skoglundh Magnus, *Competence Centre for Catalysis, KCK, Chalmers University of Technology, Göteborg, Sweden*

Plenary Lecture

08:30-09:30 **PL-7** Michel Boudart Award Lecture (2015) Prof. Freund Hans-Joachim
Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-1

Section 5. Catalysis and Environmental Protection

Chairmen: Dr. Vedyagin Aleksey, *Boreskov Institute of Catalysis, Novosibirsk, Russia*
Dr. Bukhtiyarova Marina, *MPI for Chemical Energy Conversion, Mülheim a.d. Ruhr, Germany*

Keynote Lecture

10:00-10:40 **V-KN8** Prof. Román-Leshkov Yuriy
Van de Vyver S., Lewis J.D., Román-Leshkov Yu.
Exploiting Acid-base Cooperativity in Metalloenzyme-like Lewis Acid Zeolites for Biomass Conversion
Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

Oral Presentations

10:40-11:00 **V-OP18** Calaza Florencia
Calaza F.[1], Sterrer M.[1,2], Freund H.-J.[1]
Surface Chemistry of Glycerol on Metals and Metal-Oxides as Model Catalysts for Biomass Conversion
1 - Department of Chemical Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
2 - Institute of Physics, Karl-Franzens-Universität Graz, Graz, Austria

11:00-11:20 **V-OP19** Prof. Aprile Carmela
Buaki-Sogo M.[1], Garcia H.[2], Aprile C.[1]
Ionic Liquids Based Silica Microreactors for the Efficient Conversion of Carbon Dioxide
1 - Unit of Nanomaterial Chemistry (CNano), University of Namur (UNAMUR), Department of Chemistry, Namur, Belgium
2 - Technical University of Valencia, Chemical Technology Institute (ITQ-CSIC) Valencia, Spain

11:20-11:40 **V-OP20** Dr. Demidova Yuliya
Demidova Yu.S.[1,2], Simakova I.L.[1,2], Beloshapkin S.[3], Wärnå J.[4], Suslov E.V.[5], Volcho K.P.[5], Salakhutdinov N.F.[5], Simakov A.V.[6], Murzin D.Yu.[4]
One-pot Natural Alcohol Amination Catalyzed by Gold-containing Catalysts
1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Materials & Surface Science Institute, University of Limerick, Limerick, Ireland
4 - Åbo Akademi University, Turku/Åbo, Finland
5 - Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia
6 - Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, México

11:40-12:00 **V-OP21** Dr. Nowicka Ewa
Nowicka E., Reece C., Willock D., Golunski S., Hutchings G.J.
Utilization of CO_2 in the Process of Olefins Production
Cardiff Catalysis Institute, Cardiff University, CF10 3AT Cardiff, United Kingdom

12:00-12:20 **V-OP22** Prof. Lemonidou Angeliki
Lemonidou A.A.[1,2], Yfanti V.-L.[1], Vasiliadou E.S.[1]
Selective 1,2-propanediol Formation via Tandem Reaction Cycle of Methanol Reforming-Glycerol Hydrodeoxygenation
1 - Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece
2 - Chemical Process and Energy Resources Institute (CERTH/CPERI), Thessaloniki, Greece

12:20-12:40 **V-OP23** Zacharska Monika
Zacharska M.[1,2], Bulushev D.A.[1,3], Estrada M.[4], Guo Y.[2], Beloshapkin S.[2], Kriventsov V.V.[3], Leahy J.J.[1,2], Simakov A.V.[4]
Gold Catalysts for CO-free Hydrogen Production from Formic Acid Derived from Biomass
1 - Chemical & Environmental Sciences Department, University of Limerick, Limerick, Ireland
2 - Materials & Surface Science Institute, University of Limerick, Limerick, Ireland
3 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
4 - Centro de Nanociencias y Nanotecnologia, UNAM, 22860 Ensenada, B.C., Mexico

12:40-13:00 **V-OP24** Prof. Tsodikov Mark
Tsodikov M.V.[1], Chistyakov A.V.[1], Gekhman A.E.[2], Moiseev I.I.[3]
Bimetallic Catalysts Promising in Bio-fuel Production
1 - A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia
2 - N.S. Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia
3 - I.M. Gubkin Russian State University of Petroleum and Gases, Moscow, Russia

13:00-14:30 ***Lunch***

KORSTON Ball hall-1

Evening Session

Section 1. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

Chairmen: Prof. Grünert Wolfgang, *Ruhr University Bochum, Germany*
Prof. Nam In-Sik, *Department of Chemical Engineering, School of Environmental Science and Engineering, Pohang University of Science and Techlogy (POSTECH), Pohang, Republic of Korea*

Keynote Lectures

14:30-15:10 **I-KN11** Prof. Olsbye Unni
Olsbye U., Lillerud K.P.
Catalysis in Confined Space – from Zeolites and Zeotypes to Functionalized Metal-organic Frameworks
Department of Chemistry, University of Oslo, Oslo, Norway

15:10-15:50 **I-KN12** Dr. Tatsumi Takashi
Development of New Catalytic Materials for Sustainable Production of Chemicals
Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8550, Japan

Oral Presentations

15:50-16:10 **I-OP13** Dr. Maki-Arvela Päivi
Tkacheva A., Dosmagambetova I., Mäki-Arvela P., Hachemi I., Kumar N., Eränen K., Hemming J., Smeds A., Murzin D.Y.
Surfactants from Algae Derived Feedstock: Acylation of Amino Alcohols with Fatty Acids over Zeolite Beta
Åbo Akademi University, Turku, Finland

16:10-16:30 **I-OP14** Dr. Yadav Ganapati D.
Yadav G.D., Bhanawase S.L.
A Novel Efficient Synthesis of Guaifenesin over Calcined Hydrotalcite
Department of Chemical Engineering, Institute of Chemical Technology, Matunga, Mumbai, India

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150**
(Poster set-up time 09:00 – 19:00)

Wednesday, September 2

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Schlögl Robert, *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*
Prof. Skoglundh Magnus, *Competence Centre for Catalysis, KCK, Chalmers University of Technology, Göteborg, Sweden*

Plenary Lecture

08:30-09:30 **PL-7** Michel Boudart Award Lecture (2015). Prof. Freund Hans-Joachim
Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

09:30-19:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-2

Section 2. Catalyst Preparation and Characterization

Chairmen: Prof. Mossin Susanne, *Department of Chemistry, Technical University of Denmark, Lyngby, Denmark*
Dr. Hävecker Michael, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Inorganic Chemistry, Helmholtz-Zentrum Berlin für Materialien und Energy / BESSY II, Energy Materials, Berlin, Germany*

Oral Presentations

10:00-10:20 **II-OP21** Dr. Cortés-Reyes Marina
Cortés-Reyes M., Díaz-Rey M.R., Herrera M.C., Larrubia M.A., Alemany L.J.
Cu-SAPO-34 Synthesis and in Situ Characterization. Insights into DeNOx-SCR Mechanism
Departamento de Ingeniería Química, Facultad de Ciencias, Campus de Teatinos, Universidad de Málaga, Spain

10:20-10:40 **II-OP22** Dr. Vuong T. Huyen
Vuong T.H., Radnik J., Armbruster U., Brückner A.
Structure-Reactivity Relationships in Low-temperature NH_3-SCR of NO over Highly Effective $V_2O_5/Ce_xZr_{1-x}O_2$ Catalysts
Leibniz Institute for Catalysis at the University of Rostock, Rostock, Germany

Keynote Lecture

10:40-11:20 **II-KN9** Dr. McIndoe Jason S.
Real-time Analysis of Catalytic Reactions Using Simultaneous Orthogonal Methods
Department of Chemistry, University of Victoria, Victoria, BC V8W 3V6, Canada

Oral Presentations

11:20-11:40 **II-OP23** Dr. Rout Kumar R.
Rout K.R.[1], Chen D.[1], Baido M.F[1], Fenes E.[1], Fuglerud T.[2]
Kinetics Study of Oxychlorination Process by Combined In-situ Mass- and Spatial-time Resolved UV-Visible Spectrophotometry
1 - NTNU, Norway
2 - INEOS, Norway

11:40-12:00 **II-OP24** Dr. Wang Zhendong D.
Yang W.M., Wang Z.D., Zhang B., Sun H.M., Huan M.Y., Xue M.W.
Design and Preparation of Zeolitic Catalysts for Ethylbenzene via Vapour-Phase Benzene Alkylation
Sinopec Shanghai Research Institute of Petrochemical Technology, Shanghai, China

12:00-12:20 **II-OP25** Van Haandel Lennart
Van Haandel L., Hensen E.J.M., Weber Th.
Hydrotreating Catalyst Activation under Industrial Conditions
Inorganic Materials Chemistry, Eindhoven University of Technology, Department of Chemical Engineering and Chemistry, Eindhoven, The Netherlands

12:20-12:40 **II-OP26** Pfeifer Verena
Pfeifer V.[1], Arrigo R.[1,2], Velasco-Vélez J.[1,2], Haevecker M.[1,3], Stotz E.[1], Knop-Gericke A.[1], Schlögl R.[1,2]
Development of in Situ Techniques to Monitor Oxygen Evolving Electrocatalyst Surfaces
1 - Fritz-Haber-Institut der Max-Planck-Gesellschaft, Inorganic Chemistry, Berlin, Germany
2 - Max-Planck-Institut für Chemische Energiekonversion, Heterogeneous Reactions, Mülheim a.d. Ruhr, Germany
3 - Helmholtz-Zentrum Berlin für Materialien und Energie, Catalysis for Energy, Berlin, Germany

12:40-13:00 **II-OP27** Li Hao
Li. H.[1], Anic K.[1], Rameshan C.[1], Bukhtiyarov A.V.[2], Prosvirin I.P.[2], Rupprechter G.[1]
CO_2 and H_2O (Co)adsorption on a ZrO_2 Thin Film
1 - Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

13:00-14:30 ***Lunch***

KORSTON Ball hall-2

Evening Session

Chairmen: Dr. Auroux Aline, *Université Lyon 1, CNRS, UMR 5256, IRCELYON, Institut de Recherches sur la Catalyse et l'Environnement de Lyon, Villeurbanne, France*
Dr. Cadete Santos Aires Francisco Jose, *Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256 CNRS/UCB Lyon 1, Villeurbanne, France*

Oral Presentations

14:30-14:50 **II-OP28** Schnee Josefine
Schnee J., Gaigneaux E.M.
Operando Raman and UV-Visible Spectroscopy of $H_3PW_{12}O_{40}$ in the Gas Phase Dehydration of Methanol to Dimethylether
Université catholique de Louvain, Institute of Condensed Matter and Nanosciences (IMCN/MOST), Croix du Sud 02/L7.05.17, 1348-Louvain la Neuve, Belgium

14:50-15:10 **II-OP29** Prof. Bordiga Silvia
Signorile M., Bonino F., Damin A., Bordiga S.
Raman Study of the Deactivation Products in the Methanol to Olefines Reaction: a Combined In Situ - In Silico Approach
Department of Chemistry, NIS and INSTM Reference Centre, University of Turin, Torino, Italy

15:10-15:30 **II-OP30** Prof. van Bokhoven Jeroen A.
Proff C., Fodor D., Orlando F., van Bokhoven J.A.
Where are the Active Sites in Zeolite Nano-Crystals? Influence on Post-Synthesis Treatment from Hard X-ray Depth Profiling with XPS
Institute for Chemical and Bioengineering, ETH Zurich and Paul Scherrer Institute, Villigen, Switzerland

15:30-15:50 **II-OP31** Gallas Hulin Agata
Agata G.H.[1], Thomas W.H.[2], Jerrik J.M.[1], Søren K.[1]
eTEM Investigation of Gold Nanoparticle Formation in Recrystallized Zeolite Silicalite-1
1 - Technical University of Denmark, Department of Chemistry, 2800 Kgs. Lyngby, Denmark
2 - Technical University of Denmark, Centre for Electron Nanoscopy, 2800 Kgs. Lyngby, Denmark

15:50-16:10 **II-OP32** Karim Waiz
Karim W.[1,2], Kleibert A.[2], Gobrecht J.[2], Ekinci Y.[2], van Bokhoven J.A.[1,2]
Size-dependent Redox Behaviour in Iron Observed Using Top-Down Lithography and In-Situ Single Particle Spectro-Microscopy
1 - ETH Zurich, Switzerland
2 - Paul Scherrer Institute, Switzerland

16:10-16:30 **II-OP33** Dr. Fredriksson Hans
Fredriksson H.O.A., Bu Y., Dad E., Sui H., Niemantsverdriet J.W.
Investigating Fundamental Properties of Syngas Conversion Catalysts - a Model Approach
Eindhoven University of Technology, Eindhoven

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150**
(Poster set-up time 09:00 – 19:00)

Wednesday, September 2

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Schlögl Robert, *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*
Prof. Skoglundh Magnus, *Competence Centre for Catalysis, KCK, Chalmers University of Technology, Göteborg, Sweden*

Plenary Lecture

08:30-09:30 **PL-7** Michel Boudart Award Lecture (2015). Prof. Freund Hans-Joachim
Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Pushkin hall

Section 4. Catalysis and Chemicals

Chairmen: Prof. Coman Simona, *University of Bucharest, Faculty of Chemistry, Bucharest, Romania*
Prof. Wang Ye, *State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, P.R. China*

Oral Presentations

10:00-10:20 **IV-OP21** Dr. Terent’ev Alexander
Terent’ev A.O., Krylov I.B., Vil' V.A., Zdvizhkov A.T., Sharipov M.Yu.
New Cross-dehydrogenative Coupling Reactions with Selective C-O Bond Formation
N.D. Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia

10:20-10:40 **IV-OP22** Rasmussen Dominik B.
Rasmussen D.B.[1], Christensen J.M.[1], Temel B.[2], Studt F.[3], Moses P.G.[2], Rossmeisl J.[4], Riisager A.[5], Jensen A.D.[1]
Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate on Mordenite
1 - Technical University of Denmark, Department of Chemical and Biochemical Engineering, Søltofts Plads B229, 2800 Kgs. Lyngby, Denmark
2 - Haldor Topsøe A/S, Nymøllevej 55, 2800 Kgs. Lyngby, Denmark
3 - SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA
4 - Technical University of Denmark, Department of Physics, Fysikvej B307, 2800 Kgs. Lyngby, Denmark
5 - Technical University of Denmark, Department of Chemistry, Kemitorvet B206, 2800 Kgs. Lyngby, Denmark

10:40-11:00 **IV-OP23** Dr. Liu Yue
Liu Y., Müller S., Sanchez-Sanchez M., Lercher J.
On the Mechanism for the First C-C Bond Formation in MTO Reaction
Department of Chemistry and Catalysis Research Center, Technische Universität München, Germany

11:00-11:20 **IV-OP24** Otroshchenko Tatiana
Otroshchenko T., Stoyanova M., Rodemerck U., Sokolov S., Linke D., Kondratenko E.V.
Activity Control of Supported Catalysts with Tailored Ru Nanoparticles for Non-Oxidative Propane Dehydrogenation
Leibniz Institute for Catalysis, Rostock, Germany

11:20-11:40 **IV-OP25** Dr. Martyanov Oleg
Martyanov O.N.[1,2], Chibiryaev A.M.[1,2], Kozhevnikov I.V.[1]
Methylation Reaction of Aromatic NH-heterocycles with Using Supercritical Methanol: Competitive Homogeneous and Heterogeneous Catalysis by Si-containing Compounds
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

Keynote Lecture

11:40-12:20 **IV-KN10** Prof. Hu Xile L.
Base Metal Catalysis for Cross Coupling and Addition Reactions
Laboratory of Inorganic Synthesis and Catalysis, Institute of Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Oral Presentations

12:20-12:40 **IV-OP26** Dr. Atia Hanan
Atia H.[1], Eckelt R.[1], Al-Fatesh A.S.[2], Fakeeha A.H.[2], Martin A.[1]
Effect of Promoter Addition to SBA-15 Supported Bimetallic Co-Ni Catalysts for Dry Reforming of Methane
1 - Leibniz-Institut für Katalyse, Rostock, Germany
2 - College of Engineering, King Saud University, Riyadh, Kingdom of Saudi Arabia

12:40-13:00 **IV-OP27** Dr. Zagidullin Almaz A.
Zagidullin A.A.[1], Miluykov V.A.[1], Oshchepkova E.S.[1], Sinyashin O.G.[1], Hey-Hawkins E.[2]
New Chiral Cage Phosphines for Homogeneous Asymmetric Catalysis
1 - A.E. Arbuzov Institute of Organic and Physical Chemistry, RAS, Kazan, Russia
2 - Institut für Anorganische Chemie, Universität Leipzig, Leipzig, Germany

13:00-14:30 ***Lunch***

KORSTON Pushkin hall

Evening Session

Chairmen: Dr. Taran Oxana, *Boreskov Institute of Catalysis SB RAS, Novosibirsk State Technical University, Novosibirsk, Russia*
Prof. Román-Leshkov Yuriy, *Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*

Oral Presentation

14:30-14:50 **IV-OP28** Dr. Girard Etienne
Girard E., Delcroix D., Cabiac A.
Catalytic Conversion of Cellulose to C_2-C_3 Glycols Using Heterogeneous Platinum Catalysts Supported on Cerium Oxide
IFP Energies Nouvelles, Rond-Point de l'Echangeur de Solaize, BP3, 69360 Solaize, France

14:50-15:10 **IV-OP29** Prof. Wang Ye
Wang Y.L., Deng W.P., Zhang Q.H., Wang Y.
Conversions of Cellulose and Its Derived Carbohydrates into Lactic Acid in Water Catalyzed by Al(III) and Sn(II) Dual Cations
State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P.R. China

15:10-15:30 **IV-OP30** Dr. Yokoi Toshiyuki
Otomo R, Yokoi T., Tatsumi T.
OSDA-Free Beta Zeolite with High Al Content as Efficient Catalyst for Biomass Conversion
Tokyo Institute of Technology, Yokohama, Japan

15:30-15:50 **IV-OP31** Prof. Kasaikina Olga
Kasaikina O.T., Pisarenko L.M., Zinoviev I.V.
Thermooxidative Catalytic Treatment of Biomass
N.N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia

15:50-16:30 **KN20** Award Applied Catalysis, Prof. Vasalos Iacovos
Application of Zeolite Catalysts for the Production of Clean Fossil fuels and Biofuels
Chemical Process and Energy Resources Institute, Centre for Research and Technology Hellas, Greece

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150**

(Poster set-up time 09:00 – 19:00)

Wednesday, September 2

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Schlögl Robert, *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*
Prof. Skoglundh Magnus, *Competence Centre for Catalysis, KCK, Chalmers University of Technology, Göteborg, Sweden*

Plenary Lecture

08:30-09:30 **PL-7** Michel Boudart Award Lecture (2015). Prof. Freund Hans-Joachim
Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Tolstoy hall

Section 3. Energy-related Catalysis

Chairmen: Prof. Conesa Jose C., *Instituto de Catálisis y Petroleoquímica, CSIC, Madrid, Spain*
Prof. Pidko Evgeny, *Eindhoven University of Technology, Eindhoven, the Netherlands*

Oral Presentations

10:00-10:20 **III-OP14** Castaño Pedro
Montero C., Ochoa A., Bilbao J., Gayubo A.G., Castaño P.
Surface Dynamics of Ni^0 and Coke during Ethanol Steam Reforming on a Ni/La$_2$O$_3$-alphaAl$_2$O$_3$ Catalyst
Department of Chemical Engineering. University of the Basque Country (UPV/EHU). P.O. Box: 644, 48080, Bilbao, Spain

10:20-10:40 **III-OP15** Dr. Snytnikov Pavel
Snytnikov P.V.[1,2], Sobyanin V.A.[1,2]
CO-cleanup of Hydrogen-rich Stream for LT PEM FC Feeding: Catalysts and their Performance in CO Preferential Oxidation and Methanation
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

10:40-11:00 **III-OP16** Konstantinov Grigoriy
Konstantinov G.I.[1], Tsodikov M.V.[1], Kurdymov S.S.[1], Bukhtenko O.V.[1], Maksimov Yu.V.[2], Murzin V.Yu.[3]
Catalyst with "core/ shell" Structure for Steam Methane Reforming Resistant to Presence of H$_2$S in Gas Mixture
1 - A.V. Topchiev Instiute of Petrochemical Synthesis, RAS, Moscow, Russia
2 - N.N. Semenov Institute of Chemical Physics, RAS, Moscow, Russia
3 - National Research Center "Kurchatov Institute", Moscow, Russia

11:00-11:20 **III-OP17** Angeli Sofia D.
Angeli S.D., Lemonidou A.A.
Mechanistic Implications on Low Temperature Steam Reforming of Methane over $Ni/La/CeO_2$-ZrO_2
Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece

11:20-11:40 **III-OP18** Prof. Sadykov Vladislav
Sadykov V.[1,2], Chub O.[1], Chesalov Yu.[1], Mezentseva N.[1,2], Pavlova S.[1], Arapova M.[1,3], Roger A.-C.[3], Parkhomenko K.[3], Van Veen A.C.[4]
Mechanism of Ethanol Steam Reforming over Pt/(Ni+Ru)-promoted Oxides by FTIRS In Situ
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - University of Strasbourg, Strasbourg, France
4 - University of Warwick, UK

11:40-12:00 **III-OP19** Dr. Watanabe Ryo
Watanabe R., Watanabe S., Fukuhara C.
Iron Oxide-type Structured Catalyst for Water Gas Shift Reaction
Department of Applied Chemistry and Biochemical Engineering, Graduate school of Engineering, Shizuoka University, 3-5-1, Johoku, Naka-ku, Hamamatsu, Shizuoka, Japan

12:00-12:20 **III-OP20** Dr. Mafessanti Rodolfo
Abate S.[1], Basile F.[2], Fornasari G.[2], Lombardi E.[2], Mafessanti R.[2], Vaccari A.[2]
Low Temperature CH_4 Oxy-reforming Coupled with Pd-based Membrane for an Energy-efficient Process for Syngas Production
1 - Department of Electronic Engineering, Chemistry and Industrial Eng. – DIECII - University of Messina, V.le F. Stagno D'Alcontres 31, 98166 Messina, Italy
2 - Department of Industrial Chemistry "Toso Montanari", Alma Mater Studiorum - University of Bologna, V.le Risorgimento 4, 40136 Bologna, Italy

12:20-12:40 **III-OP21** Lytkina Aleksandra
Lytkina A.A.[1], Zhilyaeva N.A.[1], Orekhova N.V.[1], Ermilova M.M.[1], Yaroslavtsev A.B.[1,2]
Effect of Ni-Cu-based Catalysts Composition and Support Structure on Hydrogen Production by Methanol Steam Reforming
1 - A.V. Topchiev Institute of Petrochemical Synthesis of the Russian Academy of Sciences, Moscow, Russia
2 - Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Moscow, Russia

12:40-13:00 **III-OP22** Dr. Lucarelli Carlo
Lucarelli C.[1], Faure R.[2], Fornasari G.[3], Gary D.[2], Molinari C.[3], Schiaroli N.[3], Vaccari A.[3]
Stability and Activity Promoters in Medium Temperature Water Gas Shift Catalysts
1 - Dipartimento di Scienza e Alta Tecnologia, Via Valleggio 9, 22100 Como, Italy
2 - Centre de Recherche Claude-Delorme, Air Liquide, B.P 126, 78354 Jouy-en-Josas, France
3 - Dipartimento di Chimica Industriale "Toso Montanari", Alma Mater Studiorum - Università di Bologna, Viale Risorgimento 4, 40136 Bologna, Italia

13:00-14:30 ***Lunch***

KORSTON Tolstoy hall

Evening Session

Chairmen: Dr. Ordomsky Vitaly, *Unité de catalyse et de chimie du solide (UMR 8181 CNRS), Université Lille 1-ENSCL-EC Lille, Bat. C3, Cité Scientifique, 59655 Villeneuve d'Ascq, France*
Dr. Snytnikov Pavel, *Novosibirsk State University, Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

14:30-14:50 **III-OP23** Dr. Bulushev Dmitri
Bulushev D.[1,2], Zacharska M.[2], Podyacheva O.[1], Jia L.[3], Kibis L.[1], Boronin A.[1], Shlyakhova E.[3], Bulusheva L.[3], Guo Y.[2], Chuvilin A.[4], Beloshapkin S.[2], Okotrub A.[3], Ramasse Q.[5], Bangert U.[2]
Effect of Nitrogen Doping of Carbon Supports for Hydrogen Production from Formic Acid Decomposition over Noble Metal Clusters and Atoms
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - University of Limerick, Ireland
3 - Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia
4 - CIC nanoGUNE Consolider, Spain
5- STFC Daresbury Laboratories, United Kingdom

14:50-15:10 **III-OP24** Prof. Ozensoy Emrah
Bulut A.[1], Yurderi M.[1], Say Z.[2], Kivrak H.[3], Gulcan M.[1], Kaya M.[4], Ozensoy E.[2], Zahmakiran M.[1]
Going Heterogeneous in the Additive-Free Hydrogen Production from Formic Acid at Room Temperature
1 - Department of Chemistry, Yuzuncu Yıl University, Van, Turkey
2 - Department of Chemistry, Bilkent University, Ankara, Turkey
3 - Department of Chemical Engineering, Yuzuncu Yıl University, Van, Turkey
4 - Department of Chemical Engineering and Applied Chemistry, Atilim University, Ankara, Turkey

15:10-15:30 **III-OP25** Dr. Millan Marcos
Puron H.[1], Pinilla J.L.[1], Yeletsky P.[2], Yakovlev V.A.[2], Saraev A.A.[2], Kaichev V.V.[2,3], Millan M.[1]
Cr-Doped Alumina as Support for NiMo Vacuum Residue Hydroprocessing Catalyst
1 - Department of Chemical Engineering, Imperial College London, London, UK
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia

15:30-15:50 **III-OP26** Dr. Frei Elias
Frei E.[1], Schumann J.[1], Kandemir T.[2], Friedrich M.[1], Trunschke A.[1], Schlögl R.[1], Lunkenbein T.[1]
The Dynamic Nature of ZnO in Industrial Cu/ZnO/Al$_2$O$_3$ Methanol Catalysts: From Minutes to Month
1 - Fritz-Haber-Institute of the Max-Planck-Society, Department of Inorganic Chemistry, Berlin, Germany
2 - Technical University Hambur-Harburg, Institute of Chemical Process Engineering, Hamburg, Germany

15:50-16:10 **III-OP27** Prof. Petrov Lachezar
Petrov L.A.[1,2], Pasupulety N.[1,2], Alhamed Y.[2,3], Alzahrani A.[2,3]
Studies on Au/Cu-Zn-Al Catalyst for Methanol Synthesis from CO_2
1 - Sabic Chair of Catalysis, Jeddah, Saudi Arabia
2 - King Abdulaziz University, Jeddah, Saudi Arabia
3 - Chemical and Materials Engineering

16:10-16:30 **III-OP28** Kirchner Johann
Kirchner J., Kureti S.
CO_2 Methanation on Iron Based Catalysts
TU Bergakademie Freiberg, Freiberg, Germany
Institute of Energy Process Engineering and Chemical Engineering, Freiberg, Germany

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150**

(Poster set-up time 09:00 – 19:00)

Wednesday, September 2

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Schlögl Robert, *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*
Prof. Skoglundh Magnus, *Competence Centre for Catalysis, KCK, Chalmers University of Technology, Göteborg, Sweden*

Plenary Lecture

08:30-09:30 **PL-7** Michel Boudart Award Lecture (2015). Prof. Freund Hans-Joachim
Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Dostoevsky hall

XI European Workshop on Innovation in Selective Oxidation

Chairmen: Prof. Centi Gabriele, *Dept. DIECII, Section Industrial Chemistry, University of Messina, ERIC aisbl and CASPE/INSTM, Messina, Italy*
Dr. Kholdeeva Oxana, *Novosibirsk State University, Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

10:00-10:20 **ISO-OP10** Solmi Stefania
Solmi S., Rozhko E., Malmusi A., Lolli A., Albonetti S., Cavani F.
Study of a New Process for the Synthesis of Adipic Acid: the Oxidative Cleavage of Trans-1,2-cyclohexanediol
Alma Mater Studiorum – Università di Bologna, Dipartimento di Chimica Industriale "Toso Montanari", Viale del Risorgimento 4, 40136 Bologna, Italy

10:20-10:40 **ISO-OP11** Dr. Odriozola Gordón José
Sayago C.M.[1,2], Carrasco C.J.[1,2], Ivanova S.[1,2], Montilla Ramos F.J.[1,2], Galindo Del Pozo A.[1,2], Odriozola Gordón J.A.[1,2]
Influence of the Ionic Liquid Presence on the Selective Oxidation of Glucose over Molybdenum Based Catalysts
1 - Instituto de Ciencia de Materiales de Sevilla, Universidad de Sevilla-CSIC, Américo Vespucio 49, 41092, Seville, Spain
2 - Departamento de Química Inorgánica, Universidad de Sevilla, Aptdo 1203, 41071 Sevilla, Spain

10:40-11:00 **ISO-OP12** Dr. Shen Wenjie
Li Y., Shen W.
Morphology-dependent Nanocatalysts: Rod-shaped Metal Oxides
Dalian Institute of Physcial Chemistry, Chinese Academy of Sciences, Dalian, China

11:00-11:20 **ISO-13** Dr. Ottenbacher Roman
Talsi E.P.[1,2], Ottenbacher R.V.[1,2], Bryliakov K.P.[1,2]
On the Mechanisms of Selective Bioinspired Oxidations Catalyzed by Aminopyridine Manganese Complexes
Novosibirsk State University, Novosibirsk, Russia
Boreskov Institute of Catalysis, Novosibirsk, Russia

11:20-11:40 **ISO-OP14** Prof. Perathoner Siglinda
Papanikolaou G., Ampelli C., Genovese C., Perathoner S., Centi G.
Catalytic Upgrading of Furfural by Oxidative Methylation over Au NPs-based Catalysts
University of Messina, Dep. of Electronic Engineering, Industrial Chemistry and Engineering, Messina, Italy

11:40-12:00 **ISO-OP15** Prof. Paul Sebastien
Grasset F.[1], Katryniok B.[1,2], Paul S.[1,2], Pera-Titus M.[3], Clacens J.-M.[3], Decampo F.[3], Dumeignil F.[1,4,5]
Selective Oxidation of 5-HMF to 2,3-diformylfuran on Intercalated VPO Catalysts
1 - Unité de Catalyse et de Chimie du Solide, UCCS, UMR CNRS 8181, Villeneuve d'Ascq, 59655, France
2 - Ecole Centrale de Lille, ECLille, Villeneuve d'Ascq, 59655, France
3 - Eco-Efficient Products and Processes Laboratory, E2P2L, UMI3463, Shanghai, 201108, China
4 - Institut Universitaire de France, IUF, Maison des Universités, 103 Bd. St Michel, Paris, 75005, France
5 - Université de Lille, Villeneuve d'Ascq, 59655, France

12:00-12:20 **ISO-OP16** Dr. Florea Mihaela
Neatu F.[1], Petrea N.[2], Petre R.[2], Sonu M.[2], Somoghi V.[3], Florea M.[1], Parvulescu V.I.[1]
Oxidation of 5-Hydroxymethyl Furfural to 2,5-diformylfuran in Aqueous Media over Heterogeneous Manganese Based Materials
1 - University of Bucharest, Department of Organic Chemistry, Biochemistry and Catalysis, Bucharest, Romania
2 - Scientific Research Centre for CBRN Defense and Ecology, Bucharest, Romania
3 - SC Stimpex SA, Bucharest, Romania

Keynote Lecture

12:20-13:00 **ISO-KN02** Prof. Kolb Gunther
Kolb G., Pennemann H.
Microstructured Reactors as Efficient Tool for the Operation of Selective Oxidation Reactions
Fraunhofer ICT-IMM, Mainz, Germany

13:00-14:30 ***Lunch***

KORSTON Dostoevsky hall

Evening Session

ISO-Discussion symposium 7. “Selective Oxidation”

Chairmen: Prof. Ruiz Patricio, *Université Catholique de Louvain, Institute of Condensed Matter and Nanosciences - IMCN, Division «Molecules, Solids and Reactivity-MOST». Croix du Sud 2, 1348 Louvain-la-Neuve, Belgique*
Prof. Cavani Fabrizio, *Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Viale Risorgimento 4, 40136 Bologna, Italy*

Oral Presentations

14:30-16:30 **1. Atomic structure and reaction mechanism/kinetics**

DS7-1
Richard M.[1], Can F.[1], Duprez D.[1], Gil S.[2], Giroir-Fendler A.[2], Bion N.[1]
Remarkable Enhancement of O_2 Activation on YSZ Surface in a Dual-Bed for Catalytic Partial Oxidation of CH_4
1 - University of Poitiers, CNRS UMR 7285, Institut des Milieux et Matériaux de Poitiers (IC2MP), 4 rue Michel Brunet TSA 51106, 86073, Poitiers Cedex9, France
2 - University of Lyon 1, CNRS UMR 5256, IRCELYON, 2 avenue Albert Einstein, F-69622, Villeurbanne, France

DS7-2
Sprung C.[1], Yablonsky G.S.[2], Schlögl R.[1], Trunschke A.[1]
A Qualitative Kinetic Analysis of Steady-State Selective Oxidation Process: Role of Water and Oxygen
1 - Fritz Haber Institute of the Max Planck Society, Department of Inorganic Chemistry, Berlin, Germany
2 - Department of Chemistry, Parks College, Saint Louis University, Saint Louis, MO, USA

DS7-3
Li G., Hensen E.J.M., Pidko E.A.
Trinuclear Copper Oxo-clusters in ZSM-5 Zeolite for Selective Methane Oxidation to Methanol
Inorganic Materials Chemistry group, Eindhoven University of Technology, Eindhoven, The Netherlands

2. Recent progress in vanadia-based catalysts of selective oxidation

DS7-4
Sushchenko E., Kharlamova T.
Structural Peculiarities and Catalytic Properties of Supported Vanadium Oxide Catalysts for Oxidative Dehydrogenation
Tomsk State University, Chemistry faculty, Tomsk, Russia

DS7-5
Malmusi A., Dellapasqua M., Velasquez Ochoa J., Cavani F.
Vanadium-Based Catalyst for Ethanol Transformation: Relation Between Structure and Catalytic Activity
Dipartimento di Chimica Industriale "Toso Montanari" - Alma Mater Studiorum - Università di Bologna, Bologna, Italy

DS7-6
Wallis P., Schönborn E., Wohlrab S., Kalevaru N., Martin A.
Silica Supported Vanadia Catalysts for Selective Methane Oxidation: Impact of Morphology and Heteroatom Doping on Catalyst Performance
Leibniz Institute for Catalysis, Rostock, Germany

3. New approaches in preparation

DS7-7
Laguna O.H.[1], Centeno M.A.[1], Boutonnet M.[2], Odriozola J.A.[1]
Gold Supported on Fe-doped Ceria Supports Prepared through the Microemulsion Method for the PROX Reaction
1 - Instituto de Ciencia de Materiales de Sevilla, Avda. Américo Vespucio, 49. CP: 41092 Seville - Spain
2 - Royal Institute of Technology (KTH). Department of Chemical Technology. Div. of Chemical Technology. Teknikringen 42, S-10044 Stockholm, Sweden

DS7-8
Dutov V.[1], Mamontov G.[1], Sobolev V.[1,2], Vodyankina O.[1]
Silica-supported Silver-containing OMS-2 Catalysts for Ethanol Oxidative Dehydrogenation
1 - Tomsk State University, Tomsk, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

DS7-9
Machado K., Mishra G.
Selective Oxidation of Cyclic-alkane, Catalyzed by Nano Size SWNTs Supported Pt and Pd Complexes Catalysts
Universidade de Trás-os-Montes e Alto Douro (UTAD), Vila Real 5001801, Portugal

DS7-10
Tyablikov I.A., Romanovsky B.V.
A Heterogeneous Single-site Organocatalyst for Alkene Epoxidation
Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

4.Photocatalytic oxidation

DS7-11
Martínez H., Páez E.A., Martínez F.
Selective Photo-Oxidation of α-pinene with dioxo-Mo(VI) complex /TiO_2 with Different Textural Properties
Cicat, Escuela de Química, UIS, Bucaramanga, Colombia

DS7-12
Arsentyev A.V.[1,2]
Study on Kinetics of Liquid Phase Photocatalytic Oxidation of Dibutyl Sulfide Over Fullerenes
1 - Novosibirsk State University, Novosibirsk, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

5. Liquid phase oxidation

DS7-13
Torozova A.S.[1,2], Doluda V.Yu.[1], Sulman E.M.[1], Murzin D.Yu.[2]
Liquid Phase Oxidation of L-sorbose over Metallic and Bimetallic Particles Stabilized in Polymer Matrix
1 - Tver State Technical University, Dep. Biotechnology and Chemistry, Tver, Russia
2 - Abo Akademi University, Turku, Finland

DS7-14
Torbina V.[1], Ivanchikova I.[1,2], Kholdeeva O.[1,2], Vodyankina O.[1]
Propylene Glycol Oxidation over Cr-MIL-101 with Tert-butyl Hydroperoxide
1 - Tomsk State University, Tomsk, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150**
(Poster set-up time 09:00 – 19:00)

Wednesday, September 2

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Schlögl Robert, *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*
Prof. Skoglundh Magnus, *Competence Centre for Catalysis, KCK, Chalmers University of Technology, Göteborg, Sweden*

Plenary Lecture

08:30-09:30 **PL-7** Michel Boudart Award Lecture (2015). Prof. Freund Hans-Joachim
Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Lermontov hall

Discussion symposium 5. "CO_2 Capture & Valorization"

Chairmen: Prof. Kegnaes Soeren, *Technical University of Denmark, Department of Chemistry, Lyngby, Denmark*
Dr. Lokteva Ekaterina, *Lomonosov Moscow State University, Moscow, Russia*

10:00-13:00 **DS5-1**
Abate S., Mebrahtu C., Perathoner S, Gentiluomo S., Giorgianni G., Centi G.
Catalytic Performance of Ni-based Catalysts Supported on λ-Al_2O_3-ZrO_2-TiO_2-CeO_2 Composite Oxide for CO_2 Methanation
University of Messina, Messina, Italy

DS5-2
Garbarino G.[1], Bellotti D.[2], Riani P.[3], Magistri L.[2], Busca G.[1]
CO_2 Methanation on Commercial Ni/Al_2O_3 and Ru/Al_2O_3 Catalysts
1 - University of Genova, DICCA Dipartimento di Ingegneria Civile Chimica e Ambientale, Genova, Italy
2 - University of Genova, DIME Dipartimento di Ingegneria Meccanica, Energetica, Gestionale e dei Trasporti, Genova, Italy
3 - University of Genova, DCCI Dipartimento di Chimica e Chimica Industriale, Genova, Italy

DS5-3
Taherimehr M.[1], Cardoso Costa Sertã J.P.[1], Kleij A.W.[2,3], Whiteoak C.J.[2], Pescarmona P.P.[1,4]
A New, Active Iron-complex Catalyst for Converting CO_2 into Cyclic Carbonates and Cross-linked Polycarbonates with Enhanced Properties
1 - COK, University of Leuven, Belgium
2 - ICIQ, Tarragona, Spain
3 - ICREA, Barcelona, Spain
4 - Chemical Engineering Department, University of Groningen, The Netherlands

DS5-4

Visconti C.G.[1], Martinelli M.[1], Falbo L.[1], Infantes-Molina A.[1], Gaeta M.[1], Lietti L.[1], Forzatti P.[1], Palo E.[2], Picutti B.[3]

CO_2 Hydrogenation to Light Olefins on a High Surface Area K-promoted Iron Catalyst

1 - Politecnico di Milano, Dipartimento di Energia, Milan, Italy
2 - KT-Kinetics Technologies SpA, Viale Castello della Magna 75, 00148 Rome, Italy
3 - Maire Tecnimont Group SpA, Via Gaetano de Castillia 6/A, 20124 Milan, Italy

DS5-5

Paksoy A.I., Aksoylu A.E.

The Analysis of Carbon Dioxide Reforming of Methane (CDRM) Performance of Co-Ce/ZrO_2 System

Bogazici University, Department of Chemical Engineering, Istanbul, Turkey

DS5-6

Bivona L.A.[1,2], Fichera O.[1], Buaki-Sogo M.[1], Fusaro L.[1], Gruttadauria M.[2], Aprile C.[1]

Novel Imidazolium Based Catalyst for the Chemical Fixation of Carbon Dioxide

1 - Unit of Nanomaterial Chemistry (CNano), University of Namur (UNAMUR), Department of Chemistry, Namur, Belgium
2 - Dipartimento di Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche (STEBICEF), Sezione di Chimica, Università di Palermo, Viale delle Scienze, Ed. 17, 90128, Palermo, Italy

DS5-7

Cadete Santos Aires F.J.[1], Aouine M.[1], Daniel C.[1], Meunier F.C.[1], Farrusseng D.[1], Epicier T.[1,2]

Real-time In situ Atomic-scale Study of the Surface Termination of Ceria Nanoparticles under Vacuum, O_2 and CO_2 Pressures by Environmental Transmission Electron Microscopy

1 - Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256 CNRS/UCB Lyon 1, 2 Avenue Albert Einstein, 69626 Villeurbanne, France
2 - Laboratoire MATEIS, UMR 5510, CNRS/INSA de Lyon, Villeurbanne Cedex, France

DS5-8

Hernández W.Y.[1], Van Oudenhove M.[2], Verberckmoes A.[2], Van Der Voort P.[1]

Au/MgO-type Catalysts for the Carbonylation of Glycerol with Urea. Effect of the Morphology and Macro/Meso-Porous Structure of the Support

1 - Center for Ordered Materials, Organometallics & Catalysis (COMOC), Department of Inorganic and Physical Chemistry, Ghent University, Ghent, Belgium
2 - Industrial Catalysis and Adsorption Technology (INCAT), Department of Industrial Technology and Construction, Faculty of Engineering & Architecture, Ghent University, Ghent, Belgium

DS5-9

Ab. Rahim M.H., Paroo I.V., Maniam G.P.

Synthesis of Organic Carbonates Using Catalyst Containing K Metal from Waste Source

Faculty of Industrial Sciences & Technology, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Kuantan, Pahang, Malaysia

DS5-10

Gabrovska M.[1], Shopska M.[1], Edreva-Kardjieva R.[1], Nikolova D.[1], Bilyarska L.[1], Crişan D.[2]

Modified Ni-Al Layered Double Hydroxides as Catalyst Precursors for Utilization of Carbon Dioxide

1 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria
2 - "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Romania

DS5-11

Eropak B.M.[1], Aksoylu A.E.[1], Çağlayan B.S.[2]

Design and Development of Efficient AC-based Adsorbents for CO_2 Removal

1 - Boğaziçi University, Department of Chemical Engineering, Istanbul, Turkey
2 - Advanced Technologies R&D Center, Boğaziçi University, Istanbul, Turkey

DS5-12

Hacioglu M., Gürkaynak Altınçekiç T., Özdemir H., Öksüzömer M.A.F.

Preperation and Characterization of Ni-based Catalysts for Oxy-CO_2 Reforming of Methane by Using Wet Impregnation Method

Department of Chemical Engineering, Istanbul University, Avcılar, Istanbul, Turkey

DS5-13

Fukuhara C.[1], Hayakawa K.[1], Murabayashi K.[2], Khono Y.[1], Watanabe R.[1]

A Honeycomb-Type Ni/CeO_2 Catalyst for CO_2 Methanation to Transform Greenhouse Gas into Useful Resources

1 - Shizuoka University, Department of Applied Chemistry and Biochemical Engineering, Graduate School of Engineering, 3-5-1 Johoku Naka-ku, Hamamatsu, Shizuoka, 432-8561, Japan
2 - Cataler corporation 7800 Chihama, Kakegawa, Shizuoka, 437-1492, Japan

DS5-14

Hillen L., Degirmenci V.

CO_2 Capture by Hierarchical Mesoporous Chabazite Type Zeolites

CenTACat, Department of Chemistry and Chemical Engineering, Queen's University, Belfast, BT9 5AG, Northern Ireland

DS5-15

Marakushev S.A., Belonogova O.V.

Autocatalytic Fixation of Carbon Dioxide

Institute of Problem of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Moscow Region, Russia

DS5-16

Calisan A., Uner D.

Surface Oxidation Mechanism of Pb-based Materials by Utilization of CO_2 as an Oxidant

Chemical Engineering Department, Middle East Technical University, Ankara, Turkey

13:00-14:30	***Lunch***

KORSTON Lermontov hall

Evening Session

Discussion symposium 8. "In Situ Measurements for Catalytic Studies: Identification of the Structure of Catalytically Active Sites"

Chairmen: Prof. Rupprechter Günther, *Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria*
Dr. Teschner Detre, *Department of Inorganic Chemistry, Fritz-Haber Institute, Berlin, Germany*

14:30-16:30 **DS8-1**
Lukashuk L.[1], Kolar E.[1], Rameshan C.[1], Teschner D.[2], Knop-Gericke A.[2], Föttinger K.[1], Rupprechter G.[1]
Mechanistic Insights into CO Oxidation and Preferential CO Oxidation over Cobalt Oxide and Promoted Cobalt Oxide Catalysts
1 - Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria
2 - Department of Inorganic Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany

DS8-2
Prosvirin I.P.[1,2], Chetyrin I.A.[1,2,3], Khudorozhkov A.K.[1,3], Bukhtiyarov V.I.[1,2,3]
In-situ XPS Study of Active Component of Pd/Al_2O_3 Catalysts in Total CH_4 Oxidation
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Research and Educational Center for Energy Efficient Catalysis in Novosibirsk National Research University, Novosibirsk, Russia

DS8-3
Bukhtiyarov A.V.[1,2], Prosvirin I.P.[1,3], Saraev A.A.[1], Klyushin A.Yu.[4], Knop-Gericke A.[4], Schlogl R.[4], Bukhtiyarov V.I.[1,2,3]
CO Oxidation on the Bimetallic Pd-Au/HOPG Catalysts: In-situ XPS and MS Investigation
1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
2 - Research and Educational Center for Energy Efficient Catalysis in Novosibirsk National Research University, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia
4 - Fritz-Haber-Institute der Max Planck Society, Berlin, Germany

DS8-4
Rameshan R.[1,2], Mayr L.[1], Penner S.[1], Franz D.[3], Vonk V.[3], Stierle A.[3], Klötzer B.[1], Knop-Gericke A.[2], Schlögl R.[2]
Carbide and Graphene Growth, Suppression and Dissolution in Ni Model Systems Studied by In-situ XPS and SXRD
1 - Institute of Physical Chemistry, University Innsbruck, Innsbruck, Austria
2 - Department of Inorganic Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany
3 - Department of Photon Science, Deutsches Elektronen Synchrotron DESY, Germany

DS8-5
Gianolio D.[1], Cibin G.[1], Parry S.A.[1], Dent A.J.[1], Kroner A.B.[2], Gibson E.K.[3], Wells P.P.[3]
B18 Capabilities for XAS In-situ Experiments in Catalysis
1 - Diamond Light Source Ltd, B18 beamline, Harwell Science and Innovation Campus, UK
2 - Diamond Light Source Ltd, Idustrial Liaison Group, Harwell Science and Innovation Campus, UK
3 - UK Catalysis Hub, RCaH, Harwell Science and Innovation Campus, Didcot, UK

DS8-6
Godiksen A.[1], Vennestrøm P.N.R.[2], Rasmussen S.B.[2], Lundegaard L.F.[2], Mossin S.[1]
In-situ EPR Spectroscopy of the NH$_3$-SCR Mechanism of Copper Chabazite
1 - Technical University of Denmark, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Kemitorvet 207, 2800 Kgs. Lyngby, Denmark
2 - Haldor Topsøe A/S, Nymøllevej 55, 2800 Kgs. Lyngby, Denmark

DS8-7
Aliyeva N.M., Mammadov E.E., Huseynova F.I., İsmailov E.H.
In Situ EMR/GC Study of the Conversion of Ethanol into Hydrocarbons on Fe-Zr/Al$_2$O$_3$ Catalysts
Institute of Petrochemical Processes, Azerbaijan National Academy of Sciences, Baku, Azerbaijan

DS8-8
Goryachev A.[1], Carla F.[2], Drnec J.[2], Onderwaater W.[2], Krause P.P.T.[3], Wonders A.H.[1], Hensen E.J.M.[1], Hofmann J.P.[1]
Synchrotron Based Operando Study of Structure Activity Relationships of Model Electrocatalysts for Water Splitting
1 - Technische Universiteit Eindhoven, Inorganic Materials Chemistry, Eindhoven, Netherlands
2 - European Synchrotron Radiation Facility, Grenoble, France
3 - Justus-Liebig-Universität Giessen, Physikalisch-Chemisches Institut, Gießen, Germany

DS8-9
Saraev A.A., Vinokurov Z.S., Shmakov A.N., Kaichev V.V., Bukhtiyarov V.I.
In Situ XRD Study of Oscillations During the Methane Oxidation over Palladium and Nickel Foils
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

DS8-10
Zheng G.[1], Polavarapu L.[1], Pastoriza-Santos I.[1], Pérez-Juste J.[1], Liz-Marzán L. M.[1,2]
Gold Nanoparticle-Loaded Filter Paper: a Recyclable Dip-Catalyst for Real-Time Reaction Monitoring by Surface Enhanced Raman Scattering
1 - Departamento de Química Física, Universidade de Vigo, Vigo, Spain
2 - Bionanoplasmonics Laboratory, CIC biomaGUNE, Spain

DS8-11

Bera P.[1], Baidya T.[2]

DRIFTS Studies of Support Effects on CO Adsorption and CO + O_2 Reaction over $Ce_{1-x-y}M_xCu_yO_{2-d}$ (M = Zr, Hf, Th)

1 - Surface Engineering Division, CSIR-National Aerospace Laboratories, Bangalore, India

2 - Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 **Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150**
(Poster set-up time 09:00 – 19:00)

Wednesday, September 2

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Schlögl Robert, *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*
Prof. Skoglundh Magnus, *Competence Centre for Catalysis, KCK, Chalmers University of Technology, Göteborg, Sweden*

Plenary Lecture

08:30-09:30 **PL-7** Michel Boudart Award Lecture (2015). Prof. Freund Hans-Joachim
Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Chekhov hall

Discussion symposium 6. "Pollution Control & Oxidation Catalysis"

Chairmen: Prof. Grünert Wolfgang, *Ruhr University Bochum, Germany*
Prof. Stakheev Alexander, *Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia*

10:00-13:00 **DS6-1**
Lopatin S.A.[1,2], Zazhigalov S.V.[1,2], Mikenin P.E.[1,2], Pisarev D.A.[1,2], Baranov D.V.[1,2,3], Zagoruiko A.N.[1,2,4]
Structured Cartridges with Glass-fiber Catalysts: New Trend in the Design of Catalytic Reactors for Pollution Control
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Research and Educational Center for Energy Efficient Catalysis, Novosibirsk State University, Novosibirsk, Russia
3 - Novosibirsk Technical State University, Novosibirsk, Russia
4 - Tomsk Polytechnic University, Tomsk, Russia

DS6-2
Gasparyan M.D., Liberman E.Y.U., Grunsky V.N., Obukhov E.
Catalysts on the Base of Ceramic Highly-porous Block-cellular Carriers
Russian Mendeleev University of Chemical Technology, Moscow, Russia

DS6-3
Jin B.F., Wei Y.C., Zhao Z., Liu J., Duan A.J.
The Synthesis Charcterization and Catalytic Performances of Three-dimensionally Ordered Macroporous x-CeO$_2$/Al$_2$O$_3$ Catalysts for Diesel Soot Combustion
State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Chang Ping, Beijing, China

DS6-4

Paul J.-F., Berrier E., Blanck D.

Are Perovskite Materials Efficient for Tree Way Catalysis? A Theoretical Study of $LaFeO_3$

Unité de Catalyse et de Chimie du Solide, Villeneuve d'Ascq, France

DS6-6

Wagloehner S., Nitzer-Noski M., Kureti S.

Soot Oxidation on Manganese Oxide Catalysts in Diesel and Gasoline Exhaust

Technical University of Freiberg, Institute of Energy Process Engineering and Chemical Engineering, Chair of Reaction Engineering, Freiberg, Germany

DS6-7

Trunfio G.[1], Di Chio R.[1], Rahim S.H.A.[1], Espro C.[1], Milone C.[1], Galvagno S.[1], Spadaro L.[2], Arena F.[1,2]

Development of MnO_x-based Catalysts for the Catalytic Wet Air Oxidation (CWAO) of Organic Pollutants

1 - Dipartimento di Ingegneria Elettronica, Chimica e Ingegneria Industriale, Università degli Studi di Messina, Viale F. Stagno D'Alcontres 31, Messina, Italy
2 - Istituto CNR-ITAE "Nicola Giordano", Salita S. Lucia 5, I-98126 S. Lucia (Messina), Italy

DS6-8

Chlala D.[1], Giraudon J.-M.[1], Nuns N.[2], Labaki M.[3], Lamonier J.-F.[1]

Attractive Route for New Hydroxyapatite Supported Calcium-Manganese Oxides for Total Oxidation of Toluene

1 - Université Lille1, UMR 8181 CNRS, UCCS, Boulevard Langevin, 59650 Villeneuve d'Ascq, France
2 - IMMCL Chevreul, Institut des Molécules et de la Matière Condensée, Lille, France
3 - Lebanese University, Laboratory of Physical Chemistry of Materials (LCPM)/PR2N, Faculty of Sciences, Fanar, BP 90656 Jdeidet El Metn, Lebanon

DS6-9

Nikbin N.[1], Austin N.[2], Christiansen M.[1], Vlachos D.G.[1], Stamatakis M.[3], Mpourmpakis G.[2]

Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters

1 - University of Delaware, Department of Chemical Engineering, Newark, Delaware, USA
2 - University of Pittsburgh, Department of Chemical Engineering, Pittsburgh, Pennsylvania, USA
3 - University College London, Department of Chemical Engineering, Torrington Pl., London WC1E 7JE, UK

DS6-10

Tabakova T.[1*], Kolentsova E.[2], Dimitrov D.[2], Petrova P.[1], Karakirova Y.[1], Avdeev G.[3], Nihtianova D.[4], Ivanov K.[2]

Effect of Au and Ag on the Performance in CO and VOCs Oxidation of Alumina Supported Cu-Mn Catalysts

1 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria
2 - Department of Chemistry, Agricultural University, Plovdiv, Bulgaria
3 - Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria
4 - Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, Sofia, Bulgaria

DS6-11

Dubkov A.A.[1,2], Carberry B.[2], Schneider M.[2], Linzen F.[2], Smirnov M.Yu.[1], Kalinkin A.V.[1], Salanov A.N.[1], Shmakov A.N.[1], Gerasimov E.Yu.[1], Bukhtiyarov V.I.[1,3]

Change in the Chemical Composition of an LNT as a Result of its Ageing in Diesel Exhaust Gases: Physical and Chemical Analysis

1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk Russia
2 - Ford Forschungszentrum Aachen GmbH, Aachen, Germany
3 - Novosibirsk State University, Novosibirsk, Russia

DS6-12

Ismagilov Z.[1,2], Parmon V.[1], Yarullin R.[3], Mazgarov A.[4], Khairulin S.[1],
Kerzhentsev M.[1], Golovanov A.[5], Vildanov A.[4], Garifullin R.[5]

The Process of H_2S Selective Catalytic Oxidation For On-site Purification of Hydrocarbon Gaseous Feedstock. Technology Demonstration at Bavly Oil Field in Republic of Tatarstan

1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia
3 - OJSC “Tatneftekhiminvestholding” Kazan, Russia
4 - OJSC “Volga research institute of hydrocarbon feed” Kazan, Russia
5 - OJSC “Tatneft”, Al`metyevsk, Russia

DS6-13

Agafonov A.A.[1,2], Lokteva E.S.[1,2], Maslakov K.I.[1,2], Strokova N.E.[1], Voronova L.V.[1]

Pd Catalysts Supported on Metal Organic Coordinated Structures in Chlorobenzene Hydrodechlorination and CO Oxidation

1 - Lomonosov Moscow State University, Chemistry Department, Moscow, Russia
2 - Institute of Hydrocarbons Processing SB RAS, Omsk, Russia

13:00-14:30	***Lunch***

KORSTON Chekhov hall

Evening Session

Chairmen: Prof. Neyman Konstantin M., *Departament de Química Física & Institut de Química Teòrica i Computacional, Universitat de Barcelona, Barcelona, Spain, Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain*
Dr. Pidko Evgeny, *Institute for Complex Molecular Systems, Inorganic Materials Chemistry, Eindhoven University of Technology, Eindhoven, the Netherlands*

Discussion symposium 9. "DFT Calculation in Catalytic Studies "

14:30-16:30 **DS9-1**
Ray K.[1], Pandey D.[1], Singh B.[2], Prasad R.[2], Deo G.[1]
A Computational Approach to Understand the Promotional Effect in Ni-Fe Bimetallic Catalyst
1 - Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India
2 - Department of Physics, Indian Institute of Technology Kanpur, Kanpur, India

DS9-2
Polynskaya Y.G., Pichugina D.A., Kuz'Menko N.E.
Propene Epoxidation with Molecular Oxygen over Gold-Silver Catalysts: Density Functional Calculations
M.V. Lomonosov Moscow State University, Moscow, Russia

DS9-3
Schimmenti R., Prestianni A., Ferrante F., Duca D.
Computational Investigation of Palladium Supported Boron Nitride Nanotube Catalysts
Università degli Studi di Palermo, Dipartimento di Fisica e Chimica, Palermo, Italy

DS9-4
Nasluzov V.A.[1], Laletina S.S.[1], Ivanova-Shor E.A.[1], Shor A.M.[1], Neyman K.M.[2,3]
A GGA+U DFT Investigation of Silver Atom, Trimer and Tetramer Supported by a Nanosized Particle $Ce_{21}O_{42}$
1 - Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia
2 - Institucio Catalana de Recerca i Estudis Avancats (ICREA), Barcelona, Spain
3 - Departament de Quimica Fisica & IQTCUB, Universitat de Barcelona, Barcelona, Spain

DS9-5
Banerjee A.[1], Gunasooriya G.T.K.K.[2], Saeys M.[2], Otyuskaya D.S.
Origin of the Spontaneous Formation of Cobalt Nano-Islands under Fischer Tropsch Conditions and Mechanistic Consequences
1 - Department of Chemical and Biomolecular Engineering, 4 Engineering Drive 4, National University of Singapore, 117576 Singapore
2 - Laboratory for Chemical Technology, Ghent University, Technologiepark 914, 9052 Gent, Belgium

DS9-6
Golosnaya M., Pichugina D., Kuz'menko N.
Quantum-Chemical Investigation Ligand-Stabilized Gold Clusters in Oxidation Reaction
M.V. Lomonosov Moscow State University, Moscow, Russia

DS9-7
Liu C., Li G., Hensen E.J. M., Pidko E.A.
Speciation of Extraframework Aluminium Species in Faujasite Zeolite: a Theoretical Perspective
Inorganic Materials Chemistry group, Eindhoven University of Technology, Eindhoven, The Netherlands

DS9-8
Avdeev V.I.[1], Bedilo A.F.[1,2], Shuvarakova E.I.[1,2]
Mechanism of Propane Oxidative Dehydrogenation on Surface Oxygen Radical Sites of VO_x/TiO_2 Catalysts
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk Institute of Technology, Moscow State University of Design and Technology, Novosibirsk, Russia

DS9-9
Goulon A.[1], Faraj A.[1], Leflaive P.[2]
Graph Machine Based Advanced Data Modelling for High-Throughput Zeolite Catalyst Screening
1 - IFP Energies nouvelles, 1 et 4 avenue de Bois-Préau, 92852 Rueil-Malmaison, France
2 - IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize, France

DS9-10
Dr. Yuan R.M.[1], Lin Z.[2]
DFT Studies on the Mechanisms of Nickel-Catalyzed Reductive Carboxylation of Styrenes Using CO_2 as the Building Block
1 - Department of Chemistry, Xiamen University, Xiamen 361005, People's Republic of China
2 - Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, People's Republic of China

DS9-11
Polo-Garzon F., Bruce D.A.
Reaction Mechanism of Dry Reforming of Methane on Rh Doped Pyrochlore Catalysts: a DFT Approach
Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, USA

16:30-17:00 ***Coffee break***

KORSTON TOWER, Combine halls: Prokofiev, Rakhmaninov, Chaikovsky, Shostakovich

17:00-19:00 Poster Session-II: II-PP1÷II-PP260, V-PP1÷V-PP150

(Poster set-up time 09:00 – 19:00)

Thursday, September 3

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Hupp Joseph, *Northwestern University, Department of Chemistry, Evanston, USA*
Dr. Bellussi Giuseppe, *Eni S.p.A, Refinding & Marketing Devision, Milanese, Italy*

Plenary Lecture

08:30-09:30 **PL-8** Prof. Skoglundh Magnus
Fundamental Studies of Metal-exchanged Zeolites for Selective Catalytic reduction of Nitrogen Oxides in Oxygen Excess
Competence Centre for Catalysis, KCK, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-1

Section 5. Catalysis and Environmental Protection

Chairmen: Prof. Khodakov Andrei Y., *UCCS, Université Lille 1-ENSCL-EC Lille, Bat. C3, Cité Scientifique, 59655 Villeneuve d'Ascq, France*
Prof. Sojka Zbigniew, *Jagiellonian University, Faculty of Chemistry, Krakow, Poland*

Keynote Lecture

10:00-10:40 **V-KN13** Prof. Nam In-Sik
Progress and Challenges in Urea/SCR Technology for Removing NO_x from Diesel Engine
Department of Chemical Engineering/School of Environmental Science and Engineering, Pohang University of Science and Techlogy (POSTECH), Pohang, Republic of Korea

Oral Presentations

10:40-11:00 **V-OP25** Prof. Grünert Wolfgang
Ellmers I.[1], Huang H.[2], Perez Velez R.[3], Brückner A.[3], Schünemann V.[2], Grünert W.[1]
NO Oxidation and Standard SCR over Fe-ZSM-5 Catalysts. Combining Moessbauer Spectroscopy and Reactivity Studies on the Search for the Active Sites
1 - Ruhr University Bochum, Bochum, Germany
2 - Universität Kaiserslautern, Kaiserslautern, Germany
3 - Leibniz-Institut für Katalyse e.V. Rostock, Rostock, Germany

11:00-11:20 **V-OP26** Dr. Moses Poul G.
Moses P.G.[1], Janssens T.V.W.[1], Falsig H.[1], Lundegaard L.F.[1], Vennestrøm P.N.R.[1], Giordanino F.[2], Borfecchia E.[2], Lamberti C.[2,3], Bordiga S.[2], Godiksen A.[4], Mossin S.[4], Beato P.[1]
The Rate Determining Step for the Selective Catalytic Reduction of NO by Ammonia
1 - Haldor Topsoe A/S, Nymøllevej 55, 2800 Lyngby, Denmark
2 - Dept. of Chemistry, NIS Centre of Excellence and INSTM Reference Center, University of Turin, Via Giuria 7, 10125 Torino, Italy
3 - Southern Federal University, Zorge Street 5, 344090 Rostov-on-Don, Russia
4 - Dept. of Chemistry, Centre of Catalysis and Sustainable Chemistry, Technical University of Denmark, Kemitorvet 207, 2800 Lyngby, Denmark

11:20-11:40 **V-OP27** Prof. Nova Isabella
Ruggeri M.P.[1], Nova I.[1], Tronconi E.[1], York A.P.E.[2]
Structure-Activity Relationship for Cu-Zeolite NH_3-SCR Catalysts
1 - Dip. Energia, Politecnico di Milano, Milano, Italy
2 - Johnson Matthey Technology Centre, Sonning Common, UK

11:40-12:00 **V-OP28** Dr. Garcia Vargas Jesus Manuel
Gil S., Garcia-Vargas J.M., Retailleau L., Giroir-Fendler A.
Influence of the Preparation Method and Used Support on the Activity of Fe-loaded Zeolites Catalysts for the NH_3-SCR of NO_x
Université Lyon 1, CNRS, UMR 5256, IRCELYON, Institut de recherches sur la catalyse et l’environnement de Lyon, 2 avenue Albert Einstein, F-69626 Villeurbanne, France

12:00-12:20 **V-OP29** Prof. Granger Pascal
Gillot S.[1,2,3], Dujardin Ch.[1,3,4], Dacquin J.-P.[1,2,3], Granger P.[1,2,3]
$CeVO_4$-based as Efficient and Stable Catalyst for NH_3 Selective Catalytic Reduction of NO_x – Application to Diesel Exhaust Gas
1 - UCCS, France
2 - University of Lille, France
3 - Cité Scientifique, 59650 Villeneuve d'Ascq, France
4 – ENSCL, France

12:20-12:40 **V-OP30** Dr. Sridhar Manasa
Sridhar M.[1,2], Ferri D.[1], van Bokhoven J. A.[1,2], Kröcher O.[1,3]
Base-promotion of Selective Decomposition of Ammonium Formate and Formic Acid over Au/TiO_2 under SCR-relevant Conditions
1 - Paul Scherrer Institut, General Energy Department, Villigen, Switzerland
2 - ETH Zurich, Institute for Chemical and Bioengineering, Switzerland
3 - École Polytechnique Fédérale de Lausanne (EPFL), Institute of Chemical Sciences and Engineering, Lausanne, Switzerland

12:40-13:00 **V-OP31** Dr. Say Zafer
Sulfur-Tolerant $BaO/ZrO_2/TiO_2/Al_2O_3$ Quaternary Mixed Oxides for $DeNO_X$ Catalysis
Say Z.[1], Mihai O.[2], Tohumeken M.[1], Ercan K.E.[1], Olsson L.[2], Ozensoy E.[1]
1 - Department of Chemistry, Bilkent University, 06800 Ankara, Turkey
2 - Chemical Reaction Engineering and Competence Centre for Catalysis, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

13:00-14:30 ***Lunch***

KORSTON Ball hall-1

Evening Session

Section 3. Energy-Related Catalysis

Chairmen: Dr. Kaichev Vasily, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Martyanov Oleg, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Keynote Lecture

14:30-15:10 **III-KN15** Prof. Rupprechter Günther
Rupprechter G., Rameshan C., Föttinger K., Suchorski Y., Bukhtiyarov A., Li H., Anic K., Wolfbeisser A., Lukashuk L.
Operando Studies on PdZn-ZnO, (Pd-)Co_3O_4 and Ni-ZrO_2: Synergies between Surface Science Based Model Systems and Technological Catalysts
Institute of Materials Chemistry, Vienna University of Technology, 1060 Vienna, Austria

Oral Presentations

15:10-15:30 **III-OP33** Dr. Arutyunov Vladimir
Arutyunov V.[1], Savchenko V.[2], Sedov I.[2], Fokin I.[2], Makaryan I.[2], Nikitin A.[1], Strekova L.[1]
Gas-phase Partial Oxidation – Catalytic Carbonylation Conception for Small-scale GTL
1 - Semenov Institute of Chemical Physics, Russ. Acad. Sci., Moscow, Russia
2 - Institute of Problems of Chemical Physics, Russ. Acad. Sci., Chernogolovka, Moscow region, Russia

15:30-15:50 **III-OP34** Dr. Simagina Valentina
Simagina V.I.[1], Netskina O.V.[1], Ozerova A.M.[1], Komova O.V.[1], Odegova G.V.[1], Kochubey D.I.[1], Kellerman D.G.[2]
Progress in the Catalysts for Small-scale Hydrogen Generators Based on Boron-containing Hydrides
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Solid State Chemistry UrB RAS, Ekaterinburg, Russia

Keynote Lecture

15:50-16:30 **III-KN16** Prof. Li Can
Photocatalytic Overall Water Splitting: Present and Future
State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian National Laboratory for Clean Energy, Dalian, China

16:30-17:00 ***Coffee break***

Chairmen: Prof. Olsbye Unni, *Department of Chemistry, University of Oslo, Oslo, Norway*
Prof. Nervi Carlo, *University of Turin, Department of Chemistry, Turin, Italy*

17:00-17:20 **III-OP35** Prof. Jayakodi Karuppiah J.
Jayakodi Karuppiah J., Young Sun Mok Y.S.
Dry Reforming of Propane over NiO-CeO_2 Loaded Fnodized Fluminum Oxide(AAO) Catalysts
Jeju National University, Department of Chemical Engineering, Jeju 690-756, South Korea

17:20-17:40 **III-OP36** Dr. Cheng Kang
Cheng K., Kang J., Zhang L., Peng X., Zhang Q., Wang Y.
Impact of Hydrocracking on Fischer-Tropsch Synthesis Selectivity: Mesoporous ZSM-5-Supported Cobalt Nanoparticles for Selective Production of C_{5-11} Isoparaffins
Collaborative Innovation Center of Chemistry for Energy Materials, State Key Laboratory of Physical Chemistry of Solid Surfaces, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005, China

17:40-18:00 **III-OP37** Chen Wei
Chen W., Zijlstra B., Filot I.A. W., Ligthart D.A.J.M., Van Hoof A.J.F., Pestman R., Hensen E.J.M.
CO Activation on Cobalt Fischer-Tropsch Catalyst
Laboratory of Inorganic Materials Chemistry, Eindhoven University of Technology
P.O. Box 315, 5600 MB Eindhoven, The Netherlands

19:30 **Banquet (restaurant PANORAMA)**

19:00 **Young scientists party**
(club "Extra Lounge" at the 25th floor of "Korston Tower" hotel)

Thursday, September 3

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Hupp Joseph, *Northwestern University, Department of Chemistry, Evanston, USA*
Dr. Bellussi Giuseppe, *Eni S.p.A, Refinding & Marketing Devision, Milanese, Italy*

Plenary Lecture

08:30-09:30 **PL-8** Prof. Skoglundh Magnus
Fundamental Studies of Metal-exchanged Zeolites for Selective Catalytic reduction of Nitrogen Oxides in Oxygen Excess
Competence Centre for Catalysis, KCK, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Ball hall-2

Section 2. Catalyst Preparation and Characterization

Chairmen: Prof. Huang Weixin, *Department of Chemical Physics, University of Science and Technology of China, Hefei, China*
Dr. Roman-Martinez M. Carmen, *Department of Inorganic Chemistry. University of Alicante, Alicante, Spain*

Oral Presentations

10:00-10:20 **II-OP34** Prof. Conesa Jose C.
Monte M.[1], Bolívar C.L.[1], Munuera G.[2], Martínez-Arias A.[1], Conesa J.C.[1]
CeO$_2$ Carrier Shape Effects on CuO$_x$/CeO$_2$ CO-PROX Catalysis: Operando X-ray Spectroscopy and DFT Modelling Studies
1 - Instituto de Catálisis y Petroleoquímica, CSIC, Marie Curie 2, 28049 Madrid, Spain
2 - Real Academia Sevillana de Ciencias, Fac. de Química, Prof. García González s/n, 41012 Sevilla, Spain

10:20-10:40 **II-OP35** Dr. Offermans Willy K.
Offermans W.K.[1], Gürtler C.[1], North M.[2], Leitner W.[3], Müller T.E.[1]
A Density Functional Theory Study on the Mechanism of the Cycloaddition of CO$_2$ and Epoxides
1 - CAT Catalytic Center, ITMC, RWTH Aachen University, Worringerweg 1, 52074 Aachen, Germany
2 - Department of Chemistry, University of York, York, United Kingdom
3 - Lehrstuhl für Technische Chemie und Petrolchemie, RWTH Aachen University, Worringerweg 1, 52074 Aachen, Germany

Keynote Lecture

10:40-11:20 **II-KN14** Prof. Neyman Konstantin
Approaching Complexity in Heterogeneous Catalysis by Density-Functional Modelling
Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain
Departament de Química Física & Institut de Química Teòrica i Computacional, Universitat de Barcelona, c/ Martí i Franquès, 1, 08028 Barcelona, Spain

Oral Presentations

11:20-11:40 **II-OP36** Dr. Pichugina Daria
Pichugina D.A., Beletskaya A.V., Kuzmenko N.E.
Effect of Structure and Composition of Gold and Gold-palladium Clusters in H_2O_2 Formation
Lomonosov Moscow State University, Department of Chemistry, Moscow, Russia

11:40-12:00 **II-OP37** Dr. Venvik Hilde J.
Svenum I.-H.[1], Vicinanza N.[2], Herron J.A.[3], Peters T.A.[1], Bredesen R.[1], Mavrikakis M.[3], Venvik H.J.[2]
Surface Phenomena Affecting the Performance of Pd-Ag Alloys
1 - SINTEF Materials and Chemistry, Trondheim, Norway
2 - Department of Chemical Engineering, NTNU, Trondheim, Norway
3 - University of Wisconsin-Madison, Madison, WI, USA

12:00-12:20 **II-OP38** Filot Ivo A.W.
Filot I.A.W.[1,2,3], Van Santen R.A.[1,2,3], Hensen E.J.M.[1,2,3]
Understanding Selectivity Issues in Rh-catalyzed CO Hydrogenation
1 - Schuit Institute of Catalysis and Institute of Complex Molecular Systems
2 - Eindhoven University of Technology, Eindhoven, The Netherlands
3 - P.O. Box 513, 5600 MB, Eindhoven, The Netherlands

12:20-12:40 **II-OP39** Saab Mohamad
Saab M., Raybaud P.
In Silico Exploration of Bimetallic Sulfides Catalysts
Direction Catalyse et Séparation, IFP Energies nouvelles, Rond-point de l'échangeur de Solaize BP 3, 69360 Solaize, France

12:40-13:00 **II-OP40** Dr. Bykova Mariya
Bykova M.V.[1,2], Rekhtina M.A.[1,2], Kaichev V.V.[1], Saraev A.A.[1], Shmakov A.N.[1], Lebedev M.Yu.[1], Venderbosch R.H.[3], Yakovlev V.A.[1]
Effect of Mo Addition on Hydrotreating Activity, Stability to Corrosion, and Physicochemical Properties of Ni-Based Catalysts for Bio-Oil Upgrading
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Biomass Technology Group B.V., 7545 PN, Josink Esweg 34, Enschede, The Netherlands

13:00-14:30 ***Lunch***

KORSTON Ball hall-2

Evening Session

Chairmen: Dr. Soler Lluís, *Institute of Energy Technologies, Universitat Politècnica de Catalunya, Barcelona, Spain*
Dr. Helveg Stig, *Haldor Topsoe A/S, Kgs. Lyngby, Denmark*

Oral Presentations

14:30-14:50 **II-OP41** Dr. Lokteva Ekaterina
Lokteva E.S.[1,2], Klokov S.V.[1,2], Golubina E.V.[1,2], Maslakov K.I.[1,2], Vasiliev K.Yu.[1,2], Antonova M.V.[1], Likholobov V.A.[2]
Pd/C Catalysts Prepared by Direct Pyrolysis of Sawdust Impregnated by Palladium Nitrate for Hydrodechlorination of Chlorobenzenes
1 - M.V. Lomonosov Moscow State University, Chemistry Department, Moscow, Russia
2 - Institute of Hydrocarbons Processing of the Siberian Branch of the RAS, Omsk, Russia

14:50-15:10 **II-OP42** Dr. Weng Weizheng Z.
Weng W.Z., Xie Y. H., Li B., Zheng Y. P., Huang C. J., Wan H. L.
Formation Mechanism of Well-Dispersed Pd Nanoparticles with High Thermal Stability on SiO_2 Using $Pd(acac)_2$ as Precursor
State Key Laboratory of Physical Chemistry of Solid Surfaces, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China

15:10-15:30 **II-OP43** Piccolo Laurent
Konuspayeva Z.[1], Afanasiev P.[1], Nguyen T.S.[1], Di Felice L.[1], Morfin F.[1], Nguyen N.T.[2], Nelayah J.[2], Ricolleau C.[2], Li Z.Y.[3], Yuan J.,[4], Berhault G.[1], Piccolo L.[1]
Au-Rh and Au-Pd Nanocatalysts Supported on Rutile Titania Nanorods: Structure and Chemical Stability
1 - Institut de Recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON), UMR 5256 CNRS & Université Claude Bernard - Lyon 1, 2 avenue Albert Einstein, 69626 Villeurbanne, France
2 - Laboratoire Matériaux et Phénomènes Quantiques (MPQ), UMR 7162 CNRS & Université Paris-Diderot, Bâtiment Condorcet, 4 rue Elsa Morante, 75205 Paris Cedex 13, France
3 - Nanoscale Physics Research Laboratory (NPRL), School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK
4- Department of Physics, University of York, Heslington, York, YO10 5DD, UK

15:30-15:50 **II-OP44** Dr. Suslova Evgeniya
Chernyak A.S., Savilov S.V., Lunin V.V., Suslova E.V.
Defectiveness of Carbon Nanomaterials as a Key Parameter of Their Effectiveness as a Support for Cobalt Catalysts in Fischer-Tropsch Synthesis
Lomonosov Moscow State University, Moscow, Russia

15:50-16:10 **II-OP45** Ruiz Patricio
Fernández C.[1], Gaigneaux E.M.[1], Bion N.[2], Duprez D.[2], Ruiz P.[1]
Proposal of a Catalytic Cooperation Model between Ru-Supported Nanoparticles in Ammonia Synthesis under Mild Reaction Conditions
1 - Université catholique de Louvain, Institute of Condensed Matter and Nanosciences - IMCN, Division «Molecules, Solids and Reactivity-MOST». Croix du Sud 2, 1348 Louvain-la-Neuve, Belgique
2 - Université de Poitiers, CNRS, UMR 7285, Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP), 4 rue Michel Brunet - TSA 51106 - 86073 Poitiers Cedex 9, Poitiers, France

16:10-16:30 **II-OP46** Dr. Penner Simon
Penner S.P.[1], Thalinger R.T.[1], Opitz A.O.[2], Schmidmair D.S.[3], Heggen M.H.[4]
Water-Gas-Shift and Methane Reactivity on Reducible Perovskite-Type Oxides
1 - University of Innsbruck, Institute for Physical Chemistry, Innsbruck, Austria
2 - Vienna University of Technology, Institute of Materials Chemistry, Vienna, Austria
3 - University of Innsbruck, Institute of Mineralogy and Petrography, Innsbruck, Austria
4 - Forschungszentrum Jülich, Ernst-Ruska Center for Electron Microscopy, Germany

16:30-17:00 ***Coffee break***

Chairmen: Dr. Smirnov Michail, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Dr. Shor Elena, *Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia*

17:00-17:20 **II-OP47** Dr. Yuan Youzhu
Duan X., Tian X., Ke J., Yuan Y.
Facile Redispersion of Sintered Au Nanoparticlces with Controllable Size for Catalytic Application
State Key Laboratory of Physical Chemistry of Solid Surfaces and National Engineering Laboratory for Green Chemical Production of Alcohols-Ethers-Esters, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

17:20-17:40 **II-OP48** Dr. Shen Wenjie
Shi Q., Li Y., Zhan E., Ta N., Shen W.
Shape Effect of TiO_2 on the Performance of VO_x/TiO_2 Catalysts for NH_3-SCR
Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

17:40-18:00 **II-OP49** Prof. Zhao Zhen
Zhang X.D., Wei Y.C., Zhao Z.
Design and Preparation of Pt-Transition Metal Oxides (TMO) Nanoparticles Supported on 3DOM Oxides with Enhanced Catalytic Activity for Soot Combustion
State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing 102249, China

19:30 **Banquet (restaurant PANORAMA)**

19:00 **Young scientists party**
(club "Extra Lounge" at the 25th floor of "Korston Tower" hotel)

Thursday, September 3

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Hupp Joseph, *Northwestern University, Department of Chemistry, Evanston, USA*
Dr. Bellussi Giuseppe, *Eni S.p.A, Refinding & Marketing Devision, Milanese, Italy*

Plenary Lecture

08:30-09:30 **PL-8** Prof. Skoglundh Magnus
Fundamental Studies of Metal-exchanged Zeolites for Selective Catalytic reduction of Nitrogen Oxides in Oxygen Excess
Competence Centre for Catalysis, KCK, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Pushkin hall

Section 3. Energy-Related Catalysis

Chairmen: Dr. Kozlova Ekaterina, *Educational Center for Energoefficient Catalysis in Novosibirsk State University, Novosibirsk State University, Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
Prof. Damyanova Sonia, *Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria*

Oral Presentations

10:00-10:20 **III-OP29** Weidler Natascha
Weidler N., Kaiser B., Jaegermann W.
Changes in the Oxidation States of Cobalt Oxides for the OER Studied by XPS and Their Correlation to the Electrochemical Activity
Technical University Darmstadt, Institute of Material Science, Jovanka-Bontschits-Str.2, Darmstadt, Germany

10:20-10:40 **III-OP30** Thalinger Ramona
Thalinger R.[1], Heggen M.[2], Schmidmair D.[3], Klötzer B.[1], Penner S.[1]
Reactivity of Metals on Perovskites ($La_{0.6}Sr_{0.4}FeO_{3-d}$ (LSF) and $SrTi_{0.7}Fe_{0.3}O_{3-d}$ (STF)) Regarding Possible SOFC Usage
1 - Institute of Physical Chemistry, University of Innsbruck, Austria
2 - Ernst Ruska-Centrum for Microscopy und Spectroscopy with Electrons, Forschungszentrum Jülich, Germany
3 - Institute of Mineralogy and Petrography, University of Innsbruck, Austria

10:40-11:00 **III-OP31** Prof. Nervi Carlo
Nervi C., Gobetto R., Minero C., Franco F., Cometto C., Sun C., Nencini L., Sordello F.
Redox Catalysts for Electrochemical CO_2 Reduction: the Role of Local Proton Source
University of Turin, Department of Chemistry, Turin, Italy

11:00-11:20 **III-OP32** Oshchepkov Alexandr
Oshchepkov A.G.[1,2,3], Bonnefont A.[3], Simonov P.A.[2], Cherstiouk O.V.[2], Pronkin S.N.[1], Parmon V.N.[2], Savinova E.R.[1]
Hydrogen Electrode Reactions over Nickel-Based Catalysts in Alkaline Medium: Influence of Composition and Structure of Ni Particles
1 - ICPEES UMR 7515-CNRS-Université de Strasbourg, France, 67087
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
3 - IC UMR 7177 CNRS-Université de Strasbourg, France, 67000

KORSTON Pushkin hall

Section 4. Catalysis and Chemicals

Chairmen: Prof. Hu Xile, *Laboratory of Inorganic Synthesis and Catalysis, Institute of Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*
Prof. Bryliakov Konstantin, *Novosibirsk State University, Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

11:20-11:40 **IV-OP34** Prof. Hulea Vasile
Hulea V.[1], Andrei R.A.[1], Fajula F.[1], Cammarano C.[1], Popa M.I.[2]
Heterogeneous Oligomerization of Ethylene over Highly Active and Stable Ni-exchanged Mesoporous Materials
1 - Charles Gerhardt Institut, Ecole Nationale Superieure de Chimie, Montpellier, France
2 - Techical University of Iasi, Iasi, Romania

11:40-12:00 **IV-OP35** Ruppel Ekaterina
Ruppel E.I.[1], Ivanchev S.S.[1], Ozerin A.N.[2]
Evolution of Catalytic Systems and Technologies of Production and Solid-state Processing of Ultra-high Molecular Weight Polyethylene with Ultra-durable and Ultra-modular Properties
1 - Boreskov Institute of Catalysis (St.Peterburg Branch), SB RAS, Saint-Petersburg, Russia
2 - Enikolopov Institute of Synthetic Polymer Materials RAS, Moscow, Russia

12:00-12:20 **IV-OP36** Dr. Parfenova Lyudmila
Parfenova L.V., Kovyazin P.V., Zakirova I.V., Khalilov L.M., Dzhemilev U.M.
Enantiomerically Pure Zirconocene Complexes in Asymmetric Alkene Carbo- and Cycloalumination
Institute of Petrochemistry and Catalysis, Russian Academy of Sciences, Ufa, Russia

12:20-12:40 **IV-OP37** Dr. Fu Gang
Fu G., Chen G.X., Zhao Y., Zheng N.F.
Tuning the Selectivity of Nanocatalysts by Using the Ligand Modification Strategy: Experiment and Theory
State Key Laboratory for Physical Chemistry of Solid Surfaces and College of Chemistry and Chemical Engineering, Xiamen University, P.R. China

12:40-13:00 **IV-OP38** Dr. Khrizanforov Mikhail
Khrizanforov M.N., Strekalova S.O., Khrizanforova V.V., Gryaznova T.V., Budnikova Y.H., Sinyashin O.G.
Electrochemical Fluoroalkylation and Phosphorylation Catalyzed by Transition Metal Complexes (Ni, Co etc.) to Avoid Chemical Oxidants or Reductants
A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, Russian Academy of Sciences, Kazan, Russia

13:00-14:30	***Lunch***

KORSTON Pushkin hall

Evening Session

Chairmen: Prof. Likholobov Vladimir, *Omsk Scientific Center SB RAS, Institute of Hydrocarbons Processing SB RAS, Omsk, Russia*
Prof. Descorme Claude, *Institut de recherches sur la catalyse et l'environnement de Lyon (IRCELYON), UMR5256 CNRS – University of Lyon, 2 avenue Albert Einstein, 69626 Villeurbanne, France*

Oral Presentations

14:30-14:50 **IV-OP39** Prof. Trifonov Alexander
Trifonov A.A., Basalov I.V., Kissel A.A., Yurova O.S.
Complexes of Rare- and Alkaline-Earth Metals for Catalytic Intermolecular Olefin Hydrophosphination and Hydroamination Reactions
Institute of Organometallic Chemistry of Russian Academy of Sciences, Nizhny Novgorod, Russian Federation

14:50-15:10 **IV-OP40** Dr. Botavina Maria
Botavina M., Martra G.
Catalysts for Resource Efficiency: Organic Carbonates from CO_2 and Alkyl or Aryl Alcohols on Cs_2O/BEA Zeolite
Department of Chemistry and Interdepartmental Centre "Nanostructured Interfaces and Surfaces – NIS" via P. Giuria 7, 10125 Torino, Italy

Keynote Lecture

15:10-15:50 **IV-KN17** Prof. Gevorgyan Vladimir
Novel Catalytic Methods for Synthesis of Organic Building Blocks and Biologically Important Heterocycles
Department of Chemistry, University of Illinois at Chicago, 845 West Taylor Street, Chicago, Illinois 60607, USA

Oral Presentations

15:50-16:10 **IV-OP41** Prof. Murzin Dmitry
Stekrova M.[1], Torozova A.[1], Mäki-Arvela P.[1], Kumar N.[1], Volcho K.[2], Salakhutdonov N.[2], Murzin D.[1]
Synthesis of Monoterpenoid Dioxinols from Isopulegol and Benzaldehyde over Heterogeneous Catalysts
1 - Åbo Akademi University, Turku, Finland
2 - Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia

16:10-16:30 **IV-OP42** Prof. Yang Qihua
Fabrication of Efficient and Stable Solid Acids via Encapsulation of PS-SO_3H within Hollow Interiors
State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

16:30-17:00 ***Coffee break***

Chairmen: Dr. Zhang Zhanguo, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba-shi, Ibaraki, Japan*
Dr. Cardenas-Lizana Fernando, *Heriot-Watt University, Chemical Engineering, Edinburgh, Scotland, United Kingdom*

Oral Presentations

17:00-17:20 **IV-OP43** Chernyshev Victor
Tarasova E.V.[1], Chernysheva A.V.[2], Chernyshev V.M.[1]
Acid-base Catalysis in the Synthesis of C-amino-1,2,4-Triazoles from Aminoguanidine and Carboxylic Acids
1 - Platov South-Russian State Polytechnic University (NPI), Novocherkassk, Russia
2 - 25th State Research Institute of Chemmotology of the Ministry of Defence of the Russian Federation, Moscow, Russia

17:20-17:40 **IV-OP44** Berenguer-Murcia Á.
Garcia-Aguilar J., Miguel-García I., Berenguer-Murcia Á., Cazorla-Amorós D.
Synthesis of Propylene Oxide with molecular O_2 over well Dispersed Ferrosilicate prepared by a One-Pot Protocol
Inorganic Chemistry Department and Materials Science Institute, Alicante University, Alecante, Spain

17:40-18:00 **IV-OP45** Dr. Auroux Aline
Stošić D.[1], Hosoglu F.[2], Bennici S.[1], Travert A.[3], Capron M.[2], Faye J.[2], Couturier J.-L.[4], Dubois J.-L.[5], Dumeignil F.[2,6], Auroux A.[1]
Synthesis of 1-Butanol and 1-Propanol from the Mixture of Methanol and Ethanol in the Presence of Hydrotalcites as Basic Catalysts
1 - Université Lyon 1, CNRS, UMR 5256, IRCELYON, Institut de Recherches sur la Catalyse et l'Environnement de Lyon, 2 Avenue Albert Einstein, F-69626 Villeurbanne, France
2 - Université Lille 1, Sciences et Technologies, Unité de Catalyse et de Chimie du Solide, UMR CNRS 8181, 59655 Villeneuve d'Ascq, Cedex France
3 - Laboratoire Catalyse et Spectrochimie, CNRS-ENSICAEN, Université de Caen, 6 Boulevard du Maréchal Juin, 14050 Caen Cedex, France
4 - ARKEMA, Centre de Recherche Rhône-Alpes, 69493 Pierre-Bénite Cedex, France

19:30 **Banquet (restaurant PANORAMA)**

19:00 **Young scientists party**
(club "Extra Lounge" at the 25th floor of "Korston Tower" hotel)

Thursday, September 3

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Hupp Joseph, *Northwestern University, Department of Chemistry, Evanston, USA*
Dr. Bellussi Giuseppe, *Eni S.p.A, Refinding & Marketing Devision, Milanese, Italy*

Plenary Lecture

08:30-09:30 **PL-8** Prof. Skoglundh Magnus
Fundamental Studies of Metal-exchanged Zeolites for Selective Catalytic reduction of Nitrogen Oxides in Oxygen Excess
Competence Centre for Catalysis, KCK, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Tolstoy hall

Section 1. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

Chairmen: Prof. Gevorgyan Vladimir, *Department of Chemistry, University of Illinois at Chicago, Chicago, Illinois, USA*
Prof. Ozensoy Emrah, *Department of Chemistry, Yuzuncu Yıl University, 65080, Van, Turkey, Ankara, Turkey*

Oral Presentations

10:00-10:20 **I-OP15** van der Wijst Cornelis
van der Wijst C.[1], Skeie Liland I.[1]., Zhu J.[1], Zhang T.[2], Wang A.[2], Chen D.[1]
Tuning the Selectivity of the Diols Produced from Cellulose with the Basic Sites of the Catalysts
1 - Norwegian University of Science and Technology, Department of Chemical Engineering, Tondheim, Norway
2 - Dalian Institute of Chemical Physics, Chinese Academy, Dalian, China

10:20-10:40 **I-OP16** Dr. Simakova Irina
Simakova I.L.[1,2], Panchenko V.N.[1], Gulyaeva Y.[1], Simonov M.[1]
Catalytic Hydrodeoxygenation of Bioderived C5 Acid into Motor Fuel Components: Kinetics and Mechanistic Study
1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

10:40-11:00 **I-OP17** Dr. Heracleous Eleni
Liakakou E.T.[1,2], Angeli S.D.[2], Triantafyllidis K.S.[1,3], Heracleous E.[1,4]
K-promoted NiMo Catalysts Supported on Activated Carbon for the Hydrogenation Reaction of CO to Higher Alcohols
1 - Chemical Process & Energy Resources Institute, CERTH, 6th km Charilaou - Thermi Road, P.O. Box 361, 57001, Thessaloniki, Greece
2 - Department of Chemical Engineering, Aristotle University of Thessaloniki, P.O. Box 1517, 54124, Thessaloniki, Greece
3 - Department of Chemistry, Aristotle University of Thessaloniki, P.O. Box 116, 54124 Thessaloniki, Greece
4 - School of Science & Technology, International Hellenic University, 14th km Thessaloniki – Moudania, 57001, Thessaloniki, Greece

11:00-11:20 **I-OP18** Dr. Ordomsky Vitaly
Ordomsky V.V., Subramanian V., Khodakov A.Y., Paul S.
Control of Chain Length Distribution of Hydrocarbons during Fischer-Tropsch Synthesis over Co Nanoparticles inside of Nanoreactors
Unité de catalyse et de chimie du solide (UMR 8181 CNRS), Université Lille 1-ENSCL-EC Lille, France

11:20-11:40 **I-OP19** Prof. Kuznetsov Boris N.
Kuznetsov B.N.[1,2], Chesnokov N.V.[1,2], Levdansky A.V.[1], Garyntseva N.V.[1], Yatsenkova O.V.[1], Grishechko L.I.[1], Celzard A.[3], Pinel C.[4]
Novel Approach to Catalytic Processing of Birch Wood Biomass to Valuable Chemical Products
1 - Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia
2 - Siberian Federal University, Krasnoyarsk, Russia
3 - Institut Jean Lamour – UMR CNRS, 7198, Epinal, rue du Merle Blanc, 27, France
4 - IRCELYON, 2 avenue Albert Einstein, F-69626 Villeurbanne Cedex, Lyon, France

11:40-12:00 **I-OP20** Dr. Tschentscher Roman
Tschentscher R., Akporiaye D.
Highly Stable and Selective Propane Dehydrogenation Catalyst
SINTEF Materials & Chemistry, Oslo, Norway

12:00-12:20 **I-OP21** McVicker Rebecca
McVicker R.U.[1], Freakley S.J.[1], Shaw G.[1], Ab Rahim M.H.[2], Forde M.M.[1], Hammond C.[1], Jenkins R.L.[1], Dimitratos N.[1], Kiely C.J.[3], Hutchings G.J.[1]
Selective Oxidation of Methane with Hydrogen Peroxide Using Gold-Palladium Nanoparticles
1 - Cardiff University, Cardiff, United Kingdom
2 - Faculty of Industrial Sciences and Technology, Universiti of Malaysia, Pahang, Malaysia
3 - Lehigh University, Bethlehem, USA

12:20-12:40 **I-OP22** Dr. Chistyakov Andrey
Chistyakov A.V.[1,2], Nikolaev S.A.[3], Zharova P.A.[1], Kriventsov V.V.[4], Tsodikov M.V.[1,2]
Ethanol Conversion into Chemicals over Au-M Containing Catalysts
1 - Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia
2 - Gubkin Russian State University of Oil and Gas, Moscow, Russia
3 - Lomonosov Moscow State University, Moscow, Russia
4 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

12:40-13:00 **I-OP23** Prof. Kogan Victor
Kogan V.M.[1], Nikulshin P.A.[2], Dorokhov V.S.[1], Permyakov E.A.[1]
Evolution and Interlayer Dynamics of Active Sites of Promoted Transition Metal Sulphide Catalysts under Hydrogen and Inert Media in the Course of Some Commercially Valuable Reactions
1 - N.D. Zelinsky Institute of Organic Chemistry, RAS, Moscow, Russia
2 - Samara State Technical University, Samara, Russia

13:00-14:30 ***Lunch***

KORSTON Tolstoy hall

Evening Session

Section 5. Catalysis and Environmental Protection

Chairmen: Prof. Granger Pascal, *Cité Scientifique, 59650 Villeneuve d'Ascq, France , University of Lille, UCCS*
Prof. Tabakova Tatyana, *Institute of Catalysis, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria*

Oral Presentations

14:30-14:50 **V-OP32** Prof. Garcia Garcia Avelina
Giménez-Mañogil J., García-García A.
Opportunities for Ceria-based Catalysts Versus Platinum Catalysts in Diesel Soot Combustion
MCMA Group, Department of Inorganic Chemistry, Faculty of Sciences, University of Alicante, Ap.99 E-03080 Alicante, Spain

14:50-15:10 **V-OP33** Dr. Porsin Andrey
Porsin A.[1], Alikin E.[2], Bukhtiyarov V.[1,3]
Low Temperature Method for Measuring Oxygen Storage Capacity of Ceria-containing Oxides
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Ecoalliance, Ltd., Novouralsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia

15:10-15:30 **V-OP34** Dr. Zheng Jinbao
Deng X., Hu X., Zheng J., Chen B.
Soot Oxidation with Ceria-zirconia Catalysts Prepared by Different Precipitant
National Engineering Laboratory for Green Chemical Production of Alcohols-Ethers-Esters, State Key Laboratory for Physical Chemistry of the solid surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

15:30-15:50 **V-OP35** Serve Adrien
Serve A.[1], Epicier T.[2], Aouine M.[3], Cadete Santos Aires F.J.[1], Tsampas M.[1], Cartoixa B.[4], Pajot K.[5], Vernoux P.[1]
Mechanistic Investigations of Soot Combustion by Ag Supported Catalysts
1 - Université de Lyon, Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256, CNRS, Université C. Bernard Lyon 1, 2 avenue A. Einstein, 69626 Villeurbanne, France
2 - Université de Lyon, MATEIS, UMR 5510, CNRS, INSA de Lyon, 69621 Villeurbanne Cedex, France
3 - Université de Lyon, Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256, CNRS, Université C. Bernard Lyon 1, 2 avenue A. Einstein, 69626 Villeurbanne, France
4 - CTI, Céramiques Techniques Industrielles, 382 Avenue du Moulinas 30340 Salindres, France
5 - PSA Peugeot Citroën, Centre technique de Vélizy, Route de Gisy 78943 Vélizy-Villacoublay, France

15:50-16:10 **V-OP36** Prof. Kotarba Andrzej
Jakubek T., Kaspera W., Legutko P., Zasada F., Piskorz W., Stelmachowski P., Indyka P., Grybos J., Sojka Z., Kotarba A.
Strong Enhancement of Desoot Activity of Transition Metal Oxides by Alkali Doping – Surface Promotion Versus Intercalation
Jagiellonian University, Faculty of Chemistry, Krakow, Poland

16:10-16:30 **V-OP37** Dr. Kureti Sven
Wagloehner S., Kureti S.
Structure-activity Relation of Iron Oxide Catalysts in Soot Oxidation
Technical University of Freiberg, Institute of Energy Process Engineering and Chemical Engineering, Chair of Reaction Engineering, Fuchsmuehlenweg 9, D-09596 Freiberg, Germany

16:30-17:00 ***Coffee break***

Chairmen: Prof. Garcia Garcia Avelina, *MCMA Group, Department of Inorganic Chemistry. Faculty of Sciences, University of Alicante, Alicante, Spain*
Dr. Kureti Sven, *Technical University of Freiberg, Institute of Energy Process Engineering and Chemical Engineering, Freiberg, Germany*

Oral Presentations

17:00-17:20 **V-OP38** Dr. Heikens S.
Heikens S.[1], Mondragon Rodriguez G.[2], Saruhan-Brings B.[2], Grünert W.[1]
Pd-doped LaFeCo Perovskites for Three-way Catalysis. Studies on Active Sites and Response to Thermal Stress
1 - Ruhr University Bochum, Bochum, Germany
2 - DLR Cologne, Köln, Germany

17:20-17:40 **V-OP39** Dr. Arandiyan Hamid
Arandiyan H., Scott J., Amal R.
Three-Dimensionally Ordered Macroporous Perovskite Catalysts: Controllable Alignments and Approach for Catalytic Applications
Particles and Catalysis Research Group, School of Chemical Engineering, The University of New South Wales, Sydney NSW 2052, Australia

17:40-18:00 **V-OP40** Dr. Tang Long
Tang L., Zhao Z., Wei Y., Liu J., Li K.
Highly Active $LaKCoO_3$ Perovskite-type Complex Oxide Catalysts over Alumina Washcoated Monolith for the Simultaneous Removal of Diesel Soot and Nitrogen Oxides
China University of Petroleum, Beijing, China

19:30 **Banquet (restaurant PANORAMA)**

19:00 **Young scientists party**
(club "Extra Lounge" at the 25th floor of "Korston Tower" hotel)

Thursday, September 3

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

Morning Session

Chairmen: Prof. Hupp Joseph, *Northwestern University, Department of Chemistry, Evanston, USA*
Dr. Bellussi Giuseppe, *Eni S.p.A, Refinding & Marketing Devision, Milanese, Italy*

Plenary Lecture

08:30-09:30 **PL-8** Prof. Skoglundh Magnus
Fundamental Studies of Metal-exchanged Zeolites for Selective Catalytic reduction of Nitrogen Oxides in Oxygen Excess
Competence Centre for Catalysis, KCK, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

10:30-11:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Dostoevsky hall

Symposium "Education in the Field of Catalysis"

Scope of discussions: Education in the field of catalysis: state of the art and possible improvements; New educational programs in the field of catalysis; Emerging topics in the field of catalysis and their reflection in educational programs; New assessment methods in the field of catalysis; New lecture courses and practical tasks; Continuous professional education in the field of catalysis; Education in the field of catalysis globally: standards and variability

Chairmen: Prof. Lunin Valery, *Moscow State University, Moscow, Russia*
Prof. Murzin Dmitry*, Åbo Akademi University, Åbo/Turku, Finland*

10:00-13:00 V. Lunin (Russia), M.V. Lomonosov Moscow State University
Introduction

1. D. Murzin (Finland), Abo/Turku University
"Teaching Heterogeneous Catalysis to Chemical Engineers"

2. M .Muhler (Germany), Ruhr-University Bochum
"Catalysis Training in Germany"

3. F. Cavani (Italy), Bologna University
"Catalysis for the Chemical Industry Taught to Industrial Chemists: Examples from the Italian Context"

4. M. Skoglundh (Sweden), Chalmers University of Technology
"Catalysis Courses at Chalmers University of Technology in Sweden"

5. J. Beltramini (Australia), The University of Queensland
"Catalysis and Reaction Engineering Training under an Australian Perspective"

6. V. Bukhtiyarov (Russia), Novosibirsk State University
"Research Training as a Necessary Part of Education in Catalysis"

7. Kh. Kharlampidi, G.Yelimanova (Russia), Kazan National Research Technological University
"From Laboratory Researches to Industrial Reactors"

8. E.J.M. Hensen (Netherland), Eindhoven University of Technology, Netherlands Institute for Research in Catalysis (NIOK)
"Education in Catalysis at the MSc and PhD Level in the Netherlands"

9. C.W. Jones (USA), Georgia Institute of Technology
"Catalysis Education in the USA"

10. Zhuravleva M.V., Zinnurova O.V., Bashkirtseva N.Yu. (Russia),
Kazan National Research Technological University, Department of Technology of basic organic and petrochemical synthesis
"Advanced Training of Catalysis Experts in Petrochemical and Refining Industries"

11. Garifzianova G.G., Tsyshevsky R.V., Khrapkovskii G.M. (Russia), Kazan National Research Technological University, department of catalysis
"Gaining Insight on Catalytic Processes from Molecular Level: Novel Course of Catalysis in KNRTU"

Discussion

13:00-14:30 ***Lunch***

KORSTON Dostoevsky hall

Evening Session

Discussion symposium 10. «Design of Gold Catalysts for Selective Processes: from Science to Real Application»

Chairmen: Prof. Mühler Martin, *Laboratory of Industrial Chemistry, Ruhr-University Bochum, Germany*
Prof. Cavani Fabrizio, *Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Bologna, Italy*

14:30-16:30 **DS10-1**
Hensen E.J.M., Song W.
Au-Cu^+ Synergy in $MgCuCr_2O_4$-Spinel Supported Gold Nanoparticles for Selective Oxidation of Alcohols and Olefins
Eindhoven University of Technology, Inorganic Materials Chemistry group, Schuit Institute of Catalysis, Eindhoven, P.O.Box 513, 5600 MB, The Netherlands

DS10-2
Castedo A.[1,2], Llorca J.[1,2], Mendoza E.[1]
Hydrogen Photoproduction in a Silicone Microreactor Loaded with Au/TiO_2
1 - Centre for Research in NanoEngineering,Universitat Politècnica de Catalunya, Barcelona, Spain
2 - Institute of Energy Technologies,Universitat Politècnica de Catalunya, Barcelona, Spain

DS10-3
Pyrjaev P.A.[1], Simonov A.N.[2], Moroz B.L.[1,3], Zyuzin D.A.[1], Kuznetsov A.N.[1], Prosvirin I.P.[1], Bukhtiyarov V.I.[1,3]
Bimetallic Catalysts Containing Palladium and Gold on Carbon Support for Hydrogen Electrooxidation: From Au Particles Coated with Submonolayers of Pd to Pd-Au Nanoalloys
1 - Boreskov Institute of Catalysis SB RASNovosibirsk, Russia
2 - School of Chemistry, Monash University, Clayton, Victoria 3800, Australia
3 - Novosibirsk State University, Novosibirsk, Russia

DS10-4

Peneau V.[1], He Q.[2], Shaw G.[1], Kiely Ch. J.[2], Hutchings Gr. J.[1], Nowicka E.[1]

Selective Oxidation of Toluene Using Noble Metals under Mild Condition

1 - Cardiff Catalysis Institute, School of Chemistry, Cardiff, CF10 3AT, UK

2 - Department of Material Science and Engineering, Lehigh University, Lehigh, PA 18015, US

DS10-5

Redina E.[1], Kirichenko O.[1], Greish A.[1], Shesterkina A.[1], Vikanova K.[2], Tkachenko O.[1], Kapustin G.[1], Kustov L.[1,3]

Catalytic Transformation of Glycerol to Lactic Acid over Au-Pt Supported Catalysts Prepared by Redox-method

1 - N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russian Federation

2 - Lomonosov Moscow State University of Fine Chemical Technologies, Moscow, Russian Federation

3 - Chemistry Department of Moscow State University, Moscow, Russian Federation

DS10-6

Manzoli M.[1], Agostini G.[2], Vindigni F.[1], Lamberti C.[1], Dimitrov D.[3], Ivanov K.[3], Tabakova T.[4]

EXAFS Study in Operando Conditions of Au/Co-doped CeO_2 Catalysts for Methanol Oxidation Reaction

1 - Department of Chemistry and NIS Interdepartmental Centre, University of Torino, Torino, Italy

2 - European Syncrotron Radiation Facility, Grenoble, France

3 - Departmemt of Chemistry, Agricultural University, Plovdiv, Bulgaria

4 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

DS10-7

Thomas L.M.[1], Lee A.F.[2], Wilson K.[2], Willock D.J.[1]

The Gold Particle Catalysed Mechanism for the Oxidation of Hydroxymethylfurfural to 2,5-Furandicarboxylic Acid: a DFT Study

1 - Cardiff University, Cardiff, United Kindom

2 - Aston University, Birmingham, United Kindom

DS10-8

Butova V.V.[1], Guda A.A.[1], Budnyk A.P.[1,2], Lamberti C.[1,2], Lomachenko K.A.[1,2], Soldatov A.V.[1]

Microwave-assistant Functionalization of MOFs with Gold Nanoparticles

1 - Southern Federal University, IRC Smart Materials, Zorge str. 5, 344090 Rostov-on-Don, Russia

2 - University of Turin, Department of Chemistry

16:30-17:00 *Coffee break*

19:30 **Banquet (restaurant PANORAMA)**

19:00 **Young scientists party**

(club "Extra Lounge" at the 25th floor of "Korston Tower" hotel)

Thursday, September 3rd

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall

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Chairmen: Prof. Hupp Joseph, *Northwestern University, Department of Chemistry, Evanston, USA*
Dr. Bellussi Giuseppe, *Eni S.p.A, Refinding & Marketing Devision, Milanese, Italy*

Plenary Lecture

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Competence Centre for Catalysis, KCK, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

09:30-10:00 ***(Break to separate Ball hall)*** ***Coffee break***

KORSTON Lermontov hall

XI European Workshop on Innovation in Selective Oxidation

Chairmen: Prof. Kolb Gunther, *Fraunhofer ICT-IMM, Mainz, Germany*
Prof. Lopez Nieto J.M., *Instituto Tecnologia Quimica, UPV-CSIC, Valencia, Spain*

Oral Presentations

10:00-10:20 **ISO-OP17** Prof. Mirodatos Claude
Serres T.[1], Alexiadis V.[2], Schuurman Y.[1], Thybaut J.W.[2], Mirodatos C.[1]
Key Parameters Controlling Selectivity and Conversion in OCM: from Experiments and Modelling, towards an Optimised Reactor Design
1 - Institut de Recherches sur la Catalyse et l'Environnement de Lyon, Université Lyon 1, CNRS, Villeurbanne, France
2 - Ghent University, Laboratory for Chemical Technology, Technologiepark 914, B-9052 Ghent, Belgium

10:20-10:40 **ISO-OP18** Dr. Sinev Mikhail
Gordienko Yu., Usmanov T., Bychkov V., Lomonosov V., Fattakhova Z., Tulenin Yu., Shashkin D., Sinev M.
Oxygen Availability and Catalytic Performance of NaWMn/SiO_2 Mixed Oxide and Its Components in Oxidative Coupling of Methane
Semenov Institute of Chemical Physics, R.A.S., Moscow, Russia

10:40-11:00 **ISO-OP19** Dr. Ivanov Dmitry V.
Ivanov D.V.[1], Isupova L.A.[1], Gerasimov E.Yu.[1,2], Dovlitova L.S.[1], Glazneva T.S.[1,2], Prosvirin I.P.[1,2]
Alkaline-earth Promoted $SrTiO_3$ and Sr_2TiO_4 in Oxidative Methane Coupling: Role of Microstructure and Surface Composition on Activity, Kinetics and Oxygen Exchange
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

11:00-11:20 **ISO-OP20** Ishikawa Satoshi I.
Ishikawa S.I.[1], Kobayashi D.K.[1], Konya T.K.[1], Ohmura S.O.[1], Murayama T.M.[1], Yasuda N.Y.[2], Sadakane M.S.[3], Ueda W.U.[1]
Redox Treatment of Orthorhombic $Mo_{29}V_{11}O_{112}$ and Relationships between the Crystal Structure, Microporosity and Catalytic Performance for the Selective Oxidation of Ethane
1 - Catalysis Research Center, Hokkaido University, Sapporo, Hokkaido, Japan JASRI/SPring-8
2 - Graduate School of Engineering, Hiroshima University, Japan

11:20-11:40 **ISO-OP21** Dr. Taran Oxana P.
Taran O.P.[1,2], Gromov N.V.[1], Zhizhina E.G.[1], Rodikova Yu.A.[1], Parmon V.N.[1,3]
The Selective Oxidation of Polysaccharides to Formic Acid at the Presence of P-Mo-V Heteropoly Acid Catalysts. The Mechanism of Reaction
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State Technical University, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia

11:40-12:00 **ISO-OP22** Dr. Marcu Ioan-Cezar
Popescu I.[1], Skoufa Z.[2], Heracleous E.[3,4], Lemonidou A.A.[2,3], Marcu I.C.[1,5]
Study of M-doped NiO (M = Li, Mg, Al, Ga, Ti, Nb) Catalysts by In situ Electrical Conductivity Measurements in Correlation with their Catalytic Performances in Ethane Oxydehydrogenation
1 - University of Bucharest, Research Center for Catalysts and Catalytic Processes, 4-12, Blv. Regina Elisabeta, 030018 Bucharest, Romania
2 - Aristotle University of Thessaloniki, Department of Chemical Engineering, University Campus, 54124 Thessaloniki, Greece
3 - Chemical Process Engineering Research Institute (CPERI), Centre for Research and Technology Hellas (CERTH), 6th km Charilaou – Thermi Road, P.O. Box 361, 57001 Thessaloniki, Greece
4 - International Hellenic University, School of Science and Technology, 14th km Thessaloniki – Moudania, 57001 Thermi, Greece
5 - University of Bucharest, Department of Organic Chemistry, Biochemistry and Catalysis, 4-12, Blv. Regina Elisabeta, 030018 Bucharest, Romania

12:00-12:20 **ISO-OP23** Dr. Pakharukov Ilya Yu.
Pakharukov I.Yu.[1,2], Bukhtiyarov V.I.[1,2], Chetyrin I.A.[1,2], Prosvirin I.P.[1,2], Parmon V.N.[1,2], Murzin Y.V.[3], Zubavichus Y.V.[3]
In-situ XPS and XAS Studies of a New Phenomenon of Kinetic Hysteresis in Selective Methane Oxidation over Platinum
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - National Research Center "Kurchatov Institute", Moscow, Russia

12:20-12:40 **ISO-OP24** Dr. Starokon Eugeny
Starokon E.V., Parfenov M.V., Pirutko L.V., Panov G.
Quasicatalytic and Catalytic Oxidation of Methane to Methanol by Nitrous Oxide over FeZSM-5 Zeolite
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russian Federation

12:40-13:00 Closing remarks

13:00-14:30	***Lunch***

KORSTON Lermontov hall

Evening Session

Discussion symposium 11. «Feasibility of Biomass Utilization for Making Fuels and Chemicals»

Chairmen: Prof. Murzin Dmitry, *Åbo Akademi University, Turku, Finland*
Dr. Sinev Mikhail, *Semenov Institute of Chemical Physics, Moscow, Russia*

14:30-16:30 **DS11-1**
Alharbi W., Brown E., Kozhevnikova E., Bond G., Kozhevnikov I.
Dehydration of Alcohols over Heteropoly Acid Catalysts in the Gas Phase
University of Liverpool, Liverpool, United Kingdom

DS11-2
Adsuar-Garcia M.D., Rufete-Beneite M., Roman-Martinez M.C.
Ru Nanoparticles on Acid-modified Carbon Materials for the Hydrolytic Hydrogenation of Cellulose
Department of Inorganic Chemistry, University of Alicante, Alicante, Spain

DS11-3
Ouanji F.[1], Kacimi M.[1], Ziyad M.[1,2], Puleo F.[3], Liotta L.F.[3]
Esterification-Neutralization-Transesterification of Waste Cooking Oil: In-situ Three-stage Method for Biodiesel Synthesis, Neutralization Step Optimization
1 - Université Mohammed V, Faculté des Sciences, Département de Chimie, Av. Ibn Battouta, BP1014, Rabat, Maroc
2 - Académie Hassan II des Sciences et Techniques, Rabat, Maroc
3 - ISMN-CNR, via Ugo La Malfa, 153, 90146, Palermo, Italy

DS11-4
Godina L.I.[1], Kirilin A.V.[1], Tokarev A.V.[1], Demidova Y.S.[2,3], Lemus J.[4], Calvo L.[4], Schubert T.[5], Gilarranz M.A.[4], Simakova I.L.[2,3], Murzin D.Y.[1]
Aqueous Phase Reforming of Xylitol over Mono- and Bimetallic Carbon-supported Catalysts
1 - Åbo Akademi University, Laboratory of Industrial Chemistry and Reaction Engineering, Biskopsgatan 8, Åbo, 20500, Finland
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia
4 - Universidad Autónoma de Madrid, 28049, Madrid, Spain
5 - FutureCarbon GmbH, Gottlieb-Keim-Strasse 60, 95448 Bayreuth, Germany

DS11-5

Varakin A., Salnikov V., Nikulshin P.

The Role of Carrier's Carbonization Degree on the HDO Conversion of the Oleic Acid over the $CoMo/C/Al_2O_3$ Catalysts

Samara State Technical University, Samara, Russia

DS11-6

Hachemi I., Mäki-Arvela P., Kumar N., Murzin Y.D.

Catalytic Hydrodeoxygenation of Microalgae Biodiesel over Sulfur-Free Nickel Supported Catalyst for the Production of Biofuels

Åbo Akademi University, Turku, Finland

DS11-7

Stepacheva A.A.[1], Sapunov V.N.[2], Nikoshvili L.Z.[1], Sulman E.M.[1], Matveeva V.G.[1]

Oils and Fats Conversion to the Second Generation of Biodiesel Using Pd-containing Catalysts

Tver Technical University, Tver, Russia
Mendeleyev University of Chemical Technology of Russia, Moscow, Russia

DS11-8

Wang C., Tian Z., Qu W., Li P., Ma H., Xu R.

Single-step Hydrotreatment of Lipids to Produce High Quality Biofuel

Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Dalian, China

DS11-9

Mielby J., Zacho S.L., Abildstrøm J.O., Kegnæs S.

Production of Bio-Renewable Chemicals Using Zeolite Encapsulated Metal Nanoparticles as Bi-functional Catalysts

DTU Chemistry, Technical University of Denmark, Kgs. Lyngby, Denmark

DS11-10

Pezoa Conte R.[1], Pham T.N.[2], Mäki-Arvela P.[1], Willför S.[3], Mikkola J.-P.[1,2]

Hydrolysis of Carbohydrates in Green Algae Using Solid Acid Catalysts

1 - Industrial Chemistry and Reaction Engineering, Johan Gadolin Process Chemistry Centre, Åbo Akademi University, FI-20500 Åbo-Turku, Finland
2 - Technical Chemistry, Department of Chemistry, Chemical-Biological Center, Umeå University, SE-901 87 Umeå, Sweden
3 - Wood and Paper Chemistry, Johan Gadolin Process Chemistry Centre, Åbo Akademi University, FI-20500 Åbo-Turku, Finland

DS11-11

Kasakov S.[1], Zhao C.[1,2], Barath E.[1], Chase Z.A.[3], Camaioni D.M.[4], Fulton J.L.[4], Vjunov A.[4], Shi H.[4], Lercher J.A.[1,4]

Glucose and Cellulose Derived Ni/C-SO_3H Catalysts for Liquid Phenol Hydrodeoxygenation

1 - Technische Universität München, München, Germany
2 - East China Normal University, Shanghai, China
3 - Washington State University, Pullman, USA
4 - Pacific Northwestern National Laboratory, Richland, USA

DS11-12
Vlasova E.N.[1,2], Aleksandrov P.V.[1,2], Deliy I.V.[1,2,3], Bukhtiyarov A.V.[1,2],
Gerasimov E.Y.[1,2], Paharukova V.P.[1,2], Bukhtiyarova G.A.[1]

Peculiarities of MoS_2/Al_2O_3, $CoMoS/Al_2O_3$ and $NiMoS/Al_2O_3$ Catalyst's Behaviour in the Hydroconversion of Aliphatic Esters and Rapeseed Oil

1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Research and Educational Center for Energy Efficient Catalysis in Novosibirsk National Research University, Novosibirsk, Russia
3 - Novosibirsk National Research University, Novosibirsk, Russia

16:30-17:00 ***Coffee break***

19:30 **Banquet (restaurant PANORAMA)**

19:00 **Young scientists party**
(club "Extra Lounge" at the 25th floor of "Korston Tower" hotel)

Friday, September 4

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall-1

Morning Session

Section 1. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

Chairmen: Prof. Gaigneaux Eric, *Universite catholique de Louvain, Belgium*
Prof. Vasalos Iacovos, *Chemical Process and Energy Resources Institute, Centre for Research and Technology Hellas, Greece*

Keynote Lecture

08:30-09:10 **I-KN18** Prof. Khodakov Andrei
Khodakov A.Y.[1], Ordomsky V.V.[1], Cai M.[1], Subramanian V.[1], Lancelot C.[1], Palcic A.[2], Valtchev V.[2], Nhut J.-M.[3], Pham-Huu C.[3], Moldovan S.[4], Ersen O.[4]
Design of Novel Hybrid Hierarchical Catalysts for Direct Synthesis of Dimethyl Ether from Syngas
1 - UCCS, Université Lille 1-ENSCL-EC Lille, Bat. C3, Cité Scientifique, 59655 Villeneuve d'Ascq, France
2 - LCS, ENSICAEN, 6 Boulevard Maréchal Juin, 14000 Caen, France
3 - ICPEES, ECPM, Université de Strasbourg, Strasbourg, France
4 - IPCMS, Université de Strasbourg, 23, rue du Loess BP 43, F-67034 Strasbourg, France

Oral Presentations

09:10-09:30 **I-OP24** Dr. Fratalocchi Laura
Fratalocchi L.[1], Visconti C.G.[1], Lietti L.[1], Tronconi E.[1], Rossini S.[2]
Taking Advantage of Mass Transfer Limitations in Egg-shell Catalysts for Intensified Fischer-Tropsch Reactors
1 - Politecnico di Milano, Dipartimento di Energia, Milano, Italy
2 - Eni, Via Maritano 26, 20097 San Donato Milanese, Italy

09:30-09:50 **I-OP25** Dr. Visconti Carlo Giorgio
Visconti C.G., Groppi G., Tronconi E.
Intensification of Strongly Endo- and Exo-Thermic Catalytic Processes through the Adoption of Highly Conductive "Packed Foams" Reactors
Politecnico di Milano, Department of Energy, Laboratory of Catalysis and Catalytic Processes, Via La Masa 34, 20156 Milano, Italy

09:50-10:10 **I-OP26** Otyuskaya Daria
Otyuskaya D.[1], Lødeng R.[2], Thybaut Joris W.[1], Marin Guy B.[1]
Microkinetics Assisted Analysis of Hydrotreating Selectivities in Fast Pyrolysis Oil Upgrading
1 - Laboratory for Chemical Technology, Ghent University, Technologiepark 914, B-9052 Gent, Belgium
2 - SINTEF Materials & Chemistry, Department of Kinetics and Catalysis, N-7465 Trondheim, Norway

10:10-10:30 **I-OP27** Dr. Benito Martin Patricia
Benito P.[1], Nuyts G.[2], Monti M.[1], De Nolf W.[2], Fornasari G.[1], Janssens K.[2], Scavetta E.[1], Vaccari A.[1]
Stable Rh Particles on Electrosynthesized Structured Catalysts
1 - University of Bologna, Dip. Chimica Industriale "Toso Montanari", Vle Risorgimento 4, 40136, Bologna, Italy
2 - University of Antwerp, Department of Chemistry, Groenenborgerlaan 171, 2020 Antwerp, Belgium

10:30-11:00 ***Coffee break***

KORSTON Ball hall-1

Section 4. Catalysis and Chemicals

Chairmen: Dr. Lokteva Ekaterina, *Lomonosov Moscow State University, Chemistry Department, Moscow, Russia*
Dr. Nartova Anna, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

11:00-11:40 **KN21** Prof. Karakhanov Eduard
Karakhanov E.[1], Maximov A.[1,2], Rosenberg E.[3]
Nanocatalyst Based on Hybrid Structured Materials: Synthesis and Application
1 - Moscow State University, Chemistry Department, Moscow, Russia
2 - Institute of Petrochemical Synthesis RAS, Moscow, Russia
3 - Department of Chemistry and Biochemistry University of Montana Missoula, Montana, 59812 United States

11:40-12:00 **IV-OP46** Dr. Trunfio Giuseppe T.
Di Chio R.[1], Trunfio G.[1], Deiana C.[2], Ivanchenko P.[2], Sakhno Y.[2], Martra G.[2], Arena F.[1]
Factors Affecting the Activity of Oxide Catalysts in the Synthesis of N-phenylpropionamide from Propanoic Acid and Aniline
1 - Dipartimento di Ingegneria Elettronica, Chimica e Ingegneria Industriale, Università degli Studi di Messina, Viale F. Stagno D'Alcontres 31, 98166 Messina, Italy
2 - University of Torino, Via P. Giuria 7, I-10125 Torino, Italy

12:00-12:20 **IV-OP47** Schaller Barbara
Schaller B.[1,2], Curtin T.[1], Leahy J.J.[1,2]
Methane to Methanol – Influencing Factors for the Direct Catalytic Low Temperature Oxidation with Copper Zeolite Catalysts
1 - Materials and Surface Science Institute, Department of Chemical and Environmental Sciences, University of Limerick, Limerick, Ireland
2 - Carbolea Research Group, Department of Chemical and Environmental Sciences, University of Limerick, Limerick, Ireland

12:20-12:40 **IV-OP48** Dr. Rose Marcus
Rose M., Pfützenreuter R.
Heterogeneously Catalyzed Aqueous Phase Amination and Isomerization of Biogenic Isohexides
Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, Aachen, Germany

12:50-13:30 **Closing ceremony** (*KORSTON Ball hall*)

13:30-15:00 ***Lunch***

Friday, September 4

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Ball hall-2

Morning Session

Section 3. Energy-Related Catalysis

Chairmen: Prof. Faria Joaquim, *LSRE-LCM, Departamento de Engenharia Química, Faculdade de Engenharia da Universidade do Porto, Porto, Portugal*
Dr. Vovk Evgeny, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia, Bilkent University, Chemistry Department, Bilkent, Ankara, Turkey*

Oral Presentations

08:30-08:50 **III-OP38** Huang Xiaoming
Huang X[1], Korányi T.I.[1], Boot M. D.[2], Hensen E.J.M.[3]
Ethanol Acts as Capping Agent and Formaldehyde Scavenger to Promote Efficient Lignin Depolymerization to Aromatics
1 - Schuit Institute of Catalysis, Inorganic Materials Chemistry Eindhoven University of Technology, The Netherlands
2 - Combustion Technology, Department of Mechanical Engineering, Eindhoven University of Technology, The Netherlands
3 - Schuit Institute of Catalysis, Inorganic Materials Chemistry Eindhoven University of Technologyniversity of Technology, The Netherlands

08:50-09:10 **III-OP39** Frusteri F.
Cannilla C., Bonura G., Feminò G., Drago Ferrante G., Frusteri F.
Biofuels Production from Glycerol and TBA using an Innovative Catalytic Membrane Reactor
National Council of Research, CNR-ITAE, via S. Lucia, 5-98126 Messina, Italy

09:10-09:50 **III-KN19** Dr. Takanabe Kazuhiro
Understanding Photocatalytic Process: Intrinsic Properties, Morphology and Timescale
Division of Physical Sciences and Engineering, KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

09:50-10:10 **III-OP40** Dr. He Jiayue
He J.[1], Renges H.[1], Barath E.[1], Mei D.[2], Lercher J.A.[1,2]
Catalytic C-O Cleavage and Hydrogenation of Diaryl Ethers in Aqueous and Apolar Phase
1 - Department of Chemistry, Technische Universität München, Lichtenbergstr.4, 85747 Garching, Germany
2 - Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA99352, USA

10:10-10:30 **III-OP41** Martinez-Espin Juan Salvador
Martinez-Espin J.S.[1,2], Westgård Erichsen M.[1], De Wispelaere K.[3], Van Speybroeck V.[3], Beato P.[2], Svelle S.[1], Olsbye U.[1]
The Effects of Methanol or Dimethyl Ether as Methylating Agent During Zeolite Catalysed Benzene Methylation
1 - Centre for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, P.O. Box 1033, Blindern, N-0315 Oslo, Norway
2 - Haldor Topsøe A/S, Nymøllevej 55, DK-2800 Kgs. Lyngby, Denmark

10:30-11:00 ***Coffee break***

Chairmen: Prof. Cunill Fidel, *Chemical Engineering Department, Faculty of Chemistry, Universitat de Barcelona, Barcelona, Spain*
Dr. Suslova Evgeniya, *Lomonosov Moscow State University, Moscow, Russia*

Oral Presentations

11:00-11:20 **III-OP42** Beretta Alessandra
Beretta A.[1], Donazzi A.[1], Pagani D.[1], Lucotti A.[2], Tommasini M.[2], Groppi G.[1], Castiglioni C.[2]
Kinetic Fnalysis and Raman Surface Characterization in the CPO of Propane, Propylene and n-C_8H_{18}
1 - Politecnico di Milano, Dipartimento di Energia, 20156, Milano, Italy
2 - Politecnico di Milano, Dipartimento di Chimica Materiali e Ingegneria Chimica, Piazza Leonardo da Vinci 32, 20133, Milano, Italy

11:20-11:40 **III-OP43** Bell Tamsin E.
Bell T.E.[1,2], Hill A.K.[1,2], Torrente-Murciano L.[1,2]
Low Temperature In-situ Hydrogen Production by Ammonia Decomposition Using Cobalt-based Catalysts
1 - Department of Chemical Engineering, University of Bath, Bath, UK
2 - Centre for Sustainable Chemical Technologies, University of Bath, Bath, UK

11:40-12:00 **III-OP44** Anton Johan
Muhler M.[1,2], Anton J.[1,2], Nebel J.[1,2], Froese C.[1,2], Kleinschmidt R.[3], Quandt T.[4], Ruland H.[1,2], Kaluza S.[5]
Na-modified Cu-Co-based Catalysts for Higher Alcohol Synthesis: Influence of Surface Composition and CoC_2 Formation
1 - Ruhr-University Bochum, Bochum, Germany
2 - Laboratory of Industrial Chemistry
3 - ThyssenKrupp Industrial Solutions
4 - Evonik Industries
5 - Fraunhofer UMSICHT

12:00-12:20 **III-OP45** Dr. Gutierrez Tinoco Oliver
Schachtl E.[1], Gutiérrez O.Y.[1], Yoo J.S.[2], Studt F.[2], Lercher J.A.[1]
Effect of Ni on the Hydrogenation Mechanism of Polyaromatic Hydrocarbons over (Ni-)MoS_2/Al_2O_3
1 - Technische Universität München, Department of Chemistry and Catalysis Research Center, Lichtenbergstraße 4, 85748 Garching, Germany
2 - SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, United States

12:20-12:40 **III-OP46** Dr. Landi Gianluca
Barbato P.S.[1], Di Benedetto A.[2], Landi G.[1], Lisi L.[1]
Structured Catalytic Honeycombs Based on Copper/Ceria for CO Preferential Oxidation in H_2-Rich Streams
1 - Research Institute on Combustion – CNR, Naples, Italy
2 - DICMAPI, University of Naples Federico II, Italy

12:50-13:30 **Closing ceremony** (*KORSTON Ball hall*)

13:30-15:00 ***Lunch***

Friday, September 4

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Pushkin hall

Morning Session

Section 2. Catalyst Preparation and Characterization

Chairmen: Prof. Zhao Zhen, *State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing, China*
Dr. Simagina Valentina, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

08:30-08:50 **II-OP50** Dr. Vereshchagin Sergei
Vereshchagin S.N.[1], Solovyov L.A.[1], Shishkina N.N.[1], Dudnikov V.A.[2], Anshits A.G.[1,3]
Oxidative Conversion of Methane Over Gd-Sr-Co-Perovskites: Structure-Activity Relationship
1 - Institute of Chemistry and Chemical Technology, Siberian Branch, Russian Academy of Sciences, Krasnoyarsk, Russia
2 - L.V. Kirensky Institute of Physics, Siberian Branch, Russian Academy of Sciences, Krasnoyarsk, Russia
3 - Siberian Federal University, Krasnoyarsk, Russia

08:50-09:10 **II-OP51** Dr. Nartova Anna V.
Nartova A.V.[1,2,3], Semikolenov S.V.[1], Bukhtiyarov A.V.[1,3], Khudorozhkov A.K.[1,3], Makarov E.M.[1,2], Kvon R.I.[1]
In Situ XPS Study of DeNOx Reactions on Platinum Catalysts: Pressure and Material Gaps
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk National Research University, Novosibirsk, Russia
3 - Research and Educational Center for Energy Efficient Catalysis in Novosibirsk National Research University, Novosibirsk, Russia

09:10-09:30 **II-OP52** Dr. Zhu Xiaochun
Zhu X.[1], Rohling R.[1], Filonenko G.[1], Mezari B.[1], Hofmann Jan P.[1], Asahina S.[2], Hensen Emiel J.M.[1]
Synthesis of Hierarchical Zeolites Using a Mono-Quaternary Ammonium Surfactant as the Mesoporogen
1 - Inorganic Materials Chemistry group, Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, The Netherlands
2 - JEOL Ltd., Akishima, Tokyo 196-8558, Japan

09:30-09:50 **II-OP53** Dr. Bion Nicolas
Fonseca J.[1], Bion N.[2], Licea Y.E.[3], Morais C.[2], Rangel M.C.[1], Duprez D.[2], Epron F.[2]
Evidence of Remarkable Redox Behaviour of Ce-doped Ordered Mesoporous Alumina at Moderate Temperature
1 - GECCAT Grupo de Estudos em Cinética e Catálise, Instituto de Química, Universidade Federal da Bahia, Campus Universitário de Ondina, Federação, 40 290-115, Salvador, Bahia, Brazil
2 - University of Poitiers, CNRS, Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP), 4 rue Michel Brunet - TSA 51106 - 86073 Poitiers, France
3 - LABCATH(Laboratório de Catálise Heterogênea) DFQ, Instituto de Química, Universidade Federal de Rio de Janeiro, Av. Athos da Silveira Ramos, 149, Rio de Janeiro, 21.949-909, Brazil

09:50-10:10 **II-OP54** van den Berg Roy
Van Den Berg R.[1], Parmentier T.E.[1], Elkjaer C.F.[2], Gommes C.J.[3], Sehested J.[2], Helveg S.[2], De Jongh P.E.[1], De Jong K.P.[1]
Support Functionalization to Retard Copper Particle Growth in the Methanol Synthesis Reaction
1 - Utrecht University, Debye Institute for Nanomaterials Science, Inorganic Chemistry and Catalysis, Universiteitsweg 99, Utrecht, Netherlands
2 - Haldor Topsoe A/S, Nymollevej 55, DK-2800 Kgs. Lyngby, Denmark
3 - University of Liege B6A, Department of Chemical Engineering, Allee de 6 aout 3, B4000 Liege, Belgium

10:10-10:30 **II-OP55** Ishutenko Darya
Ishutenko D.I., Nikulshin P.A., Pimerzin A.A.
Selective Hydrotreating of FCC Gasoline on K_x-CoMoS/Al_2O_3 Catalysts
Samara State Technical University, Samara, Russia

10:30-11:00 ***Coffee break***

Chairmen: Prof. Pescarmona Paolo, *Chemical Engineering Department, University of Groningen, The Netherlands COK, University of Leuven, Belgium*
Dr. Simakova Irina, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

11:00-11:20 **II-OP56** Dewaele Annelies
Dewaele A., Van Berlo B., Dijkmans J., Jacobs P., Sels B.
Immobilized Grubbs Catalysts on Mesoporous Materials: New Insights into Support Characteristics and Their Impact on Catalytic Activity and Product Selectivity
Center for Surface Chemistry and Catalysis, KU Leuven, Kasteelpark Arenberg 23, 3001 Leuven, Belgium

11:20-11:40 **II-OP57** Acosta Brenda
Acosta B.[1], Evangelista V.[1], Miridonov S.[2], Pestryakov A.[3], Fuentes S.[4], Simakov A.[4]
Effect of Nucleus and Shell on the Mechanism of the 4-Nitrophenol Reduction Over Aupd Based Nanoreactors
1 - Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), Posgrado en Física de Materiales, Ensenada, B. C., 22860, México
2 - Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), Departamento de Óptica, Ensenada, B. C., 22860, México
3 - Tomsk Polytechnic University, Department of Technology of Organic Substance and Polymer Materials, Tomsk, 634050, Russia
4 - Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México (CNyN-UNAM), Departamento de Nanocatálisis, Ensenada, B. C., 22860, México

11:40-12:00 **II-OP58** Prof. Lavrenov Alexander
Lavrenov A.V., Sayfulina L.F., Buluchevskiy E.A.
Direct Conversion of Ethylene to Propylene: Strategy of Catalyst Preparation
Institute of Hydrocarbons Processing of Siberian Branch Russian Academy of Sciences, Omsk, Russia

12:00-12:20 **II-OP59** Dr. Ismagilov Ilyas
Ismagilov I.[1], Matus E.[1], Kuznetsov V.[1], Sukhova O.[1], Kerzhentsev M.[1], Ismagilov Z.[1,2], Mota N.[3], Navarro R.[3], Fierro J.[3], Koekkoek A.[4], Gerritsen G.[4], Abbenhuis H.[4]
Design of Highly Efficient Catalysts for Catalytic Membrane Reactors: Study within the Framework of Demcamer Project
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia
3 - Instituto de Catálisis y Petroleoquímica, CSIC, Marie Curie 2, 28049, Madrid, Spain
4 - Hybrid Catalysis B.V., Den Dolech 2, Eindhoven 5612, AZ, the Netherlands

12:20-12:40 **II-OP60** Redekop Evgeniy
Fushimi R.[1,2], Redekop E.[3], Nyapete C.[4], Gleaves J.[5], Yablonsky G.[2]
A Kinetic Fingerprint for Distinguishing Porous Diffusion
1 - Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415, USA
2 - Parks College of Engineering, Aviation and Technology, Saint Louis University, 3450 Lindell Boulevard, Saint Louis, MO 63103, USA
3 - Department of Chemistry, University of Oslo, P.O. Box 1033 Blindern, N-0315 Oslo, Norway
4 - Department of Chemistry, Saint Louis University, 3450 Lindell Boulevard, Saint Louis, Missouri 63103, USA
5 - Department of Energy, Environmental and Chemical Engineering, Washington University in Saint Louis, Saint Louis, Missouri 63130, USA

12:50-13:30 **Closing ceremony** (*KORSTON Ball hall*)

13:30-15:00 ***Lunch***

Friday, September 4

Korston Hotel & Mall Kazan (Ershov street, 1A)

KORSTON Tolstoy hall

Morning Session

Section 5. Catalysis and Environmental Protection

Chairmen: Prof. Koehler Klaus, *Catalysis Research Center, Department of Chemistry, Technische Universität München, Garching, Germany*
Dr. Moses Poul, *Haldor Topsoe A/S, Kgs. Lyngby, Denmark*

Oral Presentations

08:30-08:50 **V-OP41** Prof. Tronconi Enrico
Ruggeri M.P., Selleri T., Nova I., Tronconi E.
Identification of Low-T Standard SCR Reaction Intermediates on Fe-, Cu-zeolite Catalysts by Chemical Trapping Techniques
Dip. Energia, Politecnico di Milano, Milano, Italy

08:50-09:10 **V-OP42** Shishkin Alexander
Shishkin A., Shwan S., Härelind H., Carlsson P.-A., Skoglundh M.
Improved Low- and High-temperature NH_3-SCR Activity over Cu-CHA Prepared by Solid-state Ion-exchange Facilitated by NH_3 and NO
Competence Centre for Catalysis, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden

09:10-09:30 **V-OP43** Dr. Pereda-Ayo B.
De La Torre U.[1], Pereda-Ayo B.[1], González-Velasco J.R.[1], Moliner M.[2], Corma A.[2]
Thermal Aging Resistance of Cu-zeolite Based Catalysts on NH_3-SCR for Lean Burn Engines Exhaust Control
1 - Department of Chemical Engineering, Faculty of Science and Technology, University of the Basque Country, P.O. Box 644, E-48080 Bilbao, Spain
2 - Instituto de Tecnología Química (UPV-CSIC), Universidad Politécnica de Valencia, Consejo Superior de Investigaciones Científicas, Valencia 46022, Spain

09:30-09:50 **V-OP44** Dr. Thogersen Joakim R.
Pedersen K.H., Castellino F., Jensen-Holm H., Thogersen J.R.
Dual Function Catalyst for SCR and CO-oxidation
Haldor Topsoe A/S, Lyngby, Denmark

09:50-10:10 **V-OP45** Alcove Silvia
Usberti N.[1], Beretta A.[1], Nash M.[2], Alcove S.[2]
A Kinetic Study of Hg Oxidation over Vanadia Based Catalyst
1 - Dipartimento di Energia, Politecnico di Milano, piazza L. da Vinci 32, 20133 Milano, Italy
2 - Johnson Matthey, Technology Center, Sonning Common, RG4 9NH, UK

10:10-10:30 **V-OP46** Dr. Thomassen Peter
Thomassen P.L., Fehrmann R., Mossin S.L.
Absorption and Oxidation of NO_x from Flue Gasses to Nitric Acid – An Atom Efficient NO_x Abatement Strategy Using Ionic Liquids
Center for Catalysis and Sustainable Chemistry, Department of Chemistry, Technical University of Denmark, Denmark

10:30-11:00 ***Coffee break***

Chairmen: Prof. Tronconi Enrico, *Dip. Energia, Politecnico di Milano, Milano, Italy*
Dr. Pinaeva Larisa, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Oral Presentations

11:00-11:20 **V-OP47** Prof. Sojka Zbigniew
Zasada F., Kaczmarczyk J., Grzybek G., Janas J., Indyka P., Grybos J., Piskorz W., Kotarba A., Sojka Z.
N_2O Decomposition over Spinel Nanocatalysts - Experimental and DFT Theoretical Approaches to Catalyst Tuning
Jagiellonian University, Faculty of Chemistry, Krakow, Poland

11:20-11:40 **V-OP48** Franken Tanja
Franken T., Palkovits R.
$K-Cu_xCo_{3-x}O_4$ as Highly Efficient Catalysts for N_2O Decomposition from HNO_3-exhaust Streams
RWTH Aachen University, Institut für Technische und Makromolekulare Chemie, Worringerweg 1, D-52074 Aachen, Germany

11:40-12:00 **V-OP49** Papista Eleni
Konsolakis M.[1], Carabineiro S.A.C.[2], Papista E.[3], Marnellos G.E.[3,4], Tavares P.B.[5], Figueiredo J.L.[2]
N_2O Decomposition over $CuO-CeO_2$ Mixed Oxides: Effect of Preparation Procedure
1 - School of Production Engineering and Management, Technical University of Crete, 73100 Chania, Crete, Greece
2 - Laboratório de Catálise e Materials (LCM), Laboratório Associado LSRE/LCM, Faculdade de Engenharia, Universidade do Porto, 4200-465 Porto, Portugal
3 - Department of Mechanical Engineering, University of Western Macedonia, GR-50100 Kozani, Greece
4 - Chemical Process & Energy Resources Institute, CERTH, 57001 Thermi, Thessaloniki, Greece
5 - CQVR Centro de Química–Vila Real, Departamento de Química, Universidade de Trás-os-Montes e Alto Douro, 5001-911 Vila Real, Portugal

12:00-12:20 **V-OP50** Zabilskiy Maxim
Zabilskiy M.[1], Djinović P.[1], Tchernychova E.[2], Erjavec B.[1], Pintar A.[1]
Catalytic Degradation of N_2O Emissions by Nanoshaped CuO/CeO_2 Materials
1 - National Institute of Chemistry, Laboratory for Environmental Sciences and Engineering, Hajdrihova 19, SI-1001 Ljubljana, Slovenia
2 - National Institute of Chemistry, Laboratory for Materials Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia

12:20-12:40 **V-OP51** Dr. Bradu Corina

Olaru A.E.[1], Capat C.[1], Frunza L.[2], Papa F.[3], Munteanu C.[3], Udrea I.[1], Bradu C.[1]

Pd-Cu Catalysts Supported on Anion Exchange Resins for the Simultaneous Catalytic Reduction of Nitrate and Reductive Dehalogenation of 4-chlorophenol from Water

1 - University of Bucharest, Research Center for Environmental Protection and Waste Management, Sos. Panduri 90, 050663 Bucharest, Romania
2 - National Institute of Materials Physics, P. O. Box MG 7, 077125 Magurele, Romania
3 - Institute of Physical Chemistry of the Romanian Academy, Spl. Independentei 202, 060021 Bucharest, Romania

12:50-13:30 **Closing ceremony** (*KORSTON Ball hall*)

13:30-15:00 ***Lunch***

Poster Presentations

Section 1. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

I-PP01
Yang W.Y., Ling F.X., Wang S.J., Shen Z.Q., Fang X.C.
Synthesis and Characterization of Core-shell Beta/MCM-22 Double-microporous Composite Zeolites
Fushun Research Institute of Petroleum and Petrochemicals, SINOPEC, Fushun, Liaoning, China

I-PP02
Fedyaeva O.N., Vostrikov A.A.
In Situ Hydrogenation and Desulfurization of Heavy Hydrocarbon Feedstocks with Addition of Zinc in Supercritical Water Flow
Kutateladze Institute of Thermophysics SB RAS, Novosibirsk, Russia

I-PP03
Vosmerikov A.[1], Korobitsyna L.[1], Sedelnikova O.[1], Zaykovskii V.[2]
Non-Oxidative Conversion of Methane into Aromatic Hydrocarbons over Mo/ZSM-5 Catalysts
1 - Institute of Petroleum Chemistry SB RAS, Tomsk, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

I-PP04
Polo-Garzon F., Bruce D.A.
Reaction Mechanism of Dry Reforming of Methane on Rh Doped Pyrochlore Catalysts: a DFT Approach
Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, USA

I-PP05
Mitina E.G.[1], Filimonov N.S.[1], Shafigulin R.V.[1], Bulanova A.V.[1], Belyakova L.D.[2], Shishkovskiy I.V.[3], Morozov Y.G.[4]
Catalytic Properties of Nanoparticles of Transition Metals in the Hydrogenation Reactions
1 - Samara State University, Samara, Russia
2 - Institute of Physical Chemistry and Electrochemistry RAS, Moscow, Russia
3 - Samara Branch of the Lebedev Physical Institute, Russian Academy of Sciences, Samara, Russia
4 - Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow Region, Russia

I-PP06
Alharbi W., Brown E., Kozhevnikova E., Bond G., Kozhevnikov I.
Dehydration of Alcohols over Heteropoly Acid Catalysts in the Gas Phase
University of Liverpool, Liverpool, United Kingdom

I-PP07
Alharbi K., Alotaibi M., Kozhevnikova E., Kozhevnikov I.
Hydrodeoxygenation of Biomass-Derived Ketones over Bifunctional Metal-Acid Catalysts in the Gas Phase
University of Liverpool, Liverpool, United Kingdom

I-PP08
Bayahia H., Kozhevnikova E., Kozhevnikov I.
Ketonisation of Carboxylic Acids over Metal Oxide and Zeolite Catalysts in the Gas Phase
University of Liverpool, Liverpool, United Kingdom

I-PP09
Dementyeva M.V.[1], Sheshko T.F.[1], Serov Y.M.[1], Shulga A.[1], Chislova I.V.[2], Zvereva I.A.[2]
The Study of Perovskite-type Ferrites: Preparation, Characterization and Application in the Catalytic Hydrogenation of Carbon Monoxide
1 - Peoples Friendship University of Russia, Faculty of Science, Physical and Colloidal Chemistry Department, Moscow, Russia
2 - Saint-Petersburg State University, Petrodvorets, Saint-Petersburg, Russia

I-PP10
Mukhtarova G.S., Efendiyeva N.K., Kasimova Z.A., Abbasov V.M., Ibrahimov H.C.
Influence of Pressure to the Hydrocracking Process of Goudron in the Presence of a Modificated Suspended Halloysite
Azerbaijan NAS Institute of Petrochemical Processes, Baku, Azerbaijan

I-PP11
Konuspayev S.R.[1], Dosmagambetova I.B.[1], Nurbayeva R.K.[2], Zhurtbayeva A.A.[1], Shensizbayeva A.B.[1], Bizhanov B.K.[1]
The New Cracking Catalysts for the Synthesis of Long Chain Paraffins α-olefins and Mixtures of Light Alkanes Conversion under Reducing Conditions
1 - al-Faraby Kazakh National University, Almaty, Kazakhstan
2 - A.B. Bekturov Institute of Chemical Sciences, Almaty, Kazakhstan

I-PP12
Pelaez R., Marin P., Ordonez S.
One-step Synthesis of Dimethyl-ether from Biogenic Syngas on Mixed Metal/Alumina Mixtures
University of Oviedo, Oviedo, Spain

I-PP13
Castedo A.[1,2], Llorca J.[1,2], Mendoza E.[1]
Hydrogen Photoproduction in a Silicone Microreactor Loaded with Au/TiO_2
1 - Centre for Research in NanoEngineering,Universitat Politècnica de Catalunya, Barcelona, Spain
2 - Institute of Energy Technologies,Universitat Politècnica de Catalunya, Barcelona, Spain

I-PP14
Memmedova M.T.
Influence of Suppores's Nature on the Activity of Hematin Catalysts
The Azerbaijan NAS Institute of Petrochemical Processes, Baku, Azerbaijan

I-PP15
Gille T., Busse O., Reschetilowski W.
Regeneration and Activation Studies with NiMo/(Al-MCM-41/ZSM-5) Catalyst System for Hydrocracking of Biogenic Residues
Technische Universität Dresden, Department of Industrial Chemistry, Dresden, Germany

I-PP16
Adsuar-Garcia M.D., Rufete-Beneite M., Roman-Martinez M.C.
Ru Nanoparticles on Acid-modified Carbon Materials for the Hydrolytic Hydrogenation of Cellulose
Department of Inorganic Chemistry, University of Alicante, Alicante, Spain

I-PP17
Kondoh H., Kitaguchi T., Nakasaka Y., Tago T., Masuda T.
Conversion of Heavy Oil into Lighter Fuels over FeO_x-Based Catalyst under Sub- and Super-Critical Water Conditions
Division of Chemical Process Engineering, Faculty of Engineering, Hokkaido University, Sapporo, Japan

I-PP18
Strigina V.A., Doluda V.Y., Skvortsov A.S., Sulman M.G., Sulman E.M.
Investigation of Furfural Hydrogenation to Furfuryl Alcohol and Tetrahydrofurfuryl Alcohol
Tver Technical University, Tver, Russia

I-PP19
Wang Y.[1,2], Sun Y.[2], Leng K.[2], Lancelot C.[1], Lamonier C.[1], Rives A.[1], Richard F.[3]
Hydrodesulfurization of Dibenzothiophene and 4,6 Dimethyldibenzothiophene over NiW Catalyst Supported over Hierarchical Mordenite
1 - University of Lille UCCS, Lille, France
2 - School of Chemical Engineering and Technology HIT, Harbin, China
3 - University of Poitiers IC2MP, Poitiers, France

I-PP20
Blashkov I., Basov L., Lisachenko A.
"Self-Sensitization" of Photocatalytic Activity of ZnO into Visible Region
St. Petersburg State University, Department of Physics, Saint-Petersburg, Russia

I-PP21
Chumachenko Y. A., Lavrenov A.V., Buluchevskii E.A., Gulyaeva T.I., Arbuzov A.B., Leontieva N.N., Ivashchenko O.V., Trenikhin M.V.
The One-step Hydrocracking of Vegetable Oil over Platinum Catalysts with Borate-containing Oxide Supports
Institute of Hydrocarbons Processing of Siberian Branch Russian Academy of Sciences, Omsk, Russia

I-PP22
Ismagilov I.[1], Matus E.[1], Kuznetsov V.[1], Sukhova O.[1], Kerzhentsev M.[1], Ismagilov Z.[1,2]
Stability of NiPd Bimetallic Catalysts in the Autothermal Reforming of Methane
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia

I-PP23
Zakarina N.A., Kim O.K., Volkova L.D., Chanysheva I.S., Dalelkhan O., Zhumadullaev D.A., Komashko L.V.
Iron Pillared Montmorillonites - Carriers of Pt-Catalysts for N-Alkanes Isomerization
Institute of Organic Catalysis and Electrochemistry after D.V. Sokolsky, Almaty, Kazakhstan

I-PP24
Mesrar F.[1], Testa M.L.[2], Brik Y.[1], Kacimi M.[1], Ziyad M.[1,3], La Parola V.[2], Liotta L.F.[2]
Acetylation of Glycerol over Mixed Zirconium Phosphate-Sulphate Catalysts
1 - Université Mohammed V, Faculté des Sciences, Département de Chimie, Av. Ibn Battouta, BP1014, Rabat, Maroc
2 - ISMN-CNR, via Ugo La Malfa, 153, 90146, Palermo, Italy
3 - Académie Hassan II des Sciences et Techniques, Rabat, Maroc

I-PP25
Shtertser N.V.[1,2], Pakharukova V.P.[1,2], Khassin A.A.[2,1]
Synthesis Features of Oxide Compounds Based on Univalent Copper of Delafossite Structure
1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Novosibirsk National Research University, Novosibirsk, Russia

I-PP26
Ouanji F.[1], Kacimi M.[1], Ziyad M.[1,2], Puleo F.[3], Liotta L.F.[3]
Esterification-Neutralization-Transesterification of Waste Cooking Oil: In-situ Three-stage Method for Biodiesel Synthesis, Neutralization Step Optimization
1 - Université Mohammed V, Faculté des Sciences, Département de Chimie, Av. Ibn Battouta, Rabat, Maroc
2 - Académie Hassan II des Sciences et Techniques, Rabat, Maroc
3 - ISMN-CNR, via Ugo La Malfa, 153, 90146, Palermo, Italy

I-PP27
Németh M.[1], Schay Z.[1], Srankó D.[1], Károlyi J.[1], Sáfrán G.[2], Sajó I.[3], Horváth A.[1]
Mechanistic Studies with Labeled $^{13}CO_2$ on Ni/ZrO_2 and Pt/ZrO_2 Dry Reforming Catalysts
1 - Centre for Energy Research, Institute for Energy Security and Environmental Safety, Department of Surface Chemistry and Catalysis, Konkoly-Thege M. street 29-33, H-1121 Budapest, Hungary
2 - Centre for Energy Research, Institute for Technical Physics and Materials Science, Thin Film Physics Department, Konkoly-Thege M. street 29-33, H-1121 Budapest, Hungary
3 - University of Pécs, Szentágothai Research Centre, Ifjúság street 20, H-7624 Pécs, Hungary

I-PP28
Belinskaya N.S., Ivanchina E.D., Ivashkina E.N., Nazarova G.Yu.
Mathematical Model of Catalytic Hydrodewaxing of Distillates
National Research Tomsk Polytechnic University, Tomsk, Russia

I-PP29
Ivanov D.P.[1], Semikolenov S.V.[1], Nartova A.V.[1,2], Fedorov V.S.[1,2], Babushkin D.E.[1], Dubkov K.A.[1]
Study of Influence of Cis-Trans Isomerization on Selective Oxidations of Alkenes by Nitrous Oxide
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

I-PP30
Naranov E.R.[1], Badeeva A.S.[1], Maximov A.L.[1,2], Karakhanov E.A.[1]
Development of New NiW Catalysts Supported on SBA-15/Zeoilte for Oil Sludge Hydrotreating
1 - Department of Chemistry, Moscow State University, Moscow, Russia
2 - Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, Russia

I-PP31
Solov'ev S.A., Egorov A.G., Egorova S.R., Lamberov A.A., Kataev A.N., Bekmukhamedov G.E.
A Numerical Investigation of the Catalyst Behaviour in Fluidized Bed Circulating Reactor
Kazan Federal University, Kazan, Russia

I-PP32
Belomestnykh I.P.[1], Krasnobaeva O.N.[2], Nosova T.A.[2], Elisarova T.A.[2], Danilov V.P.[2]
Sm, Eu Containing Hydrotalcite-like Materials as Precursors of Catalysts for Oxidative Dehydrogenation of Light Hydrocarbons
1 - Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
2 - Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow, Russia

I-PP33
Fomina O.S.[1,2], Yakhvarov D.G.[1], Sinyashin O.G.[1], Heinicke J.W.[2]
Novel α,α-phosphinoaminoacids: Synthesis, Properties and Catalytic Activity in the Ethylene Oligomerization Process
1 - A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, RAS, Kazan, Russia
2 - Institute of Biochemistry Ernst-Moritz-Arndt University of Greifswald, Greifswald, Germany

I-PP34
Gulyaeva L.[1], Shmelkova O.[1], Grudanova A.[1,2], Krasilnikova L.[1], Misko O.[1], Chernysheva E.[2], Boldushevsky R.[1,2], Asaula V.[2]
The Development of Integrated Technology for Oil and Vegetable Feedstock Processing to Produce Diesel Fuel for Arctic Climatic Zone and Jet Fuel
1 - All-Russia Research Institute of Oil Refining, JSC, Laboratory of Hydrogenated Processes and Catalysts for Motor Fuels Producing, Moscow, Russia
2 - Gubkin Russian State University of Oil and Gas, Department of Oil Refining Technology, Moscow, Russia

I-PP35
Zhiltsova E.P.[1], Lukashenko S.S.[1], Valeeva F.G.[1], Kashapov R.R.[1], Pashirova T.N.[1], Konovalov A.I.[1], Zakharova L.Ya.[1,2]
Self-Assembled Complexes of 1-Hexadecyl-4-Aza-1-Azoniabicyclo[2.2.2]Octane Bromide with Nitrates of Copper and Lanthanum as the Models of Metalloenzymes
1 - A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, Russian Academy of Sciences, Kazan, Russia
2 - Kazan National Research Technological University, Kazan, Russia

I-PP36
Aghaei P., Visconti C.G., Groppi G., Tronconi E.
Development of a General Heat Transport Model for Open-cell Metal Foams
Politecnico di Milano, Department of Energy, Laboratory of Catalysis and Catalytic Processes, Milano, Italy

I-PP37
Yeletsky P.M.[1,2], Mironenko O.O.[1], Sosnin G.A.[1,3], Yakovlev V.A.[1,2]
Selective Steam Cracking of Heavy Oil in Semibatch Reactor
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - UNICAT Ltd., Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia

I-PP38
Vasilevich A.V., Baklanova O.N., Lavrenov A.V., Likholobov V.A.
Mechanochemical Synthesis of Molybdenum Carbide: New Approach for the Hydrodesulfurization Catalysts Preparation
Institute of Hydrocarbons Processing of Siberian Branch Russian Academy of Sciences, Omsk, Russia

I-PP39
Foss L.E.[1,2], Petrukhina N.N.[3], Kayukova G.P.[1,2], Tumanyan B.P.[3], Nikolaev V.F.[1], Romanov G.V.[1,2], Vakhin A.V.[2]
Heavy Oil Upgrading in the Presence of Organic Salts of Transition Metals under Reservoir Conditions
1 - A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, RAS, Kazan, Russia
2 - Kazan Federal University, Kazan, Russia
3 - Gubkin Russian State University of Oil and Gas, Moscow, Russia

I-PP40
Simonova L.G., Zirka A.A., Isupova L.A., Reshetnikov S.I.
Influence of Catalyst Preparation Techniques on the Properties of the Cr-Mg Catalysts for Tetrachloroethylene Hydrofluorination
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

I-PP41
Sitnov S.A.[1], Vakhin A.V.[1], Petrovnina M.S.[1], Feoktistov D.A.[1], Kayukova G.P.[2], Nourgaliev D.K.[1]
Catalytic Aquathermolysis Heavy Oil in the Presence of Organometallic Complex
1 - Kazan (Volga region) Federal University, Kazan, Russia
2 - A.E. Arbuzov Institute of Organic and Physical Chemistry Kazan Scientific Centre Russian Academy of Sciences, Kazan, Russia

I-PP42
Ushakov A.E., Kozhevnikov V.L., Patrakeev M.V., Leonidov I.A., Markov A.A.
Performance of Modified Nickel Catalysts in a Catalytic Membrane Reactor for Partial Oxidation of Methane
Institute of Solid State Chemistry, Ural Branch of RAS, Ekaterinburg, Russia

I-PP43
Verboekend D., Liao Y., Schutyser W., Sels B.F.
Alkylphenols to Phenol and Olefins by Zeolite Catalysts: a Shape-Selective Process to Valorize Raw and Fossilized Lignocellulose
KU Leuven, Leuven, Belgium

I-PP44
Slyemi Samira, Barama Akila, Messaoudi Hassiba
Study of Catalytic Activity of Impregnated VMgO Catalysts in the Oxidative Dehydrogenation of Ethane
Laboratoire des Matériaux Catalytiques et Catalyse en Chimie Organique, USTHB, Faculté de Chimie, BP.32.El Alia Alger 16111 Bab-Ezzouar, Alger, Algérie

I-PP45
Onishchenko M.I.[1], Kulikov A.B.[1], Maximov A.L.[1,2]
Pt/amorphous Silica-Alumina Catalysts for Hydroconversion of C_{20}-C_{31} n-Alkanes Mixture into Fuels with Improved Cold Flow Properties
1 - A.V. Topchiev Institute of Petrochemical Synthesis, RAS (TIPS RAS), Moscow, Russia
2 - Lomonosov Moscow State University, Moscow, Russia

I-PP48
Kayukova G.P.[1,2], Gubaydullin A.T.[1], Petrov S.M.[2], Rizvanov I.H.[1], Romanov G.V.[1,2], Vahin A.V.[2], Pertukhina N.N.[3]
Change of Phase-dispersed Structure of Asphatenes in During the Hydrothermal-catalytic Conversion of Heavy Oil
1 - A.E. Arbuzov Institute of Organic and Physical Chemistry Kazan Scientific Centre Russian Academy of Sciences, Kazan, Russia
2 - Kazan (Volga region) Federal University, Kazan, Russia
3 - Gubkin Russian State University of Oil and Gas, Moscow, Russia

I-PP49

Simakova I.L.[1,2], Tarabanko V.E.[3], Chernyak M.[3], Morozov A.[3], Simonov M.[1,2]

Catalytic Conversion of Furfural into Gasoline Components

1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Institute of Chemistry and Chemical technology SB RAS, Krasnoyarsk, Russia

I-PP50

Antzara A.[1], Heracleous E.[2], Ipsakis D.[1], Silvester L.[3], Bukur D.B.[3], Lemonidou A.A.[1]

Effect of Support in NiO-based Oxygen Transfer Materials for Sorption Enhanced Chemical Looping Methane Reforming: Characterization and Reactivity Studies

1 - Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece
2 - School of Science & Technology, International Hellenic University, Thessaloniki, Greece
3 - Texas A&M University at Qatar, Chemical Engineering Program, Education city, Doha, Qatar

I-PP51

Godina L.I.[1], Kirilin A.V.[1], Tokarev A.V.[1], Demidova Y.S.[2,3], Lemus J.[4], Calvo L.[4], Schubert T.[5], Gilarranz M.A.[4], Simakova I.L.[2,3], Murzin D.Y.[1]

Aqueous Phase Reforming of Xylitol over Mono- and Bimetallic Carbon-supported Catalysts

1 - Åbo Akademi University, Laboratory of Industrial Chemistry and Reaction Engineering, Åbo, Finland
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia
4 - Universidad Autónoma de Madrid, Madrid, Spain
5 - FutureCarbon GmbH, Bayreuth, Germany

I-PP52

Lipin P.V., Potapenko O.V., Sorokina T.P., Doronin V.P.

Co-Conversion of Fatty Acids and Hydrocarbons in the Conditions of Catalytic Cracking

Institute of Hydrocarbons Processing SB RAS, Omsk, Russia

I-PP53

Semeykina V.S.[1,2,3], Polukhin A.V.[1], Parunin P.D.[1,2,3], Parkhomchuk E.V.[1,2,3], Lysikov A.I.[1,2]

Advanced Macroporous Catalysts for Heavy Oil Hydrotreating

1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Scientific Research Centre "Energy Efficient Catalysis", Novosibirsk State University, Novosibirsk, Russia

I-PP54

Varakin A., Salnikov V., Nikulshin P.

The Role of Carrier's Carbonization Degree on the HDO Conversion of the Oleic Acid over the CoMo/C/Al_2O_3 Catalysts

Samara State Technical University, Samara, Russia

I-PP55

Shelepova E.[1], Vedyagin A.[1], Mishakov I.[1,2], Noskov A.[1,2]

The Influence of Membrane Reactor Parameters on Efficiency of Hydrocarbons Dehydrogenation Process

1 - Boreskov Institute of Catalysis, Department of catalytic process engineering, Novosibirsk, Russia
2 - Novosibirsk State Technical University, Novosibirsk, Russia

I-PP56

Valdez C.E., Nechay M.R., Sparta M., Alexandrova A.N.

In Silico Design of Artificial Metalloenzymes

University of California, Los Angeles, USA

I-PP57

Bychkov V.Y.[1], Tulenin Y.P.[1], Slinko M.M.[1], Khudorozhkov A.K.[2], Bukhtiayrov V.I.[2], Korchak V.N.[1]

Self-Oscillatory Regimes of Methane Oxidation over Supported Pd Catalysts

1 - Semenov Institute of Chemical Physics RAS, Moscow, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

I-PP58
Xia W.S., Hou Y.H., Han W.C., Wan H.L.
Structure Sensitivity in $La_2O_2CO_3$ and La_2O_3 Catalysts for Oxidative Coupling of Methane
State Key Laboratory of Physical Chemistry of Solid State Surfaces, National Engineering Laboratory for Green Chemical Productions of Alcohols-Ethers-Esters, Fujian Province Key Laboratory of Theoretical and Computational Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian, P. R. China

I-PP59
Potapenko O.V., Doronin V.P., Sorokina T.P., Krol O.V., Likholobov V.A.
Mechanism of Hydrogen Transfer Reaction from Naphthenes to 1-Hexene on Y and ZSM-5 Zeolites
Institute of Hydrocarbons Processing of Siberian Branch of Russian Academy of Sciences, Omsk, Russia

I-PP60
Polo-Garzon F., Bruce D.A.
Micro-Kinetic Model of Dry Reforming of Methane on Doped Pyrochlore Catalysts
Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, USA

I-PP61
Abasov S.I., Isayeva E.S., Babayeva F.A., Agayeva S.B., Starikov R. V., Tagiyev D.B.
Catalytic Conversion of Low Molecular Alkanes with C-C Bonds Formation
The Azerbaijan NAS Institute of Petrochemical Processes, Baku, Azerbaijan

I-PP62
Asgar-Zadeh S.M.[1], Urban O.B.[1], Javadova M.N.[1], Eldarova S.G.[1], Khudiyeva I.E.[1], Alkhasli E.A.[2], Mammadov N.A.[1]
Innovative Development of Refining Sector in Azerbaijan
1 - Institute of Petrochemical Processes, National Academy of Sciences of Azerbaijan, Laboratory of Complex Refining of Petroleum and Technical and Economic Researches, Baku, Azerbaijan Republic
2 - State Oil Company of Azerbaijan Republic, SOCAR's Oil Gas Processing and Petrochemical Complex, Baku, Azerbaijan Republic

I-PP63
Yakovenko R.E., Narochnui G.B., Savost'yanov A.P.
Application of Tubular Reactor for High-Performance Fischer-Tropsch Syntehesis
Platov South-Russian State Polytechnic University (NPI), Novocherkassk, Russia

I-PP64
Sadykov V.[1,2], Bobrova L.[1], Vostrikov Z.[1], Vernilovskaya N.[1,2], Mezentseva N.[1,2]
Ethanol Steam Reforming on a Structured Heat-Conducting Catalytic Package: Modelling and Experimetal Perfomance
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

I-PP65
Hachemi I., Mäki-Arvela P., Kumar N., Murzin Y.D.
Catalytic Hydrodeoxygenation of Microalgae Biodiesel over Sulfur-Free Nickel Supported Catalyst for the Production of Biofuels
Åbo Akademi University, Turku, Finland

I-PP66
Manucharova L.A., Bakhtchadjian R., Tavadyan L.A.
Application of the Dioxo-Mo(VI) Complex Anchored on a TiO_2 in the Oxidation of DDT with Molecular Oxygen, under UV-irradiation
Nalbandyan Institute of Chemical Physics, National Academy of Sciences of the Republic of Armenia, Yerevan, Republic of Armenia

I-PP67
Samedova F.I., Gasanova R.Z., Logmanova S.B., Badavi Y.E.
Petroleum-Saturated Sands of Azerbaijan
Institute of Petrochemical Processes named after acad. Y.H. Mamedaliyev, Azerbaijan NAS, Baku, Azerbaijan

I-PP68
Dedov A.G.[1], Loktev A.S.[1], Komissarenko D.A.[1,2], Mazo G.N.[3], Shlyakhtin O.A.[3], Parkhomenko K.V.[2], Roger A.-C.[2], Mukhin I.E.[1], Lijiev M.M.[1], Moiseev I.I.[1]
Partial Oxidation and Dry Reforming of Methane to Synthasis Gas over Complex Oxide Cobaltate-based Catalysts
1 - Gubkin Russian State University of Oil and Gas, Department of General and Inorganic Chemistry, Moscow, Russia
2 - Université de Strasbourg, Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé, UMR7515 CNRS ECPM, 25 Rue Becquerel, 67087 Strasbourg, France
3 - Lomonosov Moscow State University, Chemistry Department, Moscow, Russia

I-PP69
Borshch V.N.[1], Sanin V.N.[1], Pugacheva E.V.[1], Zhuk S.Ya.[1], Andreev D.E.[1], Yukhvid V.I.[1], Eliseev O.L.[2], Kazantsev R.V.[2], Kolesnikov S.I.[3], Kolesnikov I.M.[3]
New Polymetallic Catalysts on the Base of SHS-Intermetallides for Oxidation and Reduction Processes
1 - Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow Region, Russia
2 - N.D. Zelinski Institute of Organic Chemistry RAS, Moscow, Russia
3 - I.M. Gubkin Russian State University of Oil and Gas, Moscow, Russia

I-PP70
Lamberov A.A.
Cooperation of Kazan (Volga Region) Federal University and PJSC "Nizhnekamskneftekhim" in the Development of Catalysts for the Petrochemical Industry
Kazan (Volga region) Federal University, Department of Chemistry, Kazan, Russia

I-PP71
Chu B.Z.[1], An H.[1], Truter L.A.[2], Nijhuis T.A.[2], Schouten J.C.[2], Cheng Y.[1]
Performance of Phase-pure M_1 $MoVNbTeO_x$ Catalysts with Different Post-treatments for the Oxidative Dehydrogenation of Ethane
1 - Department of Chemical Engineering, Tsinghua University, Beijing, PR China
2 - Department of Chemical Engineering and Chemistry, Laboratory of Chemical Reactor Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands

I-PP72
Stepacheva A.A.[1], Sapunov V.N.[2], Nikoshvili L.Z.[1], Sulman E.M.[1], Matveeva V.G.[1]
Oils and Fats Conversion to the Second Generation of Biodiesel Using Pd-containing Catalysts
1 - Tver Technical University, Tver, Russia
2 - Mendeleyev University of Chemical Technology of Russia, Moscow, Russia

I-PP73
Kirchmann M., Haas A., Hauber C., Böltken T.
High Throughput Testing of Naphtha Reforming Catalysts
Hte GmbH, Heidelberg, Germany

I-PP74
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2 - University of Catalysis and Inorganic Chemistry, Baku, Azerbaijan

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1 - Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia
2 - Gubkin Russian State University of Oil and Gas, Moscow, Russia
3 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
4 - Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia
5 - National Research Centre "Kurchatov Institute", Moscow, Russia

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1 - Institute of Petroleum Chemistry SB RAS, Tomsk, Russia
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2 - Technical Chemistry, Department of Chemistry, Chemical-Biological Center, Umeå University, Umeå, Sweden
3 - Wood and Paper Chemistry, Johan Gadolin Process Chemistry Centre, Åbo Akademi University, Åbo-Turku, Finland

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2 - Novosibirsk State University, Novosibirsk, Russia
3 - Scientific Research Centre "Energy Efficient Catalysis", Novosibirsk State University, Novosibirsk, Russia

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1 - Technische Universität München, München, Germany
2 - East China Normal University, Shanghai, China
3 - Washington State University, Pullman, USA
4 - Pacific Northwestern National Laboratory, Richland, USA

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1 - Southern Federal University, IRC Smart Materials, Rostov-on-Don, Russia
2 - University of Turin, Department of Chemistry, Turin, Italy

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1 - Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway
2 - SINTEF Materials and Chemistry, Trondheim, Norway

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2 - Science and Technology Application and Research Center, Dicle University, Turkey
3 - Institute of Chemical Sciences, Almaty, Kazakhstan

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3 - Ecole Centrale de Lille, 59655 Villeneuve d’Ascq, France
4 - Institut Universitaire de France, Maison Universités, 103 Boulevard Saint-Michel, Paris, France

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1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Universität Konstanz, Konstanz, Germany

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1 - Unité de Catalyse et Chimie du Solide, Villeneuve d'Ascq, France
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1 - Center for Nanomaterials and Chemical Reactions, Institute for Basic Science (IBS), Daejeon, South Korea
2 - Department of Chemistry, KAIST, Daejeon, South Korea

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1 - University of Antwerp, Antwerp, Belgium
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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Unicat Ltd, Novosibirsk, Russia

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2 - Research and Educational Center for Energy Efficient Catalysis in Novosibirsk National Research University, Novosibirsk, Russia
3 - Novosibirsk National Research University, Novosibirsk, Russia

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2 - Faculty of Science, Kasetsart University, Bangkok, Thailand

Section 2. Catalyst Preparation and Characterization

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School of Materials Science, Japan Advanced Institute of Science and Technology, Nomi, Japan

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1 - Utrecht University, Debye Institute for Nanomaterials Science, Inorganic Chemistry and Catalysis, Universiteitsweg 99, Utrecht, Netherlands
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3 - University of Liege B6A, Department of Chemical Engineering, Allee de 6 aout 3, B4000 Liege, Belgium

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National Centre for Catalysis Research and Department of Chemistry, Indian Institute of Technology-Madras, Chennai, India

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1 - Huygens-Kamerlingh Onnes Laboratory, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands
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2 - Inorganic Chemistry Department, University of Alicante, Alicante, Spain
3 - Chemical Engineering Department, University of Groningen, The Netherlands

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1 - Federal State Budgetary Educational Institution of Higher Professional Education "Kazan National Research Technological University", Kazan, Russia
2 - Technological University, Baghdad, Iraq

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Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

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3 - Université Laval, Department of Mining, Metallurgical and Materials Engineering, Québec, Canada

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2 - Department of Chemistry, University of Southampton, Highfield , Southampton, U.K.
3 - University of Poitiers, CNRS UMR 7285, Institut des Milieux et Matériaux de Poitiers (IC2MP), Poitiers, France

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3 - University of Limerick, Limerick, Ireland
4 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia

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1 - Institute of Physical Chemistry, University Innsbruck, Innsbruck, Austria
2 - Department of Inorganic Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany
3 - Department of Photon Science, Deutsches Elektronen Synchrotron DESY, Germany

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1 - International Tomography Center, SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

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1 - Lomonosov Moscow State University, Chemistry Department, Moscow, Russia
2 - Institute of Hydrocarbons Processing of the Siberian Branch of the RAS, Omsk, Russia

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1 - Institute of Energy Technologies, Universitat Politècnica de Catalunya, Barcelona, Spain
2 - Chemistry Department, Brookhaven National Laboratory, Upton, New York, USA
3 - Dipartimento di Chimica, Fisica e Ambiente, Università di Udine, Udine, Italy

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1 - Tomsk State University, Tomsk, Russia
2 - Boreskov Institute of Catalysis, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia

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1 - Institut de Chimie des Milieux et Matériaux de Poitiers, UMR 7285 CNRS, Poitiers, France
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2 - Novosibirsk State University, Novosibirsk, Russia

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2 - Kazakh-British Technical University, Almaty, Republic of Kazakhstan

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1 - Platov South-Russian State Polytechnic University (NPI), Novocherkassk, Russia
2 - Karlsruhe Institute of Technology, Karlsruhe, Germany

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Tarasov A.V., Frei E., Schumann J.

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Fritz-Haber Institut der Max-Planck Gesellschaft, Dapartment of Inorganic Chemistry, Berlin, Germany

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Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

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Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia

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1 - Hefei National Laboratory for Physical Sciences at Microscale, CAS Key Laboratory of Materials for Energy Conversion, Department of Chemical Physics, University of Science and Technology of China, Hefei, China
2 - Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia,
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1 - Institute of Petroleum Chemistry SB RAS, Tomsk, Russia
2 - Institute of Metal Physics UB RAS, Ekaterinburg, Russia
3 - Tomsk Polytechnic University, Tomsk, Russia

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1 - Institute of Hydrocarbons Processing SB RAS, Omsk, Russia
2 - Boreskov institute of catalysis SB RAS, Novosibirsk, Russia

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Lomonosov Moscow State University, Moscow, Russia

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Kazan (Volga region) Federal University, Kazan, Russia

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2 - Laboratory for Materials Chemistry, National Institute of Chemistry, Ljubljana, Slovenia

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3 - Indiana University, Indiana, USA
4 - King Abdulaziz University, Jeddah, Saudi Arabia

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Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
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2 - JSC «A.B. Bekturov Institute of chemical sciences»,, Almaty, Kazakhstan

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2 - Institute for System Dynamics and Control Theory, Irkutsk, Russia

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Bogazici University, Department of Chemical Engineering, Istanbul, Turkey

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Department of Chemical Physics, University of Science and Technology of China, Hefei, China
Hefei National Laboratory for Physical Science at the Microscale, Hefei, China
CAS Key Laboratory of Materials for Energy Conversion, Hefei, China

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1 - A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, RAS, Kazan, Russia
2 - Kazan (Volga region) Federal University, Kazan, Russia
3 - Kazan Institute of Biochemistry and Biophysics, Kazan Scientific Centre, RAS, Kazan, Russia

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1 - Research Institute on Combustion, CNR, Naples, Italy
2 - DICMAPI, University of Naples Federico II, Naples, Italy

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2 - Saint-Petersburg State University, Saint-Petersburg, Russia

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On the Physics of Intercalation of Hydrogen into Surface Nanoblisters in Pyrolytic Graphite & Epitaxial Graphene: Relevance to the Hydrogen Storage Problem
1 - I. P. Bardin Central Research Institute for Ferrous Metallurgy, G. V. Kurdjumov Institute of Metals Science and Physics, Moscow, Russia
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1 - Bilkent University, Chemistry department, Bilkent, Ankara, Turkey
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1 - Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia
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1 - A.E. Arbuzov Institute of Organic and Physical Chemistry KSC RAS, Kazan, Russia
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2 - Novosibirsk State Technical University, Novosibirsk, Russia

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1 - Institute of Chemical Physics, Academy of Sciences of Armenia, Yerevan, Armenia
2 - Institute of General and Inorganic Chemistry, Academy of Sciences of Armenia, Yerevan, Armenia

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Kvon R.I.[1], Bukhtiyarov A.V.[1,2], Nartova A.V.[1,3,2], Makarov E.M.[1,3,2], Kulagina M.A.[1,3], Shterk G.V.[1,3,2], Bukhtiyarov V.I.[1,3,2]

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MSU, Faculty of Chemistry, Moscow, Russia

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2 - Bionanoplasmonics Laboratory, CIC biomaGUNE, Spain

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Goulon A.[1], Faraj A.[1], Leflaive P.[2]

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Chemical Engineering Department, College of Engineering, King Saud University, Riyadh, KSA

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The Role of Electron-Acceptor Sites during Catalytic Dehydrochlorination of 1-Chlorobutane over Metal Oxides

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1 - Institute for Physics of Microstructures, RAS, N.Novgorod, Russia
2 - Nizhny Novgorod Alexeev State Technical University, Nizhni Novgorod, Russia

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
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1 - Southern Federal University, IRC "Smart Materials", Rostov-on-Don, Russia
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1 - Norwegian University of Science and Technology, Chemical Eng. Dept, Trondheim, Norway
2 - Technology and Projects, INEOS ChlorVinyl, Norway

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1 - St. Petersburg StateTechnological Institute (Technical University), Department of General Chemical Technology and Catalysis, St. Petersburg, Russia
2 - Abo Akademi University, Turku, Finland

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Kuznetsov V.L.[1,2], Krasnikov D.V.[1,2], Shmakov A.N.[1,2], Lapina O.B.[1], Andreev A.S.[1,2], Ishchenko A.V.[1], Prosvirin I.P.[1], Kalinkin A.V.[1], Zakharov D.N.[3], Kazakova M.A.[1,2]
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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Brookhaven National Laboratory P.O. Box 5000, Upton, NY 11973-5000, USA

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Catalytic Activity of $PCsp^3P$ Pincer Iridium Hydride Complexes in Olefines Hydroformylation and Acceptorless Alcohols Dehydrogenation: DFT and Spectroscopic Study
1 - A.N.Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia
2 - The Hebrew University of Jerusalem, Institute of Chemistry, Edmond Safra Campus, Givat Ram, 91904 Jerusalem, Israel

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D.V. Sokolsky Institute of Organic Catalyst and Electrochemistry, Almaty, Kazakhstan

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1 - D.Mendeleev University of Chemical Technology of Russia, Moscow, Russia
2 - JSC "Grodno Azot", Grodno, Republic of Belarus
3 - LLC "NIAP-KATALIZATOR", Novomoskovsk, Tula Region, Russia

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1 - Institute of Petrochemical Processes, Physical and Physical-Chemical Investigations Department, Baku, Azerbaijan
2 - Institute of Catalysis and Inorganic Chemistry, Department of Heterogeneous Catalysis, Baku, Azerbaijan

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1 - Samara State Technical University, Samara, Russia
2 - United Research and Development Centre, Moscow, Russia

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Samara State Technical University, Samara, Russia

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Larichev Yu.V.[1,2]
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1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

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Instituto Mexicano del Petróleo. Eje Central Lázaro Cárdenas No. 152. Col. San Bartolo Atepehuacan. C. P. 07730, México D. F., México

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Optimizing the Controlled Synthesis of PVP-based Carbon Supported Ru Nanoparticles: Synthesis Approaches and Characterization
1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany
4 - FutureCarbon GmbH, Bayreuth, Germany
5 - Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, México
6 - Åbo Akademi University, PCC, Turku/Åbo, Finland

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Koskin A.P.[1], Kenzhin R.M.[1], Mishakov I.V.[1,2], Vedyagin A.A[1,2]

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State Technical University, Novosibirsk, Russia

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Rotaru C.G.[1], Postole G.[2], Florea M.[1], Matei-Rutkovska F.[2], Pârvulescu V.I.[1], Gelin P.[2]

Characterization and Methane Dry Reforming Performance of CeO_2 Prepared by Modified Precipitation Route

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Precisely Controlled Synthesis of PVP- Capped Ni and Co Metal Nanoparticles

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3 - Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany
4 - FutureCarbon GmbH, Bayreuth, Germany
5 - Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, México
6 - Åbo Akademi University, PCC, Turku/Åbo, Finland

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2 - Université 20 Août-Skikda, Faculté de Technologie, Département de Pétrochimie &Génie des Procédés, BP 26, route Al-Hadaiek, 21000 Skikda, Alger, Algérie
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5 - Entreprise Nationale Sonatrach, Institut Algérien du Pétrole, Les platanes Filfila, Skikda, Alger, Algérie

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Kurtoglu K., Gubbuk I.H.

Preparation of Cu Loaded Magnetic Nanoparticle Catalyst and Its Catalytic Activity for Degradation of Azo Dyes

Selcuk University Faculty of Sciences Department of Chemistry, 42031 Campus, Konya, Turkey

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Aslan E.[1], Baslak C.[1], Hatay Patir I.[1], Kus M.[2], Ersoz M.[1]

The Photocatalytic Hydrogen Evolution by Alloyed CdTeS Nanocrystals

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2 - Department of Chemical Engineering, Selcuk University, Konya, Turkey

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Iqbal S.[1], Schonmakers D.[1], Lu L.[2], Kondrat S.A.[1], Jones D.R.[1], Wells P.P.[3], Gibson E.K.[3], Morgan D.J.[1], Kiley C.J.[2], Hutchings G.J.[1]

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2 - Department of Materials Science and Engineering, Lehigh University, Bethlehem, PA, USA
3 - The UK Catalysis Hub, Research Complex at Harwell, Harwell, Oxon, OX11 0FA, UK and University College London, Kathleen Lonsdale Materials, Department of Chemistry, Gordon Street, London, UK

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M.V. Lomonosov Moscow State University, Moscow, Russia

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1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Materials Science, Kemerovo, Russia

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1 - Azerbaijan National Academy of Sciences, Institute of Petrochemical Processes named after Yu.G. Mamedaliev, Department of "Chemistry and technology of oil and gas", Baku, Azerbaijan
2 - Leibniz Institute for Catalysis at the University of Rostock, Department of "Catalyst discovery and reaction engineering", Rostock, Germany

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1 - Belgorod State National Research University, Department of Biology and Chemistry, Belgorod, Russia
2 - Belgorod State National Research University, Shared Facilities Center "Diagnosing the Structure and Properties of Nanomaterials", Belgorod, Russia

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1 - LMCCCO, Faculty of Chemistry, USTHB, BP32 EL Alia 16111 Bab Ezzouar, Algiers, Algeria
2 - Chemistry Department, Faculty of Sciences; UHBC, BP151 Hay Es-salem, 02000, Chlef, Algeria
3 - Catalysis Science and Technology, Universiti Putra Malaysia, UPM 43400, Serdang, Selangor, Malaysia
4 - IC2MP, Université de Poitiers, 40 av. du Recteur-Pineau, 86022 Poitiers cedex, France

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1 - Moscow State University, Chemistry Department, Moscow, Russia
2 - Institute of Petrochemical Synthesis RAS, Moscow, Russia

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Institute of Petrochemical Processes of NASA, Baku, Azerbaijan

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1 - University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Department of Catalysis and Chemical Engineering, Belgrade, Republic of Serbia
2 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

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1 - Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. of Inorganic Chemistry, Berlin, Germany
2 - BASF SE
3 - ETH Zurich, Zurich Switzerland

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1 - Research and Educational Center for Energy Efficient Catalysis in Novosibirsk National Research University, Novosibirsk, Russia
2 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
3 - Tomsk State University, Tomsk, Russia

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1 - National Research Council of Italy, Institute of Science and Technology for Ceramics (CNR-ISTEC), via Granarolo 64, 48018 Faenza, Italy
2 - Department of Industrial Chemistry "Toso Montanari", Alma Mater Studiorum Università di Bologna, Viale Risorgimento 4, 40136 Bologna, Italy

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1 - Technische Universiteit Eindhoven, Inorganic Materials Chemistry, Eindhoven, Netherlands
2 - European Synchrotron Radiation Facility, Grenoble, France
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1 - Department of New Chemical Technologies and Nanomaterials, Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Moscow, Russia
2 - INFRA Technology Ltd., Moscow, Russia

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Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

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1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

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Grabchenko M.V.[1], Mamontov G.V.[1], Zaikovskii V.I.[2,3], Vodyankina O.V.[1]
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1 - Tomsk State University, Laboratory of Catalytic Research, Tomsk, Russia
2 - Institute of Catalysis SB RAS, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia

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1 - Catalysis Research Center, Department of Chemistry, Technische Universität München, Garching, Germany
2 - KAUST Catalysis Center, 4700 King Abdullah University of Science & Technology, Thuwal, 23955 6900 Kingdom of Saudi Arabia

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1 - Catalysis Research Center, Department of Chemistry, Technische Universität München, Garching, Germany
2 - KAUST Catalysis Center, 4700 King Abdullah University of Science & Technology, Thuwal, 23955 6900 Kingdom of Saudi Arabia

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Kazan national Research Technological University, Kazan, Russia

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1 - São Paulo University, Brazil
2 - Federal University of São Carlos, Brazil

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1 - Institute of Catalysis, Bulgarian Academy of Sciences, Acad. G. Bonchev str. bl. 11, Sofia 1113, Bulgaria
2 - Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Krakow, Poland

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Sergeeva T.Yu.[1,2], Sultanova E.D.[2], Mukhitova R.K.[2], Nizameev I.R.[2], Kadirov M.K.[2], Ziganshina A.Y.[2], Konovalov A.I.[2]

Application of Sodium Octacarboxylate Resorcinarenes in Synthesis of Silver Nanoparticles

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A Theoretical Study on the Effect of Active Centers of SiO_2 Surface on O_2 Interaction with Small Supported Silver Clusters

Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia

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Hydroprocessing of Heavy Crude Oil

Instituto Mexicano del Petróleo Eje Central Lázaro Cárdenas Norte, México

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2 - Haldor Topsøe A/S, Nymøllevej 55, 2800 Kgs. Lyngby, Denmark

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Institute of Petrochemical Processes, Azerbaijan National Academy of Sciences, Baku, Azerbaijan

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DFT Studies of Adsorbed N_2O and NH_3 on Pd(110)

Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

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Supporting Surfactant-hybridized $H_3PW_{12}O_{40}$ on TiO_2 to Obtain Highly Dispersed Entities for Acid Catalysis: the Undesired Coking Effect of Burning the Surfactant

Université catholique de Louvain, Institute of Condensed Matter and Nanosciences (IMCN/MOST), Belgium

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Tabakova T.[1], Papavasiliou J.[2], Ivanov I.[1], Idakiev V.[1], Avgouropoulos G.[2,3]

Effect of Dopant Nature on Low-Temperature WGS Activity of Cu-Mn Spinel Oxide Catalysts Prepared by Combustion Method

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D. Mendeleyev University of Chemical Technology of Russia, Moscow, Russia

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Kots P.A.[1], Sushkevich V.L.[1], Tyablikov O.A.[1], Ivanova I.I.[1,2]

Synthesis of Zr-BEC Zeolite Catalyst with Strong Lewis Acidity

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2 - A.V. Topchiev Institute of Petrochemical Synthesis, Russian Academy of Science, Moscow, Russia

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia

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Tver Technical University, Tver, Russia

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1 - Tver Technical University, Tver, Russia
2 - Tver State University, Tver, Russia

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CO Oxidation on the Bimetallic Pd-Au/HOPG Catalysts: in-situ XPS and MS Investigation
1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
2 - Research and Educational Center for Energy Efficient Catalysis, NSU, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia
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1 - Novosibirsk State University, Novosibirsk, Russia
2 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk Russia
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1 - Kazan National Research Technological University, department of synthetic rubber, Kazan, Russia
2 - Kazan National Research Technological University, department of General Chemical Engineering, Kazan, Russia

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1 - A.M. Butlerov Institute of Chemistry, KFU, Tatarstan Republic, Russia
2 - Association "Nizhnekamskneftekhim", Tatarstan Republic, Nizhnekamsk, Russia

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1 - Samara State Technical University, Samara, Russia
2 - Chemistry Department, M.V. Lomonosov Moscow State University, Moscow, Russia
3 - N.D. Zelinsky Institute of Organic Chemistry, RAS, Moscow, Russia

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Laboratoire de Chimie des Matériaux et Catalyse, Département de Chimie, Faculté des Sciences de Tunis. Campus Universitaire 1060 Tunis, Tunisie

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1 - Laboratoire de Chimie des Matériaux et Catalyse, Département de Chimie, Faculté des Sciences de Tunis. Campus Universitaire 1060 Tunis, Tunisie
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A GGA+U DFT Investigation of Silver Atom, Trimer and Tetramer Supported by a Nanosized Particle $Ce_{21}O_{42}$
1 - Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia
2 - Institucio Catalana de Recerca i Estudis Avancats (ICREA), Barcelona, Spain
3 - Departament de Quimica Fisica & IQTCUB, Universitat de Barcelona, Barcelona, Spain

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

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2 - Institute of Hydrocarbons Processing SB RAS, Omsk, Russia
3 - Institute of Physical Organic Chemistry NAS of Belarus, Minsk, Belarus

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1 - Kazan National Research Technological University, Kazan, Russia
2 - Kazan Federal University, Kazan, Russia

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1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
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1 - University of Bologna, Dip. Chimica Industriale "Toso Montanari", Vle Risorgimento 4, 40136, Bologna, Italy
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1 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
2 - Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia
3 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia

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1 - N.D. Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
2 - University of Torino, Department of IPM Chemistry and NIS Centre, Torino, Italy

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2 - Kazan Institute of Biochemistry and Biophysics, RAS, Kazan, Russia

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A.M. Prokhorov General Physics Institute RAS, Department of Technologies and Measurements on Atomic Scale, Moscow, Russia

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Omsk State Technical University, Omsk, Russia
3 - Institute of Hydrocarbons Processing, SB RAS, Omsk, Russia

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1 - Kocaeli University, Department of Chemical Engineering, Kocaeli, Turkey
2 - AYARGEM, Alternative Fuels R&D Center, Kocaeli University, Kocaeli, Turkey
3 - Turkish Petroleum Refineries Corporation, R&D Department, Izmit, Turkey

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1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
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Yelimanova G.G.[1], Smolin R.A.[2], Batyrshin N.N.[1], Kharlampidi Kh.E.[1]
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1 - Kazan National Research Technological University, Kazan Russia
2 - United Research and Development Center, Kazan, Russia

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Boronin A.I.[1,2], Slavinskaya E.M.[1,2], Gulyaev R.V.[1,2], Zaikovskii A.V.[3], Smovzh D.V.[3], Novopashin S.A.[3]
Plasma-arc Synthesis of PdCeSnC Composites for Preparation of Highly Active Pd/CeO$_2$-SnO$_2$ Catalysts for Low-Temperature CO Oxidation
1 - Novosibirsk State University, Novosibirsk, Russia
2 - Boreskov Institute of Catalysis, Novosibirsk, Russia
3 - Kutateladze Institute of Thermophysics, Novosibirsk, Russia

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Universidade Federal de São Carlos, Brazil

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ECAT Company, Perm, Russia

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1 - Laboratory of Industrial Chemistry, Process Centre, Abo Academi University Fin-2050 Turku/Abo, Finland
2 - The Department of General Chemical Technology and Catalysis, and Laboratory of Catalytic Technologies, St. Petersburg State Technological Institute (Technical University), Saint-Petersburg, Russia

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3 - Research and Educational Center for Energy Efficient Catalysis in Novosibirsk National Research University, Novosibirsk, Russia

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Inst. Ciencia de Materiales de Sevilla and Universidad de Sevilla, Seville, Spain

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2 - Grupo de Catálisis, Departamento de Química, Universidad del Cauca, Popayán Calle 5 No. 4-70, Colombia
3 - Servicios Técnicos de Investigación, Facultad de Ciencias, Universidad de Alicante, Alicante, España

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D.V. Sokolsky Institute of Organic Catalysis and Electrochemistry, Almaty, Kazakhstan

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Semenov Institute of Chemical Physics RAS, Moscow, Russia

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Institute for Problems of Chemical and Energetic Technologies SB RAS, Biysk, Altai krai, Russia

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2 - Institute of Technical Physics and Materials Science, Centre for Energy Research, Hungarian Academy of Sciences, Budapest, Hungary

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Federal University of Campina Grande, Academic Unit of Chemical Engineering, Campina Grande, PB, Brazil

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Membrane Zeolite MCM-22/γ-Alumina Applied to the Adsorption Capacity of the Gasoline

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Kazan National Research Technological University, Department of Catalysis 420015, Kazan, Russia

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Influence of Zink on the Formation and Properties of Catalysts Pt/Mg(Zn)AlO$_x$ Obtained from the Layered Hydroxides

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3 - Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia
4 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

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Textural Properties of Iron-Based Catalysts Supported on Mesoporous Silica SBA-15 Synthesized with Different Silica Source

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2 - Federal University of Ceará, Brazil

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Soybean Oil Transesterification Applying Iron-Based Catalysts Supported on Mesoporous Silica SBA-15

Federal University of Campina Grande, Campina Grande, Brazil

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Samara State Technical University, Samara, Russia

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1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
2 - Rzhanov Institute of Semiconductor Physics, Novosibirsk, Russia

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1 - A.V. Topchiev Institute of Petrochemical Synthesis, RAS, Moscow, Russia
2 - Gubkin Russian State University of Oil and Gas, Moscow, Russia
3 - Moscow State University, Dep. of Chemistry, Moscow, Russia

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Development of New Materials Laboratory-LABNOV, Federal University of Campina Grande, Department of Chemical Engineer, Av. Aprígio Veloso, 58109-970 Campina Grande, Brazil

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1 - Département de Chimie, Faculté des Sciences et Sciences Appliquées, Université Akli Mohand Oulhadj de bouira, Algeria
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1 - Bashkir State University, Department of chemistry, Ufa, Russia
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Dudkina Yu.B.[1], Gryaznova T.V.[1], Davydov N.A.[1], Mustafina A.R.[1], Vicic D.A.[2], Budnikova Yu.H.[1]
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1 - A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, RAS, Kazan, Russia
2 - Department of Chemistry, Lehigh University, 6 East Packer Avenue, Bethlehem, Pennsylvania18015, United States

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Lomonosov Moscow State University, Moscow, Russia

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Mechanism of Propane Oxidative Dehydrogenation on Surface Oxygen Radical Sites of VO_x/TiO_2 Catalysts
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2 - Novosibirsk Institute of Technology, Moscow State University of Design and Technology, Novosibirsk, Russia

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Middle East Technical University, Chemical Engineering Department, Ankara, Turkey

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1 - Lomonosov Moscow State University, Department of Chemistry, Moscow, Russia
2 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

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Catalytic Activity of Palladium Complexes Based on Tridentate Ligands with Ancillary Sulfur Donor Groups in the Suzuki Cross-Coupling
1 - A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russia
2 - N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia

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Djaidja A.[1,2], Messaoudi H.[1], Slyemi S.[1], Barama A.[1]
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Samara State Technical University, Samara, Russia

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Crucial Role of the Graphene Edges for CNT Formation during the Preparation of Metal/Carbon Catalysts
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Boytsova O.[1,2], Baranchikov A.[1], Ivanov V.[1]
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1 - Kurankov Institute of General and Inorganic Chemistry RAS, Moscow, Russia
2 - Lomonosov Moscow State University, Moscow, Russia

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DRIFTS Studies of Support Effects on CO Adsorption and CO + O_2 Reaction over $Ce_{1-x-y}M_xCu_yO_{2-d}$ (M = Zr, Hf, Th)
1 - Surface Engineering Division, CSIR-National Aerospace Laboratories, Bangalore, India
2 - Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India

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Department of Chemistry, University of Antioquia, Medellin, Colombia

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In Situ X-ray Absorption Spectroscopy and X-ray Powder Diffraction for Temperature- and Pressure-Dependent Hydride Phase Formation in Supported Pd nanocatalysts
1 - Southern Federal University, Rostov-on-Don, Russia
2 - Department of Chemistry, University of Torino, Italy
3 - ESRF, Grenoble, France
4 - ChimetSpA, Arezzo
5 - ETH Zurich, Switzerland
6 - PSI, Villigen, Switzerland

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Catalytic Performance of a Polyoxometalate/Reduced Graphene Oxide Composite in Degradation of Methylene Blue
1 - Necmettin Erbakan University A.K. Education Faculty, Department of Science Education, Konya, Turkey
2 - Selcuk University, Science Faculty, Department of Chemistry, Turkey
3 - Necmettin Erbakan University A.K. Education Faculty, Department of Chemistry Education, Konya, Turkey

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Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

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1 - Diamond Light Source Ltd, B18 beamline, Harwell Science and Innovation Campus, UK
2 - Diamond Light Source Ltd, Idustrial Liaison Group, Harwell Science and Innovation Campus, UK
3 - UK Catalysis Hub, RCaH, Harwell Science and Innovation Campus, OX11 0DE, Didcot, UK

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Department of Inorganic Chemistry, Fritz Haber Institute of the Max Plank Society, Berlin, Germany

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Panova Y.[1], Kashin A.[2], Vorobev M.[3], Ananikov V.[1,2]
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1 - Saint-Petersburg State University Institute of Chemistry, Petrodvorets, Russia
2 - N.D. Zelensky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia
3 - Saint-Petersburg State University, St.Petersburg, Russia

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1 - SABIC, Oxygenates & Aromatics Global Technology, Jubail 31961, Saudi Arabia
2 - Schuit Institute of Catalysis, Laboratory of Inorganic Materials Chemistry, Eindhoven University of Technology, Eindhoven, The Netherlands
3 - University of Cambridge, Department of Chemistry Lensfield Road, Cambridge, CB2 1EW

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Catalytic Performance in Isopropanol Decomposition over $H_{3+X}PMO_{12-X}V_XO_{40}$ Heteropolyacids Supported on Mesoporous Molecular Sieve HMS
1 - Laboratoire LCPMM, Département de Chimie, Faculté des Sciences, U.Blida, route de Soumaa BP Blida, Algeria
2 - Laboratoire de Chimie du Gaz Naturel, Faculté de Chimie, USTHB 109 El-Alia Bab Ezzouar, Alger-Algérie

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Inorganic Materials Chemistry group, Eindhoven University of Technology, Eindhoven, The Netherlands

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Department of Chemical Engineering, Istanbul University, Avcılar, Istanbul, Turkey

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk National Research State University, Novosibirsk, Russia

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Mechanistic Insights into CO Oxidation and Preferential CO Oxidation over Cobalt Oxide and Promoted Cobalt Oxide Catalysts
1 - Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria
2 - Department of Inorganic Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany

Section 3. Energy-Related Catalysis

III-PP01
Takahashi A., Fujitani T.
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Research Institute for Innovation in Sustainable Chemistry, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan

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Hybrid Membrane-catalytic Reactor for Synthesis Gas and Pure Hydrogen Co-production by Dry Reforming of Methane and Ethanol
1 - A.V. Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, Russia
2 - Institute of Structural Macrokinetics and Materials Science, Russian Academy of Sciences, Chernogolovka, Chernogolovka, Moscow Region, Russia

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Institut de Recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON), UMR 5256 CNRS & Université Claude Bernard - Lyon 1, 2 avenue Albert Einstein, 69626 Villeurbanne, France

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Syngas Production via Combined H_2O and CO_2 Reforming of Coke Oven Gas over La-promoted $Ni/MgAl_2O_4$ Catalyst
Yonsei University, Department of Environmental Engineering, 234 Maeji, Heungeop, Wonju, Gangwon-do, 2210-710 Republic of Korea

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Conesa J.C.
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Instituto de Catálisis y Petroleoquímica, CSIC, Madrid, Spain

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Striegler K.[1], Kasprick M.[1], Benndorf G.[2], Bertmer M.[2], Gläser R.[3]
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1 - Universtät Leipzig, Faculty of Chemistry and Mineralogy, Institute of Chemical Technology, Leipzig, Germany
2 - Universtät Leipzig, Faculty of Physics and Earth Science, Institute for Experimental Physics II, Leipzig, Germany
3 - Universtät Leipzig, Faculty of Chemistry and Mineralogy, Institute of Chemical Technology, Leipzig, Germany

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Institute of High-Temperature Electrochemistry of the Urals Branch of the Russian Academy of Sciences, Yekaterinburg, Russia

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Foil of the Pd-In-Ru alloy for the Membrane Technology of Preparing High-purity Hydrogen
1 - Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences, Moscow, Russia
2 - Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Russia

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Asalieva E.Yu.[1,2], Sineva L.V.[1,3], Gryaznov K.O.[1,4], Kulchakovskaya E.V.[1], Mordkovich V.Z.[1,3]
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1 - Technological Institute for Superhard and Novel Carbon Materials, Moscow, Russia
2 - Lomonosov Moscow State University, Moscow, Russia
3 - INFRA Technology Ltd, Moscow, Russia
4 - Lomonosov Moscow State University of Fine Chemical Technologies, Moscow, Russia

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Gold Catalysts on Y-modified Ceria for CO-free Hydrogen Production Via WGSR and PROX
1 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria
2 - Istituto per lo Studio di Materiali Nanostrutturati, CNR, I- 90146 Palermo, Italy
3 - Universidad Nacional Autónoma de México, P. 04510 México D.F., Mexico
4 - Department of Chemical Engineering, University of Patras, Patras, Greece
5 - Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

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São Paulo University, Brazil

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São Paulo University, Brazil

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São Paulo University, Brazil

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Department of Inorganic Chemistry, University of Alicante, Alicante, Spain

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1 - Pontificia Universidade Católica do Rio de Janeiro, Brazil
2 - Universidade Federal Fluminense, Brazil

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1 - Universidad de Guanajuato. División de Ciencias Naturales y Exactas. Noria alta S/N, Col. Noria Alta 36050. Guanajuato, Guanjuato. México
2 - Università degli Studi di Firenze. Dipartimento di Chimica e CSGI. Sesto Fiorentino, Firenze. Italia
3 - Universidad Autónoma Metropolitana. División de Ciencias Básicas e Ingeniería. Av. San Rafael Atlixco No. 186, Col. Vicentina 09340, Distrito Federal, México

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Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences, Moscow, Russia

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1 - Martin-Luther-University Halle-Wittenberg, Halle, Germany
2 - Ruhr-University Bochum, Bochum, Germany
3 - Leibniz-Institut für Katalyse e.V. an der Universität Rostock (LIKAT), Rostock, Germany

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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia

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A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center of Russian Academy of Sciences, Kazan, Russia

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National Institute of Advanced Industrial Science and Technology (AIST), Onogawa 16-1, Tsukuba-shi, Ibaraki 305-8569, Japan

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2 - Université Lille1, UMR 8181 CNRS, UCCS, Boulevard Langevin, 59650 Villeneuve d'Ascq, France

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1 - Russian Academy of Sciences, Metallurgy and Material Science Institute named after Baikov A.A., Moscow, Russia
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1 - Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany
2 - MPI for Chemical Energy Conversion, Mülheim-a.-d.-Ruhr, Germany

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1 - Samara State Technical University, Samara, Russia
2 - Chemistry Department, M.V. Lomonosov Moscow State University, Moscow, Russia

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University of Messina, Dep. of Electronic Engineering, Industrial Chemistry and Engineering, Italy

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1 - Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/BC/01, 1060 Vienna, Austria
2 - MAX IV Laboratory, Lund University, Ole Römersväg 1, SE-221 00 Lund, Sweden

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1 - Institute of Chemical and Engineering Sciences, ASTAR, Singapore
2 - Department of Materials Science and Engineering, National University of Singapore, Singapore

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A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia

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Instituto de Ciencia de Materiales de Sevilla.Centro Mixto CSIC-Universidad de Sevilla,Av. Américo Vespucio 49, 41092 Sevilla, Spain

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1 - Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia
2 - Faculty of Chemistry, Moscow State University, Moscow, Russia

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Department of Chemical Engineering, Boğaziçi University, Istanbul, Turkey

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1 - CSIR-NEERI, Nagpur, India
2 - Indian Institute of Science Bangalore, India

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United Research and Development Centre, Moscow, Russia

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3 - Instituto de Tecnología Química (Universidad Politécnica de Valencia - Consejo Superior de Investigaciones Científicas), Avenida de los Naranjos s/n.46022 Valencia, Spain

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Korovin E.Y.[1,2,3], Kozlov D.V.[1,2,3], Besov A.S.[1,2,3]

Photocatalytic Acetone Vapor Oxidation over TiO_2 under Controlled Periodic Illumination. Experimental and Modeling Study

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3 - Research and Educational Centre for Energoefficient Catalysis (NSU), Novosibirsk, Russia

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Pyrjaev P.A.[1], Simonov A.N.[2], Moroz B.L.[1,3], Zyuzin D.A.[1], Kuznetsov A.N.[1], Prosvirin I.P.[1], Bukhtiyarov V.I.[1,3]

Bimetallic Catalysts Containing Palladium and Gold on Carbon Support for Hydrogen Electrooxidation: From Au Particles Coated with Submonolayers of Pd to Pd-Au Nanoalloys

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3 - Novosibirsk State University, Novosibirsk, Russia

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3D Ordered Macroporous Ti-based Catalysts: Design, Synthesis and High Catalytic Activity for the Photoreduction of CO_2 with Water to Mechane

State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing, China

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Tsyganenko A.

Advances in Catalyst Characterization by FTIR spectroscopy

V.A. Fock Institute of Physics, St.Petersburg State University, St.Petersburg, Russia

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Keller V.[1], Pichot V.[2], Minetti Q.[1]

New Nanodiamonds/TiO_2 Composite Materials for the Solar Energy Conversion into Hydrogen by Water Splitting

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Szíjjártó G.P., Tálas E., Pászti Z., Mihályi J., Bálint S., Tompos A.,Boráth I.

Pt-SnO_x-TiO_2 Catalysts for Methanol Photocatalytic Reforming: Influence of Co-catalysts on the Hydrogen Production

Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Magyar Tudósok körútja 2, H-1117 Budapest, Hungary

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Striegler K.[1], Richter D.[1], Benndorf G.[2], Gläser R.[3]

New Approaches for Solar Fuel from Suspended Photocatalysts

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2 - Universtät Leipzig, Faculty of Physics and Earth Science, Institute for Experimental Physics II, Leipzig, Germany
3 - Universtät Leipzig, Faculty of Chemistry and Mineralogy, Institute of Chemical Technology, Leipzig, Germany

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Synthesis of Mesoporous SnO_2 as Anode for PEMFCs

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3 - S.C. STIMPEX S.A., Bucharest, Romania
4 - University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis, Bucharest, Romania
5 - National Institute of Materials Physics, Bucharest, Romania

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Ni-based Catalysts for Methane dry Reforming: EXAFS, TEM and DRIFT Investigation on the Au/Pt/Pd Effects

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2 - DUBBLE, European Synchrotron Radiation Facility (ESRF), B.P. 220, F-38043 Grenoble, France
3 - 3Netherlands Organization for Scientific Research (NWO) Grenoble CEDEX, France
4 - University of Namur (UNAMUR), 61 rue de Bruxelles, B-5000 Namur, Belgium
5 - CSIC, C/Marie Curie 2, Cantoblanco, 28049, Madrid, Spain

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Mansur A.J., Vallezi Paladino L.A.

Catalysts (NiMg)AlO_x + CeO_2 Derived of Hydrotalcite Type Structures Applied to Dry Reforming of Biogas

Federal University of São Carlos, Chemical Engineering Department, Brazil

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Mondal T.[1], Pant K.K.[1], Dalai A.K.[2]

Role of Rh as a Promoter on the Activity of Ni/CeO_2-ZrO_2 Catalyst for Oxidative Steam Reforming of Bio-ethanol

1 - Indian Institute of Technology Delhi, Department of Chemical Engineering, Hauz Khas, New Delhi, India
2 - University of Saskatchewan, Department of Chemical and Biochemical Engineering, Saskatoon, Canada

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Smal E.A.[1,2], Mezentseva N.V.[1,2], Sadykov V.A.[1,2], Krieger T.A.[1], Rogov V.A.[1,2], Simonov M.N.[1], Larina T.V.[1]

Ethanol Steam Reforming over $Mn_xCr_{3-x}O_4$-based Spinel-type Oxide

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Fedotov A.[1], Antonov D.[1], Tsodikov M.[1], Uvarov V.[2]

Syngas and Hydrogen Production by Dry and Steam Reforming of Methane and Fermentation Products on Porous Ceramic Membrane-Catalytic Ni-Co-containing Converters

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Karuppiah J., Mok Y.S.

Dry Reforming of Propane over CeO_2/Ni-foam Catalysts

Jeju National University, Department of Chemical Engineering, Jeju 690-756, South Korea

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Samoilov A.V.[1], Kirillov V.A.[1], Kuzin N.A.[1], Shigarov A.B.[1], Taleb A.[2], Markides C.N.[2]

A Catalytic Heater for an External Combustion Engine

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2 - Clean Energy Process Laboratory, Department of Chemical Engineering, Imperial College London, London, UK

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Braga A.H.[1], Batista J.B.O.[1], Damyanova S.[2], Bueno J.M.C.[1]
Ethanol Steam Reforming to Hydrogen over CoNi-based Catalysts
1 - Universidade Federal de São Carlos, Departamento de Engenharia Química, São Carlos, São Paulo, Brazil
2 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

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1 - Chemical Engineering Department, University of Malaga, Malaga, Spain
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1 - Laboratoire Catalyse et Spectrochimie, CNRS, EnsiCaen, University of Caen, Caen, France
2 - Institut de Recherches sur la Catalyse et l'Environnement de Lyon, Université Lyon 1, CNRS, Villeurbanne, France
3 - Unité de Catalyse et de Chimie du Solide, USTL-ENSCL-EC Lille, Villeneuve d'Ascq, France

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3 - Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

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2 - Department of Chemical Engineering, University of Patras, Patras, Greece

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2 - Novosibirsk State University, Novosibirsk, Russia
3 - Research and Educational Center for Energy Efficient Catalysis, Novosibirsk State University, Novosibirsk, Russia

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1 - Dipartimento di Ingegneria Industriale via Giovanni Gronchi 18, Università di L'Aquila. L'Aquila, Italy
2 - Institut de la Matière Condensée et des Nanoscience.Université Catolique de Louvain Croix du Sud 2 Louvain –la-Neuve B-1348 Belgique

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Tokyo University of Agriculture and Technology, Japan

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2 - ESICB, Kyoto University, Kyoto Daigaku Katsura, Saikyo, Kyoto, 615-8520, Japan
3 - JST PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan

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2 - Dipartimento di Chimica Industriale "Toso Montanari", Alma Mater Studiorum - Università di Bologna, Viale Risorgimento 4, 40136 Bologna, Italia

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2 - Lab. Catalysis & Spectrochemistry, ENSICAEN, Caen, France

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INCAPE; FIQ; UNL

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University of Brasilia, Brazilia, Brazil

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1 - Faculty of Chemical & Natural Resources Engineering, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Gambang, Pahang, Malaysia
2 - Center of Excellent For Advanced Research in Fluid Flow (CARIFF), Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Gambang, Kuantan, Pahang, Malaysia

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1 - Department of Chemical Engineering. University of the Basque Country (UPV/EHU), Bilbao, Spain
2 - NMR Service, SGIKER, University of the Basque Country (UPV/EHU), "Joxe Mari Korta" Center, Tolosa Hiribidea, 72, 20018. San Sebastian, Spain
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1 - Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark
2 - DONG Energy, Denmark

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1 - Ruhr University Bochum, Bochum, Germany
2 - Martin-Luther-Universität Halle, Germany
3 - Leibniz-Institut für Katalyse e.V. Rostock, Rostock, Germany
4 - tascon GmbH Münster, Germany
5 - ION-TOF GmbH Münster, Germany
6 - Huntsman Pigments Krefeld, Germany
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1 - Department of Chemical Engineering, University of Patras, Patras, Greece
2 - Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece
3 - Department of Chemistry, University of Patras, Patras, Greece

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2 - University of Barcelona (UB), Department of Electronics, Marti i Franquès 1, 08028, Barcelona, Spain

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1 - Department of Environmental and Chemical Engineering, University of Calabria, Rende (CS), Italy
2 - Department of Civil Engineering, Energy, Environment and Materials, Mediterranea University, Reggio Calabria, Italy
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1 - Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences; H-1117 Budapest, Magyar tudósok körútja 2, Hungary
2 - Instituto de Catálisis y Petroleoquímica, CSIC. C/Marie Curie 2, 28049, Madrid, Spain

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School of Science and Engineering, Teesside University, Borough Road, Middlesbrough, TS1 3BA, UK

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2 - Scania AB, Materials Technology, Engine Performance and Emissions, Södertälje, Sweden
3 - Institute for the Study of Nanostructured Materials, Palermo, Italy

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2 - Research and Educational Center for Energy Efficient Catalysis, Novosibirsk National Research University, Novosibirsk, Russia
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2 - Novosibirsk State University, Novosibirsk, Russia
3 - Institute of Powder Metallurgy, Minsk, Belarus
4 - Unversity of Strasbourg, Strasbourg, France

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1 - Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, México
2 - Instituto de Catálisis y Petroleoquímica, CSIC, c/Marie Curie 2, Cantoblanco, 28049 Madrid, Spain

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1 - NANOMAC – Chemical Engineering, Univ. of Queensland, Brisbane, QLD 4072, Australia
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2 - Novosibirsk State University, Novosibirsk, Russia
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1 - University of Genova, DICCA Dipartimento di Ingegneria Civile Chimica e Ambientale, Genova, Italy
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2 - Novosibirsk State University, Novosibirsk, Russia
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D.V. Sokolsky Institute of Organic Catalysis and Electrochemistry, Almaty, Kazakhstan

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2 - IBEROL- Sociedade Ibérica de Biocombustívei e Oleaginosas S.A., Quinta da Hortinha–Alhandra Vila Franca de Xira, 2601-908, Portugal

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Boğaziçi University, Department of Chemical Engineering, Istanbul, Turkey

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University of Salerno, Department of Industrial Engineering, Fisciano (SA), Italy

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Instituto de Ciencia de Materiales de Sevilla (IMCSE), Centro Mixto US/CSIC, Avda, Américo Vespucio 49, 41092 Sevilla, España

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Department of Chemical Engineering and Materials Science/Environmental Technology Research Center, Yuan Ze University, Chung-Li City, Tao-Yuan County, Taiwan

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Teesside University, School of Science and Engineering, Middlesbrough, Tees Valley, TS1 3BA, UK

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3 - IRCELYON, UMR5256 CNRS-Universitè Lyon 1, 2 Avenue Albert Einstein, 69626 Villeurbanne cedex, France

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2 - INFRA Technology Ltd., Moscow, Russia
3 - Department of Chemical Technology and New Materials, Moscow State University, Moscow, Russia

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2 - Dip.to di Ingegneria Civile, Chimica e Ambientale, Università di Genova, Genova, Italy

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1 - Korea Institute of Energy Research, Clean Fuel Laboratory, 152 Gajeong-Ro, Yuseong-Gu, Daejeon 305-343, Republic of Korea
2 - University of Science and Technology, Department of Advanced Energy Technology, 217 Gajeong-Ro, Yuseong-Gu, Daejeon 305-350, Republic of Korea
3 - Chungnam National University, Graduate School of Energy Science and Technology, 99 Daehak-Ro, Yuseong-Gu, Daejeon 306-764, Republic of Korea

Section 4. Catalysis and Chemicals

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Azerbaijan State Oil Academy, Baku, Azerbaijan Republic

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Chemical Engineering Department, College of Engineering King Saud University P.O. Box 800, Riyadh 11421, Kingdom of Saudi Arabia

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1 - King Abdulaziz City for Science and Technology 1, National Center for Petrochemical Technology, P.O.Box 6086, Riyadh 11442, Kingdom of Saudi Arabia
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1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia

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Bivona L.A.[1,2], Quertinmont F.[1], Beejapur H.A.[2], Giacalone F.[2], Buaki-Sogo M.[1], Gruttadauria M.[2], Aprile C.[1]
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1 - Unit of Nanomaterial Chemistry (CNano), University of Namur (UNAMUR), Department of Chemistry, Rue de Bruxelles 61, 5000 Namur, Belgium
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Universidad de Antioquia, Medelín, Colombia

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1 - Lomonosov Moscow State University of Fine Chemical Technologies, Moscow, Russia
2 - A.V. Topchiev Institute of Petrochemical Synthesis, RAS, Moscow, Russia
3 - Institute for Physical-Chemical Medicine, Moscow, Russia

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1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
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1 - Irkutsk State Technical University, Irkutsk, Russia
2 - A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, Irkutsk, Russia

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1 - Instituto Nacional de Catalisis y Petroquimica, INCAPE, Sgo. del Estero 2654, Santa Fe, Argentina
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1 - Bashkir State University, Department of chemistry, Ufa, Russia
2 - Institute of Chemistry of RAS, Ufa, Russia

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Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia

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The First Example of Catalytic Tandem Interaction N-allyl-N-arylamines with Diazocompounds: Aza-Claisen Rearrangement – Carbenation

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2 - Bashkir State University, the Faculty of Chemistry, Ufa, Russia
3 - Zelinsky Institute of Organic Chemistry, RAS, Moscow, Russia
4 - Ufa State Aviation Technical University, Ufa, Russia

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2 - Clean Energy & Chemical Engineering, UST, Daejeon, Korea

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Indian Institute of Technology Delhi, New Delhi, India

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Budnikova Y.H.

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A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan ScientificCenter, RAS, Kazan, Russia

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Institute of Structural Macrokinetics and Materials Science Russian Academy of Sciences, Chernogolovka, Russia

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Kazan National Research Technological University, Institute of Polymers, Kazan, Russia

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Riga Technical University, Institute of Applied Chemistry, Riga, Latvia

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University of Bucharest, Faculty of Chemistry, Buchasert, Romania

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University of Bucharest, Faculty of Chemistry, Buchasert, Romania

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1 - Kazan National Research Technological University, Kazan, Russia
2 - Alexander Butlerov Institute of Chemistry, Kazan (Volga Region) Federal University, Kazan, Russia
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1 - State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, P. R. China
2 - School of Chemical and Biomedical Engineering, Nanyang Technological University Singapore, Singapore

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1 - Novosibirsk State University, Novosibirsk, Russia
2 - Boreskov Institute of Catalysis, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia

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1 - Tomsk Polytechnic University, Tomsk, Russia
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1 - Institute of Petrochemical Processes named after Academician Y.H.Mamedaliyev, Baku, Azerbaijan
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Hamdy Saad Mohamed[1,2], Berg O.[3], Mul J.[2]
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2 - Chemistry Department, Science College, King Khalid University, Abha, Saudi Arabia
3 - Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands

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2 - Novosibirsk State Technical University, Novosibirsk, Russia
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2 - Alexander Butlerov Institute of Chemistry, Kazan (Volga Region) Federal University, Kazan, Russia
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1 - Industrial Catalysis and Adsorption Technology, Ghent University, Department of Industrial Technology and Construction, Valentin Vaerwyckweg 1 9000 Ghent, Belgium
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1 - Leibniz Institute for Catalysis, Rostock, Germany
2 - National Chemical Laboratory, Pune, India
3 - Mojj Eng. Syst. Ltd, Pune, India

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1 - Catalysis Laboratory, Indian Institute of Chemical Technology, Hyderabad, India
2 - Leibniz-Institut für Katalyse an der Universität Rostock e.V., Rostock, Germany

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1 - Selcuk University, Science Faculty, Department of Chemistry, Konya, Turkey
2 - Necmettin Erbakan University, Deparment of Science Education, Faculty of Education, Konya, Turkey

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2 - Tomsk Polytechnic University, Tomsk, Russia
3 - Universidad Autónoma de Baja California, Ensenada, México
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1 - Universidade Federal de Minas Gerais, Belo Horizonte 31270-901, Brazil
2 - University of Liverpool, Liverpool, UK

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Kuznetsov V.L.[1,2,3], Krasnikov D.V.[1,2], Kazakova M.A.[1,2], Moseenkov S.I.[1], Smirnova T.E.[3], Suslyaev V.I.[3], Dorofeev I.O.[3]
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2 - Novosibirsk State University, Novosibirsk, Russia
3 - National Tomsk State University, Tomsk, Russia

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1 - Moscow State University, Chemical Department, Moscow, Russia
2 - Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russia

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1 - Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia
2 - Institute of Petroleum Chemistry SB RAS, Tomsk, Russia

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1 - Bilkent University, Department of Chemistry, Ankara, Turkey
2 - Baylor University, Department of Chemistry & Biochemistry, Waco, TX, 76798, USA

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1 - University of Lille UCCS, France
2 - Arkéma Groupement de recherches de Lacq, France

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1 - Department of Chemical Engineering, Aristotle University of Thessaloniki, University campus, Thessaloniki, Greece
2 - Chemical Process & Energy Resources Institute, CERTH, Thessaloniki, Greece

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Department of Chemical Engineering and Materials Science/Environmental Technology Research Center, Yuan Ze University, Taiwan

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University of Bologna, dep. of Industrial Chemistry, Bologna, Italy

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1 - Instituto de Investigaciones en Catálisis y Petroquímica, INCAPE, Colectora Ruta Nac. Nº 168 Km. 0 – Paraje El Pozo, Santa Fe (3000), Argentina
2 - Facultad de Ciencias, Universidad de Alicante, Apartado 99, E-03080 Alicante, Spain

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1 - Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Chernogolovka, Moscow Region, Russia
2 - Faculty of fundamental physical and chemical engineering, Moscow State University, Moscow, Russia

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Mäki-Arvela P.[1], Torozova A.[1], Stekrova M.[1], Kumar N.[1], Aho A.[1], Heinmaa I.[2], Volcho K.P.[3], Salakhutdinov N.F.[3], Murzin D.Yu.[1]
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1 - Process Chemistry Centre, Åbo Akademi University, Turku/Åbo, Finland
2 - Institute of Chemical Physics and Biophysics, Tallinn, Estonia
3 - N.N. Vorozhtsov Institute of Organic Chemistry, RAS, Novosibirsk, Russia

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Mari M.[1], Cavani F.[1], Kuenzle N.[2], Hanselmann P.[2], Janssen M.[2]
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1 - Università di Bologna, dipartimento di Chimica Industriale Toso Montanari, Bologna, Italy
2 - Lonza Ltd, Visp, Switzerland

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Mashkovsky I.S.[1], Markov P.V.[1], Bragina G.O.[1], Baeva G.N.[1], Tkachenko O.P.[1], Kozitsyna N.Yu.[2], Vargaftik M.N.[2], Stakheev A.Yu.[1]
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1 - Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
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Tver Technical University, Tver, Russia

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Melián Rodríguez M.[1,2], Saravanamurugan S.[1,2], Kegnæs S.[1,2], Riisager A.[1,2]
Catalytic Oxidation of Veratryl Alcohol – a β-O-4 Lignin Model Compound - to Veratraldehyde
1 - Technical University of Denmark, Kgs. Lyngby, Denmark
2 - Centre for Catalysis and Sustainable Chemistry, Kgs. Lyngby, Denmark

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Zhu Y.[1], Li X.[2], Adrian K.T.[2], Ding J.[2], Xue J.M.[2]
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1 - Institute of Chemical and Engineering Sciences, Jurong Island, Singapore
2 - Department of Materials Sciences & Engineering, National University of Singapore, Singapore

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Mishanin I.I.[1], Lunin V.V.[1,2], Bogdan V.I.[1,2]
Oxidative Dehydrogenation of Ethane on MoVTeNbO Catalysts
1 - Lomonosov Moscow State University, Moscow, Russia
2 - Zelinsky Institute of Organic Chemistry, Moscow, Russia

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Modvig A.E.[1,2], Fristrup P.[1], Riisager A.[1,2]
Oxidative Catalytic Upgrading of Biomass-derived Glycolaldehyde to Glycolics
1 - Technical University of Denmark, Kgs. Lyngby, Denmark
2 - Centre for Catalysis and Sustainable Chemistry, Kgs. Lyngby, Denmark

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Kazan National Research Technological University, Department of General Chemical Technology, Kazan, Russia

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University of Limerick, Limerick, Ireland
Materials and Surface Science Institute, University of Limerick, Limerick, Ireland
Carbolea Research Group, University of Limerick, Limerick, Ireland

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Selective Hydrogenation of 2-methyl-3-butyne-2-ol Catalyzed by Embedded Polymer-protected PdZn Nanoparticles
1 - Boreskov Institute of Catalysis, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia

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University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis, Bd. Regina Elisabeta 4-12, Bucharest 030016, Romania

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University of Oviedo, Oviedo, Spain

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Ivanovo State University of Chemistry and Technology, Research Institute for Thermodynamics and Kinetics of Chemical Processes, Dep. of Physical and Colloid Chemistry, Ivanovo, Russia

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1 - D.V. Sokolsky Institute of Organic Catalysis and Electrochemistry, Almaty, Kazakhstan
2 - Research Institute of New Chemical Technologies and Materials, Almaty, Kazakhstan

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Peneau V.[1], He Q.[2], Shaw G.[1], Kiely Ch. J.[2], Hutchings Gr. J.[1], Nowicka E.[1]
Selective Oxidation of Toluene Using Noble Metals under Mild Condition
1 - Cardiff Catalysis Institute, School of Chemistry, Cardiff, UK
2 - Department of Material Science and Engineering, Lehigh University, Lehigh, PA, US

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Peng B., Ember E.E., Lercher J.A.
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Lehrstuhl II für Technische Chemie and Catalysis Research Center, Department of Chemistry, Technische Universität München, Garching, Germany

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Abba M.O., Pereñiguez R., Caballero A.

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Instituto de Ciencia de Materiales de Sevilla and Dpto. Química Inorgánica (CSIC-Universidad de Sevilla). Av. Américo Vespucio, 49, 41092 Seville, Spain

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1 - Kazan National Research Technological University, Kazan, Russia
2 - A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan, Russia

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Phung T.K., Garbarino G., Busca G.

Ethanol Conversion to Useful Products: Ethylene, Diethyl Ether, Higher Hydrocarbons, Acetaldehyde and Acetone

University of Genova, Department of Civil, Chemical and Environmental Engineering, Genova, Italy

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Podolean I., Coman S.M., Parvulescu V.I.

Synthesis of Platform Molecules from Cellulose over Bifunctional Magnetic Nanocatalysts

University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis, Bdul. Regina Elisabeta, 4-12, Bucharest, Romania

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Rajkhowa T., Thybaut J.W., Marin G.B.

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Laboratory for Chemical Technology, Ghent University, Technologiepark 914, B-9052 Gent, Belgium

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Tver Technical University, Tver, Russia

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Catalytic Transformation of Glycerol to Lactic Acid over Au-Pt Supported Catalysts Prepared by Redox-method

1 - N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia
2 - Lomonosov Moscow State University of Fine Chemical Technologies, Moscow, Russia
3 - Chemistry Department of Moscow State University, Moscow, Russia

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Rodikova Y.A., Zhizhina E.G., Pai Z.P.

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Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

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Rodygin K.S.[1], Ananikov V.P.[2]

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2 - N.D. Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences. Moscow, Russia

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1 - Tver Technical University, Tver, Russia
2 - Åbo Akademi University, Åbo, Finland

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Irkutsk State University, institution, Chemistry Department, Irkutsk, Russia

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1 - St. Petersburg State Technological Institute (Technical University), Laboratory of Catalytic Technologies, St.Petersburg, Russia
2 - St. Petersburg State Technological Institute (Technical University), Resource-Saving Department, Moskovsky St.Petersburg, Russia
3 - St. Petersburg State Technological Institute (Technical University),General Chemical Technology and Catalist Department, St.Petersburg, Russia

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1 - Peoples Friendship University of Russia, Faculty of Science, Physical and Colloidal Chemistry Department, Moscow, Russia
2 - Saint-Petersburg State University, Petrodvorets, Saint-Petersburg, Russia

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2 - Moscow State University, Dep. of Chemistry, Moscow, Russia
3 – LECO, Russia

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In Situ Synthesis of Unsupported Transition Metal Sulfide Catalysts for Hydrodearomatization Processes
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2 - Moscow State University, Dep. of Chemistry, Moscow, Russia

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2 - Novosibirsk State University, Novosibirsk, Russia
3 - Universitat Rovira i Vigili Marcel lí Domingo s/n, 43007 Tarragona, Spain

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1 - Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Km. 107 Carretera Tijuana a Ensenada, C.P. 22860, Ensenada, Baja California, México
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3 - Materials & Surface Science Institute, University of Limerick, Limerick, Ireland
4 - Laboratory of Industrial Chemistry and Reaction Engineering, Process Chemistry Centre, ÅboAcademi University, FI-20500 Åbo/Turku, Finland

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Tshwane University of Technology, Department of Chemical, Metallurgical and Materials Engineering, Private Bag X680, Pretoria 001, Republic of South Africa

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2 - Novosibirsk State University, Novosibirsk, Russia

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Effect of Technological Parameters on the Process of Epichlorohydrin Synthesis
1 - Moscow State University of Fine Chemical Technologies, Moscow, Russia
2 - Nizhni Novgorod State Technical University, Nizhni Novgorod, Russia
3 - R&D Engineering Centre "Syntez", Moscow, Russia

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Tver Technical University, Tver, Russia

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Lomonosov Moscow State University, Moscow, Russia

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Tashkent Chemical Technological Institute, Tashkent, Uzbekistan

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1 - Cardiff University, Cardiff, United Kindom
2 - Aston University, Birmingham, United Kindom

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Paul S.[1,2], Heyte S.[1,3], Thuriot Roukos J.[1], Araque Marin M.[1,2], Dumeignil F.[1,3,4]
REALCAT: A New High-throughput Platform Dedicated to the R&D in Catalysis for Biorefineries
1 - Unité de Catalyse et de Chimie du Solide, UCCS, UMR CNRS 8181, Villeneuve d'Ascq, 59655, France
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3 - Université de Lille, Villeneuve d'Ascq, 59655, France
4 - Institut Universitaire de France, IUF, Maison des Universités, 103 Bd. St Michel, Paris, 75005, France

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Insights on the Mechanism for the Transformation of Ethanol on Basic Oxides (Lebedev and Guerbet Reactions)
1 - Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Bologna, Italy
2 - Dipartimento di Scienze ed Alta Tecnologia, Università degli Studi dell'Insubria, Como, Italy

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Yaroslavl State Technical University, Chemical Engineering Department, Yaroslavl, Russia

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1 - Institute of Petroleum Chemistry, Siberian Branch of the Russian Academy of Sciences, Tomsk, Russia
2 - Institute of Catalysis, SB RAS, Novosibirsk, Russia

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Beijing Key Laboratory of Green Reaction Engineering and Technology, Department of Chemical Engineering, Tsinghua University, Beijing, China

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Dossumov K.[1], Yergaziyeva G.Y.[2], Myltykbayeva L.K.[2], Mironenko A.V.[2]
Modified Nickel Catalysts for Oxidation of Methane
1 - Centre of Physic-Chemical analysis and investigation methods, Almaty, Kazakhstan
2 - The Institute of Combustion Problems, Almaty, Kazakhstan

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Suyunbayev U., Yergaziyeva G., Zhumagazin A.
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Institute of Combustion Problems, Almaty, Kazakhstan

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Kanagawa University, Yokohama, Japan

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Moscow State Academy of Fine Chemical Technology (MITHT), Moscow, Russia

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Alkayeva Y.[1], Shutilov A.[2,3,4], Zenkovets G.[2,3]
Microwave Assisted Heterogeneous Vapor-Phase Oxidation of 3-picoline to Nicotinic Acid over Vanadium–titanium Oxide Catalytic System
1 - Fordham University, New York, United States
2 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
3 - Novosibirsk State University, Novosibirsk, Russia
4 - Novosibirsk State Technical University, Novosibirsk, Russia

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Instituto de Catálisis y Petroquímica, UNL-CONICET, Sgo del Estero 2654, Sta Fe (3000), Argentina

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Study of the Reaction Network of Fischer-Tropsch Synthesis by Multicomponent Steady-State Isotopic Transient Kinetic Analysis
1 - Norwegian University of Science and Technology, Trondheim, Norway
2 - SINTEF Materials and Chemistry

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Lee K.A.[1], Moon D.J.[2], Park N.C.[3], Kim Y. Ch.[3]
The Characteristics of Phosphoric Acid Modified Niobia Catalysts in the Gas Phase Glycerol Dehydration
1 - Department of Chemicals Engineering, Chonnam National University, 77 Youngbong-ro, Buk-gu Gwangiu 500-757, Republic of Korea
2 - Korea Institute Science and Technology, Hwarangno 14-gil 5, Seongbuk-gu Seoul 136-791, Republic of Korea
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Kim N.Y.[1,2], Jung J.-S.[1,3], Park J.I.[1], Ramesh S.[1], Kim S.W.[1,3], Ahn B.S.[1,3], Lee K.Y.[2], Moon D. J.[1,3]
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1 - Clean Energy Research Center, KIST, Seoul, Korea
2 - Department of Biological & Chemical Engineering, Korea University, Seoul, Korea
3 - Clean Energy & Chemical Engineering, UST, Daejeon, Kore

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Sub G.G.[1], Moon D.J.[2], Park N.C.[3], Kim Y.C.[3]
Kinetics for Hydrogen Production from Glycerol Steam Reforming Reaction Using Ni-Fe-Ce/Al_2O_3
1 - Department of Chemicals Engineering, Chonnam National University, 77 Youngbong-ro, Buk-gu Gwangiu 500-757, Republic of Korea
2 - Korea Institute Science and Technology, Hwarangno 14-gil 5, Seongbuk-gu Seoul 136-791, Republic of Korea
3 - Faculty of Applied Chemical Engineering and the Research Institute For Catalysis, Chonnam National University, 77 Youngbong-ro, Buk-gu Gwangju 500-757, Republic of Korea

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Heterogeneous Lipase-Active Biocatalysts for Oil Triglycerides' Hydrolysis and Interesterification
Boreskov Institute of Catalysis, Novosibirsk, Russia

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Highly Selective Catalysts for Synthesis of Alkylaromatic Hydroperoxides and Prospects of Their Industrial Application
1 - Tomsk State University, Tomsk, Russia,
2 - Yaroslavl State Technical University, Yaroslavl, Russia,
3 - Kazan State Technological University, Kazan, Russia

Section 5. Catalysis and Environmental Protection

V-PP01
Lopatin S.A.[1,2], Zazhigalov S.V.[1,2], Mikenin P.E.[1,2], Pisarev D.A.[1,2], Baranov D.V.[1,2,3], Zagoruiko A.N.[1,2,4]
Structured Cartridges with Glass-fiber Catalysts: New Trend in the Design of Catalytic Reactors for Pollution Control
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Research and Educational Center for Energy Efficient Catalysis, Novosibirsk State University, Novosibirsk, Russia
3 - Novosibirsk Technical State University, Novosibirsk, Russia
4 - Tomsk Polytechnic University, Tomsk, Russia

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Gasparyan M.D., Liberman E.Y.U., Grunsky V.N., Obukhov E.
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Russian Mendeleev University of Chemical Technology, Moscow, Russia

V-PP03
Jin B.F., Wei Y.C., Zhao Z., Liu J., Duan A.J.
The Synthesis Charcterization and Catalytic Performances of Three-dimensionally Ordered Macroporous x-CeO_2/Al_2O_3 Catalysts for Diesel Soot Combustion
State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Chang Ping, Beijing, China

V-PP04
Paul J.-F., Berrier E., Blanck D.
Are Perovskite Materials Efficient for Tree Way Catalysis? A Theoretical Study of $LaFeO_3$
Unité de Catalyse et de Chimie du Solide, Villeneuve d'Ascq, France

V-PP06
Wagloehner S., Nitzer-Noski M., Kureti S.
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Technical University of Freiberg, Institute of Energy Process Engineering and Chemical Engineering, Chair of Reaction Engineering, Freiberg, Germany

V-PP07
Trunfio G.[1], Di Chio R.[1], Rahim S.H.A.[1], Espro C.[1], Milone C.[1], Galvagno S.[1], Spadaro L.[2], Arena F.[1,2]
Development of MnO_x-based Catalysts for the Catalytic Wet Air Oxidation (CWAO) of Organic Pollutants
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V-PP08
Chlala D.[1], Giraudon J.-M.[1], Nuns N.[2], Labaki M.[3], Lamonier J.-F.[1]
Attractive Route for New Hydroxyapatite Supported Calcium-manganese Oxides for Total Oxidation of Toluene
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2 - IMMCL Chevreul, Institut des Molécules et de la Matière Condensée, Lille, France
3 - Lebanese University, Laboratory of Physical Chemistry of Materials (LCPM)/PR2N, Faculty of Sciences, Fanar, BP 90656 Jdeidet El Metn, Lebanon

V-PP09
Nikbin N.[1], Austin N.[2], Christiansen M.[1], Vlachos D.G.[1], Stamatakis M.[3], Mpourmpakis G.[2]
Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters
1 - University of Delaware, Department of Chemical Engineering, Newark, Delaware, USA
2 - University of Pittsburgh, Department of Chemical Engineering, Pittsburgh, Pennsylvania, USA
3 - University College London, Department of Chemical Engineering, Torrington Pl., London WC1E 7JE, UK

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Tabakova T.[1], Kolentsova E.[2], Dimitrov D.[2], Petrova P.[1], Karakirova Y.[1], Avdeev G.[3], Nihtianova D.[4], Ivanov K.[2]

Effect of Au and Ag on the Performance in CO and VOCs Oxidation of Alumina Supported Cu-Mn Catalysts

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2 - Department of Chemistry, Agricultural University, Plovdiv, Bulgaria
3 - Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria
4 - Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, Sofia, Bulgaria

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Dubkov A.A.[1,2], Carberry B.[2], Schneider M.[2], Linzen F.[2], Smirnov M.Yu.[1], Kalinkin A.V.[1], Salanov A.N.[1], Shmakov A.N.[1], Gerasimov E.Yu.[1], Bukhtiyarov V.I.[1,3]

Change in the Chemical Composition of an LNT as a Result of its Ageing in Diesel Exhaust Gases: Physical and Chemical Analysis

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2 - Ford Forschungszentrum Aachen GmbH, Aachen, Germany
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V-PP12

Ismagilov Z.[1,2], Parmon V.[1], Yarullin R.[3], Mazgarov A.[4], Khairulin S.[1], Kerzhentsev M.[1], Golovanov A.[5], Vildanov A.[4], Garifullin R.[5]

The Process of H_2S Selective Catalytic Oxidation for On-site Purification of Hydrocarbon Gaseous Feedstock. Technology Demonstration at Bavly Oil Field in Republic of Tatarstan

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2 - Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia
3 - OJSC "Tatneftekhiminvestholding", Kazan, Russian Federation
4 - OJSC "Volga research institute of hydrocarbon feed"35-A N. Ershov Str., 420045 Kazan, Russia
5 - OJSC "Tatneft", Al`metyevsk, Russia

V-PP13

Agafonov A.A.[1,2], Lokteva E.S.[1,2], Maslakov K.I.[1,2], Strokova N.E.[1], Voronova L.V.[1]

Pd Catalysts Supported on Metal Organic Coordinated Structures in Chlorobenzene Hydrodechlorination and CO Oxidation

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2 - Institute of Hydrocarbons Processing of the Siberian Branch of the RAS, Omsk, Russia

V-PP14

Taherimehr M.[1], Cardoso Costa Sertã J.P.[1], Kleij A.W.[2,3], Whiteoak C.J.[2], Pescarmona P.P.[1,4]

A New, Active Iron-complex Catalyst for Converting CO_2 into Cyclic Carbonates and Cross-linked Polycarbonates with Enhanced Properties

1 - COK, University of Leuven, Belgium
2 - ICIQ, Tarragona, Spain
3 - ICREA, Barcelona, Spain
4 - Chemical Engineering Department, University of Groningen, The Netherlands

V-PP15

Mironenko A., Kazieva A., Mansurov Z., Kudyarova Z.

Design of Catalysts of Carbon Dioxide Conversion of Methane

The Institute of Combustion Problems, Almaty, Kazakhstan

V-PP16

Gabrovska M.[1], Shopska M.[1], Edreva-Kardjieva R.[1], Nikolova D.[1], Bilyarska L.[1], Crişan D.[2]

Modified Ni-Al Layered Double Hydroxides as Catalyst Precursors for Utilization of Carbon Dioxide

1 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria
2 - "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania

V-PP17
Xie S., Wang Y., Zhang Q., Wang Y.
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State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

V-PP18
Eropak B.M.[1], Aksoylu A.E.[1], Çağlayan B.S.[2]
Design and Development of Efficient AC-based Adsorbents for CO_2 Removal
1 - Boğaziçi University, Department of Chemical Engineering, Istanbul, Turkey
2 - Advanced Technologies R&D Center, Boğaziçi University, Istanbul, Turkey

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Hacioglu M., Gürkaynak Altınçekiç T., Özdemir H., Öksüzömer M.A.F.
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Department of Chemical Engineering, Istanbul University, Avcılar, Istanbul, Turkey

V-PP20
Fukuhara C.[1], Hayakawa K.[1], Murabayashi K.[2], Khono Y.[1], Watanabe R.[1]
A Honeycomb-Type Ni/CeO_2 Catalyst for CO_2 Methanation to Transform Greenhouse Gas into Useful Resources
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V-PP21
Hillen L., Degirmenci V.
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CenTACat, Department of Chemistry and Chemical Engineering, Queen's University, Belfast, BT9 5AG, Northern Ireland

V-PP22
Marakushev S.A., Belonogova O.V.
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Institute of Problem of Chemical Physics, RAS, Chernogolovka, Moscow Region, Russia

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Calisan A., Uner D.
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Chemical Engineering Department, Middle East Technical University, Ankara, Turkey

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Gaynanova G.A., Yackevich E.I., Lukashenko S.S., Mirgorodskaya A.B., Zakharova L.Ya.
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A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, Russian Academy of Sciences, Kazan, Russia

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Gaynanova G.A.[1], Vagapova G.I.[1], Valeeva F.G.[1], Galkina I.V.[2], Zakharova L.Ya.[1], Sinyashin O.G.[1]
Supramolecular Catalytic System Based on Amphiphilic Triphenylphosphonium Bromide for the Hydrolysis of Phosphorus Acid Esters
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V-PP26
Dossumov K.[1], Yergazieva G.Y.[2], Telbayeva M.M.[2], Tayrabekova S.[3], Kalihanov K.[3], Suyunbayev U.[2]
Modified by Lanthanum Cerium - containing Catalysts for Converting Bio-Ethanol into Ethylene
1 - Centre of Physic Chemical methods of investigation and analysis, Almaty, Kazakhstan
2 - The Institute of Combustion Problems, Almaty, Kazakhstan
3 - Kazakh National University named Al-Farabi, Almaty, Kazakhstan

V-PP27
Demirel S.E., Aksoylu A.E.
An In-situ FTIR-DRIFTS Study on Carbon Dioxide Reforming of Methane on Pt-Ni/Al_2O_3
Department of Chemical Engineering, Bogazici University, Istanbul, Turkey

V-PP28
Erşahin S.[1], Çağlayan B.S.[1,2], Aksoylu A. E.[1]
An Experimental Study on Characterization and Mixed Reforming Performance of Co-Based Bimetallic Catalysts
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2 - Advanced Technologies R&D Center, Boğaziçi University, Bebek, Istanbul, Turkey

V-PP29
Yashnik S.A.[1], Taran O.P.[1,2], Ismagilov Z.R.[1,3], Parmon V.N.[1,4]
DR UV-Vis Study of Copper(II) Oxo/Peroxocomplexes in Cu-substituted ZSM-5
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State Technical University, Novosibirsk, Russia
3 - Institute of Coal Chemistry and Material Science, Kemerovo, Russia
4 - Novosibirsk State University, Novosibirsk, Russia

V-PP30
Mikenin P.E.[1,2], Lopatin S.A.[1,2], Zazhigalov S.V.[1,2], Pisarev D.A.[1,2], Baranov D.V.[1,2,3], Zagoruiko A.N.[1,2,4]
Structured Glass-fiber Catalysts for Selective Oxidation of H_2S
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3 - Novosibirsk Technical State University, Novosibirsk, Russia
4 - Tomsk Polytechnic University, Tomsk, Russia

V-PP31
Kolobov N.S.[1,2,3], Selishchev D.S.[1,2,3], Kozlov D.V.[1,2,3]
Photocatalytic Oxidation of CO over TiO_2 Modified by Noble Metals
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2 - Novosibirsk State University, Novosibirsk, Russia
3 - Research and Educational Centre for Energoefficient Catalysis (NSU), Novosibirsk, Russia

V-PP32
Carberry B.[1], Schneider M.[1], Ukropec R.[1], Boerensen C.[1], Dubkov A.A.[2,1]
Characterization of the Automotive Exhaust Gas Aftertreatment Catalysts with Flow Chemisorption Methods
1 - Ford Forschungszentrum Aachen GmbH, Aachen, Germany
2 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk Russia

V-PP33
Sokolov S.[1], Bychkov V.Yu.[2], Rodemerck U.[1], Stoyanova M.[1], Linke D.[1], Kondratenko E.V.[1]
Kinetic and Mechanistic Studies of Dehydrogenation of Propane and Isobutane Assisted by High-Throughput Tools
1 - Leibniz Institute for Catalysis, Albert-Einstein-Str. 29A D-18059 Rostock, Germany
2 - Semenov Institute of Chemical Physics, Moscow, Russia

V-PP35
Gil'mundinov Sh.A., Sassykova L.R., Massenova A.T., Bunin V.N., Rakhmetova K.S.
Catalytic Neutralization of Toxic Emissions of Furnaces of Oil Heating
D.V. Sokolskii Institute of Organic Catalysis and Electrochemistry, Laboratory of Catalytic Synthesis, Almaty, Kazakhstan

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Study of the Interaction of Chloroform and Hydrogen with the Metallic Species in Precious Metals Supported Catalysts for the Hydrodechlorination of Chloroform
Departamento de Química-Física Aplicada, Sección de Ingeniería Química, Universidad Autónoma de Madrid, C/Francisco Tomás y Valiente nº5, Campus de Cantoblanco, 28049 Madrid, Spain

V-PP37
Orge C.A., Pereira M.F.R., Faria J.L.
Mineralization of Aniline and Reactive Dye Blue 5 Solutions by Photocatalytic Ozonation
LSRE-LCM, Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

V-PP38
Rejeb R.[1], Kalfallah B.L.[1], Delahay G.[2]
Mixed MoTi-pillared Clay as a Catalyst for Selective Catalytic Reduction of NO by NH_3
1 - Laboratoire de Chimie des Matériaux et Catalyse, Département de Chimie, Faculté des Sciences de Tunis. Campus Universitaire 1060 Tunis, Tunisie
2 - Institut Charles Gerhardt Montpellier, UMR 5253, CNRS-UM2-ENSCM-UM1, Equipe MACS, Ecole Nationale Supérieure de Chimie, 8, rue Ecole Normale 34296 Montpellier Cedex 5, France

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Chagas C.A., Schmal M.
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Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

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Hirayama J.[1], Kamiya Y.[2]
Photocatalytic Reduction of Nitrate to Nitrogen in Water under Visible Light Irradiation in the Presence of $Pt/SrTiO_3$:Rh Photocatalyst and $SnPd/Al_2O_3$ Non-photocatalyst
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2 - Research Faculty of Environmental Earth Science, Hokkaido University, Sapporo, Japan

V-PP41
Todorova S.[1], Stefanov P.[2], Naydenov A.[2], Tzaneva B.[3], Stoyanova D.[2]
Co, La and Ce Modified $Pd\text{-}Al_2O_3$ - Catalysts for Methane Combustion
1 - Institute of Catalysis, Bulgarian Acad. of Sciences, Sofia, Bulgaria
2 - Institute of General and Inorganic Chemistry, Bulgarian Acad. of Sciences, Sofia, Bulgaria
3 - Technical University of Sofia, Sofia, Bulgaria

V-PP42
Jirátová K.[1], Balabánová J.[1], Kovanda F.[2], Obalová L.[3]
Deep Ethanol Oxidation over Nanosized Co-Mn-Al Mixed Oxides Supported on Pelletized Magnesia-alumina
1 - Institute of Chemical Process Fundamentals of the Czech Academy of Sciences, Praha, Czech Republic
2 - University of Chemistry and Technology, Praha, Czech Republic
3 - Institute of Environmental Technology, VŠB - Technical University of Ostrava, Czech Republic

V-PP43
Lee T.H.[1], Seong Y.B.[1], Lee J.W.[1], Kim M.J.[1], Park C.J.[1], Choi W.Y.[1], Lee T.J.[1], Park N.-K.[2], Baek J.-I.[3], Lee J.B.[3]
Synthesis of Macro-porous Cu-Sn-Zr Catalyst for SO_2 Reduction
1 - Yeungnam University, Chemical Engineering, Gyeongsan, Republic of Korea
2 - Yeungnam University, Institute of Clean Technology, Republic of Korea
3 - Korea Electric Power Research Institute, Republic of Korea

V-PP44

Jáuregui Haza U.J.[1], Abreu Zamora M.A.[1], González Labrada K.[2], Robaina León Y.[1], Valdés Callado M.[1]

Degradation of Paracetamol by Homogeneous Catalytic Photo-Fenton Process in an Open Channel Reactor

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2 - Instituto Superior Politécnico José Antonio Echeverría, La Habana, Cuba

V-PP45

Pitault I.[1], Gelin P.[2], Fiani E.[3], Meille V.[4], Bornette F.[4], Vanoye L.[4], Soufi J.[4,2]

Catalytic Oxidation of Polycyclic Aromatic Hydrocarbons (PAH) over Zeolite Type Catalysts: Effect of Si/Al Ratio, Structure and Acidity

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3 - ADEME Agence de l'Environnement de la Maîtrise de l'Energie, 20 avenue du Gresillé 49004 Angers Cedex01, France
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Vilasi P.[1,2], Vernoux P.[1], Briois P.[2], Billard A.[2], Arab Pour Yazdi M.[2]

Synthesis and Catalytic Performances of Nanostructured Lanthanum Cobaltite Catalytic Thin Films Prepared by Physical Vapour Deposition

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V-PP47

Montecchio F.[1], Delin J.[2], Kaijser P.[2], Mills J.[3], Engvall K.[1], Lanza R.[1]

Photocatalytic and Ozone Combined UV Treatment for VOCs Abatement at Trace Concentrations

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2 - Scandinavian Centriair AB, Industrivägen 39, 433 61 Sävedalen, Sweden
3 - Techniair Ltd, Tudor Cottage Calleywell Lane, Aldington, Ashford, Kent TN25 7DU, United Kingdom

V-PP48

Maksimchuk N.V., Ivanchikova I.D., Ayupov A.B., Kholdeeva O.A.

Direct synthesis of cyclic carbonates by oxidative carboxylation of styrenes over Ti-containing catalysts

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V-PP49

Ilichev I.S.[1], Radbil A.B.[1], Kozlov I.A.[2], Ignatov A.V.[2], Semyonycheva L.L.[3], Novoselov A.S.[3]

Hydrogenation of Terpineol to Dihydroterpineol over Various Catalysts

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2 - CJSC "Russkiy katalizator", Nizhniy Novgorod, Russia
3 - Achevskiy State University of Nizhniy Novgorod, Research Institute of Chemistry, Nizhniy Novgorod, Russia

V-PP50

Sevinç A.[1,2], Karakaş G.[1], Atamer İ.B.[2]

Catalyst for Complete Oxidation of Nitrogen Containing Samples

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2 - Terralab A.S., Ankara, Turkey

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Akopian A.V., Rakhmanov E.V., Grigoriev D.A., Anisimov A.V.

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Chemistry Faculty of Lomonosov Moscow State University, Moscow, Russia

V-PP52
Alikin E.A.
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Ecoaliance Ltd, Novouralsk, Russia

V-PP53
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Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia

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Cortés-Reyes M.[1], De La Torre U.[2], Pereda-Ayo B.[2], Herrera M.C.[1], Larrubia M.A.[1], González-Velasco J.R.[2], Alemany L.J.[1]
Analysis of Performance of a Bimodal Cu-CHA as SCR Catalyst Coupled in a NSR-SCR Dual System
1 - Departamento de Ingeniería Química, Facultad de Ciencias, Campus de Teatinos, Universidad de Málaga, E-29071, Spain
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V-PP55
Kryuchkova T.A.[1], Khairullina I.A.[1], Sheshko T.F.[1], Serov Y.M.[1], Chislova I.V.[2], Zvereva I.A.[2]
$(Gd,Sr)_{n+1}Fe_nO_{3n+1}$ Catalysts Applied in Dry (Carbon Dioxide) Methane Reforming
1 - Peoples Friendship University of Russia, Faculty of Science, Physical and Colloidal Chemistry Department, Moscow, Russia
2 - Saint-Petersburg State University, Petrodvorets, Saint-Petersburg, Russia

V-PP56
Fahami A.R., Nova I., Tronconi E.
Mechanistic Kinetic Modeling of NO Oxidation over a Commercial Cu-Zeolite Catalyst for Diesel Exhaust Aftertreatment
Dip.Energia, Politecnico di Milano, Milan, Italy

V-PP57
Selleri T.[1], Nova I.[1], Tronconi E.[1], Weibel M..[2], Schmeißer V.[2]
Modelling Hydrocarbon Deactivation of SCR Zeolite Catalysts
1 - Dip.Energia, Politecnico di Milano, Milan, Italy
2 - Daimler AG

V-PP58
Bertolucci E.[1], Raspolli Galletti A.M.[2], Axet M.R.[3], Serp P.[3]
Green Synthesis of Ruthenium Nanoparticles on Magnetic Carbon Nanostructures and Their Use for the Selective Hydrogenation of Nitroaromatics
1 - Scuola Normale Superiore of Pisa, Italy
2 - University of Pisa, Department of Chemistry and Industrial Chemistry, Italy
3 - University of Toulouse, Laboratoire de Chimie de Coordination composante ENSIACET, France

V-PP59
Gu S.Y., Wu L.H., Chen H.N.
Catalytic Wet Oxidation of Organic Wastewater over TiO_2 Supported Ru-Pt Bimetallic Catalysts
Sinopec Shanghai Research Institute of Petrochemical Technology, Shanghai, China

V-PP60
Zheng J., Meyer S., Köhler K.
Decomposition of N_2O by Ruthenium Catalysts: Influence of the Support
Catalysis Research Center, Department of Chemistry, Technische Universität München, Lichtenbergstraße 4, 85748 Garching, Germany

V-PP61
Patino Y.[1], Pilevar S.[2], De Wael K.[2], Diaz E.[1], Ordonez S.[1]
Catalytic Effect of Carbon Nanotubes in the Electrochemical Reduction of Nalidixic Acid
1 - University of Oviedo, Oviedo, Spain
2 - University of Antwerpen, Antwerpen, Belgium

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Diaz M., Lima E.
Perturbing the Surface Polarity of Cellulose to Improve its Catalytic Conversion to Glucose
Instituto de Investigaciones en Materiales, UNAM, Mexico, Mexico

V-PP63
San Jose-Alonso D., Illan-Gomez M.J., Roman-Martinez M.C.
Co Catalysts for the Dry Reforming of Biogas
Department of Inorganic Chemistry, University of Alicante, Alicante, Spain

V-PP64
Perez-Coronado A.M., Calvo L., Alonso N., Heras F., Rodriguez J.J., Gilarranz M.A.
Pd Nanoparticles via Water in Oil Microemulsion as Catalyst for Nitrite Reduction
Sección de Ingeniería Química, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid, Spain

V-PP65
Borges D.G.[1], Moores A.[2], Assaf J.M.[1]
$CaO/CoFe_2O_4$ Synthesized by Citrate Precursor Method for Transesterification Reaction
1 - Laboratory of Catalysis, Department of Chemical Engineering, São Carlos Federal University, São Carlos-SP, Brazil
2 - Center for Green Chemistry and Catalysis, Department of Chemistry, McGill University, Montreal-QC, Canada

V-PP66
Manzoli M.[1], Agostini G.[2], Vindigni F.[1], Lamberti C.[1], Dimitrov D.[3], Ivanov K.[3], Tabakova T.[4]
EXAFS Study in Operando Conditions of Au/Co-doped CeO_2 Catalysts for Methanol Oxidation Reaction
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2 - European Syncrotron Radiation Facility, Grenoble, France
3 - Departmemt of Chemistry, Agricultural University, Plovdiv, Bulgaria
4 - Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria

V-PP67
Zazi A.[1,2], Gonzalez-dela Cruz V.M[3,2], Halliche D.[1], Holgado J.P.[3], Caballero A.[3], Bachari K.[4], Saadi A.[1], Tezkratt S.[2], Cherifi O.[1]
Effect Promoter of Cobalt on the Catalyst Ni-Mg-Al Obtained via Hydrotalcites for the Dry Reforming of the Methane
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4 - Centre de Recherches Scientifiques (CRAPC), BP 248, 16004 Alger, Algeria

V-PP68
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On the Correlations between Redox Properties and Catalytic Performances of $Ce_xPr_{1-x}O_{2-\delta}$ Catalysts Towards Environmentally Relevant Oxidation Reactions
1 - MCMA Group, Department of Inorganic Chemistry. Faculty of Sciences. University of Alicante. Ap.99 E-03080 Alicante, Spain
2 - Faculty of Sciences. University of Cádiz. Campus Río San Pedro, Puerto Real, Spain

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Giménez-Mañogil J., García-García A.
Identifying the Nature of the Copper Entities over Ceria-based Supports to Promote Diesel Soot Combustion: Synergistic Effects
MCMA Group, Department of Inorganic Chemistry. Faculty of Sciences. University of Alicante. Ap.99 E-03080 Alicante, Spain

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Quiles-Díaz S., Giménez-Mañogil J., García-García A.
Catalytic Performance of 2%$CuO/Ce_{0.8}Zr_{0.2}O_2$ Loaded over SiC-DPF in NOx-assisted Combustion of Diesel Soot
MCMA Group, Department of Inorganic Chemistry. Faculty of Sciences. University of Alicante. Alicante, Spain

V-PP71
Papa F.[1], Balint I.[1], Negrila C[2], Olaru E.A.[3], Munteanu C.[1], Zgura I.[2], Bradu C.[3]
Pd-Cu Nanostructured Catalysts for Water Phase Reduction of Nitrates. Influence of the Support and of the pH
1 - Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania
2 - National Institute of Materials Physics, Magurele, Romania
3 - University of Bucharest, Research Center for Environmental Protection and Waste Management, Sos. Panduri 90, 050663 Bucharest, Romania

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Cruceanu A.[1], Zavoianu R.[1], Pavel O.D.[1], Florea M.[1], Bradu C.[2], Olaru E.[2]
Red Mud Catalysts for Sulphide Oxidation in Wastewater
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2 - PROTMED research centre, University of Bucharest, Bucharest, Romania

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Barrera A.[1], Padilla F.[1], Tzompantzi F.[2], López-Gaona A.[2], Castellanos S. G.[1]
Photocatalytic Activity in the Degradation of Phenol over Zn^{2+}:Al^{3+}:W^{6+} Layered Double Hydroxide Prepared by Coprecipitation
1 - Universidad de Guadalajara, CUCI, Laboratorio de nanomateriales catalíticos, Ocotlán, Jalisco, México
2 - Universidad Autónoma Metropolitana-Iztapalapa, Depto. de Química, México D.F., México

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Barrera A.[1], Salazar K.G.[1], Tzompantzi F.[2], Padilla F.J.[1], Castellanos S.G.[1], López-Gaona A.[2]
Photodegradation of Phenol over Al_2O_3-Nd_2O_3 Nanomaterials Doped with Fe, Mg, and Zn Oxide
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Yahya R.[1], Craven M.[1], Kozhevnikova E.[1], Steiner A.[1], Kozhevnikov I.[1], Samunual P.[2], Bergbreiter D.[2]
Polyisobutylene Oligomer-bound Polyoxometalates as Efficient and Recyclable Catalysts for Biphasic Oxidations with Hydrogen Peroxide
1 - University of Liverpool, Liverpool, UK
2 -Texas A&M University, USA

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Benadda A.[1], Rahou S.[1], Barama A.[1], Djadoun A.[2]
Catalytic Combustion of Toluene over MnO_x-CeO_2 Mixed Oxides
1 - LMCCCO, Faculté de Chimie, USTHB, Algiers, Algeria
2 - Laboratoire de Géophysique, FSTGAT, USTHB, Algiers, Algeria

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Klyushina A.[1], Obalová L.[1], Karásková K.[2], Jirátová K.[3]

Effect of Preparation Method on Catalytic Properties of Co-Mn-Al Mixed Oxide for N_2O Decomposition

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Obalová L.[1], Karásková K.[1], Kovanda F.[2], Jirátová K.[3], Šrámek J.[4], Kustrowski P.[5], Chromčáková Ž.[1], Pacultová K.[1], Kočí K.[1], Borovec K.[1], Dej M.[1]

K/Co_4MnAlO_x Catalyst for N_2O Abatement from Nitric Acid Plant Waste Gases – Results of Pilot Plant-scale Testing

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5 - Jagiellonian University, Krakow, Poland

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Yuan R.M.[1], Lin Z.[2]

DFT Studies on the Mechanisms of Nickel-Catalyzed Reductive Carboxylation of Styrenes Using CO_2 as the Building Block

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2 - Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, People's Republic of China

V-PP80

Lee J.W.[1], Lee T.H.[1], Seong Y.B.[1], Kim M.J.[1], Park C.J.[1], Choi W.Y.[1], Park N.-K.[2], Lee T.J.[1], Chang W.C. [3], Choi H.-Y.[4]

Catalytic Decomposition of NF_3 Exhausted in Semiconductor Manufacturing Process over γ-Al_2O_3 Catalyst with H_2O or without H_2O

1 - Yeungnam University, Chemical Engineering, Gyung San, Republic of Korea
2 - Yeungnam University, Institute of Clean Technology, Republic of Korea
3 - KOCAT Incorporated
4 - Institute for Advanced Engineering

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Krivoruchenko D.S.[1], Stakheev A.Yu.[1], Bokarev D.A.[1], Telegina N.S.[1], Kustov A.L.[2], Thøgersen J.R.[2]

"Bifunctional" [Mn-Ce/Fe-zeolite] Catalysts for Selective Catalytic Reduction of NO_x by NH_3 at Low Temperature

1 - N.D. Zelinsky Institute of Organic Chemistry, Moscow, Russia
2 - Haldor Topsøe A/S, Denmark

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Barsukov D.V., Subbotina I.R.

Increase of CO Photocatalytic Oxidation Rate on Titania under Moderate H_2O Coverages

Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia

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Zharmagambetova A.K., Auyezkhanova A.S., Altynbekova K.A.

Supported Polymer-Metal Comlexes for n-Octane Oxidation by Hydrogen Peroxide under Mild Conditions

D. Sokolskii Institute of Organic Catalysis & Electrochemistry, Almaty, Kazakhstan

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Yashnik S.A.[1], Salnikov A.V.[1], Kerzhentsev M.A.[1], Ismagilov Z.R.[1,2], Jin Y.[3], Koseoglu O.R.[3]
Sorption of Sulfur-containing Molecules on CuZnAl-O Catalysts from Model and Straight-run Diesel Fuel
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia
3 - Saudi Aramco, Research and Development Center, Dhahran, Kingdom of Saudi Arabia

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Shuvarakova E.I.[1,2], Bedilo A.F.[1,2], Mishakov I.V.[1,3], Vedyagin A.A.[1,3]
Role of Electron-Acceptor Sites during Destructive Sorption of CF_2Cl_2 over MgO and VO_x/MgO Aerogels
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk Institute of Technology, Moscow State University of Design and Technology, Novosibirsk, Russia
3 - Novosibirsk State Technical University, Novosibirsk, Russia

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Mytareva A.I.[1], Stakheev A.Yu.[1], Bokarev D.A.[1], Kustov A.L.[2], Thøgersen J.R.[2]
The Synergistic Effect for [RedOx + Zeolite] CombiCat in NH_3-SCR: Contributions of Different Pathways to the Overall Mechanism
1 - Zelinsky Institute of Organic Chemistry, Moscow, Russian Federation
2 - Research & Development, Haldor Topsøe A/S, Lyngby, Denmark

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Bogdan V.I.[1,2], Koklin A.E.[1], Kustov A.L.[2,1], Lunin V.V.[2,1]
Conversion of Lignin Catalyzed with Sub- and Supercritical Water
1 - Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia
2 - Moscow State University, Chemical Department, Moscow, Russia

V-PP88
Koklin A.E.[1], Kondratyuk A.V.[1,2], Lunin V.V.[1,2], Bogdan V.I.[1,2]
Aqueous Phase Hydrodeoxygenation of Phenol on Bifunctional Catalyst Systems: Ru/C and Acids
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2 - Lomonosov Moscow State University, Moscow, Russia

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Gaidai N.A.[1], Luu C.L.[2], Nguyen T.[3], Hoang T.C.[2], Ha C.A.[3], Ho S.T.[2], Agafonov Yu.A.[1], Lapidus A.L.[1]
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1 - JSC Managing company "Biochemical Holding "Orgkhim", Nizhniy Novgorod, Russia
2 - Institute of Chemical Technology, Vietnam Academy of Science and Technology, Ho Chi Minh, Vietnam
3 - HoChiMinhCity University of Technology, Vietnam

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Serov N.Yu., Shtyrlin V.G.
Catalytic Flow Syntheses of Oligopeptides in the Glycine – Trimetaphosphate – Imidazole System
Kazan Federal University, A.M. Butlerov Chemistry Institute, Kazan, Russia

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Rakhmatullina A.P.[1], Bogachyova T.M.[2], Satbaeva N.S.[1]
A Study of Glycolysis of Polyethylene Terephthalate Waste in the Presence of Catalyst for the Production of bis(2-hydroxyethyl)terephthalate
1 - Kazan National Research Technological University, department of synthetic rubber, Kazan, Russia
2 - Kazan National Research Technological University, department of General Chemical Engineering, Russia

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Sagdeev A.[1], Galimova A.[1], Gumerov F.[2]
The Aluminum Oxide Active Catalyst's Regeneration Using Supercritical Carbon Dioxide
1 - Nizhnekamsk Chemical Technological Institute (branch institute) of the Kazan National Research Technological University, Nizhnekamsk, Russia
2 - Federal State Budgetary Educational Institution of Higher Professional Education "Kazan National Research Technological University", Kazan, Russia

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Salyakhova M.A., Pukhacheva E.N., Zaripova V.M., Uvaev V.V.
The Composite Rubberized Material with Coated Photocatalytic Layer
Open Joint Stock Company "Kazan Chemical Research Institute", Kazan, Russia

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Bachurikhin A.L.[1,2], Efendiev M.S.[1,2]
Electromagnetic Catalytic Reactor of Water Treating from Oils and Hydrocarbons
1 - Zelinsky N.D. Institute of Organic Chemistry of the Russian Academy of Science, Moscow, Russia
2 - OJSC DagNefteProduct, Makhachkala City, Russia

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Ermolaev I.S.[1,2], Ermolaev V.S.[1,2], Mordkovich V.Z.[1,2]
Optimization of Catalytic Gas-To-Liquid Technology for Better Carbon Efficiency
1 - Technological Institute for Superhard And Novel Carbon Materials, Moscow, Russia
2 - INFRA Technology, Moscow, Russia

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Abate S., Mebrahtu C., Perathoner S, Gentiluomo S., Giorgianni G., Centi G.
Catalytic Performance of Ni-based Catalysts Supported on λ-Al_2O_3-ZrO_2-TiO_2-CeO_2 Composite Oxide for CO_2 Methanation
University of Messina, Messina, Italy

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Fodil Cherif N.[1,2], Fares A.[1,2], Barama A.[1]
Preparation of Cobalt Titanate Nanoparticles and the Study of Their Photocatalytic Behaviors
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2 - Centre de Recherche Scientifique et Technique en Analyses Physico-Chimiques CRAPC, Bou-Ismail, Tipasa

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Visconti C.G.[1], Martinelli M.[1], Falbo L.[1], Infantes-Molina A.[1], Gaeta M.[1], Lietti L.[1], Forzatti P.[1], Palo E.[2], Picutti B.[3]
CO_2 Hydrogenation to Light Olefins on a High Surface Area K-promoted Iron Catalyst
1 - Politecnico di Milano, Dipartimento di Energia, Milan, Italy
2 - KT-Kinetics Technologies SpA, Rome, Italy
3 - Maire Tecnimont Group SpA, Milan, Italy

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Paksoy A.I., Aksoylu A.E.
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Bogazici University, Department of Chemical Engineering, Istanbul, Turkey

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Bivona L.A.[1,2], Fichera O.[1], Buaki-Sogo M.[1], Fusaro L.[1], Gruttadauria M.[2], Aprile C.[1]
Novel Imidazolium Based Catalyst for the Chemical Fixation of Carbon Dioxide
1 - Unit of Nanomaterial Chemistry (CNano), University of Namur (UNAMUR), Department of Chemistry, Namur, Belgium
2 - Dipartimento di Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche (STEBICEF), Sezione di Chimica, Università di Palermo, Palermo, Italy

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Cadete Santos Aires F.J.[1], Aouine M.[1], Daniel C.[1], Meunier F.C.[1], Farrusseng D.[1], Epicier T.[1,2]
Real-time In situ Atomic-scale Study of the Surface Termination of Ceria Nanoparticles under Vacuum, O_2 and CO_2 Pressures by Environmental Transmission Electron Microscopy
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Au/MgO-type Catalysts for the Carbonylation of Glycerol with Urea. Effect of the Morphology and Macro/Meso-Porous Structure of the Support
1 - Center for Ordered Materials, Organometallics & Catalysis (COMOC), Department of Inorganic and Physical Chemistry, Ghent University, Ghent, Belgium
2 - Industrial Catalysis and Adsorption Technology (INCAT), Department of Industrial Technology and Construction, Faculty of Engineering & Architecture, Ghent University, Ghent, Belgium

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Ab. Rahim M.H., Paroo I.V., Maniam G.P.
Synthesis of Organic Carbonates Using Catalyst Containing K Metal from Waste Source
Faculty of Industrial Sciences & Technology, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Kuantan, Pahang, Malaysia

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Chemical Technologies for Environmental Sustainability Group, Department of Chemical Engineering, Faculty of Science and Technology, University of the Basque Country UPV/EHU , P.O. Box 644, E-48080 Bilbao, Spain

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Department of Chemical Engineering, Faculty of Science and Technology, University of the Basque Country, UPV/EHU, P.O. Box 664, E-48080 Bilbao, Spain

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Lin K.-S., Chiang C.L., Adhikari A.K.
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Department of Chemical Engineering and Materials Science/Environmental Technology Research Center, Yuan Ze University, Chung-Li City, Tao-Yuan County, Taiwan

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Sagdeev A.A.[1], Gallyamov R.F.[1], Sagdeev K.A.[1], Gumerov F.M.[2]
Regeneration of the Hydrogenation Catalysts by Supercritical Fliud Extraction
1 - Nizhnekamsk Chemical Technological Institute, Nizhnekamsk, Russia
2 - Kazan National Research Technological University, Kazan, Russia

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Selen Çağlayan B.[1,2], Aksoylu A.E.[1]
CO_2 Adsorption Kinetics on Chemically Modified Activated Carbon
1 - Department of Chemical Engineering, Bogazici University, Bebek, Istanbul, Turkey
2 - Advanced Technologies R&D Center, Bogazici University, Bebek, Istanbul, Turkey

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Mendeleev University of Chemical Technology of Russia, Moscow, Russia

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Shoen A.[1,2,3], Dacquin J.-Ph.[1,2,3], Dujardin Ch.[1,3,4], Granger P.[1,2,3]
Perovskite-based Catalysts as Alternative to Commercial Three-Way-Catalysts? – Impact of Cu and Ca Doping and Optimisation of Surface Properties
1 – UCCS
2 - University of Lille, France
3 - Cité Scientifique, 59650 Villeneuve d'Ascq, France
4 – ENSCL, France

V-PP112
Salbidegoitia J.A., Fuentes E.G., Gonzalez-Marcos M.P., Gonzalez-Velasco J.R.
Effect of Desilication of HY Zeolite in Pt/HY Catalysts for Polystyrene Hydrocracking
Group of Chemical Technologies for Environmental Sustainability, Department of Chemical Engineering, Faculty of Science and Technology, The University of the Basque Country, UPV/EHU. Bilbao, Spain

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Shutilov A.[1,2,3], Pakharukov I.[1,2], Oleynik A.[1,3], Zenkovets G.[1,2]
Study of Supported Pt/TiO_2 Catalysts with Enhanced Activity in CO Oxidation
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3 - Novosibirsk State Technical University, Novosibirsk, Russia

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Taran O.[1,2], Yashnik S.[1], Ayusheev A.[1], Prihod'ko R.[3], Ismagilov Z.[1], Goncharuk V.[3], Parmon V.[1,4]
Composite Carbon /Zeolite Adsorbent-catalysts for Organic Containing Wastewater Purification Using Wet Peroxide Oxidation
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3 - Dumansky Institute of Colloid and Water Chemistry NASU, Kiev, Ukraine
4 - Novosibirsk State University, Novosibirsk, Russia

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Pachatouridou E.[1,2], Iliopoulou E.[1], Konsolakis M.[2], Yentekakis I.V.[3]
Effect of SO_2 on N_2O Decomposition over Ir Catalysts Supported on CeO_2-Modified Al_2O_3
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Artioli N.[1], Solt H.[1], Bazin P.[1], Aureau D.[2], Etcheberry A.[2], Rousseau S.[3], Blanchard G.[3], Moral N.[4], Busardo D.[5], Bruma A.[6], Malo S.[6], Daturi M.[1]
Highly Active Nanocatalysts by Ion Beam Surface Modification
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Group of Chemical Technologies for Environmental Sustainability, Department of Chemical Engineering, Faculty of Science and Technology, The University of the Basque Country, UPV/EHU. Bilbao, Spain

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Technical University of Freiberg, Institute of Energy Process Engineering and Chemical Engineering, Chair of Reaction Engineering, Freiberg, Germany

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Department of Chemical Engineering, Faculty of Science and Technology, University of Basque Country, Bilbao, Spain

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Selective Oxidation and Hydrogenation of CO over Precious Metal Catalysts for Fuel Cell Applications
School of Chemistry and Physics, University of KwaZulu-Natal, Westville, Durban, South Africa

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Dip. Energia, Politecnico di Milano, Milan, Italy

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Ribeiro R.S.[1], Silva A.M.T.[2], Faria J.L.[2], Gomes H.T.[1]
Magnetic Carbon Xerogels for the Catalytic Wet Peroxide Oxidation of 4-Nitrophenol Solutions
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Mahardiani L.[1], Kamiya Y.[2]
Acceleration of Catalytic Ozonation of Ammonium Ion in Water over Cobalt Oxide Catalyst by Repeated Use
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Ercan K.E.[1], Say Z.[1], Vovk E.I.[1,2], Pantaleo G.[3], Liotta L.[3], Venezia A.[3], Ozensoy E.[1]
Novel Hybrid Perovskite Catalysts for DeNOx Applications
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3 - CNR-Institute for the Study of Nanostructured Materials (ISMN), 90146, Palermo, Italy

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NH_3-SCR and NH_3 Oxidation over V-based Catalysts: Design of "High-Efficiency" NH_3-SCR Reactor for Stationary Applications
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Tomsk State University, Tomsk, Russia

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Mendeleev University of Chemical Technology of Russia, Moscow, Russia

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Zagaynov I.V.[1], Liberman E.Yu.[2]
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1 - A.A. Baikov Institute of Metallurgy and Materials Science, Moscow, Russia
2 - D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

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al-Faraby Kazakh National University, Almaty, Kazakhstan

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Khusnutdinova J.R.[1], Gellrich U.[2], Milstein D.[2]
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1 - Okinawa Institute of Science and Technology Graduate University, 1919-1 Tancha, Onna-son, Kunigami-gun, Okinawa, 904-0495 Japan
2 - Department of Organic Chemistry, Weizmann Institute of Science, Rehovot, Israel

V-PP131
Bal H., Demirhan C.D., Aksoylu A.E.
Effects of La and Ce Promotion on CDRM Performance of Co-Ni/ZrO_2 Catalysts
Department of Chemical Engineering, Boğaziçi University, Istanbul, Turkey

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Selishchev D.S.[1,2,3], Kozlov D.V.[1,2,3]
Photocatalytic Oxidation of Diethyl Sulfide Vapor over TiO_2 Deposited on Porous Supports
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3 - Research and Educational Centre for Energoefficient Catalysis (NSU), Novosibirsk, Russia

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Pinaeva L.G.[1], Ivanov D.V.[1], Sadovskaya E.M.[1,2], Isupova L.A.[1]
High Temperature N_2O Decomposition over Massive and Supported Mixed Oxides: Principles of Activity Regulation
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V-PP134
Kolinko P.[1,2], Lyulyukin M.[1], Besov A.[1,2], Parkhomchuk E.[1,2,3], Kozlov D.[1,2,3]
Development of the Methods for Fast Catalytic Air Purification from CWAs
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia,
3 - Research and Educational Centre for Energoefficient Catalysis (Novosibirsk State University), Novosibirsk, Russia

V-PP135
Vedyagin A.A.[1,2], Volodin A.M.[1], Stoyanovskii V.O.[1], Kenzhin R.M.[1], Mishakov I.V.[1,2], Plyusnin P.E.[3], Shubin Yu.V.[3]
Stabilization Effect of Pd–Rh Alloyed Nanoparticles in Three-way Catalysts
1 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 - Novosibirsk State University, Novosibirsk, Russia
3 - Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

V-PP136
Venezia A.M.[1], Pantaleo G.[1], La Parola V.[1], Deganello F.[1], Singha R.K[2], Bal R.[2]
Synthesis Effect on CH_4 Partial Oxidation over Ni-CeO_2 Catalysts
1 - Institute of Nanostructured Materials, CNR, Palermo, Italy
2 - Indian Institute of Petroleum, Dehradun, Uttaranchal, India

V-PP137
Khobragade R.[1], Saravanan G.[1], Rayalu S.[1], Bakardjieva S.[2], Subrt J.[2], Labhasetwar N.[1]
Improved Diesel Soot Oxidation Performance of Manganese-substituted Strontium Ferrite
1 - CSIR-NEERI, Nagpur, India
2 - IIC, ASCR

V-PP138
Hansen K.K.
Selective Elecrochemical Reduction of NO_x
Technical University of Denmark, Denmark

V-PP139
Belskaya O.B.[1,2], Mironenko R.M.[1], Rodionov V.A.[1], Talsi V.P.[1], Sysolyatin S.V.[3], Likholobov V.A.[1,2]
Hydrogenation of 2,4,6-trinitrobenzoic Acid on Pd/Sibunit Catalysts
1 - Institute of Hydrocarbons Processing SB RAS, Omsk, Russia
2 - Omsk State Technical University, Omsk, Russia
3 - Institute for Problems of Chemical and Energetic Technologies SB RAS, Biysk, Altai krai, Russia

V-PP140
Altunina L.K., Svarovskaya L.I., Guseva Yu.Z.
Biocatalytic Generation of Oil-Displacing Systems in Low-Temperature Reservoirs of Viscosity Oil
Institute of Petroleum Chemistry Siberian Branch of the Russian Academy of Sciences, Tomsk, Russia

V-PP141
Matveyeva A.N., Pakhomov N.A.
The Rehydration of Centrifugal Thermal Activation Products of Gibbsite – the Industrial Waste of Catalyst KDM
St. Petersburg State Institute of Technology (Technical University), Department of General Chemical Technology and Catalysis, Saint-Petersburg, Russia

V-PP142
Tkachenko I.S.[1,2], Tkachenko S.N.[1,3], Egorova G.V.[1], Lunin V.V.[1], Golosman E.Z.[4], Lokteva E.S.[1,2], Likholobov V.A.[2]
Iron –Containing Catalysts from By-Products of Underground Water Ozonation
1 - Lomonosov Moscow State University, Chemistry Department, Moscow, Russia
2 - Institute of Hydrocarbons Processing of the Siberian Branch of the RAS, Omsk, Russia
3 - LLC NVF 'TIMIS', Moscow, Russia
4 - LLC "NIAP –CATALYZATOR", Novomoskovsk, Tula Region, Russia

V-PP143
Garcia-Aguilar J., Miguel-García I., Berenguer-Murcia Á., Cazorla-Amorós D.
Sol-Gel Synthesis of Robust Silica Monoliths by Interfacial Solution/Precipitation Reactions: Application in the Preferential Oxidation of Carbon Monoxide
Inorganic Chemistry Department and Materials Science Institute, Alicante University, Alicante, Spain

V-PP144
Tabari T., Uner D.
Photocatalytic Removal of NO under Visible Light Irradiation over Sol-Gel Synthesized $PbTiO_3$ Nanoparticles
Chemical Engineering Department, Middle East Technical University, Ankara, Turkey

V-PP146
Nagieva I.T[1,2], Gasanova L.M[2], Nasirova U.V[2], Nagiev T.M[1,2]
Coherent Synchronized Monooxidation of Ethylene by Hydrogen Peroxide on a Biomimetic Catalyst
1 - Baku State University, Baku, Azerbaijan Republic
2 - Nagiev Institute of Catalysis and Inorganic Chemistry, National Academy of Sciences of Azerbaijan, Baku, Azerbaijan Republic

V-PP147
Casanovas Grau A., Llorca Piqué J.
Hydrogen Production from Olive Mill Wastewater through Steam Reforming. Catalyst Development
Institute of Energy Technologies. Technical University of Catalonia, Barcelona, Spain

V-PP148
Khaleel A., Nawaz M.
Bulk Mixed Al-transition Metal Oxide Catalysts for Enhanced Oxidation of 1,2-dichloroethane
UAEU, Al-Ain, UAE

V-PP149
Tudorache M., Gheorghe A., Parvulescu V.I.
Green Alternative for Guideline Monoterpenoids to Value-added Products – Tailored the Biocatalytic Transformation of α-pinene
University of Bucharest, Bucharest, Romania

V-PP150
Kurtoglu K., Gubbuk I.H., Akgemci E.G..
Characterization and Application in Catalytic Reduction of MB of $Fe_3O_4SiO_2Ni$ Nanoparticles
Necmettin Erbakan University, Faculty of Ahmet Kelesoglu Education Chemistry, Department of Chemistry, Konya, Turkey

XI European Workshop on Innovation in Selective Oxidation (ISO ‘15) "Selectivity in Oxidation: Key to new resources valorization"

ISO-PP01
Li G., Hensen E.J.M., Pidko E.A.
Trinuclear Copper Oxo-clusters in ZSM-5 Zeolite for Selective Methane Oxidation to Methanol
Inorganic Materials Chemistry group, Eindhoven University of Technology, Eindhoven, The Netherlands

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Richard M.[1], Can F.[1], Duprez D.[1], Gil S.[2], Giroir-Fendler A.[2], Bion N.[1]
Remarkable Enhancement of O_2 Activation on YSZ Surface in a Dual-Bed for Catalytic Partial Oxidation of CH_4
1 - University of Poitiers, CNRS UMR 7285, Institut des Milieux et Matériaux de Poitiers (IC2MP), 4 rue Michel Brunet TSA 51106, 86073, Poitiers Cedex 9, France
2 - University of Lyon 1, CNRS UMR 5256, IRCELYON, 2 avenue Albert Einstein, Villeurbanne, France

ISO-PP03
Sprung C.[1], Yablonsky G.S.[2], Schlögl R.[1], Trunschke A.[1]
A Qualitative Kinetic Analysis of Steady-State Selective Oxidation Process: Role of Water and Oxygen
1 - Fritz Haber Institute of the Max Planck Society, Dept. of Inorganic Chemistry, Berlin, Germany
2 - Department of Chemistry, Parks College, Saint Louis University, Saint Louis, MO, USA

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Bakaev V.A.[1], Vershinin N.N.[1], Berestenko V.I.[1], Efimov O.N.[1], Kabachkov E.N.[1,2], Kurkin E.N.[1,2]
Nanomaterial Based Catalysts for Low-temperature Oxidation of Carbon Monoxide
1 - Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Chernogolovka, Moscow region, Russia
2 - Scientific Center in Chernogolovka, RAS, Chernogolovka, Moscow region, Russia

ISO-PP05
Laguna O.H.[1], Centeno M.A.[1], Boutonnet M.[2], Odriozola J.A.[1]
Gold Supported on Fe-doped Ceria Supports Prepared through the Microemulsion Method for the PROX Reaction
1 - Instituto de Ciencia de Materiales de Sevilla, Avda. Américo Vespucio, 49. CP: 41092 Seville - Spain
2 - Royal Institute of Technology (KTH). Department of Chemical Technology. Div. of Chemical Technology. Teknikringen 42, S-10044 Stockholm, Sweden

ISO-PP06
Dutov V.[1], Mamontov G.[1], Sobolev V.[1,2], Vodyankina O.[1]
Silica-supported Silver-containing OMS-2 Catalysts for Ethanol Oxidative Dehydrogenation
1 - Tomsk State University, Tomsk, Russia
2 - Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

ISO-PP07
Tyablikov I.A., Romanovsky B.V.
A Heterogeneous Single-site Organocatalyst for Alkene Epoxidation
Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

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Martínez H., Páez E.A., Martínez F.
Selective Photo-Oxidation of α-pinene with dioxo-Mo(VI) complex /TiO_2 with Different Textural Properties
Cicat, Escuela de Química, UIS, Bucaramanga, Colombia

ISO-PP09
Arsentyev A.V., Vorontsov A.V.
Study on Kinetics of Liquid Phase Photocatalytic Oxidation of Dibutyl Sulfide Over Fullerenes
Novosibirsk State University, Novosibirsk, Russia
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

ISO-PP10
Torozova A.S.[1,2], Doluda V.Yu.[1], Sulman E.M.[1], Murzin D.Yu.[2]
Liquid Phase Oxidation of L-sorbose over Metallic and Bimetallic Particles Stabilized in Polymer Matrix
1 - Tver State Technical University, Dep. Biotechnology and Chemistry, Tver, Russia
2 - Abo Akademi University, Turku, Finland

ISO-PP11
Torbina V.[1], Ivanchikova I.[1,2], Kholdeeva O.[1,2], Vodyankina O.[1]
Propylene Glycol Oxidation over Cr-MIL-101 with Tert-butyl Hydroperoxide
1 - Tomsk State University, Tomsk, Russia
2 - Boreskov Institute of Catalysis, Novosibirsk, Russia

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Schwach P., Tarasov A., Willinger M., Schlögl R., Trunschke A.
Influence of Pre-treatment on the Oxidative Coupling of Methane over MgO Catalysts
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

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Podolean I., Papuc B., Parvulescu V.I., Coman S.M.
New Insights in the Catalytic Oxidation of Levulinic Acid to Succinic Acid
University of Bucharest, Faculty of Chemistry, Bucharest, Romania

ISO-PP14
Malmusi A., Dellapasqua M., Velasquez Ochoa J., Cavani F.
Vanadium-Based Catalyst for Ethanol Transformation: Relation Between Structure and Catalytic Activity
Dipartimento di Chimica Industriale "Toso Montanari" - Alma Mater Studiorum - Università di Bologna, Bologna, Italy

ISO-PP15
Gumina B.[1], Cannilla C.[2], Spadaro L.[2], Di Chio R.[1], Trunfio G.[1], Arena F.[1]
Structure and Reactivity of Nanostructured MnO_x Catalysts in the Liquid Phase Selective Oxidation of Benzyl Alcohol with Oxygen
1 - Dipartimento di Ingegneria Elettronica, Chimica e Ingegneria Industriale, Università degli Studi di Messina, Messina, Italy
2 - Istituto CNR-ITAE "Nicola Giordano", Messina, Italy

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Sushchenko E., Kharlamova T.
Structural Peculiarities and Catalytic Properties of Supported Vanadium Oxide Catalysts for Oxidative Dehydrogenation
Tomsk State University, Chemistry faculty, Tomsk, Russia

ISO-PP17
Wallis P., Schönborn E., Wohlrab S., Kalevaru N., Martin A.
Silica Supported Vanadia Catalysts for Selective Methane Oxidation: Impact of Morphology and Heteroatom Doping on Catalyst Performance
Leibniz Institute for Catalysis, Rostock, Germany

ISO-PP18
Machado K., Mishra G.
Selective Oxidation of Cyclic-alkane, Catalyzed by Nano Size SWNTs Supported Pt and Pd Complexes Catalysts
Universidade de Trás-os-Montes e Alto Douro (UTAD), Vila Real 5001801, Portugal

ISO-PP19
Shimanskaya E.I., Doluda V.Yu., Sulman E.M.
Catalytic Synthesis of 2-methyl-1,4-naphthoquinone in 1%Au/HPS Presence
Tver Technical University, Tver, Russia

ISO-PP20
Liu Q.L., Li J.M., Zhao Z., Gao M.L., Liu J.
Mo-incorporated KIT-6 Mesoporous Silica Catalysts with High Performance for the Selective Oxidation of Propane to Acrolein
State Key Laboratory of Heavy Oil, College of Science, China University of Petroleum, Beijing, China

ISO-PP21
Solsona B.[1], Dejoz A.[1], Vazquez M.I.[1], Lopez Nieto J.M.[2], Soriano M.D.[3], Concepcion P.[2], Cecilia J.A.[3], Jimenez Jimenez J.[3], Rodríguez Castellon E.[3]
Oxidative Dehydrogenation of Ethane on NiO supported on Pillared Clays
1 - Universitat de Valencia, Spain
2 - ITQ (UPV-CSIC), Spain
3 - Universidad de Málaga, Spain

ISO-PP22
Alotaibi M.[1,2], Kalevaru V.N.[1], Almegren H.[2], Alkinany M.[2], Martin A.[1]
Gas Phase Hydroxylation of Benzene to Phenol over M (Co, Ni, Cu, Zn)/ZSM-5 Using Nitrous Oxide
1 - Leibniz Institute for Catalysis at University of Rostock, Rostock, Germany
2 - Petroleum and petrochemicals Research Institute, King Abdulaziz City for Science and Technology, Saudi Arabia

ISO-PP23
Gogol V.V., Pichugina D.A., Ku'zmenko N.E.
DFT Study of the Interaction of CO and $O_2$with Gold-Copper Tetrahedral Bimetallic Clusters
M.V. Lomonosov Moscow State University, Moscow, Russia

ISO-PP24
Benyounes A.[1,2], Ouanji F.[2], Ziyad M.[3], Kacimi M.[2], Serp P.[1]
Selective Isopropyl Alcohol Oxidation on Palladium and Ruthenium Catalysts Supported on Amphiphilic Hybrid Carbon Nanotubes
1 - Laboratoire de Chimie de Coordination UPR CNRS 8241, composante ENSIACET, Université de Toulouse, 4 allée Emile Monso - CS 44362, 31030 Toulouse Cedex 4, France
2 - Laboratory of Physical Chemistry of Materials, Catalysis and Environnement (URAC26), Department of Chemistry, Faculty of Science, University of Mohammed V-Agdal, CS 1014 Rabat, Morocco
3 - Hassan II Academy of Science and Technology, CS 10000 Mohammed VI -Ex Imam Malik, Km 11, Rabat, Morocco

ISO-PP25
Dorofeeva N.V.[1,2], Vodyankina O.V.[1], Sobolev V.I.[1,3], Koltunov K.Yu.[3,4]
Ethanol Transformation over Cu-containing Zirconium Phosphate
1 - Tomsk State University, Tomsk, Russia
2 - Tomsk Polytechnic University, Tomsk, Russia
3 - Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
4 - Novosibirsk State University, Novosibirsk, Russia

ISO-PP26
Lomonosov V.I.[1], Gordienko Yu.A.[1,2], Usmanov T.R.[1,3], Sinev M.Yu.[1]
Kinetic Conjugation Effects during C_1-C_2-hydrocarbon Oxidation in the Conditions of Methane Oxidative Coupling
1 - Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia
2 - ZAO «SCHAG» company, department of chemical technology, Moscow, Russia
3 - Lomonosov Moscow University of Fine Chemical Technology, Moscow, Russia

ISO-PP27
Gryaznova T.V., Dudkina Y.B., Budnikova Y.H., Sinyshin O.G.
Metal-catalyzed Electrochemical Oxidative Phosphonation of Azoles
A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center of Russian Academy of Sciences, Kazan, Russia

EUROPACAT XII

SHORT ABSTRACTS

Plenary Lectures

PL-1

Catalysis in Organic Chemistry: from Butlerov to these Days

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Mechanistic studies have revealed fascinating nature of catalytic reactions that are now ubiquitously employed in modern organic chemistry. A variety of metal species are generated during well-known catalytic reactions [1-4]. In fact, mononuclear metal complexes, metal clusters and nanoparticles are easily accessible on catalyst activation stage or during the course of the catalytic reaction. Formation of "cocktail" of metal species in solution is not uncommon starting with wide variety of different metal precursors (pre-catalysts) [3]. Recent studies provided important evidence on unusual reactivity of small metal clusters, especially the properties connected with "superatomic" structural units [2].

Another important point is evolution of the metal catalyst during catalytic reaction. Evolution of metal complexes in homogeneous catalysis as well as evolution of supported metal catalysts under heterogeneous conditions are the processes of paramount importance. Understanding the nature of these processes is required to achieve selective transforamtions and to develop stable and recyclable catalysts.

Design of new generation of adaptive catalytic systems to facilitate transformations in organic synthesis will be presented and discussed with a focus on development of organic synthesis procedures performed with "atomic precision" [5].

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PL-2

Enhancing Catalytic Rates in Constraints – from Acid-base to Metal Catalyzed Reactions

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Understanding the elementary steps in acid-base and metal catalyzed organic transformations is a key for improving existing and developing new catalysts and process routes for nearly all energy related chemical conversions. Solid acids and bases with nanopores such as zeolites act as solid Brønsted and Lewis acids being excellent model as well as industrial catalysts with well-defined acid-base sites and a well-defined reaction space around the sites. Within the pores of molecular sieves reacting molecules are constrained in a reaction space, which can be subtly adjusted via direct synthesis, as well as via the addition of cations, oxidic clusters or organic fragments. The impact of such changes on mono- and bimolecular reactions such as elimination reactions of alcohols, cracking and alkylation of hydrocarbons are discussed for gas and liquid phase reactions.

Experimental methods to define the state of the reacting molecules combined with detailed kinetic analysis and theory will be used to explain the principal contributions of the interactions and the confinement to determine reaction rates. The chemical environment in these pores also influences metal catalyzed hydrogenation and hydrogenolysis via new pathways enabled by the proximity of metals and Brønsted acid sites. Using examples for catalyzed reactions in gas and liquid phase, it will be shown that the reactivity can be drastically increased by tailoring the space around the active site.

PL-3

Fossil and Renewable Energy: the Turning Point of the Liquid Fuels Production

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Energy, as well as food and water is a basic need for survival. Over the past 150 years, the energy availability guaranteed first by coal and then by oil and gas, has supported the growth of the world population to the current level of 7 billion people. The increase of population prompted the demand of basic needs and therefore the exploitation of planetary resources, impacting on their availability and increasing the environmental pressure.

Today the availability of energy sources and the effects on the environment generated by their use, are among the main critical issues that humanity faces. The production and trade of energy resources are often linked to events with important socio-economical impact, just remember the effects generated by the discovery and exploitation of shale-gas and shale-oil and then by the fall in oil prices. The strong concern on climate change and environmental effects of entropic activity is pushing the majority of nations to react through shared actions, but the conflicting requirements of developed countries and those under development are slowing down the effectiveness of these processes. At the recent UN climate conference held in Lima last December (COP-20), weak progress have been made. It was reconfirmed the principle of common but differentiated responsibility, already introduced in the first United Nations Framework Convention on Climate Change in 1992, which states that every nation must take action to mitigate the climate change according to its own financial and infrastructural capability. It was also introduced a tool (Lost & Damage) through which developing countries particularly vulnerable to the consequences of climate change will be able to receive financial compensation for natural disasters now inevitable, but the main differences between the parties were not reconciled and the most important decisions have been postponed to the next conference in Paris in December 2015. The European Union countries are facing the consequences of these changes with the addition of local problems. The production of liquid fuels in Europe has suffered from an economical point of view from 2008 until the second half of 2014, when the drop in oil prices has given breath for the refinery industry. The problems of this sector are generated by the progressive reduction in fuel demand, by the entry of not negligible amount of bio-fuels, by the obsolescence of the European refining system, characterized by a relatively large number of medium/small refineries and by the high cost of energy. Although since 2007, 14 plants have been closed, persists in Europe overcapacity of refining that endangers other production sites. This crisis is structural in its nature and therefore major interventions targeted to balance supply and demand are required as well as new technological solutions. A reduction of refining capacity appears unavoidable, but at the same time the production of bio-fuels matching the technical and environmental needs, the efficiency improvement of refining technologies to pursue the reduction of energy consumption and the total conversion of crude oil in good quality middle distillates must be strongly pursued. The disciplines most involved by these needs are catalysis, materials science and process engineering. In this presentation some recent results related to the production of bio-fuels and to the total conversion of the oil barrel to middle distillates will be presented and discussed trying to highlight the prospects and the opportunities that science and technology can offer for the mitigation of the problems exposed.

PL-4

Catalysis Using Supported Gold and Gold Palladium Nanoparticles

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Gold catalysis has become a well-established field of endeavour. Much still remains to be discovered in this interesting research field, but to date much progress has been made. In this lecture recent preparation strategies to make supported nanoparticles will be described and discussed. These will involve the use of colloidal and impregnation methods. Monometallic gold catalysts will be discussed together with bimetallic gold palladium and trimetallic gold palladium platinum catalysts.

The first part of the talk will discuss the use of carbon-supported gold nanoparticles for the hydrochlorination of acetylene.[1] This is one of the original reactions where the high activity of gold catalysts was first observed.[2] Details of the catalyst characterisation will be described showing the evolution of the catalyst structure as it is exposed to the reaction conditions. Using detailed aberration-corrected STEM together with X-ray photoelectron spectroscopy the important features of this catalyst will be explored.

In the second part the preparation of bimetallic gold palladium and gold platinum catalysts will be described for the oxidation of alcohols, the activation of C-H bonds[3] and the direct synthesis of hydrogen peroxide.[4] In the final part the preparation and use of the more complex trimetallic nanoparticles will be discussed.[5] One particular example concerns the oxidation of benzyl alcohol as when using supported gold palladium nanoparticles toluene can be observed as a by-product. This by-product can be switched off in two ways. First the design of the bimetallic catalyst support is crucial and the interfacial sites are considered to be important for the selective oxidation to benzaldehyde. Oxides that maximise the interfacial contact give lower toluene formation and with MgO and ZnO in particular no toluene formation is observed although high activities for selective oxidation are observed. Secondly, addition of platinum to the gold palladium bimetallic also swiches off toluene formation. The origins of these effects will be discussed.

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PL-5

Mesoporous Metal-Organic Frameworks as Platforms for Single-site Heterogeneous Catalysts

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AIM (ALD In MOFs) is an emerging synthesis technique that provides access to well-defined arrays of non-aggregating, monodisperse, and organic-capping-ligand-free clusters of metal atoms, metal-oxides/hydroxides, and metal-sulfides. The technique entails adapting atomic-layer-deposition (ALD) chemistry to mesoporous metal-organic framework materials that present suitable node- or linker-based reaction sites. By using multiple, individually self-limiting, ALD growth cycles, clusters of varying, predetermined size, and clusters comprising mixed compositions can be synthesized. In some cases the obtained clusters lack stable analogues in conventional heterogeneous catalyst synthesis chemistry, in part due to a propensity for conventionally synthesized clusters to aggregate under typical conditions for catalysis of gas-phase reactions. As one might guess, the properties of AIM-synthesized clusters and the associated porous-MOF scaffolds render the clusters readily accessible to candidate molecular reactants. The clusters, in many cases, display high catalytic activity for both gas-phase and condensed-phase reactions reactions. Notably, excellent steam stability and moderate thermal stability (temperatures to ca. 350 oC) can be obtained with appropriately designed MOFs This presentation will center on one or two case studies, including AIM-MOF synthesis, structural characterization, catalytic activity, and computationally informed analysis of mechanisms of catalysis.

Because the catalytic clusters comprising nodes and subsequently installed metal atoms are monodisperse, both coordinatively and in terms of cluster size, the resulting ensembles are amenable to structural and functional characterization with a level of precision previously associated mainly with single crystal metal or metal-oxide surfaces. The porosity of the MOF scaffold, however, makes the catalyst arrays three-dimensional and greatly increases the number of active sites relative to two-dimensional arrays. In addition to boosting overall catalytic activity, the presentation of monodisperse catalysts in 3D rather than 2D arrays greatly facilitates structural and functional characterization.

This presentation will touch on catalyst characterization, including in operando characterization. The characterization methods include DRIFTS, EXAFS, total X-ray scattering and pair-distribution-function analysis, single-crystal X-ray diffraction, and energy-dispersive microscopy. Both structural characterization and functional characterization are facilitated by comparative computational modeling and simulations.

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PL-6

Dynamics in Heterogeneous Catalysis

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Heterogeneous catalysis carries its name from the concept of a well-defined heterogeneous interface between the catalyst surface and the reactant environment. The processes of adsorption, desorption and reaction between adsorbates describes the overall reaction. Under conditions where adsorption dominates the overall reaction such an interface can be clearly identified and studied by many techniques.

Under conditions of high performance catalysis with significant turnover this definition becomes increasingly difficult. Strong structural modifications of the solid surface are involved in such reactive states. We identify the transformation of a sharp interface into a termination layer with substantially different structural and chemical properties than the bulk. In certain cases even the bulk underneath a sub-surface region of the solid undergoes reaction-induced transformations.

These phenomena are at the center of the so-called gaps in catalysis science. They describe catalysts as chemically dynamical systems interacting with the molecular dynamics of the reactants. Under such conditions the definition of active sites as elements of the bulk structure of a catalyst material becomes questionable as well as the concept of a surface where all constituents are active. Consequently the metrics of "activity" becomes a challenge. The often-practiced structural analysis of a catalyst outside its reaction environment describe a state of the system as far apart from the reacting state as "models" constructed from a-priori assumptions about the nature of the active state.

The contribution illustrates the role of in-situ techniques in discovering and analyzing such active states of catalysts. In consequence we may realize that the distinct difference between homogeneous and heterogeneous catalysis gradually vanishes under the unified concept of a dynamical active site resulting from catalyst-reactant interactions.

PL-7

Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level

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Our understanding of catalysis, and in particular heterogeneous catalysis, is to a large extend based on the investigation of model systems. The enormous success of metal single crystal model surface chemistry, pioneered by physical chemists, is an outstanding example. Increasing the complexity of the models towards supported nanoparticles, resembling a real disperse metal catalyst, allows one to catch in the model some of the important aspects that cannot be covered by single crystals alone. One of the more important aspects is the support particle interface. We have developed strategies to prepare such model systems based on single crystalline oxide films, which are used as supports for metal, and oxide nanoparticles, which may be studied at the atomic level using the tools developed in surface science.

However, those oxide films may also serve as reaction partners themselves, as they are models for SMSI states of metal catalyst. Using such model systems, we are able to study a number of fundamental questions of potential interest, such as reactivity as a function of particle size and structure, influence of support modification, as well as of the environment, i.e. ultra-vacuum or ambient conditions, onto reactivity.

The thin oxide film approach allows us to prepare and study amorphous silica as well as 2D-zeolites. Those systems, in spite of their complexity, do lend themselves to theoretical modelling as has been demonstrated.

PL-8

Fundamental Studies of Metal-exchanged Zeolites for Selective Catalytic reduction of Nitrogen Oxides in Oxygen Excess

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Selective catalytic reduction with ammonia (NH_3-SCR) is a well-established and effective method to eliminate nitrogen oxides (NO_x) in oxygen excess for stationary and mobile applications. For the latter case vanadia supported on titania was the first NH_3-SCR catalyst that was commercialized. This catalyst is highly effective around 350-450°C, however at lower or higher temperatures, the efficiency of the catalyst to reduce NO_x decreases. Furthermore, problems like toxicity of volatile vanadium compounds and high activity to oxidize sulfur dioxide have promoted the development of alternative catalysts. Zeolite systems are in this connection interesting candidates. Presently, iron- and copper-exchanged zeolite structures are the most attractive alternatives to the traditional vanadia-based SCR catalyst. However, several challenges arise when using metal-exchanged zeolites in exhaust gas after-treatment systems for vehicles. Two of the more important issues are the hydrothermal stability and the tolerance against chemical poisoning. Furthermore, the possibility to control the distribution of the metal species in the zeolite by thermal treatment during the preparation or after deactivation is another important aspect of metal-exchanged zeolite structures.

The first part of this lecture will focus on iron-exchanged zeolite beta, Fe-BEA, as NH_3-SCR catalyst. The deactivation of Fe-BEA after hydrothermal treatment, and phosphorous and potassium exposure has been studied experimentally and by kinetic modeling as well as activation and regeneration of the catalyst using hydrogen treatment. The fundamental mechanisms for thermal and chemical degradation of Fe-BEA will be presented and discussed. Furthermore, the activation and regeneration of the catalyst by hydrogen exposure will be discussed. The second part of the lecture will focus on copper-exchanged zeolite structures. The solid-state ion-exchange of different types of zeolite structures from copper oxides has been studied experimentally in different atmospheres. It is shown that the copperexchange is possible at unprecedented low temperatures, as low as 250°C, when facilitated by ammonia. The influence of the treatment conditions on the copper-exchange and the mechanism of the ion-exchange process will be presented and discussed. Such copperexchanged zeolite structures with high copper loading are potentially interesting catalysts for a number of technical applications.

Keynote Lectures

V-KN1

Catalytic Wastewater Treatment

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Although the water resource is not exhaustible, the water quality must be preserved, which does represent a major challenge for the coming decades. Water is extremely useful on a daily basis for many different industrial, agricultural and domestic applications. As a result of all these different uses, a wide variety of waste effluents is being produced everyday all over the world. The lecture will concentrate on such wastewater but not on the treatments involved upon the production of drinking water. While conventional wastewater treatment plants, mainly based on biological processes, are quite efficient for the purification of low concentrated, non-toxic and biodegradable wastewater, new solutions had to be imagined for the treatment of toxic and/or non-biodegradable and/or highly concentrated effluents.

Many different approaches have been investigated, numerous combinations have been tested but none of the alternatives developed up to now might be considered as universal. None of them is really better than the other: the more tools in the toolbox, the better.

Before selecting one technology over another, many different parameters have to be considered including the composition of the effluent, the concentration of the pollutants, the physical and chemical characteristics of the wastewater (pH, ionic force, turbidity, etc.), the volumes to be treated, as well as some engineering and economical aspects, etc. The final objective of the treatment is also to be taken into account, i.e. whether the pollutants should be totally mineralized or the treated effluents should only be made biodegradable or the organic content should be recovered to produce new chemicals and/or materials.

Among the possibilities, catalytic processes may play a crucial role, especially when the reaction conditions need to be made milder and/or when the process has to be ran faster and/or whenever selectivity issues are of major concern. Again, different options have been evaluated, including both reduction and oxidation processes.

Key examples taken from the recent literature will be presented all along the lecture, trying to combine different aspects and approaches, going from the development of innovative catalytic materials till the mechanistic information. Looking at the reduction processes, both the hydrodehalogenation and the catalytic reduction reactions will be briefly reviewed and the major challenges to be overcome will be highlighted both in terms of material science or catalytic efficiency (activity and selectivity). Finally, most catalytic oxidation processes will be listed, especially the advanced oxidation processes (AOPs), involving the hydroxyl radicals as the active oxygenated species; and the catalytic wet air oxidation for the most complex type of effluents. The main achievements and the key issues in the different fields will be identified.

II-KN2

Lewis Acid-base Catalysts for the Synthesis of Fine Chemicals

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Particle size is one of the key parameters determining the electronic properties, and as a direct consequence, the catalytic behavior of the supported metals. Sub-nanometric particles were already reported to exhibit beneficial Lewis acid properties for the control of both the activity and selectivity in reactions of importance [1]. However, specific Lewis properties can also be induced in nano-supported metal catalysts.

Based on this importance, the synthesis of metal and alloy nanoparticles of controlled size and shape become a hot topic. Unique properties at the interface between molecular structures and bulk materials can be thus induced following a rational design [2]. Typically, this occurs under strong reduction conditions and requires the presence of a stabilizer able to preserve the above properties.

The aim of this lecture is to present the synthesis of different Lewis acid-base catalysts for the synthesis of fine chemicals. First part will discuss metal- (Pd, Ru, Au, Pt, Ir) and alloy- (Pd-Au) nanoparticles and their catalytic behavior, focusing on the selectivity effects induced after their immobilization onto inorganic carriers. The preparation of the catalysts exhibiting metal Lewis acidity was carried out using several routes: i) the reduction of inorganic metal salts with Na[$AlEt_3H$] or Na[BH_4] [3-8] followed by the embedding of the resulted colloids in inorganic matrix supports using the sol-gel techniques (SiO_2, ZrO_2, SiO_2-Ta_2O_5]; ii) reduction of the organometallic complexes under supercritical CO_2 conditions followed by the ionic liquid stabilization of the resulted nano-particles [9]; iii) ionic exchange and deposition/precipitation of the noble metals onto zeolites and metal oxides [10-11]; and iv) impregnation of noble metals onto oxifluoride supports [12].

Second part will consider Lewis nano-base catalysts prepared via hydrolysis of $Mg(OCH_3)_2$ in a methanol–toluene mixture.

The characterization of these catalysts evidenced in all the cases the presence of the Lewis acid or basic centers. The concentration of these centers was correlated with other properties as particle size and shape, dispersion, etc that were determined using an ensemble of techniques: adsorption-desortption of N_2 at 77K, *in situ* FTIR measurements, DR-UV-Vis, SAXS, XRD, XPS, SEM, TEM, Mossbauer spectroscopy, etc. [2-6].

Finally, the talk will try to associate all these characteristics with the selectivity effects. The effect of the *Lewis acidity* in nano-particles was checked in various reactions like hydrogenation of C=C bonds in simple molecules like styrene or different cycloalkenes, hydrogenolysis of complex molecules like 1,1a,6,10b-tetrahydro-1,6-methanodibenzo[a,e]cyclopropa[c] cycloheptenes, diastereoselective hydrogenation of C=O versus C=C in un-saturated aldehydes and ketones like cinnamaldehyde or prostaglandin derivatives, or reduction of nitric oxides with hydrocarbons. The modification of the supported metal nano-particles by asymmetric ligands like Synphos and cinchonidine will be also discussed comparatively with the homogeneous systems in the selective hydrogenolysis of bicyclo[2.2.2]oct-7-enes and hydrogenation of ethyl pyruvate. The effect of *Lewis basicity* was checked in transesterification reactions.

Conclusions

A correct electron density in metal nanoparticles may lead to very high selectivities, and even activities, in complex reactions. Since there are still many reactions for which the selectivity levels are un-satisfactory future developments in the preparation control of such catalysts are necessary.

Acknowledgements

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IV-KN3

Design of Supported Molecular Catalysts for Organic Synthesis

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1 Introduction

Molecular rhodium metal-ligand complex catalysts are a highly versatile class of catalysts used in both bulk chemical production (e.g. hydroformylation) and in the synthesis (e.g. asymmetric hydrogenation) of high value complex organic molecules, such as pharmaceuticals. In all cases, due to the cost of rhodium and in the latter case the ligands, achievement of high turnover numbers (TONs) is critical. This has led to the exploration of methodologies to increase the TONs of these catalysts by catalyst recovery and recycle. This presentation will describe our development of supported asymmetric dirhodium complex catalysts for cyclopropanations and C-H activation mediated catalytic coupling reactions [1,2]. The catalyst behavior, including reaction and substrate scope, will be initially described in batch reactions. Subsequently, a new design of a flow reactor for deployment of solid catalysts based on polymer/oxide hollow fibers will be described [3].

2 Experimental/methodology

A silica-grafted analogue of the well-known $Rh_2(DOSP)_4$ catalyst that reacts donor-acceptor diazonium compounds with various coupling partners via carbene-mediated reactions was prepared as described in the literature [2]. The obtained catalysts were used in an array of asymmetric cyclopropenation and cyclopropanation reactions, as well as coupling reactions that proceed via catalytic C-H activation, including (i) tandem ylide formation/[2,3] sigmatropic rearrangements with allylic and propargylic alcohols and (ii) combined C–H functionalization/Cope rearrangements in a batch reactor.

Cellulose acetate / oxide composite hollow fibers were also prepared as microfluidic flow reactors [3]. The oxide particles included porous silica particles as well as zeolites. To the silica particles, well-defined molecular catalysts could be grafted, and both an organocatalyst (primary aminopropyl fragments) and organometallic catalyst ($Rh_2(DOSP)_4$ analogue described above) were grafted to the silica particles within the fibers. The fibers were then used as flow reactors for an array of reaction types important in organic synthesis, including a deprotection reaction (BrØnsted acid zeolite), a coupling reaction (aminopropyl catalyst), and a series of asymmetric coupling reactions (dirhodium carneoid catalysts).

3 Results and discussion

A wide array of asymmetric coupling reactions were conducted using both the silica-supported dirhodium carbenoid catalyst in batch, with product yields and ee's being comparable in most cases (Fig 1).

Three catalysts were also incorporated into composite polymer/oxide hollow fibers. The fibers containing acidic ZSM-5 zeolite are demonstrated to effect the deprotection of benzaldehyde dimethyl acetal in flow. In addition, fibers containing silica-grafted aminopropyl organocatalysts are shown to efficiently catalyse the Kneovenagel condensation of benzalde- hyde and malononitrile in flow. Finally, the dirhodium carbenoid catalyst is demonstrated to catalyse some of the same reactions studied in batch in flow. Fig. 2, below, shows that excellent performance was obtained in flow even after 1000 turnovers were achieved.

Fig 1. Array of products obtained in asymmetric cyclopropanations, cyclopropenations, as well as C-H coupling reactions catalysed by dirhodium carbenoid catalysts.

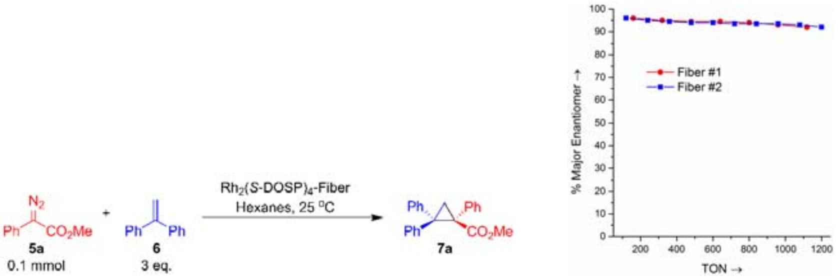

Fig 2. Asymmetric cyclopropanation in flow using dirhodium carbenoid catalyst over 1000 turnovers.

4 Conclusions

A new supported dirhodium carbenoid catalyst supported on porous silica is reported for a variety of asymmetric coupling reactions. This catalyst shows good activity and selectivity, closely paralleling the performance of the parent homogeneous catalyst, $Rh_2(DOSP)_4$. The catalyst is exploited in both batch reactions and in a novel, polymer/oxide hollow fiber microfluidic reactor. The hollow fiber reactor is demonstrated to be a new mode of facilitating catalyst-reagent contacting while carrying out organic synthesis in flow.

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III-KN4

Catalysis to Produce Solar Fuels. Status and Challenges

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1 Introduction

Realize a sustainable, resource-efficient and low-carbon economy is a major current challenge for society [1,2], but there are main issues to couple the renewable energy sources with the actual energy infrastructure, even considering smart grids. All renewable energy sources except biomass still suffering of major problems of storage and transport at long distance, as well as integration in the industrial production chain. CO_2 conversion to (liquid) fuels using renewable energy sources, e.g. the production of solar fuels, appears as the preferable and more sustainable solution to above problems and to avoid very large investments. The chemical (re)use of CO_2 using renewable energy thus become a key aspect towards the more general goal of resource and energy efficiency, because combines the reuse of a waste and of a relevant carbon sources to the reduction of fossil fuel use as well as GHG and pollutants emissions [3,4]. At the same time, catalysis to produce solar fuels has a major impact in reshaping the future of chemical production and low-carbon bioeconomy. We limit discussion here to the concept of solar fuels as those deriving from the conversion of CO_2 using renewable source of energy to synthetize the products of reaction [5].

2 The impact on scenario for sustainable energy/chemical production

There are many major changes in the chemical production, necessary to respond to the request of a resource and energy efficient sustainable future and to move to a low carbon economy. The use of alternative raw materials is between these driving forces. Biomass as chemical feedstock, (re)use of CO_2, waste valorisation, use of renewable energy, use of fossil fuels alternative to oil (actually accounting for majority of petrochemistry production), from shale gas to coal, are between these driving elements [2,3]. There is a change from the current (oil-centred) petrochemistry to the future of chemical production based on a larger use of alternative raw materials and of renewable energy sources. The lecture will shortly introduce this changing scenario and the impact on moving to solar fuels in this general panorama [3,4].

Solar fuels are a key element to move to a low-carbon bioeconomy [6]. Depending on the model for biorefineries, different options may be possible to integrate bio- and solar-refineries. In the energy biorefinery, where biofuels are the characterizing element, the utilization of CO_2 and renewable energy has the main scope to decrease the carbon footprint and at the same time increase the productivity in energy products. In biorefineries where chemicals are the main product (biofactories) the scope is instead different and the target is the optimal integration of CO_2 utilization within the value chain. However, a range of different other cases are also possible. The lecture will shortly discuss some of the possibilities for new sustainable biorefineries and the opportunities to integrate renewable energy sources in the biorefinery production (solar biorefineries).

There is a changing panorama for bio-based production, with new opportunities offered by the integrated utilization of CO_2 and renewable energy to move to a sustainable and low-carbon bioeconomy.

3 Options and opportunities for solar fuels

There are four main options to implement solar fuels and realize energy efficiency:

- A resource & energy efficiency chemical production, with the objective to reduce the use of fossil fuels as raw material and energy vectors, and to introduce renewable energy in the chemical production chain [2-4].
- Import unexploited renewable energy (RE) resources, via renewable H_2 (water electrolysis) using remote RE sources and CO_2 conversion to methanol or other CO_2-derived energy vectors, and production of solar fuels and chemicals [7].
- Local storage on RE in smart grids, with the main example being power-to-gas (CO_2 to CH_4) [8].
- Develop artificial leaves, in a long-term, for distributed production [9,10].

The lecture will comment these options, their status and opportunities.

4 Moving to artificial leaves

After analysing the motivations why chemical energy storage is the key for a sustainable use of solar energy, and some of the recent progresses in producing solar fuels and related devices, the discussion will be focused on the analysis of the critical elements of artificial leaves to consider for the development of next-generation solar photoelectrocatalytic (PEC) devices [9,10]. There are many challenges to be addressed to realize with good efficiency this process, from the challenges in the electrocatalysts to the understanding of the coupling of the fast processes of charge separation with the slower (at least three order of magnitude) processes of catalytic reduction and charge transfer [11,12]. There is the need to understand this chemistry and to analyse the role of advanced design in nanomaterial to control these processes. Transport processes and reactions at the interface are often dominating the overall performances. Thus, the development of the single components should proceed in parallel with the device development, and not separate as currently. Integrated nano-engineering of materials and devices is the challenge to address properly above problem and to enable the practical implementation of artificial leaf-type devices [13-15]

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V-KN5

Carbon Dioxide as Carbon Source for the Energetic and Chemical Value Chain: Challenges and Opportunities for Catalysis

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The finite resources of fossil feedstock together with the increase in anthropogenic emission of carbon dioxide (CO_2) are a major concern of global importance. The use of CO_2 as carbon source offers the possibility to contribute to sustainable processes at the interface of the energy and chemical supply chains.

This presentation highlights some of the key scientific challenges associated with these concepts and demonstrates how catalysis research combining molecular and engineering sciences provides key contributions to this area. The general aspects and current trends in academia and industry [1] are illustrated with examples concerning the development, application, and mechanistic understanding of catalysts and catalytic systems for the selective conversions of CO_2 to formic acid [2] and higher carboxylic acids [3], to methanol [4] and for methylation [5], and for polyurethane synthesis [6]. Possible applications include the use of CO_2 as C1-building block for fuels and polymers, as well as for chemicals and pharmaceuticals.

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II-KN6

Electron Microscopy Advances in Catalysis

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In recent years, electron microscopy has made significant progress for the study of solid materials at the atomic-scale. Advancements in electron optics and data acquisition methods have made electron microscopy capable of delivering images with sub-Ångström resolution and single-atom sensitivity [1-3]. Parallel developments of gas cells, sample stages and micro-electro-mechanical system devices have made high-resolution electron microscopy available for *in situ* observations of solid materials during exposure to reactive gas environments at pressures up to atmospheric levels and temperatures of up to several hundred centigrade [4-6]. It is desirable to take advantage of these emerging technologies in the study of heterogeneous catalysts because they provide unique information about surface structures and dynamics.

In this contribution, I will outline advances in electron microscopy that enable observations of catalysts at atomic-resolution and in catalytically meaningful environments. Their application will be illustrated with studies within e.g. hydrotreating, methanol synthesis and diesel automotive exhaust abatement catalysis [1-11]. Moreover, it will be discussed how the atomic-scale observations can beneficially be combined with reactivity data, calculated or measured, from simpler model systems. Hereby, the description of the dynamic functions and properties of catalysts can be extended with information that is specific to the exposed surface sites, which, in general, should contribute to the continued development of new and better catalysts.

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IV-KN7

Chemical Photocatalysis Using Visible Light

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The use of visible light for organic synthesis is a very old idea: More than 100 years ago the Italian chemist Giacomo Ciamician discovered and promoted the field. Recently, photoredox chemistry mediated by metal complexes, such as ruthenium-trisbipyridine, or organic dyes, such as eosin or perylenediimides, gained enormous interest for applications in organic synthesis.

We present some of the recent results using photoredox catalysis with visible light from our laboratory including photooxidations, oxidative C-C bond formation and arylation reactions utilizing one or two photons for activation.

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V-KN8

Exploiting Acid-base Cooperativity in Metalloenzyme-like Lewis Acid Zeolites for Biomass Conversion

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1 Introduction

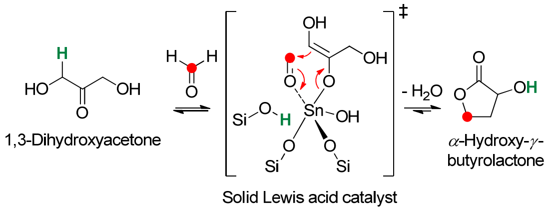
In our efforts to shift away from traditional petroleum-based raw materials to supply fuels and chemicals, biomass has emerged as an attractive renewable carbon-containing feedstock. Its complex chemical diversity has created daunting challenges that require the implementation of robust, active, and selective catalysts to effectively transform it into useful products. In this lecture, new developments in the use of Lewis acid zeolites will be presented in the context of converting biomass-derived oxygenates into value-added products. Specific examples will be presented highlighting the role that catalytic pairs play in enhancing the activation of targeted functional groups, achieving cooperative catalysis, or promoting one-pot cascade reaction sequences. Lewis/Brønsted acid pairs will be discussed in the context of hydrolysis/transfer hydrogenation cascades for the conversion of furfural into gamma-valerolactone, while Lewis acid/base pairs will be discussed in the context of cooperative C-C coupling of oxygenates, including coupling of hydroxyacetone with formaldehyde to form α-hydroxy-γ-butyrolactone (HBL), i.e. a chemical intermediate used for production of pharmaceuticals.[2]

2 Experimental/methodology

Reactivity studies were performed in batch and flow reactors at between 80 and 160 °C using 1,4-dioxane, toluene, water or acetone as solvents, and a metal:oxygenate ratio of 1:100 and a oxygenate:formaldehyde ratio of 1:3 [1]. Sn-Beta was synthesized based on a procedure reported by Corma et al. [3]. Details on the characterization of the catalysts can be found in publication [4].

3 Results and discussion

As a representative example of C-C coupling, the production of HBL will be discussed in more detail. Sn-Beta zeolites effectively catalyze the C–C coupling reaction between DHA and formaldehyde, yielding up to 60 % HBL at 98% conversion after 3 h [1]. Byproducts observed were lactic acid and (1,3-dioxolan-4-yl)methanol. The conversion pathway of DHA into HBL involves consecutive aldol condensation, 1,2-hydride shift, dehydration, intramolecular hemiacetal and keto–enol tautomerization reactions. Of particular importance in this pathway is the aldol condensation step, as our reactivity studies, coupled with spectroscopic and computational analyses, corroborate a mechanism involving soft enolization of DHA followed by an aldol addition of formaldehyde to the Sn-enolate intermediate, generating erythrulose as an intermediate species. More specifically, in our proposed mechanism, the framework Sn atom polarizes the carbonyl group of DHA, resulting in a substantial increase in the acidity of the α-proton. This proton can be removed by the basic oxygen atom connected to Sn, generating a Sn-enolate intermediate and a silanol group (Scheme 1). Coordination of the oxygen atom of formaldehyde to the Sn center induces polarization in the molecule, further enhancing its reactivity by increasing the electrophilicity of the aldehyde carbon



Scheme 1. Proposed soft enolization pathway for the catalytic C–C coupling between DHA and formaldehyde using Sn-Beta zeolites.

Formation of the aldol addition product erythrulose as a reaction intermediate in the production of HBL was substantiated by using it as a reactant in place of DHA. A reaction of erythrulose with Sn-Beta under identical conditions as those used for DHA generated a 24% HBL yield, thus confirming that erythrulose can undergo the suggested transformation. To further support our hypothesis, isotopically labeled formaldehyde was reacted with DHA in the presence of Sn-Beta and investigated using GC-MS and 13C NMR. The mass spectrum of the product mixture agrees with that obtained from the reaction with unlabeled formaldehyde, but is shifted by m/z = 1 to higher m/z ratios. Specifically, the main fragment ion at m/z 58, corresponding to the resonantly stabilized species 13CH2=CH–CH+–OH, indicates that HBL contains the 13C label at the C4 position. This was corroborated by 13C NMR, which showed a main resonance at δ = 65.2 ppm corresponding to the C4 atom. The highly selective incorporation of 13C atoms can indeed be rationalized by considering the proposed C–C bond formation mechanism. Formation of erythrulose is calculated to proceed exothermically with a ΔG0 value of 0.4 kJ mol−1, which, although slightly positive, compares favorably to 16.8 kJ mol−1 for the previously proposed aldol condensation of pyruvic aldehyde with formaldehyde into 4-hydroxy-2-oxobutanal [4]. The estimated ΔG0 values of the ring closure and 1,2-hydride shift are -49.1 and -57.0 kJ mol−1, respectively, strengthening the feasibility of the reaction mechanism shown in Scheme 1. Although this abstract is not meant to divulge detailed spectral data, we note that we were also able to observe formation of C5 sugars, indicating the occurrence of two consecutive aldol condensation reactions

4 Conclusions

Catalytic pairs represent a powerful, yet relatively unexplored, strategy for the selective activation of oxygenates. Akin to metalloenzymes, Lewis acid zeolites can be engineered to feature catalytic pairs and catalyze reactions with high activity under mild conditions. In particular, the development of catalytic C–C bond formation schemes based on renewable substrates is of importance to define sustainable paradigms for chemical manufacture. With a few exceptions, aldol condensation reactions between biomass-derived platform chemicals using heterogeneous Lewis acid zeolites have received little attention so far.

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II-KN9

Real-time Analysis of Catalytic Reactions Using Simultaneous Orthogonal Methods

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Powerful insights into catalytic mechanisms can be acquired through direct observation of intermediates while the reaction is being carried out. Numerous spectroscopic and kinetic tools have been utilized for this purpose, and our focus has been on developing real-time methodologies to allow electrospray ionization mass spectrometry (ESI-MS) to reliably perform this task in real time. Fast and sensitive and with a high dynamic range, ESI-MS is capable of handling the complex soup of components that is an evolving catalytic reaction. With the use of charged tagged substrates and continuous infusion of sample, the reactants, products, byproducts, catalyst resting state, decomposition products and abundant intermediates can be measured simultaneously and reproducibly at a sampling rate of 1 s^{-1}. However, by offloading the task of assessing reaction progress to an orthogonal method, the overall dynamic range can be increased to over 5 orders of magnitude, i.e. real time analysis of species present at part-per-million levels during reactions performed at typical concentrations (0.1 M). Examples of our approach will be presented in the context of a variety of transition-metal catalyzed reactions, including various palladium-catalyzed cross-coupling reactions and rhodium-catalyzed hydrogenation and hydroacylation reactions.

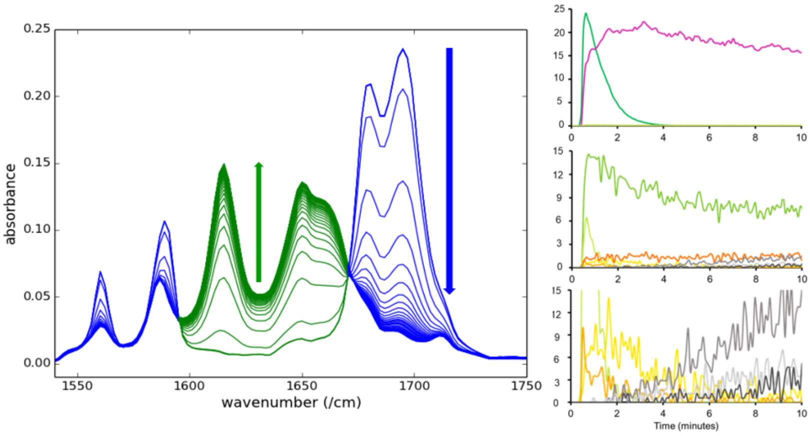

Figure 1. Complementary real-time spectroscopic and spectrometric data from a catalytic reaction.

IV-KN10

Base Metal Catalysis for Cross Coupling and Addition Reactions

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1 Introduction

The advancement of catalysis has had a significant impact on society. As chemists strive to improve the efficiency of chemical synthesis and to enable green and renewable energy conversion and storage technologies, fundamental research in catalysis is as important today as at any time in the past. Base metal catalysis, where the catalysts contain only elements abundant in the earth's crust, offers potential advantages in cost, availability, scalability, and sometimes compatibility with health and the environment. In this talk, I will present our recent work in base metal catalyzed cross coupling reactions and functionalization of alkenes and alkynes.

2 Experimental/methodology

Cross coupling of alkyl halides is challenging because metal alkyl intermediate species are prone to unproductive beta-H elimination. We have applied Ni, Cu, and Fe-based catalysts for these reactions. We also employ well-defined metal complexes as mechanistic probes.

Alkynes and alkynes are readily available and inexpensive feedstock chemicals. We have developed Fe and Cu catalysis to transform these unsaturated molecules into higher-valued compounds through addition reactions.

3 Results and discussion

We developed a well-defined Ni catalyst, Nickamine, that catalyzes the alkyl-alkyl, alkyl-aryl, and alkyl-alkynyl Kumada coupling of activated alkyl halides, as well as direct alkylation of alkynes and heterocycles (Figure 1).[1-5] The mechanism of these reactions was thoroughly studied using radical probes, kinetics and DFT computations.[6,7] We also studied the mechanism of analogous Fe-catalyzed alkyl-aryl Kumada coupling using defined Fe pincer complexes.[8] A common bimetallic oxidative addition reaction pathway involving alkyl radical intermediates was found for these coupling reactions.

We discovered that Fe catalysts could be used to promote the 1,2-addition of perfluoroalkyl iodides to alkynes and alkenes.[9] The resulting perfluoroalkylated alkyl and alkenyl iodides could be further functionalized by cross coupling reactions. Further investigation showed that copper catalysis can be used to promote the 1,2-addition of alpha-carbonyl iodides to alkynes,[10] resulting beta,gamma-unsaturated ketones which are an important class of organic molecules.

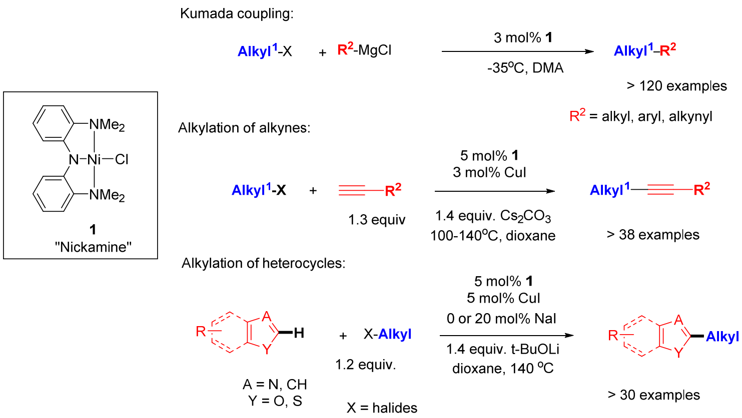

Fig. 1. Cross coupling-type reactions catalyzed by Nickamine.

4 Conclusions

We have developed efficient base metal catalysis for some important organic reactions such as cross coupling and alkene and alkyne functionalization. The complex mechanism of these reactions is started to be elucidated, showing unique features compared with precious metal catalysis.

Acknowledgements

We thank the EPFL, the Swiss National Science Foundation, and the European Research Council for financial support.

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I-KN11

Catalysis in Confined Space – from Zeolites and Zeotypes to Functionalized Metal-organic Frameworks

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More than a decade of systematic studies of zeolite- and zeotype-catalysed reactions have revealed how confinement effects may alter the rates of individual reactions, as well as the selectivity of complex reaction networks (see e.g. [1-2]).
A parallel, large research effort is targeting another class of nanoporous solids, metal-organic frameworks (MOFs), as a next generation sorbents and catalysts. Ideally, MOFs offer a wide variety of functionalities and pore sizes. However, synthesis as well as chemical, thermal and mechanical stability issues may restrict their applicability. In this lecture, focus will be set on the Zr-MOF series developed at UiO [3-5]. Studies of chemical stability and mechanical strength, catalyst formulation and catalyst performance (ethene oligomerisation, CO_2 reduction) will be presented.

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I-KN12

Development of New Catalytic Materials for Sustainable Production of Chemicals

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Our comfortable modern life is supported by numerous chemical, in particular petrochemical, products. At present, petrochemical industry is based on lower olefins that are produced by thermal cracking of petroleum naphtha in Southeast Asia and Europe. We need to develop the methods for manufacturing chemical products from more substantial fossil resources if possible, and for the long term, preferably from renewable resources.

To develop new technologies of efficient and sustainable production of lower olefins that could replace the conventional thermal cracking process**,** we have tried to improve the catalytic performance of zeolites in catalytic naphtha cracking that occurs at much lower temperature and gives higher selectivity for propylene than thermal naphtha cracking. The critical matter is the elongation of catalyst duration time. There are two main causes for the activity loss, coke deposition and dealumination. Several methods for mitigating the deactivation have been developed.

Because of the shale gas revolution, the use of methane as chemical feedstock as well as fuels is attracting widespread attention. At this time methanol is considered as getting more available chemical feedstock. While methanol production through direct oxidation of methane is extremely difficult, it is worth challenging. In any case, methanol to olefins (MTO) reaction is a promising route to the lower olefins. In this reaction, the deactivation as a result of coke deposition is a critical problem. For the MTO reaction a large number of zeolites were screened and we have found CIT-1 (**CON**) zeolite is promising for selectively converting methanol to propylene and butenes without serious loss of activity.

While fossil fuels will be the dominant factor in the future energy and chemicals scenario for a couple of decades to come, we need to develop methods of alternative chemicals production. Compared to petroleum and natural gas, biomass has low H/C and high O/C ratios and low calorific value. Thus biomass could be useful for the production of chemical products that are not manufactured on a massive scale in the current petrochemical industry. It has long been recognized that 5-hydroxymethylfurfural (HMF) is a bio-based “platform” material for producing useful chemicals. Increasing research interest has been paid to the synthesis of HMF from sugars, particularly from glucose. We have found an effective transformation of glucose to HMF over Beta zeolite by finely tuning acid properties. The high Brønsted/Lewis acid ratio is a key factor for selective production of HMF from glucose. Meanwhile, a great deal of effort has been devoted to the production of sorbitol, as bio-based feedstock, from cellulose. For example, sorbitol can be converted to isosorbide (1,4:3,6-dianhydrosorbitol) through double intramolecular dehydration. Isosorbide can be used to produce polymers such as polyester and polycarbonate; Poly-(ethylene-co-isosorbide)- terephthalate is a bio-based alternative to polyethylene terephthalate (PET). Isosorbide can also replace bisphenol A in the production of polycarbonate and epoxy resins. We have developed highly active zeolite catalysts for the dehydration of sorbitol to isosorbide in water.

For a future sustainable chemicals scenario, it may be desirable to develop efficient methods for utilizing CO_2 by using renewable energy, which could be the ultimate goal. Photocatalytic decomposition of water by visible light, which accounts for a great majority of sunlight, is an enormous challenge and it is absolutely necessary to activate the research in this field. In Japan a 10-year METI (Ministry of Economy, Trade and Industry)-sponsored national project that targets the recycling CO_2 by using solar H_2 started in 2012. This project is named ARPChem (Artficial Photosynthesis of Chemicals). At this moment this project focuses on the production of light olefins as chemical feedstock. We are developing the process consisting of methanol synthesis from CO_2 and H_2, followed by the MTO reaction catalyzed by zeolites.

V-KN13

Progress and Challenges in Urea/SCR Technology for Removing NOx from Diesel Engine

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The advent of energy-efficient automotive diesel engine has significantly reduced its fuel consumption and CO_2 emission to atmosphere in recent decades [1]. From an environmental point of view, however, the emissions of atmospheric pollutants including nitrogen oxides (NOx) from the diesel engine become a primary concern, while CO and HCs can be readily oxidized by a diesel oxidation catalyst (DOC) commonly installed into diesel after-treatment system under lean operating condition. The abatement of NOx from the diesel engine exhaust is thus one of the critical issues for the commercial implementation of the modern energy-efficient diesel engine technology.

Among promising NOx reduction technologies currently available, the LNT and the SCR technologies are the two leading ones despite their inherent shortcomings still remaining as important technical issues to be resolved [2-3]. A practical advantage of the urea/SCR technology over the LNT rests on the fact that it does not require the use of a large amount of noble metals and complex engine controls which is the essential requirement for the LNT technology [4]. The HC/SCR technology lags behind due primarily to its insufficient low-temperature activity and narrow temperature window on top of its poor tolerance toward H_2O and SO_2 [5].

The urea/SCR technology is undoubtedly one of the commercially proven, reliable and available technologies to meet the stringent worldwide environmental regulations including EURO VI and SULEV for reducing NOx emissions from diesel engine [1,6-7]. The V_2O_5/TiO_2 catalyst has been employed as the conventional SCR catalyst especially for the removal of NOx from stationary sources [8,9]. However, V_2O_5/TiO_2 may not be active in the diesel exhaust temperature ranging from 150~250 ^{o}C for light duty diesel engine to 200~350 ^{o}C for heavy duty one, and zeolite based-catalysts including ZSM5 and SSZ13 have then been regarded as the promising urea/SCR catalyst to be directly applied to the diesel after-treatment system [10-12]. In recent years, a number of efforts for further improving the low-temperature activity as well as the stability of the urea/SCR catalysts have been underway for their implementation to the next generation vehicles equipped with the advanced diesel engines.

In this presentation, the progress and challenges in the urea/SCR technology to remove NOx from diesel engine will be reviewed in the topics ranging from the underlying catalysis to the recent research trend and commercial applications. Included in the discussion will be the promoted V_2O_5/TiO_2 catalyst by the modification of catalyst support [13,14] as well as the bimetallic catalyst systems aimed at improving the low temperature activity of the current urea/SCR catalysts and their catalytic characteristics [15,16]. In addition, the local environment of active sites in CuSSZ13, currently regarded as the most promising low-temperature SCR catalyst, will be discussed by ESR and XANES studies in order to understand its strong thermal stability [17]. Also presented will be the tolerance of CuSSZ13 toward CO_2, recently reported as a new deactivating precursor for the urea/SCR catalyst [18].

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II-KN14

Approaching Complexity in Heterogeneous Catalysis by Density-Functional Modelling

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1 Introduction

Key elements of nanomaterials for current and prospective applications often consist of many thousands of different atoms and thus remain inaccessible for the first-principles (based on Density Functional Theory, DFT) computations due to their size and complexity. However, such systems could be quite realistically represented by computationally tractable smaller model nanoparticles and their aggregates, whose surface structure and reactivity reveal only weak or monotonic size dependence.

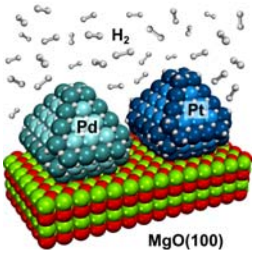

Fig. 1. Models for studies of hydrogen absorption in MgO(100)-supported 1.6 nm large Pd_{127} and Pt_{127} particles with surfaces saturated by hydrogen [8].

2 Results and discussion

We address various problems related to approaching complexity of multicomponent nanomaterials for heterogeneous catalysis and energy technologies in the frameworks of DFT electronic structure modelling.

Among the discussed questions are:

(*i*) To what extent commonly used slab models represent surface properties of metal and metal-oxide nanostructures?
(*ii*) How to design and handle more realistic models?
(*iii*) How significant are interactions at the interface of metal nanoparticles with supporting oxide materials of different kinds and degrees of ordering?
(*iv*) How important are surface coverage effects?
(*v*) Are there reliable ways to computationally optimize chemical ordering of metal components in sufficiently large bimetallic nanoparticles?

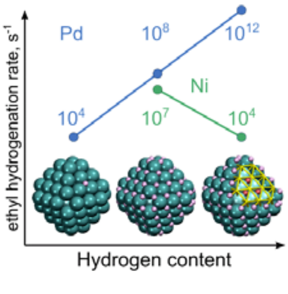

Fig. 2. Subsurface hydrogen can modify the stability and the reactivity of the adsorbed hydrogen in two different ways: in the presence of subsurface H a representative reaction of ethyl hydrogenation is calculated to be strongly accelerated on Pd (Pt), but slowed down on Ni (Rh) [7].

3 Conclusions

The presented results illustrate the current state of advanced theoretical models in heterogeneous catalysis. A general conclusion is that to provide realistic enough description of complex experimentally relevant catalytic systems and processes at affordable computing cost, the models need to be *as simple as possible, but not simpler*.

Acknowledgements

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III-KN15

Operando Studies on PdZn-ZnO, (Pd-)Co_3O_4 and Ni-ZrO_2: Synergies between Surface Science Based Model Systems and Technological Catalysts

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Our group´s philosophy is to study catalytic surface reactions on heterogeneous catalysts *via a two-fold approach,* employing both *surface science based planar model catalysts* as well as *industrial-grade catalysts* [1-3]. For both, the focus is on examining *active functioning catalysts* under *operando* conditions, at (near) ambient pressure and at elevated temperature (Figure 1).

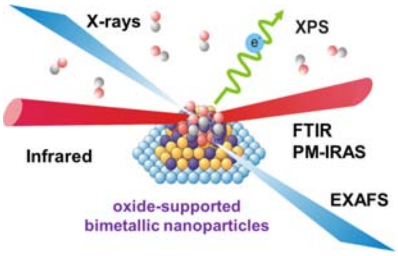

Figure 1. Schematics of spectroscopic studies of functioning catalysts; from [3].

In particular for ultrahigh vacuum (UHV) based model catalysts that has been a challenge, requiring application of *in situ surface spectroscopy*, such as sum frequency generation (SFG) laser spectroscopy, polarization-modulation infrared reflection absorption spectroscopy (PM-IRAS) and near ambient pressure x-ray photoelectron spectroscopy (NAP-XPS) [1]. To image ("see") ongoing surface reactions by *in situ surface microscopy*, photoemission electron microscopy (PEEM) was applied to polycrystalline samples [2]. For technological catalysts, analogous *operando* studies were performed by Fourier transform infrared spectroscopy (FTIR), x-ray absorption spectroscopy (XAS), near ambient pressure x-ray photoelectron spectroscopy (NAP-XPS), and x-ray diffraction (XRD) [3]. Most of the operando studies were performed at synchrotron sources (BESSY (DE), MaxLab (SE), SLS (CH)), and in lock-step with theory.

This two-fold approach yields a better "*holistic*" view of the catalytically relevant atomic and electronic surface structures of catalysts, as well as of molecular details that steer reaction activity and, even more important, reaction selectivity. Comparing surface science based single crystals with nanoparticle model catalysts elucidates the *materials gap*, and comparing UHV to ambient pressure studies reveals the *pressure gap*. In particular, synergisms between studies on model and technological catalysts often provide access to atomistic details.

Among the systems studied are
i) hydrogen generation by methanol steam reforming on alloy (intermetallic) catalysts, i.e. PdZn surface alloys on Pd(111) single crystals [4] and PdZn nanoparticles supported on ZnO [3],
ii) CO oxidation on noble metals [2], thin films and commercial cobalt oxides (Co_3O_4 and CoO),
iii) CO and water adsorption, and methane reforming on Ni-ZrO_2, employing an ultrathin ZrO_2 trilayer (O-Zr-O) film on $Pt_3Zr(0001)$ [5] as well as commercial ZrO_2 as support [6].
The combined studies provide detailed mechanistic insight, e.g. on i) the effect of PdZn thickness, surface corrugation and valence band structure on selectivity, ii) locally-resolved catalytic ignition, surface oxide formation/reduction, oxygen vacancy formation as well as carbon balance, iii) electronic structure of ultrathin oxides, and gas-induced oxide and nanoparticle reconstructions. Very recently, we have applied the operando NAP-XPS approach to examine electrochemical water splitting on perovskite-type electrodes under potential control, elucidating polarization-driven changes of surface composition and their effect on reaction kinetics [7].

Acknowledgements
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III-KN16

Photocatalytic Overall Water Splitting: Present and Future

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This lecture presents the research progress on solar fuel productions from photocatalytic and photoelectrocatalytic (PEC) processes with the emphasis on the fundamental understanding of the semiconductor-based photocatalytic and photoelectrocatalytic water splitting for solar fuel production.
The great challenge of energy conversion photocatalysis lies in its complicated processes including light absorption (harvesting), charge separation and migration, and redox reactions. In order to gain high photon energy conversion efficiency, a photocatalyst or photocatalytic system must harmonically guarantee high efficiencies of all these three processes instead one of them. Semiconductors with appropriate phase junctions have been demonstrated to be an efficient approach for achieving efficient charge separation [1]. Cocatalysts play important roles in the assembly of efficient semiconductor photocatalyst. It has been conceptually demonstrated Pt-PdS/CdS dual cocatalyst system can achieve 93% H_2 evolution activity in the presence of sacrificial reagents under visible light irradiation (l>420 nm) [2,3]. Recently, it has been also demonstrated that electrons and holes can be spatially separated on the {010} and {110} facets of $BiVO_4$ crystal [4]. It has been demonstrated that the intrinsic nature of charge separation between different facets of $BiVO_4$ together with the synergetic effect of dual-cocatalysts plays key role in photocatalytic activity enhancement [5]. This work opens up a new avenue for the assembly of semiconductor crystal based artificial photosynthesis system by selectively loading of dual cocatalysts on the different facets.
Alternative approaches other than powdered semiconductor system should be also highly considered, such as photoelectrochemical (PEC) and solar cell coupled with water electrolysis catalyst systems. A Ta_3N_5 photoanode coated with ferrihydrite (Fh) layer on which Co_3O_4 water oxidation cocatalyst ($Co_3O_4/Fh/Ta_3N_5$) was deposited, could yield a photocurrent of 5.2 $mAcm^{-2}$ at a potential of 1.23 V vs. RHE under AM 1.5G simulated sunlight irradiation. And remarkably, about 94% of the initial activity could be maintained even after 6 h irradiation, which is due to the avoidance of the corrosion of Ta_3N_5 via. efficient hole storage and transfer by the Fh layer [6]. A self-biased photoelectrochemical–photovoltaic coupled system consisting of FeOOH/Mo:$BiVO_4$ photoanode and a Pt/p-Si solar-cell-based photocathode showed h_{STH} of 2.5% under parallel irradiation [7].

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IV-KN17

Novel Catalytic Methods for Synthesis of Organic Building Blocks and Biologically Important Heterocycles

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We have developed a set of novel efficient transition metal-catalyzed annulation and cycloisomerization methodologies for synthesis of multisubstituted carbo- and heterocycles [1-22]. Traditionally, regioselective synthesis of carbo- and heterocycles possessing various functional groups is not a trivial task. We have shown, however, that incorporation of migrating step(s) in the cyclization cascade often helps solving this problem. Thus, it was found that in the presence of Cu-, Ag-, and Au catalysts, a number of groups, such as Hal-, RS-, AcO-, TsO-, Ar-, and SiR_3 could undergo 1,2- or 1,3-migration, or in some cases even double migration, which allows for expeditious synthesis of densely-functionalized carbo- and heterocycles, which are not easily accessible via existing techniques. Most of these transformations proceed via metal-stabilized carbene intermediates. The validity of vinylidene- and carbene intermediates in some of these cascade reactions was tested by means of DFT calculations. We have also developed new tri-component coupling reactions toward expeditious assembly of aminoindoline, aminoindole, and imidazopyridine cores. These methods were used for synthesis of libraries of small heterocyclic molecules for wide biological screening.

The scope of these transformations will be demonstrated and the mechanisms will be discussed.

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I-KN18

Design of Novel Hybrid Hierarchical Catalysts for Direct Synthesis

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1 Introduction

Dimethyl ether (DME) is one of the most promising environmentally optimized alternatives to conventional fossil fuels due to its high cetane index, low emission of CO, NO_x and particulates and reduced noise. DME can also be used as a substitute for liquefied petroleum gas (LPG). DME is biodegradable; it has low toxicity and does not corrode any metals. In addition, DME is an important intermediate for the production of useful chemicals (i.e. methyl acetate and dimethyl sulphate) and petrochemicals (light olefins, BTX aromatics). In the industry, DME can be produced from syngas using either two-stage or single-stage direct technologies. The two-stage technology is currently considered as the most mature route. In the first stage, syngas is converted into methanol over copper based catalysts. In the second stage, methanol is dehydrated into DME over acid catalysts. The maximum syngas conversion to methanol is limited by thermodynamics especially at high temperatures. The single-stage direct DME synthesis overcomes these thermodynamic constraints and leads to higher per-pass CO conversions and higher DME productivity. The direct DME synthesis, however, requires an efficient bifunctional catalyst. The crucial issue in catalyst design for direct DME synthesis is optimisation of the catalyst composition and interaction between methanol synthesis and methanol dehydration active phases. Direct DME synthesis faces several challenges. First, the catalyst activity can be improved for more efficient manufacturing. Second, because of very fast reaction of carbon monoxide with released water, significant amounts of CO_2 are produced. This leads to lower carbon efficiency. Third, the activity of the DME synthesis catalyst decreases with time on stream. The catalyst deactivation affects both copper and acid catalyst sites. The deactivation phenomena may include copper oxidation, sintering, coke deposition, contamination by impurities in syngas, etc.

Zeolite based catalysts have several advantages for methanol dehydration to DME relevant to more conventional oxide catalysts. However, the low back-diffusion of DME through the zeolite crystals could lead to post-reactions yielding undesirable by-products and carbonaceous residues. The latter induces plugging of the catalyst's pores and thus progressive deactivation. Therefore it is of interest to develop new zeolite catalytic system with a hierarchical porosity, i.e. micropores connected from each other with a network of meso- or macropores, in order to facilitate the reactant access and product removal.

The present work addresses design of efficient bifunctional catalysts on the basis of copper and hierarchical ZSM-5 zeolites for direct DME synthesis from syngas. In particular, the lecture is devoted to the strategies relevant to the control of catalyst activity, selectivity and stability.

Experimental/methodology

The $CuO–ZnO–Al_2O_3$ precursor was prepared by co-precipitation. A series of ZSM-5 zeolites were prepared from Na_2O - SiO_2 -Al_2O_3-TPAOH - H_2O systems. The hierarchical structure was created using sacrificial templates and treatment with HF_2^-. The hybrid catalysts were prepared using kneading. The catalysts were characterized both *ex-situ* using BET, SEM, TEM, XPS, TPR TPO, FTIR with adsorbed molecular probes (CO, Py, lutidine). The catalytic performance was evaluated in a fixed-bed millireactor. The *operando* XRD/XANES/EXAFS synchrotron experiments were carried out at the ESRF (SNBL beamlines) using a high pressure capillary cell with simultaneous on-line MS analysis of reaction products.

Results and discussion

Strategies for the activity control

DME, methanol, hydrocarbons, carbon dioxide and water are major products of carbon monoxide hydrogenation over hydride copper-zeolite catalysts. The activity depends on both concentrations of copper active phase and acid sites in zeolites. Our detailed study revealed a strong correlation between the zeolite crystallite sizes and reaction rate. At the same concentration of copper active sites, higher reaction rate is systematically observed over the catalysts containing smaller zeolite crystallites. The equilibrium of carbon monoxide hydrogenation shifts to methanol, because of rapid transfer of methanol molecules for dehydration to the acid site of the zeolite.

Strategies for the selectivity control

Our results suggest that higher concentration of Bronsted acid sites favours DME selectivity and suppress yields of methanol. Carbon dioxide is undesirable products of DME direct synthesis. Carbon dioxide produces in secondary reactions, its selectivity increases with higher carbon monoxide conversion. Two strategies are proposed to decrease the CO_2 selectivity in direct DME synthesis. The first one involves catalyst promotion which might affect the rate of elementary steps of different reactions. Promotion with tin for example resulted in a noticeable drop in carbon dioxide production. The presence of tin in the catalysts seems to considerably slow down the water gas-shift reaction leading to CO_2. The second strategy focuses on the protecting of the active sites for methanol synthesis from exposure to water. Water gas shift reaction in the bifuncntional catalysts for direct DME synthesis occurs on copper phases. Encapsulation of copper in hydrophobic silica nanospheres could result in a decrease in the CO_2 selectivities and enhanced DME productivity.

Strategies for the stability control

A combination of *ex-situ* and *operando* XAS characterization uncovered that copper is present in metallic form under a wide range of operating conditions. Copper sintering could be a major reason for the deactivation of hybrid hierarchical catalysts. The sintering phenomena are significantly accelerated in the presence of co-fed water. Copper sintering results in a decrease in the number of active sites for methanol synthesis. In addition the migration of copper nanoparticles can plug the porous structure of zeolite and reduce the concentration of acid sites for methanol dehydration. Copper sintering is accelerated by higher concentration of Bronsted acid sites on the external surface of zeolite. The *operando* experiments conducted under realistic conditions of DME synthesis did not reveal any noticeable copper oxidation. No significant carbon deposition was also observed. Catalyst deactivation can be accelerated by the heat spots, the reaction is exothermic. The strategies for the catalysts stability control developed in this work address reducing the concentration of Bronstend acid sites on the external surface of zeolite by sylilation or shaping the catalysts on silicon carbide host matrix with high thermoconductivity.

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III-KN19

Understanding Photocatalytic Process: Intrinsic Properties, Morphology and Timescale

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Introduction

Solar energy conversion is must to compensate the gap between energy production and its demand which is increasing with years [1]. A large scale energy generation from solar energy is only achieved by collection of solar spectrum at large scale. Overall water splitting using heterogeneous photocatalysts using a single semiconductor enables to directly generate H_2 from photo-reactor and is one of the most economical technologies in large-scale production of solar fuels [2]. The efficient photocatalyst materials are essential to make this process feasible for future technology. The potential scheme of photocatalytic process at different scale is depicted in Figure 1.

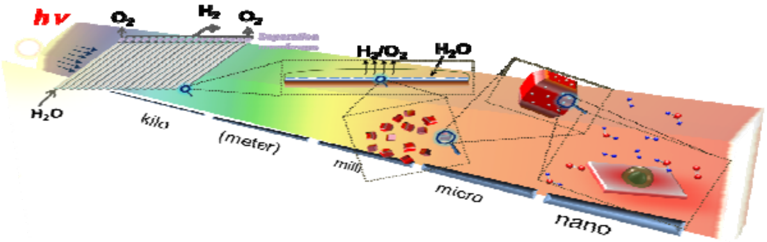

Fig. 1. A schematic of basic concept of overall water splitting at different scale.

Discussion

The photocatalysis involves multiple steps of the photophysical and electroccatalytic processes, as depicted by Figure 2. The photocatalytic reaction is initiated by the excited charge carriers (electrons and holes) that are generated by the absorption of the photons in the semiconductor materials (photocatalysts) [3]. Both the generated electrons and the holes move to the surface of the photocatalytic materials and subsequently initiate their respective redox reactions [3]. The photocatalytic process fully utilizes the electronic configuration occurring at the metal–semiconductor and semiconductor–electrolyte interfaces by constructing band structures (the formation of band bending and barriers) [4,5], preferably without introducing p–n junctions that generally increase the process cost. This electronic structure is essential in enhancing the charge separation and in achieving a highly efficient photocatalytic process because the photophysical process, including the generation and recombination of the excited carriers, occurs on a significantly shorter time scale (femto- to-microseconds) than surface electrocatalytic reactions, unless the process is separated effectively (microseconds to several seconds) [3]. The design of the photocatalysts should be focused on the following points [6]:

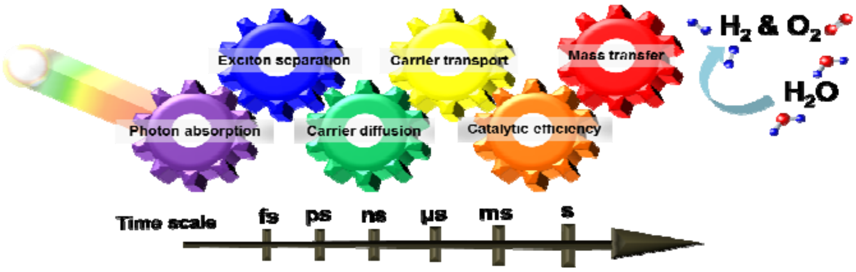

Fig. 2. Six sequential properties that require attentions to achieve efficient photocatalytic water splitting.

1) Select suitable elements to be used as photocatalysts that possess the suitable band positions and band gaps with high absorption coefficients and low exciton binding energy;
2) Synthesize highly crystalline bulk photocatalysts throughout the particle with appropriate concentrations of the majority carriers;
3) Construct band bending in such a way to improve charge separation;
4) Develop highly active cocatalysts for surface electrocatalysis;
5) Effectively locate the sites and maximize the concentrations of the reduction/oxidation cocatalysts on the photocatalyst surfaces.
6) Optimize solution condition for improved water redox reactions (pH, electrolyte etc.).

To understand the properties that affect photocatalytic process, various forms of photocatalytic materials are needed [7]. For example, thin film configuration is effective to measure absorption properties, such as absorption coefficient, refractive index, dielectric constant, and charge carrier concentration, carrier mobility, carrier lifetime and diffusion length. Calculations including density functional theory provide useful information, such as electronic structure (direct/indirect band gap), absorption coefficient, exciton binding energy, and dielectric constant. Photoelectrochemical configuration is effective to measure photoelectrochemical performance at different potential (Fermi level) and at different excitation wavelength. Semiconductor-electrochemistry is also effective to learn flat-band potential and majority carrier concentrations of the semiconductor. Measurements of the electrocatalytic performance give information of overpotential required for the respective redox reactions, and concentration gradient and diffusion of electrolyte. As a consequence of these parameters, photocatalytic powder configuration can only measure hydrogen and/or oxygen with and without sacrificial reagents [8].

To achieve efficient photocatalysis for overall water splitting, all of the parameters discussed above should be improved because the overall efficiency is obtained as the multiplication of all these fundamental efficiencies. Accumulation of knowledge from solid-state physics to electrochemistry and multidisciplinary approach to conduct various measurements are inevitable to fully understand the photocatalysis and to improve the efficiency.

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KN20

Application of Zeolite Catalysts for the Production of Clean Fossil Fuels and Biofuels

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Transportation fuels are one of the most important energy carriers used in internal combustion or jet engines. Diesel and gasoline are the key fuels in use today and in the foreseeable future. Zeolites have played a major role in the manufacturing of both fuels for over half a century. In this presentation emphasis will be placed on Fluid Catalytic Cracking (FCC), the workhorse process for the refining industry for many years. We will briefly examine the evolution of the FCC process by reviewing the progress dictated by environmental requirements such as reduction in the carbon dioxide and sulfur dioxide emissions in the refinery and the requirements set by the clean air act for reducing the auto exhaust emissions.

Although future developments in refining catalysts have the potential to play a major role in reducing the carbon footprint of fossil fuels, it is necessary to reduce the carbon intensity (gr CO2e per MJ fuel consumed) of transportation fuels via the gradual introduction of alternative fuels such as electricity/hydrogen and biofuels. Among the biofuels of great interest are hydrocarbon type fuels, because they are compatible with existing infrastructure and internal combustion engines. Main fuels in this category include: Hydrogenated Vegetable Oil (HVO), Fischer Tropsch Liquids and transportation fuels derived from Biomass Thermal Pyrolysis or Biomass Catalytic Pyrolysis.

It will be shown that zeolite catalysts play a major role in upgrading Fischer Tropsch Liquids and producing diesel, aviation fuel and naphtha. Emphasis will be placed on the use of ZSM-5 for the Biomass Catalytic Pyrolysis process, where biomass is processed in a Circulating Fluid Bed reactor using a ZSM-5 catalyst both as heat carrier and as a catalyst for the in situ upgrading of the pyrolysis vapors. Finally, future research directions to improve the economics of biomass derived hydrocarbons will briefly be discussed.

KN21

Nanocatalyst Based on Hybrid Structured Materials: Synthesis and Application

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1 Introduction

The catalyst containing nanoparticles demonstrate high selectivity and activity, recyclable and thus meet the requirements for green catalysts technological application. The principal problem arising at nanoparticles synthesis and their application in catalysis is necessity to stabilize and control their size. The main approaches to solve this problem are incorporation of metal nanoparticles in channels of solid supports with regular structure. Designing novel support materials, having a regular structure and capable of binding the substrate molecule selectively, could be considered as one of the most promising area for creating of new selective catalysts [1-3]. We report herein a number of different approaches for design new hybrid materials for hydrogenation catalysts based on metal nanoparticles and structured supports [2-5].

2 Experimental

The synthesis of hybrid mesoporous supports and catalytic experiments on hydrogenation were carried out as described in [3-6].

3 Results and Discussion

As a catalysts we synthesized a number of hybrid materials (Fig.1-2):

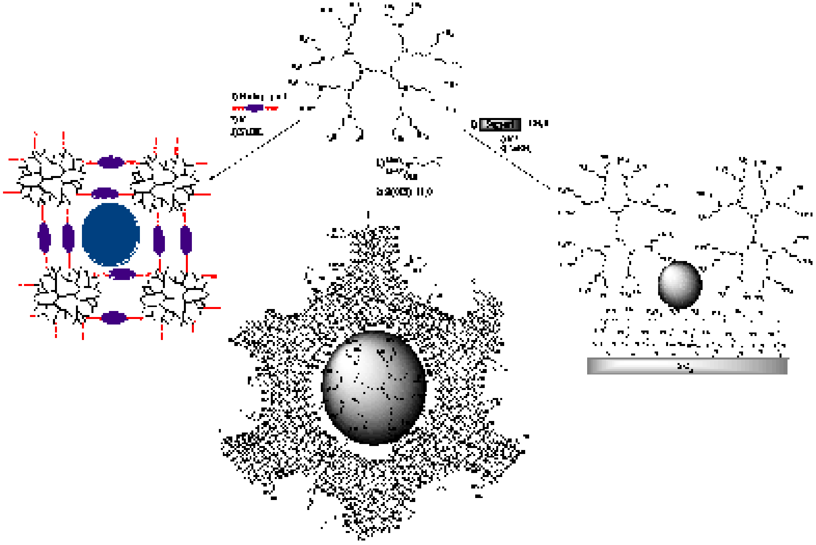

Fig 1. Preparation of hybrid catalyst on the base of dendrimers

1 - The heterogeneous organic supports synthesized by the covalent binding of dendrimers using diepoxide and diisocianate. Approach includes prior cross-linking of the dendrimers with subsequent encapsulation of metal nanoparticles. Depending on the generation of the dendrimer, one can obtain particles differing in size (1–4 nm), which may significantly affect the process of catalytic reactions.

2 - The microporous materials synthesized by sol-gel methods in situ using dendrimers. The preliminary modification of the dendrimer terminal aminogroups by the silyl-containing linkers and synthesis of mesoporous silica channels in presence of a template using sol-gel method and grafting the modified dendrimers to the silica surface formed *in situ*.

3 - The combination of silica polyamine composite (SPC) hybrids with dendrimers to provide an easy route to stabilization of nanoparticles on the silica surface, **E.**g. polypropyleneimine (PPI) dendrimers of the third generation that have been covalently grafted to a silica surface modified with polyallylamine (PAA) have been synthesized.

4 - Organic polymers with highly ordered mesoporous structure modified by functional groups (resol based mesoporous materials and mesoporous aromatic frameworks). The nanoparticles were included into pores.

5 - The nanopartilces of Pd, Rh, Ru, Pt were encapsulated into the materials using impregnation- reduction method. All materials obtained were identified by the TEM, XPS, FTIR, NMR MAS methods. The size of the particles was shown to be 2-5 nm and could be regulated by the structure of support.

6 - The catalysts synthesized showed superior activity and selectivity in the hydrogenation of different unsaturated and aromatics compounds. The Pd nanocatalysts demonstrated high efficiency in selective semihydrogenation of phenylacetylene to styrene, dienes to monoenes. The turnover number exceeded the 100000 h-1. Ruthenium and Rhodium catalysts exhibit high activity in the hydrogenation of aromatics and phenols. The hybrid catalysts displayed high resistance to metal leaching and could be widely used in green solvents

Conclusions

Catalysts based on metal nanoparticles encapsulated into different types of structured hybrid matrices were synthesized. The materials displayed high activity and substrate selectivity in the hydrogenation of various substrates,

Acknowledgments

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Oral Presentations
Section 1. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

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I-OP01
Layered Zeolite SRZ-21 for Cumene Production

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A layered zeolite with MWW structure, named as SRZ-21, is prepared by using the mixture of organic silane and inorganic silica as the raw materials. SRZ-21 could be prepared at a wider Si/Al mole ratio range. The X-ray diffraction and nuclear magnetic resonance results prove that the layered structure remains unchanged after calcinations and the organic silicon species mainly locates between the layers of zeolite crystal. Transmission electron microscopy images reveal that the thickness of the single-layer of the SRZ-21 zeolite is around 2.6 nm, which is much thinner than that of the MCM-22. The catalytic performances demonstrate that SRZ-21 has excellent activity, selectivity and stability for benzene alkylation reaction with propylene, and also is a good catalyst candidate for diisopropylbenzene transalkylation reaction for the cumene production.

I-OP02
Relationship between the Crystal Morphology and Acidity of the *BEA-type Zeolites and the Resistance to Coke Formation during Ethanol to Hydrocarbons Transformation

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Three *BEA zeolites (Si/Al ~ 20) with crystallite size ranging from micrometer to nanometer were synthesized (one micro-crystal, one nano-crystal and one nano-sponge) in order to establish a relation between the textural properties of the catalyst and it's lifetime.

I-OP03
Gold-based Yolk-shell Nanoreactors. Enhancement of Catalytic Performance via Gold Cores Decoration with Ceria or Pd

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Herein, we described the novel way for synthesis of highly effective and stable gold-based yolk-shell nanoreactors for the 4-nitrophenol reduction and CO oxidation.

I-OP04
Tuning the Catalytic Activity of Pt and PtCo Nanoparticles by Acidic Mixed-oxide Supports

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Our recent advances in the catalytic application of monometallic and bimetallic nanoparticles (NPs) supported on several silica mixed oxides of different acidity are here presented. Pt and Co NPs and bimetallic PtCo NPs have been synthesized and deposited (1 wt.%) on silica modified with 5 wt.% of Al, Nb, Ti, and Zr. The obtained samples have been characterized by several surface techniques to study the textural properties and metal dispersion; acidic properties were evaluated by base titrations in different liquids in order to provide measurements of both *intrinsic* and *effective* acidity.

The support chosen for MNPs may direct the selectivity of the transformation of HMF into valuable products. Mild *effective* acidity of the support (i.e. Nb/SiO_2) seems more suitable for enhancing the catalytic action of MNPs and depressing the unknown by-product formation. The most active catalyst (Co-Nb/SiO_2) was also the most selective toward hydroxymethyl furan di-ether (HMFDE) with 77% selectivity.

I-OP05

Selective Catalysis with Metal Nanoparticles Encapsulated in Porous Materials

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Here we present the progress that has been made on the synthesis of metal nanoparticles confined in different porous materials and their application in catalysis.

We have tested all obtained materials as catalysts in the different selective oxidation and hydrogenation reactions. Furthermore, we have characterized the prepared materials with various techniques including SEM, in situ TEM, STEM, TEM tomography, XPS, XRF, BET and XRD among others.

In conclusion, we have developed several simple and effective methods for encapsulation of metal nanoparticles in different porous materials. The methods are cost-effective, practical, and result in a narrow size distribution of small nanoparticles that are situated inside the porous materials. Furthermore, the materials showed catalytic activity and selectivity in a number of test reactions.

I-OP06

Ethene Oligomerization in Ni-based Zeolites: Experimental and Theoretical Investigations of the Reaction Mechanism

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Nickel-based zeolites are promising materials for heterogeneous catalysis of ethene oligomerization. While both Ni^+ and Ni^{2+} have been proposed as active sites for this reaction, the mechanism is still unknown and the activity of such materials was shown to be very low compared to conventional homogeneous catalysts. Therefore, ethene oligomerization in nickel-containing zeolites is investigated in this work by combining computer simulation and experimental work. A catalytic cycle analogous to the Cossee-Arlman mechanism used in homogeneous catalysis is proposed. Micro-kinetic modeling shows that desorption of the higher alkene products is the limiting step in typical reaction conditions (150 °C, atmospheric pressure). This hypothesis was supported by operando IR spectroscopy and catalytic testing, showing buildup of long alkyl chains until blocking of the pores and rapid deactivation of the catalyst. The work provides a starting point for identifying rate-limiting factors with the aim of improving the performance of these materials.

I-OP07

Synthesis, Characterization and Catalytic Study of Ni supported Apatite-type Lanthanum Silicates in Glycerol Steam Reforming Reaction

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Although rare earth apatites have attracted interest as promising solid oxide fuel cell electrolytes, over the last years their catalytic application studies are increased. For the glycerol steam reforming reaction Ni appears as the most promising active metal, due to its property to promote the C–C rupture. In this study, $La_{9.83}Si_{6-x-y}Fe_xAl_yO_{26\pm\delta}$, apatites were successfully prepared by solid state reaction and characterized for their structural properties. These materials were impregnated with Ni and were systematically studied for their catalytic activity in the glycerol steam reforming reaction (GSRM). Ni/apatite catalysts provided a glycerol conversion close to 100% for the whole range of temperatures and a higher H_2 concentration at the gaseous products even for low temperatures, ranging between 25 and 40 % v/v for 500-750 °C. The performance of Ni/ATLS catalysts in the GSRM reaction exhibited higher performance in comparison with Al_2O_3 supported Ni catalysts even from lower temperatures.

I-OP08

Renewable Feedstocks for Refineries & Conventional Sulfided Catalysts

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Processing of renewables in refineries has to be intensified to meet the targets set by the European Union. Triglycerides from waste sources and bio-oils are the most promising feedstocks. Renewable origin, use of non-food feedstocks and low sulphur content in products are the main benefits of using these feedstocks. CoMoS catalysts were found to be active and stable catalysts in long term upgrading of triglycerides to diesel-range hydrocarbons. In addition, bio-oil conversion has been demonstrated as a feasible future source of fuels. Commercial CoMoS and NiMoS catalysts were used in a fixed bed reactor with a non-isothermal profile. High content of oxygenated compounds and high content of water in bio-oil resulted in need for maintaining sulfane partial pressure. The increased H_2S concentration allowed to extend catalyst lifetime and also positively affected the final product quality. The product consisted typically of gasoline and diesel-like fractions.

I-OP09

Towards Efficient Hydrodeoxygenation on Transition Metal Phosphides

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In order to explore intrinsic catalytic properties of phosphides with high specific surface areas, two series of W-, Mo-, and Ni-phosphides were synthesized, one prepared by the conventional TPR, the other (CA-) prepared by a route based on the addition of citric acid in the synthesis. Hydrodeoxygenation (HDO) of palmitic acid as a model compound for algae based feedstocks was studied on the synthesized metal phosphides. The use of citric acid during the synthesis leads to smaller crystals and higher specific surface areas of the CA- compared to the TPR-phosphides. This leads to higher intrinsic activity and higher selectivity to HDO route.

I-OP10

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Catalytic Oxidative Desulfurization of Diesel Fuel as an Alternative to and Combination with HDS Process

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Compounds of the DBT family are rather resistant to removal by HDS, but they are easier oxidized by active oxygen than thiophenes.

The goal of this work is to study in detail ODS of heterocyclic sulfur-compounds in gas-vapor phase over CuZnAl-O and Cu/CeO_2 catalysts. The oxidant (O_2 and O_3), molar ratio O_2/S, LHSV, GHSV and temperature were varied within a wide range for the purpose of increasing sulfur removal efficiency. The data on the efficiency of the gas-phase desulfurization of hydrocarbon fuels will be compared with the literature data on their peroxide oxidation.

The gas phase oxidative desulfurization of refractory sulfur compounds with air was shown to be feasible at atmospheric pressure and temperatures 350-400°C. The reactivity of different sulfur containing molecules in ODS over catalysts increased in the sequence: thiophene<DBT<DMDBT. During this process heterocyclic sulfur-compounds transform to sulfur dioxide, and hydrocarbon fragments are oxidized to carbon dioxide and water.

I-OP11

Hydrotreatment Catalysts for Bio-oil and Lipids Processing into Valuable Chemicals and Biofuels

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The new catalytic technologies of biomass processing should play a key role in the bioenergetics and chemical industry evolution. In Boreskov Institute of Catalysis (BIC) the investigations are carried out aimed at the development of heterogeneous hydrotreatment catalysts for competent processing of biomass derivatives into valuble chemicals and biofuels. The following catalytic systems are of primary interest: catalysts for selective hydrogenation and complete hydrodeoxygenation of bio-oil components, hydrocracking catalysts for lipids processing into green diesel and kerosene, and catalysts for fatty alcohols production via selective hydrogenation of lipids derivatives. Each bio-feedstock has certain peculiarities for processing and as a result definite requirements to the catalysts are established. The latest results of catalysts investigation in the above mentioned types of biomass processing are reported about.

I-OP12

Aldol Condensation of Biomass Derived Aldehydes: Comparison of the Reactivity of Furfural and Hydroximethylfurfural

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The different behaviour of the two main biomass-derived aldehydes - furfural and hydroxymethylfurfural (HMF) - as reactants in the aldol condensation with acetone is studied in this work. Substantial differences have been observed between both starting compounds, being the Mg-Zr mixed oxides the most active catalyst for the furfural condensation (63 % of C13) but the MgAl mixed oxides for the HMF one (27 % of C15). The low solubility of C15 adduct hinders the direct comparison of reaction results, being necessary the use of bifunctional catalysts (Pd/MgZr and Pd/MgAl) and reducing atmosphere to increase its solubility and to prevent the massive precipitation of this fraction. This drawback is not observed in the case of C13 (furfural condensation adduct), which does not present solubility problems at reaction conditions. The more complex mechanism and the higher number of interactions involved between 5-HMF and the catalytic surface justify the lower selectivities obtained in this condensation.

I-OP13

Surfactants from Algae Derived Feedstock: Acylation of Amino Alcohols with Fatty Acids over Zeolite Beta

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Utilization of lipids from algae, which contain also proteins and sugars, is of growing interest. Biocompatible surfactants derived from fatty acids, such as N-alkyl amides, have several application areas in pharmaceuticals and cosmetics. The aim of this work is to study catalytic acylation of amino alcohols with fatty acids. Brønsted acidic zeolite H-Beta-22 was used as a catalyst. Several feedstock, such as stearic acid, methyl palmitate and technical grade oleic, were used together with ethanolamine, alaninol and leucinol. Conversion in the amidation of technical grade oleic and stearic acids was 74% and 94%, respectively within 3 h. Selectivity to the desired amide was also relatively high with oleic acid, over 73% and only small amounts of aminoalkylesters were formed. Ester amides containing 38 C atoms in the case of oleic acid and ethanolamine, when both amino- and hydroxyl groups react in 2-aminoethanol with two fatty acid molecules, were also formed. The amidation of *Chlorella* based biodiesel synthesized via *in situ* transesterification with methanol and sulphuric acid as a catalyst was also demonstrated.

I-OP15

Tuning the Selectivity of the Diols Produced from Cellulose with the Basic Sites of the Catalysts

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Ni-Zn catalysts supported on carbon nanotubes were tested for the direct catalytic conversion of cellulose to diols. Ni-Zn catalysts are highly basic and the basic property of the catalysts is the key parameter for product selectivity. Results show a correlation between the yield of the C_3 products and the amount of basic sites per gram catalyst. A clear decrease in the amount of basic sites per gram catalyst was observed with an increase in reduction temperature. The increase in C_3 yield is attributed to the increase in isomerization of glucose to fructose. This provides principles for rational design of catalysts to tune the product distribution.

I-OP16

Catalytic Hydrodeoxygenation of Bioderived C5 Acid into Motor Fuel Components: Kinetics and Mechanistic Study

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C5 acid conversion through the intermolecular coupling into 5-nonanone with CO_2 and water releasing followed by hydrodeoxygenation into *n*-nonane over Pd and Pt catalysts in reductive atmosphere was studied. Spectroscopic methods (FTIR and UV-Vis *in situ*) were applied to study a feasible mechanism of ketonization still debated in the literature. Both catalytic reactions were explored separately in order to be performed thereafter in a cascade mode over the best bifunctional catalyst, which turned out to be Pt(Pd)/M_xO_y. Higher activity of ZrO_2 and CeO_2/ZrO_2 in C5 acid decaboxylative coupling in H_2 atmosphere compared to that in N_2 was found. Kinetic regularities and size effect of 5-nonanone hydrodeoxygenation over Pd and Pt on Zr and Ce/Zr oxides was elucidated. FTIR and UV-Vis study allowed to identify different carboxylates adsorption forms and to reveal their key role in the ketonization mechanism. The reaction conditions were found provided C9 alkane yield more than 80%.

I-OP17

K-promoted NiMo Catalysts Supported on Activated Carbon for the Hydrogenation Reaction of CO to Higher Alcohols

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In this study, the hydrogenation of CO to higher alcohols was investigated over K-promoted bimetallic nickel-molybdenum oxide-based catalysts supported on activated carbon, focusing on the effect of acidity. The use of activated carbon as support was found to be beneficial for the formation of higher alcohols, probably due to transformation of the active $NiMoO_4$ phase from alpha to beta. Acid-pretreatment of the activated carbon support prior to impregnation led to increased activity which can be ascribed to better dispersion of the active phase on the support and therefore higher exposure of active Ni-O-Mo sites. A clear correlation between CO conversion and acidity was established for all investigated catalysts, demonstrating that Ni-O-Mo entities with acidic properties constitute the active centres for CO activation. Overall, a 35wt% K-NiMo catalyst supported on acid-pretreated high surface area carbon exhibited the optimum performance, with space time yield of 141.5 mg/$g_{catalyst}$/h to oxygenates at 280°C.

I-OP18

Control of Chain Length Distribution of Hydrocarbons during Fischer-Tropsch Synthesis over Co Nanoparticles inside of Nanoreactors

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One of the main problems of the Fischer-Tropsch (FT) synthesis is too broad distribution of the produced hydrocarbons due to the Anderson-Schulz-Flory law resulting in a non-selective formation of any hydrocarbons. This work is directed on the solution of this problem by application of nanoreactors with encapsulated metal nanoparticles inside. Our results show that encapsulation of Co nanoparticles in nanosize silica spheres results in increase of the activity and stability with shift of the chain length distribution of hydrocarbons to lower values in comparison with FT synthesis over conventionally prepared impregnated catalyst. The high activity is the result of well dispersed Co inside of nanoreactors with low interaction with the material of support. High stability is the result of low segregation of metal due to encapsulation inside of nanoreactors. The shift to short chain hydrocarbons is due to the restriction of the chain growth by the walls of nanoreactors.

I-OP19

Novel Approach to Catalytic Processing of Birch Wood Biomass to Valuable Chemical Products

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The presentation describes a novel approach to wasteless processing of birch-wood biomass, based on integration of catalytic methods of wood components conversion to xylose, microcrystalline cellulose (MCC), sulfates of MCC, organic and carbon aerogels. Hydrolysis of birch wood hemicelluloses to xylose at 120 °C was accelerated by sulfated carbon and zeolite SBA-15 catalysts. Suspended TiO_2 catalyst was used for prehydrolized wood fractionation on MCC and soluble lignin by H_2O_2 at 100 °C. MCC sulfates were firstly obtained with the use of green sulfation agent – mixture of sulfamic acid and basic catalyst urea. Porous organic and carbon aerogels with unique properties were firstly synthesized from soluble lignin-formaldehyde mixtures. Based on kinetic studies the optimal conditions of birch wood fractionation on xylose, MCC and soluble lignin were established. For characterization of obtained products the methods of HPLC, GC-MS, FTIR, NMR, XRD, SEM, AFM, BET were used.

I-OP20

Highly Stable and Selective Propane Dehydrogenation Catalyst

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PtSnZn catalysts on hydrotalcite-based oxide supports were prepared using scalable methods and tested for propane dehydrogenation. The catalysts showed superior long-term stability, stability against sintering and selectivity towards propylene. Coke deposits consist of two species: a) adsorbed oligomers that can be removed upon steam addition; b) char which can only be removed by oxidative treatment.

The effect of steam loading, temperature and pressure on the conversion and selectivity is discussed.

I-OP21

Selective Oxidation of Methane with Hydrogen Peroxide Using Gold-Palladium Nanoparticles

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Au-Pd nanoparticles have been found to be effective catalysts for the selective low temperature oxidation of methane using hydrogen peroxide as the oxidant. The primary product of the reaction is methyl hydroperoxide which is generated through the reaction of H_2O_2 and $\bullet CH_3$. In this work the effect of both the supporting material and the choice of catalyst preparation method on catalyst activity are investigated.

I-OP22

Ethanol Conversion into Chemicals over Au-M Containing Catalysts

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Direct catalytic valorization of ethanol either to olefins fractions C_3-C_8 or 1-butanol, 1-hexanol and 1-octanol over Au-Cu and Au-Ni containing catalysts was studied. Selectivity of 1-butanol formation was 75 %. First time ever over heterogeneous catalysts the reaction of ethanol and iso-propanol was carried on resulted in 3-methyl-2-butanol formation that is precursor of valuable monomer – isoprene. The peculiarities of the reaction mechanism are discussed, with the specific surface and electronic features of the prepared catalysts being considered. Found that growing the Au particles by forming the mixed MO/Au (M- Cu, Ni) particles resulted in an increased aim products selectivity.

I-OP23

Evolution and Interlayer Dynamics of Active Sites of Promoted Transition Metal Sulphide Catalysts under Hydrogen and Inert Media in the Course of Some Commercially Valuable Reactions

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According to the suggested dynamic model, neighboring layers of the multilayered MoS_2 crystallite exchange sulfur between Mo- and S-edges placed one under another in the course of permanent reduction–sulfidation processes under hydrogen atmosphere. When the sulfur atoms bonded to Co atoms leave the reduced edge of the layer, the atoms of the promoter also move along the sulfur atoms from one layer to an adjacent layer of higher sulfidation state. Then the process reverses. Such oscillations occur until the sulfur organic compound adsorbs on the vacancy on the reduced edge. The frequency of the oscillations determines catalytic activity of the CoMoS slab. Thiophene adsorption makes transfer of a promoter to the neighboring slab improbable because the electron density of thiophene sulfur compensates the extra positive charge on the Mo atom appeared after H_2S removal. When thiophene adsorbs on the vacancy of the CoMoS site the proton linked to Co moves to the SH group of the neighboring layer forming the H_2S which desorbs from this layer and new vacancy is formed. This model explains the reasons of the electron transfer from atom of promoter to Mo and different locations of the active sites responsible for hydrogenation and desulfurization on a promoted Mo-sulfide slab. A method to evaluate the efficiency of CoMoS catalysts for HDS of various types of crudes has been developed. Now these findings obtain their explanations within the developed dynamic model.

The suggested model gives a basis to develop criteria to evaluate the efficiency of the catalyst activity in hydrotreating of various types of crude oil.

I-OP24

Taking Advantage of Mass Transfer Limitations in Egg-shell Catalysts for Intensified Fischer-Tropsch Reactors

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A small Co/Al_2O_3 eggshell-type Fischer-Tropsch catalyst, with a diameter of 600microns, and a diffusive length of 58microns, was prepared by following an innovative impregnation method. Such method is based on the protection of the support pores with an organic liquid and on the control of the impregnation time. A fraction of such catalyst was grinded and sieved in the range 75-100microns for comparison purposes. Both the catalysts were tested in the FTS at condition relevant to industrial operations. Eggshell sample shows very interesting catalytic performances, characterized by higher CO conversion, slightly higher C_{25+} selectivity, lower olefin content in the products and higher alcohol content than the powder sample. These results are explained by considering the presence of weak mass transfer restrictions in the case of eggshell sample and point out that small eggshell catalysts have the potential to intensify the operations of fixed-bed reactors for the Fischer-Tropsch synthesis.

I-OP25

Intensification of Strongly Endo- and Exo-Thermic Catalytic Processes through the Adoption of Highly Conductive "Packed Foams" Reactors

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In this work we have investigated the concept of highly conductive "packed foams" reactors. In such reactors, the catalyst is loaded in the form of small pellets (e.g. microspheres) packed in the voids of open-cell metallic foams (or sponges). In particular, we have assessed the heat transfer performances of packed sponges and we have compared them to those of conventional packed beds of pellets and of bare open-cell foams. We have found that "packed foams" may be particularly advantageous in compact reactors requiring short tubes, in view of their flow-independent, conductive heat transfer mechanism (controlled by the highly conductive open foam substrate) which adds to the convective heat transfer typical of packed-beds of pellets. A circuit of equivalent resistances has been identified to describe the heat transfer mechanisms within packed foams.

I-OP26

Microkinetics Assisted Analysis of Hydrotreating Selectivities in Fast Pyrolysis Oil Upgrading

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In recent years, due to the depletion of fossil resources and environmental concerns, biomass valorization via fast pyrolysis has emerged as an attractive alternative route for chemicals and fuels production. While a lot has already been done in the field of fast pyrolysis itself, bio-oil hydrotreatment still represents significant challenges.

A non-sulfided 15wt.%Co-3.8wt.%Mo/Al_2O_3 was used as a catalyst and has a relatively low cost in comparison to noble metal catalysts and doesn't require sulphiding pretreatment as do conventional hydrotreating catalysts. Anisole was used as a model compound for assessing the various elementary steps by systematically varying the operating temperature, pressure and inlet composition at different space times. Mainly demethylation and isomerization were observed rather than hydrogenation or hydrodeoxygenation, even at very high anisole conversions. This behavior was quantitatively described by an elementary reaction network, providing key insight in the reaction mechanism as well as a basis for further catalyst design.

I-OP27

Stable Rh Particles on Electrosynthesized Structured Catalysts

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Rh structured catalysts for the catalytic partial oxidation of CH_4 to syngas, coated on FeCrAlloy foams, were prepared by thermal decomposition of electrosynthesized hydrotalcite-type compounds. The metal particle size distribution, coating thickness and activity of Rh-structured catalysts were optimized by modifying the Rh/Mg/Al atomic ratio percent (a.r.%) and total metal concentration in the electrolytic solution as well as by inclusion of Ni as second active phase.

Catalysts with smaller, more dispersed and stabilized Rh metallic particles in the coating, and therefore improved catalytic performances, were prepared by tailoring both the Rh content (Rh/Mg/Al = 5/70/25 a.r.%) and concentration of metals (0.06M) in the electrolytic solution. The formation of bimetallic RhNi particles largely increased the activity, although the stability has to be still improved.

Section 2. Catalyst Preparation and Characterization

II-OP01

Combining Operando Spectroscopy and Chemometrics to Understand Changes in the Active and Deactivating Species During the Methanol-to-Olefins Reaction over H-SSZ-13

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In this contribution we present a powerful approach to discriminate between the hydrocarbon species, which are contributing to the activity and deactivation of a H-SSZ-13 catalyst during the methanol-to-olefins (MTO) reaction. This combines an operando UV/Vis spectroscopy setup with a chemometrical analysis of the spectroscopic data by using a non-negative matrix factorization method. This methodology reveals that the reaction temperature affects to a great extent the nature of both the hydrocarbon species active in the MTO reaction and the hydrocarbon species deactivating the catalyst material. These results provide important fundamental insight into the MTO reaction and deactivation mechanisms.

II-OP02

Elucidation of the Mechanism of Hydrothermal Synthesis of Zeolite Catalysts Using Ex-situ and In situ Approaches

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The potential of the *in situ* MAS NMR techniques for the unravel of the mechanism of hydrothermal synthesis of zeolite catalysts has been demonstrated on the examples of synthesis of Al-, Zr- and Sn-BEA materials. The techniques is shown to give insight into the mechanism of the main steps of synthesis, including, gel formation, gel aging, crystal nucleation, growth and recrystallation; to provide information on the kinetics of each reaction step; to enable detection intermediate species stable only under hydrothermal conditions. The comparison of the results of *in situ* MAS NMR experiments with *ex situ* studies performed using XRD, SEM, TEM, IR and adsorption techniques outlined that the kinetic parameters obtained using both approaches are in good agreement. Combination of these two approaches will lead to fast progress in understanding the mechanisms of synthesis of different solids and therefore will facilitate the development of novel advanced materials.

II-OP04

Methane Activation on In-Modified ZSM-5 Zeolite. Solid-State NMR Characterization of the Pathways of the Alkane Transformation to Surface Species

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In this paper, we have analyzed in situ the kinetics of H/D exchange of methane with Brønsted acid sites of zeolite H-ZSM-5 modified with indium (In^+/H-ZSM-5 and InO^+/H-ZSM-5) by ^1H MAS NMR and compared this kinetics with the kinetics on the pure acid form of zeolite H-ZSM-5. Surface species formed from methane at elevated temperature have been monitored with ^{13}C CP/MAS NMR spectroscopy. This approach to the study of methane activation on heterogeneous catalysts allowed us to establish some peculiarities of methane activation by Brønsted acid sites and by indium species of In^+/H-ZSM-5 and InO^+/H-ZSM-5 zeolites, identify reaction intermediates and clarify the pathway of methane involvement in the reaction of ethylene aromatization or the alkylation of benzene with methane.

II-OP06

Dispersion and Orientation of Zeolite ZSM-5 Crystallites within a Fluid Catalytic Cracking Catalyst Particle

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Fluid catalytic cracking (FCC) is of great industrial importance in crude oil refinery. The FCC catalyst particles are a complex mixture of various components to ensure the catalytic performance (inside a zeolite) and its resistance to chemical and mechanical deactivation. Locating the various components in a catalyst particle is challenging and may involve the degradation of the particle.

The anisotropic nature of absorption and emission of elongated molecules entrapped inside zeolite channels was employed to selectively visualize the zeolite component within the matrix of an industrial FCC catalyst particle. Confocal fluorescence microscopy views the inner volume of the intact catalyst particle and is selective to (anisotropic) crystalline material and allows its location, size distribution, and orientation in three dimensions. This selective visualization may serve as a post-synthesis quality control on the dispersion and quantity of zeolite ZSM-5 crystallites inside a single FCC particle.

II-OP07

Parahydrogen-Induced Polarization in Heterogeneous Catalytic Processes

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Nowadays parahydrogen-induced polarization (PHIP) in heterogeneous hydrogenations has clearly proven its viability. While this sub-field of hyperpolarization in magnetic resonance is still in its infancy, at this point the demonstration that many types of heterogeneous catalysts have an intrinsic ability to produce PHIP is quite an important and encouraging achievement. Heterogeneous processes may have certain limitations, but they also have many advantages over their homogeneous counterparts. In this respect, PHIP appears to be a more direct way to catalyst-free hyperpolarized liquids and solutes, and quite likely the only way to utilize parahydrogen to produce hyperpolarized gases. It is also expected that PHIP could become a useful tool in the mechanistic studies of heterogeneous catalytic processes.

II-OP08

Selective Hydrogenation Processes over Novel Fiberglass Based Catalysts

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New results on the preparation of palladium fiberglass catalysts, their characterization by means of XPS, STEM and HS-LEIS, as well as kinetic and mechanistic data on selective hydrogenation of acetylene followed from SSITKA are presented. The effective ways of confining 1 nm Pd clusters in the subsurface layers of glass and increasing their concentration were developed. Namely, these small clusters were shown to be responsible for high catalyst performance. The SSITKA study using ^{13}C labeled acetylene clearly demonstrated that gas-phase ethylene was not involved in the reaction even at its very high excess. This fact was explained by the ability of glass to absorb predominantly such readily polarizable molecules like acetylene, but not ethylene. As a result, at a complete acetylene conversion our single-component Pd/FG catalyst demonstrates high selectivity (the ethylene increment of 60 %), which is higher than that of commercial bimetallic one.

II-OP09

Dependence of Catalytic Activity of Palladium Nanoparticles on Stabilization Models

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Palladium nanoparticles (PdNPs) are widely used as the catalyst in palladium catalysed reactions such as Suzuki cross-coupling. The problem of nanoparticles aggregation could be solved by using sterically hindered phosphonium ionic liquids (PILs) as stabilizers.

The influence of PdNP stabilizer on the catalytic reaction is significant. Modelling of NP's stabilization process admits to find out the optimal reaction conditions.

A number of synthesized PILs was tested as the stabilizers of PdNPs in Suzuki cross-coupling of 1,3,5-tribromobenzene and phenylboronic acid. It was found that size distribution and arrangement of PdNPs are determined by nature of the coating agent as well as its concentration in reaction mixture. Rational design and concentration control of these salts allows separating the contribution of steric and electrostatic factors in PdNPs stabilization.

II-OP10

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Selective Ethylene Trimerization by Titanium Complexes Bearing Phenoxy-Imine Ligands with Pendant arm: NMR and EPR Spectroscopic Study of the Reaction Intermediates

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The catalyst systems, for selective trimerization of ethylene are of great industrial and academic interest, since 1-hexene is used as a comonomer for linear-low-density polyethylene production. The titanium(IV) complex $LTiCl_3$ bearing a substituted phenoxy-imine ligand L activated with MAO produced 1-hexene with high activity and selectivity. The presented work is aimed at NMR and EPR spectroscopic study of the Ti(IV), Ti(III) and Ti(II) species formed upon activation of the pre-catalyst $LTi^{IV}Cl_3$ with various activators (MAO, MMAO, $AlR_3/[CPh_3]^+[B(C_6F_5)_4]^-$, R = Me, Et, ^{i}Bu) to elucidate possible role of the observed titanium species in ethylene trimerization and polymerization reactions. It was found that Ti(IV) complexes $[LTi^{IV}Me_2]^+[A]^-$, and Ti(II) complexes of the type $[LTi^{II}(S)]^+[A]^-$ ($[A]^-$ = counter ion, S = solvent or vacancy) participate in the selective ethylene trimerization process, whereas Ti(III) species of the type $[LTi^{III}(\mu\text{-}H)(\mu\text{-}Cl)Al^iBu_2]^+[MeMMAO]^-$ and $[LTi^{III}(\mu\text{-}Me)(\mu\text{-}Cl)Al^iBu_2]^+[MeMMAO]^-$ can promote undesirable PE formation.

II-OP11

Chemistry of the Active Metal Center in the Selective Catalytic Reduction of NO by NH_3

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A new reaction scheme for the SCR reaction is presented. The scheme is relevant for copper exchanged zeolites and adaptable to iron exchanged zeolites and vanadia (V_2O_5) on TiO_2. It is compatible with previous suggestions but is the first to fully comply with the constraints usually put upon chemically consistent reaction schemes at moderate temperatures. The fast SCR reaction is shown to be an integral part of the standard SCR cycle.
The cycle is followed on Cu-SSZ-13 by several spectroscopic methods under *in-situ* conditions showing the spectroscopic fingerprint of both the fully oxidized resting state and the fully reduced resting state of the catalyst. The implications of this cycle on the chemistry of the active metal center will be investigated and presented.

II-OP12

Novel Preparation of Reverse Model Catalyst for CO Oidation and H_2O Dissociation

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The nature of the support-catalyst interaction and the influence of the boundary between a metal-catalyst and a support could be crucial for understanding the working mechanism of a catalyst. These questions can be addressed through design of a reverse catalyst. Here we report the developed procedures of novel reverse catalysts preparation using atomic layer deposition, which are providing the precise control of chemical composition and morphology of reverse catalysts. The reactivity of reverse model catalysts FeO and Al_2O_3 Pt(111), Pd(111) and Cu(111) were tested for CO oxidation and H_2O dissociation. CO adsorbed in the vicinity of the oxide islands was identified as an active species of the $CO+O_2$ reaction lowering temperature threshold. The oxides demonstrated the critical role in water dissociation.

II-OP13

Dynamic High-Resolution Study of the Structural Evolution of Ag Nanoparticles during Carbon Gasification within an Aberration-Corrected Environmental Transmission Electron Microscope

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Gasification of carbon can be achieved, in the presence of metal catalysts supported on solid carbon materials, at high temperature in oxidative environments.) On structured materials such as graphite or graphene these trenches tend to be rather 2D at the surface of the material ("pacman effect"). In this work we have studied the gasification of a non-structured material (amorphous carbon) by silver nanoparticles (Ag-NPs) in presence of oxygen and at variable temperatures in an aberration corrected Environmental TEM at atomic resolution.
We were particularly interested on the dynamic structural evolution of the Ag-NPs observed in real-time. Gasification rate slows when the Ag-NPs transform from initial hexagonal structure to fcc; concurrently the Ag-NPs shrink rapidly. The dynamic real-time high resolution images associated with local EELS measurements allowed to propose a mechanism for the observed phenomena; however the motor behind the hexagonal to fcc transition still remains to be clarified.

II-OP14

Atomic-Resolution Imaging of Environmental Catalysts

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In recent years transmission electron microscopy has made considerable progress that is beneficial to heterogeneous catalysis. Here, we demonstrate such advances on two catalysts for environmental purposes: Co-promoted MoS_2 for hydrodesulfurization processes in oil refining, and V_2O_5/TiO_2 for selective catalytic reduction of nitrogen oxides in automotive exhaust abatement. Imaging of these catalysts has long remained particularly challenging as the active phases are atomically dispersed on the support.
Through careful control of the imaging conditions and sample environment in the microscope, the structure and composition of these catalysts could be characterized at resolutions and sensitivities on the atomic scale. For the MoS_2 catalyst this has allowed the localization of individual promoter atoms. For V_2O_5/TiO_2, we can show that imaging must be performed *in-situ* under an oxygen atmosphere to retain the relevant oxidation state.
These characterizations of industrial-style catalysts open up important opportunities for making connection with results from simple model systems.

II-OP15

Operando Spatially- and Time-Resolved XES Andvalence-to-Core-XES for the Characterization of Fe- and Cu-Zeolite Catalysts for NH_3-SCR of NOx

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We are presenting the application of novel *operando* spectroscopic techniques, in particular high energy resolved X-ray absorption spectroscopy and X-ray emission spectroscopy to study the mechanism of selective catalytic reduction of NOx over metal-exchanged zeolites as well as to obtain oxidation state of active sites for the SCR modelling. In addition, spatially-resolved XAS was used which uncovered gradients of Fe / Cu oxidation state and coordination number depending on the reaction conditions. Time-resolved XAS allowed monitoring oxidation state dynamics of Fe / Cu sites during transients NH_3 concentration experiments and during simulation of the temperature transients such as New European Driving Cycle. Finally, valence-to-core XES allowed identification of structure of NOx and NH_3 species adsorbed on Fe / Cu sites and provided an evidence for a different intermediate species over Fe- and Cu-zeolites.

II-OP16

Novel Research platforms ISISS and EMIL at BESSY II: In Situ Surface Characterization of Catalysts by Synchrotron Based Near Ambient Pressure X-ray Electron Spectroscopy

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The ISISS facility at the synchrotron radiation source BESSY II is dedicated to *in situ* characterisation of gas/solid and liquid/solid interfaces of functional materials by near ambient pressure XPS (NAP-XPS) and variable pressure soft-XAS (vP-XAS). The dynamic formation of the electronic surface structure by interaction with the ambient gas under equilibrium will be exemplified by a study of the technically relevant alkane oxidation catalyst vanadyl pyrophosphate. In addition to the determination of composition and vanadium oxidation state also semiconductor properties like work function changes and Fermi level pinning and their dependence on the gas composition have been studied illustrating the importance of the electronic factor in catalysis. Furthermore, vP-XAS studies (≤1000mbar) will be shown to discuss the pressure dependence of complex alkane oxidation reactions. The novel EMIL facility and prospects of innovative ambient pressure and liquid flow reaction cells based on low kinetic energy electron transparent membranes will be discussed.

II-OP17

Mechanism for Selective Oxidation of Ethanol over V-Ti Catalyst

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The selective oxidation of ethanol to acetaldehyde and acetic acid over a monolayer V_2O_5/TiO_2 catalyst has been studied *in situ* using Fourier transform infrared spectroscopy and near ambient-pressure X-ray photoelectron spectroscopy. The data were complemented by temperature–programmed reaction spectroscopy and kinetic measurements in a flow reactor. Based on the obtained data the mechanism for the oxidation of ethanol over vanadia-titania catalysts is developed.

II-OP18

What are the Active Sites of Gold in CO Oxidation Reaction?

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Since the 90's, Au catalysis has attracted a lot of attention; however, the active sites of Au catalysts are still not well understood. Here we report a systematic study of the activation mechanism of Au in CO oxidation using *in-situ* and *ex-situ* techniques. Our *in-situ* measurements show that the oxidation of extended Au surfaces by O_3 treatment is accompanied by the formation of a metastable surface oxide; however, Au-oxide does not directly participate in CO oxidation over Au catalysts. Au NPs on oxygen-free supports remain inactive regardless of the NPs' size and the type of the support. In contrast, Au NPs on transition metal oxides show high catalytic activity, which depends on the method of preparation. Our findings suggest that Au NPs are activated via Strong Metal Support Interactions, assuming a strong influence of the support on the electronic Au structure through charge transfer and stabilization of low-coordinated Au atoms.

II-OP19

Ceria Supported Gold Catalysts: Mechanistic Studies of CO Oxidation Using a Combined Operando Approach

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Ceria supported gold catalysts show a high activity and stability in low-temperature CO oxidation. However, the influence of active support materials such as ceria on the catalytic properties of gold nanoparticles is not well understood. In this context, we employ *operando* spectroscopy to study the room temperature oxidation of CO over ceria supported gold catalysts. Combined operando Raman and UV/Vis spectroscopy, *quasi in situ* X-ray photoelectron spectroscopy (XPS) and *operando* diffuse reflectance infrared spectroscopy (DRIFTS) are used.

In particular, *operando* Raman and IR data demonstrate the potential of a complementary vibrational spectroscopic approach to elucidate the mode of operation of Au/CeO_2 catalysts in CO oxidation. Depending on the gas environment (oxidative, reaction, reductive) a distinct spectral signature of adsorbed CO, carbonate, formate, hydroxyl and peroxide species as well as ceria phonons is observed allowing for new insight regarding the presence of reaction intermediates and the role of the support.

II-OP20

Reactivity of Oxygen in Methanol Partial Oxidation over Au(111) Model Catalyst Surface

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The partial oxidation and alcohols oxidative coupling on gold requires the presence of adsorbed atomic oxygen. Although molecular O_2 does not dissociate on the gold surface, atomic oxygen layers can be prepared by ozone decomposition. In the current work, we investigated the different oxygen species on the Au(111) model catalyst surface and their reactivities in methanol partial oxidation. Adsorbed oxygen layers prepared at various temperatures reveal drastically different reactivities towards methanol: the oxygen layers prepared at 140 K demonstrate higher activity than that of 460 K. With increasing temperature, the active oxygen species were observed to transform into inactive oxygen. The XPS and TPD analysis of oxygen layers reveal the presence of inactive subsurface oxygen at higher temperatures. Current results are critically important for the molecular understanding of the fundamental aspects of oxidative catalysis by gold.

II-OP21

Cu-SAPO-34 Synthesis and in Situ Characterization. Insights into DeNOx-SCR Mechanism

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Selective catalytic reduction (SCR) is, recently, proposed as an advanced technology to reduce NO_x from lean-burn engines vehicles. The copper exchanged zeolites have been shown as suitable materials for this technology. However, the interest in one-pot synthesis of these catalysts has increased. A series of silicoaluminophosphates has been synthesized, characterized and analyzed in SCR reaction conditions. It has been observed that the synthesis and the gel composition influence the textural properties as well as the copper oxidation states ratio in zeolitic materials. The variation of the synthesis parameters yields a material with high cristallinity, constant ammonia retention capacity in the operation window of SCR technology and a suitable Cu(I)/Cu(II) ratio to ensure the efficient selective catalytic reduction of NO_x with NH_3 and avoid co-side products.

II-OP22

Structure-Reactivity Relationships in Low-temperature NH_3-SCR of NO over Highly Effective $V_2O_5/Ce_xZr_{1-x}O_2$ Catalysts

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Different prepared 5% V_2O_5/ $Ce_xZr_{1-x}O_2$ (x = 1, 0.9, 0.8, 0.7, 0.5, 0.3 and 0) catalysts were been characterized with regard to phase composition, structure and valence state of vanadium sites as well as the surface properties using XRD, ICP, XPS, BET, UV-Vis-DRS and EPR. *In situ* UV-Vis-DRS and EPR were also applied under catalytic reaction conditions, partly *in situ* UV-vis-DRS monitoring the absorbance at 700 nm to elucidate the behavior of VO_x species. The combined characterization techniques revealed that highly dispersed V^{5+} species on both 5VZr and $5VCe_7Zr_3$ catalysts are more active than 5VCe catalyst containing exclusively V^{4+}. However, 5VZr contains a significant amount of tetrahedral VO_4 sites while octahedrally coordinated V is dominating on the mixed support. Fitting of the time-dependent redox behavior of the V sites by a first-order rate law revealed the presence of two types of oxidized and reduced VO_x species under reducing and oxidizing conditions in all these catalysts. *In situ* EPR studies of the highest active 5 % V2O5/$Ce_{0.7}Zr_{0.3}O_2$ under NH_3-SCR feed indicate the presence of V^{4+} in states of low activity (150°C) while exclusively V^{5+} is present in states of high activity (250°C).

II-OP23

Kinetics Study of Oxychlorination Process by Combined in-situ Mass- and Spatial-time Resolved UV-Visible Spectrophotometry

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To obtain mechanistic insight into the active sites of industrial catalyst used inside industrial plants, and comprehensive spatial-time quantitative- and qualitative analysis of reaction kinetics is an extremely hard task that is rarely achieved. In situ operando combined UV-Vis spectrophotometry has been explored to study the reducibility of Cu-phases on $CuCl_2/\gamma$-Al_2O_3 catalyst during oxychlorination reaction cycle, and quantitative spatial-time kinetic data of the oxychlorination process including redox reaction of Cu catalysts was recorded by mass spectrometry and spatial-time resolved UV-Vis spectrophotometry. It has been found that the active phase of the $CuCl_2$/ γ-Al_2O_3 is altered along the catalyst bed during the steady state and CuCl phase of the catalyst dominates on surface. The catalyst oxidation step is found to be rate determining step at the given reaction conditions. Based on the quantitative study of kinetics, a kinetic model can be developed to map Cu^{II}/Cu^{I} in both spatial- and time scales of a reactor.

II-OP24

Design and Preparation of Zeolitic Catalysts for Ethylbenzene via Vapour-Phase Benzene Alkylation

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Based on the diversity of raw materials, design and preparation of three ZSM-5 zeolitic catalysts for vapour-phase benzene alkylation processes using pure ethylene, bio-ethanol and FCC off-gas as alkylation agents to manufacture ethylbenzene were carried out. Nano-sized ZSM-5 zeolite after steam treatment was used as the active component in pure ethylene process. Then, with combination of an extra phosphoric acid treatment to enhance the stability of the active sites, nano-sized ZSM-5 zeolite can be utilized in the bio-ethanol process. For benzene alkylation process using FCC off-gas, oriented ZSM-5 zeolite was synthesized and shaped into cylindrical catalyst with abundant macropores and mesopores to facilitate materials diffusion. Moreover, hydrothermal treatment and acid leaching modification were carried out to remove the Lewis acid site to inhibit side reactions. The above mentioned ZSM-5 catalysts are commercialized and exhibit good industrial performance.

II-OP25

Hydrotreating Catalyst Activation under Industrial Conditions

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The activation of Co-Mo hydrotreating catalysts was followed by *in situ* XAS under conditions close to industrial practice. It is demonstrated that active phase genesis strongly depends on activation parameters and precursor composition.
Activation in a model diesel feed led to rapid active phase genesis, initiated by thermal decomposition of organosulfides in the feed. The influence of organic additives with varying chelating propensity for the precursor metals on the catalytic performance indicated that an optimum interaction of the promoter and the active phase was achieved for catalyst precursors prepared with weakly chelating ligands. It is proposed that the reducibility of Mo in the precursor is the key parameter that determines the efficient formation of the active 'Co-Mo-S' phase.

II-OP26

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Development of in Situ Techniques to Monitor Oxygen Evolving Electrocatalyst Surfaces

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Being a low carbon technology, hydrogen production from water electrolysis is especially appealing nowadays. For the design of suitable electrode materials, it is crucial to understand the structural transformation of electrocatalyst surfaces upon the sluggish oxygen evolution reaction (OER). To monitor changes in the electronic structure of electrocatalysts while the OER proceeds, we have therefore designed an electrochemical cell that can be integrated into a Near-Ambient-Pressure X-ray Photoelectron Spectroscopy (NAP-XPS) setup. The Nafion®-cell utilizes the proton exchange membrane Nafion® to separate a liquid from the XPS measurement chamber. While the OER is driven by an externally connected potentiostat, XP spectra of the oxygen electrode can be recorded simultaneously. The development of this *in situ* cell is a step towards bridging the pressure gap between classical XPS measurements in UHV and electrochemical measurements in aqueous electrolytes.

II-OP27

CO_2 and H_2O (Co)adsorption on a ZrO_2 Thin Film

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Being a carbon source, the utilization of carbon dioxide (CO_2) became attractive from both an environmental and economical perspective. However, CO_2 is a very stable molecule, thus to induce a reaction the activation of CO_2 by catalysts is required. One way of activating CO_2 is dry reforming of methane (CH_4), when CH_4 is reformed by CO_2 on Ni or Pt particles supported by zirconia (ZrO_2). Such activation can occur on the ZrO_2 or on the interfacial sites. We have employed in situ X-ray Photoelectron Spectroscopy, in situ Infrared Reflection Absorption Spectroscopy and Temperature Programmed Desorption in order to examine the adsorption of CO_2 (and H_2O) on ZrO_2 ultrathin film. Our study shows that CO_2 adsorbs only weakly on ZrO_2 ultrathin film and desorbs at low temperature. H_2O can activate CO_2 via hydrogenation and leads to the formation of formaldehyde, dioxymethylene and formate on the ZrO_2 surface.

II-OP28

Operando Raman and UV-Visible Spectroscopy of $H_3PW_{12}O_{40}$ in the Gas Phase Dehydration of Methanol to Dimethylether

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The main issue in heteropolyacid-based catalysis of gas phase reactions is their deactivation due to the formation of coke (carbonaceous depostits). In our work, we investigate the catalytic activity of $H_3PW_{12}O_{40}$, the most acidic Keggin-type heteropolyacid, in the gas phase dehydration of methanol to dimethylether. The latter is nowadays seen as one of the most important and promising renewable fuels for the future. During the temperature programmed reaction up to 350°C, the conversion of methanol over $H_3PW_{12}O_{40}$ (800 mg) is of 3%, 65% and 90% at respectively 100°C, 150°C and 200 to 350°C. Up to 200°C, the selectivity to dimethylether is around 90%. From 200°C on, it drops. Byproducts as methane, ethylene and propylene are then detected. Herein, we demonstrate via *operando* Raman and UV-Visible characterization that such changes in the selectivity to dimethylether over $H_3PW_{12}O_{40}$ are related to the amount of coke produced and to the latter's degree of disorganization.

II-OP29

Raman Study of the Deactivation Products in the Methanol to Olefines Reaction: a Combined In Situ - in Silico Approach

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Methanol to Olefines (MTO) reaction is a process which relevance is increasing in the last years. One of the main limitations affecting MTO is the relatively fast catalysts deactivation, due to coking, i.e. mainly methylated benzenes and polycyclic aromatic hydrocarbons.

To get a better knowledge in the deactivation of MTO catalysts, the characterization of spent catalysts performed by UV Raman spectroscopy has been coupled to the simulation. Different zeolites have been deactivated under different reaction and their Raman spectra have been compared with ones of selected reference molecules. Moreover their vibrational spectra have been simulated by ab initio calculation, also computing the Resonant Raman intensities in order to allow an easier understanding of the experimental data.

The combination of experimental and simulated UV Raman spectra can represent an interesting tool in the characterization of the deactivation species in the MTO reaction, increasing the understanding of deactivation pathways in MTO.

II-OP30

Where are the Active Sites in Zeolite Nano-Crystals? Influence on Post-Synthesis Treatment from Hard X-ray Depth Profiling with XPS

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The aluminum distribution within crystals of zeolite ZSM-5 was quantitatively determined by depth profiling using XPS. Subtle differences in synthesis parameters yield a different extend of aluminum enrichment at the surface and the crystal bulk. This then leads to very different zeolite structure after base leaching and hollow single zeolite crystals can be obtained. The measurements also unambiguously identify dissolution and redistribution of aluminum and silicon atoms during base leaching.

II-OP31

eTEM Investigation of Gold Nanoparticle Formation in Recrystallized Zeolite Silicalite-1

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The preparation of gold nanoparticle encapsulated zeolite silicalite-1 is reported. The zeolites are modified by a recrystallization process (desilication), which creates voids and mesopores inside the crystal structure of individual particles. This additional porosity facilitates the formation of gold nanoparticles inside the zeolite channels upon wet impregnation. Environmental Transmission Electron Microscopy (eTEM) is applied for the characterization of the material with the emphasis on the process of *in-situ* nanoparticle formation inside the zeolite channels, sintering stability at elevated temperatures, and the reactivity of the material in the simple oxidation reaction. Furthermore, the influence of degree of desilication and temperature of desilication on the recrystallized material is investigated. Variation in choice of gold precursor and water content for impregnation of the recrystallized silicalite-1 are examined in terms of size of nanoparticles and their distribution inside the zeolite framework.

II-OP32

Size-dependent Redox Behaviour in Iron Observed Using Top-Down Lithography and In-Situ Single Particle Spectro-Microscopy

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Shape and size of nanoparticles considerably affect catalytic activity. Their synthesis in a controlled manner resulting in well-defined shape and size as well as their characterization at the single particle level will help gaining deeper insight into chemical mechanisms and elucidating size and shape effects. The mechanism of oxidation of iron has extensively been investigated in the past and studies have concluded that the behavior of bulk iron is different from nanoparticles but knowledge about the behavior in nanoscale is limited. To determine size-dependent redox behaviour in iron, we fabricated model systems using top-down nanolithography enabling nanoparticles of well-defined size and order. Single particle spectro-microscopy was performed simultaneously on different sizes using using X-ray photoemission electron microscopy (PEEM) and effect of particle size in oxidation of iron nanoparticles has been determined. Based on the kinetics and thermodynamic stability, reaction mechanism for the interconversion of oxides in iron nanoparticles is proposed.

II-OP33

Investigating Fundamental Properties of Syngas Conversion Catalysts - a Model Approach

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Methanol and Fischer-Tropsch synthesis are well-established, commercially used catalytic processes. Yet, our understanding of the catalysts, and in particular their de-activation mechanisms is incomplete. The reasons for this are the complexity of the reaction itself and of the catalysts, containing promoter and support materials as well as three-dimensional, random distributions of the catalyst materials in pores. In contrast, on flat model systems, catalyst properties as well as gas composition and temperature can be precisely controlled and measured. Therefore, changes in catalyst oxidation state, stability towards sintering and contact between the various catalyst components can be accurately studied. We demonstrate the fabrication of model catalysts using physical vapour deposition and wet-chemical approaches. These catalysts have been characterized and tested using XPS, TEM and in-situ UV-vis and mass spectroscopy. The strength of the approach was demonstrated in several experiments, including in-situ catalyst oxidation/reduction and sintering of syngas conversion catalysts.

II-OP34

CeO_2 Carrier Shape Effects on CuO_x/CeO_2 CO-PROX Catalysis: Operando X-ray Spectroscopy and DFT Modelling Studies

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Synchrotron-based spectroscopies together with DFT modelling are used to analyze the particular behaviour presented by CuO_x/CeO_2 catalysts active in CO-PROX reaction when they are supported on ceria nanocubes presenting the more reactive (001) surface, as compared with catalysts supported on ceria nanospheres. Surface-sensitive XANES at Cu L_3 edge confirm previous data from operando DRIFTS and activity measurements indicating that in nanocube-supported CuO the deep reduction of this oxide, necessary for H_2 activation, is hindered (thus improving CO-PROX selectivity), in agreement with DFT-derived data on the energy needed to form anion vacancies. Cu K edge EXAFS reveals a more distorted Cu environment when CuO is supported on ceria nanocubes, also in agreement with both XRD results and DFT data which show in that case higher CuO-CeO_2 adhesion energy and a strong distortion of the CuO structure.

II-OP35

A Density Functional Theory Study on the Mechanism of the Cycloaddition of CO_2 and Epoxides

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Depending on applied conditions and the choice of catalyst, the cycloaddition of carbon dioxide and epoxides leads to cyclic carbonates or polyethercarbonates. Both possible products represent valuable, industrial compounds. Most current catalysts for the cycloaddition, which are used in industrial processes, require the use of high reaction temperatures and/or high pressures of carbon dioxide. Systems based on tetrabutylammonium bromide and oxo bridged bimetallic aluminum complexes have been identified as catalysts for the cycloaddition of carbon dioxide and epoxides at atmospheric pressure and close to room temperature. It has been anticipated that these oxo bridged bimetallic aluminum complexes act as Lewis acid and a likely mechanism has been proposed. Inspired by this, we started density functional theory calculations to model the proposed mechanism in silico. We predicted by DFT and found experimentally the existence of $[\{Al(salen)\}_2(\mu\text{-}CO_3)]$. This complex can react with propylene oxide to propylene carbonate and likely plays a role in the catalysis. The focus of the modelling is to elucidate this role.

II-OP36

Effect of Structure and Composition of Gold and Gold-palladium Clusters in H_2O_2 Formation

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The DFT simulation of H_2O_2 formation from H_2 and O_2 on gold and gold-palladium clusters was performed. The Au_n, $Au_{n-1}Pd$ (n=8, 20, 32), Au_4Pd_4, $AuPd_7$ clusters was considered as the active sites of catalysts. Based on physical chemistry formalism, the conditions of the activity and selectivity of the H_2O_2 formation are supposed. The gold clusters demonstrate low activity in hydrogen peroxide formation. A Pd atom surrounded by gold atoms in AuPd clusters facilitates H_2O_2 synthesis.

II-OP37

Surface Phenomena Affecting the Performance of Pd-Ag Alloys

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In order to investigate adsorption and dissociation of H_2 on PdAg alloy surfaces a combined experimental and theoretical study of surface phenomena affecting hydrogen transport through PdAg membranes has been performed. The experimental results indicate that the structure and compositions, as affected by combined thermal treatment and exposure, affect the surface phenomena controlling permeation kinetics. The calculations compare bulk to Pd-terminated Pd3Ag(111) to elucidate how the H_2 adsorption and dissociation in presence of CO may be affected by the surface composition.

II-OP38
Understanding Selectivity Issues in Rh-catalyzed CO Hydrogenation

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Density functional theory calculations were performed to investigate all elementary reaction steps relevant to CO hydrogenation over Rh. From the obtained dataset, rate constants were constructed using the Eyring equation and microkinetics simulations were performed. In these simulations, a Degree of Rate Control analysis as well as a Degree of Selectivity Control analysis were performed to investigate the propensity of the individual elementary reaction steps on the overall activity and selectivity of CO hydrogenation over Rh. Our study reveals that (i) CO dissociation does not limit the reaction rate nor the selectivity and (ii) ethanol is formed by C+CO coupling followed by a complex series of hydrogenation and dehydrogenation reactions. Ethanol selectivity can be improved by decreasing the rate of CH_x hydrogenation that promotes methane formation. These insights will be discussed in the frame of promoter effects described in literature.

II-OP39
In Silico Exploration of Bimetallic Sulfides Catalysts

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Hydrodesulfurization (HDS) is one of the crucial catalytic process of industrial refining to produce clean fuels. Contrary to Co and Ni promoters of the CoMoS and NiMoS active phases industrially used in HDS catalysts, the structural, electronic, and energetic descriptors of MeMoS phases of the other 3d transition metals (Me) are poorly quantified. In order to provide such relevant descriptors of the catalytic activity, we systematically investigate MeMoS phases by using density functional theory calculations coupled with a thermodynamic model. We determine the equilibrium structures (S-coverages) and edge energy of the MeMoS nano-crystallites a function of the position of Me in the 3d transition metals row and as a function of the sulfo-reductive conditions. In addition, magneto-structure effects are found to play a key role in the stability of MeMoS edges with Me= Cr, Mn and Fe but these effects also depend on the S-coverages.

II-OP40
Effect of Mo Addition on Hydrotreating Activity, Stability to Corrosion, and Physicochemical Properties of Ni-Based Catalysts for Bio-Oil Upgrading

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A series of NiCuMo(X)/SiO_2 sol-gel catalysts (X as Mo/Ni atomic ratio) has been studied in hydrotreatment of guaiacol (GUA) to clarify the effect of different Mo content on the catalysts performance in the target process. GUA conversion over NiCuMo(X)/SiO_2 catalysts was shown to proceed through the two main routes: HDO and HYD route − with benzene and methoxycyclohexanoles as the main intermediates, correspondingly. Increasing of Mo content allowed higher contribution of HDO route into GUA transformations, the final product always being cyclohexane. The catalysts stability after glacial acetic acid treatment was shown to increase noticeably with Mo content. According to the catalysts characterization by physicochemical methods, their corrosion resistance and changes in HDO selectivities could be associated with the change of active component nature: electronic effects between Mo^0 and Ni^0, and the presence of coordinatively unsaturated Mo species, which could play a significant role in activation of Oxy-organics.

II-OP41
Pd/C Catalysts Prepared by Direct Pyrolysis of Sawdust Impregnated by Palladium Nitrate for Hydrodechlorination of Chlorobenzenes

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Pyrolysis of sawdust impregnated with $Pd(NO_3)_2$ in inert atmosphere is an appropriate way to produce Pd/C catalysts containing nanoparticles of Pd^0 (XPS data) in the narrow particle size range on the carbon support of biomorphic structure. Such systems are active in gas-phase hydrodechlorination of chlorobenzene in continuous flow system with packed bed of catalyst, and liquid-phase hydrodechlorination of polychlorinated benzenes. Pretreatment of sawdust by soaking in water, with or without sonification, and by hydrothermal water treatment provides significant increase of S_{BET} (up to 225 m^2/g) at a concurrent widening of Pd particle size distribution. Both the presence of alkali-earth metals in Pd/C due to the use of biotemplate, and modification with Co addition improve catalytic properties.

II-OP42

Formation Mechanism of Well-Dispersed Pd Nanoparticles with High Thermal Stability on SiO_2 Using $Pd(acac)_2$ as Precursor

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We report the synthesis of a well-dispersed Pd/SiO_2 catalyst with Pd loadings between 0.5 and 8 wt% by using a simple impregnation method with $Pd(acac)_2$ as precursor. Formation of single layer of $Pd(acac)_2$ on SiO_2 surface through the hydrogen bond interaction of silanol group with $Pd(acac)_2$ in the impregnation step is crucial to the final formation of well-dispersed Pd nanoparticles on SiO_2. When a silica supported $Pd(acac)_2$ sample was heated to ~200 °C in air, the single layer of $Pd(acac)_2$ on SiO_2 surface decomposed into the metallic Pd nanoparticles with an average size of about 2.8 nm. The resulting Pd nanoparticles demonstrated superior stability against sintering at high temperature. The mean size of Pd particles remains at approximately 3 nm even after calcination at 800 °C. This straight forward procedure can also be used in the synthesis of other sinter-resistant metal catalysts supported on SiO_2 such as Ni/SiO_2 and $Rh\text{-}CeO_2/SiO_2$.

II-OP43

Au-Rh and Au-Pd Nanocatalysts Supported on Rutile Titania Nanorods: Structure and Chemical Stability

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Au-Rh and Au-Pd nanoparticles (NPs) were synthesized by colloidal chemical reduction and immobilized on hydrothermally-prepared rutile titania nanorods. The catalysts were characterized by aberration-corrected (S)TEM, XPS and FTIR, and were evaluated in the hydrogenation of tetralin in the presence of H_2S. Reduction in H_2 at 350 °C was found efficient for removing the polyvinyl alcohol (PVA) surfactant while preserving the size (3 nm), shape and bimetallic nature of the NPs. While Au-Pd as-prepared NPs are alloyed at the atomic scale, Au-Rh ones contain randomly distributed single-phase domains. Pre-reduction generates a well-defined segregated structure with Rh located at the interface between Au and TiO_2. Both titania and gold increase the resistance of Rh and Pd to surface oxidation. Furthermore, although detrimental to initial tetralin hydrogenation activity, gold stabilizes the NPs against surface sulfidation, leading to increased catalytic performances of the Au-alloyed systems as compared to their monometallic counterparts.

II-OP44

Defectiveness of Carbon Nanomaterials as a Key Parameter of Their Effectiveness as a Support for Cobalt Catalysts in Fischer-Tropsch Synthesis

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New nitrogen-doped carbon materials were synthesized and characterized. These materials were tested as Co catalysts supports in Fischer-Tropsch synthesis. The correlation between «defectiveness» of carbon nanomaterials and catalytic characteristics was found.

II-OP45

Proposal of a Catalytic Cooperation Model between Ru-Supported Nanoparticles in Ammonia Synthesis under Mild Reaction Conditions

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According to previous results, a broad size distribution of Ru-supported nanoparticles is required for a high activity in ammonia synthesis under mild reaction conditions. In this work we reach a broad distribution of sizes by mixing different RuO_2 colloidal suspensions, before impregnation on alumina, which promotes a higher catalytic activity. Kinetic studies, 'in situ' characterizations and H/D isotopic exchange experiments were performed on catalysts containing small Ru nanoparticles and catalysts containing larger particles, in order to elucidate the mechanism of catalytic cooperation. Clear evidence is presented of a mechanism involving migration of H atoms from large to small Ru nanoparticles, which is expected to improve the catalytic performance by promoting the hydrogenation of adsorbed NH_x species and the release of active sites.

II-OP46

Water-Gas-Shift and Methane Reactivity on Reducible Perovskite-Type Oxides

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A comparative study of activity for hydrogen oxidation, water-gas shift and methane reforming was performed on two perovskitic materials $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ (LSF) and $SrTi_{0.7}Fe_{0.3}O_{3-\delta}$ (STF). Impedance measurements on LSF thin film model electrodes revealed a high surface activity of the material in oxidizing and reducing atmospheres. On powder samples the (inverse) water-gas shift reactivity starts at about 450°C on both LSF and STF. Total oxidation of methane to CO_2 with reactive lattice oxygen on fully oxidized samples was observed on LSF and STF. The catalytic activity of both perovskite-type oxides is strongly dependent on the degree of reduction and the associated reactivity of the remaining lattice oxygen. Investigation of the structural state of the after each step of a full catalytic cycle including oxidative and reductive activation revealed no changes in the SrO-termination after a catalytic inverse water-gas shift reaction up to 600°C, but a different surface and bulk reactivity.

II-OP47

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Facile Redispersion of Sintered Au Nanoparticlces with Controllable Size for Catalytic Application

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Downsizing larger Au particles into tiny ones with controllable size is still a challenge topic. Here, we report that Au nanoparticles (Au NPs) on activated carbon with uniformly distribution and controllable size are generated from the sintered Au NPs through a reverse agglomeration (redispersion) process using appreciate alkyl halides under mild conditions. The process is related to the C–X bond dissociation energy and the significant adsorption of iodic species on the Au NPs. A new protocol for size controlling and predicting the redispersion efficiency of Au NPs was established by correlation with the C–X bond dissociation energy of alkyl halides. The findings may pave the way for the facile regeneration of sintered Au-based catalysts for practical applications. The regenerated Au/C catalyst could almost recover its activity for the hydrochlorination of acetylene.

II-OP48

Shape Effect of TiO_2 on the Performance of VO_x/TiO_2 Catalysts for NH_3-SCR

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The shape effect of TiO_2 on the catalytic performance of VO_X/TiO_2 catalyst for selective reduction of NO with NH_3 was investigated. TiO_2 nanosheets that exposed 74% {001} facets and TiO_2 nanospindles enclosed with 81% {101} facets were hydrothermally synthesized with the aid of F^- and CH_3COO^-, respectively. After loading vanadia at monolayer dispersion, the {001} facets of TiO_2 nanosheets favored the generation of octahedral vanadia species, whereas the {101} facets on TiO_2 nanospindles resulted in tetrahedral VO_x species. As a consequence, the VO_x/TiO_2-nanosheets showed a significantly higher activity for selective reduction of NO by NH_3 than the VO_x/TiO_2-nanospindles, primarily because of the active vanadia species in octahedral coordination environment on the {001} facet of TiO_2. This result demonstrates the importance of morphology in the preparing efficient VO_x/TiO_2 catalysts.

II-OP49

Design and Preparation of Pt-Transition Metal Oxides (TMO) Nanoparticles Supported on 3DOM Oxides with Enhanced Catalytic Activity for Soot Combustion

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Soot particle emitted from diesel engine vehicles is one of probable precursors to damage the human health. Development of catalysts, which decrease the emission amount of diesel soot, is one of the focus research topics in the field of environmental catalysis. To design a synthesize high-performance material of catalytic activity, understanding the properties affecting catalytic performance is of great importance. The key challenge is to find effective catalysts for soot combustion that operates at low temperatures. A number of researches show that transition metal oxides (TMO: Ti, Mn, V, Cr, Fe, Co, Ni, Cu, Zn, Ce, etc.) are one of the key components in auto-exhaust treatment catalysts. 3DOM structure oxides will be a valuable and promising catalyst system not only for diesel soot combustion due to their good catalytic properties and big pore sizes but also for catalytic oxidation of hazardous macromolecule organic compounds. However, the catalytic performance is limited by the intrinsic activity of metal oxide. Noble metal nanoparticles are possible choices for enhancing the intrinsic catalytic activety of 3DOM metal oxides. Among the reported catalysts for soot oxidation, Pt-based catalysts are still the best catalytic system, and are also only currently commercialized for practical conditions. The catalytic performance of Pt nanocrystals can be finely tuned by transition metal oxides (TMO) due to the strong metal-oxides interaction. Thus, the shape-controlled synthesis of Pt-TMO nanoparticles over 3DOM Al_2O_3 support is a promising route for enhancing their catalytic activities.

Synthesis of monodispersed PMMA microsphere, assembly template, and preparation of 3DOM Oxide (e.g., Al_2O_3, ZrO_2) supports by colloidal crystal template (CCT) were method described previously. 3DOM Al_2O_3-supported Pt-TMO nanoparticle (NPs) catalysts were synthsized by one-pot process of the gas bubbling-assisted membrane reduction-precipitation (GBMR/P) method just developed in our lab. The typical preparative procedures were described as follows: 3DOM Al_2O_3 support and TMO precursor were also introduced into the H_2PtCl_6 solution (Beaker I). The mixture solution was driven by a peristaltic pump. A reductant solution ($NaBH_4$) in Beaker II was injected to the membrane reactor with two ceramic membrane tubes (Φ 3 mm × 160 mm) by a constant flow pump. Meantime, the hydrogen gas was also injected by the two other membrane tubes. The $NaBH_4$ solution was infiltrated through the abundant holes (d=40 nm) on the wall of the ceramic tubes into the glass tube reactor, where the reduction of metal ions occurred immediately when the two solutions met. After complete consumption of the $NaBH_4$ solution, the precipitation agent ($NH_3 \cdot H_2O$) was added into Beaker II and was injected to the membrane reactor same as the reductant agent by a constant flow pump. The synthesis process was stopped after complete consumption of the precipitation agent solution. The final products were calcined in an oven at 500 °C for 1 h and the desired 3DOM Pt-TMO/oxide catalysts were obtained.

Fig. 1 shows SEM (A), TEM (B), STEM (C) and HRTEM (D) images of 3DOM Pt-$CeO_{2-\delta}$/oxide catalysts. The SEM image exhibits that the macroporous material contains a skeleton surrounding uniform close-packed periodic voids with the average diameter of 260±10 nm. The wall thicknesses observed from SEM images are 30±5 nm. 3DOM structures with overlapped pores can be also clearly observed by TEM and STEM images in Fig. 1(B-C). The spherical platinum nanoparticles are anchored evenly over the surface of 3DOM oxide host, and all Pt particles are highly dispersed (Fig. 1C). One Pt nanoparticles on the surface of 3DOM oxide were covered by the $CeO_{2-\delta}$ nano-sheet and formed the core-shell structural Pt-$CeO_{2-\delta}$ nanoparticles (Fig. 1D). The ordered nanostructure with Pt-$CeO_{2-\delta}$ core-shell-type nanoparticles would provide abundant catalytic active sites with low- coordinatively unsaturated ceric cation duo to the maximal contact region of $CeO_{2-\delta}$(shell)-Pt(core)-oxide (support) nanojunction system. Therefore, 3DOM Pt-$CeO_{2-\delta}$/oxide catalysts show high catalytic activities (T_{50}, 340 °C) for diesel soot combustion under the loose contact between soot and catalysts.

The catalysts of 3DOM oxides-supported Pt-TMO nanoparticles were synthesized successfully by one-pot GBMR/P method. The mutifunctional materials, which combine both advantages of 3DOM structure and nanoparticles with the maximal contact region of TMO(shell)-Pt(core)-oxides(support) nanojunction system, may be useful for fundamental research on metal-support synergetic effect and potential practical applications in the catalytic oxidation of solid particles.

II-OP50

Oxidative Conversion of Methane Over Gd-Sr-Co-Perovskites: Structure-Activity Relationship

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A number of $Gd_xSr_{1-x}CoO_{3-\delta}$ (x=0.5-0.9) monophase perovskites with ordered and disordered Gd^{3+}/Sr^{2+} ions and oxygen vacancy sites was prepared and characterized by XRD, full-profile crystal structure analysis, O_2 TPD, H_2 TPR; catalytic properties were determined at 360-850°C in reaction of methane deep oxidation to CO_2 and oxidative coupling of methane (OCM) to C_2-hydrocarbons. Cubic phases with disordered Gd/Sr cations were found to be up to five times more active in the reaction of methane combustion and less selective in OCM than tetragonal perovskite phases with ordered distribution of Gd^{3+}/Sr^{2+} ions over the A-sites of the crystal lattice. The observed difference in catalytic performance was attributed to weakly bound mobile oxygen, presented on A-site disordered perovskites.

II-OP51

In situ XPS Study of DeNOx Reactions on Platinum Catalysts: Pressure and Material Gaps

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The results of *in situ* X-ray photoelectron spectroscopy study obtained for special model catalyst Pt/AlOx/FeCrAl with isotopic kinetic studies on Pt/γ-Al_2O_3 of the NO involved reactions (NO decomposition, NO+CO, NO+C_3H_6) modeling process of car exhaust neutralization are presented. The details of catalyst activation and deactivation as well as details of catalytic reactions were studied and the explanations of obtained effects were proposed. The principal difference of surface layer composition between supported and bulk catalysts is shown. It was assumed that alumina support is involved into considered reactions. Applied approach bridges the pressure and material gap between model and real catalysts and provides information very useful for the practical catalysis.

II-OP52

Synthesis of Hierarchical Zeolites Using a Mono-Quaternary Ammonium Surfactant as the Mesoporogen

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Most of the successful approaches of hierarchical zeolite synthesis are based on bottom-up approaches involving self-assembly processes between complex and, therefore, expensive surfactants and silicates. Although such materials yield model systems for catalysis studies, their synthesis is not amenable to scale-up because of materials cost. Herein we present a successful and scalable dual-templating strategy. It is based on the use of a very cheap and simple-to-prepare amphiphilic surfactant containing a single N-methylpiperidine head group as quaternary ammonium center. We show how it can be used in concert with conventional zeolite structure-directing agents to efficiently downsize microporous domains in SSZ-13 zeolite. This approach is not only very effective as only small amounts of the template need to be added to the synthesis gel, but it also leads to materials with excellent catalytic performance.

II-OP53

Evidence of Remarkable Redox Behaviour of Ce-doped Ordered Mesoporous Alumina at Moderate Temperature

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Cerium-based materials are extensively studied because of their remarkable properties that make them interesting for a wide scope of catalytic applications. The importance of CeO_2 is linked to its oxygen storage capacity and mobility, due to the two stable valence states of the Ce^{4+}/Ce^{3+} couple. These properties are improved when the crystallite size of ceria decreases since over pure ceria the phenomenon is limited to the surface and sub-surface layers. In the present study, we performed a series of cerium-doped mesoporous alumina employing the Evaporation Induced Self Assembly (EISA) route and we particularly investigated the redox behaviour of these large surface mixed oxides by using advanced characterization techniques.

We demonstrated by XANES and OSCC techniques that the high reduction rate of the solids observed at 400°C is reversible. Such properties make these mixed oxides very interesting supports of catalysts for selective oxidation reactions.

II-OP54

Support Functionalization to Retard Copper Particle Growth in the Methanol Synthesis Reaction

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The introduction of amine groups on silica retarded copper particle growth in the methanol synthesis reaction. *In-situ* TEM suggested a slightly smaller contact angle of copper on amine-functionalized silica and hence an increased interaction between the particles and the support to be responsible for the improved thermal stability.

II-OP55

Selective Hydrotreating of FCC Gasoline on K_x-CoMoS/Al_2O_3 Catalysts

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Catalytic properties of industrial and laboratory (K)-CoMoS/Al_2O_3 catalysts synthesized with the use of molybdenum heteropolycompound in hydrotreating of FCC gasoline were compared. Synthesized catalysts were characterized with the use of the following techniques: low-temperature nitrogen adsorption, Raman spectroscopy, X-ray photoelectron spectroscopy, high-resolution transmission electron microscopy, NH_3-TPD, H_2-TPR. Catalytic activity examination was carried out in hydrotreating of heavy fraction of FCC gasoline. The performance of synthesized catalysts was estimated with conversions of sulfur and olefinic compounds and HDS/HYD selectivity that calculated as a ratio of hydrodesulfurization (HDS) and hydrogenation (HYD) rate constants. For all catalysts kinetic characteristics such as reaction order, activation energy and preexponential factor were also calculated It was established that modifying TMS catalysts with alkali metal leads not only to changing of physical-chemical characteristics but also catalytic properties and kinetic characteristics as well. Using potassium in catalyst synthesis results in changing of both active sites nature and amount.

II-OP56

Immobilized Grubbs Catalysts on Mesoporous Materials: New Insights into Support Characteristics and Their Impact on Catalytic Activity and Product Selectivity

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The best support characteristics for immobilization of the Hoveyda-Grubbs catalyst 2 (HG2) were defined to obtain a maximal activity in the ring-opening ring-closing metathesis (RO-RCM) of cyclooctene. This was accomplished by scrutinizing textural and structural parameters of the support, as well as investigating surface properties like surface adsorption, silanol density and catalyst loading. Mesoporous silica MCM-41 and TUD-1 were found to answer these conditions best. Furthermore typical heterogeneous aspects like continuous reactions and pore diffusion limitations (PDL) were examined. MCM-41 (2 nm pores) is more prone to PDL compared to TUD-1 (15 nm pores) at high Ru loadings. This phenomenon originates from linear polymer obstruction and is even more pronounced in cage-like pore systems. As a consequence, this affects product selectivity. The optimal support-catalyst system is used to unravel the reaction pathways of RO-RCM of cyclooctene to cyclic oligomers under heterogeneous catalysis conditions. Based on the mechanism, differences were highlighted between homo- and heterogeneous reactions and diverse pore architectures.

II-OP57

Effect of Nucleus and Shell on the Mechanism of the 4-Nitrophenol Reduction Over AuPd Based Nanoreactors

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The effect of nucleus and shell on the mechanism of the 4-nitrophenol reduction into 4-aminiphenol over AuPd based nanoreactors was examined using on line UV-Vis spectroscopy and principal component analysis. It was found that the presence of AuPd species on the surface of nanoreactor's nuclei favors the reduction steps while oxide shell participates in the reaction mechanism provoking indirect route of the 4-aminophenol formation through condensation of intermediates.

II-OP58

Direct Conversion of Ethylene to Propylene: Strategy of Catalyst Preparation

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There is an increasing worldwide demand for propylene due to a higher demand for polypropylene than polyethylene. Direct conversion of ethylene to propylene without any addition of other hydrocarbons is the most desirable route, but no single catalyst with high ethylene conversion and propylene selectivity has been found so far. The aim of our studies is preparation a new PdO-Re_2O_7 catalyst, based on SO_4^{2-}/ZrO_2 for the direct conversion of ethylene to propylene at mild conditions (reaction temperature up to 100°C, atmospheric pressure). Special attention is paid to the influence of the supported metal oxide (PdO, Re_2O_7) content, to the support nature and to the several the preparation procedures of PdO-$Re_2O_7/SO_4^{2-}/ZrO_2$ catalysts. A series of supported Pd-Re catalysts showed high propylene yield (42.4-55.2 wt. % at 40°C and 49.8-62.1 wt. % at 80°C), and that the initial activity depends on the Re_2O_7 content in the catalysts.

II-OP59

Design of Highly Efficient Catalysts for Catalytic Membrane Reactors: Study within the Framework of Demcamer Project

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DEMCAMER - DEsign and Manufacturing of CAtalytic Membrane Reactors by developing new nano-architectured catalytic and selective membrane materials" is a collaborative project, the aim of which is to develop innovative multifunctional catalytic membrane reactors based on new nano-architectured catalysts and selective membrane materials to improve their performance, durability, cost effectiveness and sustainability (lower environmental impact and use of new raw materials) over four selected chemical processes for pure hydrogen, liquid hydrocarbons and ethylene production [http://www.demcamer.org]. The research activity of the team from Boreskov Institute of Catalysis within the framework of DEMCAMER focused on the development of novel catalyst materials for autothermal reforming (ATR) and oxidative coupling of methane (OCM) as well as quantum-chemical modeling. The rational preparation procedures and optimal compositions of catalysts for ATR of CH_4 and OCM have been developed and structure-property-performance relationships were identified. The proposed catalysts showed values of activity, selectivity and stability in compliance with the DEMCAMER target.

II-OP60

A Kinetic Fingerprint for Distinguishing Porous Diffusion

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A unique characterization technique is presented that can be used to distinguish the internal/external features of a nanoporous material. Under the vacuum pulse response conditions of a TAP (Temporal Analysis of Products) experiment reactor transport is well-defined Knudsen diffusion and the number of collisions of a diffusing probe molecule with the active material is low. As a result, we observe that only molecules with a finite surface lifetime will have the opportunity to enter the pore structure. When the size of the probe molecule is similar to that of the pore size, and energy barrier exists for entering the pore. An adsorption model for porous diffusion is presented that separates adsorption on the external surface from the kinetic process of entering the pore. Experimental data is described in terms this adsorption model for the diffusion of a series of small hydrocarbon molecules in the HKUST-1 metal organic framework.

Section 3. Energy-Related Catalysis

III-OP01

Spinel Mn-Co oxide in N-doped Carbon Nanotubes as Bifunctional Electrocatalyst

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We demonstrate the synthesis of spinel Mn-Co oxide nanoparticles partially embedded in N-doped carbon nanotubes (NCNTs), which were used as bifunctional electrocatalysts for oxygen reduction/evolution reactions (ORR/OER) under alkaline conditions. The synthesis was achieved by catalytic growth of NCNTs using Co-Mn oxides as catalyst and subsequent oxidative treatments: (1) oxidation under flowing air by moving the reactor into a furnace and withdrawing it from the heating zone after 5 min, which causes opening and rupture of the CNTs through oxidation and thermal stress; (2) oxidation in HNO_3 vapor at 200 °C, which oxidizes both the residual growth catalysts and the NCNTs leading to more hydrophilic surface. Due to a cooperative effect from the nitrogen groups in NCNT and the spinel Mn-Co oxide particles, the capability of the resulting catalysts to electrolyze both the ORR and the OER becomes tremendously enhanced producing exceptionally active bifunctional catalysts for reversible oxygen electrodes.

III-OP02

Efficient Nanostructured in Photocathodes for Water Reduction through Optimization of Interface Energetics and Structure

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The "Holy Grail" of solar energy conversion and storage is efficient photoelectrolysis of water using semiconductors to store solar energy in the simplest chemical bond, namely that of H_2. P-InP with a bandgap well-matched to the solar spectrum is a good candidate for photoelectrochemical hydrogen production from water. Herein, we optimized the interface energetics by depositing a thin layer of heavily doped n^+-InP on top of a p-InP substrate. X-ray photoelectron spectroscopy and Mott-Schottky measurements proved the positive shift of band-edge after n^+-InP layer deposition in vacuum and electrolyte, respectively. As a consequence, the onset potential reaches 0.85 V. A moth-eye-like antireflection layer created on the top of electrode help to increase the short-circuit current up to 28 $mAcm^{-2}$. Together, these modifications led to a photoelectrode efficiency of 15.5%, which is the highest one for PEC water reduction reported for single junction PEC cells so far.

III-OP03

Novel Photocatalysts Based on $Cd_{1-x}Zn_xS/Zn(OH)_2$: Activation during the Hydrogen Evolution from Aqueous Solutions of Ethanol

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Rapid depletion of natural raw hydrocarbons (oil, gas, and coal) determines an acute need to identify and develop alternative energy sources. The unique properties of hydrogen make it a versatile and environmentally friendly chemical energy carrier, suitable for use in all types of heat engines and power generation devices. The photocatalytic splitting of water using the energy of visible part of solar light is a very attractive way for the hydrogen production. Recently there has been a tendency to use available organic substances as electron donors for the photocatalytic hydrogen evolution. In this research, novel composite photocatalysts $Pt/Cd_{1-x}Zn_xS/ZnO/Zn(OH)_2$ with a high activity under visible light were proposed. The activation of the photocatalyst during the photocatalytic hydrogen evolution from alkaline aqueous solutions of ethanol was observed. The activation is likely caused by formation of ε–$Zn(OH)_2$ in a basic media.

III-OP04

The Role of Co-catalysts in Photoelectrochemical Versus Photocatalytic Water Splitting: CoO_x on $LaTiO_2N$

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The idea to produce environmentally friendly fuel by direct conversion of solar energy into hydrogen is gaining increasing attention. For this purpose the implementation of water splitting in a technological large-scale solution is desirable. Several concepts have been proposed [1]: One of them is the use of photocatalytically active particles to produce H_2 and O_2, another one is based on the photoelectrochemical cell. To enhance the performance of the photocatalyst, co-catalysts were used in both, photocatalytic and the photoelectrochemical setups. For O_2 production $LaTiO_2N$ is well-studied photocatalyst [2], while Co oxides were found to be very active co-catalysts [2]. However, it is not entirely clear, whether co-catalysts act on the kinetics of the oxygen evolution reaction or facilitate mainly the charge separation. In this contribution, we investigate whether CoO_x co-catalysts deposited on $LaTiO_2N$ serve the same function in a photocatalytic setup compared to a photoelectrochemical setup.

III-OP05

Photocatalytic Overall Water Splitting using Ga_2O_3 with Various Phase Compositions Loaded with Rh-free Co-Catalysts

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Ga_2O_3 materials with various phase compositions and structures have been synthesized by precipitation and CVS and compared to commercial β-Ga_2O_3. A significant influence of the structural properties on the overall water splitting performance was determined. The Ga_2O_3 catalysts are as active or more active than commercial Ga_2O_3 and exhibit a significant higher stability. A ternary non-noble metal co-catalyst was found to be comparably active to a Rh-containing photocatalyst.

III-OP06

Synthesis and Reactivity of Au/g-C_3N_4/TiO_2 Nanocomposites for Water-Splitting under Solar Light Illumination

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The aim of this study is the control and the optimization of the synthesis of Au/g-C_3N_4/TiO_2 nanocomposites applied to H_2 production from water dissociation under solar light irradiation. An important step lies in the optimization of the composite in terms of g-C_3N_4/TiO_2 ratio and Au content. These experimental parameters have also been correlated to the photocatalytic activity toward H_2 production. Furthermore, the Au nanoparticles deposition method has been optimized to achieve deposition yield higher than 80% on TiO_2, g-C_3N_4 and g-C_3N_4/TiO_2 surfaces. The photocatalytic composites exhibit enhanced activity under solar light irradiation, compared to Au/g-C_3N_4 and Au/TiO_2.

III-OP07

Efficient Solar Production of Methane from CO_2 and H_2 Using Nickel Catalysts

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The sunlight-induced reduction of CO_2 by H_2 has been studied using a series of n- and p-type semiconductors as potential photocatalysts. It has been proven that whereas classical n-type semiconductors are inactive for the reduction of CO_2, the reaction proceeds efficiently to CH_4 on p-type semiconductors, being nickel-based materials the most active photocatalysts. The conversion of CO_2 is essentially quantitative under simulated solar light at short reaction times ($\leq$ 1 h) on nanopowdered NiO or Ni/$SiO_2 \cdot Al_2O_3$ photocatalysts. Furthermore, the selectivity to CH_4 approaches 100%. Dark thermal experiments were conducted and photoactivity spectra were recorded, proving that light absorption by the nickel catalysts is actually initiating the reactions. In fact, UV-free visible light can also promote the process. Regarding the photocatalytic materials, both particle sizes and presence of the silica-alumina support were observed to profoundly affect the reaction outcomes.

III-OP09

IrNiOx-based Oxide Thin-Films and Metal-Oxide Hybrid Core-Shell Nanoparticles as Efficient Electrocatalysts of Oxygen Evolution

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Water electrolysis combined with renewable electric power generation technologies is expected to emerge as a low-emission method for storing excess electricity. The challenge in electrocatalytic water splitting is the high overpotential required for the anodic oxygen evolution reaction (OER). Relatively low overpotential is attainable in acid electrolyzers using RuO_x and IrO_x-based electrocatalysts, however they are expensive and of limited sustainability. In this contribution, we address the challenges related to noble metal content and durability of water splitting catalysts by presenting a low-Ir content OER catalyst on a corrosion-stable oxide support with excellent electrochemical performance and durability. The catalyst is based on dealloyed and surface oxidized $IrNi_{3.3}$ nanoparticles (with IrNi@IrO_x core-shell structure) supported on high surface area mesoporous Sb-doped SnO_2. Activity, stability and characterization results will be discussed.

III-OP10

Partial Oxidation of Methane to Methanol with Bismuth-Based Photocatalysts

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Bi_2WO_6 and $BiVO_4$ were evaluated as photocatalysts in the selective oxidation of methane to methanol. CO_2, CH_3OH and C_2H_6 formed by a parallel coupling reaction were obtained as only products. Higher methane conversions and CO_2 concentrations were initially obtained with Bi_2WO_6, while better selectivity to methanol was observed with $BiVO_4$. Moreover, the influence of several scavengers and additives was also studied. The presence of Fe^{3+} species tends to increase the concentration of ·OH radicals and thus favors the complete oxidation of methane to CO_2. Conversely, nitrite ions have a positive effect on the selectivity by acting as UV filter and ·OH scavenger, thus completely inhibiting the formation of C_2H_6 and the total oxidation reaction. In this sense, $BiVO_4$ emerges as good alternative material in this process because of its lower oxidizing power, closely related to its band configuration.

III-OP11

Photocatalytic Hydrogen Evolution from Aqueous Solutions of Na_2S/Na_2SO_3 under Visible Light Irradiation of Nonstoichiometric Silver Sulfide Nanoparticles

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A method for the synthesis of nonstoichiometric silver sulfide nanoparticles which are catalytically active under visible light irradiation (450 nm) has been suggested and explored. The photocatalysts were characterized by UV–vis spectroscopy, high-resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and low-temperature N_2 adsorption–desorption techniques. The catalytic activity of nonstoichiometric silver sulfide nanoparticles was measured by the photocatalytic evolution of hydrogen from the aqueous solution of Na_2S/Na_2SO_3. High photocatalytic activity is measured for all samples with excess of silver nanoparticles. Higher photostability of nonstoichiometric silver sulfide nanoparticles stabilized by EDTA in compare to non-stabilized nanoparticles were found. This effect can be explained by nonstoichiometry and crystalline silver impurities on the surface of stabilized silver sulfide nanoparticles.

III-OP12

CO_2 Conversion into Solar Fuels

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The massive release of CO_2 to the atmosphere is believed to result in considerable climate changes, therefore a great deal of effort is being put to reduce its concentration in the atmosphere and to prevent its emissions. Solar energy, which is an abundant, clean and sustainable resource, can be used to photocatalytically convert CO_2 into a solar fuel. Solar fuels derived from CO_2 can contribute to neutralize the carbon balance into the atmosphere and can be converted into easily transportable liquid chemicals, such as CH_3OH. In this work, composites prepared from graphene oxide (GO) and titanium dioxide (TiO_2) are applied to the photocatalytic water reduction of CO_2 into renewable fuels. The effect of copper metal as co-catalyst will be assessed and its influence on the photocatalytic reaction inferred. It is found that the selectivity towards methanol formation is linked to the presence of Cu on the photocatalysts, while the visible light photo-response is assigned to the presence of GO.

III-OP13

Photocatalytic Pathways for Hydrogen Production from Biomass over UV- and Visible-Light Responsive Materials

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Sunlight-driven hydrogen production from readily-available biomass-derived resources (‘photocatalytic reforming’) is a promising route to supply a non-polluting, carbon-neutral energy storage medium. We have conducted a systematic study of the kinetics of photocatalytic reforming of a series of alcohol and polyol model compounds aiming at a comprehensive and general understanding of the reaction pathways of the respective anodic half-reactions over co-catalyst decorated semiconductors. We establish the existence of multiple reaction pathways and different reaction selectivities in dependence of the nature of the semiconductor by comparison of TiO_2-based photocatalysts and visible-light responsive oxynitride photoabsorbers (e.g. GaN:ZnO solid solutions). Investigations with systematically varied reactant structure (e.g. from methanol via ethylene glycol, glycerol to higher molecular weight compounds) revealed that a common set of intermediates is generated towards full mineralization (formation of CO_2).

III-OP14

Surface Dynamics of Ni^0 and Coke during Ethanol Steam Reforming on a Ni/La_2O_3-alphaAl_2O_3 Catalyst

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Steam Reforming of Ethanol is an attractive route for H_2 production, due to its increasing demand. In this work, we have studied the morphologic and compositional dynamics of Ni and coke phases on a Ni/La_2O_3–αAl_2O_3 catalyst during the process. Our aims are establishing a relationship among these dynamics and contribute to the understanding of the catalyst deactivation. The experiments were carried out in a fluidized bed reactor, at 500 ºC, steam/ethanol ratio = 3, $W/F_0 = 0.09\ g_{cat}\cdot min/g_{EtOH}$ and time on stream from 1.5 to 20 h. The dynamic changes of composition and morphology of Ni and coke were characterized by several techniques, as these changes are strongly correlated with the deactivation performance of the catalyst. Three stages are differentiated during a kinetic run, whose duration depends on the operating conditions and that occur in parallel with the growth of Ni-carbides, filamentous and pyrolytic coke.

III-OP15

CO-cleanup of Hydrogen-rich Stream for LT PEM FC Feeding: Catalysts and their Performance in CO Preferential Oxidation and Methanation

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The present report summarizes the results obtained during a systematic study of catalysts, their performances and fundamental principles of the preferential CO oxidation and preferential CO methanation reactions. CO PROX was studied over supported noble mono-metal based catalysts, supported bimetallic systems prepared with the use of double complex salts, and copper-ceria catalysts. CO MET was studied over nickel-based catalysts. The role of nickel precursor was investigated and the positive effect of chlorine on the catalyst selectivity was demonstrated. The catalysts were characterized by BET, XRD, XPS, TEM, EDX, TPR and TPD techniques.

Catalytic performance of the prepared systems in a form of grains in the fixed-bed continuous flow reactor was studied. The Cu/CeO_2 catalysts were coated on the surface of microchanel reactors and investigated in CO PROX. The structured Ni/CeO_2 catalysts supported over corrugated metal gauzes were studied in CO MET reaction in milli-channel reactor.

The effect of internal diffusion was estimated and the optimum grain size/coating thickness was found.

III-OP16

Catalyst with "core/ shell" Structure for Steam Methane Reforming Resistant to Presence of H_2S in Gas Mixture

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Results of studies on the activity of the Ni-containing catalyst in the steam reforming of methane (SRM) process are presented. It is established that the catalyst shows high activity in SRM, stability to coke formation and resistance to H_2S presence in the reaction gas mixture. The catalyst was prepared on the basis of mixed oxides separated from layered vermiculite. The structure and the phase composition of catalytically active components were investigated by XAFS, XRD, EDX, TEM and Moessbauer spectroscopy. It is found that the active components of catalyst are represented by clusters with core-shell configuration where FeNi alloy is a core (~10 nm) surrounded by superparamagnetic γ-Fe_2O_3 shell (1- 4 nm). These clusters are distributed in the mixed spinel $Mg(Fe,Al)_2O_4$ matrix. It is suggested that clusters of FeNi alloy are active in SRM while superparamagnetic γ-Fe_2O_3 particles are active in the oxidative decomposition of H_2S.

III-OP17

Mechanistic Implications on Low Temperature Steam Reforming of Methane over $Ni/La/CeO_2$-ZrO_2

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Low temperature reforming of methane combined with hydrogen-selective membrane offers significant advantages in terms of sustainability. The mechanism of methane steam reforming in the low temperature range (<550 ºC) is investigated over $Ni/La/CeO_2$-ZrO_2. H_2-TPR showed that the catalyst can be fully reduced within the temperature range of operation allowing the reduction process being conducted without the need of further heating of the reactor. At the same temperature range the catalyst showed maximum oxygen mobility as determined by oxygen isotopic exchange tests, which might contribute to the high activity and coke resistance of the catalyst. Temperature programmed methane decomposition showed that lattice oxygen of the partially reduced support participates in the reaction scheme.

III-OP18

Mechanism of Ethanol Steam Reforming over Pt/(Ni+Ru)-promoted Oxides by FTIRS in Situ

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Mechanism of ethanol steam reforming into syngas over Pt/ $Pr_{0.15}Sm_{0.15}Ce_{0.35}Zr_{0.35}O_2$ and 10wt.% $LaNi_{0.95}Ru_{0.05}O_3/Mg\text{-}Al_2O_3$ catalysts was studied by in situ FTIRS. Surface species (ethoxy, adsorbed ethanol, acetaldehyde, acetate) were identified and their thermal stability and reactivity were estimated. Transformation of ethoxy species by dehydrogenation is a fast step, while the rate-determining stage is the C-C bond rupture in thus formed acetaldehyde at metal sites. Acetate species are spectators, while transformation of ethoxy species on acid sites of alumina-supported catalyst produces C_2H_4 and $(C_2H_5)_2O$ via dehydration route.

III-OP19

Iron Oxide-type Structured Catalyst for Water Gas Shift Reaction

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The iron oxide-based material has been focused on as the promising catalyst for water gas shift reaction (WGS). This work was purposed to develop the iron oxide-based structured catalyst for WGS reaction.The prepared iron oxide on the aluminum plate had the characteristic morphology; the circular sheet of iron oxide was deposited on the aluminum plate. To promote the WGS performance of the iron oxide structured catalyst, a small amount of Pd and K was loaded on the iron oxide. As a result, a high activity was obtained on $Pd/K/FeO_x/Al$-plate. The synergistic effect was observed among the Pd, K and iron oxide components.

III-OP20

Low Temperature CH_4 Oxy-reforming Coupled with Pd-based Membrane for an Energy-efficient Process for Syngas Production

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Catalysts for reforming processes are generally affected by sintering and carbon formation. CH_4 oxy-reforming is the combination of SRM and CPO reactions in order to generate heat within the catalytic bed allowing to carry out the process at 750°C, at low residence times and S/C ratios.

$Ce_{0.5}Zr_{0.5}O_2$ support is synthesized through inverse microemulsion and impregnated with Rh (1 wt%). This catalyst exhibits an high activity in all of the conditions, reaching CH_4 conversions close or coincident with those calculated at equilibrium. Its high stability is also demonstrated, confirming the hypothesis asserting that the oxygen mobility of $Ce_{0.5}Zr_{0.5}O_2$ phase can increase the catalyst stability.

Combining oxy-reforming with a Pd dense membrane downstream the reactor, is possible to separate selectively H_2 from the outlet gas mixture. A stream of pure H_2 is obtained, but the H_2 efficiency must be improved using a sweep gas in order to raise up the separation driving force.

III-OP21

Effect of Ni-Cu-based Catalysts Composition and Support Structure on Hydrogen Production by Methanol Steam Reforming

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Hydrogen production via PEM fuel cells presents an eminently suitable alternative to internal combustion engines. Methanol steam reforming is a promising way to produce high-pure hydrogen for fuel cell from biomass.

New catalysts ($Ni_{0.8}\text{-}Cu_{0.2}/ZrO_2$, $Ni_{0.2}\text{-}Cu_{0.8}/ZrO_2$) were developed for the methanol steam reforming process. It was confirmed that obtained catalysts are active in MSR reaction. Catalysts showed good stability without apparent deactivation during the testing. It was shown also, that support structure has the main influence on composites activity, while the nature of a dominant metal affected on the selectivity of the resulting catalysts. The influence of support structure on the mechanism of MSR reaction was discussed. The most active and selective catalyst was the amorphous sample $Ni_{0.2}\text{-}Cu_{0.8}/ZrO_2$. The most probable mechanism of MSR process is bifunctional and includes simultaneous water adsorption on ZrO_2 support and alcohol adsorption on metal catalyst.

III-OP22

Stability and Activity Promoters in Medium Temperature Water Gas Shift Catalysts

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H_2 is considered as the main clean fuel of the future and is also a relevant raw material in chemical and petrochemical industry. One of the largest sources of H_2 is the Water Gas Shift (WGS) reaction currently performed in two reactors, although recently, the industrial interest moved towards new catalysts able to operate at medium temperature (MTS), that allow to operate in only one reactor and with low steam/dry gas (S/DG) ratios. In this paper it was investigated the effect of Ce, La and Zr to promote chemical-physical properties and catalytic activity in a Cu/Zn/Al MTS catalyst. It was observed that mainly La and Zr promoted the thermal stability, with a similar trend also for Cu surface area and dispersion. This effect resulted in significant increase of CO conversion in operating condition of industrial interest, with a good stability in time.

III-OP23

Effect of Nitrogen Doping of Carbon Supports for Hydrogen Production from Formic Acid Decomposition over Noble Metal Clusters and Atoms

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Effects of N-doping of carbon nanofibers and mesoporous graphene like carbon were studied for hydrogen production by decomposition of formic acid over Pt, Pd and Ru clusters of less than 3 nm size. N-doping of the supports (6-7 at.% N) provides a considerable increase of the formic acid decomposition rate (up to 10 times for Pt), selectivity to hydrogen (from 96.2 to 99.5% for Pt) and resistance to CO inhibition. This could be related to the presence of electron-deficient clusters and isolated atoms of metals stabilized by pyridinic nitrogen on the open edge graphene sites; these can dehydrogenate an intermediate adduct of formic acid with pyridinic nitrogen ($>NH^+HCOO^-$) to give hydrogen and carbon dioxide. The N-doped Pd and Pt catalysts showed the highest activity in the hydrogen production.

III-OP24

Going Heterogeneous in the Additive-Free Hydrogen Production from Formic Acid at Room Temperature

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Formic acid (HCOOH) has a great potential as a safe and a convenient hydrogen carrier for fuel cell applications. However efficient and CO-free hydrogen production through the decomposition of formic acid at low temperatures (< 363 K) in the absence of additives constitutes a major challenge. Herein, we present a new heterogeneous catalyst system comprised of bimetallic PdAg alloy and MnOx nanoparticles supported on amine-grafted silica facilitating the liberation of hydrogen at room temperature through the dehydrogenation of formic acid in the absence of any additives with unprecedented activity, converging to that of the existing state of the art homogenous catalysts. This superior catalytic system enables facile catalyst recovery and very high stability against agglomeration, leaching and CO poisoning. Current heterogeneous catalytic architecture presents itself as an excellent contender for clean hydrogen production via room-temperature additive-free dehydrogenation of formic acid in on-board hydrogen fuel cell applications.

III-OP25

Cr-Doped Alumina as Support for NiMo Vacuum Residue Hydroprocessing Catalyst

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Mesoporous alumina was doped with Cr using a coprecipitation method in order to prepare a support for hydrocracking catalysts. NiMo catalysts were prepared by impregnation on alumina (NiMo/Al_2O_3) and Cr-doped alumina (NiMo/Al_2O_3-Cr) and characterised. The presence of Cr in the support led to a better dispersion of NiMo and lower metal reduction temperatures as determined by temperature-programmed reduction (TPR) and X-ray photoelectron spectroscopy (XPS). As a consequence, a larger number of metal active sites was available in reduced form at operating conditions. The textural properties remained relatively unaffected by the coprecipitation of Cr together with the alumina. The catalysts were tested in their activity towards hydrodeasphaltenisation reactions using vacuum residue as feed in a batch reactor in two successive one-hour experiments involving reutilisation of the catalysts with fresh feed. It was found that Cr not only aided metal dispersion in catalyst synthesis but also coke dispersion during reaction, leading to sustained catalytic activity despite NiMo/Al_2O_3-Cr having a larger amount of coke deposits. Spent catalysts had a reduction in surface area and pore volume when compared to the fresh materials. Spent NiMo/Al_2O_3 catalysts had a decrease in average pore diameter (APD) whereas NiMo/Al_2O_3-Cr maintained the fresh material APD. NiMo/Al_2O_3-Cr could accommodate higher coke yields without significant variation in its textural properties.

III-OP26

The Dynamic Nature of ZnO in Industrial Cu/ZnO/Al_2O_3 Methanol Catalysts: From Minutes to Month

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Methanol has the potential to play a key role in the energy system of the future as a synthetic fuel[1]. The industrial catalysts consist mainly of Cu/ZnO/Al_2O_3, with a defective Cu surface in contact with Zn, enriched at the surface[2]. In this work, we report on the dynamic nature of ZnO, from a layered ZnO modification [5] to ZnO crystallites at different time scale and influences like pressure, temperature and gas atmosphere. We investigated the catalyst by quasi insitu neutron diffraction, HRTEM and DRIFTS etc. in full depth and found out, that ZnO is changing enormously in many facets, and identified a layered, graphitic ZnO modification by complementary methods at an industrial relevant catalyst[3,4]. To control the dynamic of ZnO is crucial for the development of more stable catalysts.

III-OP27

Studies on Au/Cu-Zn-Al Catalyst for Methanol Synthesis from CO_2

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Methanol synthesis from CO_2 via gas phase hydrogenation was carried out on Au/Cu-Zn-Al catalysts. The base Cu-Zn-Al with different Cu content was synthesized by rapid precipitation method and subsequently gold, 1-3 wt% was deposited on the base Cu-Zn-Al by deposition precipitation method. Solid catalysts investigated in this study were characterized by BET surface area, XRD, HR-TEM, XPS and CO_2, CO and H_2-TPD techniques. Formation of methanol in this study was influenced by the copper content in base Cu-Zn-Al and also on gold loading. Among the catalysts studied 1Au/C_4ZA (1 wt% Au supported on Cu: Zn: Al=4:1:1 mole ratio) exhibited maximum methanol yield of 16% mass. Among the catalysts studied the decreasing order of CO_2 conversion is as follows: 1Au/C_4ZA > 0.5Au/C_4ZA> C_4ZA> 3Au/C_4ZA at GHSV 7000 h^{-1}. The greater methanol yield on 1Au/C_4ZA attributed to; i) H_2 spill over by Au to adjacent copper in Cu-Zn-Al ii) higher adsorption capacities to H_2 and CO on Au-Cu-Zn-Al iii) surface Cu/Au ratio. To the best of our knowledge, this is the first report for gold influence on Cu-Zn-Al system in CO_2 hydrogenation process.

III-OP28

CO_2 Methanation on Iron Based Catalysts

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Our studies focus on the CO_2 methanation on iron based catalysts in order to substitute traditional Ni catalysts. We achieved high CH_4 yields in the temperature range between 250 and 450 °C, whereas the CO_2 fraction was varied from 0.1 to 20 vol.%. Moreover, phase transformation and morphology was examined during methanation by using in situ X-ray diffraction. Consequently, a correlation of structure and activity was obtained revealing high methanation activity of metallic iron. Additionally, the formation of carbonaceous bulk and surface species was found to be crucial for the methanation reaction. The nature of carbon species deposited on the catalyst strongly depended on the physicochemical properties of the precursor.

III-OP29

Changes in the Oxidation States of Cobalt Oxides for the OER Studied by XPS and their Correlation to the Electrochemical Activity

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Here we present CoO_x/Ti deposited by thermal chemical vapor deposition (CVD) and plasma enhanced CVD. We report electrochemical (EC), photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) measurements. The electrochemical behavior was coupled with the electronic structure by recording XP spectra after each electrochemical treatment (conditioning and cyclovoltammetry). We found that the electrochemical behavior of CoO_x/Ti depends on the preparation method and the resulting electronic structure. Thermal deposition leads to the formation of a Co(II)Oxide which undergoes during the conditioning a transformation to Co(II)Co(III)O_x. This change in oxidation state is coupled with an decrease in overpotential from η=0,57 to η=0,43V at 5mA/cm^2. Plasma deposited Co(III)-dominated mixed CoO_x has a lower onset potential from the beginning but transforms partly into Co(II) during the OER which increase overpotential from η=0,44 to η= 0,50V at 5mA/cm^2. It can be summarized that the Co(III)-state is observed as the active species and further investigations were done to stabilize this state.

III-OP30

Reactivity of Metals on Perovskites ($La_{0.6}Sr_{0.4}FeO_{3-d}$ (LSF) and $SrTi_{0.7}Fe_{0.3}O_{3-d}$ (STF)) Regarding Possible SOFC Usage

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The reactivity of two different perovskites, LSF ($La_{0.6}Sr_{0.4}FeO_{3-d}$) and STF ($SrTi_{0.7}Fe_{0.3}O_{3-d}$), was investigated regarding a possible usage as anode material for SOFC (solid oxide fuel cell) application.
The reactions were performed in a quartz batch reactor. The gas phase composition was monitored by mass spectroscopy.
The pure perovskites showed only inverse water gas shift reactivity but no methanation or methane reforming activity. Ttherefore both perovskites were impregnated with metals (Ni, Rh and Co). Comparing Ni-STF and Ni-LSF, the former showed a better methanation behaviour concerning activity and selectivity. The reaction also starts at lower temperatures about 250 °C. In the case of Ni-LSF the inverse water gas shift reaction is competing with the methanation reaction. Furthermore Ni-LSF is not as stable as Ni-STF.

III-OP31

Redox Catalysts for Electrochemical CO_2 Reduction: the Role of Local Proton Source

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The effects of the highly fluorescent 4-piperidinyl-1,8- naphthalimide (PNI) chromophore on the CO_2 reduction catalytic properties of rhenium-based catalysts are investigated. The electro- and photocatalytic CO_2 reduction features of [Re(CO)$_3$(bpy)Cl] (bpy = 2,2'-bipyridine) are compared with the activity of [Re(CO)$_3$(phen–PNI)Cl] (phen = 1,10-phenanthroline), which is known for its long excited-state lifetime. The effect of a local proton source on the activity of a bromotricarbonyl Mn redox catalyst for CO_2 reduction has been investigated. The electrochemical behaviour of the novel complex [fac-Mn(dhbpy)(CO)$_3$Br] (dhbpy = 4-phenyl-6-(1,3-dihydroxybenzen-2-yl) 2,2'-bipyridine), containing two acidic OH groups in the proximity of the metal centre, under a CO_2 atmosphere showed a sustained catalysis in homogeneous solution even in the absence of Brønsted acids.

III-OP32

Hydrogen Electrode Reactions over Nickel-Based Catalysts in Alkaline Medium: Influence of Composition and Structure of Ni Particles

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Activity of (electro)catalysts is known to be strongly influenced by the composition and structure of the particles. After contact with air the surface of metallic Ni is oxidized to form several layers of NiO covered by α-Ni(OH)$_2$, which further transform into β-Ni(OH)$_2$. We demonstrate the influence of NiO/Ni(OH)$_2$ species on the activity of Ni in the hydrogen electrode reactions in alkaline media. Electrodeposited Ni nanoparticles with different sizes was studied and compared with polycrystalline Ni disk electrode. Preparing of bimetallic Ni-based materials provides another way of changing the activity of Ni. We demonstrate the enhanced activity of carbon supported NiCu/C catalysts for the hydrogen oxidation/evolution reactions. We also developed a kinetic meanfield model which provides some insights into the mechanism of the hydrogen electrode reactions.

III-OP33

Gas-phase Partial Oxidation – Catalytic Carbonylation Conception for Small-scale GTL

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Despite the significant progress in industrial GTL technologies, even the world class GTL plants demonstrate only marginal limits of profitability. The main reason is the high expenditures for existing technologies of syngas production. Therefore, there are no expectations of the significant increase of traditional GTL in the nearest future. To increase the possibilities for practical application of gas chemistry two alternatives can be suggested. The first one is decreasing the cost of syngas, e.g. by matrix conversion of hydrocarbon gases. But the more evident is the developing of alternative "without syngas" GTL routes via direct partial oxidation or oxy-cracking of hydrocarbons with subsequent catalytic carbonylation and/or oligomerization of oxidation products. The paper discusses some alternative GTL routes of such kind alongside with possibilities to regulate the ratio of oxidation products depending on desired carbonylation processes.

III-OP34

Progress in the Catalysts for Small-scale Hydrogen Generators Based on Boron-containing Hydrides

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For safe operation of electronic devices, high-energy sources are needed. A promising solution is use of portable PEM fuel cells. It requires creation of systems for storage and generation of high-purity H_2. Generation of large amounts of hydrogen over a prolonged time is best achieved in a hydrogen generator (HG) with a flow reactor where a concentrated solution of hydride ($NaBH_4$, NH_3BH_3) passes through a fixed bed of granular catalyst. In this case, granulated Co-Ru catalyst is the most promising. HG with a batch reactor operating with solid pellets of mixture of $NaBH_4$ and active cobalt catalyst is needed for a short-time generation of H_2 which is important when charging batteries in the field. The active cobalt catalysts are formed from cobalt compounds directly in the in the reaction medium of boron-containing hydrides hydrolysis. Their structure was established using a set of modern physical methods, including EXAFS and neutron scattering.

III-OP35

Dry Reforming of Propane over NiO-CeO_2 Loaded Fnodized Fluminum Oxide(AAO) Catalysts

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The dry reforming of propane with CO_2 was carried out in a thermo-catalytic reactor. The catalytic performance of AAO supported catalysts with various nickel and Ceria loadings at different reaction temperatures. The obtained results show that both C_3H_8 and CO_2 conversions increased with increasing ceria loading up to 80%(0.8M) and 20% (0.2M) NiO/CeO_2-AAO catalysts showed the highest activity for dry reforming reaction. The prepared catalysts were characterized by XRD, FESEM, TEM, EDX dot-mapping, and BET analysis. The results of catalyst testing revealed that the catalysts with higher ceria loading catalyst (0.2M NiO+0.8M CeO_2) have superior catalytic performance for activity and stability than other loading. Although Ni-based catalysts have been intensively employed in reforming reactions, they commonly suffer severe deactivation due to sintering of metal particles and carbon deposition. After 12 h under stream at 540°C, CeO_2/AAO catalysts, showed a stable operation in presence of a deposited amorphous carbon. The main advantage of a plated catalyst is effective heat exchange and the formation of the NiO and CeO_2–bimetallic oxides on AAO support, which brings about the improvement in catalytic activity.

III-OP36

Impact of Hydrocracking on Fischer-Tropsch Synthesis Selectivity: Mesoporous ZSM-5-Supported Cobalt Nanoparticles for Selective Production of C_{5-11} Isoparaffins

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Bifunctional Fischer–Tropsch (FT) catalysts that couple uniform-sized Co nanoparticles for CO hydrogenation and mesoporous zeolites for hydrocracking/isomerization reactions were found to be promising for the direct production of gasoline-range ($C_{5–11}$) hydrocarbons from syngas. The Brønsted acidity results in hydrocracking/isomerization of the heavier hydrocarbons formed on Co nanoparticles, while the mesoporosity contributes to suppressing the formation of lighter ($C_{1–4}$) hydrocarbons. The selectivity for $C_{5–11}$ hydrocarbons could reach about 70% with a ratio of isoparaffins to *n*-paraffins of approximately 2.3 over this catalyst, and the former is markedly higher than the maximum value (ca. 45%) expected from the Anderson–Schulz–Flory distribution. By using *n*-hexadecane as a model compound, it was clarified that both the acidity and mesoporosity play key roles in controlling the hydrocracking reactions and thus contribute to the improved product selectivity in FT synthesis.

III-OP37

CO Activation on Cobalt Fischer-Tropsch Catalyst

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Transient kinetic experiments (SSITKA, chemical transient kinetics and $^{12}C^{16}O/^{13}C^{18}O$ isotope scrambling) are combined with first-principle based microkinetic modeling (MKM) to investigate the mechanism of CO activation that initiates the Fischer-Tropsch reaction. Together with MKM, the transient data can be interpreted in terms of the mechanism of both direct and H-assisted CO dissociation. Degree of rate control analysis suggests that CH_2O dissociation controls the overall rate for Co(0001) surface, and CO dissociation and CH_3 hydrogenation control the rate on Co(1121). Combined transient data show better correspondence of direct CO dissociation with the kinetics than hydrogen assisted CO dissociation does. This result was confirmed by transient data fitting. By $^{12}C^{16}O/^{13}C^{18}O$ isotope scrambling, we found that the CO scrambling TOF is close to that of the methanation, indicating that direct CO dissociation is the main mechanism of CO activation. Combined, these results highlight the importance of direct CO dissociation on Co nanoparticles.

III-OP38

Ethanol Acts as Capping Agent and Formaldehyde Scavenger to Promote Efficient Lignin Depolymerization to Aromatics

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Obtaining renewable fuels and chemicals from lignin presents an important challenge to the use of lignocellulosic biomass to meet sustainability and energy goals. We developed a thermocatalytic process for the depolymerization of lignin in supercritical ethanol over $CuMgAlO_x$ catalyst; this process delivers high yields of mainly alkylated mono-aromatics (60–86%, depending on the lignin used) with a significant degree of deoxygenation. We revealed new mechanistic insights about lignin depolymerization and highlighted the role of alcohol solvents In addition to its role as a capping agent and hydrogen source, ethanol also acts as formaldehyde scavenger that reacts with the formaldehyde formed from methoxy group cleavage from the lignin during supercritical ethanol-mediated reactions, which explains why ethanol is a better solvent than methanol for lignin depolymerization. We believe that these insights provide new impetus for the design of better processes to valorize lignin.

III-OP39

Biofuels Production from Glycerol and TBA using an Innovative Catalytic Membrane Reactor

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Glycerol *poly*-*tert*-butyl ethers can be produced by etherification of glycerol with *tert*-butyl alcohol (TBA) by employing an acid catalyst. This synthesis represents a new route for the oxygenated additives production for diesel fuels. Since the reaction is controlled by equilibrium and water is formed as *by*-product, irrespectively from the catalyst used, the reaching of high glycerol conversion and *poly*-ethers yield is limited by thermodynamic constraints. A study regarding the optimization of the reaction conditions is reported by exploiting an innovative batch reactor coupled with a permselective membrane to remove the water from the reaction medium and to promote the formation of *poly*-ethers. By setting the appropriate reaction parameters and employing a proper solid catalyst (Hyflon/SiO_2), it is possible to carry out the etherification of glycerol with TBA to obtain, in one step, an ethers mixture without glycerol containing about 80 wt.% of *di*- and *tri*-ethers suitable to be added to diesel fuel.

III-OP40

Catalytic C-O Cleavage and Hydrogenation of Diaryl Ethers in Aqueous and Apolar Phase

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The effects of substituted groups and solvents on the catalytic conversion of three di-aryl ethers (diphenyl ether (-H), di-*p*-tolyl ether ($-CH_3$) and 4,4'-dihydroxydiphenyl ether (-OH)) over Ni/SiO_2 in aqueous and apolar phase (*n*-hexane) have been investigated. Two competitive parallel reaction routes (C-O bond cleavage and hydrogenation) occur over Ni/SiO_2 under the reaction conditions. The substituted groups and solvents affect not only reaction pathways and the selectivities to C-O bond cleavage and hydrogenation, but also reaction rates via altering the reactant solubilities, solvent-reactant interactions, as well as by competitive solvent/reactant adsorption on the Ni surface. In aqueous phase, the reaction rates of C-O cleavage or hydrogenation follow the order of $TOF_{\text{4,4'-dihydroxyldiphenyl ether}} > TOF_{\text{diphenyl ether}} > TOF_{\text{di-}p\text{-tolyl ether}}$. The reaction rates follow the order of $TOF_{\text{di-}p\text{-tolyl ether}} > TOF_{\text{diphenyl ether}} > TOF_{\text{4,4'-dihydroxyldiphenyl ether}}$ in apolar phase.

III-OP41

The Effects of Methanol or Dimethyl Ether as Methylating Agent During Zeolite Catalysed Benzene Methylation

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Microporous zeolites and zeotypes are effective catalysts in aromatics transformations due to their acidity and shape selectivity. In this contribution, the methylation of benzene by methanol and dimethyl ether has been compared by experimental and theoretical methods. The study has been performed over two zeolites with different topology, H-ZSM-5 (MFI) and H-SSZ-24 (AFI), and an isostructural zeotype with lower acid strength, H-SAPO-5 (AFI). Methylation rates were significantly higher for dimethyl ether at 250 and 300°C. Remarkable selectivity differences were observed. The use of methanol led to high diphenylmethane yields in all catalysts, while dimethyl ether led to more selective methylation of benzene. The formation of diphenylmethanes is apparently accompanied by elimination of H_2 rather than alkane formation. Molecular dynamics simulations reveal different stability and reactivity of co-adsorbed complexes of methanol or dimethyl ether with aromatics. Further experimental and theoretical studies to elucidate the reaction mechanisms are ongoing.

III-OP42

Kinetic Analysis and Raman Surface Characterization in the CPO of Propane, Propylene and n-C_8H_{18}

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Fuel flexibility is a major goal of the Catalytic Partial Oxidation (CPO) for small-scale production of H_2: the reformer is required to process fuels ranging from NG and LPG, up to logistic and biomass-derived fuels. The main drawbacks are the high temperatures reached by the catalyst (>1000°C) and the formation of C-deposits. In this work, we analyze the CPO of C_3H_8, C_3H_6 (C_{2+} coke-forming fuel) and n-C_8H_{18} (logistic fuel) performed on Rh/αAl_2O_3 catalysts: the formation of C-species as a function of temperature is analyzed by combining kinetic investigations in an annular reactor with Raman measurements of the catalyst surface. The combined application of these techniques allows to individuate the nature of the catalytic site for the fuel activation (O-O, O- or - pairs) as well as the tendency of the fuel to from C.

III-OP43

Low Temperature In-situ Hydrogen Production by Ammonia Decomposition Using Cobalt-based Catalysts

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The use of chemical molecules, such as ammonia, as hydrogen vectors has the potential to unlock a pseudo hydrogen economy overcoming the transport and storage issues associated with the use of hydrogen in fuel cells. While we have currently demonstrated the low temperature decomposition of ammonia at 180ºC using ruthenium-based catalysts, our current efforts are based on the use of more readily available and cheaper metals such as cobalt. In this work, we demonstrate that the optimum cobalt nanoparticle size is well below the optimum 3-5 nm particles in the ruthenium case, demonstrating the importance of stabilising small cobalt particles on microporous and/or nanostructured supports such as γ-Al_2O_3 nanorods.

III-OP44

Na-modified Cu-Co-based Catalysts for Higher Alcohol Synthesis: Influence of Surface Composition and CoC_2 Formation

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Na-modified bimetallic Cu-Co-based catalysts for HAS were successfully prepared by coprecipitation and subsequent alkali loading by incipient wetness impregnation. The thorough characterization of the reduced and spent state enabled the evaluation of different catalyst properties and their correlation with the performance in HAS. The initial deactivation observed for the Na-free catalysts is explained by strong surface modifications under reaction conditions. In contrast, the surface composition is stabilized in the presence of the Na promoter resulting in a constant degree of conversion and a constant product distribution during HAS. Obviously, the presence of alkali promoters favors the carbidization of Co, which is assumed to improve the catalyst properties with respect to deactivation and product distribution.

III-OP45

Effect of Ni on the Hydrogenation Mechanism of Polyaromatic Hydrocarbons over (Ni-)MoS_2/Al_2O_3

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The study focuses on the effect of Ni as promoter on (Ni-)$MoS_2/\gamma\text{-}Al_2O_3$ catalysts. Combined IR and isotopic H-D exchange experiments showed that the concentration of active surface hydrogen increased by 30% in presence of Ni. Kinetic investigations of the hydrogenation of phenanthrene display differences in the hydrogen and H_2S reaction orders of Ni-$MoS_2/\gamma\text{-}Al_2O_3$, pointing to a change of the rate determining step. In combination with DFT calculations it was concluded, that Ni drives the reaction towards deep hydrogenation by increasing the coverage of active SH species plus optimizing phenanthrene adsorption on Ni-promoted MoS_2 edges.

III-OP46

Structured Catalytic Honeycombs Based on Copper/Ceria for CO Preferential Oxidation in H_2-Rich Streams

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In this work we systematically study the effect of the preparation method of slurries and of geometrical features (as cell density) and thermal conductivity of the substrate material on the activity of monolithic catalysts towards CO-PROX reaction. CuO/CeO_2 monoliths were successfully prepared and tested in CO-PROX reaction. At high conversion (i.e. under the most interesting reaction conditions) monoliths show improved performance with respect to powder catalyst, providing higher catalyst efficiency. Slurry composition affects catalytic layer adhesion and activity towards CO-PROX. Wet milling and colloidal ceria addition reduce the mean particle dimension of the powder used to prepare the slurry improving the specific surface area (ie. larger copper dispersion), but resulting in a partial intrusion of the washcoat into the cordierite macropores. The monolith performance can be optimized by engineering the catalytic systems and, in particular, by increasing the cell density and thermal conductivity of the substrate.

Section 4. Catalysis and Chemicals

IV-OP01

Selectivity in the Liquid-Phase Hydrogenation of 5-Hydroxymethyl Furfural over Ni-Al Catalysts

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Dehydrations of biomassderived sugars generate platform chemicals, such as 5-hydroxymethyl furfural. The liquid phase hydrogenation of 5-hydroxymethyl furfural was studied over $Ni_{1-x}Al_x$ catalysts ($0.2 \leq x \leq 0.45$) based on hydrotalcite like compounds. Temperature (80-140°C), pressure (20-60bars) and solvent (water, methanol) had a strong effect on the catalytic response. 100% yield of tetrahydrofuran-2,5-diyldimethanol was obtained when working at low temperature (80°C). An increase in temperature, to 140°C, was associated with a shift of selectivity. In water, the combined hydrogenation and ring rearrangement generate the formation of 3-hydroxymethylcyclopentanone. When working in methanol, we observed the etherification of the intermediate furan-2,5-diyldimethanol with formation of 2,5-bis(methoxymethyl)furan. We observed for the first time the formation of ether furan and cyclopentanone derivative over Ni catalysts.

IV-OP02

Liquid-Phase Hydrogenation of Benzaldehyde and Furfural over Pd/C and Ru/C Catalysts

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The study has revealed that the nature of carbon support (i.e. structure and physicochemical characteristics such as texture and acid-base properties) affects the formation and state of supported metal in the Pd/C and Ru/C samples as well as its catalytic properties in hydrogenation of benzaldehyde in ethanol medium and furfural in aqueous medium.

IV-OP03

Sustainable "Hydrogen Free" Catalytic Hydrogenation: From Concept to Reality

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Hydrogenation as a core catalytic operation in synthetic organic chemistry is typically operated in excess of pressurised gaseous H_2 to maximise product yield. Over 95% of global H_2 production is fossil fuel based with a pressing demand for alternative sources with enhanced efficiencies. A step change in catalytic hydrogenation must tackle H_2 utilisation and a completely new approach is urgently needed for sustainable chemical production. We establish the viability of novel coupling and cross-coupling catalytic dehydrogenation (as a source of reactive hydrogen) with hydrogenation. Cu/SiO_2 is effective in dehydrogenation and we demonstrate catalytic synergy between Au and Cu in reaction coupling with orders of magnitude enhanced H_2 utilisation, elevated selective hydrogenation rate and simultaneous production of several high value products. Our coupled system avoids the use of compressed H_2 from non-renewable sources with critical safety and long term supply implications for large scale production.

IV-OP04

Conversion of Furfuryl Alcohol into 2-methylfuran at Room Temperature Using Pd/TiO_2 Catalyst

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The selective hydrogenation of Furfuryl alcohol into 2-Methylfuran was investigated at room temperature using Palladium supported catalysts. $Pd\text{-}TiO_2$ catalysts can be very effective for the selective synthesis of 2-Methylfuran at room temperature and very low pressure of hydrogen. The effect of various reaction conditions (pressure, catalyst amount, and solvent) was discussed.

IV-OP05

Transition Metal Oxides Nanoparticles on Activated Carbon Fibres as Efficient Catalyst for Nitroarenes Reduction under Mild Conditions

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We report the catalysts based on transition metal oxides (Fe_2O_3, Co_3O_4, CeO_2, and NiO) supported on activated carbon fibres (ACF) developed for selective CTH of functionalized nitroarenes to corresponding anilines. Highly dispersed metal oxide NPs (2-4 nm) stabilized within ACF micropores were tested in CTH of nitroarenes with different substituents (-OCH_3, -CH_3, -H, -Cl, -$CH=CH_2$) using N_2H_4 as a reducing agent under mild conditions (T = 333 K: P = 1 bar). Extremely high yields (>99 %) of the desired products were achieved. The challenging reduction of nitrostyrene to vinylaniline was successfully performed over Co_3O_4/ACF with a selectivity of >99 % at full nitrostyrene conversion.

IV-OP06

Oxidation, Oxidative Esterification and Ammoxidation of Acrolein over Metal Oxides: Do These Reactions Include Nucleophilic Acyl Substitution?

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It is known that nucleophilic acyl substitution in the RCOX compounds (X = Hal, OCOR, and other “good leaving” groups) is a fundamental and energetically favorable route to carboxylic acid derivatives. When water, alcohols and ammonia are used as nucleophiles, carboxylic acids, esters and amides (or nitriles) are obtained, respectively. On the other hand, the same products are derived from aldehydes upon their catalytic aerobic oxidation, on condition that water, alcohols and ammonia are present in the feed gas. Therefore, one can surmise that nucleophilic substitution reactions are involved intrinsically in the catalytic oxidation reactions. In agreement with this hypothesis we have shown, as an example, that the selfsame catalyst, MoVTeNb mixed oxides, enables successful oxidation, oxidative esterification and ammoxidation of acrolein. In addition, the concept was considered in the view of established organic and general chemistry principals.

IV-OP07

Highly Enantioselective Oxidation of Olefins and Thioethers with H_2O_2 Mediated by Chiral Titanium(IV) Complexes

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Highly enantioselective epoxidation of olefins (with up to 99.8 % *ee*) and oxidation of thioethers (up to 98.5 % *ee*) with “green” H_2O_2 on novel chiral titanium(IV) salan and salalen complexes is reported. The effects of steric bulk and electronic properties of chiral ligands on the enantioselectivity of oxidations have been examined. Mechanistic studies reveal distinct mechanisms operating in those processes: stepwise mechanism for epoxidations and concerted one for sulfoxidations. The epoxidation on Ti-salan complexes is rate-limited by coordination of the olefin to the electrophilic titanium peroxo active species, while sulfoxidation on Ti-salalen complexes is rate-limited by generation of the titanium peroxo species upon reaction of the catalyst with H_2O_2. For the first time, non-linear temperature dependence of enantioselectivity (isoinversion behavior) has been documented for the asymmetric sulfoxidation reactions, with T_{inv} of 273…283 K, which temperature range may be recommended for preparative catalytic sulfoxidations.

IV-OP08

Catalytic Performance of Fluidizable Binder-free Mo/HZSM-5 Catalyst in the Non-oxidative Methane Conversion to Benzene at Severe Conditions

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With a high selectivity to benzene up to 70% the non-oxidative CH_4 dehydroaromatization over Mo/HZSM-5 provides a new route of direct conversion of methane resources toward valuable chemicals. However, due to serious coke formation the catalyst has to be operated in a continuous regeneration mode for maintaining its high activity. Thus a two-bed type of circulating fluidized bed reactor system was proposed and a binder-free, fluidizable Mo/HZSM-5 catalyst was developed for realization of industrial application of this new reaction system. In this study, the catalytic performance of this binder-free catalyst was evaluated in either a micro fixed-bed reactor, or a micro fluidized-bed or a two-bed type circulating fluidized bed system at the practically required severe conditions of 1073 and 10,000 mL/g/h. The results have demonstrated that this catalyst can offer a long-term stable aromatics formation activity under either periodic or continuous regeneration mode.

IV-OP09

Direct Dimethyl Ether Synthesis from Synthesis Gas: the Influence of Methanol Dehydration on Methanol Synthesis Reaction

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Direct dimethyl ether (DME) synthesis from synthesis gas is studied with regards to the effect that combining methanol synthesis and dehydration in a single reactor can have on the catalytic performance. For this, the influence of operating conditions (space velocity, temperature, pressure, time-on-stream and syngas composition) on activity, selectivity and stability of the catalyst was studied and compared for methanol synthesis, methanol dehydration and direct DME synthesis. Results confirm the advantage of direct DME synthesis over the two-step process at conditions where syngas conversion to methanol is thermodynamically limited. However, results suggest that combining methanol synthesis and dehydration has a negative effect on the methanol formation kinetics, which can be observed at conditions where the effect of the reverse reaction on methanol synthesis is negligible. The origin of the observed phenomena is further investigated by introducing the dehydration products (DME and H_2O) into the methanol synthesis feed.

IV-OP10

Methanol to Hydrocarbons over ZSM-5: Diffusion and the External Particle Surface

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The methanol to hydrocarbons process (MTH) is a valuable means by which to balance the use of fossil and renewable resources, providing a wide range of hydrocarbons from either renewable or fossil-derived methanol. We explore the contributing roles of internal and external acidity and hydrocarbon diffusion in ZSM-5 catalysts with respect to the conversion, selectivity and deactivation during the MTH reaction using a range of characterisation techniques, with particular focus on tapered element oscillating microbalance and pulsed field gradient NMR studies.

IV-OP11

Insights in the Reaction Mechanism for HMF Oxidation to FDCA over Bimetallic Au/Pd Nanoparticles

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This work deals with the oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA) using supported Pd-Au nanoparticles. The active phase composition was shown to be crucial for FDCA formation. Indeed, both Au and Pd nanoparticles formed 5-hydroxymethyl-2-furancarboxylic acid (HMFCA) under the studied conditions; however, with Pd HMFCA was not further transformed, while Au and bimetallic Pd-Au systems both catalysed its oxidation to FDCA.
The thermal treatment of Pd-Au catalysts considerably modified their catalytic activity, because Pd atoms concentrated onto the outer part of nanoparticles. The resulting morphology showed a different reaction path for FDCA formation compared to the untreated catalyst, with an important contribution of the Cannizzaro reaction. PVP-protected Pd-Au nanoparticles with different structures (either alloy or core-shell morphology) were synthesized and their reactivity tested in order to confirm the presence of different mechanisms for HMF oxidation, depending on whether the active phase preferentially exposes either Pd or Au atoms.

IV-OP12

Noble Metal Nanoparticles Supported on Carbon-based Materials as Catalysts for 5-HMF Oxidation to FDCA

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2,5-furandicarboxylic acid (FDCA) can be produced by 5-hydroxymethylfurfural (5-HMF) oxidation and has been selected as a building block chemical for the production of bio-based polymers. In the present study, the oxidation of 5-HMF in mild reaction conditions has been performed (100°C, 8 bar O_2) and water was used as a solvent (pH 9). The catalysts investigated were noble metal catalysts supported on carbon and polymeric materials and, accordingly to the preparation method, different particle sizes were achieved. Au, Pt and Pd showed high selectivity to the oxidation products of 5-HMF, while Ru produced low yields of the desired product. The most active catalyst prepared was Au(PVA)/C with particle size between 2 and 5 nm (95% FDCA after 8 hours), while Au/C with smaller particle size was totally inactive. Hydrophilic sulfonated polyacrylates (DAE25), inaccessible to fructose, are promising as supports for catalysts suitable for the one-pot reaction from fructose to FDCA.

IV-OP13

Catalytic Applications of Palladium Nanoparticles-supported Nanocomposites in Carbonylation Reactions

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Supported palladium nanoparticles (Pd NPs) have been widely used as efficient catalysts in organic conversions such as Suzuki-Miyaura cross-coupling reactions due to their high activity and recyclability [1,2]. We have successfully loaded Pd-NPs on varying supports such as metal organic frame works (MOF), cyclic poly(*L*-lactide)-clay, carbon nanotubes and graphene oxides to form Pd NPs-supported nanocomposites [3-7]. The prepared nanocomposites have been used as catalysts for carbonylation of various aryl halides to form corresponding amides and ketones, repectively (see Eqs. 1-2). These catalysts show high activity and good recyclability. Detail synthesis and activity will be presented.
Ar–X (X = Cl, Br, I) + CO + HNRR′ → Ar–CO–NRR′ ……………………(Eq 1)
Ar–I + CO + Ar′–$B(OH)_2$ → Ar–CO–Ar′ ……………………………..…(Eq 2)

IV-OP14

Hydrogenation Reactions in Aqueous Media Catalysed by Pd and Pt Green Nanoparticles

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We prepared and characterized a series of twelve NPs using two metals (Pd and Pt) with six different water-soluble lignins.
We investigated the different catalytic activity of Pt and Pd NPs towards the hydrogenation of allyl alcohols in mild conditions (water media, 20 °C, 1 atm).
The conversion of allyl alcohol with Pd NPs was quantitative. However, the main reaction product, was always propionaldehyde, the isomerization product of allyl alcohol.
At the contrary, when we put allyl alcohol with Pt NPs in aqueous solution, 1-propanol (in solution), propene and propane (in gas phase) were found.
Finally we tested also 2-buten-1-ol and 3-methyl-2-buten-1-ol. With both metal NPs, we observed lower conversions with allyl alcohol while 3-methyl-2-buten-1-ol showed the higher reactivity.
In presence of Pd NPs, we observed always C=C hydrogenation, isomerization and double bond migration products; in the case of Pt NPs only saturated alcohols and hydrocarbons were detected.

IV-OP15

Room Temperature Glucose Isomerization in Sn-BEA: on the Role of Diffusion under Practical Reaction Conditions

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The zeolite-catalyzed isomerization of carbohydrates is of topical interest in biomass valorization research. Diffusion limitations of the sugar molecules into the micropores of zeolites may have strong influence on catalyst performance. We investigated the effects of diffusion in the zeolite-catalyzed isomerization of carbohydrates. By using in-situ ^{13}C-MAS NMR on Sn-BEA impregnated with $^{13}C_1$-glucose, we found that under solventless conditions glucose is converted after impregnation of dehydrated Sn-BEA at room temperature, while in the case of hydrated Sn-BEA the reaction proceeds much slower. Our results point to the determining role of solvent exchange processes and diffusion limitations on the catalytic reactivity of Lewis acid zeolites in glucose activation. We extended our study of mass transport effects by assessing the reactivity of Sn-functionalized 10-MR MCM-22/ITQ-2 and 12-MR, 1-dimensional MOR. We find that the reactivity of these materials towards 1,3-dihydroxyacetone and glucose is adversely affected by diffusion limitations compared to Sn-BEA.

IV-OP16

A Theoretical Perspective on the Role of Cooperativity in Glucose Activation by Lewis Acid Zeolite and Oxide Catalysts

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The mechanism of glucose isomerization by Sn-BEA zeolite and surface of WO_3 oxide was studied by periodic DFT calculations. In both systems, the favourable reaction mechanisms involve a cooperative action of the Lewis acidic sites and neighbouring proton donors at the rate-determining H-shift step. Alternative pathways promoted solely by the Lewis acidic centres proceed with much higher activation energies. The proposed mechanisms closely resemble the way homogeneous catalysts and enzymatic systems promote such a reaction. The activation of glucose by bio- and chemocatalysts involves the dynamic and cooperative action of their active sites towards selective glucose transformation. These fundamental insights pave the way towards a generic reactivity concept of carbohydrate activation.

IV-OP17

New Insights in the Catalytic Conversion of Sugars with Sn-Beta

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This study focuses on increasing the selectivity to methyl lactate from carbohydrates using stannosilicates as heterogeneous catalyst. The presence of alkali metal ions was found to have a promoting effect on the yield of methyl lactate from sugars at 170°C, resulting in an increase in yield from sucrose from 30 to 75% using Sn-Beta. It was found that the alkali source could both be added to the catalyst during synthesis, but also directly to the solvent during reaction. The beneficial effect applies not only to Sn-Beta prepared by the fluoride route, but also to Sn-Beta prepared by post-treatment of a dealuminated commercial zeolite and to other non-zeolithic stannosilicates such as Sn-MCM-41 and Sn-SBA-15. These findings make it possible to expand on the catalyst portfolio and get a better understanding of the reaction system.

IV-OP18

Mg-Al Hydrotalcites with Tailored Structure as Efficient Catalysts for Glucose Isomerization into Fructose

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Mg-Al hydrotalcites with various Mg-to-Al molar ratios, texture and morphology were synthesized by co-precipitation and studied as catalysts for the isomerization of glucose into fructose. Preparation was conducted at different parameters such as pH during co-precipitation, aging temperature and solvent. The catalysts were characterized by ICP-OES, N_2 sorption, sorption of acrylic acid, XRD, TG-DSC, and SEM. Variation of synthesis procedure allows controlling properties such as crystallite size, dispersion of primary particles and morphology of their agglomerates. Composition and structure of hydrotalcites impact the basicity, while performance of the catalysts dramatically depends on the concentration of basic sites. The best fructose yields up to 30% with 89% selectivity were obtained over materials synthesized in (i) aqueous medium at pH 10 and (ii) aqueous-ethanol mixture at pH 9.5. Although some leaching of magnesium occurred, the hydrotalcites could be recycled without loss of activity and selectivity.

IV-OP19

Liquid Phase Oxidation of Glucose to Gluconic Acid over Supported Metal Catalysts

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The metal catalyzed liquid-phase oxidation of glucose to gluconic acid is widely studied, since the latter is a fine chemical used as water soluble cleansing agent and additive for food and beverages. At alkaline pH and at 70°C under 3 bar O_2, the best results are obtained with Au supported on the mesoporous carbon SX with full conversion and good yield of gluconic acid (90%). Even using air as oxidizing agent the Au/SX catalysts give good results in terms of conversion (~100%) and yield of gluconic acid (~90%). Some catalyst systems were also tested at neutral pH, using pure oxygen as oxidizing agent. With Au(1wt%)/ZnO at 70°C the conversion is ~55% with a selectivity of ~90%, while at RT the values of conversion and selectivity to gluconic acid are respectively ~40% and ~80%, with lower amount of gluconic acid produced (~30%).

IV-OP20

Efficient Carbon Based Catalysts with Acid Sites and Magnetic Properties for Starch Valorization to Bio-chemicals

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Along with cellulose, starch is an important raw material for the synthesis of levulinic acid (LA). Many studies were done in homogeneous acid catalysis but the use of mineral acids presents a series of drawbacks. Solid acid catalysts represent an alternative to such systems, but progress is still insignificant, and new active and selective solid catalyst systems wait to be discovered and developed. In this context, the main objective of this work was the design and development of carbon based catalysts (i.e., MWCNT and graphene) with acid sites and magnetic properties, suitable for the starch conversion into chemicals. Obtained results indicated the GO@SO_3CF_3 sample as more active and selective than MNP@MWCNT-SO_3H sample. Interesting enough, the reaction selectively to either lactic (49%) or levulinic acid (60%) is not controlled by the L/B acid sites ratio but by the reaction conditions.

IV-OP21

New Cross-dehydrogenative Coupling Reactions with Selective C-O Bond Formation

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The cross-dehydrogenative C-C coupling was studied in most detail; the C-N, C-P, and C-O cross-coupling reactions are less well developed. It is difficult to achieve high selectivity in the cross-dehydrogenative C-O coupling because the starting compounds are prone to side oxidation and fragmentation reactions giving, for example, alcohols and carbonyl compounds. In this work we found cross-dehydrogenative C–O coupling of 1,3-dicarbonyl compounds and their heteroanalogs with oximes, hydroxyamides, and peroxides.

IV-OP22

Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate on Mordenite

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Ketene is a reaction intermediate in the carbonylation of dimethyl ether to methyl acetate over Mordenite. The formation of ketene is predicted by our detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid, when D_2O is introduced in the feed during the carbonylation reaction.

IV-OP23

On the Mechanism for the First C-C Bond Formation in MTO Reaction

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Catalytic conversion of methanol to hydrocarbons (MTH) on acidic zeolite is an important process in respect of gasoline (MTG) and olefin (MTO) production. The mechanism for the first C-C bond formation is still unclear despite of diverse proposals. We detected acetic acid and methyl acetate as potential intermediates in MTO. In parallel, an increase of MTO reaction rate was observed in the presence of CO. Therefore, we propose that the first C-C bond is formed through carbonylation of surface methoxy groups, generating surface acetyl groups, which transform further into the first ethylene and propylene.

IV-OP24

Activity Control of Supported Catalysts with Tailored Ru Nanoparticles for Non-Oxidative Propane Dehydrogenation

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Owing to large reserves of shale gas and growing demand for propene, non-oxidative propane dehydrogenation (PDH) to propene is now playing an important role in the chemical industry. However, industrially applied Pt-based catalysts are expensive, while their CrO_x-based counterparts are toxic. Therefore, the purpose of the present study was to develop alternative catalysts, which are free on the above drawbacks. In this contribution we introduce novel PDH catalysts comprising commercial supports and well-defined (1 nm) Ru nanoparticles (NP) with an overall metal loading of only 0.05 wt.%. The kind of support was found to crucially influence the catalyst activity. H_2-TPR results indicate that supported Ru NP influence support reducibility that might be responsible for the catalytic activity. Ru/La_2O_3-ZrO_2 showed both higher formation rate and space time yield of propene compared to an industrial Pt-Sn/Al_2O_3 analogue. Such results appear promising from an applied viewpoint and provide fundamental insights for developing active and selective PDH catalysts.

IV-OP25

Methylation Reaction of Aromatic NH-heterocycles with Using Supercritical Methanol: Competitive Homogeneous and Heterogeneous Catalysis by Si-containing Compounds

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Experimental data obtained point to the mixed and competitive heterogeneous–homogeneous catalytic effect of Si-containing compounds on the methylation reaction of some aromatic NH-heterocycles with methanol at 350°C without additional methylating reagents. The starting SiO_2-containing material (quartz, Pyrex glass or silica gel) reacts with methanol at supercritical conditions to form *in-situ* tetramethyl orthosilicate (TMOS). Both solid SiO_2 and liquid TMOS have demonstrated the pronounced and comparable catalytic effect.

IV-OP26

Effect of Promoter Addition to SBA-15 Supported Bimetallic Co-Ni Catalysts for Dry Reforming of Methane

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DRM was investigated over Co-Ni bimetallic supported on Sc, Mg, and La- SBA-15 catalyst with the aim to minimize carbon deposition. The fresh and spent prepared catalysts were characterized using N_2-adsorption, XRD, TGA, TEM and TPR. Results showed a CH_4 conversion of 73 and 76%, respectively, during the first 6 h and a slight decrease during 25 h to 66 and 73%, respectively. It seems that the stability of the Sc catalyst could be due to the generation of non-deactivating carbon deposits. The type of carbon deposition and/or location of carbon might be the reason for the deactivation of the catalysts.

IV-OP27

New Chiral Cage Phosphines for Homogeneous Asymmetric Catalysis

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The increasing demand to produce enantiomerically pure pharmaceuticals, agrochemicals, flavours and other fine chemicals has advanced the field of asymmetric catalytic technologies. Ligands with optically active phosphorus(III) centres have been used to some extent in transition metal-catalysed enantioselective reactions. Chiral cage phosphines are characterised by the presence of a chiral non-racemizable phosphorus atom situated at the bridgehead of a bicyclic system. The effectiveness of cage phosphines as weak, bulky ligands have been demonstrated in different asymmetric homogeneous catalysis with *ee*'s > 99% [1].

IV-OP28

Catalytic Conversion of Cellulose to C_2-C_3 Glycols Using Heterogeneous Platinum Catalysts Supported on Cerium Oxide

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Cellulose, the most abundant and non-food carbohydrate source on earth, has attracted considerable attention for the production of bio-sourced platform molecules. In particular, the interest for C_2-C_3 glycols has been driven by the increasing demand for ethylene glycol and bio-based polyethylene terephtalate (PET) in the packaging industry. Original dual catalytic systems combining homogeneous and heterogeneous catalysts based on basic oxides were screened for the conversion of cellulose to C_2-C_3 glycols. This dual approach associates the advantages of a homogeneous catalyst –selectivity and enhanced solid substrate-catalyst contact– and those of a heterogeneous one –stability and recyclability This communication aims to illustrate the great potential of such catalytic systems to achieve high selectivities in ethylene and propylene glycols (EG and PG) from cellulose. A specific focus on a cerium oxide-based catalytic system and its role in reaction mechanisms will be presented.

IV-OP29

Conversions of Cellulose and Its Derived Carbohydrates into Lactic Acid in Water Catalyzed by Al(III) and Sn(II) Dual Cations

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The development of new routes for direct transformation of cellulose into high-valued chemicals such as lactic acid is of great importance for establishing sustainable chemical processes. Herein, we report our recent finding that the combination of Al^{III} and Sn^{II} dual cations work efficiently for the direct conversion of cellulose into lactic acid in water. A lactic acid yield of 66% was attained from cellulose at 463 K. Our studies revealed that the formation of lactic acid underwent three key tandem reaction steps from glucose, i.e., the isomerization of glucose to fructose, the retro-aldol fragmentation of fructose into trioes, and the isomerization of trioes to lactic acid. We clarified that Al^{III} was responsible for the isomerization of both glucose and trioes, while Sn^{II} played a significant role in the retro-aldol fragmentation of fructose to trioes.

IV-OP30

OSDA-Free Beta Zeolite with High Al Content as Efficient Catalyst for Biomass Conversion

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A route to producing useful chemicals from biomass by using “green” zeolite catalysts has been successfully developed. Organic structure-directing-agent (OSDA)-free Beta zeolite with a high Al content exhibited a remarkably high catalytic performance in the conversion of glucose to 5-hydroxymethylfurfural (HMF) by virtue of its appropriate acid properties; A sufficient number of Lewis acid sites was generated by calcination of the NH_4-form zeolite with the original Brønsted acid sites substantially maintained, resulting in the high Brønsted/Lewis acid ratio and the proximity of both acid sites.

IV-OP31

Thermooxidative Catalytic Treatment of Biomass

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The new catalytic oxidative treatment of biomass is suggested. The colloid catalyst, based on iron (III) oxides, together with hydrogen peroxide as oxidants realizes the oxidative destruction of lignobiomass under atmospheric pressure at mild temperature. The oxidative destruction of biomass results in formation of organic acids and other low molecular oxidation products derived from lignin, hemicellulose, cellulose, lipoproteins and sugars; the solid product constitutes of cellulose and its derivatives. The yield and quality of the solid product depends on biomass nature, reagents concentration ratio (biomass, catalyst, hydrogen peroxide), and oxidation process duration. In this work, the possibilities of the treatment to process lignocellulosic biomass of different origin (rice and oat straw, wood sawdust, peat, olive press cake) in reaction vessels of different sizes have been studied. The main attention is brought to develop waste-free and environmentally friendly features of catalytic treatment and to reveal the optimal conditions for biomass treatment.

IV-OP34

Heterogeneous Oligomerization of Ethylene over Highly Active and Stable Ni-exchanged Mesoporous Materials

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Ni-AlMCM-41 and Ni-AlSBA-15 oligomerization catalysts (2-2.6 wt% Ni and Si/Al = 7-9) were prepared and characterized by various techniques, including powder X-ray diffraction, N2 sorption, TEM, ^{27}Al and ^{29}Si MAS NMR. Both types of materials exhibited outstanding catalytic behavior in the oligomerization reaction of ethylene. At 150 °C and 3.5 MPa, in both batch and flow mode, the catalysts were highly active (up to 175 g of oligomers per gram of catalyst per hour), selective (C4, C6, C8, and C10 olefins, no cracking products) and stable (high conversion during 80 h on-stream). These performances were superior to those exhibited by other Ni-based heterogeneous catalysts. A mechanistic pathway involving metallacyclic intermediates is supported by the experimental results.

IV-OP35

Evolution of Catalytic Systems and Technologies of Production and Solid-state Processing of Ultra-high Molecular Weight Polyethylene with Ultra-durable and Ultra-modular Properties

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The question of the evolution of catalytic systems used in the production of ultra high molecular weight polyethylene is reviewed. It is shown that increasing requirements for production technology (living polymerization mechanism, improving the morphology of the resulting reactor powders, simplifying the processing conditions) was associated with the expansion of the catalyst systems from modified Ziegler—Natt's multicenter catalytic systems to a single site metallocene catalyst systems and postmetallocene. The requirements for the choice of the polymerization conditions which provide receiving reactor powders of ultra high molecular weight polyethylene with improved processability, including solid-phase processing in ultra-durable and ultra-modular product, were formulated.

IV-OP36

Enantiomerically Pure Zirconocene Complexes in Asymmetric Alkene Carbo- and Cycloalumination

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The catalytic action of enantiomerically pure conformationally rigid and non-rigid complexes Zr in the reaction of alkenes of various structures with organoaluminum compounds has been studied. The effect of intramolecular exchange between conformers of substituted bis-indenyl Zr η^5-complexes on the reaction chemo- and enantioselectivity was shown.

IV-OP37

Tuning the Selectivity of Nanocatalysts by Using the Ligand Modification Strategy: Experiment and Theory

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Surface ligand modification could open a new door to enhance the selectivity for selective hydrogenation reaction over noble metal nanocatalyst. In this contribution, we provide several examples, such as chemoselective hydrogenation of α, β-unsaturated aldehydes, selective hydrogenation of nitroaromatics and selective hydrogenation of benzyl substituted olefins. Based on comprehensive structural characterizations and DFT calculation, it is clearly revealed that simple organic modification could precisely shape the selectivity through steric and/or electronic effects. In addition, adsorbed H atom could also be viewed as surface modifier, which significantly affects the nature of the surface and controls the selectivity.

IV-OP38

Electrochemical Fluoroalkylation and Phosphorylation Catalyzed by Transition Metal Complexes (Ni, Co etc.) to Avoid Chemical Oxidants or Reductants

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As a result, a one-step catalytic method for aromatic perfluoroalkylation with metal complexes electrochemical reduction under mild conditions with decisive role of the sacrificial anode metal ion has been developed. This technique was tested with various catalysts and anode metals. Some laws of this reaction were discovered. Some regularities of this reaction, such as the linear dependence of Ar-R_F yield vs reduction potential of the catalyst, the copper anode fundamental importance for the selective formation of the cross-coupling product, which confirms the important role of transmetallation step in the catalytic cycle, were shown.

New approach to C-H bonds of aromatic substrates phosphorylation, based on nickel, cobalt or manganese complex in the high oxidation states generation and regeneration on the electrode was proposed. New methods of organofluorine and organophosphorus compounds synthesis can find possible practical application for biologically active, hydrophobic or plasticizing compounds production.

IV-OP39

Complexes of Rare- and Alkaline-Earth Metals for Catalytic Intermolecular Olefin Hydrophosphination and Hydroamination Reactions

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Rare-earth complexes proved to be efficient catalysts for a wide range of transformations of unsaturated substrates (polymerization, hydroamination, hydrosilylation, hydroboration etc).

The synthesis and characterization of heteroleptic alkyl, hydrido, amido rare-earth (+2 and +3) and alkaline-earth complexes supported by various N,N-, N,N,N,N-, N,N,O-, N_2,O_4-, N,N,P(O)-ligands as well as their catalytic activity in intermolecular olefin hydrophosphination and hydroamination will be reported. The new complexes afford highly active, chemoselective and, in the case of monoadditions, 100% *anti*-Markovnikov regiospecific catalysts (down to 0.04 mol-% loading) for the hydrophosphination of styrene with $PhPH_2$ under mild conditions. The highest TOF 330 h^{-1} at 60 °C was observed for Yb(II) amido complex. These complexes also turned out to be efficient precatalysts for the intermolecular hydroamination of styrene and pyrrolidine.

IV-OP40

Catalysts for Resource Efficiency: Organic Carbonates from CO_2 and Alkyl or Aryl Alcohols on Cs_2O/BEA Zeolite

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Modifying BEA zeolites with both Cs^+ exchanged ions and Cs-oxide like nanospecies it is possible to increase their basic properties and their capacity for CO_2 activation. Cs/BEA catalyst with Cs/Al ratio = 1.6 was tested in the reaction between alkyl C_1-C_4 and aryl (catechol) alcohols and CO_2. The ability of the alkyl C_1-C_4 alcohols to form the corresponding organic carbonates depends on the length of the alkyl chains – it decrease with the increase of the alkyl chains length. Conversely, larger but rigid aromatic ring of catechol appeared as an active substance in the reaction with CO_2 for the production of the carbonate.

IV-OP41

Synthesis of Monoterpenoid Dioxinols from Isopulegol and Benzaldehyde over Heterogeneous Catalysts

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New biologically active substances are synthesized from a variety of compounds isolated from natural sources. It has been published that compounds with benzodioxin framework can possess promising analgesic activity. Compounds with the mentioned structure were synthesized by the reaction between *cis*-verbenol oxide and aromatic aldehydes in the presence of an excess of montmorillonite clay.

In the current research, syntheses of compounds with the desired benzodioxin framework were investigated. Besides verbenol oxide also substrates with analogous structure, namely isopulegol and 3-methyl-6-(prop-1-en-2-yl)cyclohex-3-ene-1,2-diol, were tested in the reaction with benzaldehyde.

In the present work zeolite Beta-150 was modified by iron, characterized and tested per se and in the modified form for syntheses of compounds with the desired benzodioxin framework.

Addition reactions were observed to be influenced by the structure of substrate as well as by physico-chemical properties of the catalysts.

Detailed kinetic analyses and reaction mechanisms will be discussed in the final work.

IV-OP42

Fabrication of Efficient and Stable Solid Acids via Encapsulation of PS-SO_3H within Hollow Interiors

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Efficient and stable solid acids have been successfully synthesized by sulfonation of polystyrene (PS) in the hollow interiors of silica-based hollow nanostructure. It was found that larger and smaller inner void space results in the formation of PS-SO_3H-SiO_2 respectively with double-shell (DSNs) and yolk-double-shell nanostructure (YDSNs). PS-SO_3H-SiO_2 with DSNs and YDSNs nanostructure shows comparable activity and is more active than Amberlyst-15 in the esterification reaction. PS-SO_3H-SiO_2 with YDSNs nanostructure affords higher activity than that with DSNs nanostructure in the Friedel-Crafts alkylation of toluene with 1-hexene, which is mainly attributed to the fact that unique YDSNs nanostructure could slow down the swelling rate of PS-SO_3H during the catalytic process. More importantly, PS-SO_3H-SiO_2 with YDSNs nanostructure showed much higher recycle stability than Amberlyst-15 in the Friedel-Crafts alkylation of toluene with 1-hexene, probably due to the high thermal stability of sulfonic acid group and unique YDSNs nanostructure.

IV-OP43

Acid-base Catalysis in the Synthesis of C-amino-1,2,4-Triazoles from Aminoguanidine and Carboxylic Acids

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C-amino-1,2,4-triazoles (AT) are employed as multifunctional reagents for the production of pesticides, medicaments, pigments, corrosion inhibitors, energetic materials, *etc*. One of the promising approaches to the synthesis of AT is based on the two-step reaction of aminoguanidine with carboxylic acids which proceeds through the formation of intermediate 2-guanyl hydrazides. Although this method has received industrial application for the preparation of some AT (R = H, COOH), yields of many AT in the reactions of aminoguanidine with many carboxylic acids are poor, and, therefore, the method needs to be improved. The report describes the results of our studies of the mechanisms, thermodynamic and kinetic parameters of the reaction between aminoguanidine and carboxylic acids as well as new elaborated approaches to the catalytic synthesis of 3-substituted 5-amino-1,2,4-triazoles.

IV-OP44

Synthesis of Propylene Oxide with molecular O_2 over well Dispersed Ferrosilicate prepared by a One-Pot Protocol

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In this study, we have developed a one-step synthesis catalyst based on very well dispersed iron single sites on a silica structure. The catalyst has been tested in propylene epoxidation reaction, using two different atmospheres H_2/O_2 and O_2 to evaluate the behavior of the catalyst.
Propylene Epoxidation. The catalytic tests are performed in a quartz tube reactor with a feed composition O_2/C_3H_6 (10 % each) and He as carrier gas (GHSV= 10000 ml $h^{-1}g^{-1}$ in all cases). The temperature is raised up to 500ºC at 3ºC/min.
A novel catalyst has been synthetized for propylene epoxidation with molecular O_2 and H_2/O_2 mixtures with a good performance, due to the very well dispersed iron single-sites on the silica support. Additional characterization (FTIR and UV-VIS) is mandatory to get insights into the reaction mechanism that is taking place in the presence of the catalyst.

IV-OP45

Synthesis of 1-Butanol and 1-Propanol from the Mixture of Methanol and Ethanol in the Presence of Hydrotalcites as Basic Catalysts

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Synthesis of 'Guerbet' alcohols is a reaction of great importance for enhancing the potential of biomass derived chemistry. Here, hydrotalcite catalysts (Mg/Al = 2, 3, 4, 5, 6, 7) were prepared by the ultrasound assisted coprecipitation method. The synthesized solids have been characterized in terms of their structural, textural, and surface properties, including the acid-base and red-ox features, by a variety of techniques (BET, XRD, TG, and TPR). The strength, strength distribution, and number of acid and base sites were estimated by adsorption microcalorimetry measurements of ammonia and sulphur dioxide, whereas their nature was evaluated by FTIR of adsorbed CO_2 and pyridine. Furthermore, a variation of 'Guerbet' reaction, using a mixture of methanol and ethanol in order to produce two valuable products for the chemical industry, namely 1-propanol and 1-butanol in gas phase was performed. Special attention was devoted to the relationship between surface acidity-basicity and catalytic activity.

IV-OP46

Factors Affecting the Activity of Oxide Catalysts in the Synthesis of N-phenylpropionamide from Propanoic Acid and Aniline

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Amidic group synthesis is a fundamental step for the manufacture of a variety of biological compounds and innovative materials. The main industrial processes relying on reaction between amines and activated carboxylic acids precursors or on the direct condensation between carboxylic acids and amines at high temperature, actual synthesis suffer from serious economic and environmental drawbacks. Then, the direct catalytic synthesis of amides from ammines and acids has been recently indicated as a major Green Chemistry issue. Comparative studies of the reactivity pattern of commercial and lab-made oxide catalysts (γ-Al_2O_3, CeO_2, ZrO_2, TiO_2) in the synthesis of N-phenylpropionamide (T, 383K) from aniline and propanoic acid allows to relate physico-chemical properties with catalytic functionality. 0^{th}-order kinetic dependence on reagents concentration suggests that the amidation reaction proceeds via a L-H path kinetically controlled by desorption steps (r.d.s.), while the formation of bidentate, bridging and unidentate carboxylate intermediates account for different amidation functionalities.

IV-OP47

Methane to Methanol – Influencing Factors for the Direct Catalytic Low Temperature Oxidation with Copper Zeolite Catalysts

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Methanol is a flexible key component for several alternative fuels. A catalytic method for direct partial oxidation of methane to methanol using molecular oxygen at low temperatures was developed. This research is focusing on copper zeolite catalysts which were found to be active for this catalytic oxidation reaction. It was found that the catalytic performance of methane oxidation is influenced by several factors such as catalyst preparation techniques and diverse pre-treatment steps. Experiments have shown that catalysts with the same metal loadings, achieved through different preparation procedures have different effects on the product yields. Calcination studies found that the reaction is more efficient when the catalyst is calcined in-situ. Contamination with air after calcination and pre-reaction was found to affect the product yield.

IV-OP48

Heterogeneously Catalyzed Aqueous Phase Amination and Isomerization of Biogenic Isohexides

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The replacement of monomers by novel biomass-derived building blocks is of major importance for the utilization of renewable resources in polymers production. We report a heterogeneously catalyzed conversion of the hydroxyl groups of bifunctional isohexides by amination to the corresponding diamines. Compared to conventional alcohol amination in the gas phase this reaction is carried out at temperatures below 200°C in aqueous solutions of the substrates. Different catalysts were screened, reaction condition optimized and the reaction kinetics were investigated to gain an understanding of the reaction path via the dehydrogenation, imine-formation and hydrogenation to the amine. An unusual effect of stereoselectivity due to the different configuration of the hydroxyl groups was observed and investigated in detail. Overall, this work poses a foundation for the future development of commercial processes for the production of isohexide-based amine monomers as well as of aqueous phase amination processes of biogenic alcohols in general.

Section 5. Catalysis and Environmental Protection

V-OP01

Highly Accessible TiO_2 Nanoparticles Embedded at the Surface of SiO_2 for the Photocatalytic Degradation of Pollutants under Visible and UV Radiation

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A new synthesis method was developed to prepare a series of TiO_2/SiO_2 composites in which TiO_2 nanoparticles are embedded at the surface of SiO_2. The method is based on the use of activated carbon as template. The obtained materials display high surface area and well-dispersed, highly accessible TiO_2 domains. These features led to a higher photocatalytic activity than the TiO_2 P25 benchmark in the degradation of pollutants both under UV and visible radiation. The activity in visible light stems from residual C atoms of the carbon template.

V-OP02

Photocatalytic Activity of the Uranyl Modified Titania, Silica and Alumina under Visible Light Irradiation

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Photocatalysis is a promising method for destruction of various toxic pollutants. TiO_2 is the most active heterogeneous photocatalyst which is playing an important role in many industrial and technological processes. Unfortunately pure TiO_2 is active only under the mild UV irradiation ($\lambda<400$ nm) which occupies only about 4% of the solar light spectrum. In order to utilize solar light efficiently in the visible region ($\lambda>420$ nm) which covers large range of the solar spectrum, the development of visible-light-driven photocatalysts has started over last decades.

It is well known that uranyl ions in water could be synthesized by visible light and after excitation the oxidizing potential of uranyl ions becomes as high as 2,6-2,7 V. At the same time the gas phase photocatalytic oxidation of organic species with uranyl-modified photocatalysts is weakly investigated. The influence of spectral characteristics, uranyl quantity and nature of the support were the subject of current research.

V-OP03

Combining the Photocatalyst Pt/TiO_2 and the Non-photocatalyst $SnPd/Al_2O_3$ for Effective Photocatalytic Purification of Groundwater Polluted with Nitrate

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We investigated photocatalytic reduction of NO_3^- in real groundwater in the presence of a photocatalyst Pt/TiO_2 and a non-photocatalyst $SnPd/Al_2O_3$, which were dispersed in the groundwater, under irradiation at $\lambda > 300$ nm, with glucose as a hole scavenger. NO_3^- in the groundwater completely and selectively decomposed to N_2 (83%) after 120 h over the Pt/TiO_2-$SnPd/Al_2O_3$ system in combination with photooxidative pretreatment of the groundwater over Pt/TiO_2 to decompose organic compounds. The decomposition rate of NO_3^- in the groundwater was still slower than that in an aqueous NO_3^- solution even after the pretreatment of the groundwater. The lower photocatalytic performance was due to poisoning of Pt/TiO_2 with sulfate and silicate ions and poisoning of $SnPd/Al_2O_3$ with polymerized silicate ions. On the other hand, cations, including Na^+, K^+, Mg^{2+}, and Ca^{2+}, in the groundwater did not affect the photocatalytic and catalytic performances of the system.

V-OP04

Hierarchically Porous Fe-silicalites for Total Oxidation of Organic Molecules

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Series of hierarchical Fe-silicalites were prepared by two approaches: template synthesis and patterning Fe-silicalite nanocrystals. The synthesized samples were characterized by a number of methods: laser diffraction analysis, X-ray diffraction, scanning and transmission electron microscopy, energy-dispersive X-ray spectroscopy, argon and nitrogen adsorption measurements, inductively coupled plasma optical emission spectrometry, UV visible diffuse reflectance spectroscopy and temperature-programmed desorption of ammonia. Hierarchically porous Fe-silicalites were tested in total liquid phase catalytic oxidation of different organic molecules, including phenol, the natural polymer – lignin, macrolide antibiotic – clarithromycin lactobionate and metal ion complexing agent – EDTA by H_2O_2 at low temperatures (298-323 K) compared with Fe-silicalite microspheres and homogeneous Fenton reagent. Performances of hierarchical Fe-silicalites in oxidation of large organic molecules by hydrogen peroxide were significantly improved *vs.* the reference Fe-silicalite microbeads, resulted from increasing catalytic sites accessibility.

V-OP05

CO_2 Methanation on Commercial Ni/Al_2O_3 and Ru/Al_2O_3 Catalysts

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CO_2 hydrogenation was successfully carried out on commercial Ni/Al_2O_3 and Ru/Al_2O_3 catalysts. Both catalysts were fully characterised by the use of XRD, IR, UV-vis, H_2-TPR, FE-SEM before and after reaction. Ru/Al_2O_3 is an excellent catalyst for CO_2 methanation, arriving at 96% methane yield with no CO coproduction at 573 K at 30000 h^{-1} GHSV in excess hydrogen. Moreover, at 648 K is completely selective to methane while Ni-based catalysts reveals already CO coproduction. Kinetic orders of reactant partial pressure were successfully determined for both catalysts. A different behaviour of the two catalysts was observed during activation, since only Ru/Al_2O_3 catalyst must be conditioned on stream, simple reduction in hydrogen is not giving rise to a fully active catalyst. This behaviour suggests that activation implies not only reduction but also other chemical conversion. Ru/Al_2O_3 catalyst was not deactivated after nine cycles thus may be adopted in intermittent condition operations.

V-OP06

CO_x Hydrogenation on Promoted Iron Based Catalysts: the Key Role of the Potassium on the Process Selectivity

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The hydrogenation of CO_2 to hydrocarbons is a potential solution to convert a primary green-house-molecule into added value products. It is known that the addition of potassium to Fe-based catalysts improve the selectivity to long-chain hydrocarbons during CO hydrogenation, but no information are available for CO_2 containing streams. In this work, Fe-catalysts with different K/Fe atomic ratios were tested in presence of $H_2/CO_2/N_2$, $H_2/CO/N_2$ and $H_2/CO/CO_2$ mixtures. During CO_2 hydrogenation, K was found to have a dramatic effect on the product selectivity. Indeed high K-loadings promote the chain growth process and inhibit the secondary reactions of primary olefins. These results were explained in terms of K-effects in stabilizing surface iron carbides and considering the K role as electron donor, able to affect the relative adsorption strengths of H_2, CO and CO_2.

V-OP07

Conversion of CO and H_2 to Liquid Hydrocarbons via Dimethyl Ether on Zeolit Catalysts

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TIPS RAS has developed the technology of highly selective preparation of the gasoline range hydrocarbons from CO and H_2 via oxygenates (DME and methanol) which is an analog process to the one of TIGAS by Haldor Topsoe company, which uses synthesis gas with the ratio of $H_2/CO=1$. Advantage of the method developed in TIPS RAS is ability to use the synthesis gas of practically any composition with achievement of high conversion of synthesis gas for pass. The advantages of this technology can also be attributed to the flexibility in the orientation of the final product, taking into account characteristics and needs of a particular oil field. Depending on the process conditions can be obtained as high-octane gasoline and the mixture of hydrocarbons with a low aromatic content, which is essentially analogous to a light synthetic oil, which can be used as a product of processing of associated petroleum gas for injection into the pipeline.

V-OP08

Performing Industrial Scale Steam Reforming of CO_2-rich Gas

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Use of traditional nickel catalyst for reforming of CO_2-rich gas has been demonstrated on industrial scale plants with a dry synthesis gas production up to 133,000 Nm^3/h, but this requires a co-feed of large amounts of water. The technology is challenged due to the low H/C ratio of a reforming feed with high CO_2 content, which implies that a high potential for carbon formation exists. Developing of technology for this field is closely related to more traditional steam methane reforming (SMR), as reaction mechanism and kinetics are comparable. With increased resistance toward carbon formation, the SPARG (sulfur passivated reforming) process or noble metal catalysts have been demonstrated in industrial scale, showing that operation is possible at very severe conditions for reforming of feedstocks with high CO_2 concentrations and only a minor co-feed of water.

V-OP09

Methanol Synthesis from Steel Mill Gases

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Methanol synthesis is performed over a Clariant industrial catalyst. The methanol synthesis is carried out using different gas compositions. Catalyst testing is performed at the temperature range of 190 – 260ºC and pressure of 15 – 30 bars. The first set of measurement was carried out at different temperatures, pressure of 30 bar and space velocity of 4800 h^{-1}. It was shown that CO_2 conversion and methanol yield increase with temperature since the reaction rate is higher at higher temperature. However, selectivity to methanol decreases, that can be explained by two competitive reactions: methanol synthesis and reverse water gas shift reaction which have different thermal effects, high temperature results in higher contribution of reverse water gas shift reaction. The stability test with benzene in the feed gas was done at 250ºC, 15 bars and 4800 h^{-1} for 250 hours. The methanol rate practically does not change during the experiment, that confirms stability of the catalyst at the chosen reaction conditions.

V-OP10

Molybdenum-based Catalysts for the Biogas Dry Reforming

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Methanisation is an alternate way widely implemented because it produces biogas from organic waste digestion. This gas contains CH_4 and CO_2 and the major advantage for the utilization of biogas is the consumption of the two main greenhouse gases for the production of syngas (H_2, CO), which could be industrially attractive for the Fischer-Tropsch process, eventually setting up a promising waste-to-liquids fuel substitute. The major inconvenient is the presence of hydrogen sulphide, an impurity in the above-mentioned biogas. In this context, it is of great interest to design a catalyst with the potential to maintain its activity in the presence of sulphur and/or in a sulphided state.The Mo catalysts have shown some very promising features for the DRM in the presence of sulphur. They also exhibited higher stability to carbon deposition. Metallic promoters were used to enhance the catalyst thermal stability and help suppressing carbon deposition.

V-OP11

Stepwise Tuning of Multi-sites CuZnZr-HZSM5 Catalysts for Direct DME Synthesis from CO_2-H_2 Mixtures

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The perspective of using CO_2 as "carbon source" for producing methanol and/or dimethylether (DME) looks very attractive since their potential alternative use to traditional crude oil derived fuels. The properties of CuZnZr-HZSM5 catalysts were investigated in order to shed lights into the requirements necessary to design a multifunctional catalyst active in one-step synthesis of DME by CO_2 hydrogenation reaction. With respect to the conventional physical mixing between methanol catalyst and zeolite, the incorporation of metal-oxide and acid sites in a single system can enhance the CO_2 conversion, also allowing a higher rate of MeOH formation/dehydration on neighbour surface sites.

V-OP12

New Fiberglass Based Pt Catalyst for VOC and CVOC Removal

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The highly dispersed Pt species were stabilized in the bulk of Zr-silicate glass. By means of STEM-HAADF and XPS with ion etching it was shown that positively charged 1-1.5 *nm* Pt clusters are located at a depth of 10-20 *nm*. In spite of a very low noble metal content (0.01-0.02%), the Pt/FG catalysts revealed a higher performance in both VOC and CVOC abatement in comparison with conventional ones containing 30-60 times more platinum. In particular, the catalyst almost completely destructed the dioxin up to acceptable level of 0.4 ppb. Moreover, the TOF was 5-10 times higher as compared with the alumina-, or silica-supported Pt catalysts. The SSITKA study showed that molecular oxygen species activated on metal clusters are involved in deep oxidation of hydrocarbons. The high performance of the fiberglass catalyst in VOC removal was successfully confirmed at the industrial level.

V-OP13

Synergetic Effect of Pd Addition on Catalytic Behaviour of Monolithic Catalysts for Diesel Vehicle Emission Control

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We early demonstrated synergetic effect of Pt and manganese oxides which allows decreasing the Pt loading to 0.7-1.05 g/L in the catalytic system for diesel engine exhaust treatment. Here, we are reporting our study of the effect of Pd addition into Pt-MnO_x-Al_2O_3 monolithic catalysts on their catalytic activity and stability in hydrocarbon and CO oxidation.

The synergetic effect in catalytic activity is observed also at Pd addition into Pt-MnO_x-Al_2O_3 catalyst. As result, new diesel exhaust catalyst contains a Pt loading as low as 0.17 g/L at the Pd loading of 0.35 g/L. The PtPd-MnO_x-Al_2O_3 catalyst has high activity in low temperature oxidation of light hydrocarbons and high thermal stability.

We are discussing also Redox properties (TPR-H_2), particles size and morphology (HRTEM), and interaction of nanoscale Pt/Pd particles with Mn-modified alumina (chemical differentiating dissolution) in order to explain a positive effect of Pd on catalytic behaviour of Pt-Mn-alumina catalyst.

V-OP14

Propane Oxidation over Pd/Al_2O_3: Selectivity, Activity and Size Effect

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Propane oxidation reaction over Pd/Al_2O_3 catalysts with different Pd nanoparticles sizes was studied in this work. The dependence of catalytic activity from several parameters such as the reaction temperature and C_3H_8:O_2 ratio in inlet gaseous mixture was revealed. The increase of TOF values with particles size growth was found for propane combustion reaction. It is shown that reaction path can be changed from total oxidation to steam conversion of propane in CH_x-rich mixtures and at higher temperatures. Moreover, the selectivity towards CO in steam conversion reaction is higher for the catalyst with the smallest mean diameter of palladium nanoparticles. XPS in-situ was used to show that palladium active state in propane oxidation reaction is mixed Pd^0-PdO state. Furthermore, Pd^0/PdO ratio in the active component straightly correlates with TOF values for the total propane oxidation reaction.

V-OP15

Methane Oxidation over Palladium: On the Mechanism in Rich Methane-Oxygen Mixtures at High Temperatures

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The major environmental concern of natural gas fueled engines is the methane slip into the atmosphere. Therefore palladium-based catalysts are widely used in gas-engine emission control systems to guarantee lowest levels of methane pollution. This work presents a first part of a newly formulated surface reaction mechanism focusing on the oxidation of methane over the reduced palladium surface. The mechanism is evaluated through numerical simulation and comparison with experimentally obtained spatially-resolved species concentration profiles in a Pd/Al_2O_3 coated honeycomb monolith channel at various carbon-to-oxygen feed ratios. Both the numerical and experimental investigations show that methane is first converted through a total oxidation zone before partial, total oxidation and steam reforming reactions participate concerted further downstream in the catalyst channel. The developed multi-step surface reaction kinetics on reduced palladium, predicts all features of the experimental spatially-resolved species profiles.

V-OP16

Hierarchical Pd/ZSM-5 Catalysts for Methane Oxidation in the Presence of Steam

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Catalytic methane oxidation is applied in exhaust gas treatment to reduce unburnt methane emissions in stationary combustion processes as well as in natural gas vehicles to mitigate the severe greenhouse effect of methane. Pd/zeolite catalysts are reported to provide higher activity than the commonly used Pd/Al_2O_3, but suffer from rapid deactivation under reaction conditions and in the presence of steam, mainly due to sintering and formation of inactive $Pd(OH)_2$.

In this work a novel approach is proposed with the aim to inhibit sintering of Pd particles dispersed on zeolite support. Small Pd clusters are stabilized within constricted mesopores of ZSM-5 obtained by desilication with NaOH in the presence of tetrapropylammonium bromide.

The catalytic activity of Pd on parent and desilicated zeolites was very similar under dry conditions. However, in the presence of water vapour desilicated zeolites had 50-70°C lower light-off temperature compared to the parent zeolite.

V-OP17

Mixed Ionic-electronic Conducting Catalysts for Catalysed Gasoline Particulate Filter

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Future changes in Europe regulation (Euro 6c in 2017) concerning particle matter (PM) abatement will probably lead to the implementation of filter devices in direct injection gasoline (GDI) engines. Catalyzed-Gasoline Particulate Filter (cGPF) can be combined with conventional three way converter (TWC) to meet pollutants standards. Electro-promoted nano-dispersed catalysts for vehicles exhaust after-treatment is getting growing attention since they can combine electrochemical promotion of catalysis and high metallic active site availability. Nano-cell catalysts are composed of nano-electrodes (two different natures of metallic nanoparticles) supported on a mixed ionic-electronic conductor (MIEC). Washcoated MIEC-based catalysts inside mini-GPFs have been tested for GDI exhaust aftertreatment using a bench scale plant. The presence of a membrane in GPFs modifies both, their catalytic and filtering performance. The impact of the membrane, the catalyst loading and location as well as the presence of soot particles on the catalytic properties will be discussed.

V-OP18

Surface Chemistry of Glycerol on Metals and Metal-Oxides as Model Catalysts for Biomass Conversion

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Employing renewable sources from biomass to produce chemicals and energy is one of the most important technological approaches to solve the energy crisis, thus developing the concept of biorefineries. When obtaining biodiesel from biomass conversion, about 10 % of the reaction by-product is glycerol. Therefore, is mandatory to search for new processes to upgrade this by-product into more valuable chemicals. By combining several surface science techniques we studied the adsorption and reactivity of glycerol with metal single crystals and metal oxide model catalysts. This polyalcohol reacts on Pd surfaces producing CO and H_2 (good reforming catalyst). The presence of oxygen on Pd opens up other decomposition pathways where more aldehyde is observed. The Au surface presents no reactivity, but it can be boosted up with chemisorbed oxygen (RCOOH). Atomistic level understanding can be reached from surface science studies which can be then applied for the development of new catalytic materials.

V-OP19

Ionic Liquids Based Silica Microreactors for the Efficient Conversion of Carbon Dioxide

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Transformation of CO_2 into high added value products is an interesting topic since CO_2 is a non-toxic, renewable and easily available source of carbon. Among these valued products, cyclic carbonates and polycarbonates stand out. The reaction usually needs from a catalyst able to activate either the carbon dioxide, either the epoxide or both. At this purpose, ionic liquids have demonstrated a good catalytic activity to overcome CO_2 transformation in homogeneous [3, 4] and in heterogeneous conditions. Over the years, different strategies for ionic liquids heterogeneization have been proposed. In this work, a novel heterogeneization strategy where a double alkyl chain imidazolium ionic liquid is polymerized as liposome-like structure and used as template for the synthesis of mesoporous silica is presented. The hybrid silica microreactors with a porous shell and accessible imidazolium core displayed excellent performances in the synthesis of cyclic carbonates via chemical fixation of carbon dioxide into various epoxides.

V-OP20

One-pot Natural Alcohol Amination Catalyzed by Gold-containing Catalysts

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The one-pot terpene alcohol amination, which is of high practical importance for the synthesis of complicated amines with specific physiological properties, was systematically studied in the presence of gold catalysts to obtain the knowledge about the key parameters determining the catalytic performance. The catalytic activity and product distribution were shown to be strongly dependent on the support properties, namely acidity and basicity, and conditions of the catalysts pretreatment. The Au/ZrO_2 catalyst pretreated under oxidizing atmosphere was observed to be rather active resulting in total conversion of myrtenol and selectivity to corresponding amine of about 53%. The reaction kinetics was modeled based on mechanistic considerations with the catalyst deactivation step included in the mechanism.

V-OP21

Utilization of CO_2 in the Process of Olefins Production

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Production of olefins is a very crucial and relevant reaction . Utilization of CO_2, especially as a mild oxidant, has received considerable attention recently By combining those 2 aspects, we proposed oxidative dehydrogenation of propane with the use of CO_2. Here we proposed the use of Pd -Ce based catalyst, to achieve high conversion and selectivity in this reaction. Studies involving TAP measurements over 5%Pd/$Ce_{0.25}Zr_{0.25}Al_{0.5}O_{1.75}$ clearly showed CO production from CO_2 at temperature higher than 300°C.The role of CO_2 in reverse water gas shift reaction as well as in oxidative dehydrogenation via Mars van Krevelen mechanism will be fully presented. The most active catalyst has been fully characterized using several techniques, e.g.: TEM, EXAFS and TPRDO. Also DRIFT analysis with CO_2 and CO will be presented.

V-OP22

Selective 1,2-propanediol Formation via Tandem Reaction Cycle of Methanol Reforming-glycerol Hydrodeoxygenation

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A tandem catalytic cycle of methanol aqueous phase reforming-glycerol hydrodeoxygenation targeted to 1,2-propanediol formation under inert conditions is investigated. Methanol aqueous-phase reforming provides the H_2 which sequentially drives the deoxygenation of glycerol. This cascade system is effectively catalysed by a CuZnAl catalyst and under the optimum reaction conditions glycerol is selectively converted to 1,2-propanediol with high yields (74.3%). Reusability studies showed moderate initial deactivation and further stabilization after three reaction cycles. Moreover, reactants intrinsic rate slightly vary upon reuse, revealing the structural integrity of the nature of the active sites. Exploration of the reaction pathways indicated that glycerol hydrodeoxygenation primarily proceeds via a dehydration-hydrogenation mechanism (via hydroxyacetone as intermediate). However, contribution of the glyceraldehyde route (dehydrogenation-dehydration-hydrogenation) to 1,2-propanediol formation cannot be excluded.

V-OP23

Gold Catalysts for CO-free Hydrogen Production from Formic Acid Derived from Biomass

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Formic acid (FA) is a non-toxic by-product of biomass cellulose hydrolysis used for production of levulinic acid.
We showed for the first time that Al_2O_3 is a better support than MgO, CeO_2, ZrO_2 and La_2O_3 supports to stabilize active Au species for hydrogen production from FA decomposition and doping of the Au catalyst with potassium ions leads to a considerable improvement of the catalytic performance. Thus, a 3 wt.% Au/Al_2O_3 catalyst with 3 wt.% of K is an effective and stable (>26 h) catalyst for the FA decomposition at low temperature (<360 K). It provides CO free hydrogen production.
The K-doping effect could be explained by the presence of K+ ions in FA liquid condensed in the catalyst's pores, which stabilize formate ions in the solution providing a different mechanism of FA conversion through these ions as compared to the undoped catalyst.

V-OP24

Bimetallic Catalysts Promising in Bio-fuel Production

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The paper presents the results of studies on direct catalytic conversion of primary biomass products into hydrocarbon fuels components. Ethanol, 2-methylpropanol-1, 3-methylbutanol-1, mixture of fermentation organic products, glycerol, rapeseed oil and wood cellulose were used as a feed. With the use of industrial and laboratory bimetallic catalysts based on alumina and zeolite supports original approaches to the selective conversion of bio-substrates into alkanes, olefins, aromatics and naphthenic hydrocarbons components of gasoline and diesel fractions were elaborated. It was found the novel reaction of hydrocarbon skeleton cross-condensation of ethanol combine together with another bio alcohols, glycerol and acetone into hydrocarbons makes it possible to substantially extend the range of renewable raw materials for fuels production. It was manner to combine conversion of products fermentation and rapeseed oil mixture to alkane-aromatic gasoline and kerosene fractions without loaded of molecular hydrogen was created. Hydrogen is need for rapeseed oil hydrogenate deoxygenation was forming inner of the reaction zone during coupled reaction carrying out of ethanol aromatization. It was shown that rapeseed oil can be selectivity converts to narrow C3 and C18 alkane-olefin fractions and H_2O with used of $Pt\text{-}Sn/Al_2O_3$ catalysts.
With using of XAFS, X-Ray, TEM HR as well as kinetics and FDT methods it was studied active components structure evolution and mechanistic aspects of bio-substrates conversion.

V-OP25

NO Oxidation and Standard SCR over Fe-ZSM-5 Catalysts. Combining Moessbauer Spectroscopy and Reactivity Studies on the Search for the Active Sites

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Active sites of NO oxidation and standard SCR over Fe-ZSM-5 have been investigated by combining catalytic studies on conventional and ^{57}Fe-enriched samples with post-mortem low-temperature Mössbauer spectroscopy. Investigation of reaction rates depending on Fe content suggest that NO oxidation is catalyzed by a small minority of the iron present while there are two different site types for standard SCR: isolated sites remaining three-valent in reaction medium, and small oligomeric Fe oxo clusters. Mössbauer measurements at 5 K under low and high external field were analyzed with 5 signals representing different species: Fe^{III} in antiferromagnetically coupled clusters (particles), high-spin Fe^{II}, two signals representing three isolated Fe^{III} oxo ions, oligomeric clusters with (pseudo)paramagnetic behavior and diamagnetic structures, the latter most likely to be identified with $Fe^{III}\text{-O-}Fe^{III}$ sites discussed in literature. The role of the observed species in SCR catalysis will be discussed.

V-OP26

The Rate Determining Step for the Selective Catalytic Reduction of NO by Ammonia

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A reaction scheme for the SCR reaction is constructed, in which only stable molecules are adsorbed and desorbed from the catalyst, and which describes the overall stoichiometry of the NH_3-SCR reaction correctly. By example of a Cu-CHA catalyst, the stability of the intermediates appearing in the reaction scheme and the transition state energies of relevant reaction steps have been verified by combination of density functional theory (DFT) and EPR, IR and X-ray Spectroscopy. From the reaction scheme, it can be determined that the rate determining step for NH3-SCR over a Cu-CHA catalyst is the activation of NO by O_2 on a Cu^+ site, and that this is not in contradiction to a very low rate for NO oxidation to NO_2 in the absence of ammonia. The reaction scheme further provides new insights in the role of several reaction intermediates, resulting in a deeper understanding of the NH_3-SCR reaction.

V-OP27

Structure-Activity Relationship for Cu-zeolite NH_3-SCR Catalysts

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Cu-zeolites are considered the most efficient SCR catalysts due to high activity at low temperature. The relationship between SCR performance and zeolite structure is analyzed for three different Cu-zeolites (Cu-BETA, Cu-SSZ-13, and Cu-SAPO-34) by steady state and transient kinetic experiments and by in-situ DRIFT spectroscopy. The results suggest that the zeolite structure has a crucial role in determining the stability and reactivity of the reaction intermediates of SCR reactions.

V-OP28

Influence of the Preparation Method and Used Support on the Activity of Fe-loaded Zeolites Catalysts for the NH_3-SCR of NO_x

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A series of Fe-loaded zeolites catalysts were prepared by impregnation and in-situ hydrothermal synthesis, and the influence of the preparation method and the support used (ZSM-5, Beta and LTL) on the SCR-NH_3 activity was studied. These catalysts after aged were characterized by N_2 adsorption, ICP, RMN, XRD, XPS and TEM analysis. Iron species on the surface were assigned to the Fe^{3+} ions and the small amount of Fe^{2+} in the case of the hydrothermal catalysts, whereas the impregnated catalysts presented the formation of Fe_3O_4 oxides, which resulted in difference in SCR activity. The hydrothermal catalysts presented higher activity, N_2 selectivity and lower N_2O formation than the impregnated one. This could be a consequence of the partial pores blockage of the zeolite and the Fe_3O_4 oxides formation, when the impregnated method was used. Moreover, the framework structure and/or pore geometry of the used support was crucial for determining the SCR activity.

V-OP29

$CeVO_4$-based as Efficient and Stable Catalyst for NH_3 Selective Catalytic Reduction of NO_x – Application to Diesel Exhaust Gas

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Reduction of NO_x by NH_3 is recognized as the most efficient technology for practical application for both stationary and mobile sources. However commercial V_2O_5–WO_3/TiO_2 or V_2O_5–MoO_3/TiO_2 can suffer from vanadium toxicity due to the presence of V_2O_5. By contrast, cerium orthovanadate material ($CeVO_4$) has interesting properties related to the stabilization of Ce^{3+} and V^{5+} cations in tetragonal zircon-type structure. This compound is also active in oxidation reaction thanks to its reducibility. In the present study we investigated the catalytic behaviour of $CeVO_4$ in the Selective Catalytic Reduction of NO_x by ammonia. Particular attention was focused on the impact of synthesis procedure and thermal ageing treatments on the catalytic activity in standard SCR, fast SCR and NO_2 SCR conditions.

V-OP30

Base-promotion of Selective Decomposition of Ammonium Formate and Formic Acid over Au/TiO_2 under SCR-relevant Conditions

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A systematic study investigating the influence of ammonia on formic acid decomposition over Au/TiO_2 under SCR-relevant conditions revealed a significant promotional effect on the rates and CO_2 selectivity. Analogously, it was demonstrated that such a gas-phase basic-reactant effect can be realized as a catalytic effect by introducing a base metal oxide (La_2O_3) to the catalyst. However, both forms of the base-induced promotional effect were contingent on the presence of gold. These findings are important for the application of formate-based alternative ammonia precursors for SCR.

V-OP31

Sulfur-Tolerant BaO/ZrO_2/TiO_2/Al_2O_3 Quaternary Mixed Oxides for DeNOx Catalysis

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It is apparent that although high BaO loadings favor higher NOx storage capacity (NSC), they also render the NSR/LNT catalyst more prone to sulfur poisoning. By, designing a catalyst with a proper support material (e.g. AZT) and functionalized with intermediate BaO loadings (e.g. 8 wt% BaO), a sulfur tolerant NSR/LNT system with a satisfactory NSC can be achieved. This hypothesis is tested in quantitative flow reactor measurements performed under realistic catalytic conditions suggesting that Pt/8BaO/AZT catalyst shows a superior NSC at 573 K upon sulfur poisoning and subsequent regeneration, surpassing the catalytic performances of all of the currently investigated materials including the conventional Pt/20BaO/Al benchmark catalyst.

V-OP32

Opportunities for Ceria-based Catalysts Versus Platinum Catalysts in Diesel Soot Combustion

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The overall aim of this research is to conduct a systematic study of the ceria-zirconia and 2% Cu/ceria-zirconia catalytic activities for soot combustion, comparing to a commercial Pt/alumina catalyst in order to explore the opportunities of ceria-based catalysts versus noble metal supported catalysts for this application.

The catalysts were characterized by N_2 adsorption-desorption isotherms at -196ºC, XRD, Raman spectroscopy, XPS and H_2-TPR. Activity tests were performed towards NO oxidation to NO_2 (from 25ºC to 700ºC) and diesel soot combustion under NOx/O_2 and O_2 atmospheres, in ramp mode (from 25ºC to 700ºC) and isothermal conditions (400ºC, 425ºC and 450ºC).

The results revealed that copper is well-dispersed onto the ceria-zirconia support. A very low loading of copper improves the reducibility of the catalyst and increases significantly the activity for the NO oxidation to NO_2. Remarkably, copper/ceria-zirconia shows a higher soot combustion rate than the Pt-based catalyst (under NOx/O_2, at 450ºC).

V-OP33

Low Temperature Method for Measuring Oxygen Storage Capacity of Ceria-containing Oxides

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A new method of investigation of oxygen storage capacity (OSC) of ceria-containing oxides in a wide range of temperature is considered. Usually, the approach is based on using CO oxidation with oxygen released from the lattice of ceria-containing oxides. However, the low activity of ceria in this reaction at low temperature limits the whole process of OSC measurement. Therefore, the new method suggests the addition to a ceria-containing oxide of a more active catalyst Pt/Al_2O_3 to facilitate the CO oxidation step. A correlation between OSC and effectiveness of TWC is also presented. The method allows studying the OSC at lower temperatures. The results are utterly essential for the understanding the behavior of TWC and thus for their development.

V-OP34

Soot Oxidation with Ceria-zirconia Catalysts Prepared by Different Precipitant

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Ce-Zr catalysts were successfully synthesized based on co-precipitation method using precipitants. The as-prepared catalysts with controlled particle size exhibited different oxidation activity towards soot. It is expected that the precipitant can modify the interaction of Ce with Zr. Moreover, the suitable interaction is beneficial for increasing the quantity of absorbed oxygen species on the surface of catalyst, and in turn improves the catalytic performance.

V-OP35

Mechanistic Investigations of Soot Combustion by Ag Supported Catalysts

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Silver is known for its ability to oxidize soot thus being an interesting element for diesel particle filter regeneration. We investigated the mechanism behind soot oxidation by silver-supported catalysts. Those were prepared by aqueous impregnation of supports such as zirconia, silica, ceria-zirconia and yttria-stabilized zirconia (YSZ, an ionic conductor) by silver nitrate. We performed various characterizations such as in-situ E-TEM observations, isotopic exchanges and propene cracking to understand the synergy between silver and support toward soot oxidation. Cycled soot-oxidation experiments were also conducted to investigate the stability of silver over time. The presence of 1%wt of silver on the surface of YSZ allows lower oxidation temperature even in poor contact conditions between soot and catalyst. E-TEM observations indicate the important role of mobile silver nanoparticles, actually tunneling through the soot and consuming it. Stability of Ag-nanoparticles over the support appears to be an issue, as the nanoparticles sinter and evaporate when all the soot is consumed.

V-OP36

Strong Enhancement of DeSoot Activity of Transition Metal Oxides by Alkali Doping – Surface Promotion Versus Intercalation

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The aim of this study is to develop an innovative robust catalytic material for soot combustion in the low temperature regime. The proposed materials are comprised of 3*d*-metal (manganese, iron, cobalt) oxides, surface decorated or intercalated by alkali, which act as promoters. The study focuses on the exploration of the key parameters governing the catalytic process: surface alkali dispersion, formation of new phases (nanostructurization), soot-catalyst interaction, topology of the soot molecular framework and the influence on the Fermi level caused by alkali doping. The methodology combining the experimental investigations and DFT molecular modeling allows for the establishment of rational principles for designing the optimal soot oxidation catalysts. Based on the experimental (XRD, XRF, RS, XPS, TEM/EDX) and molecular modeling results an integral picture of the soot combustion process over alkali promoted manganese (layered birnessite KMn_4O_8 and cryptomelane KMn_8O_{16}), iron (layered $K_2Fe_{22}O_{34}$, tunneled $KFeO_2$) and cobalt (layered $KCoO_2$) catalysts was developed.

V-OP37

Structure-activity Relation of Iron Oxide Catalysts in Soot Oxidation

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Particulate filters are widely used for the abatement of soot from the exhaust of diesel engines. However, the trapped soot has to be removed from the filters to avoid backpressure issues. In this concern, the present paper addresses the structure-activity relation of iron oxide catalysts for soot oxidation. Structural features of the different iron oxide samples are systematically evaluated by a series of physical-chemical characterisation tools, while the catalytic performance is assessed based upon temperature programmed oxidation studies using tight contact catalytic/soot mixtures. The correlation of structure and activity shows Lewis acid sites and moderate crystallinity of the catalysts to be crucial. These results coincide with mechanistic studies thus representing the base for the targeted design of advanced catalysts.

V-OP38

Pd-doped LaFeCo Perovskites for Three-way Catalysis. Studies on Active Sites and Response to Thermal Stress

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Noble-metal (e. d. Pd) doped perovskites have been recommended as “intelligent” three-way catalysts (TWC), which segregate Pd^0 under rich conditions and resorb Pd^{2+} in the lattice under lean conditions on the time scale of λ fluctuations. We present a study with $LaFe_{0.65}Co_{0.35-x}Pd_xO_3$, which was exposed to redox treatments at 400, 650, and 900 °C. Catalytic data were measured under stoichiometric, rich, and lean conditions, and under simulated λ cycling, samples were characterized by XRD, nitrogen physisorption, TPR, and XAFS.

Activity in oxidation reactions was related to the BET surface area, being probably dominated by Co(Fe) sites. The perovskite was strongly activated for NO reduction (and likewise N_2O decompostion) by redox cycling at 400 °C, which created Pd alloy particles with Co(Fe). There was no complete re-incorporation upon Pd reoxidation at any temperature. The perovskite strongly responded to fluctuations of feed composition. The stability claimed in literature could not be reproduced.

V-OP39

Three-Dimensionally Ordered Macroporous Perovskite Catalysts: Controllable Alignments and Approach for Catalytic Applications

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The facile dual-template preparation of 3DOM-m $La_xCe_{1-x}CoO_3$ (LCCO) with formation of highly crystalline mesoporous walls by employing polymethyl methacrylate (PMMA) microspheres as hard template and of its supported Pt nanoparticles (NPs) by adopting the gas-bubbling cetyltrimethyl ammonium bromide (CTAB)-assisted reduction route. It was found that the obtained *x* wt% Pt/3DOM-m $La_xCe_{1-x}CoO_3$ catalysts have attracted much attention because of their unique properties, such as high surface areas, controllable compositions, crystallinity, thermal and chemical stability, high porosities, narrow pore size distributions as well as their excellent catalytic performance for oxidation of hydrocarbons .

V-OP40

Highly Active $LaKCoO_3$ Perovskite-type Complex Oxide Catalysts over Alumina Washcoated Monolith for the Simultaneous Removal of Diesel Soot and Nitrogen Oxides

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Novel cordierite-monolith-supported $LaCoO_3/Al_2O_3$ catalysts were prepared with $LaCoO_3$ nano-catalysts on porous hollow aluminum oxide nanoparticles as washcoat and monolithic cordierite as the monolithic ceramic substrate. The coating of porous hollow aluminum oxide nanoparticles could increase the surface area of monolithic cordierite for approach 200 times and also endue the coated layer with engineered porous hollow structure.

Finally, the catalytic activity for the simultaneous removal of soot and nitrogen oxides was evaluated by a technique of the temperature-programmed oxidation reaction. In the $LaCoO_3$ catalyst, the partial substitution of La^{3+} at A-site by alkali metal K^+ enhanced the catalytic activity for the oxidation of soot particle and reduction of NOx. The activity of cordierite-monolith-supported $LaKCoO_3/Al_2O_3$ was assayed in the simultaneous removal of soot (carbon black) and NOx. The new combined system of cordierite-monolith-supported $LaKCoO_3/Al_2O_3$ catalysts shows high catalytic performance, the emmitions of PM, CO, hydrocarbon can meet the need for the Chinese National V standard under different conditions, NOx emissions decreased, and can reach the Chinese National IV standard.

V-OP41

Identification of low-T Standard SCR Reaction Intermediates on Fe-, Cu-zeolite Catalysts by Chemical Trapping Techniques

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The low temperature mechanism of the Standard SCR of NO with NH_3 is still debated. The utilization of BaO/Al_2O_3 in physical mixture with metal promoted zeolite catalysts (chemical trapping) enables the stabilization of NOx intermediates and their direct observation via ex situ IR spectroscopy and other techniques. Based on multiple evidence, nitrites are detected and identified as the primary intermediates in the oxidative activation of NO over both Fe- and Cu-zeolites.

V-OP42

Improved Low- and High-temperature NH_3-SCR Activity over Cu-CHA Prepared by Solid-state Ion-exchange Facilitated by NH_3 and NO

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This presentation will focus on optimizing the copper oxide concentration used in the physical mixture before treatment. Furthermore, we are showing that Cu-CHA prepared by [NO+NH_3]-SSIE can possess relatively high activity both for low- and high-temperature NH_3-SCR compared to Cu-CHA prepared by conventional aqueous-based ion-exchange, even by using lower copper content [3]. The study shows that the 2.0% Cu-CHA sample prepared by the [NO+NH_3]-SSIE method possesses the highest NH_3-SCR activity among the studied catalysts.

V-OP43

Thermal Aging Resistance of Cu-zeolite based Catalysts on NH_3-SCR for Lean Burn Engines Exhaust Control

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Copper supported ZSM5 and BETA zeolites and Cu-Chabazite catalysts have been prepared and tested in NH_3-SCR reaction for NO_x removal in lean burn engines exhausts. Fresh and hydrothermally aged catalysts were submitted to different characterization techniques, including NH_3-TPD, H_2-TPR, N_2 adsorption-desorption to quantify evolution of their physico-chamical catalytic properties. The superior performance of Cu-Chabazite both in NO_x conversion and selectivity to N_2, especially after accelerated hydrothermal aging, for NH_3-SCR reaction is demonstrated. The main advantage corresponds with practically total NO_x conversion in a wider temperature window, from 220 to 380ºC, which is practically maintained after severe aging treatment. On the other hand, the aging environment provokes a significant decrease in the catalytic activity of Cu-ZSM5 and Cu-BETA at any temperature. Direct relationship between the activity loss and reduction in BET surface, acidity and surface reducibility provoked by the thermal aging are found.

V-OP44

Dual Function Catalyst for SCR and CO-oxidation

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Haldor Topsoe has developed DNX® GTC-802, a dual function catalyst for combined cycle gas turbines with the same SCR activity as an SCR-only catalyst but with CO oxidation functionality as well. In this way both NOx and CO removal can be achieved with a significantly reduced catalyst volume, thus decreasing the pressure drop as well as the SO_2 oxidation and this in turn is beneficial for both overall plant efficiency and maintenance. The dual function catalyst can also in certain cases simplify the retrofitting of plants with SCR-only but that have to comply with CO emission limits, i.e. it may simply replace the existing SCR catalyst in the HRSG. The dual function catalyst provides an option for VOC removal as well.

V-OP45

A Kinetic Study of Hg Oxidation over Vanadia Based Catalyst

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Among the various air pollutants emitted from coal-fired power plants, elemental mercury is a major environmental issue that has attracted considerable attention in recent years. It is now well known in literature that the presence of a SCR-DeNO$_X$ unit affects mercury speciation, since the SCR catalyst favors the highly desired conversion of Hg^0 to the ionic species Hg^{2+} in the presence of HCl. Several studies have investigated Hg oxidation over V-based catalysts; a number of macroscopic kinetic effects have been unanimously recognized, but the mechanism and kinetics behind them are still under study. This work aims at deepening the comprehension of the complex surface interactions that occur on the SCR catalyst in the presence of NO (whose effect has been reported by other studies to be either positive or negative) and HCl under different operating temperatures as the initial step toward a systematic kinetic investigation of this complex reacting system.

V-OP46

Absorption and Oxidation of NOx from Flue Gasses to Nitric Acid – An Atom Efficient NO_x Abatement Strategy Using Ionic Liquids

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Formation of NO_x during high temperature combustion with air is inevitable and of increasing environmental concern. There are several working techniques for removing NOx utilising transition metal catalysts. However, these catalysts are prone to poisoning from alkaline aerosols formed when firing biomass, waste or other cruder fuels. This work presents an alternative method, in which ionic liquids (ILs) are used to absorb and oxidise the NOx into a valuable bulk chemical, nitric acid. This work investigates the mechanism involved in the reaction, as well as the kinetics. The reaction has been followed *in-situ* by ATR-FTIR spectroscopy and several intermediates are proposed in this work, as well a catalytic cycle describing the reaction. Excellent reversible of the reaction is observed despite formation of nitric acid in an IL with little or no water present.

V-OP47

N_2O Decomposition over Spinel Nanocatalysts - Experimental and DFT Theoretical Approaches to Catalyst Tuning

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Faceted spinel nanocrystals are excellent model catalysts exhibiting high *de*N_2O reactivity. We synthesized Mn_3O_4, Fe_3O_4 and Co_3O_4 samples of controlled nanograin size and morphology, and characterized them with XRD, XPS, RS, UV-Vis, FE-SEM/HR-TEM/EDX/EELS, and TPR/TPO techniques. The experiments were supported by DFT modeling. The catalytic performance of all nanospinels was analyzed in terms of their redox properties probed by TPR/TPO and pulsed CO/O_2 surface titration and work function measurements. Selective replacement of the constituent Fe, Mn and Co cations by non-redox Mg^{2+} and Al^{3+}, revealed that the octahedral ions, play the role of prime active sites in deN_2O reaction. The catalytic performance and the redox properties of the investigated spinels were discussed in terms of the spin and charge transfer dynamics for M^{2+}/M^{3+} and M^{3+}/M^{4+} redox couples. The obtained results allowed for an in-depth rational account for the catalytic behavior of the manganese, iron, and cobalt spinels in N_2O decomposition.

V-OP48

K-$Cu_xCo_{3-x}O_4$ as Highly Efficient Catalysts for N_2O Decomposition from HNO_3-exhaust Streams

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Herein, we present copper cobalt mixed spinels as highly active catalysts for decomposing N_2O from tail gases of HNO_3 production. These catalysts stand out due to its high conversions in ideal ($T_{100\%}$ = 330 °C) and real reaction conditions ($T_{100\%}$ = 490 °C) (1000 ppm N_2O + 200 ppm NO + 2 % O_2 + 0.5 % H_2O) even at high GHSV. Furthermore, it shows outstanding catalytic stability. In our contribution we enlighten the influence of the amount of Cu in $Cu_xCo_{3-x}O_4$ on the catalytic activity and illustrate how the activity can be enhanced by the use of dopants. Furthermore, we elucidate the effect of the single gases on the activity during N_2O decomposition and show how the active species can be reduced. Introducing this catalyst after the $DeNO_x$ stage in the HNO_3 plant could reduce the operating temperatures in the DeN_2O stage to temperatures as low as 330 °C.

V-OP49

N_2O Decomposition over CuO-CeO_2 Mixed Oxides: Effect of Preparation Procedure

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Nitrous oxide (N_2O) is one of the most significant greenhouse gases, severely contributing to the depletion of the stratospheric ozone layer. Therefore, considerable efforts have been devoted on the N_2O abatement from anthropogenic sources, with the catalytic decomposition to be considered as one of the most promising technologies. Despite of the excellent catalytic performance of noble metals-based catalysts, recently it has been shown that CuO-CeO_2 mixed oxides confer a synergistic effect toward enhanced reducibility and catalytic performance. The present work is focused on the N_2O decomposition over bare or mixed CeO_2 and CuO oxides catalysts, prepared by different routes (impregnation, precipitation, exo-templating). The obtained results revealed the superiority of Cu-Ce mixed oxides prepared by precipitation compared to all other composites, which can be ascribed to its excellent redox properties linked to Ce^{4+}/Ce^{3+} and Cu^{2+}/Cu^{+} redox couples.

V-OP50

Catalytic Degradation of N_2O Emissions by Nanoshaped CuO/CeO_2 Materials

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The main purpose of this work was to investigate in detail the influence of nanoparticle shape and exposed crystal planes of CeO_2 supports on catalytic property of CuO/CeO_2 solids in low temperature N_2O degradation. Prepared materials were thoroughly characterized by N_2-sorption, SEM, HR-TEM, XRD, H_2-TPR, *in-situ* DRIFTS and *operando* DR UV-Vis techniques. We have shown that activity of CuO/CeO_2 materials in catalytic N_2O degradation depends on both shape induced activity of CeO_2 ([100] and [110] facets are more reactive) and its BET surface area. Sample containing 4 wt. % of Cu on CeO_2 nanorods exhibited highest activity per copper loading (3.8 mol $N_2O/(mol_{Cu}$ h) at 375 °C). Developed catalysts are stable for 100 h even in the presence of NO, O_2 and H_2O, which makes them appealing for potential industrial application. By using surface-sensitive *operando* techniques, the mechanism of studied reaction over CuO/CeO_2 catalyst was proposed.

V-OP51

Pd-Cu Catalysts Supported on Anion Exchange Resins for the Simultaneous Catalytic Reduction of Nitrate and Reductive Dehalogenation of 4-chlorophenol from Water

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Water pollution with fertilizers and pesticides becomes a major problem worldwide. Organochlorine compounds (pesticides and their degradation byproducts) have been detected adjacent to nitrates in ground and surface water from agricultural areas. This work is focused on simultaneous removal of nitrate and organochlorine compounds from aqueous media through a catalytic reduction process, which could contribute to the protection and remediation of natural water resources.In this purpose, a bimetallic catalyst Pd-Cu supported on an anion exchange resin (*A-520E-Purolite*) was prepared by successive deposition of the metals (2%Pd et 0.5%Cu). In the first step, palladium was introduced by ion exchange with the functional groups $–N(CH_3)_3^+Cl^-$ present onto the styrene–divinylbenzene polymeric matrix of the resin, using as precursor the $[PdCl_4]^{2-}$ complex. In order to enhance the interaction Pd-Cu, the second component was deposited by a controlled surface reaction, in which Cu^{2+} was reduced by the hydrogen adsorbed on the pre-reduced Pd surface. The morphological and structural characterisation of the catalyst was achieved by means of: Scanning Electron Microscopy with Energy Dispersive X-ray spectroscopy (SEM-EDX), X-Ray Diffraction analysis (XRD), X-Ray Photoelectron Spectroscopy (XPS) and microphotography. The catalytic tests were carried out in a continuous flow system with a fixed bed reactor (0.4 g catalyst) in which the aqueous solution (0.25-1.0 $mL.min^{-1}$) circulates concurrently with the hydrogen flow (25-100 $mL.min^{-1}$). Firstly, the catalyst was tested in the reduction of NO_3^- (100 $mg.L^{-1}$). When the steady-state was attained, depending on operational parameters, the conversion of nitrate reached 95%, with 93% selectivity on N_2. The hydrodechlorination of 4-chlorophenol (50 $mg.L^{-1}$) in the presence of nitrate was almost complete (conversion higher than 98%) while conversion of nitrate was maintained the same with only a very small decrease in selectivity.

Poster Presentations
Section 1. Novel Catalytic Materials and Processes for Securing Supplies of Raw Materials

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I-PP01

Synthesis and Characterization of Core-shell Beta/MCM-22 Double-microporous Composite Zeolites

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Using Beta zeolites as core crystals, the core-shell Beta/MCM-22 composite zeolites with uniform morphology were successfully synthesized by hydrothermal synthesis. The zeolites showed uniform structured composite zeolite particle morphology. Beta and MCM-22 zeolites acted as core and shell, respectively. The total acid amount of Beta/MCM-22 is between Beta and MCM-22. Medium acid distribution of the composite reaches 40.1% higher than Beta and MCM-22, 30.0%, 38.2%, respectively. The ratios of Brönsted acid and Lewis acid are increased markedly (C_B/C_L=13.80). The surface energy, Si-OH groups and surficial positive charges of Beta zeolites are enriched through Ar-H_2 plasma surface treatment, and these were the inner reasons of uniform morphology core-shell Beta/MCM-22 composite zeolites.

I-PP02

In Situ Hydrogenation and Desulfurization of Heavy Hydrocarbon Feedstocks with Addition of Zinc in Supercritical Water Flow

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Hydrogenation and desulfurization of oxygen-free bitumen, sulfur-rich asphaltite, and liptobiolith coal in supercritical water flow (400°C,30 MPa) in the presence of zinc shavings and also zinc sulfidation by supercritical hydrogen sulfide without and with addition of water (400°C, P^0_{H2S}=11.8-15.2 MPa) are studied. It is shown that addition of zinc shavings to this heavy hydrocarbon feedstocks resulted in increase in the yield of light hydrocarbons and decrease in the amount of H_2S. Based on the data on yield and composition of conversion products mechanisms of their formation are proposed. Catalytic effect of water on zinc sulfidation is found out.

I-PP03

Non-Oxidative Conversion of Methane into Aromatic Hydrocarbons over Mo/ZSM-5 Catalysts

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Non-oxidative methane conversion into aromatic hydrocarbons on zeolites ZSM-5 modified with MoO_3, Mo_2C and Mo nanopowders is studied. The microstructure, composition and acid properties of Mo/ZSM-5 catalysts are investigated by high-resolution transmission electron microscopy, energy-dispersive X-ray analysis, and programmed thermal desorption of ammonia. The method of Mo introduction into the zeolites is important for the preparation of the Mo/ZSM-5 catalysts. An addition of Mo nanopowder is resulted in preparation of the most active catalyst samples.

I-PP04

Reaction Mechanism of Dry Reforming of Methane on Rh Doped Pyrochlore Catalysts: a DFT Approach

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The dry reforming of methane (DRM) using CO_2 has long been considered a viable method for converting methane into syngas, which can then be readily used in the production of a variety of chemicals and particularly liquid fuels. $La_2Zr_2O_7$ (LZ) is a pyrochlore structure which has shown good long term thermal stability, so that efforts have been made to tailor its catalytic properties, showing Rh as a promising dopant to enhance catalytic performance for DRM. We use density functional theory (DFT) to describe the reaction mechanism of DRM on the planes (011) and (111) of 2 wt% Rh-substituted LZ. It was found that Rh decreases activation barriers, among them the barrier for CHO dehydrogenation, which makes the plane (111) catalytically active for DRM. Our results show the limiting reaction step on the CH_4 dehydrogenation path, which agrees with lower conversions for CH_4 compared to CO_2, as observed experimentally by collaborators.

I-PP05

Catalytic Properties of Nanoparticles of Transition Metals in the Hydrogenation Reactions

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This paper studies the catalytic activity of transition metal nanoparticles - nickel and copper obtained by different methods in the hydrogenation of unsaturated and aromatic hydrocarbons.

I-PP06

Dehydration of Alcohols over Heteropoly Acid Catalysts in the Gas Phase

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Dehydration of methanol and ethanol was studied at a gas-solid interface over a wide range of solid Brønsted acid catalysts based on Keggin heteropoly acids (HPAs), focussing on the formation of dimethyl (DME) and diethyl ethers. These, especially DME, are foreseen to play important role in the future energy sector. The catalysts included $H_3PW_{12}O_{40}$ (HPW) and $H_4SiW_{12}O_{40}$ supported on SiO_2, TiO_2, Nb_2O_5 and ZrO_2, as well as bulk acidic Cs salts of HPW. Isopropanol dehydration was also studied in order to gain mechanistic insights. A fairly good correlation between the catalyst activity (turnover frequency) and the catalyst acid strength (enthalpy of ammonia adsorption) was established, which demonstrates that Brønsted acid sites play important role in these reactions. Kinetics of isopropanol dehydration and ^{1}H NMR point to different chemical structure of acid sites in bulk and supported HPA catalysts, resulting in differing reaction mechanisms.

I-PP07

Hydrodeoxygenation of Biomass-Derived Ketones over Bifunctional Metal-Acid Catalysts in the Gas Phase

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Gas-phase hydrogenation of aliphatic and aromatic ketones to alkanes was investigated using bifunctional metal-acid catalysis. The catalysts were comprised of a metal (Pt, Ru, Ni, Cu) supported on acidic caesium salt of tungstophosphoric heteropoly acid $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ (CsPW) and Pt supported on zeolites (HZSM-5, HY, HBeta). The reaction occurred via ketone-to-alcohol hydrogenation on metal sites followed by dehydration of alcohol to alkene on acid sites and finally hydrogenation of alkene to alkane on metal sites. Catalyst activity decreased in the order: Pt > Ru >> Ni > Cu. Pt/CsPW showed the highest catalytic activity, giving almost 100% alkane yield at 100°C and 1 bar H_2 pressure. Evidence is provided that the reaction is limited by ketone-to-alcohol hydrogenation.

I-PP08

Ketonisation of Carboxylic Acids over Metal Oxide and Zeolite Catalysts in the Gas Phase

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Ketonisation of carboxylic acids is employed as a clean method for the synthesis of ketones and upgrading biomass-derived oxygenates, e.g., bio-oil obtained from fast pyrolysis of biomass. Zn-Cr oxides are demonstrated to be active and durable catalysts for the gas-phase ketonisation of acetic and propionic acids at 300-400°C to form acetone and 3-pentanone, respectively. Zn-Cr(10:1) oxide exhibits best performance, exceeding that of ZnO and Cr_2O_3. FTIR shows that carboxylic acid is adsorbed dissociatively on Zn-Cr oxide to form a bridging surface metal carboxylate. A ketonisation mechanism via β-ketoacid intermediate route is proposed. Silicalite-1 is an environmentally benign non-metal ketonisation catalyst. Ketone selectivity is increased by base treatment generating silanol nests in silicalite-1, as evidenced by FTIR.

I-PP09

The Study of Perovskite-type Ferrites: Preparation, Characterization and Application in the Catalytic Hydrogenation of Carbon Monoxide

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New complex perovskite ferrites was obtained ($An + {}_1BnO_{3n+1}$, where n = 1,2,3, ..., ∞, A = Gd, Sr, B = Fe). It was found that the oxides synthesized by the ceramic technology are in the microcrystalline state with Fe + 3 in one magnetically ordered state, and by the sol-gel method - in the nanocrystalline state and heterovalent Fe^{+3}, Fe^{+4} with oxygen vacancies. Catalytic performances are obtained in the hydrogenation of carbon monoxide. The relationship was found between the catalytic activity and physico-chemical properties of ferrites.

I-PP10

Influence of Pressure to the Hydrocracking Process of Goudron in the Presence of a Modificated Suspended Halloysite

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The main results of hydrocracking of goudron under reduced pressure in the presence of a suspended catalyst have been analyzed. It was investigate the influence of pressure to hydrocracking process of goudron. It was determined that with increasing from 0.5 to 4 MPa the yield of light oil products increased from 47,0 to 58% mass. So that, the yield of gasoline decrease from 30 % to 27 %, but the yield of diesel fraction increased from 16 % to 30,52 %. Further, at the increasing pressure from 4 MPa to 6 MPa the yield of light oil products increased a few, but amount of cock is decrease from 13 % to 9 %. The change of pressure also influence to the hydrocarbon composition of obtaining products.

I-PP11

The New Cracking Catalysts for the Synthesis of Long Chain Paraffins α-olefins and Mixtures of Light Alkanes Conversion under Reducing Conditions

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Combination of synthetic GIC with decationized natural zeolite consisting of clinoptilolite and WPAS there have been obtained paraffin cracking catalysts for the synthesis of long-chain α-olefins. Cracking was carried out in a reaction-regeneration mode at the fixed bed at temperatures 450-550ºC and atmospheric pressure.

A mixture of light alkanes simulating passing gases and fatty oil refinery gases are converted under reducing conditions to produce a mixture of light olefins and hydrogen disequilibrium mode. There were prepared and tested 3% Ru, Pt, Pd, supported on γ-Al_2O_3 in the conversion of a mixture of light alkanes into a flow system at a stationary bed of catalyst in the temperature range 350-500°C and atmospheric pressure in the four modes with clean gas and in the presence of hydrogen and water.

I-PP12

One-step Synthesis of Dimethyl-ether from Biogenic Syngas on Mixed Metal/Alumina Mixtures

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An alternative procedure for obtaining DME from biogenic syngas is presented in this work. Mechanical mixtures of a commercial methanol synthesis catalyst (alumina supported Cu-Zn oxides) and γ-alumina were used as catalysts. Experiments were performed at 523-543 K, 3 MPa and 0.1-0.2 mol/h·g space velocity. Results obtained shows that this system is highly selective for DME formation (close to 70 %, not depending on the obtained CO conversion), with minor methanol formation. Deactivation studies suggest that observed decrease on CO conversion is mainly related with the stability of the metal oxides catalyst (copper sintering and re-oxidation), whereas alumina chemical properties (specially distribution of acid sites) does not change during the reaction.

I-PP13

Hydrogen Photoproduction in a Silicone Microreactor Loaded with Au/TiO_2

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The photogeneration of hydrogen at room temperature from water-ethanol mixtures has been tested under dynamic conditions in a silicone microreactor loaded with Au/TiO_2. The advantages of using a silicone microreactor are flexibility and low cost while maintaining high UV transparency. We have manufactured polydimethylsiloxane (PDMS) microreactors containing channels of 500 µm in diameter by designing patterns with a 3D printer. This design allows a high degree of process intensification, with an optimum mass transfer and a good light penetration. The channels have been coated with ca. 0.5 mg cm^{-2} of Au/TiO_2 (1-2 wt% Au). Several operational conditions have been selected for the photoproduction of hydrogen, including UV dose (0-20 mW cm^{-2}), contact time (5000-10000 h^{-1}), catalyst load, and water-ethanol ratio (1-100% C_2H_5OH). The results show an easy operation and a significant enhancement of the hydrogen photoproduction rate compared with conventional photoreactors.

I-PP14

Influence of Suppores's Nature on the Activity of Hematin Catalysts

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The production of various intermediate petrochemical products and liquid fuels from natural gas by catalytic procedures is an important problem related to high effectiveness chemical technologies. One of the pressing problems and rapidly developing domains of modern applied catalysis is oxidative activation of methane, which is main component of natural gas and the lower olefins.

Metalloporphyrin-based catalytic models of monooxygenases were used in many works. These studies showed that, monooxygenase model reactions largely occurred in nonaqueous solvents, and the active center in such reactions was hemin characterized by the formation of an intermediate, in which the hematin form was naturally absent.

In this work, the influence of support properties on the activity of hematin-containing (biomimetic) catalysts in methane hydroxylation by hydrogen peroxide was investigated. Biomimetic catalysts were prepared by the adsorption of hematin on the granulated neutral and activated Al_2O_3, zeolite NaX and synthtic amorphous magnesium- and chromium-containing aluminosilicates (AlSiMg and AlSiCr, respectively). It was established, that aluminosilicate-based biomimetic catalysts are more active in methane hydroxylation than those on Al_2O_3 and zeolite. $PPFe^{3+}OH/AlSiCr$, which is most active in the catalase reaction, shows considerably lower monooxygenase activity in comparison with $PPFe^{3+}OH/AlSiMg$.

I-PP15

Regeneration and Activation Studies with NiMo/(Al-MCM-41/ZSM-5) Catalyst System for Hydrocracking of Biogenic Residues

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The bifunctional catalyst system can be used for the selective catalytic conversion of vegetable oil by hydrocracking. Thereby high olefin yields could be reached but deactivation of catalysts is a major problem. Accordingly, regeneration and activation of used catalyst samples are necessary. Furthermore, conversion of non-food sustainables, like biogenic residues is of particular interest.

The present work studies the influence of regeneration and activation of NiMo/(Al-MCM-41/ZSM-5) on catalytic properties in hydrocracking of biogenic residues. In this context, special attention is directed to product distribution (especially the yield of light olefins), deactivation of the synthesized catalyst sample and shortening of regeneration program.

The conversion of biogenic residue results in high yields of gaseous hydrocarbons at temperatures of 500°C, WHSV of 5 h^{-1} and pressure of 5 bars. These gaseous products consist mainly of light olefins (C_2-C_6). In this way valuable base chemicals could be produced from waste materials. The yield of olefins could keep at constant level by different regeneration programs for over 24 hydrocracking tests. Furthermore, the time of regeneration and activation steps were significantly reduced.

I-PP16

Ru Nanoparticles on Acid-modified Carbon Materials for the Hydrolytic Hydrogenation of Cellulose

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Cellulose is one of the most abundant compounds of biomass and it can be converted to fuels and other chemical products by means of hydrolytic hydrogenation. This reaction involves two steps: hydrolysis, which requires an acidic catalyst and hydrogenation for which a noble metal is necessary. For such a purpose bifunctional catalysts have been prepared consisting of ruthenium nanoparticles supported on carbon materials that have been modified with acid functionalities, either created by oxidation or by the anchorage of a heteropolyacid.

The prepared bifunctional catalysts give an acceptable cellulose conversion and good selectivity to sorbitol. Among the tested catalysts, the one prepared with the support having the highest developed surface chemistry is the most active.

I-PP17

Conversion of Heavy Oil into Lighter Fuels over FeO_x-Based Catalyst under Sub- and Super-Critical Water Conditions

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FeOx-based catalysts have been developed and upgrading of oil sand bitumen was conducted under sub- and super-critical water conditions using a fixed-bed flow type reactor. The reaction was conducted at 693 K under an atmospheric pressure to super-critical conditions. Heavy components were effectively decomposed over the catalyst without any deactivation. Total yield of lighter components was reached to 70 mol%-C at 19.0 MPa. Moreover, in sub- and super-critical water conditions, coke amount deposited on the catalyst was much lower than that under an atmospheric pressure condition. Accordingly, upgrading of heavy oil over the FeOx-based catalysts under sub- and super-critical water conditions was effective in producing lighter fuels.

I-PP18

Investigation of Furfural Hydrogenation to Furfuryl Alcohol and Tetrahydrofurfuryl Alcohol

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This work is devoted to furfural hydrogenation under H_2 over hypercrosslinked polystyrene-supported 3% Ru catalysts. During the investigation furfuryl and tetrahydrofurfuryl alcohol was found to be the main product of hydrogenation reaction, also and the intermediate products of reaction were found. The maximum conversion obtained over hypercrosslinked polystyrene-supported 3% Ru catalysts at 383 K and 6 MPa was 99.1% with 1.4% and 60.7% selectivity to furfuryl alcohol and tetrahydrofurfuryl alcohol.

I-PP19

Hydrodesulfurization of Dibenzothiophene and 4,6 Dimethyldibenzothiophene over NiW Catalyst Supported over Hierarchical Mordenite

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The utilization of acidic supports has been suggested to improve HDS catalytic performance, in particular by enabling isomerization of the alkyl substituents in sulfur refractory compounds. Hierarchical zeolites have attracted much attention because of the introduction of additional mesopores in an initial strong acid support. In the present work, the catalytic performance of NiW catalysts supported on mordenite (HM) and hierarchical mordenite (HM-M) evaluated in HDS of dibenzothiophene (DBT) and 4,6-dimethyldibenzothiophene (4,6-DMDBT) are reported and compared with that of an alumina supported catalyst. NiW/Al_2O_3 exhibited better HDS activity than NiW/HM and NiW/HM-M in the HDS of DBT. However, its activity was greatly inhibited in the HDS reaction of 4,6-DMDBT where NiW/HM and NiW/HM-M displayed maintained catalytic performance, in relation with additional reaction routes like isomerization. NiW/HM-M exhibited the highest catalytic performances for 4,6-DMDBT HDS showing the potential interest of hierarchical zeolites as support for deep desulfurization.

I-PP20

"Self-Sensitization" of Photocatalytic Activity of ZnO into Visible Region

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We have studied an environmentally important reaction $CO + NO \xrightarrow{h\nu} CO_2 + 1/2\,N_2$ (1) on the "self-sensitizated" ZnO photocatalyst under the activation in the visible region. The reaction (1) is really photocatalytic. The spectral activation region for the reaction (1) is shifted from the UV edge (385 nm) of ZnO to the visible light up to $\lambda > 570$ nm due to the intrinsic point defects of F-type which form a near-surface 2D structure. The mechanism of the reaction kinetics and the energy schemes of the active centers are presented.

I-PP21

The One-step Hydrocracking of Vegetable Oil over Platinum Catalysts with Borate-containing Oxide Supports

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The main objective of this research was studying the effect of the nature oxide supports (γ-Al_2O_3, ZrO_2, B_2O_3-Al_2O_3, B_2O_3-ZrO_2) on the properties of bifunctional Pt-containing catalysts for hydrocracking of vegetable oil.

The catalytic tests were carried out in a continuous flow fixed bed reactor at temperature of 380°C, pressure of 4.0 MPa. The WHSV of feed was 1.0 h^{-1}. The H_2/feed ratio was 1400 (v/v). The time on stream was 20 h. The purified sunflower oil was used as the feedstock.

It is shown that as effective catalysts of vegetable oils hydrocracking can be used supported Pt-containing system based on both individual and borate-containing alumina and zirconia. The use of catalysts Pt/B_2O_3-Al_2O_3 and Pt /ZrO_2-B_2O_3 is more preferably due to the formation of iso- and cycloalkanes, which potentially providing good low temperature properties of diesel fuels.

I-PP22

Stability of NiPd Bimetallic Catalysts in the Autothermal Reforming of Methane

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Autothermal reforming (ATR) of hydrocarbons is the most promising process for hydrogen production. This work is devoted to the study of the effect of support composition (x/Al_2O_3, x = CeO_2, ZrO_2, La_2O_3, $Ce_{0.5}Zr_{0.5}O_2$, $La_2O_3/Ce_{0.5}Zr_{0.5}O_2$) and preparation mode (co-impregnation, sequential impregnation) on the stability of NiPd bimetallic catalysts in the ATR of CH_4. The directional regulation of Red-Ox properties, structure and particle size of Ni-containing active component by means of variation of support composition and preparation mode provides the development of an active and stable NiPd bimetallic catalyst. Developed catalyst formulation $10Ni0.2Pd/10Ce_{0.5}Zr_{0.5}O_2/Al_2O_3$ prepared under optimized conditions shows high activity (CH_4 conversion ~100%, H_2 yield > 80%), stability (time on stream 100 h), resistance to carbon formation and resistance to deactivation by sulfur. The best performance of the optimized catalyst can be associated with peculiarity of NiPd particles structure and the optimal ratio between Ni^{2+} species with different ability for reduction.

I-PP23

Iron Pillared Montmorillonites - Carriers of Pt-Catalysts for N-Alkanes Isomerization

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The purpose of work was the determination of the physical-chemical characteristics of the Pt-catalysts on Fe-pillared montmorillonite with varying content of platinum (0.1 and 0.35%) and their catalytic activity in the reaction of n-hexane isomerization.

Pt-catalysts based on iron-pillared H-montmorillonite in Na- and Ca-forms were studied by BET, XRD, TPD of ammonia, elemental analysis, electronic and IR spectroscopy. For the preparation.

The catalysts were tested in the isomerization of n-hexane at 250-400^{0}C, P=1atm, molar ratio of $H_2:C_6H_{14}=3.5$,ω- 0.82 hour^{-1}. Conversion of n-hexane under atmospheric pressure in isomerization correlates with the total amount of strong and medium a.c. Pt-supported catalysts on FeNaHMM have more higher activity compared with the results of FeCaHMM. It has been shown that the increased acidity of Fe (2.5) NaHMM-contact leads to increased cracking and reduced selectivity by C_6-isomers. The relative number of disubstituted isomers formed on 0.35%Pt-catalysts is less than on 0.1% -contacts. The results indicate the formation of nanodispersed Pt particles on the surface of Fe-pillared MM and a strong interaction between the supported metal and carrier with formation of intermetallic compounds and oxides. It is concluded that the effect of dispersion of platinum particles on the direction of the isomerization process.

I-PP24

Acetylation of Glycerol over Mixed Zirconium Phosphate-Sulphate Catalysts

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In the present work the acetylation of glycerol over zirconium phosphates and mixed zirconium phosphate sulphate catalysts was investigated. In details, the catalysts with formula $Zr_3(PO_4)_4$, α-$Zr(HPO_4)_2$ and ZrP_2O_7 and $Zr_2(PO_4)_2SO_4$ have been prepared. Characterizations by XRD, FT-IR, NH_3-TPD were performed. Moreover, XPS analyses were carried out over the most active samples. The surface chemical composition in terms of P/Zr and S/Zr atomic ratios was monitored in the fresh and used catalysts. The glycerol acetylation reactions were performed by using a mass ratio of catalyst/glycerol equal to 5wt% and molar ratio acetic acid/glycerol corresponding to 3:1. The products were analysed by GC-MS. Recycling experiments up to 5 cycles were performed over the most active catalysts. Over the most active catalyst, $Zr_2(PO_4)_2SO_4$, 96% of glycerol conversion was obtained in 1h and full conversion after 3h. $Zr_3(PO_4)_4$, ZrP_2O_7 and α-$Zr(HPO_4)_2$ were less performing giving about 85-90% of glycerol conversion after 3h.

I-PP25

Synthesis Features of Oxide Compounds Based on Univalent Copper of Delafossite Structure

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Well crystallized delafossite $CuMO_2$ could be prepared by solid state reaction at temperatures exceeding 1000°C. However, the literature describes methods for obtaining at low temperatures, for example, synthesis using aluminum nitrate or hydrothermal synthesis. We tried this methods and thermal treatment of joint co-precipitated oxyhydroxides in this research. So, preparation of copper oxide compounds with delafossite structure is possible even at rather low temperatures. Dispersion suitable for the catalytic applications can be achieved. However, further research is needed to improve the phase purity of the samples.

I-PP26

Esterification-Neutralization-Transesterification of Waste Cooking Oil: In-situ Three-stage Method for Biodiesel Synthesis, Neutralization Step Optimization

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Biodiesel is a promising renewable fuel alternative to fossil oil. For the biodiesel production from low-cost feedstock, it is required to reduce the FFAs concentration below the allowed limits prior to biodiesel manufacturing. In order to produce biodiesel with high acidity feedstock, in-situ three-stage method was performed. It is based on a first in-situ esterification using sulfuric acid as catalyst followed by neutralization and transesterification performed by using lime stone as neutralizing agent and basic catalyst. Neutralization was the crucial step. The present work was devoted to the optimization of the neutralization step. The results show that the conversion was complete and reached around 96 % in the three-stage method. The ^{1}H-NMR, ^{13}C-NMR, FT-IR and GC analyses of the final product confirmed that the properties of the biodiesel produced by the in-situ three-stage method comply with the European standards.

I-PP27

Mechanistic Studies with Labeled $^{13}CO_2$ on Ni/ZrO_2 and Pt/ZrO_2 Dry Reforming Catalysts

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Methane dry reforming (DRM) was studied over 1%Ni/ZrO_2, 3%Ni/ZrO_2 and 1%Pt/ZrO_2 catalysts. The catalysts were prepared by impregnation with the addition of Na and characterized by TEM, XRD, XPS and DRIFTS methods. The presence of Na was suggested to induce the appearance of unique bridged CO sites during CO chemisorption in DRIFTS measurements for all samples and to cause BE shift in XPS spectrum of the highly dispersed Pt/ZrO_2. Catalytic investigations - at atmospheric pressure in plug flow reactor - showed that 3%Ni/ZrO_2 was the most active but coke was deposited on its surface measured by the subsequent temperature programmed oxidation (TPO) measurements. Experiments under sub atmospheric pressure (~50 mbar) in a closed loop circulation system using $^{13}CO_2$ revealed that Ni and Pt catalysts had the same initial reaction pathways; on 3%Ni/ZrO_2 the surface carbon species from CH_4 and $^{13}CO_2$ scrambled at 600°C and methane dissociation was found reversible.

I-PP28

Mathematical Model of Catalytic Hydrodewaxing of Distillates

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One of the varieties of light hydrocracking is hydrodewaxing of distillates. It represents light hydrocracking (breakage) of n-paraffin hydrocarbons in order to produce diesel fuel with improved low-temperature properties. The purpose of the process is producing of winter arctic diesel fuel with very low freezing point (from -18 to -68 °C). A polyfunctional zeolite-containing catalyst is used in this process. The work is devoted to mathematical model of the process development.

I-PP29

Study of Influence of Cis-Trans Isomerization on Selective Oxidations of Alkenes by Nitrous Oxide

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In the present work the influence of cis-trans isomerization of heptane-3 on reactivity of C=C bond of alkenes towards N_2O as well as the contribution of the reaction route with the break of the initial double bounds were studied. It was shown that both cis- and trans-heptane isomers perform very similar reactivity. At the same time for trans-hepten-3 the contribution of the route with C-C bound break is approximately three times higher comparing with cis-heptane-3. The study reveals the common regularities of the oxidation of compounds with C=C bounds by nitrous oxide. The observed difference in contribution of the reaction route with C-C bound break for the olefins confirms the results obtained for rubbers previously.

I-PP30

Development of New NiW Catalysts Supported on SBA-15/Zeoilte for Oil Sludge Hydrotreating

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NiW sulfided catalysts based on micro-mesoporous composite materials SBA-15/zeolite with the zeolite-β, ZSM-5 structures and SBA-15 mesoporous structure were synthesized and used as catalyst support for hydrotreating of oil sludge. The supports and catalysts were characterized by various techniques including XRD, nitrogen adsorption, TPD NH_3, TEM, ^{27}Al MAS NMR. The characterization results showed that NiW/SBA-15/ZSM-5 and NiW/SBA-15/zeolite-β had high activity, and demonstrated more hydrocracking activity than NiW/SBA-15 and NiW/Al_2O_3. The high activity of SBA-15/zeolite supported catalysts in oil sludge hydrotreating might be attributed to the combination of open mesoporous structure and the large amounts of acid sites.

I-PP31

A Numerical Investigation of the Catalyst Behaviour in Fluidized Bed Circulating Reactor

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Fluidized bed reactors are widely used in the petrochemical industry, in particular for the isobutane dehydrogenation process with fine particles of the chromia-alumina catalyst. An injection of hot catalyst particles is needed for sustenance the temperature of the reaction. The main objective is effective heating of the fluidized bed region with the highest concentration of catalyst. In the large reactors the structural elements (lattice) are used for breaking gas bubbles and active mixing of gas and catalyst. In present paper the motion of solid catalyst particles with a size of 20-200 microns in isobutane dehydrogenation reactor model was investigated. Geometrically reactor is5.1 m in internal diameter and 17.4 m in height, partitioned by ten distributive lattice of angle-type with an area of free section of 30%. A vertical pipe is placed in the center part of reactor for the supplying of heated catalyst. Calculations of hydrodynamic and heat transfer processes in the reactor were carried out by numerical methods using computers with special attention to the flow near the walls in reactor.

I-PP32

Sm, Eu Containing Hydrotalcite-like Materials as Precursors of Catalysts for Oxidative Dehydrogenation of Light Hydrocarbons

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The results of complex investigation of the process of oxidative dehydrogenation of light alkane are presented. The new hydroxosalts which have a layered structure of hydrotalcite type with Sm and Eu were synthesized. These hydroxosalts were used as precursors for oxidative dehydrogenation of ethane, propane and isobutane. The oxidative dehydrogenation was studied in the presence of CO_2 and mixture of CO_2+O_2. A strong dependence of the yield and selectivity of alkanes loading and the conditions of heat treatment were observed. The optimum reaction conditions for formation of alkenes have been determined. It was shown that introduction of Sm and Eu results in an increase of olefins yield and selectivity to olefins.

I-PP33

Novel α,α-phosphinoaminoacids: Synthesis, Properties and Catalytic Activity in the Ethylene Oligomerization Process

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The generation of the active nickel catalysts was performed by reaction of oxidative addition of synthesized new N-substituted α-diphenylphosphino-α-aminoacids to the electrochemically generated nickel(0) complexes as in case of previously described organonickel sigma-bonded complexes. Showed the kinetics and mechanism of three-component condensation reaction of secondary phosphine, primary amine and glyoxylic acid hydrate in diethyl ether or methanol allowed an easy access to N-monosubstituted diphenylphosphinoglycines.

The diphenylphosphinoglycines and diphenylphosphinoglycolates possess the P-C-C(O)-O structure motif of the diphenylphosphinoacetic acid which is known to form active nickel catalysts for the ethylene oligomerization. Screening tests of the catalytic activity of the new phosphinoglycines in combination with complex $[Ni_0(COD)_2]$ (where COD= 1,5 cyclooctadiene) led likewise to oligo/polymerization of ethylene with high selectivity for linear products with methyl and vinyl end groups.

I-PP34

The Development of Integrated Technology for Oil and Vegetable Feedstock Processing to Produce Diesel Fuel for Arctic Climatic Zone and Jet Fuel

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In the work was shown the possibility of the use of pyrolysis liquid products of biomass and synthetic oil, obtained through the biomass gasification stage together with the oil fractions for the production of diesel fuels for arctic conditions and jet fuels by hydroconversion and isodewaxing processes.

As a result of co-processing of pyrolysis liquid products of plant biomass and oil feedstock by processes of the hydroconversion and isodewaxing can be produced the winter diesel fuel with filterability temperature limit equal to minus 32 according to standard GOST R 55475-2013.

Processing of synthetic oil in a mixture with petroleum diesel distillate by isodewaxing process allows obtaining jet fuel brand JET-A1 and diesel fuel for arctic conditions of EN 590:2009 "Automotive fuels – Diesel – Requirements and test methods".

I-PP35

Self-Assembled Complexes of 1-Hexadecyl-4-Aza-1-Azoniabicyclo[2.2.2]Octane Bromide with Nitrates of Copper and Lanthanum as the Models of Metalloenzymes

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Aggregation, adsorption and solubilization of aqueous solutions of the complexes of 1-hexadecyl-4-aza-1-azoniabicyclo[2.2.2]octane bromide with nitrates of transition metals (Cu^{2+}, La^{3+}) have been investigated by methods of tensiometry, conductometry, spectrophotometry (solubilization of water-insoluble dye Orange OT). The critical micelle concentration, the parameters of adsorption of surfactants at the water-air interface and the solubilization capacity of the micelles toward the hydrophobic substrate were determined.

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I-PP36

Development of a General Heat Transport Model for Open-cell Metal Foams

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The main interest of this work is to describe a general model determining the governing contributions of the heat transfer parameters related to the metal foams properties in the heat transfer experiments under fluid flow conditions typical for catalytic reactors. Therefore, such a model can describe the variation of heat transfer parameters based on the different metal foam characteristics at different experimental conditions.

I-PP37

Selective Steam Cracking of Heavy Oil in Semibatch Reactor

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The work is devoted to investigation of catalytic steam cracking of heavy oil (Tatarstan, Russia) at 425 – 450 ºC with elicitation of such subprocesses as just thermocracking and steam cracking without catalyst. In the case of the catalytic steam cracking 10 % $Fe_2O_3/\gamma\text{-}Al_2O_3$ impregnated catalyst was used. It was obtained, that introducing of water into the thermocracking of the heavy oil has led to significant increase of liquid products (from 60 to 75 wt %) with simultaneous decrease of gases and coke. Introducing the catalyst has led to increase of H : C ratio from 1.70 in HO to 1.78 in the liquid products of the catalytic steam cracking.

I-PP38

Mechanochemical Synthesis of Molybdenum Carbide: New Approach for the Hydrodesulfurization Catalysts Preparation

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In this work of molybdenum carbides were prepared using the mechanochemical synthesis. The structure and catalyst activity of the molybdenum carbides were also studied.

Two series of samples were synthesized through mechanochemical synthesis both under air and inert atmosphere. Mechanochemical synthesis was carried out using a AGO-2 type planetary high energy ball mill with stainless steel vials and balls under air atmosphere. The rotation speed of the mill was 1000 rpm and the ball-to-powder mass ratio was about 40:1. The model feedstock for testing of samples in the hydrodesulfurization was a heptane solution of 1 wt% and 4.7 wt% dibenzothiophene containing.

I-PP39

Heavy Oil Upgrading in the Presence of Organic Salts of Transition Metals under Reservoir Conditions

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Physical modeling of heavy oil aquathermolysis was studied at temperatures of 250; 300 and 350°C, with carboxylates of nickel and cobalt metals used as oil soluble catalysts. We have found that at 300ºC light components content increases by 15 times during the period from the initial boiling point to 125°C and the content of resins drops by 1.8 times which leads to a decrease in viscosity from 3390.0 to 310.2 mPas at 20°C.

I-PP40

Influence of Catalyst Preparation Techniques on the Properties of the Cr-Mg Catalysts for Tetrachloroethylene Hydrofluorination

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The effect of the chromium-magnesium precursor preparation techniques (mixing, co-precipitation, precipitation) on physicochemical (the BET surface area, the total pore volume, the mean pore diameter) and catalysts activity in the gas-phase hydrofluorination of perchloroethylene to pentafluoroethane was studied. It was obtained, that more active catalyst was prepared by wet mixing of the solid carrier MgF_2 with a solution of $CrCl_3$. The precursor contained 6.1% chromium, and the BET specific surface area was equal to 60 m^2/g.

Kinetic regularities have been studied for the most active catalyst. Based on the experimental data, the pathway of perchloroethylene fluorination with HF over a 6.1% chromium–magnesium oxide catalyst was identified. The process involves several consecutive reactions for the formation of main fluorination products and parallel reactions for the formation of by-products.

I-PP41

Catalytic Aquathermolysis Heavy Oil in the Presence of Organometallic Complex

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Synthesized a new catalyst for an intensification of steam carrying thermal method of heavy oil production, using available domestic raw materials. Organometallic catalyst is a complex (the precursor), based on iron oxide, soluble in polar and non-polar liquids.

Found that the use of this catalyst showed high efficacy in the hydrogenolysis and hydrogenation of resinous-asphaltene compounds heavy oil. It was established that the catalyst promotes the formation of light fractions, thus reducing the viscosity of heavy oil.

I-PP42

Performance of Modified Nickel Catalysts in a Catalytic Membrane Reactor for Partial Oxidation of Methane

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The atmospheric pressure experiments were carried out at 850-950°C for 300-700 h. The methane conversion over modified catalysts was about 97% while selectivity for CO exceeded 95%. The after test inspections of the catalysts did not reveal any significant formation of soot or/and coke.

I-PP43

Alkylphenols to Phenol and Olefins by Zeolite Catalysts: a Shape-Selective Process to Valorize Raw and Fossilized Lignocellulose

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The conversion of alkylphenols to phenol and olefins is presented as a key step in the upgrading of raw (wood) and fossilized (coal) lignocellulose. An exceptional catalytic performance is achieved by application of acidic shape-selective zeolites (e.g. H-ZSM-5) in the dealkylation of 4-*n*-propylphenol, yielding selectively (>95%) phenol and propylene. Importantly, the catalytic stability can only be maintained when water is co-fed during the reaction. In this contribution we highlight the nature of the role water plays, and extrapolate it to other reactions. In addition, the influence of the length, branching, and position of the alkyl moiety is studied and related to the composition, pore-size, and pore connectivity of the zeolite. Accordingly, light is shed on the exact nature of the active site, its location, abundance, and strength.

I-PP44

Study of Catalytic Activity of Impregnated VMgO Catalysts in the Oxidative Dehydrogenation of Ethane

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V-Mg-O catalysts (Mg/V=4.5) were prepared by impregnation of $Mg(OH)_2$ or commercial MgO with aqueous solution of ammonium metavanadate NH_4VO_3 at pH=11. The catalysts, calcined at 550 and 650°C, were characterized by XRD, FTIR, TPR and H2-HT-DRX and tested in the oxidative dehydrogenation (ODH) of ethane (Tr=450°C and $C_2H_6/O_2=2$). XRD and FTIR analysis show for all samples, the formation of a mixture of crystalline phases: $Mg_3(VO_4)_2$, α-$Mg_2V_2O_7$ and MgO with $Mg_3V_2O_8$ as the major phase. H_2-HT-XRD analysis shows that the $Mg_3V_2O_8$ phase, formed at ambient temperature, remained stable up to 625°C. The TPR profiles show one step of vanadium reduction which correspond to the passage from vanadium tetrahedral coordination (V^{5+} in $Mg_3V_2O_8$ phase) to a cubic spinel phase MgV_2O_4 containing V^{3+}. The V-Mg-O samples were active and selective in ODH of ethane (up to 99% of ethylene selectivity). These good performances are attributed to the predominance of $Mg_3V_2O_8$ orthovanadate in the mixture.

I-PP45

Pt/amorphous Silica-Alumina Catalysts for Hydroconversion of C_{20}-C_{31} n-Alkanes Mixture into Fuels with Improved Cold Flow Properties

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Traditionally, winter diesel and jet fuel produced from petroleum feedstocks. However, “gas to liquid” technology produces long-chain *n*-alkanes that is a good feedstock for diesel and aviation fuels components production. Bifunctional catalysts with acidic and hydrogenation functions are taraditionaly used for *n*-alkanes hydrocracking and hydroisomerization.

So, it was investigated the behavior of Pt-containing catalysts based on acidic amorphous silica in the hydroconversion of the model feed containing C_{20}-C_{31} *n*-alkanes to obtain kerosene and diesel fractions having improved cold flow properties. The synthesized Pt/amorphous silica-alumina catalyst provides the formation of branched alkanes of diesel fraction from C_{20}-C_{31} *n*-alkanes that is a key factor of good cold flow fuel properties. At high conversion level up to 90% it is possible to produce up to 50 wt.% of diesel fraction.

I-PP48

Change of Phase-dispersed Structure of Asphatenes in During the Hydrothermal-catalytic Conversion of Heavy Oil

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Heavy oil Ashalchinskoye field and its conversion products obtained in the medium of water vapor in the presence of natural iron catalyst - hematite were investigated. Asphaltenes investigated using complex physical and chemical methods.

Shows the effect of temperature and water content on the formation and stability of the phase-dispersed structure of asphaltenes in hydrothermal-catalytic process in the presence of catalyst - iron oxide.

I-PP49

Catalytic Conversion of Furfural into Gasoline Components

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Furfural is the main industrial product of pentose carbohydrates hydrolysis, however development of biofuels of the furfural platform has started to be discussed only recently. Alkylfurfuryl ethers, namely butylfurfuryl ether, propylfurfuryl ether, 2-methylfuran, and furfuryl alcohol offer high anti-knocking activity (blending research octane numbers (BRON) above 100), and may be applied as components of biofuels. 2-methylfuran was successfully tested in the mixtures with gasoline in car engines. The aim of this work is to study furfural catalytic hydrogenation over Cu-Ru/C and Pt/C catalysts in alcohol solutions to produce alkylfurfuryl ethers. It was shown that furfural hydrogenation in alcohol media is accompanied by formation of acetals. Both products, furfural and furfuryl acetals, are hydrogenated, and the acetals give the corresponding ethers. In such way catalytic hydrogenation of furfuryl acetals was found to be an alternative and a promising method to produce corresponding furfuryl ethers with rather good yields.

I-PP50

Effect of Support in NiO-based Oxygen Transfer Materials for Sorption Enhanced Chemical Looping Methane Reforming: Characterization and Reactivity Studies

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Sorption-enhanced chemical looping reforming is an innovative process aiming at the production of pure H_2 and sequestration-ready CO_2 stream with minimum energy requirements. Herein we investigate the effect of support (SiO_2, TiO_2, Al_2O_3, ZrO_2) in NiO-based oxygen transfer materials under conventional and chemical looping reforming conditions. Reduction in CH_4 led to high reduction degrees (>94%) for NiO/ZrO_2 and NiO/SiO_2. NiO/Al_2O_3 and NiO/TiO_2 demonstrated lower reducibility due to strong metal-support interaction. Subsequent exposure to air resulted in complete re-oxidation of NiO over all materials. Under conventional reforming conditions, reduced NiO/Al_2O_3 and NiO/ZrO_2 displayed high activity with <8% deactivation after 10h. NiO/SiO_2 and NiO/TiO_2 however proved to be inactive probably due to easy re-oxidation of metallic nickel in the presence of steam. The two promising materials were tested in chemical looping reforming. NiO/ZrO_2 exhibited good activity with more than 80% initial CH_4 conversion and less than 2% deactivation after 20 redox cycles.

I-PP51

Aqueous Phase Reforming of Xylitol over Mono- and Bimetallic Carbon-supported Catalysts

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Aqueous phase reforming is an advantageous technology, which allows hydrogen and alkanes production from carbohydrates obtained from abundant biomass sources. This process is beneficially compared with steam reforming, since aqueous solutions of feedstock are converted at moderate temperatures (190-250°C) and slightly elevated pressures, keeping the reaction in a liquid phase. Thus, less energy is spent for heating, no evaporation is needed, and undesirable reactions of coke formation are suppressed. The catalysts used for the APR process should have high hydrothermal stability, which determines the choice of carbon as the support material. In the current study metal screening is performed for different carbon-supported catalysts. The following issues are discussed: activity for xylitol conversion, selectivity to hydrogen and alkanes, and stability in long-term experiments.

I-PP52

Co-Conversion of Fatty Acids and Hydrocarbons in the Conditions of Catalytic Cracking

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Effective way to identify patterns of transformation real bio raw material is study the behavior of the individual compounds under catalytic cracking. Conversion various model compounds of bio-oil in conditions of cracking investigated in the works. The authors described the direction of transformations oxygenate hydrocarbons, belonging to different classes.

The present work was aimed at studying the transformation of fatty acids and various hydrocarbons under catalytic cracking. The study co-conversion oleic acid with hydrocarbons demonstrates that the unsaturated fatty acid may provide both a promoting effect on the cracking of hydrocarbons and to suppress their transformation. Researches of transformation of hydrocarbon-stearic acid indicate that the mechanism promoting action of fatty acid on cracking of hydrocarbons is similar as in the case of oleic acid. However, at high content of stearic acid in model mixtures sharp reduction conversion of hydrocarbon not observed.

I-PP53

Advanced Macroporous Catalysts for Heavy Oil Hydrotreating

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A set of CoMoNi catalysts supported on alumina and sepiolite-like mineral have been studied in heavy tatar oil hydrotreating in a fixed bed reactor. To elucidate the effect of macroporous texture and phase composition of the support all the samples have been investigated by XRD, XPS, XFS, SEM, TEM, mercury porosimetry and N_2 low-temperature adsorption methods. Despite a plenty of factors being relevant for high catalytic activity, the macroporous texture was shown to be of great importance in this process.

I-PP54

The Role of Carrier's Carbonization Degree on the HDO Conversion of the Oleic Acid over the CoMo/C/Al_2O_3 Catalysts

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The report presents the results of the research and development of new hydrotreating catalysts for hydroprocessing of various hydrocarbon raw feeds using heteropolyacids and chelating agents. New approaches for creating TMS catalysts were developed. Simultaneous use of Co_2Mo_{10}HPA and chelating agents allows to change significantly the promotion ratio and morphology of CoMoS active phase type II and, thereby, catalyst properties in HDS and HYD reactions. New catalysts for (i) deep diesel hydrotreating, (ii) selective hydrotreating of FCC gasoline with saving octane number, and (ii) deep VGO hydrotreating were developed.

I-PP55

The Influence of Membrane Reactor Parameters on Efficiency of Hydrocarbons Dehydrogenation Process

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Dehydrogenation of saturated hydrocarbons is known to be the key route to yield the monomers despite on having the strong endothermic and equilibrium limitations. The oxidative dehydrogenation (ODH) is free of latter restrictions but characterized with low product selectivity. The use of the catalytic membrane reactor (CMR) with additional hydrogen oxidation permits one to combine the advantages of conventional dehydrogenation and oxidative dehydrogenation processes. In this case the endothermic and exothermic processes are supposed to take place within the different compartments of the membrane reactor (so called thermodynamically "conjugated" reactions). The impact of membrane reactor parameters on performance of dehydrogenation processes has been theoretically investigated and compared with the tubular reactor.

The dehydrogenation processes of ethane, propane and ethylbenzene were considered. The theoretical study was implemented by means of mathematical modeling.

The use of the membrane reactor combined with hydrogen oxidation was found to be the most effective way to produce olefins via dehydrogenation process. Carrying out the dehydrogenation process in conjugated membrane reactor enables attainment of very high hydrocarbon conversions (98-100%) at considerably lower temperatures (500°C for ethane, 550°C for propane, and 600°C for ethylbenzene). Using the membrane reactor permits one to increase the conversion value by the selective hydrogen removal from the reaction zone and to shift the equilibrium towards the products.

I-PP56

In Silico Design of Artificial Metalloenzymes

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Considering how well Nature does metalloenzymatic catalysis, t is most inviting to borrow Nature's strategies for our own, non-natural catalytic goals. Having more synthetic capabilities than living cells, we also can operate a broader scope of catalytic metals, potent but potentially non-physiological. However, the goal is formidable, from both theoretical and experimental standpoints. We will present out new computational tools for metalloenzymes design. The first one is a very efficient sampling technique that mixes the quantum mechanical (QM) treatment of the metal site and discrete molecular dynamics (DMD) for aggressive sampling of the protein. QM/DMD is then coupled to protein design, which thus starts including the quantum effects on the metal into the design process, as is required for transition metals. We also have a fast searching engine for the identification of appropriate natural protein scaffolds to hold our designed active sites. These tools have been extensively tested for prediction of metalloprotein structural and electronic responses to metal installation, removal, and replacement. With this arsenal at hand, we made our first attempts at metalloenzyme design, both conservative and more ambitious.

I-PP57

Self-Oscillatory Regimes of Methane Oxidation over Supported Pd Catalysts

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Self-oscillations of methane oxidation rate over Pd catalysts are usually observed in methane-rich reaction mixtures. The oscillations are interesting to understand the methane oxidation mechanism, but they are detrimental for industrial catalysis. Self-oscillations and temperature hysteresises during methane oxidation over Pd/Al_2O_3 catalysts were studied both in a tubular quartz flow reactor and a combined thermogravimetric-mass-spectrometric setup. Temperature ranges of self-oscillation regimes were measured and shown to shorten with a decreasing of Pd particle size. The catalyst weight and gaseous components oscillations were detected and the results allowed to reveal the nature of Pd variations during the oscillation cycle: periodic oxidation-reduction of Pd and carbon accumulation-removal as PdC_x. An extremal relationship between the catalytic activity and Pd oxidation degree x of PdO_x was found: Pd activity is maximum at x=0; it drops to minimum and gradually increases with x rise from 0 to 0.3.

I-PP58

Structure Sensitivity in $La_2O_2CO_3$ and La_2O_3 Catalysts for Oxidative Coupling of Methane

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Methane is main component of nature (shale) gas. It is chemically stable and its activation often requires high temperatures, which lead to its deep transformation into the undesirable products such as CO and CO_2, and then it is significant and challengeable to develop efficient catalysts for the selective transformation of methane. In this work, we have synthesized $La_2O_2CO_3$ (and La_2O_3) samples with different morphologies (rod- and plate-shape) at nanometers, and found that one of the rod-like samples shows the highest catalytic properties in oxidative coupling of methane (OCM) at low temperatures (420-500°C), and its specific activity is at least 20 times higher than another rod-like sample. This difference is corresponding to O_2-TPD results, and can be attributed to the crystallographic facets exposed. Among the exposed facets, (110), (1-20) and (2-10) facets have relatively loose atomic configuration, which can improve the activity and the selectivity of the catalysts for OCM.

I-PP59

Mechanism of Hydrogen Transfer Reaction from Naphthenes to 1-Hexene on Y and ZSM-5 Zeolites

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Intermolecular hydrogen transfer reactions are important in the transformation of hydrocarbons in catalytic cracking, alkylation and isomerization processes. To determine the mechanism of hydrogen transfer from naphthene (donor) to 1-hexene (acceptor) transformations of mixtures containing deuterated hydrocarbons on Y and ZSM-5 zeolites were investigated.

The reaction product composition is characterized by the occurrence of two competing reactions – cracking and hydrogen transfer. Cracking reactions occur predominantly at monomolecular mechanism on HZSM-5 zeolite. Bimolecular hydrogen transfer reaction from naphthene to olefin catalyzed by large pore zeolite HREY. The mechanism of hydrogen transfer from deuterated naphthene to olefin suggests four steps: 1) activation of the olefin molecule on Brensted acid sites and carbocation formation, 2) reacting of the carbocation (on surface) with a hydrogen donor molecule (hydride-ion transfer step), 3) desorption of paraffin with a single deuterium atom and formation surface carbocation, 4) decomposition of the carbocation with restoration of active site.

I-PP60

Micro-Kinetic Model of Dry Reforming of Methane on Doped Pyrochlore Catalysts

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The dry reforming of methane (DRM) using CO_2 has long been considered a viable method for converting methane into syngas, which can then be readily used in the production of a variety of chemicals and particularly liquid fuels. $La_2Zr_2O_7$ (LZ) is a pyrochlore structure which has shown good long term thermal stability, so that efforts have been made to tailor its catalytic properties, showing Rh as a promising dopant to enhance catalytic performance for DRM. By using DFT, the plane (111) was found to be catalytically stable and CHO dehydrogenation identified as the rate limiting step. A micro-kinetic model was built and successfully reproduced the experimental H_2/CO ratios for 2% and 5% Rh-doped pyrochlores. This model can then be used to predict how a reduction in a specific activation barrier would affect the overall reaction performance, so that an optimized catalyst can be suggested, synthesized and tested.

I-PP61

Catalytic Conversion of Low Molecular Alkanes with C-C Bonds Formation

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Interactions between methane-propane, propane-benzene as well as bimolecular isomerization of n-butane, n-hexane and mixtures thereof over Ni/MOR/SO_4^{2-}/ZrO_2 at 150-400ºC, atmospheric pressure and GHSV 350-1500 h^{-1} are studied.

Lowering of the process temperature facilitates the methane involvement to the propane alkylation. The methane substitution to benzene and application of H-form zeolites as an acid catalysts allow obtaining isopropylbenzene at 180-200ºC.

The activation of C-C bonds formation in the studied reactions is explained by valence unsaturated oxygen atoms appearance in the catalytic systems, which are stabilized by pulling hydride ions from lower alkanes molecules. A possible mechanism for the new C-C bonds formation in the studied reactions is proposed.

I-PP62

Innovative Development of Refining Sector in Azerbaijan

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Results of the studies conducted in the Institute of Petrochemical Processes on developing prospective complex refining schemes have been presented with consideration for features of Azerbaijani crudes, energy and petrochemical infrastructure, prospective demands on the quality of the products and market structure. The advantage of the integration processes have been identified by analyzing various options that consider individual and joint operation of fuel and lube profiled refineries, integration between refining and petrochemicals and integration between refining, gas processing and petrochemicals within the single fuel and energy complex. Based on calculations maximum profitability of a refinery is 17%, while in refining-petrochemicals integration scenario it rises to 25% and to 35% if gas processing is integrated with refining and petrochemicals.

I-PP63

Application of Tubular Reactor for High-Performance Fischer-Tropsch Syntehesis

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Problems of application of tubular reactor for high-performance Fischer-Tropsch synthesis at high gas volume rates (3000-5000 h^{-1}) are considered. A possibility for maintenance of quasi-isothermal regime by tuning gas flow turbulency is demonstrated. Corresponding heat transfer intensification can be distinguished by rising gas flow rate from 0.1 to 10 m/s in the reactor tube.

I-PP64

Ethanol Steam Reforming on a Structured Heat-Conducting Catalytic Package: Modelling and Experimetal Perfomance

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In this work, experimental and numerical studies of ethanol steam reforming (ESR) over a structured package consisted of five stacked microchannel corundum – protected Fechraloy plates covered with a layer of $Ni+Ru/Sm_{0.15}Pr_{0.15}Ce_{0.35}Zr_{0.35}O_2$ active composition have been performed.

I-PP65

Catalytic Hydrodeoxygenation of Microalgae Biodiesel over Sulfur-Free Nickel Supported Catalyst for the Production of Biofuels

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Microalgae is a convenient lipid resource with a high growing rate and is a potential feedstock for diesel-range hydrocarbons. In situ transesterification was performed in order to extract Chlorella microalgae and transform it to fatty acids methyl esters (FAME). Due to a high content of oxygen, an upgrading step is required. Non-precious metal catalysts particularly Ni supported materials are beginning to attract attention as feasible catalysts for the conversion of lipids into fuel-like hydrocarbons via deCOx. Hydrodeoxygenation of FAME over Ni/H-Y catalyst was performed in a semi-batch reactor at 300 °C in hydrogen at the total pressure of 30 bar. The catalyst was synthesized by a wet-impregnation method and characterized by N_2-physisorption, NH_3-TPD, CO_2-TPD, SEM, EDXA, TEM.
The results revealed that Ni/H-Y allowed a complete conversion of FAME in approximately 2 hours resulting in diesel-range aliphatic hydrocarbons. Ni catalyst exhibited a two-fold higher selectivity to hydrodeoxygenation than to decarboxylation.

I-PP66

Application of the Dioxo-Mo(VI) Complex Anchored on a TiO_2 in the Oxidation of DDT with Molecular Oxygen, under UV-irradiation

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The feasibility of the photocatalytic oxidation of DDT (1,1,1-Trichloro-2,2-bis(4-chlorophenyl)ethane) by the dioxo-Mo^{VI}-dichloro [4,4′-dicarboxylato-2,2′-bipyridine] complex, anchored on TiO_2, in the presence of O_2 has been tested under UV-irradiation (λ= 253.7nm), in acetonitrile solution. It has been shown that the reaction has catalytic character. Conversion of DDT to dicofol (2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethanol) and a number of other chlorinated and non-chlorinated products, reaches up to 32% during 32 h. The main primary reaction by oxo-atom transfer from dioxo-Mo complex to the bibenzylic carbon atom of DDT is the formation of dicofol (21%). The catalytic cycle is performed via the re-oxidation of Mo^{IV} of the anchored complex into Mo^{VI} (apparently, by formation of oxo-peroxo moieties) by molecular oxygen, in “dark” reaction.

I-PP67

Petroleum-Saturated Sands of Azerbaijan

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The rational refining of the alternative sources of heavy and superheavy hydrocarbon feedstock is the urgent one. In this connection it is required to perform investigations with allowance for specific conditions.
By the method of solvent extraction from oil-saturated sand deposits of Balakhany and Mashtaga organic part was isolated, which has a high density (1143.9 kg/m^3 at 20ºC), high resin-asphaltene substances (14.2%) and low (0.906) paraffin contents. It contains Ni; Fe; Zn; Mn; Cr; Mg; Pb; Co, etc.
As a result of the fractionation of extraction products and compounding following narrow fractions of oil products were obtained, % (w): boiling up to 180ºC - 13; 180-240ºC – 7.5; 240-350ºC – 4.3; 350-500ºC - 32.6; above 500ºC - 42.6.
In IPCP of Azerbaijan NAS there have been carried out the investigations of rational use of the Azerbaijan bituminous sands of Kirmaky deposit with obtaining valuable oil products including base oil with VI 80-96.

I-PP68

Partial Oxidation and Dry Reforming of Methane to Synthesis Gas over Complex Oxide Cobaltate-based Catalysts

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Perovskite-like materials - $Nd_{2-x}Ca_xCoO_4$ (x = 1 and 0.75) and $La_{2-x}Sr_xCoO_4$ (x = 1 and 0.75) were investigated in partial oxidation of methane to syngas. It was found that $NdCaCoO_4$-derived catalysts demonstrated selectivity to CO and H_2 close to 100% with CH_4 conversion near 90%. Moreover, long time on stream test revealed $NdCaCoO_4$ worked at least 140h without any trend to deactivation. It was observed by XRD and SEM that $NdCaCoO_4$ results in the formation of finely dispersed Nd_2O_3, CaO and Co metal during reaction. $La_{2-x}Sr_xCoO_4$-derived catalysts were less active and selective most likely due to their structure stability and easiness to reoxidation. The most active $NdCaCoO_4$ was also investigated in dry reforming of methane showing CH_4 and CO_2 conversion near 96 and 93%, respectively. The time on stream test over $NdCaCoO_4$ catalyst revealed that CH_4 and CO_2 conversions were constant at least for 30h.

I-PP69

New Polymetallic Catalysts on the Base of SHS-Intermetallides for Oxidation and Reduction Processes

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Multifunctional polymetallic catalysts produced from complex SHS-intermetallides of transition metals and rare earths were investigated. Two-level oxo-metallic nanostructures of 10-100 nm were typical features of their surface. The catalysts were highly active in the processes of deep oxidation, Fischer-Tropsch (FT) and hydrodesulfurization (HDS). No preliminary activation of the catalysts for the FT and HDS processes was required.

I-PP70

Cooperation of Kazan (Volga Region) Federal University and PJSC "Nizhnekamskneftekhim" in the Development of Catalysts for the Petrochemical Industry

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FGAOU VPO "Kazan (Volga region) Federal University" works closely with the petrochemical enterprises of Tatarstan. The report provides examples of successful joint works and plans to deepen mutually beneficial cooperation.

I-PP71

Performance of Phase-pure M_1 $MoVNbTeO_x$ Catalysts with Different Post-treatments for the Oxidative Dehydrogenation of Ethane

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Phase-pure M1 $MoVTeNbO_x$ catalysts with different post-treatments have been prepared from the same precursor slurry by hydrothermal synthesis and used to study the key factors influencing their performance in the oxidative dehydrogenation of ethane (ODHE) process. A hydrogen peroxide treatment increased the V^{5+}concentration which can improve the catalytic activity and stability in comparison with the steam treatment. A post-treatment with oxalic acid improved the catalyst surface area but caused some vanadium leaching. The phase-pure M1 catalyst calcined at 650 ºC and purified by H_2O_2 showed the best catalyst productivity of 0.77 kg_{C2H4}/kg_{cat}/h at 73% ethane conversion and 85% ethylene selectivity in ODHE process. We further prepared the phase-pure M1 catalyst on metal-ceramic complex substrates by a dip-coating method. The performance of the M1-PVA catalyst plate in a micro-channel reactor approached an ethane conversion of ~ 60% and ethylene selectivity of ~ 85% with a high catalyst productivity of 0.64 kg_{C2H4}/kg_{cat}/h.

I-PP72

Oils and Fats Conversion to the Second Generation of Biodiesel Using Pd-containing Catalysts

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In this work the investigation of fatty acids hydrodeoxygenation was done. The kinetic curves based on the experimental data were investigated by the method of transformation, which consist of the linear transformation of reaction time by the multiplication of reaction time by the coefficient η.

I-PP73

High Throughput Testing of Naphtha Reforming Catalysts

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Herein, we present the latest developments of high throughput technology for testing catalytic naphtha reforming catalysts in 16 parallel reactors under industrially relevant conditions to yield reformate with a constant research octane number (RON). The presentation includes information on appropriate test protocols and the required analytical setup to analyse complex multi-component feeds and products. Based on the Paraffins / Iso-paraffins / Aromatics / Naphthenes / Olefins (PIANO) distribution research octane numbers (RONs) are calculated. In connection with a fully automated data evaluation it will be shown that catalysts can be precisely characterized and differentiated by activity, selectivity and deactivation. The temperature is adjusted automatically for each of the 16 parallel reactors to keep the RON of the reformate or C_{5+} at a constant specified target value for time on streams up to 1000h.

I-PP74

How Small Catalyst Crystallites Can Be: The Case of Anatase

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With the purpose to investigate the smallest anatase nanoparticles we created models of such nanoparticles with size starting from a single elementary cell and up to 3 nm exposing (001), (010) and (101) facets and containing various amounts of chemisorbed water molecules. The title question is solved using XRD patterns of the nanoparticles. Electronic and structural properties as well as their adsorption behavior is studied with the help of DFT and modern semiempirical methods. It is clearly demonstrated that there is a minimal size of nanoparticles in order for them to show crystallinity measured with XRD and EXAFS. The structure of small nanoparticles is very sensitive to the composition of their surface and distribution of hydroxyl groups over it. The crystalline core - amorphous shell structure is typical and agrees well to the experimental data. Even for ideal anatase NP, there is a strong inherent surface heterogeneity.

I-PP75
Catalytic Decomposition of Ammonium Nitrate on Cores of Oil Breeds

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We present herein the results of catalytic activity study of cores (basalts, clays, sandstones) in ammonium nitrate decomposition. The influence of the ratio of used reagents on ammonium nitrate conversion is investigated at different conditions.
It has been shown that the dependence of degree of NH_4NO_3 decomposition on the ratio of nitric and formic acids represents a curve with a maximum in a point corresponding to the molar ratio HNO_3: HCOOH = 2.7. The found value of the maximum is the general for various ratios of nitric acid and ammonium nitrate. The catalytic activity of core oil-bearing rocks of different nature observed in the reaction of decomposition of ammonium nitrate for the first time. Activity of natural samples exceeds that of commercial Pt/Al_2O_3catalyst. The observed regularities are explained on the basis of the proposed mechanism of the reaction.

I-PP76
Areas of Growth of PJSC «Nizhnekamskneftekhim»

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The petrochemical complex of the Republic of Tatarstan has the required scientific, educational and industrial facilities for establishing itself as one of the catalyst production centers in our country. An example of the efficient work of the scientists, specialists of PJSC «Nizhnekamskneftekhim » and Kazan (Privolzhskiy University on organizing the production of high technology, import substituting products is given. New catalysts provide higher level of processing hydrocarbon feedstock, process independence of rubber production.

I-PP77
Sensitization of Wide-Bandgap Oxides ZnO and TiO_2 to the Visible Region Using Intrinsic Point Defects, Surface 2D Nanostructures and Composites ZnO/Si, TiO_2/Si

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We investigate the sensitization of ZnO and TiO_2 using their intrinsic colored defects, 2D “core-shell” nanostructures ZnO/ZnO_{1-x}, TiO_2/TiO_{2-x} and composites ZnO/Si, TiO_2/Si. Photocatalytic reactions of $NO + CO = 1/2N_2 + CO_2$ and photo-induced isotope oxygen, as well as photo-adsorption/desorption of simple molecules (H_2, O_2, CO, CO_2, N_xO_y) are studied.

I-PP78
Comparing Alkylation of 3,4 Dimethylphenol with Propanols and Propenes into Oxide Catalyst

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In this report the comparing results of catalytic alkylation 3,4 dimethylphenol with propanol and propene into cobalt ferrite oxide catalyst was shown, as result the regularities in reaction was identified. The main and side conversion that took place in catalysis condition was defined.

I-PP79
Knowledge Extraction for Oxidative Coupling of Methane from Publications in the Literature

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Oxidative coupling of methane (OCM) reaction plays an important role in industry. OCM reaction yield seems to depend on very large number of variables such as catalyst type, preparation and operation conditions. A huge amount of experimental data was generated in literature. Due to the complexity of relations between variables and yield, we need more systematic and effective approaches to extract knowledge from the published literature such as data mining. In this work, a large database for the lanthanum based catalysts on OCM reaction was constructed by using the published data in the literature, and analyzed using support vector machines technique to develop a model to predict the results of the experimental conditions, which are not yet studied. The results were quite satisfactory indicating that such works can help to improve experimental works by helping to identify the most suitable conditions for high performance.

I-PP80

Pt-Sn Catalysts for Biomass Conversion into Fuel Components and Chemicals

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Over Pt-Sn containing catalysts during ethanol or rapeseed oil conversion the C-O hydrogenating selectivity significantly increases. Optimal conditions for effective ethanol conversion into hydrocarbons C_3-C_8 were found. The most prospect catalyst for biosubstrates conversion was found to be $1Pt\text{-}5Sn/Al_2O_3$. During ethanol conversion aim fraction yield of alkanes and olefins C3-C8 was 50 wt.%. During rapeseed oil conversion under 400 °C a aliphatic hydrocarbons C_3-C_{18} were obtained with total yield about 99% calculated on passed carbon. Noted that only two fractions of C_3 and C_{18} hydrocarbons selectively formed. Obtained results allow minimizing loss of initial carbon weight due to cancelation of carboxyl fragment of fatty acids and glycerol conversion into methane and carbon oxides. Olefins C_{18} were found in products composition. Its yield was 23 wt.% of which 7-10 wt.% were linear alpha olefins. This result made rapeseed oil conversion over $1Pt\text{-}5Sn/Al_2O_3$ catalyst prospective for fuel components and monomers production.

I-PP81

Novel Catalytic Route for the Oxidative Dehydrogenation of Ethane and Propane over CeO_2-based Catalysts

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This work reports a novel route for the oxidation dehydrogenation of C_3H_8 to C_3H_6 and C_2H_6 to C_2H_4 at moderate temperatures in the presence of HCl. CeO_2 nanorod was found to be an efficient catalyst and the modification of CeO_2 by MoO_x or MnO_x further enhanced the formation of C_3H_6 or C_2H_4. The 8 wt% MoO_x–CeO_2 catalyst provided a C_3H_6 yield of ~50% and the 8 wt% MnO_x–CeO_2 catalyst provided a C_2H_4 yield of ~75%. We suggest that the redox between Ce^{4+} and Ce^{3+} plays a key role in the activation of HCl to form an active Cl species for lower alkane activation.

I-PP82

Single-step Hydrotreatment of Lipids to Produce High Quality Biofuel

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Lipids can be converted to biodiesel or biojet fuel via hydrotreatment process. Generally, the existing technology consists of two steps, in which the deoxygenation of lipids to *n*-alkanes and isomerization of *n*-alkanes to *iso*-alkanes are carried out separately, and this will consume considerable hydrogen and energy. To combine the deoxygenation and isomerization reactions in a single step is attractive. However, big amount of water produced in the deoxygenation reaction will poison the isomerization catalyst, which make the single-step process very difficult to be carried out. In this work, a single-step hydrotreatment process for producing biodiesel or biojet fuel from lipids by using bifunctional catalysts was devised, and mechanism of the reactions and structure-activity relationship of the catalysts were also discussed. Under the drive of traditional energy consumption, this single-step hydrotreatment processes will provide new solutions for effective conversion of biomass to liquid fuels.

I-PP83

Bulk Carbonaceous Catalysts of Heavy Hydrocarbon Feedstock Processing

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The subject of this work was to determine the catalytic activity of nanocarbon systems in the process of thermal cracking of petroleum fractions and thereof residues in synchronous restructuring of oil dispersion system under ultrasonication.

I-PP84

Structure of the Ferrospheres Globules Active in the Total Oxidation and Oxidative Coupling of Methane

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In order to elucidate possible influence of the morphology of globules and microstructure of the catalytic active phase on the different OCM performance we thoroughly characterized high calcium ferrospheres with the Fe_2O_3 content in the range of 76–98 wt% in terms of their composition, morphology, microstructure of the iron containing phases and catalytic properties. The detailed analysis of the obtained results including chemical composition of individual ferrospheres of different morphological types allows us to conclude that the globules with high Al_2O_3 and MgO content and skeletal-dendritic structure are responsible for the deep oxidation of methane. The reaction OCM takes place on the sheet-like type globules with high CaO content. The block-like type globules have a low activity in both reactions.

I-PP86

Production of Bio-Renewable Chemicals Using Zeolite Encapsulated Metal Nanoparticles as Bi-functional Catalysts

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Here, we present the latest results from our on-going investigations of zeolite encapsulated metal nanoparticles and their activity and selectivity as bi-functional catalysts for the direct production of MIBK from acetone. In this reaction, the zeolite facilitates the acid catalyzed aldol condensation of acetone to mesityl oxide, while the metal nanoparticles (Ni, Pd or Pt) catalyze the following hydrogenation to MIBK. Furthermore, we present a new and simple method to encapsulate metal nanoparticles in zeolites. Although encapsulated metal nanoparticles have many potential applications, previous attempts to encapsulate metal nanoparticles in zeolites have relied on expensive additives and complex synthetic procedures. Until now, the exploration and exploitation of zeolite encapsulated metal nanoparticles has therefore remained very limited. In contrast, our method is simple, effective and scalable and we therefore hope that impregnation of recrystallized zeolites may become a useful tool in the development of new and efficient bi-functional heterogeneous catalysts.

I-PP87

The Role of Cobalt Sulphide Particles in Alumina Supported CoMo HDT Catalysts

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The objective of the research was to investigate the effect of the modifying alumina surface with cobalt sulphide on the physicochemical characteristics of the CoMoS active phase formed from $Co_2Mo_{10}HPA$ as well as catalytic properties of the $Co_2Mo_{10}/Co_x/Al_2O_3$ catalysts. Moreover, the role of cobalt sulphide particles on the surface of alumina supported CoMo-catalysts and the assumption about hydrogen spillover over catalyst surface from cobalt sulphide particles to CoMoS phase crystallites were studied.

Obtained results, also, make it possible to reassess the role of cobalt sulphide particles in HDT catalysts.

I-PP88

Influence of Cu and Mo on Catalytic Activity of Modified Ni Based Catalysts in Hydrodeoxygenation Process of Plant Lipids

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Renewable biofuels are needed to partially displace petroleum derived transport fuels and diversify local energy source in some region. Removing of oxygen from esters (biodiesel) and triglycerides by hydrodeoxygenation is required for production of hydrocarbons – biofuels competitive with conventional fossil derived fuels. The aim of this study is the investigation of hydrodeoxygenation of esters in the presence of Ni-containing catalysts modified by Cu and Mo. Correlations between molybdenum and copper content, structure and surface of the Ni based catalysts and their activity in the hydrodeoxygenation reaction of esters were observed. It was shown that catalytic activity correlate with the content of Mo^{4+} form on the surface of Ni-Cu-Mo catalysts and Ni/Cu relation in the content of the Ni-Cu catalysts.

I-PP89

Effect of Mesoporosity and Acidity on the Hydroconversion of n-Hexadecane over Pt/based Catalysts

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Production of hydrocarbons by the gasification of biomass and subsequent Fischer–Tropsch (FT) reaction is a very promising route for renewable fuel production. The F-T process produces F-T waxes, which are then upgraded by hydrocracking. Hydrocracking is carried out over bifunctional catalysts composed by a hydrogenating–dehydrogenating component (usually a highly dispersed noble metal) supported on an acidic carrier, which provides the cracking/isomerization function. The current work aims to investigate the effect of acidity and mesoporosity of Pt/based catalysts (supported on conventional or mesoporous ZSM-5 carrier or a mesoporous silica/alumina) on the hydrocracking of F-T waxes using n-decahexane as the model compound. Introduction of mesoporosity in ZSM-5 led to changes in Brönsted and Lewis acid sites distribution. Evaluation of Pt/ZSM-5 catalysts performance showed significant differentiations in activity. Decreased acidity led to less active material, while the presence of mesoporosity additionally affected selectivity, slightly enhancing formation levels of C_4-C_6 products

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I-PP90

Hydrolysis of Carbohydrates in Green Algae Using Solid Acid Catalysts

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Algae are known to grow at high rates compared to terrestrial plants that contain comparable amounts of carbohydrates by weight. Consequently, this renders them attractive under a biorefinery concept. In this work the green algae *Ulva rigida*, containing about 40 wt-% of carbohydrates, was treated with the solid acid catalyst Amberlyst 70, equivalent to 0.01 mol-H^+eq./L, continuous stirring at 800 rpm and 90°C for 259 h. Different physicochemical methods such as OEC, TMG and EDXA were used to characterize the solid residue, and GC techniques for carbohydrates analyzes. The results show relatively fast carbohydrate release, 63.4 wt-% in 259 hours, but slow carbohydrate hydrolysis to monomers, 13.6 wt-% in 259 hours. The residual solid contained 4.0 wt-% of carbohydrates. The present results show great potential for sugars production, although more experiments using different catalysts, slightly increase of temperature and use of pressurized reactors are required to optimize the monomer yields.

I-PP91

Mesoporous Zeolites Synthesised with In Situ Generated Carbon Template

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Zeolites are among the most widely used industrial catalysts. However, the presence of micropores inside zeolites might result in an unacceptably slow diffusion of reactants and products to and from the active sites located inside the zeolite. Several strategies have been proposed to overcome this challenge, a multitude of these require though costly reagents or are time consuming, so a new approach is needed.

Here, we present a versatile method for the preparation of zeolites with an additional mesoporous system. This is done using *in situ* generation of a carbon template, directly onto the silica raw material. The carbon template is later removed by combustion, leaving mesopores. This method allows for careful control of the porosity of the mesoporous zeolite, and it does not depend on the availability of specialized carbon templates. The effect of the mesoporosity generated by this *in situ* carbon templating was tested in hydrocracking of n-octane.

I-PP92

Study of Biforming Process on CoMoNi Catalyst by Accelerator Mass Spectrometry

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Heavy oil upgrading technologies usually use two groups of methods: carbon rejection methods (delayed coking, fluid coking etc.) and hydrogen addition methods (H-Oil, LC-fining etc.). Nevertheless, there are exist some alternative ways of oil refining that look promising but are not investigated well for using in industrial scales. One of them is biforming process – process of integration of hydrocarbon gases in liquid hydrocarbons. In this paper the biforming process was investigated on mesoporous CoMoNi catalyst with the presence of ^{14}C marked methane. The methane integration was analyzed by acceleration mass spectrometry (AMS) of ^{14}C content in biforming products. During the work, the method of ^{14}C analysis in oils has been set. Authors showed that biforming process do not proceed with following parameters in methane atmosphere: 420°C, 15MPa, LHSV $1h^{-1}$, CoMoNi mesoporous catalyst.

I-PP93

Synthesis of Alcohols and their Conversion in Reactive and Inert Gases on Alkali Modified Molybdenum Disulphide Catalysts

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Molybdenum-based sulphide catalytic systems are promising for production of alcohols from CO and H_2. The model of interlayer dynamic nature of the active sites of transition metal sulphide catalysts was taken as a conceptual basis for the work. The application of the interlayer concept as a generalized approach to synthesis of alcohols makes it possible to explain the experimental structure-properties correlations and to optimize the catalyst composition for these processes. The principles were developed for the preparation of efficient sulphide catalysts based on molybdenum promoted with cobalt and modified by potassium for the synthesis of alcohols from syngas.

I-PP94

Glucose and Cellulose Derived Ni/C-SO_3H Catalysts for Liquid Phenol Hydrodeoxygenation

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Sulfonated carbons were explored as functionalized supports for Ni nanoparticles to hydrodeoxygenate (HDO) phenol. The dual-functional Ni catalysts supported on sulfonated carbon (Ni/C-SO_3H) showed high rates for phenol hydrodeoxygenation in liquid hexadecane, but not in water. While the C-SO_3H supports were active for cyclohexanol dehydration in hexadecane and water, Ni/C-SO_3H only catalysed the reduction of phenol to cyclohexanol in water. The state of 3–5 nm grafted Ni particles was analysed by in situ X-ray absorption spectroscopy. The results show that the metallic Ni was rapidly formed in situ without detectable leaching to the aqueous phase, suggesting that just the acid functions on Ni/C-SO_3H are inhibited in the presence of water. Using in situ IR spectroscopy, it was shown that even in hexadecane, phenol HDO is limited by the dehydration step. The minimum addition of 7 wt % C-SO_3H to the most active of the Ni/C-SO_3H catalysts enabled nearly quantitative conversion of phenol and the highest selectivity (90 %) towards cyclohexane in 6 h, at temperatures as low as 473 K, suggesting that the proximity to Ni limits the acid properties of the support.

I-PP95

Role of Nb in Formation of MoVTeNb Catalyst for Propane Ammoxidation

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To date, the problem of oil gas utilization and industrial processing of its components (methane, ethane and propane) is very actual. This issue is closely connected with the need to develop new power saving technologies in petrochemical industry. In light of this, the development of relevant manufacturing process of acrylonitrile from inexpensive and abundant propane instead propylene is challenging and economically is attractive. MoVTeNbO catalysts are reported [1, 2] to be the most efficient catalysts for the ammooxidation of propane to acrylonitrile. The role of Nb in the formation of the structure of these catalysts is still under debate. The work object is to elucidate of Nb effect on the phase composition and catalytic function in selective conversion of propane.

I-PP97

The Polypropylene Based Composites Produced by Using Pre-adsorbed Catalyst on the Surface of Carbon Nanotubes

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We investigated the possibility of producing composite materials based on multi-wall carbon nanotubes and polypropylene (MWCNTs/PP) by the in situ polymerization of propylene using Ti-Mg catalysts, pre-adsorbed on the surface of MWCNTs. Complex of physical and chemical methods revealed that the polymerization of polypropylene on these catalysts leads to the formation of enlarged PP blocks formed by the interaction of PP molecules with the surface of nanotubes.

I-PP98

Transition Metal Oxides on Heterogeneous Fenton-like Systems with Thermal and Enzyme Peroxidase Catalytic Activity for Pollutant Degradation

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Easy-handle and stable synthetic nanoparticles (Nps) and mesoporous micrometric materials made from transition metal oxides and its momtmorillonite clay composites were obtained using different precipitation routes. The ability of these materials for the catalytic degradation of some model pollutants in water solutions were successfully evaluated as a result of active Fenton like heterogeneous reaction mechanism or calculating the activation energy (Ea) after thermal degradation process from a model Arrhenius equation in optimized experimental conditions.

Magnetite and clay metallic oxides composites including those with grinded zero-valent iron showed peroxidase enzyme activity. The experimental evaluation model in this case was the efficiency of radioactive electrophilic iodination reaction of aromatics amino acids in a model protein bovine serum albumin (BSA).

Artificial peroxidase enzyme activity was determined using both, H_2O_2 and SCN^- natural enzyme substrates with excellent results.

I-PP99

Microwave-assistant Functionalization of MOFs with Gold Nanoparticles

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Present investigation is focused on development of a microwave-assistant solvothermal synthesis in order to grow gold nanoparticles inside the MOF structures – $Cu_3(BTC)_2$ and Fe(BTC) (BTC – benzene-1,3,5-tricarboxilic acid), and inside the ZIF-8. For synthesis, we used MOFs obtained in our laboratory and commercially available Basolite C300 and Basolite F300. Gold nanoparticles were obtained inside porous materials from $HAuCl_4$ and sodium citrate in the microwave oven. So we have developed the microwave-assistant solvothermal synthesis, which allowed as to functionalize three MOFs – $Cu_3(BTC)_2$, Fe(BTC), and ZIF-8 with gold nanoparticles with diameters in 5-13 nm range. Variations in time of mixing of the reagents allowing to optimize the penetration depth of gold into the porous matrix. Obtained materials have good stability and may be applied for catalytic tests.

I-PP100

On the Origin and State of Ni and Fe Species as Catalysts for the Initiation of Metal Dusting Corrosion

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Ni-based industrial alloy samples were pretreated at high temperatures in steam/inert atmosphere, followed by exposure to syngas mixtures with either simplified ('*infinite*') or more-industrially relevant ('*finite*') carbon activity (a_c), in order to reveal catalytic phenomena critical to the unwanted carbon formation that initiates metal dusting corrosion. The resulting surfaces and carbonaceous products were studied via optical-microscopy, SEM, TEM/EDS, XPS and depth profile analysis by AES under ion-sputtering. Varying pre-oxidation conditions provide Cr and Al rich surface oxide layers that strongly differ in thickness and composition, which clearly affects the propensity to form carbon on the surface under *infinite* a_c conditions. Experiments under *finite* a_c demonstrate further the kinetic control of the carbon forming reactions. The detailed characterization establishes the role of reducible Ni/Fe species in the oxide layer matrix.

I-PP101

Towards the Application of New Ionic Liquids Based Ru(II) Catalysts in Transfer Hydrogenation Reactions

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At the present time, searching new efficient catalysts for petro chemistry and organic synthesis, which meet sustainability, is the topical task for the improvement of oil refining. Ionic liquids (IL) and transition metal complexes based on them satisfy these requirements.

Herein we report about mild reaction conditions (82^{0}C, atm. pressure) for the transfer hydrogenation of ketones using Ru/IL catalysts $[Ru((Ph_2PO)\text{-}C_7H_{14}N_2Cl)(\eta^6\text{-arene})Cl_2]Cl$ and $[Ru((Cy_2PO)\text{-}C_7H_{14}N_2Cl)(\eta^6\text{-arene})Cl_2]Cl$ (arene: benzene, *p*-cymene).

The catalytic activities dependent on the groups (phenyl and cyclohexyl) on the phosphorus atom, conversely not to depend on the arene moieties bound to metal center. Ru/IL systems appeared to be active and efficient catalysts leading to nearly quantitative conversions. This transfer hydrogenation process uses non-gaseous hydrogen donors, such as iso-propanol, and may be applied for acetophenone reduction, a byproduct in the SMPO process of ethylbenzene and propene conversion to styrene and propylene oxide.

I-PP103

Syngas Production from CH_4 and CO_2 over Ni-based Nanocomposites Catalysts at Mild Conditions

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Ni-based catalysts (Ce-Ni-O, Ni-Mg-Al-O) were successfully prepared by coprecipitation method for the efficient and sustainable syngas production from methane and carbon dioxide. The influence of different parameters was studied, such as the Ni loading, the concentration of the reactants, the reaction temperature (600°C-800°C) and the pretreatment temperature. An almost linear increase between the metal loading and the conversion of the reactants is obtained, however, an optimized system can be proposed with high activity and selectivity. At the mild temperature of 600°C high conversions i.e. 58% for CH_4 and 66% for CO_2 are obtained at the stable state on Ni-Mg-Al-O compound (10 mg) with a high selectivity (H_2/CO ratio of 0.81) with reactants concentration at 20 %. The catalysts were characterized to find correlations between catalytic activity and physico-chemical properties. All the catalysts correspond to nanomaterials with small average particles size and well dispersion of Ni species.

I-PP104

Identification and Kinetic Tracing of Catalyst Intermediates by Complementary Spectroscopic Methods, Applied to the Resting States of Olefin-Polymerization Catalysts

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The structural characterization of reactive intermediates, which arise in the course of a catalytic reaction, and the kinetic tracing of their concentration profiles are ongoing tasks in all fields of catalysis research. NMR spectroscopy can generally provide superb structural information concerning catalyst species present in homogeneously dissolved catalyst systems, but the time resolution of this method is often insufficient to follow the time-course of a rapidly proceeding catalyst reaction. UV-vis spectroscopy, on the other hand, can generally provide only very limited structural information but this method can, in principle, be tuned so as to provide an almost unlimited time-resolution. To elucidate catalytic processes in structural as well as kinetic terms, it would thus appear desirable to combine both of these complementary spectroscopy methods. In the following, we describe the application of this approach toward full characterization of several zirconocene-based catalyst systems used for the polymerization of α-olefins.

I-PP106

Density Functional Theory Study of Alcohol Amination Reaction on Monoclinic Zirconia Surfaces

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In the actual environmental awareness, the N-alkylation of alcohols with amines or ammonia is particularly attractive because of the availability of various types of alcohols (which can be bio-sourced) and the fact that water is the main by-product. Metal-Supported Oxide catalytic family offers promising properties for alcohols amination. However, the role played by the oxide surfaces in this catalytic process is not precisely understood. We are thus interested in a monoclinic zirconia phase to probe with DFT calculations the reactivity of small molecules at this oxide surfaces. For ethanol amination with ammonia over ZrO_2, we demonstrated that the Eley-rideal nucleophilic substitution mechanism has lower activation barrier than the Langmuir-Hinshelwood one. We also showed that the reactivity is relatively poor at the bare ZrO_2 surfaces and highlighted the important role played by the coadsorbed water molecule. These calculations demonstrate that water can assist alcohol amination and also alcohol dehydrogenation.

I-PP107

Ethylbenzene Hydroisomerization over an EU-1 Zeolite Generated in Presence of a Multivalent Surfactant Capping Agent

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The capping effect of a multivalent cationic surfactant was successfully used in the synthesis of EU-1 zeolite nanocrystals with decreasing crystal size. The formation of nanocrystals was attributed to the strong binding effect of the surfactant molecules on the substrate surfaces, whereas the microporous architecture was still directed by the conventional structure-directing agent. The samples were tested in the presence of a metallic phase in the industrially important ethylbenzene hydroisomerization. Catalytic results demonstrated the remarkable impact of generating an EU-1 zeolite with a larger and easily accessible outer surface (152 m^2/g), exhibiting a higher concentration of active acid sites, compared to the bulk counterpart (62 m^2/g). The catalyst revealed a two-fold increase of conversion compared to a bulk sample, with no detrimental effects being observed in the obtained isomerization yields.

I-PP108

Catalytic Oxidation of α-Alkenes C_8-C_{12} to Carboxylic Acids

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The possibility of carboxylic acids (heptanoic, nonanoic and undecanoic) obtaining by α-alkenes oxidation with 30% aqueous hydrogen peroxide as oxidant in two-phase medium was investigated. Tungsten peroxopolyoxo complexes $Q\{PO_4[WO(O_2)_2]_4\}$ (where Q^+– $[MeOct^n{}_3N]^+$, $[CetPy]^+$ or $[Bu^n{}_4N]^+$) as phase-transfer catalysts were used in the processes.

I-PP109

Innovative Catalyst Design for Improved Catalytic Properties for Methanol-to-Olefins Reaction

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By replacing packed beds of catalyst pellets or powders by a structured catalyst, the performance of the reactions that suffer from mass and heat transfer limitations can be significantly improved. However the architecture of the porous support material will have an impact on the catalytic properties of the final catalyst. By using robocasting, periodic and highly reproducible support structures, with high mechanical properties and low pressure drop were synthesized. These support with different architecture were wash coated with ZSM-5 and catalytically evaluated in the methanol-to-olefins reaction. The results of catalytic tests show an increase in activity and selectivity to the desired light olefins in case of using structured catalysts. Robocasting could become an interesting tool for the development of innovative catalytic structures with improved mass and heat transfer properties. Further improvement can be made by optimizing the porosity, unit cell size and further design of the channels of the structures.

I-PP110

Development of Technology for Catalytic Neutralization of Toxic Waste Gas Impurities

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Polyoxide Ni-Cu-Cr/2% Ce/θ-Al_2O_3 catalyst with desired properties on carriers for deep oxidation of hydrocarbons - toluene, xylene, styrene, ethyl acetate, butyl acetate, isobutanol, formaldehyde, acetone, ethanol, etc., which have a toxic effect on living organisms and flora, was developed. It has been shown that the synthesized polyoxide Ni-Cu-Cr catalyst supported on 2% Ce/θ-Al_2O_3 provides 98.8% toluene conversion up to CO_2 at space velocity 5×10^3 h^{-1}, temperature 723-773 K and content of toluene 320 mg/m^3 in the initial mixture.

I-PP111

Asphaltene Aggregation Processes in the Crude Oils

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Asphaltenes extracted from tatar oil have been studied by SAXS. It was found that the asphaltene aggregates in the toluene solution without any additives have elongate shapes and wide sizes distribution with characteristic size about several nm. The influence of more than 30 chemical additives on the asphaltene aggregation process has been studied. It was found that additives could increase, decrease or not affect on the asphaltene particle sizes. In presentation will discussed possible mechanisms of interaction additives with asphaltene aggregates.

I-PP112

Peculiarities of MoS_2/Al_2O_3, $CoMoS/Al_2O_3$ and $NiMoS/Al_2O_3$ Catalyst's Behaviour in the Hydroconversion of Aliphatic Esters and Rapeseed Oil

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The work presents the results of comparative study of MoS_2/Al_2O_3, $CoMoS/Al_2O_3$ and $NiMoS/Al_2O_3$ catalysts in the aliphatic ethers hydro conversion and in the hydrotreating of rapeseed oil (RSO) and its mixtures with the straight-run gasoil (SRGO). The selectivity of aliphatic ether and RSO transformation depends on the composition of sulphide phase and the reaction conditions. The un-promoted MoS_2/Al_2O_3 catalyst turns the reaction to HDO route, avoiding the formation of C_{15} hydrocarbons and CO/CO_2 molecules. The $CoMo/Al_2O_3$ and $NiMo/Al_2O_3$ catalysts gave C_{16} and C_{15} hydrocarbons. The RSO addition decreased the activity of $CoMoS/Al_2O_3$ catalysts but had no effect on the activity of $NiMoS/Al_2O_3$ in the HDS and HDN reaction. The CO molecules formed as a result of RSO hydroconversion can be considered as a main inhibitor of $CoMoS/Al_2O_3$ catalyst's activity. So, the chemical composition of sulphide phases effects strongly on the behaviour of sulfided catalysts in the hydrotreating of triglyceride-based feedstocks.

I-PP113

HMS Supported $H_4PMo_{11}VO_{40}$ Catalysts for the Isopropanol Decomposition Reaction

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HPAs were supported on silicate mesopourous HMS by dry impregnation method with 3wt.% loading. Various techniques including: Elemental analysis, XRD, FT-IR-DRIFT, N_2 physisorption, TG-DTA and SEM analysis were used to characterize the fresh catalysts. Catalytic performances of supported HPAs were compared to those of HPAs bulk in the isopropanol decomposition reaction to propene, diisopropylether and acetone products at 75°C. The supported HPAs showed better dispersion of heteropolyacids on the HMS surface. A sensitive decrease of the HMS support surface area was observed in the presence of $H_4PMo_{11}VO_{40}$ clusters. By TG-TDA analysis, HPA-HMS catalyst showed a higher thermal stability than pure HPA.High catalytic performances were obtained for HPA-HMS catalyst. These results could be related to the high dispersion of HPA on the support.

The Effect of K- and Mn- Promoters on N-doped Carbon Nanotube-Supported Iron Nanoparticles for CO_2 hydrogenation

I-PP114

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CO_2 hydrogenation over iron catalyst without promoter resulted in high methane selectivity and low olefin selectivity. However, it was possible to suppress methane formation and to enhance C_{3+} selectivity as well as olefin selectivity by doping with small amounts of potassium. The catalysts promoted with Mn achieved a higher stability than the unpromoted catalyst. By increasing the residence time in the reaction zone, the selectivity towards hydrocarbons was increased considerably, while the selectivity of CO was decreased. The addition of both K and Mn enhanced the catalytic activity and stability of iron catalysts in CO_2 hydrogenation.

Section 2. Catalyst Preparation and Characterization

II-PP01

Capped Co-promoted Pd/AlOOH Catalysts in Dehydrogenation of Formic Acid for Hydrogenation of Maleic Anhydride

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Capped Co-promoted Pd nanoparticles (NPs) supported on boehmite (AlOOH) were synthesized under hydrothermal conditions to explore the catalysis for hydrogenation of petroleum-derived maleic anhydride (MAn) using biomass-derived formic acid (FA) as a hydrogen source. Among various bimetallic CoPd catalysts, *N*,*N*-dimethyldodecylamine *N*-oxide (DDAO)-capped bimetallic CoPd NPs supported on AlOOH (denoted as CoPd-DDAO/AlOOH) exhibited superior catalysis and excellent reusability without leaching of metal elements.

In CoPd-DDAO/AlOOH, STEM-EDS mapping confirmed the homogeneity of Co and Pd element in each NP with uniform compositional distribution. XRD, XPS and XAS supported the Co-Pd interactions whereas XPS and XAS advocated the partial electron exchange in the supported bimetallic CoPd-DDAO NPs to control the electron density on Pd active centers in the catalyst.

In summary, significant catalysis by CoPd-DDAO/AlOOH for the hydrogenation of MAn using FA are described in this presentation based on electronic/geometric modifications caused by Co-Pd alloying in the presence of DDAO capping agent.

II-PP02

In-Situ TEM and Electron Tomography: Revealing the Location and the Mechanism of Formation of Copper Particles

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The formation and location of copper nanoparticles on silica, synthesized via co-precipitation or incipient wetness impregnation, were studied with *in-situ* TEM and Electron Tomography. Partial entrapment of the copper particles, originated during the reduction of a co-precipitated copper silicate, resulted in a higher thermal stability in the methanol synthesis reaction.

II-PP03

Effect of the PdFe Alloy in the Catalysis of Water Gas Shift Reaction

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In this work, we present a controlled synthesis of 1-wt% Pd/Al_2O_3 and 1-wt% PdFe/Al_2O_3 nanocatalysts. We studied the effect of adding Fe to Pd in the catalysis of water gas shif (WGS) reaction. Also, conventional 1-wt% Pd/Al_2O_3 and PdFe/Al_2O_3 catalysts were prepared for comparison. TEM images of the PdFe alloy show uniform nanoparticles of approximately 5 nm in diameter. In the CO chemisorption measurements, the PdFe/Al_2O_3 show low palladium dispersion that can be due the formation of alloy. The PdFe/Al_2O_3 catalyst show higher rates compared to Pd/Al_2O_3 catalysts. We successfully demonstrated the synthesis of PdFe alloy nanoparticles and deposited on alumina. The addition of Fe to Pd catalysts increase the rates for WGS reaction compared to Pd catalysts. These findings were important because can lead to better understanding of the alloy effect in catalytic reactions.

II-PP05

Atomic Scale Understanding of Hydrodesulfurization Catalysis Using High-Pressure Scanning Tunneling Microscopy

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During hydrodesulfurization (HDS), sulfur is removed from crude oil over a MoS_2 catalyst supported on Υ-Al_2O_3. The catalyst is generated *in situ* from a MoO_3 precursor using a sulfur-rich feedstock (sulfidation). Stronger requirements on sulfur levels in fossil fuels and decreased quality of crude oil has inspired continuing interest in improved understanding of the process. While a combination of spectroscopy and microscopy methods have generated a good understanding of the atomic structure of the catalyst and its precursor, little is known about their dynamics under reaction conditions.

Here, we introduce a new model system, MoO_3 on an alumina film on NiAl(110), which allows us to study the detailed nature of the MoO_3–alumina bond using a scanning tunnelling microscope (STM). With our high-pressure STM, we have performed *operando* experiments, following the dynamics of the atomic structure of the catalyst under reaction conditions.

II-PP06

A Novel Synthesis Strategy in Supercritical CO_2 for the Preparation of Nanostructured Ce-Pr Mixed Oxide with Enhanced Catalytic Properties

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The use of supercritical CO_2 as reaction medium was coupled to a tailored reactor design to produce a nanostructured Ce-Pr mixed oxide with high surface area and with high dispersion of Pr within the mixed oxide. This material displayed much superior catalytic performance in the oxidation of CO compared to pure CeO_2 and PrO_2 synthesised with the same approach, and also compared to oxides with the same composition but prepared with a conventional synthesis method. This novel synthesis method is of general applicability and, therefore, is also promising for the preparation of other mixed oxide catalysts.

II-PP07

Synthesis and Regeneration of Different Catalysts with the Supercritical Fluid Technology

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The research of possibility of using supercritical carbon dioxide in the synthesis and regeneration of various catalysts was carried out. The optimum parameters under which the palladium catalyst synthesis process using an organic complex of palladium chloride and regeneration of nickel-molybdenum catalyst held most effectively are determined.

II-PP08

Solvation Shell of Platinum Complexes in Solutions According to EXAFS Data

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Using EXAFS and Raman spectroscopy the structure of the solvation shell of hexachloroplatinate complexes in dimethylsulfoxide (DMSO) and water solutions over a wide range of concentration and aging time were studied. The experimental results clearly reveal that chlorine atoms are in the platinum atoms surrounding. Hydrolysis processes and direct interactions of platinum atoms are not observed. A tightly bound solvation shell covers the platinum complexes. Regardless of the solvent origin, solution concentrations and aging times, EXAFS curves of radial distribution function (RDF) exhibit maximums in the region 3.7-4.4 Å. These maximums belong to oxygen atoms of the solvation shell.

II-PP09

Synthesis of Catalytically Active Mesoporous Aluminosilicates without the Use of Templates

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Developed a method of sol-gel synthesis of mesoporous aluminosilicate based on the use of oligomeric esters of orthosilicic acid (ES-40) and an alcohol solution of aluminum nitrate. The method allows to obtain mesoporous aluminosilicates having a narrow pore size distribution. Obtained aluminosilicates exhibit high catalytic activity in the oligomerization of 1-octene with a high yield of trimers.

II-PP10

Tuning of the Copper-Zirconia and Palladium-Zirconium Phase Boundary for CO_2-Selective Methanol Steam Reforming

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Zirconia copper catalysts for methanol steam reforming are known for higher CO_2-selectivity than the technically used Cu-Zn system. We investigated the beneficial Cu-Zr bi-functionality in order to distinguish synergistic phase boundary effects such as improved Cu redox chemistry, improved surface hydroxylation and also structural modifications of Cu itself e.g. by dopant-induced strain effects. "Real" and "inverse" UHV model catalysts have been prepared applying several methods such as a self-developed sputter technique, ALD/CVD using the organometallic precursor Zr-t-butoxide as well as thermal evaporation for Cu. Characterization including XPS, LEIS, AES, HREELS and STM and catalytic experiments in the UHV-attached high pressure batch reactor allowed to correlate chemical/structural surface information with catalytic performance.
For Palladium, a very unusual and potentially beneficial redox-behavior of Zr^0/Zr^{4+} was investigated "ex-situ" and "in-situ" using NAP-XPS. The described redox-reversibility of Zr is subject to be an active state for several catalytic reaction, e.g. for Methanol decomposition.

II-PP11

Activated Reactive Synthesis, a Flexible Route to Produce Manganese Oxides with Improved Textural, Redox and Catalytic Properties

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Seeking for effective and low cost materials for low temperature Volatile Organic Compounds (VOCs) removal remains an important industrial challenge. Manganese oxides and especially cryptomelane have been identified as promising catalysts for this purpose. This paper deals with a promising "solvent free" synthesis route, for the preparation of nanostructured cryptomelane. Commercial cryptomelane was used for the synthesis of activated oxides by activated reactive synthesis process, involving two successive steps, a high energy ball milling (HEBM) and low energy ball milling (LEBM). The restructuring of a pre-crystallized manganese oxide via reactive grinding process allowed to generate cryptomelane with high surface area after particles de-agglomeration step occurring during the LEBM process. Redox properties were found also to be promoted at low temperature by the material microstructure. Hence specific activity of cryptomelane in VOCs (formaldehyde or toluene) oxidation was found to be enhanced when the LEBM process was applied to the catalyst.

II-PP12

Ternary and Quaternary Interstitial Nitrides for Ammonia Synthesis

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In this presentation, a sol-gel Pechini route will be shown to be effective in the preparation of phase pure Ni2Mo3N catalysts exhibiting high activity for ammonia synthesis. Both ammonolysis and direct reaction with the N2/H2 reaction mixture are suitable for nitridation of the precursor, with the latter offering advantages in terms of large scale application where ammonolysis is not favoured due to issues relating to heat transfer. In contrast to the Pechini method based route, Ni2Mo3N samples prepared from a NiMoO4 precursor yield materials which are inactive for ammonia synthesis. In addition to reaction data, the results of isotopic nitrogen exchange studies will be presented and correlated with activity for ammonia synthesis. The possibility of a Mars-van Krevelen mechanism for the material active in ammonia synthesis will be discussed. Further studies extended to investigate novel quaternary catalysts will also be outlined.

II-PP14

Kinetic Classification for the Coupled Reactions. New Oportunities of Catalytic Systems Design

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The kinetic classification of coupled reactions is proposed. This classification includes one-route and multiroute mechanisms. A one-route coupled reaction mechanism includes consecutive elementary steps leading to two (or more) different products. This reaction is described by one stoichiometric equation. Multiroute coupled reactions are described by a number of independent stoichiometric equations and may be chain and non-chain processes. The principle of kinetic conjugation (PKC) is formulated on the basis of Shilov's theory of coupled reactions and modern kinetic theory of multiroute reactions. The approach to catalytic systems design on the base of PKC includes purposeful selection of catalytic systems using information about probable mechanisms of desirable products formation from available starting reagents.

II-PP15

Tailored Synthesis of Palladium Nanoparticles on Carbon Nanofibers for Different Catalytic Applications

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The paper is devoted to the development and study of the different procedures of the palladium nanoparticles stabilization by means of CNFs and N-CNFs. It was shown that a combination of a proper precursor and N-CNFs allowed to control the size of supported Pd nanoparticles and improve the activity of catalysts in reactions of formic acid decomposition and hydrogenation of nitrobenzene.

II-PP16

Synthesis of Bimetallic PdAg Nanoparticle Arrays by the Diblock Copolymer Micelle Approach: a Way to Synthesize Supported Catalysts with Controlled Size, Composition and Spacing

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Bimetallic nanoparticles (NPs) display unique properties drastically different from those of the corresponding single-component particles. These properties are assumed to result from both the electronic and structural effects of the bimetallic NP. As these properties depend also on the preparation conditions, the synthesis of bimetallic NPs with accurately controlled structures and compositions is essential to obtaining advanced materials for electronic, magnetic, optic and catalytic properties.

In the present study, 2D ordered arrays of bimetallic PdAg NPs were successfully synthesized via the copolymer micelle approach and characterized by various spectroscopic and microscopic characterization methods.

The copolymer micelle approach is an excellent method to obtain ordered arrays of bimetallic NPs supported on flat surfaces with controlled sizes, spacing and compositions. These collections of NPs can be used as model catalysts (for COV abatement in the case of PdAg) where important parameters that influence their catalytic behaviour can be finely monitored and modulated.

II-PP17

Influence of Platinum Anion Complexes Composition on Their Anchoring on Magnesium – Aluminum Layered Hydroxides

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The study investigates the anchoring of platinum complexes with different composition and geometry ($[PtCl_6]^{2-}$, $[PtCl_4]^{2-}$, $[Pt_3(CO)_6]_n^{2-}$) on magnesium – aluminum layered hydroxides (LDH-MgAl) with different Mg/Al ratio (Mg/Al = 2, 3, 4). Catalytic properties of $Pt/MgAlO_x$ were tested in propane dehydrogenation.

It has been found that composition and geometry of platinum complexes as well as Mg/Al ratio in LDH-MgAl have a significant effect on anchoring of complexes onto support and on dispersion, electronic state of the platinum sites and their activity in propane dehydrogenation. Complexes $[PtCl_6]^{2-}$ fixated in interlayer space by electrostatic interaction with positively charged LDH-MgAl layers without significant hydrolysis of the complexes. Adsorption of complexes $[PtCl_4]^{2-}$ is accompanied by their hydrolysis upon contact with basic support with possibility of coordination of $[PtCl_4]^{2-}$ with hydroxyl groups of the LDH-MgAl. No adsorption of platinum carbonyl complexes $[Pt_3(CO)_6]_n^{2-}$ occurred on LDH-MgAl owing to steric difficulties. When $[Pt_3(CO)_6]_n^{2-}$ anchore on $MgAlO_x$ decrease of complexes size took place.

Propane conversion and propylene yield decrease with increase Mg/Al ratio for catalysts made from chloride precursors. Propane conversion, platinum dispersion and stability of catalysts obtained from platinum carbonyl complexes were above respective characteristics for samples, made using chloride precursors.

II-PP18

An Acidity Study of Encapsulated Heteropolyacids in a Sol-Gel Silica Matrix for a Green Friedel-Crafts Alkylation

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A heterogeneous acid catalyst active in the Friedel-Crafts alkylation was prepared. Different amounts (11% to 40% w/w) of Keggin type tungstophosphoric acid (HPW) were encapsulated in a silica matrix using the sol-gel method. Tungsten-oxygen vibration bands measured by IR spectroscopy confirmed the presence of HPW in the support. Almost no leaching of HPW in ethanol was observed by UV-vis spectroscopy after the Soxhlet extraction, suggesting that the Keggin structure was firmly incorporated into the silica matrix. Acidity measurements were performed using pyridine adsorption and temperature programmed desorption in order to determine the amount and type of acid sites on the catalyst surface. The maximum amount of Brönsted acid sites was reached in the sample containing the 30% of HPW. The samples were tested in the resorcinol alkylation with methyl-tert-butylether to give 4-tert-butylresorcinol and 4,6-di-tert-butylresorcinol. The catalytic activity was found to increase with the number of Brönsted acid sites.

II-PP19

Carbide and Graphene Growth, Suppression and Dissolution in Ni Model Systems Studied by in-situ XPS and SXRD

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In catalysis, the activity and selectivity of the entire catalytic entitity can be modified by carbon in connection with metal-support interaction. The stability of Ni-based anode materials in Solid Oxide Fuel Cells (SOFC) can be enhanced by carbon management, when they are exposed to hydrocarbon rich fuel gas. Carbon managment requires the understanding of the adsorption, migration, dissolution and resegregation of carbon on the catalyst, as well as of the structural and electronical properties of different scenarios of C-distribution.

The role of the clock-reconstructed Ni(111) surface carbide regarding further C-growth and dissolution is tested and experimental data are compared to the structural models proposed in the literature. In our work, we focus on the behavior of Carbon on different Nickel systems in the temperature region of 300K to 800 K.

Structure modelling of SXRD data to confirm the most plausible configurations of unrotated graphene on Ni(111) will be presented.

II-PP20

Effect of the Preparation Method of $La_{1-x}Sr_xFeO_3$ Perovskites on N_2O Decomposition

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In this work, the N_2O decomposition has been studied over perovskites $La_{1-x}Sr_xFeO_3$ synthesized through two different methods: (i) sol-gel auto-combustion and (ii) wet impregnation of metal nitrates on chiral silica as a substrate. The non porous perovskites $La_{1-x}Sr_xFeO_3$ through sol-gel auto-combustion combustion show higher activity that the mesoporous perovskites prepared through the wet impregnation. Moreover, the effect of the properties of the solids on catalytic activity was examined. The higher specific surface area and the chiral morphology of the silica support did not improve the catalytic properties of the system $La_{1-x}Sr_xFeO_3$.

II-PP21

Hidden Resources of Electron Scattering at Surface and in the Bulk of a Solid: an Exploratory Research

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The resonant core level excitation under the tuneable synchrotron irradiation results in specific responses forming the grounds of advanced EXAFS, XAS and XES methods. The report highlights similar effects provided by handy routine techniques of elastic electron scattering and X-ray photoelectron spectroscopy. An integrated electronic structure of chemically bound atoms at surface, including adsorbed species or in the bulk originally holds a set of cells for the resonant energy absorption such as intra- and interband electron transitions, plasmon oscillations, ionization of valent states, etc. The model experiments have shown that both inelastic electron scatterings, at surface and in the bulk follow similar rules. Furthermore, it is a common occurrence that the core level excitation is accompanied by using above cells to form an additional multichannel route for the nonradiative energy dissipation. An event comes true on condition that both, the core and coupled electrons belong to the same configuration.

II-PP22

Surface Defects: Evaluation the Gap between Structure and Catalytic Activity

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The quantitative correlation between structure and activity of catalytic centres at solid surface has been performed within a suggested model. The sum of bonds lost by adjacent atoms forming an adsorption site as compared with bulk atoms is taken for evaluation the local surface imperfection, while the reaction enthalpy at that site is considered as a measure of activity. Semi-empirical calculations have revealed that surface defects provide weakly bound, but inclined to hydrogenation state of atomic nitrogen that makes the grain boundary to be the center for sustained surface wave nucleation during $NO+H_2$ reaction on the Rh tip. The sum of lost bonds predicted for optimal catalytic center of Fe atoms in NH_3 synthesis coincides with that of C_7-cite as responsible for largest activity of the Fe(111) single crystal among others. The same approach can be applied to any other adsorption or catalytic process exhibiting high surface sensitivity.

II-PP23

Design of Ceramometal Cu-Al Catalyst with Egg-Shell Microstructure for Water-Gas Shift Reaction

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Water-gas shift reaction (WGS) is one of the primary industrial reactions of hydrogen production. One of the main problem of low temperature shift is the low activity of conventional catalyst per volume of the catalyst bed. The possible way to increase the volume activity is the use of ceramometal catalysts with enhanced real and loading density. In the presented work a new CuAl-based catalyst prepared through the stage of mechanical alloying of Cu-Al powders was developed. The detailed study of the structural, textural, surface and other physical properties in comparison with catalytic properties of cermet CuAlO/CuAl catalysts has been carried out. It was found that TOF values of some cermet catalyst are higher than for conventional CuZnAl oxide catalyst. The structure sensitivity of cermets has been discussed.

II-PP24

Parahydrogen-Induced Polarization (PHIP): a Superior Tool for Mechanistic Studies of Heterogeneous Catalytic Reactions

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Parahydrogen-Induced Polarization (PHIP) is a very informative method for mechanistic and kinetic investigations of catalytic reactions involving hydrogen.

In this work PHIP technique was used for investigation of heterogeneous hydrogenation of α,β-unsaturated carbonyl compounds and vinyl acetate. The existence of route of pairwise hydrogen addition to C=C bonds of acrolein, crotonaldehyde and vinyl acetate over several supported metal catalysts was demonstrated. In hydrogenation of acrolein and vinyl acetate over Rh catalysts the formation of hyperpolarized 2-butene from adsorbed vinyl species was observed. In propene-d6 hydrogenation the H/D-exchange via hydrogen addition with subsequent dehydrogenation was demonstrated. It was shown for the first time that PHIP effects can be observed in heterogeneous hydrogenations over bulk metals and metal oxides. Also PHIP technique was used for kinetic studies of heterogeneous hydrogenations. The influence of hydrogen pressure and reaction temperature on the rate of pairwise and non-pairwise routes of hydrogen addition was investigated.

II-PP26

Biomorphous $CeZrO_2$ and $CuO-CeZrO_2$ Catalysts for Low-temperature CO Oxidation

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Ceria-zirconia catalysts modified with CuO are promising systems for low-temperature CO oxidation. In this work pine sawdust and organic surfactant (CTAB) were compared as templates to create mesoporous structure for $CeZrO_2$ and $CuO-CeZrO_2$ catalysts.

In this paper it was shown that catalytic systems obtained using different templates have similar phase composition, but a different extent of crystallinity of ceria-zirconia oxide (it is higher for the $CuO/CeZrO_2$ (CTAB) and lower for $CuO/CeZrO_2$ (SD)). Moreover, it was shown that the catalysts contain separate phase of CuO with the traces of Cu_2O. Modification of $CeZrO_2$ with Cu oxide leads to the significant decrease of the temperature of CO oxidation, from 250 to 100°C and less. Therefore the sawdust which is the waste in timber industry could be effectively used as the template for active ceria-zirconia catalysts instead of organic templates.

II-PP27

Ethanol Steam Reforming over RhPd Supported on Nanoshaped CeO_2

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One of the challenges of ethanol steam reforming (ESR) to produce hydrogen (H_2) is how to employ lower temperatures and improve the efficiency of ESR, in order to scale down the ESR for diverse forthcoming applications. In the last two decades, a myriad of supported metals have been investigated as potential catalysts for ESR. Among them, the bimetallic Rh-Pd system supported over CeO_2 has shown an outstanding catalytic performance for ESR. Here we report a systematic study of the ESR reaction over RhPd nanoparticles supported on ceria with different morphologies (nanocubes, nanorods and nanopolyhedra), analyzing their catalytic performance and using several characterization tools (operando X-ray diffraction, electron microscopy, etc.) in order to investigate the role of the oxide morphology and the importance of the size and synthetic routes to load RhPd nanoparticles onto ceria supports.

II-PP28

Design and Synthesis of Supported Vanadium Catalysts for Oxidative Dehydrogenation of Hydrocarbons

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Lanthanum orthosilicates with an apatite structure can be a possible matrix for isolated tetrahedral vanadium oxide species, which presence is commonly supposed to be essential for maintaining high conversion and selectivity in the ODH of lower alkenes. However, a tailor-made design of materials with desired properties requires developing of controlled synthesis method based upon understanding general physicochemical regularities at each stage of the selected preparation technique. In the present work, the peculiarities of genesis of the structure and texture of lanthanum silicates in the course of synthesis by co-precipitation were examined. The possible mechanism of the apatite-type lanthanum silicate formation is considered. Given the peculiarities of their formation via co-precipitation, the vanadium catalysts based on amorphous and crystalline lanthanum orthosilicates will be also prepared by co-precipitation as well as wetness impregnation methods. Their structure peculiarities and catalytic properties in ODH of propane will be examined.

II-PP30

The Interaction of Model NSR Catalysts BaO/MO$_2$ and Pt-BaO/MO$_2$ (MO$_2$ = TiO$_2$, ZrO$_2$, TiO$_2$-ZrO$_2$) with NO$_2$

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NSR catalysts are used for nitrogen oxides neutralization in exhaust gases by storage in the form of nitrites and nitrates with following reduction to nitrogen. In this paper we studied the interaction of model NSR-systems BaO/MO$_2$ and Pt-BaO/MO$_2$ (M = TiO$_2$, ZrO$_2$, TiO$_2$-ZrO$_2$) with NO$_2$ using XPS. NSR samples were prepared in the form of thin films (10-15 nm) of supporting material on FeCrAlloy substrates with BaO and Pt deposited on the supports. Treatment in NO$_2$ produced by lead nitrate decomposition was performed at pressure of 3×10^{-6} mbar and a sample kept at room temperature. NSR samples react with NO$_2$ to form successively barium nitrite and nitrate. At that, two new states of platinum are formed: metallic particles with dissolved oxygen and platinum oxide PtO$_2$. After the annealing in vacuum at 500ºC, Pt particles become larger that makes their oxidation more difficult.

II-PP31

Location, Toxicity and Growth Mechanism of Coke on Hierarchical MOR Zeolites

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The aim of this work is to establish a relation between the textural properties of different hierarchical HMOR zeolites and the toxicity, location composition of coke formed during the propylene oligomerisation.

II-PP32

Computational Investigation of Palladium Supported Boron Nitride Nanotube Catalysts

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Due to their unique thermal, chemical and mechanical stability boron nitride based nanotube (BNNT) derivatives are suitable for high temperature technologies and catalysis. BNNTs supported metal nanoparticles have been already studied as catalyst for the selective oxidation of lactose showing high activity and selectivity. In this case it has been showed that the chemical nature of the support could affect the degree of dispersion and size of the dispersed nanoparticle, ruling the reaction activity and selectivity. A computational study could elucidate how the interactions between metals and BNNTs affect the growth of metal clusters. In this study the interaction of Pd$_2$, Pd$_3$, Pd$_4$ and Pd$_{30}$ clusters with a single walled BNNT was modelled by an UFF/DFT ONIOM approach. The adsorption behaviour of the oxygenate D-glucopyranose species on the larger cluster was also carried out to model a medium-complex biomass derived molecule.

II-PP33

Peculiarities of Controlled Synthesis of Highly Efficient Cu-Containing Catalyst for Methanol Synthesis

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The obtained results and recently published data suggest that the active state of Cu-Zn-containing methanol synthesis catalysts is an extremely complicated system, which includes defective metallic particles that strongly interact with the supporting defective ZnO phase in the form of epitaxial bonding and are at least partially decorated by amorphous oxide overlayer [1, 2]. Both the metallic nanoparticles and the oxide support have mixed (Cu-Zn) composition and are defective. Al^{3+}(Cr^{3+}) cations are not merely structural promoter, however, directly affect the specific activity of the active sites.
The intimate interaction of Cu-Zn species may only be possible as the result of their genesis from mixed Cu-Zn oxide phases. Solubility Cu^{2+} in ZnO can be dramatically increased by anionic modification of the mixed oxide structure. Promotion of the oxide structures by small quantities of Al^{3+}(Cr^{3+}) cations can further expand solubility ranges and thermal stability of the catalyst. Evolution of anionic admixtures due to overheating the mixed oxide beyond the threshold of their thermal stability (*ca.* 380-400^{0}C) leads to decomposition and recrystallization of mixed oxides, causing the decrement of the catalytic activity in methanol synthesis. The most natural way for production of anion-modified mixed oxide is decomposition of mixed hydroxycarbonates at moderate temperatures.

II-PP34

Effect of Catalyst Preparation on the Selective Hydrogenation of Canola Oil over Low Percentage Pd/Diatomite Catalysts

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Hydrogenated vegetable oils contain high contents of *trans*-fatty acids. Because of the increased health concern about *trans*-fatty acids, new hydrogenations have been studied to seek ways for substantial reduction of the *trans*-fatty acids in the hydrogenated products. In this research, activated diatomite has distinctive properties as a support for hydrogenation catalysts. We are preparing adsorption method to synthesize low percentage 0.2% of Pd/Diatomite catalyst. It was utilized for hydrogenation of canola oil in industrial pilot testing, at temperature 90°C and 0.5MPa pressure and compared to commercial nickel catalyst (Pricat-9910) at 150°C, 0.5MPa pressure agitation of 800 rpm for 160 min. The changes in iodine value, fatty acid composition, *trans*-fatty acids, melting point and solid fat content were investigated on partial hydrogenated canola oil. The results show that the 0.2% Pd/D catalyst is the most active compared to the commercial catalyst. Lower hydrogenation temperature used 0.2% Pd/D catalyst, significant reducing the formation of *trans*- content by 13% in fat.

II-PP35

Metal-free N-doped Carbon Networks as Hydrogenation Catalysts: a Computational Study

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A computational study concerning metal-free hydrogenation catalysts based on N-doped carbon networks. Different models and theoretical approaches were employed in order to obtain a complete picture of the H_2 fragmentation on two kinds of substitutional defect, namely 4N and 3N defects framed within different models of carbon networks. The influence of the π-system and of the curvature on the ergonicity associated to the H_2 bond cleavage were analyzed. It was found that increasing the number of the benzene rings, surrounding the defects, the ergonicity of the reaction increases whereas the curvature of the carbon network scarcely affects the same property. The catalytic hydrogenation mechanism involving the C_6H_5-NO_2 and C_6H_5-CN molecules was also studied. In some details, a pronounced difference in the adsorption processes on the title networks characterizing the C_6H_5-NO_2 and C_6H_5-CN molecules was outlined.

II-PP36

Enhanced Catalytic Performance of Ni-Fe Alloy in Methane Dry Reforming: Role of Fe

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A series of bimetallic Ni-Fe/$MgAl_2O_4$ catalysts with Fe/Ni molar ratios between 0 and 1.5, are examined for methane dry reforming from 923 to 1073 K and a CH_4/CO_2 ratio of 1. The evolution of the catalyst structure during H_2-TPR, CO_2-TPO, and dry reforming is examined using time-resolved in situ XRD. During H_2-TPR, Fe_2O_3 and NiO are reduced to Fe and Ni up to 973 K. Higher temperatures lead to Ni-Fe alloy formation. The alloy remains stable up to 900 K under CO_2-TPO and is decomposed to Ni and Fe_3O_4 at higher temperatures. The Ni-Fe alloy is the active phase. Fe partially segregates from the alloy forming FeO_x during reaction. Lower amounts of accumulated carbon were observed on Fe-promoted samples. The process of dry reforming on Ni-Fe catalysts follows Mars-Van Krevelen mechanism: CO_2 oxidizes Fe to FeO_x and CH_4 is activated on Ni sites to form H_2 and surface carbon. The latter was reoxidized by lattice oxygen from FeO_x, producing CO.

II-PP37

Hybrid SILP Catalysts Based on Carbon Materials

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SILP (“Supported Ionic Liquid Phase”) catalysts have been prepared using a Rh complex as active species and different IL ([bmim]PF_6] loadings. Several carbon materials of different morphology and textural properties have been used as support. The catalysts have been tested in the hydrogenation of cyclohexene and they have shown to be active and reusable. In some cases the SILP catalysts are more active than the analogous biphasic system and even more active than the homogeneous system. There is a notable effect of the support properties on the stability of the supported IL phase and on the catalytic activity. The best results have been obtained with a commercial activated that has a broad pore size distribution.

II-PP38

Influence of the Support Nature on Palladium Activity in Liquid-Phase Hydrogenation of C=C Bond in Molecules with Polar and Non-Polar Substituents

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The main question involved in this work concern with correct support choice at the step of catalyst design as it might influence catalytic performance due to metal-support interaction caused either by electronic state of metal or by specific interaction between solution compounds and support surface. Palladium catalysts supported on inorganic solids of various nature were tested in hydrogenation reactions of substituted olefins (cyclohexene and maleic acid) in aliphatic alcohols and water as solvents. According the XPS data no correlation between Pd electronic state and its specific catalytic activity was found. Irrespective to the content of water in aliphatic alcohol solvent specific catalytic activity of supported Pd in cyclohexene hydrogenation depend on support material nature. The trend of this change doesn’t agree with analogous trend in maleic acid hydrogenation. The structure sensitivity of the reactions occurs only after high-temperature reduction of Pd with H_2 at 400°C.

II-PP39

Electrochemical Alternating Current Synthesis of Composite Materials for Catalysis

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The “one-pot” electrochemical preparation method of composite materials (Pt/C, Pt/SnO_x-C, Pt/NiO-C, Pt/γ-Al_2O_3, Cu_2O-ZnO) based on metal oxidation and dispergation under alternating current was used. As-prepared materials can be effectively used as electrocatalysts in fuel cells, diesel oxidation catalysts and photocatalysts in technologies of purification of water as well as in the processes of organic compounds oxidation.

II-PP40

On Combined Reactivity and Thermogravimetric Study of CO and CO_2 Hydrogenation to Methanol over Cu Based Catalyst

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Catalysts for conversion of CO_2 into chemicals and fuels are an important building block for sustainable usage of energy resources and feedstock in chemical industries. This work aims to illustrate the potential of the thermogravimetric technique combined with activity measurements in studying reaction intermediates and mechanistic aspects. One of the promising reactions of industrial relevance used for CO_2 conversion is methanol synthesis over Cu – based catalyst:

$CO_2+3H_2 \leftrightarrows CH_3OH+H_2O$

The reactivity measurements in steady and transient state in combination with surface titration experiments were performed for the analysis of stable surface intermediates and exploring the nature of the active catalytic site with respect to the specific catalyst. The instant study elucidates the working principle of two realistic high performance catalysts with respect to the adsorbates accumulated during the steady state under reaction conditions (30bar, 250°C) in CO or CO_2 gas feeds.

II-PP41

Alumina Exsiccates Prepared via CTA Technology

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The main goal of the paper is investigation of eta and gamma based alumina exsiccates (phase composition, acid and base properties, porosity and durability of granules, static and dynamic capacities) prepared via CTA technology depending on row hydroxides (bayerite or pseudo boehmite structured) and nature of electrolytes (acid or base) used for pastes preparation.

II-PP42

Textural and Transport Properties of Hydrotreatment Catalysts (γ-aluminas) Characterised by ^{129}Xe-NMR Spectroscopy

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In the context of current environmental regulations, the optimization of hydrotreatment (HDT) catalysts is of crucial interest. HDT catalyst consists of a mesoporous support (γ-alumina) impregnated by an active metal phase. The knowledge of textural properties of the support is determinant for optimizing transport properties of the impregnation solutions, reactants and products. Based on the great sensitivity of the highly polarizable electronic cloud of the xenon atom to its environment, the ^{129}Xe NMR has proved to be a very useful technique to study the porosity of microporous and mesoporous solids like zeolites and silicas. Combining the results of different NMR measurements, it is possible to characterize the textural and transport properties of aluminas: i) the chemical shift of Xe adsorbed measured by 1D NMR experiments has been correlated to the pore diameter and ii) 2D exchange measurements allows to describe the pore connectivity.

II-PP43

Organoboron Nanoparticles Catalityc Properties: the Substrate Effect

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The substrate effect on catalytic properties of organoboron nanoparticles (OBN) deposited on the SiO_2, Al_2O_3 and HOPG was investigated on the example of ammonia decomposition reaction. OBN deposited on HOPG achieve the highest rate of the ammonia decomposition. Catalytic activity ratio for OBN on HOPG, Al_2O_3, SiO_2 substrates is 1.00 : 0.82 : 0.43 relatively. It was shown that the difference in catalytic properties of deposited OBN is due to potential differences between the particles and the substrates causing organoboron nanoparticles charging. Measured at room temperature potential difference of the particles and the substrates is -0.6, -0.2 and 0.0 V for SiO_2, Al_2O_3 and HOPG relatively. Reaction mechanism elucidating the OBN catalytic effect on different substrates was presented.

II-PP44

The Influence of Support Properties on State of Supported CrO_x and Activity of Chromium Oxide Catalysts in Dehydrogenation of Hydrocarbons

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Catalytic dehydrogenation is the widely used method of olefin production. Cr-containing catalysts are the main type of materials for dehydrogenation of C_3-C_5 hydrocarbons. Support properties and preparation conditions define the state of supported chromium and its catalytic properties. The state of active component may be controlled by changing of support nature or by introduction of modifying additives.

It was shown that states of chromium depend on the nature of support. The combination of properties in mixed supports allowed us to control the state and activity of supported chromium, which can be considered as the foundation for the preparation of efficient Cr-containing catalysts for dehydrogenation of hydrocarbons.

II-PP45

Characterization and Mobility of the Different Protonic Species in Anhydrous and Hydrated 12-Tungstophosphoric Acid Studied by Solid State ^{2}H NMR

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Mobility of the different protonic apecies in Anhydrous and hydrated 12-Tungstophosphoric acid was characterized by solid state ^{2}H NMR. It was demonstrated that in fully anhydrous HPA there are two types of surface protons. The ones rapidly flipping, being localized on the bridged xygen sites, and the ones involved into relatively fast migration over the surface oxygens of the Keggin anion. Below 423 K the population of fast migrating protons is low, but almost all surface protons are rapidly diffusing over the Keggin-anion surface at T > 503 K by hopping between neighboring oxygens. At low hydration levels (n < 6) the TPA surface protons interacts with water to form $[D_3O]^+$ and $[D_5O_2]^+$ ions. The analysis of the evolution of spin relaxation times with temperature for different spectral species allowed quantify the kinetic parameters of the $[D_3O]^+$ ion formation/decomposition and to characterize the mobility of the OD, D_2O, and $[D_3O]^+$ species.

II-PP46

Differences in the Location of Guest Molecules within Zeolite Pores As Revealed by Multilaser Excitation Confocal Fluorescence Microscopy: Which Molecule Is Where?

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Zeolites are an important group of heterogeneous catalysts, which are for example employed in the Fluid Catalytic Cracking (FCC) process (such as zeolite Y and ZSM-5). Their internal pore architecture makes these catalysts selective for reactants, products, and transition states.

A systematic polarised fluorescence confocal microscopic investigation was presented for three batches of large coffin-shaped ZSM-5 crystals. These crystals were strictly oriented with respect to the recorded polarisation plane of emission light and elongated molecules have been formed due to the acid catalysed oligomerisation of the probe molecule 4-fluorostyrene. The observation of polarised emission was linked to structural features, and the location of dimeric carbocationic species inside straight and sinusoidal zeolite channels was distinguished. Fluorescence spectra were extracted (translated into the third dimension) from which it was possible to discriminate the same dimeric carbocationic species situated inside straight and sinusoidal zeolite channels, respectively, based on their spectroscopic features.

II-PP48

Active Cu Structure for Water-Gas-Shift Reaction

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We report the successful synthesis of uniform Cu nanocrystals with various shapes preferentially exposing different crystal planes and their catalytic activity in the WGS reaction. The structures of Cu nanocrystals were characterized by SEM, TEM/HRTEM, in-situ XRD, XPS, operando-DRIFTS, TPRS. Our results clearly demonstrate that the Cu(100) surface is the active structure for the WGS reaction. Via the combination of in-situ experimental measurements and DFT calculations, the reaction mechanism of the WGS reaction on the Cu surface was revealed.

II-PP49

Enhancing Catalytic Performance of Au/TiO_2 Catalyst in Propylene Epoxidation with O_2 and H_2 via Tuning TiO_2 Morphology

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Propylene epoxidation with O_2 and H_2 catalyzed by Au/TiO_2 catalysts is a promising green route to produce propylene oxide. We herewith report that the catalytic performance of Au/TiO_2 catalysts can be significantly enhanced via tuning the morphology of TiO_2 support. Au/TiO_2 catalyst employing anatase TiO_2 nanocrystals predominantly enclosed with {001} facets acquires a propylene oxide yield of more than 40% higher than traditional Au/P25 catalyst. The ensemble consisting of intimately-contacting Au$^{\delta-}$ species and Ti^{4+} species with weak chemisorption strength is active to catalyze propylene epoxidation with O_2 and H_2 to propylene oxide. These results unambiguously demonstrate strong morphology effect of TiO_2 support on the Au-TiO_2 interaction and catalytic performance of Au/TiO_2 catalysts and provide a strategy of morphology engineering to optimize the catalytic performance of Au/TiO_2 catalysts for the green propylene oxide production.

II-PP51

Oxidative Dehydrogenation of Propane over Hydroxyapatites Substituted with Mg^{2+} and SiO_4^{4-} Ions

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The synthesis of HA modified by Mg^{2+} and SiO_4^{4-} ions was performed to determine the modifying effect of ions on the acid and catalytic properties for oxidative dehydrogenation of propane. The acidity of the surface was determined by low temperature FTIR spectroscopy of adsorbed CO. It was found that the introduction of Mg^{2+} and SiO_4^{4-} ions into the structure of HA did not alter the hydroxyapatite structure, but it led to increased surface acid properties. The sample modified by magnesium showed the highest activity and selectivity in the oxidative dehydrogenation of propane. The achieved total selectivity in the formation of ethylene and propylene at 550ºC over this catalyst was 57% at conversion of 17%.

II-PP52

Evolutions of the Surface Structure and Catalytic Performance of PtRu/C and PtRu/Al_2O_3 during Thermal Treatments

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The changes of the surface structure thus the catalytic properties of PtRu bimetallic catalysts during thermal treatment under H_2 at different temperature were studied. It was found migration of Pt to the surface occurred when the treatment temperature was increased. The electronic interactions between Pt and Ru became stronger with increased treatment temperature, and electrons would be transferred from Pt to Ru. When used in the oxidation of CO and benzyl alcohol, opposite relationships between the activity and treatment temperature for these two reactions were observed. With the increase in treatment temperature, the activity for CO oxidation increased, while that for the oxidation of benzyl alcohol decreased, and it was also observed the amount of oxidized Pt species during the reactions increased. Based on these results, it can be concluded that oxidized Pt species is favorite to CO oxidation, while metallic Pt to oxidation of benzyl alcohol respectively.

II-PP53

Photoactive Coatings Based on Titanium Dioxide Formed by Plasma-Electrolytic and Anodic Oxidation

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The improving of photoactive and photocatalytic properties of TDO in an important task, especially in the environmental aspect, and there, in the foundation, in two directions: the formation of nanostructured film coating TDO and its doping.
There are methods of plasma-electrolytic oxidation (PEO) and anodic oxidation (AO) lets form the oxidizing metal (Ti), but also include a film component of forming electrolyte and also receive and regulate nanotubular structures TDO and use it as a photocatalyst or a template for modify its photoactive properties. Under the conditions of formation of coatings by the PEO-method volume of generated photocurrents is a linear function of the concentration of content of dopants in coatings. The samples of nanotubular TDO are generated photocurrents due here in the introduction of Pt-nanoparticles of TDO-nanotubes with decreased recombination of photogenerated of electrons and holes. Photoactivity of samples of doped PEO-coatings differ from undoped samples more than order.

II-PP54

The Role of Etch Pits in Catalytic Etching of Platinum Catalyst Gauzes in Ammonia Oxidation

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Detailed investigation of the surface microstructure of platinum catalyst gauzes after 50 hours of treatment in the NH_3+O_2 reaction mixture revealed fragments of wires with different etching degrees demonstrating development of catalytic etching. On fragments with minimum etching, pores, cavities and etch pits were observed at grain boundaries, whereas crystallite plains with the height ~ 100 nm and many etch pits with the size of 50-150 nm were observed on the surface of the grains. A continuous layer of crystallites with the size of 3-16 μm having internal penetrating pores with the diameter of 1-5 μm was observed on the fragment with maximum etching. We believe that the NH_3 oxidation on metal atoms located on surface defects (grain boundaries, dislocations) results in weakening of bonds between these atoms. As a result, the mobility of the atoms increases, they migrate and are gradually incorporated into crystal plains on the grain surfaces.

II-PP55

Solid-phase Synthesis of Intercalated Compounds of Molybdenum Disulfide

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The subject of this work was researching of possibility of intercalation during mechanical activation of molybdenum disulfide in the presence of polar liquids, as well as the determination of the activity of catalysts in the model reaction of hydrogenolysis of DBT.

II-PP56

Interactions in Catalytic System Ru-Rb-C (Sibunit) for Low-temperature Ammonia Synthesis Investigated by EXAFS

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It is known that ruthenium-alkali metals-carbon support system is highly active in ammonia synthesis. The aim of this work is the investigation of structural changes in the Ru-Rb-Sibunit system, which take place on different stages of catalyst preparation.

A set, consisting the samples 4%Ru/Sibunit after drying, after hydrogen reduction, and the samples 4%Ru-8.5%Rb/Sibunit after steps of drying, activation, reduction and after reaction of NH_3 synthesis was prepared.

It is shown by EXAFS that ruthenium in the Ru/Sibunit catalyst after drying presents in monatomic state. In the Ru-Rb/Sibunit catalyst after reduction active compound presents as metallic ruthenium. Absence of Ru-Rb distance indicated that ruthenium and rubidium are located mainly separate from each other.

II-PP57

Influence of Carbon Nanotubes Oxidation on the Co/CNT Structure and Catalytic Activity in CO Hydrogenation

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In this work we studied the influence of CNT oxidation on the morphology and catalytic activity of Co/CNT catalysts. Multiwall CNT were synthesized by catalytic chemical vapor deposition method, then boiled in nitric acid during 1-15 h and studied by BET, Raman spectroscopy, XPS and TGA-MS. Maxima of the defectiveness, BET surface area and surface oxygen content were obtained at 9 h oxidation. Catalysts were prepared using impregnation of Co nitrate ethanol solution for the Co loading of 15 wt. In situ reduced samples (H_2, 400°C, 4 h) were tested in CO hydrogenation conditions (220°C, 1 bar, H_2:CO=2.1:1, 70 h) in a fix-bed reactor. The dependences of catalytic activity and selectivity from Co/CNT structure were obtained in present work. Reduced and treated catalysts were studied by TEM. It was found that Co particle size decreases and CO conversion increases with increase of oxygen content.

II-PP59

Hydrothermal Treatment of Gamma Alumina: Mechanisms and Effects on Catalytic Properties

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For some catalytic processes it is necessary to increase the acidity of γ-alumina for the synthesis of catalysts with perfect activity. It is known that hydrothermal treatment is an alternative method for the modification of alumina acidity. This process accompanied by a formation of boehmite, however, the cause of the additional active sites have not been identified.

Shown that the transition alumina→boehmite occures in solid phase. After 1–3 h of hydrothermal treatment, secondary aggregates of the starting aluminum oxide are dispersed, which leads to an increase in the specific surface area. In the process, the content of acid centers and the activity of the samples in the skeletal isomerization of *n*-butenes on strong Lewis acid centers also grow. It is assumed that boehmite forms layer by layer from surface of alumina primary particles. From this viewpoint, the pore structure and acidity distribution changes attributed.

II-PP60

Multifunctional Bimetallic Transition Metal Catalysts for Stable and Selective Methane Dry Reforming

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This study investigates stable and selective reforming of CH_4 with CO_2 with bimetallic transition metal catalysts containing Ni, Co, W and Fe, deposited over ordered mesoporous Al_2O_3. The function of neighboring CeO_2-ZrO_2 clusters is to continuously supply oxygen species and gasify the coke.

TEM characterization confirmed ordered mesoporous structure of AlCZ support. After active metal deposition, the ordered mesoporous structure was maintained. High dispersion of active metals clusters (below 5 nm) over the surface of the alumina matrix was achieved.

Catalytic results were most promising for NiFe/AlCZ and CoFe/AlCZ catalysts. These materials exhibited stable activity during the 20 h TOS and H_2/CO ratios which are very close to the equilibrium values. On the other hand, a noticeable deactivation of NiW/AlCZ and CoW/AlCZ catalysts was identified. Also, a significantly lower H_2/CO ratio over these catalysts indicates the dominance of WGS reaction, which consumes a substantial part of H_2 to produce water.

II-PP61

Magnetically Separable Metal Nanoparticles as Effective Reusable Hydrogenation Catalysts

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In this work we report several approaches to synthesis of iron oxide MNPs and their use as support for palladium-containing catalysts of alkynol hydrogenation: thermal decomposition of iron-containing precursor; ligand exchange method using functional acids containing multiple double bonds; functionalization of MNP surface with polyphenylenepyridyl dendrons or dendrimers. All the synthesized Pd/MNPs catalysts were shown to be promising in alkynol hydrogenation (up to 98% of selectivity at 95% of a substrate conversion, along with extremely high activity were achieved).

II-PP63

Characterization of Electron-Acceptor Sites on the Surface of Sulfated and Chlorinated Alumina by EPR Using Spin Probes

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Alumina modification with sulfates was found to result in a gradual increase of the concentration of electron-acceptor sites characterized using the formation of radical cations from aromatic molecules with different ionization potentials. The strongest electron-acceptor sites tested with toluene immediately after adsorption were only detected with a concentration of SO_3 not less than 4%. The weakest sites tested with perylene presented on the surface of all the samples, with their concentration on 12% SO_3 sample being 3×10^{19} g^{-1}. Chlorination only led to minor growth of the concentration of the weak sites. Recommendations on the use of spin probes for testing electron-acceptor sites with different strength are suggested. A mechanism of the polycondensation of aromatic probes on the surface electron-acceptor sites explaining experimental results and possible structures of such sites were proposed.

II-PP64

X-Ray Diffraction Methods for Nano-Scale Structural Studies of Catalytic Materials

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Structural diagnostics of catalytic materials is related with an ability to study nano-scale structures. There is significant drawback with common XRD methods, since they probe well-crystallized materials. Alternative effective approaches take into account both the Bragg and diffuse scattering appeared in the XRD pattern. The structure of nanocrystalline phases can be determined using radial distribution function (RDF) of electron density or pair distribution function (PDF) method and direct modelling XRD patterns by the Debye Function Analysis (DFA). The possibilities of these methods to probe structure of catalytic materials are shown for some examples: 1) structural study of nanocrystalline γ-Ga_2O_3 oxide; 2) determination of local atomic structure of supported platinum in Pt/γ-Al_2O_3 catalysts.

II-PP65

Design of Active and Selective Catalyst Systems on the Basis of Clinoptilolite for Hydrocarbon Cracking

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Modification of natural zeolite of Shankanay field by different by nature acids showed the stages of formation of the activity and selectivity of the catalyst. Treatment by mineral acids leads to carrying away ions of the alkali and alkaline earth metals from the surface of zeolite. Treatment by organic acids wash out iron ions, by forming a soluble complex with iron compounds, which prevents carbonization by iron ions catalyzing the formation of carbon from hydrocarbons. Modification of zeolite by HPA leads to a deep loosening of the surface, which leads to a sharp increase in the specific surface area.

II-PP66

Effect of Oxygen Bulk Diffusion in Nickel on Self-Sustained Oscillations in the Catalytic Oxidation of Methane

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The model of methane oxidation over nickel was amended with a step of diffusion of oxygen from the nickel surface into its volume, and the influence of this step on the characteristics of the oscillatory regime was studied. Solutions obtained in the models with and without diffusion of oxygen into nickel were compared. In the self-oscillatory regime of the reaction, the concentration of subsurface oxygen was found to oscillate synchronously with concentrations of reaction products. The addition of the oxygen diffusion into the model leads to the appearance of an induction period, which is consistent with experimental data.

II-PP67

SEM and EDX Characterization of $Mn/Na_2WO_4/SiO_2$ Catalyst for Oxidative Coupling of Methane

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The oxidative coupling of methane (OCM) into ethane and ethylene has been widespread process for the last few decades, since there is a huge chemical demand in the industry for ethylene. For this purpose, several studies have been conducted in order to obtain possible commercial OCM catalyst. In the current study, SEM and EDX characterization of $Mn/Na_2WO_4/SiO_2$ catalyst for the OCM in various forms and structures (prepared by various methods such as incipient to wetness impregnation, sol-gel and hydrothermal synthesis) were investigated. The characterization results showed that the dispersion of Mn and Na_2WO_4 metals over catalyst surface were different in different forms of the catalysts, and this affects the catalytic activity and C_2 (ethane and ethylene) yield.

II-PP68

Significant Enhancement Effect of PVP Capping Ligands on Catalytic Activity of Cu_2O Octahedra in CO Oxidation

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All previously-reported capping ligands exert the surface-blocking effect to decrease the catalytic activity. However, we found PVP significantly enhance the catalytic activity of Cu_2O octahedra in CO oxidation. During the reaction, PVP partially decomposes with the breaking of the N-C bond of the N-CH-CH_2 moiety and the remaining group can enhance the O_2 adsorption on the Cu_2O octahedra surface to improve the catalytic activity. These results reveal that proper capping ligands can significantly enhanced the activity of catalytic reactions in gas phase and open a new window to research the catalysis of nanocrystals.

II-PP69

Development of Hybrid Nanocomposites by Immobilization of Metal Nanoparticles on the Supramolecular and Polymer Matrices of Resorcinarene Derivatives

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Synthesis of highly stable, water-dispersible metal-nanoparticle was achieved by employing of molecular and supramolecular assemblies of resorcinarene in water. The nanoparticles are obtained with controlled size and high catalytic activity. The synthesis and catalytic properties of the hybrid nanocomposites will be discussed in the presentation.

II-PP70

Kinetically Modelled Temperature Programmed Desorption of CO_2 as a Powerful Tool for Identification and Quantification of Sites of Copper/ceria Catalysts for CO-PROX

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This work deals with a combined (experimental/modelling) technique, we named Kinetically Modelled Temperature Programmed Desorption (KM-TPD) using CO_2 as probe molecule, used to identify and quantify the different sites of copper-ceria catalysts. Three sites were identified: i) cerium centres deeply modified by interaction with copper active towards CO oxidation, ii) not modified cerium centres and iii) copper centres in supported copper oxide active for H_2 oxidation, respectively. We changed both the CuO load and the catalyst preparation technique, thus providing different copper dispersion. Copper content and interaction with the ceria significantly affect the catalytic activity and selectivity to CO_2. The qualitative and quantitative evaluation of sites active for CO and H_2 oxidation very well agrees with the catalytic performance in CO-PROX of catalysts suggesting that this technique may be useful for kinetic study.

II-PP71

Photocatalytic Activity of Al-doped TiO_2

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Metal doping is a promising way to enhance the activity of photocatalysts. The optimal metal dopant concentration for a catalyst of a given particle size was shown to vary from 0.01% to 1% independently on the metal dopant nature. In the present work a series of Al-doped titanium dioxide samples synthesized by sol- gel method was studied. Surface characterization was carried out by SEM, Raman spectroscopy, X-ray phase analysis and FTIR spectroscopy of adsorbed CO. Specific surface area was measured by BET method. Photoactivity was evaluated by phenol decomposition under irradiation in aqueous suspension.

The dependence of initial phenol decomposition rate for the samples on the weight percentage of aluminum dopant manifests a maximum at 0.5% of Al content and shows the activity higher than for commercial P25 TiO_2. The highest activity seems to be due to the optimal balance between particle size and aluminum concentration.

II-PP72

On the Physics of Intercalation of Hydrogen into Surface Nanoblisters in Pyrolytic Graphite & Epitaxial Graphene: Relevance to the Hydrogen Storage Problem

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There is a number of recent data on the surface nanoblister formation in highly oriented pyrolytic graphite (HOPG) and epitaxial graphene under hydrogenation in atomic gaseous hydrogen (without catalysts). The process physics has been yet not enough studied.

In the present study, the results {Nechaev et al. (2014)} of the thermodynamic analysis of some recent experimental data are considered.

The very recent experimental data {Geim et al. (2014)} show that a hydrogen atom can not pass through a perfect graphene network. The analysis {Nechaev et al. (2014)} of a number of experimental data show that a hydrogen atom can pass through permeable defects in graphene, i.e. grain boundaries, their triple junctions and/or others.

The "thermodynamic forces" and energetics of forming of graphene nanoblisters (under atomic hydrogen treatment, without catalysts) in the surface HOPG layers and epitaxial graphenes have been quantitatively described, particularly, conditions of the thermal-elastic thermodynamic equilibrium. The physics of intercalation of H2 gaseous nanophase of a high density into graphene nanoblisters have been revealed. It can be used for solving of the very current problem of the hydrogen on-board efficient and safety storage.

II-PP73

On the Spillover Effect Manifestation When the Solid Hydrogen Intercalation into Hydrogenated Graphite Nanofibers: Relevance to the Hydrogen Storage Problem

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The spillover effect manifestation in hydrogenated carbon-based nanomaterials has been not enough studied up to nowadays. In this connection, the thermodynamic analysis {Nechaev et al (2014)} of the related STM, AFM and other experimental data on hydrogenation of high oriented pyrolytic graphite (without catalysts), epitaxial graphenes (without catalysts) and graphite nanofibers (with catalysts) has been done.

Such analysis has shown that the spillover effect is obviously manifested in data {Gupta et al. (2004)} and data {Park et al. (1999)} on hydrogenation of graphite nanofibers (with metallic catalysts), resulting in intercalation of the solid molecular hydrogen nanophase.

It is related to solving of the current problem of the hydrogen on-board efficient storage.

II-PP75

Oxidation of n-heptane over Sphere Catalysts with a Composition of TiO_2-SiO_2-M_xO_y, where M is Co or Ni

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The preparation technique of new composite catalytic materials in the form of hollow spheres was developed. TiO_2-SiO_2 composites were modified by nickel and cobalt. After annealing, the spatial structure of sphere samples was studied by X-ray microtomography on a digital 3D microtomograph. The state of the cations of transition elements and titanium was characterized by UV-Vis DR spectroscopy. The catalysts were tested in the oxidation of n-heptane. It was found that besides the destructive oxidation, the oxidative dehydrogenation of n-heptane and formation of partial oxidation products such as ketones and esters took place. The selectivity towards the partial oxidation products at 400-450ºC reaches 63% on Ni modified catalyst.

II-PP76

C-C Bond Activation in Acetaldehyde Oxidation on Au(111)

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In the current study, partial oxidation of acetaldehyde on oxygen pre-covered Au(111) single crystal model catalyst surface has been investigated. It has been demonstrated that for low oxygen coverages, two different partial oxidation products namely, methyl acetate and acetic acid can be generated without the formation of significant quantities of carbon dioxide. Since the formation of methyl acetate as the oxidative coupling reaction product implies C-C bond cleavage; it was demonstrated that oxygen pre-covered Au(111) single crystal model catalyst surface can activate C-C bonds. In addition to the generation of these products; indications of the polymerization of acetaldehyde on the gold surface were also observed as an additional catalytic route competing with the partial and total oxidation pathways. The interplay between the partial oxidation, total oxidation and polymerization pathways reveals the complex catalytic chemistry associated with the interaction between the acetaldehyde and atomic oxygen on the gold catalyst surfaces.

II-PP78

Commercial Experience of Operating FCC Unit with Low Catalyst-to-feed Ratio and the Reduced REO Content in the Catalysts

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The distinguishing feature of one of the commercial FCC units is a high potential for the reactor throughput, which determines a low value of catalyst-to-feed ratio.

Enhancement of the catalytic cracking capacity led to the implementation of catalysts with reduced REO content and increased quality and quantity of zeolite component in the sample for the purpose of maintaining constant basic product yields at decreased catalyst-to-feed ratio without considerable reconstruction of the unit equipment.

The report also describes the commercial experience of the replacement of cracking catalyst with catalyst containing significantly reduced amount of REO (lower than 0.1 wt%).

II-PP79

Tuning the Catalytic Activity of Palladium Nanoparticles by Modification Phosphonium Ionic Liquid Structure

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Palladium nanoparticles (PdNPs) stabilized by ionic liquids have been successfully used in catalysis. Phosphonium ionic liquids (PILs) especially sterically hindered ones have been less studied.

Catalytic activity of PdNPs depends on their size as well as on their environment in the solution. The interactions between nanoparticle and stabilizer molecules are important for understanding the mechanism of the nanoparticle stabilization. The PIL structure primarily determines the supramolecular organization of the PIL/Pd/solvent system and as a consequence the efficiency of the catalytic composition.

We have found that varying the length of the linear alkyl substituent of the sterically hindered phosphonium salt allows tuning catalytic activity of PdNPs in Suzuki reaction. There was also shown that the balance between electrostatic and steric stabilization is necessary for the formation of stable and active PdNPs.

II-PP80

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Advantages of Ultrasonic Spray Pyrolysis to Prepare Catalysts for Carbon Nanofiber Synthesis

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Ultrasonic spray pyrolysis of water solutions was employed to prepare catalyst (NiO-CuO/10%MgO) for carbon nanofiber synthesis. A domestic humidifier as atomizer and electric precipitator for product capturing were used as parts of experimental set-up. Diameter of spherical-shaped secondary particles (0.2–5 microns) was proved to depend on concentration of precursor solution (0.1-5 mas. % of salts). The simplicity of setup installation along with easy control of particle size of synthesized catalysts makes such method very attractive. Comparison with conventionally prepared catalyst (co-precipitation, mechanochemical activation) in the reaction of butane decomposition at 700 °C was made. CNF obtained from USP-prepared catalysts was characterized by narrow size distribution and relatively high yield.

II-PP81

Modification by Sn as a Key Factor in Thermal Stability of Pd-ceria Based Catalysts for Low-temperature CO Oxidation

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Using the procedure of oncoming precipitation the Pd/CeO_2-SnO_2 catalysts for low temperature CO oxidation were synthesized for the first time. These catalysts are characterized by high activity with unusually high thermal stability at temperatures up to 1000 °C. Formation of microdomain structure is shown to provide high thermal stability of catalytically active phases including the surface PdO_x(s)/Pd–O–Ce(s) species which determine the reaction rate.

II-PP82

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Application of the Nanopowders of Ni, Co and Their Alloy Prepared by a Method of Plasma-Mechanochemistry for the Reaction of the Carbon Dioxide Conversion of Methane

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The nanopowders of Ni and Co metals and their alloy were prepared by plasma-mechanochemical method, and the activity of catalysts on their basis was studied in the carbon dioxide conversion of methane (CDCM) at atmospheric pressure. It was found that the catalytic activity of Ni nanopowder rapidly decreased because of the blocking of its surface by coking products. Powder of Co showed lower but stable activity, which gradually decreased as a result of coking only 300 h after the onset of reaction. A Ni–Co alloy is an active and selective catalyst for CDCM. Its catalytic activity appeared at 400°C; at 870°C, conversion reached 90% and remained unchanged for 500 h. The initial activity was restored by the regeneration of a catalyst based on the Ni–Co alloy with molecular hydrogen for several hours at 400°C.

II-PP83

Effective Acidities of Heterogeneous Catalysts in Various Liquids in Relation with their Catalytic Activity

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Our recent results on the *effective* acidities of several catalysts and supports measured in various liquids, like water, methanol, 2-propanol, hydro-alcoholic mixtures, among others, and the observed relations with catalytic activity in some liquid-solid reactions of biomass valorization, running in the same liquids, are presented. For such measurements, basic solutions of 2-phenylethylamine, chosen as molecular probe, in the selected liquid, have been injected in a home-modified liquid-chromatographic line in which the solid acid sample had been put in a column-sample holder. The measurements can be carried out according with a complete recirculation mode or according with a pulse method. Amount of acid sites and percent of strong acid sites could be determined in any kind of liquid.

The sample studied are bulk and supported acid catalysts (niobium oxide and niobium phosphate and other synthesized catalytic material: a ternary NbPSi compound, and several mixed silica oxide materials used as supports).

II-PP84

New Heterogeneous Catalysts for Free Radical Generation

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Cationic surfactants (S+) are found to form mixed micelles together with amphiphilic hydroperoxides and catalyse decomposition of hydroperoxides into free radicals.The development of catalytic systems for radical generation based on this property of cationic surfactants is presented. Heterogeneous catalysts prepared by adsorption of S+ on montmorillonite, microcrystalline cellulose, and chitosan, were studied by means of microcalorimetry as complex initiators for radical polymerization of styrene containing cumene hydroperoxide. The catalytic activities of prepared catalysts were tested in the model reaction of limonene oxidation as well. Unlike a less adsorption of cationic surfactants on cellulose, the initiation rates (R_i) with this catalyst were established as the highest R_i for both polymerization and oxidation processes. The increase of catalytic effect of cationic surfactant on the cellulose surface and the role of hydroperoxide nature in colloid catalytic system are discussed.

II-PP85

High Active Cr-Al Oxides Catalyst for the Ozone Friendly Freons Synthesis: Pretreatment Conditions and Kinetic Study

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The physicochemical properties of Cr_2O_3/γ- Al_2O_3 catalysts obtained by heat treatment of the sample (precursor) in nitrogen and air between 110 and 600°C and their influence on the catalytic activity in tetrachloroethylene hydrofluorination was studied by the TA, TPD, X-ray diffraction, BET, and DRS methods. It was shown that the temperature and gas composition of precursor pretreatment strong effect on the specific surface area and activity of the catalysts. The $CrO_{1.9}$ compounds are more active than $CrO_{1.5}$. For more active catalyst sample kinetic study was performed.

II-PP86

A Computational Approach to Understand the Promotional Effect in Ni-Fe Bimetallic Catalyst

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A specific Ni to Fe ratio in supported Ni-Fe catalysts enhanced the catalytic activity of the CO_2 hydrogenation reaction relative to supported Ni catalysts. Experimental evidence of alloy formation was established in the supported Ni–Fe catalysts. The formation of alloys was the basis of assessing the catalyst by Density Functional Theory, which has been used for electronic characterization of metal and alloy surfaces. Various electronic properties based on d-electron density of states (DOS) of surface Ni atoms were computed for Ni(111), Ni_3Fe(111) and NiFe(111) surfaces. Lowering of d-band center, upper d-band edge, and DOS at Fermi level in Ni_3Fe and NiFe surfaces occurred, indicating perturbation of the electronic environment of the surface Ni. A consequence of the lowering suggested weaker adsorption on the alloys compared to pure Ni. Thus, formation of a suitable alloy gave rise to an optimum value of d-DOS based properties, which improved the catalytic activity.

II-PP87

Origin of the Spontaneous Formation of Cobalt Nano-Islands under Fischer Tropsch Conditions and Mechanistic Consequences

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Cobalt catalysts undergo a massive reconstruction under Fischer-Tropsch conditions, resulting in the formation of nano-islands containing about 28 Co atoms. Using density functional theory, we show that the reconstruction is driven by the strong and synergistic adsorption of aromatic square-planar carbon and CO at the step sites. The local aromaticity of the Co_4C unit limits the carbon step coverage to 50%, and hydrogenation of CO to CH is found to be relatively facile at the remaining step sites. The CH species then diffuse to the terraces sites where chain growth takes place via the CO insertion mechanism.

II-PP88

Instrumentally Induced Differential Charging Effect in XPS – Turning Drawback to Advantage

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The employing of instrumentally induced surface charging for X-Ray Photoelectron Spectroscopy investigation of supported metal catalysts is described. The interpretation of the observed effects in XPS spectra of conductive, poorly conductive and non-conductive specimens (Sibunit, tantalum and tungsten oxides, alpha-alumina) is discussed. The obtained results prove that such ad hoc approach gives the exclusive additional information on the population density of metal nanoparticles at the non-conductive support surface, and – with a priori knowledge about metal loading – allows estimating the average size of such particles directly from the spectroscopic data.

II-PP89

Kinetics of Activation Fischer-Tropsch Iron-Based Catalysts under CO and CO/H_2 Flows

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Fischer-Tropsch synthesis (FTS) is an alternative method to produce a variety of chemicals as hydrocarbons and oxygenate from syngas. Both cobalt and iron are used as FTS catalysts, but iron is more preferable because of their low cost, high resistance to poisons and possibility to work under low H_2/CO ratio. It is known that iron carbides are active phases in FTS iron-based catalyst. Recently, it was established that activity and selectivity of iron catalyst depend on the composition of the mixture by which catalyst activated, but the reasons are still unclear.

In our research, we investigated the kinetics of carburization FTS iron catalysts in the atmosphere of both carbon monoxide and syngas ($CO:H_2 = 1:1$) by *in situ* magnetometric method. It was shown that the composition of activation mixture dramatically effects on the kinetics of carburization FTS iron-based catalysts. The size effect of activation processes was established.

II-PP90

Gold Nanoparticle-Loaded Filter Paper: a Recyclable Dip-Catalyst for Real-Time Reaction Monitoring by Surface Enhanced Raman Scattering

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Taking their advantage of low-cost, and mesoporous fibers and so on, cellulose filter paper based hybrid materials have developed for the sensing and diagnostics. However, their application in catalysis has not been well explored yet. Herein, we demonstrated a novel strategy, robust and recyclable ‘dip-catalyst’ based on a gold nanoparticle (Au NP)-loaded filter paper composite, prepared by a simple dip-coating process using concentrated Au NP suspensions in toluene. Oleylamine-capped Au nanoparticles, dispersed in an organic solvent, strongly adsorbed on cellulose filter paper, which shows a great ability to wick fluids due to its microfiber structure. Strong van der Waals forces and hydrophobic interactions between the particles and the substrate lead to nanoparticle immobilization, with no desorption upon further immersion in any solvent. While performing as catalysts, the composites display excellent surface enhanced Raman scattering (SERS) efficiency, allowing the real-time monitoring of chemical reactions.

II-PP91

Graph Machine Based Advanced Data Modelling for High-Throughput Zeolite Catalyst Screening

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Zeolites are widely used as catalysts in the refining and petrochemical industries. However the lack of accurate models for predicting hydrocarbons adsorption on molecular sieves prevents using these models for statistical learning together with high throughput experimentation.

This work aims at developing a QSAR (Quantitative Structure Activity Relationship) model for zeolite catalysis having a new structure. This model is used within a high throughput iterative screening loop to determine hydrocarbons adsorption enthalpies on different molecular sieves.

II-PP92

Catalytic Methane Decomposition using Iron-Lanthanum Catalysts: Effect of Fe Loading on Activity Performance

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Thermo-catalytic methane decomposition is gaining momentum in the area of heterogeneous catalysis whereby methane can be employed to generate clean fuel hydrogen as well as valuable carbon nanomaterial. Lanthanum supported iron based catalysts were prepared by impregnation method to study the catalytic performance of as prepared catalysts in a micro-activity tubular fixed bed reactor. Effect of metal loading was studied as well. The activity results revealed that 40% Fe/La$_2$O$_3$ showed better activity compared with the other catalysts. The catalysts were characterized using BET and TGA.

II-PP93

Temperature-Programmed vs. Isothermal Pulsed Oxidation of Graphene Formed on Pt/Mg(Al)O$_x$ Dehydrogenation Catalysts

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Graphene deposition and subsequent oxidation was studied on a highly-active Pt/Mg(Al)Ox catalyst using TPO, TAP, HRTEM, and Raman. The results indicate that even chemically-uniform carbon deposits may exhibit complex oxidation kinetics which are governed by a reaction/transport interplay. Readily accessible graphene burns off from Pt as well as support at <700 K, while the residual carbon deposits survive around large Pt nanoparticles and inaccessible packets of the support surface up to 800 K.

II-PP94

The Role of Electron-Acceptor Sites during Catalytic Dehydrochlorination of 1-Chlorobutane over Metal Oxides

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In this study we characterized weak electron-acceptor sites formed during 1-chlorobutane dehydrochlorination over several MgO and Al$_2$O$_3$ samples using perylene and anthracene as spin probes. This is the first ever study where the concentrations of electron-acceptor sites were measured during a catalytic reaction. It is shown that the concentration of weak elector-acceptor sites correlates with the catalytic activity. The obtained results indicate that weak electron-acceptor sites tested using perylene may be the active sites accounting for 1-chlorobutane dehydrochlorination in the active state of the catalysts. It seems to be very important to study possible correlations between the concentrations of electron-acceptor sites and catalytic activity of various catalytic reactions believed to take place on surface acid sites to elucidate the possible role of electron-acceptor sites in these reactions.

II-PP96

Surface Electron-Acceptor Sites: Their Structure and Role in Catalytic and Solid-State Reactions

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According to the results of our DFT simulations, the experimentally observed high electron affinity of solid acid catalysts can be explained assuming that dissociation to the positive and negative charges occurs on their surface during activation. The resulting sites are remarkably similar in their properties to the species resulting from the electrolytic dissociation of strong homogeneous acids and superacids and accounting for their reactivity. For the first time the concentrations of electron-acceptor sites were measured during catalytic and solid-state reactions. The experimental correlations between the concentrations of the electron-acceptor sites and the catalytic activity in reactions catalyzed by acids suggest that these reactions are likely to occur on such sites rather than on more abundant traditional acid sites. Such sites also seem to be responsible for at least some bulk solid-state reactions.

II-PP97

Direct Imaging of Octahedral Distortion in a Complex Molybdenum Vanadium Mixed Oxide

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Nowadays Cs corrected TEMs are powerful enough to obtain point resolution below 50 pm. However, direct imaging of light elements next to heavy elements remains complex. In probe corrected scanning transmission electron microscopy recent developments tackle this challenge, resulting in the revival of the annular bright field (ABF) detector. In contrary to the contrast detected by the high angle annular dark field method, the ABF detector is also sensitive to light elements.

Using the ABF detector, we investigated orthorhombic (Mo,V) oxides crystallized in a structure analog to the M1 structure of MoVTeNb oxide. The obtained micrographs were compared with Rietveld refined X-ray diffraction and electron paramagnetic resonance data. Furthermore we directly measured metal-oxygen bond angles and discussed the oxidation states of the metal centers.

Seeing where the atoms are, generates in particular in heterogeneous catalysis a deeper understanding of the functionality of materials on the way towards tailor-made catalysts.

II-PP98

State and the Catalytic Properties of Cu/ZSM-5 in Selective NO Reduction with Propane

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Catalytic properties of the Cu/ZSM-5 catalyst prepared by ion exchange of the HZSM-5 with aqueous ammonia solution of copper nitrate can be tuned by varying the nature of copper precursor (CC I or CC III). These factors have a significant effect on the copper species located on the surface of zeolite. In the SCR of NO with propane the highest reaction rate per gram of Cu attainable on the catalyst prepared from CC I. This due to the optimum size of Cu^{2+} oxide clusters, which ensures that a large proportion of the active component is have an optimum degree of covalence for the given process involved in the reaction and the copper–oxygen bonds.

II-PP99

In Situ XRD Study of Oscillations during the Methane Oxidation over Palladium and Nickel Foils

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Self-sustained oscillations in the methane oxidation over a Pd and Ni foils were studied in situ using time-resolved XRD. Regular oscillations of a relaxation type were observed at the atmospheric pressure in oxygen-deficient conditions in a temperature range of 350–500°C in the case of Pd and in a temperature range of 650-900°C in the case of Ni. During the oscillations the periodic changes of XRD reflex intensities corresponding to Pd, PdO, and “PdCx-like” phases or Ni and NiO phases were accompanied by synchronous variations of the catalyst temperature. The study has clearly confirmed that the originating of oscillations in the catalytic oxidation of methane in both the cases is determined by the periodic oxidation/reduction of the catalyst.

II-PP100

Temperature Behayiour of the Silane and Germane Molecule Fractures Adsorbed by a Growth Surface in an Epitaxial Process

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In the limits of the kinetic approach based on data of technological experiments, the range of characteristic rates of decomposition of disilane, silane and germane radical molecules adsorbed on the surface during the growth of an epitaxial layer is determined. These parameters are very important for estimation of the interfaces blurring in a two-phase system. The temperature dependences of the decomposition rate of hydride molecules exhibit an unusual activationless behavior in the growth temperature range. The form of the observed dependences is determined by the pyrolysis model and conditions of transferred of hydrogen from an adsorbed molecule onto the surface of the growing layer. It is demonstrated that the basic features of the behavior of the decomposition rate of hydride molecules are controlled by the specifics of the interaction of the hydride molecular beam with the growth surface under conditions of low and high degrees of bonding of hydrogen to free surface bonds.

II-PP101

Model Systems for Co Fischer-Tropsch Catalysts

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In Fischer – Tropsch synthesis (FTS), natural gas, biomass or coal are converted to liquid fuels via synthesis gas. Alkali metals (AM) can be introduced during the preparation of the catalyst or from the synthesis gas feedstock, especially if derived from biomass. AM impurities on supported Co catalysts are reported to considerably decrease the FTS activity, even at very low loadings/concentrations. Adsorption studies of FTS relevant adsorbates on cobalt (Co) single crystals, with and without predeposited AM have been performed, with Scanning Tunneling Microscopy (STM). The effect of the AM on restructuring and relevant adorbates have been targeted. Changes to the adsorption phenomena occuring during exposure to FTS relevant adsorbates have been observed on Co surfaces with submonolayer amounts of AM. The precise distribution of AM on the surface requires further studies to be determined. Relevant modelling investigations with Density Functional Theory (DFT) will be presented together with the experimental findings.

II-PP102

Synthesis of Zeolites from Fly Ashes for Potential Applicationin Environmental Problems

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The disposal of fly ashes represents a serious economic and environmental problem for many industries that use electric power plants. Using the department of Antioquia (Colombia) as example, almost all the fly ashes are generated by food, textile and mining industries, and are disposed of as landfill. However, new ways of utilizing fly ashes has been growing. One of the main approach is the conversion of fly ash into zeolite. Its applications as ionic exchange are very useful for the metal absorption of poison metals. Herein we evaluated the chromium adsorption onto surface of zeolites synthetized through fly ashes of different sources.

II-PP103

Spin Probes for Characterization of Active Sites on the Surface of Oxide Catalysts and Prediction of Their Catalytic Activity

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In this communication we discuss the applications of spin probes for characterization of diamagnetic surface active sites of oxide catalysts. The main goal of these studies is to develop spin probe techniques for determination and characterization of surface active sites that account for catalytic activity of oxide catalysts. We used donor molecules with different ionization potentials (chlorobenzene, toluene, anthracene, perylene) for characterization of electron-acceptor sites with different strengths. Acceptor molecules with different electron affinities (nitrobenzene, 1,3,5-trinitrobenzene) were used for characterization of electron-donor sites. Lewis acid sites were studied using adsorption of stable nitroxyl radicals TEMPO and TEMPONE from toluene solutions. NO is another spin probe that proved to be convenient for characterization of Lewis acid sites and Fe(II) ions. EPR silent oxygen radical anions O^- on the surface of MgO and CaO were revealed using the formation of complexes with molecular oxygen, which are reliably detected by EPR.

II-PP104

Cr-doped Silica Porous Monolith as a Model for Experimental and Theoretical Studies of Phillips Catalyst

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The determination of the structure of the active sites of the Phillips catalyst remains difficult, although constitutive knowledge has been accumulated on simplified systems. The set of silica mesoporous monoliths with high surface area and with Cr loading in the 0.01-0.5 wt% range was produced by one-pot sol-gel method. Despite extremely low Cr loading, the FTIR of CO probes revealed the known families of surface Cr sites. These species readily react at RT with ethylene condensed into the pores, causing a fast growth of polyethylene. A systematic study of dehydroxylation state of the surface on the Cr(II)/SiO_2 samples activated in the 550–750 °C temperature interval was performed in terms of distribution of fully isolated and weakly interacting hydroxyl groups. Experimental observations allowed for development of cluster models of Cr_A and Cr_B sites and the results of DFT calculations are satisfactorily reproduced the main experimental data.

II-PP105

Rational Design of Cu-based Catalyst of Oxychlorination Process by Combined in-situ Mass- and Spatial-time Resolved UV-Visible Spectroscopy

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Oxychlorination of ethylene is the most important route to produce 1, 2-dichloroethane (EDC), which is a key step for poly-vinyl chloride (PVC) [1]. In commercial ethylene oxychlorination reactors, gaseous ethylene, HCl and air react with $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst at a temperature range of 217 ^{0}C-257 ^{0}C and a pressure 5-6 atm.
The $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst is effective in the oxychlorination of ethylene because $CuCl_2$ can catalyze the conversion of HCl to chlorine. In the literature [2], it has been shown that by feeding the three reactants separately, the oxychlorination reaction is catalyzed by a highly dispersed $CuCl_2$ phase and thereby follows a three step redox mechanism:
Step 1. Reduction of $CuCl_2$ to CuCl.
Step 2. Oxidation of CuCl to form an oxy-chloride.
Step 3. Hydrochlorination of the oxy-chloride using HCl to form $CuCl_2$ and H_2O.
In-situ spectroscopy is an approach to monitor online the physicochemical phenomena of the catalyst material in a reactor [3]. The results from such in-situ study at industrial relevant conditions provide detailed insight into the working principles of the catalytic material. So that it would then be possible to improve the existing catalyst formulations or design completely new catalysts, which are more active and/or selective. In the past [4], an operando XANES and EXAFS have been performed to monitor the Cu^{II} to Cu^{I} transformation in the ethylene oxychlorination environment on the $CuCl_2/\gamma\text{-}Al_2O_3$. It has been found that the rate determining step of the overall process (1) is the CuCl oxidation (3). It is noted that the XANES and EXAFS are performed in transition mode, i.e., the catalyst layer is very thin and the space velocity is very high. Therefore, it is difficult for the detailed kinetic study. Hence, we developed an operando set-up to study kinetics of the reaction including catalyst active component involved by combined UV/Vis- and mass spectroscopy, where the reaction conditions and flow can be well controlled in the normal fixed bed reactor.
A strategy of combined transient and steady-state kinetic study was employed. The transient kinetic study was performed for individual reaction steps such as the reduction, oxidation and hydrochlorination steps in the catalytic cycle of oxychlorination process. The UV-Vis spectroscopic technique in the reactor focuses on the same spot of a catalyst in a reactor under true reaction conditions and is capable of delivering sub second time resolution. However, in the overall reaction study, the UV-Vis focuses on the same spot of catalysts in the reactor first until the process reached steady-state to get the time resolved kinetic data. After that the whole catalyst bed of the reactor is scanned by UV-Vis spectroscopy to measure the active Cu^{II} along the reactor axis.
First experiments have been performed by using $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst for individual steps of the oxychlorination process. The change of Cu state from Cu^{II} to Cu^{I} has been studied by the use of UV-Vis spectroscopy, whereas the reaction rate, conversion has been calculated by Mass spectroscopy. It has been found that the rate determining step of the overall process is the CuCl oxidation step. Results obtained from oxychlorination of ethylene on CuCl2/ $\gamma\text{-}Al_2O_3$ catalyst, showed a lower reaction rate on the oxidation step (step2) than the reduction step (step1), which leads to deactivation of catalyst due to the excess amount of intermediate (CuCl). Therefore, CeO_2 is used as promoter to enhance the catalytic performance of the reaction by reducing the reaction rate at the reduction step (step1) in one hand and increasing the oxidation rate on the other hand. Various weight percentages of Ceria (1, 3 and 5 wt %) doped with $CuCl_2$/ $\gamma\text{-}Al_2O_3$ is been used in several cycles.
UV-VIS and Mass Spectroscopies, combined with laboratory techniques made it possible to have a good understanding in kinetic behaviour of the active phase and effects of CeO_2 as promoter for the catalyst. Results show that even low concentrations of ceria in $CuCl_2/\gamma\text{-}Al_2O_3$ can highly enhance catalytic performance of the catalyst however high concentration of CeO_2 has negative impacts on activity of the catalyst.

II-PP106

Controllable Metal Dusting of Ni-M Alloys: New Opportunities for Design of Self-organized Catalysts and Synthesis of Carbon Nanomaterials

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Bimetallic alloys Ni_{1-x}-M_x (M=Co, Cu, Fe, Cr, Mo; x=0.01÷0.5) were synthesized by various methods (coprecipitation, mechanochemical activation) to be used as precursors for preparation of self-organized catalysts active in production of carbon nanomaterials. Suggested approach is based on metal dusting (MD) of Ni-based alloys in aggressive reaction atmosphere containing chlorinated hydrocarbons and H_2. Ni-Mo precursor was found to give the most active catalyst while the best stabilizing effect was elucidated for the addition of Cr.

Disintegration of starting alloys results in formation of the active metallic sites catalyzing multi-directional growth of carbon fibers of submicron diameter and segmented morphology. Due to defective structure, the obtained carbon product is characterized with high surface area (up to 400 m^2/g) and porosity (0.5-0.8 cm^3/g).

The effect of M and its concentration in Ni-M precursor upon catalytic activity and structural peculiarities of CNM product being formed will be discussed in details.

II-PP108

Characterization of the Catalysts with Atomically Dispersed Pd and Rh on Alumina

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Recent experimental studies have demonstrated that atomically dispersed or ionic clusters of precious metals show the highest activity in a number of oxidation reactions. Concentration of intrinsic centers on a surface of γ-Al_2O_3 that are capable to stabilize the supported precious metals in atomic and cluster forms is not that great and usually does not exceed 0.5 wt. % by metal. In the case of Pd and Rh containing catalytic systems there are two main processes known to be responsible for catalyst deactivation. The first one refers to the sintering of dispersed Pd while another process is related to the bulk diffusion of Rh ions into support. The present study aims in a developing of spectroscopic optical, EPR and catalytic (ethane hydrogenolysis) methods for characterization of Pd and Rh state on alumina-based catalysts containing ultra-low concentrations (as low as 0.02 wt. %) of the supported metals.

II-PP109

Novel Catalysts for Selective C≡C Bond Hydrogenation Based on Metal-organic Framework MIL-53(Al) as a Host Matrix for Pd Nanoparticles

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Selective semihydrogenation of an acetylenic function is a demanding task. During the last decade the metal-organic framewoks (MOFs) received a considerable attention as metal carriers for heterogeneous catalysis, which enable fine tuning the activity and selectivity of the resulted heterogeneous systems. In this study we explored the catalytic performance the novel catalysts on the basis of Pd nanoparticles encapsulated in microporous metal-organic framework MIL-53(Al) in the hydrogenation of diphenylacetylene (DPA) as the model substrate. Al^{3+}-derived microporous phenylenecarboxylate frameworks, i.e. MIL-53 (Al(OH)bdc, bdc = benzene-1,4-dicarboxylate) was utilized for Pd deposition.

The synthesized MIL-53 derived catalysts demonstrate high activity and excellent selectivity in semihydrogenation of diphenylacetylene in a liquid phase. Our study revealed a strong impact of both parent framework activation conditions and Pd NP reduction temperature on the catalytic performance of Pd@MIL-53(Al) nanocomposites.

II-PP110

Effect of the Synthesis Route on NO_x Storage over Ceria/Zirconia based-Mixed Oxides in LNT Applications

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In this current study, structural evolution of ternary ($CeO_2/ZrO_2/Al_2O_3$) mixed oxides was monitored as a function of temperature by means of XRD, Raman and BET. Moreover, NO_x adsorption capabilities of the materials were investigated by means of in-situ FTIR and TPD techniques. TPD and in-situ FTIR analysis indicated that simultaneous impregnation route of CeO_2 and ZrO_2 (i.e. Pt/(CeZr)/Al) exhibited superior performance as compared to the subsequent impregnation (i.e. Pt/Ce/Zr/Al).

II-PP111

Choice and Validation of the Promoting Additives on the Zeolite Catalysts of Isobutane Alkylation

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The process of optimize technology for the synthesis of zeolite catalysts for producing high-octane gasoline, to increase their stability, activity, and reduction of coke formation processes investigated the effect of promoting additives such as Cs^+, La^{3+}, Ca^{2+}, Ce^{3+}, Ni^{2+}, Zr^{4+}. It is established that the introduction of a certain type of cation (monocation form of catalyst), and the combination with the introduction of two or more (polycation form) allows to control the availability of the porous structure can influence the formation of active sites of the zeolite catalysts, acid-base characteristics, activity and thus modeling direction selectivity of the process.

II-PP112

In Situ and Ex Situ Studies of Bimetallic Catalysts Activation for Multiwalled Carbon Nanotubes Growth

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In the present paper, we study the formation of the active component of the different bimetallic catalyst (Fe-Co, Co-Mn, Fe-Mo, Co-Mo) during MWCNT growth using in situ synchrotron radiation X-ray diffraction analysis (SRXRD) and in situ XPS in combination with ex situ and in situ high speed HRTEM, solid-state 59Co NMR, gas chromatography. HRTEM, Raman data, thermal dependence of conductivity and magnetoresistance measurements were used for the characterization of relationship between MWCNT defectiveness and catalyst composition.

II-PP113

Catalytic Activity of PCsp^{3}P Pincer Iridium Hydride Complexes in Olefines Hydroformylation and Acceptorless Alcohols Dehydrogenation: DFT and Spectroscopic Study

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Bifunctional dibenzobarrelene-based PC(sp^3)P pincer iridium complex **1** is an efficient catalyst in acceptorless dehydrogenation of alcohols and hydrogenation/hydroformylation of alkenes. The results of variable temperature IR and NMR (^{1}H, ^{31}P) analysis of **1** and its analogue – COOEt substituted complex **2** in different media (dichloromethane, toluene, DMSO, and mixed solvents) in combination with the quantum chemical (DFT/M06; AIM) calculations imply flexibility of the dibenzobarrelene-based scaffold unprecedented for conventional pincer ligands. Both the complex **1** and its counterpart **2** prefer facial configuration of the PCP ligand with P-Ir-P angle of ca. 100º. Such geometries are dictated by stabilizing Ir···O interaction and differ by the mutual arrangement of the H and Cl ligands. The complexes show dynamic equilibrium between two most stable *fac*-isomers, which can be transformed into the meridional ones in the presence of coordinating additives (CH_3CN, DMSO or CO, but not Et_3N), some of which have been used as auxiliary base in catalytic alcohols dehydrogenation. The mechanism of the H_2 activation and C-H bond formation involves intramolecular cooperation between the structurally remote CH_2OH functionality and the metal center and proceeds without the change of the oxidation state of the metal. Model IR studies of *i*PrOH dehydrogenation show higher activity of *fac*-isomer relative to *mer*-one which is further facilitated by addition of Et_3N.

II-PP115

Novel Surface Oxide on Pt(111) as the Active Phase for NO and CO Oxidation

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Platinum finds its main application as a car catalyst to control the emission of exhaust gases. Despite platinum's wide use for catalytic oxidation, the active surface phase under oxygen-rich reaction conditions is still highly debated.

For the Pt(111) surface, the facet lowest in energy, it is also not clear what the relevant structure is under oxygen-rich reaction conditions. Both a bare metallic surface, a surface oxide and bulk α-PtO_2 have been found to be stable in different experiments. With the high-pressure, high-temperature reactorSTM, we have studied the oxidation of Pt(111) and have found a stable surface oxide that assembles in a 'spoke wheel' superstructure at 1 bar O_2 at 430 K. This surface oxide was also studied during NO oxidation and CO oxidation under reaction conditions.

II-PP116

Thermally Stable Multicomponent Manganese Catalyst for Deep Oxidation of Methane

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It was established that MnREEAEE catalyst supported on 2 % Ce/θ-Al_2O_3 has a higher thermal stability (up to 1473 K) and specific activity in the reaction of deep oxidation of methane, compared to known catalysts (IC-40 and Ni-Cu-Cr/2 % Ce/θ-Al_2O_3) which are used for purification of gases from organic substances and combustion of CH_4. The results indicate the real possibility of practical use of thermally stable up to 1473 K MnREEAEE/2 % Ce/θ-Al_2O_3 catalyst for utilization of lean mixtures of CH_4 in catalytic heat generators. The developed catalyst does not concede to known analogues both in activity and thermal stability, where perovskites and manganese hexaaluminates were used.

II-PP117

Thermostable Cu-containing Catalyst with Grafted Active Component for the Dehydrogenation of Cyclohexanol to Cyclohexanone

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The technology of cyclohexanol dehydrogenation catalyst was developed, allowing us to obtain the copper coating with much finer particles of active component compared to analogues. The catalyst was prepared by deposition of copper from an aqueous solution of its ammonium carbonate complex on the silica support. Measurement of activity and selectivity of catalyst samples was performed in flow type setting laboratory at 250°C, atmospheric pressure, the volumetric feed rates 1.0 h-1 (middle results for 64 working hours). The new catalyst is superior by conversion and thermal stability of BASF sample, and the selectivity of K-CO catalyst. According to the firm “Zud Chemie” the extension of dehydrogenation selectivity of 1.0% provides annual economical effect more than U.S. $ 1.2 million per unit.

II-PP118

Hydrogenation of Benzene in the Presence of Nickel Nanocatalysts Immobilized on Chitosan

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Hydrogenation of benzene with chitosan-nickel nanocatalyst was performed at room temperature and atmospheric pressure. The obtained polymer-immobilized nickel nanoparticles show high activity in hydrogenation reaction of benzene and maintain it in repeated cycles. Catalytic properties of nanocomposites depend on producing conditions which impact on the size of the formed nickel nanoparticles.

II-PP119

Key Magnetic Intermediates in Rhenium-based Olefins Metathesis Catalytic Systems

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In this report the results of studies of magnetic intermediates and reactions with their participation in rhenium-based catalytic systems of olefin metathesis are given. Paramagnetic rhenium complexes are identified in olefin metathesis catalyst systems based on complexes of mono-, bi-, hexa -nuclear compounds: $Re(CO)_5X$**;** $Re_2X_4(CH3COO)_4 \cdot 2H_2O$, $[DMFAH]_2Re_6X_{14}$, where (X=Cl, Br). EPR signals with magnetic resonance parameters (MRP): $g_o = 2.070$, A_o ($^{185,187}Re$) =321 G at 300K and $g_I = 2.135$, $g_\perp = 2.067$, $\langle g_o \rangle = 2.098$, $A_\parallel$ ($^{185,187}Re$) =469 G, $A_\perp$ ($^{185,187}Re$) =271 G, <A ($^{185,187}Re$)> =337 G at 77K are registered for the products of the reaction of $Re(CO)_5Br$ with $(C_2H_5)_3Al$ in n- heptane solution. These values of MRP belong to low spin complexes of rhenium with total spin S=1/2 and square-pyramidal structure of a local environment. Results of this work show that in all cases the interaction of rhenium complexes with aluminiumorganic compounds in solution leads to stable at room temperature paramagnetic complexes with total spin S=1/2 and highly covalent Re-C bond. The formation of paramagnetic rhenium complexes with $Re=CH_2$ bond and total electron spin S = 1/2 is established. The presented spectra are the first direct observation of paramagnetic rhenium intermediates in the catalytic systems for olefin metathesis.

II-PP120

Dibenzothiophene Hydrogenolysis on Zinc Modified Ni-MoW/Al_2O_3 Hydrotreating Catalysts

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A line of Ni-MoW/Al_2O_3 catalysts was synthesized by means of wetness impregnation method from aqua solution of Ni, Mo and W compounds ($Ni(NO_3)_2 \cdot 6H_2O$, $H_3PMo_{12}O_{40} \cdot 17H_2O$, $H_3PW_{12}O_{40} \cdot 29H_2O$). Introduction of ZnO was carried out with different methods. Catalytic activity was determined in a bench-scale flow reactor unit in the hydrogenolysis of dibenzothiophene. ZnO modification of Al_2O_3 surface changes the morphology of NiMoW(S)/Al_2O_3 catalysts sulfide phases. Modification of Al_2O_3 with ZnO in amounts of 0.5-1.0 wt. %, followed by introduction of active phase precursors, increases DBT HDS activity from 38 to 54%. Impregnation of dried NiMoW/Al_2O_3 catalysts with solution of $Zn(CH_3COO)_2$ decreases the activity (the minimum of activity in this case was found for NiMoW/Al_2O_3 modified with 0.5 wt.% of ZnO). Parallel introduction of Zn, Ni, Mo and W decreases the catalysts activities in all cases.

II-PP121

Hydrotreating of Vacuum Gas Oil on NiMo/P-γ-Al_2O_3 Catalysts

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Modification of hydrotreating catalysts carrier was carried out with phosphoric acid water solution by wetness impregnation method (P_2O_5 content 0,5, 1, 2 and 5 wt. %), followed by draying and calcination. Modified carrier was impregnated with water solution of active phase precursors (Mo, Ni(Co)) on the second stage of synthesis. The optimum amount of P_2O_5 for modification of vacuum gas oil hydrotreating catalyst was found. The relationships between HDS, HYD PAH, HYD olefins and P_2O_5 content for NiMo/P-γ-Al_2O_3 catalysts were determinated. The maximum of HDS activity was found for catalyst, contained 2.0 wt. % of P_2O_5.

II-PP122

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Progress in the SAXS Study of Supported Metal Catalysts and Porous Composite Materials

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It has been proposed to use new masking liquids with a relatively low X-ray radiation absorption for SAXS study of complex materials. In presentation will be discussed prospects and restrictions of new technique, examples of their application to study some catalysts and porous composites. Using these liquids we achieved very good agreement between the SAXS and TEM data. The SAXS technique employing such masking liquids can be used as a quick analytical method for determining the particle size distributions of supported metals. Fluorocarbon liquids can eliminate the scattering signal from any support with the density of 2.8 g/cm^3 or less.

II-PP123

Silica Poisoning Effect on HDT Catalysts Processing Light Coker Naphtha

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γ-alumina-based HDT catalysts used as silicon traps adsorb more efficiently silicon compounds from naphtha till saturation, which occurs at a relatively low concentration (5-10 wt%). As the silicon content in the catalyst increases, the surface is progressively deactivated, mainly affecting the hydrodenitrogenation and hydrogenation activity. According to the aforementioned, the deactivation of HDT catalysts was investigated by means of a fraction of naphtha doped with silicone oil with different concentrations, which was used to contaminate the catalysts. The presence of silicon species was detected by ^{29}Si NMR and FTIR spectroscopies. The Si-O-Al formation was evidenced by the B/L ratio measured for the doped HDT catalysts. The results obtained for the deactivation of HDT catalysts exposed to high silicon contents show that this factor plays a major role in the loss of activity.

II-PP124

Optimizing the Controlled Synthesis of PVP-based Carbon Supported Ru Nanoparticles: Synthesis Approaches and Characterization

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Nowadays nanosized metal nanoparticles (NPs) attract a lot of attention due to their unique chemical and physical properties. In particular, a colloidal method based on immobilization of colloidal metal NPs over different types of supports is an effective alternative approach to the synthesis of supported metal catalysts with well-defined particles. The purpose of the current work is to explore regularities of ruthenium NPs formation via polyol reduction and to determine key parameters for the synthesis of Ru NPs with a controllable particle size allowing further preparation of heterogeneous catalysts for different catalytic application, e.g. aqueous phase reforming (APR) of bioderived sugar and sugar alcohols. Different strategies to prepare Ru NPs of different size with narrow particle size distribution were applied. The influence of synthesis variables, such as reduction conditions, microwave irradiation, the ratio between Ru and stabilizing agent (PVP), and the initial Ru concentration on the particle size was studied.

II-PP125

Sulfated Perfluoropolymer on Carbon Nanofibers Composites: Preparation, Acidity and Catalytic Activity in the Gas-Phase Benzene Nitration

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Sulfated perfluoropolymers supported on carbon nanofibers are shown to be active and stable catalysts for gas-phase benzene nitration. The best catalyst exhibits 99.9% selectivity to nitrobenzene with concentration of by-products (mainly nitrophenols) less than 300 ppm.

II-PP126

Characterization and Methane Dry Reforming Performance of CeO_2 Prepared by Modified Precipitation Route

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Cerium oxide catalysts for fuel cells application were synthesized via precipitation and modified precipitation routes where the effect of H_2O_2 and/or cetyltrimethylammonium bromide (CTAB) addition in the precipitation step has been investigated. Microstructure and reduction–reoxidation properties of the oxides were analyzed by XRD, Raman, TPR-H_2, TPR-CH_4 and TPO. The catalytic properties were investigated in dry reforming of methane between 750 and 900 °C under stoichiometric and oxidizing conditions. A material exploitable for applications in catalysis and solid oxide fuel cells (SOFCs) was obtained by modifying the precipitation route via the addition of H_2O_2 (CeO_2_H_2O_2). Compared to materials synthesized conventionally or by using CTAB, CeO_2_H_2O_2 exhibited the best thermal stability, least surface loss under high temperatures operation (e.g. 900 °C), superior stability with respect to bulk redox properties when alternating between oxidizing and reducing treatments, and highest catalytic activity and resistance to deposition of graphitic carbon.

II-PP127

Precisely Controlled Synthesis of PVP- Capped Ni and Co Metal Nanoparticles

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Colloidal Ni and Co nanoparticles were synthesized by a modified polyol method using sodium borohydride as a reducing agent. The influence of a gas atmosphere and a reduction temperature on nanoparticles formation was studied. A series of Co and Ni nanoparticles with the average particle sizes 1.8÷2.8 and 2.6÷9.8 nm were obtained, respectively, by varying synthesis conditions. Nanoparticle size was found to increase with the increase of the reduction temperature. The oxidative atmosphere was shown to favour nanoparticles growth as it was demonstrated in the case of nickel.

II-PP128

Syngas Production via Dry Reforming of Methane over $NiAl_xFe_{2-x}O_4$ Oxides: Synthesis, Characterization and Reactivity Study

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The reforming of methane to syngas using CO_2 instead of steam is an attractive route, including from the point of view of sustainability because it uses two greenhouse gases. Compared to noble metals, Ni-catalysts are cheap but very easily deactivated by coking. Ni-based mixed oxides structurally well-defined like perovskites and spinels are being studied because they possibly make solid solutions and allow to vary the composition and thus the catalytic properties. In this study, the textural, structural and catalytic properties of nickel ferrite aluminate samples prepared by coprecipitation method, using nitrates and chlorides salts as precursor, are presented.

II-PP129

Preparation of Cu Loaded Magnetic Nanoparticle Catalyst and Its Catalytic Activity for Degradation of Azo Dyes

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In this study, $Fe_3O_4@SiO_2$-*Cu* nanoparticles for catalytic reduction of azo dye pollutants are prepared. This nanoparticles exhibit enhanced catalytic reduction efficiency for azo dyes compared with those of pure *Cu* or Fe_3O_4 nanoparticles, and can also be rapidly separated from aqueous solution using a magnet. Synthesized magnetic nanoparticles were characterized by different techniques including X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared (FT-IR) spectroscopy and thermal analysis (TGA). The degradation efficiency was found to depend essentially on initial dye concentration, solution pH and the catalyst loading. Study of the catalytic activity of $Fe_3O_4@SiO_2$-*Cu* was conducted at the laboratory temperature.

II-PP130

The Photocatalytic Hydrogen Evolution by Alloyed CdTeS Nanocrystals

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In recent years, photocatalytic water splitting using solar energy has become a promising approach for clean, environmentally friendly and low-cost production of hydrogen. So far, numerous active semiconductor-based photocatalysts and their composites have been developed for the photocatalytic hydrogen production reactions because of their suitable physical and photochemical properties. In the present investigation, photocatalytic generation of hydrogen by using 3-mercaptopropionic acid capped CdTe and CdTeS alloy nanocrystals have been investigated under visible-light irradiation in the aqueous solution by using at the pH 4.65 ascorbic acid solution as a sacrificial electron donor and $CoCl_2.6H_2O$ as an artificial catalyst. The photocatalytic hydrogen evolution activities of CdTe and CdTeS alloy nanocrystals are contrasted. CdTeS alloy nanocrystals was found to display higher photocatalytic activity than the sole CdTe nanocrystals. More importantly, no noticeable decrease in the activity of CdTe and CdTeS alloy nanocrystals was observed during the photocatalytic hydrogen evolution for at least 12 h.

II-PP131

Ruthenium Nanoparticles Supported on Carbon – an Active Catalyst for the Hydrogenation of Lactic Acid to Form 1,2-Propane Diol

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The hydrogenation of lactic acid to 1,2-propanediol using a series of 5wt.% Ru/C. Catalysts prepared by standard impregnation using a range of carbon supports were compared with a catalyst obtained commercially. The catalysts were tested for their activity in an autoclave and characterised using XRD, TPR, TEM, XPS, and EXAFS. The support effect on the dispersion of the ruthenium nanoparticles is discussed.

II-PP132

First Principles Study of Oxygen Adsorption and Dissociation on Au-Ag Clusters in the Propylene Epoxidation Reaction

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The development of nanostructured catalysts of selective oxidation is of exceptional significance for science and chemical technology. It is generally accepted that gold is inert, however nanostructured gold exhibits high catalytic activity. The electronic properties of gold nanoparticles change with doping heteroatoms. Thus, if we replace one or more gold atoms by silver atoms, will we obtain synergetic effects in oxygen activation?

The main goal of our research is quantum chemical analysis of the structure and electronic properties of $Au_{20-x}Ag_x$ (x=0, 1, 4, 16, 19), and the simulation of the reaction of oxygen and the bimetallic clusters. Calculations are performed in the framework of DFT/PBE approach with relativistic all electron basis set, using supercomputer SKIF MSU "Chebyshev".

In the present work we considered tetrahedral Au_{20} and Ag_{20} clusters, their mono-doped analogs ($Au_{19}Ag$ and $Ag_{19}Au$), as well as core-shell clusters Au_4Ag_{16} and $Au_{16}Ag_4$. The stability and reactivity of these clusters are predicted by the calculation of IP, EA, E_b and HOMO−LUMO gap. With the increase of the silver content in the bimetallic Au−Ag clusters values of IP, EA, and HOMO−LUMO gap decrease. Silver tends to occupy the facet position in the bimetallic cluster and gold tends to occupy the apex position. Strong correlation between the cluster activity in oxygen activation and the content of silver atoms in cluster is observed. Oxygen activation and dissociation on Au−Ag clusters are more favorable on edge atoms.

II-PP135

The Effect of Hydrolysis Temperature on the Textural Properties of Nanoscale Rutile

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The effect of $TiCl_4$ hydrolysis temperature on the textural properties of the resulting rutile and on the changes of these properties upon calcination was studied. The mercury porosimetry, BET, SEM and TEM studies have revealed that nanoscale rutile obtained by thermolysis of titanium tetrachloride has a multi-level packing of the particles with a heterogeneous pore structure. Raising the temperature of rutile synthesis increases the fraction of mesopores and decreases the fraction of micro- and macropores in rutile samples. As shown by the textural study of the samples upon calcination in the temperature range of 100-1000°C, the temperature mode is the key factor that produces changes at different levels of the hierarchical system and determines features of the porous structure of nanoscale rutile.

II-PP136

Propene Epoxidation with Molecular Oxygen over Gold-Silver Catalysts: Density Functional Calculations

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Propylene oxide is important product in chemistry industry. Recently, considerable progress has been made in the epoxidation of propene with molecular oxygen over coinage metal catalysts such as Au and Ag.

The main goal of this study was to investigate of the structure of the active centre of the silver and gold-silver clusters on the reaction mechanism. We have performed DFT/PBE calculation with program PRIRODA.

As a model of clusters, we consider extra stable tetrahedral Ag_{20} and $Ag_{19}Au$ clusters containing one gold atom on the top, edge, or facet. Before the study of the reaction mechanism, we calculated propylene and oxygen adsorption on Ag_{20} and $Ag_{19}Au$ clusters. Simulation the pathway of propylene oxidation has shown that the reaction goes through the formation of a five-membered oxametallacycle consisting of two metal atoms and a −O−C−C− fragment and four-membered oxametallacycle including a single metal atom and −O−C− fragment.

II-PP137

A Comparative Study of Methanol Conversion to Light Olefins over SAPO-34 Prepared via Conventional and Ultrasound Assisted Hydrothermal Methods

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A comparative synthesis of SAPO-34 was carried out via conventional and ultrasound assisted hydrothermal methods and tested toward methanol conversion to light olefins. XRD patterns showed suitable crystalline structure of sonochemically synthesized SAPO-34 and its nanoscale structure. Catalytic performance tests of synthesized SAPO-34 toward methanol to light olefins conversion showed higher activity of sonochemically synthesized SAPO-34. Olefins yield of sonochemically synthesized SAPO-34 was higher than that of the conventional SAPO-34.

II-PP138

Stabilization of Transition Metal Ions in Unstable Oxidation State in the Matrix of Layered Double Hydroxides with the Structure of Hydrotalcite

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The present article is concerned with the study of systems of co-precipitated hydroxides of magnesium (II), aluminum (III) and nickel (III). Such systems may exhibit unusual redox, catalytic and other properties therefore their synthesis might be of interest.
LDHs containing Ni^{3+} ions in the structure of metal hydroxide layers were synthesised by co-precipitation from the aqueous solutions of mixtures of magnesium, aluminium and nickel salts in oxidizing media. Atomic ratio Al^{3+}:Ni^{3+}in the co-precipitated samples was varied in a wide range. The formation of single phase product was shown to be possible with a substitution of up to 25% aluminium ions for nickel in the structure of hydrotalcite. Thus the introduction of cations in the structure of hydrotalcite allows to stabilize them in unstable oxidation state.

II-PP139

Modeling the Mechanism of Surface Stages of Vapor Phase Catalytic Oxidation of 4-Methylpyridine

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Heterogeneous vapour phase catalytic oxidation of 4-methylpyridine is a new efficient and ecology friendly technology of isonicotinic acid (INA), feedstock for the synthesis of a number of antituberculosis drugs.
Kinetic calculations show that INA arises via stage of forming 4-pyridine carbaldehyde. Part of the acid is decarboxylated until pyridine. When water concentration increases the velocity constant of the aldehyde conversion into acid dramatically rises. Chemisorption on a catalyst's surface water creates the new acid centres capable to interact with heteroatom of nitrogen of a substratum.
The cluster approach and the program Gaussian-09 W were used to model both the 4-methylpyridine chemisorption on the vanadia catalysts surface. It is shown that the promotional effect of the modifier oxide on the vanadia catalytic activity is caused with increasing of nucleophilicity (proton affinity) of vanadium bonded oxygen and reduction enthalpy of deprotonation of the oxidized methyl group of the chemisorbed 4-methylpyridine.

II-PP140

Effect of the Preparation Method of Nano-Titanium Pyrophosphate on Catalytic Properties: The Conversion of n-Butane

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Titanium pyrophosphates are used in the conversion of n-butane. TiPO catalysts were prepared, by used several methods then characterized and tested in ODH of n-butane. Catalyst were characterized by X-ray diffraction, FTIR, DTA-TG, BET and TPD-NH_3, FESEM to characterise structural and textural surfaces properties. The effect of the preparation method in conversion of n-butane into butenes has been investigated.
The P:Ti ratios obtained from chemical analysis were close to the theoretical ones. Samples show low surface areas. The FTIR spectrum shows titanium pyrophosphate frequencies. In XRD spectra we identify the phase TiP_2O_7 (JCPDS 00-038-1468) in TiPO-2-A and TiPO-2-S samples. The DTA-TG curves show that samples are stable up 600°C. FE-SEM monographs show agglomerate spherical nanoparticles. The ODH reaction of n-butane gives the best yield (12.07) obtained over TiPO-2-S catalyst, with a conversion of 28.12% and selectivity of butenes 42.95%. The best performance is observed at 450 °C and for a reaction time (35 min). All catalysts are activated over time.

II-PP141

Relationship between Surface Acid/Base Sites of Solid Catalysts and Their Catalytic Activity in Biomass Derived Reactions

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The determination of the acid-base properties of solid catalysts in the same media as used during the catalytic reaction is fundamental to correlate the catalytic activity to the surface properties.
Correct evaluation of reliable experimental data from titration calorimetry for systems with well-defined initial state and with controlled addition of a base titrant results in differential heats of surface processes. Results allowed to discriminate the active acid sites of catalysts in water by their strength and to assess that their relative acid strength is changing with reaction medium (gas phase or liquid medium).
This work has well demonstrated that for reactions performed in water or any other liquid solvent the number and the strength of accessible acidic/basic sites can be different, depending strongly on the solvent-solid bondings.

II-PP142

Selective Hydrogenation of Phenylacetylene to Styrene over Pd-Fe/SiO_2 Effect of Catalyst Preparation

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Selective hydrogenation of alkynes to alkenes, without further reduction to alkanes, is of particular importance in the production of polymers. The Pd-Fe_3O_4/SiO_2 systems are known to be catalytically active and selective in the hydrogenation of phenylacetylene to styrene, yet alloyed Pd-Fe NPs exhibit a decrease in TOF as compared with Pd NPs. In this work, the catalysts were prepared by simultaneous or consecutive deposition of the metal precursors on the silica carriers followed by different thermal treatments. The XRD analysis revealed the formation of the Pd^0, α-Fe_2O_3, and Fe_3O_4 phases after calcination of the samples at 240–260ºC, as well as the Pd-rich alloys and the Fe^0 phase after reduction at 400ºC. The TPR analysis confirmed the strong interaction of Pd with Fe species and alloy formation. The catalytic behavior of the Pd-Fe/SiO_2 system is strongly dependent on the catalyst preparation variables that change the Pd particle size and Pd-Fe alloying.

II-PP143

Bimetallic PdRu Nanocatalysts for the Hydrogenation of Phenols

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Hybrid bimetallic catalyst based on the PdRu nanoparticles, encapsulated into cross-linked dendrimer networks, was synthesized using a co-complexation method. Mean particles size was 2-2.5 nm. The catalyst obtained was successfully tested in the hydrogenation of phenols. It was found out, that the presence of palladium in the alloy increased the selectivity on cyclohexanone in the hydrogenation of phenol. Replacement of phenol to more hydrophobic anisole and phenethole resulted in the drastical decrease in activity and in the formation of the hydrogenolysis (benzene, cyclohexane) and deoxygenation (phenol) products. Introducing the alkylic substituents to the aromatic ring of phenol also led to the decrease in conversion. The main reaction products were corresponding substituted derivates of cyclohexanol. The polar hydrophilic hydroquinone and resorcinol, vice versa, were converted faster than phenol.

II-PP144

Hybrid Bimetallic RhRu and PdRh Nanocatalysts: Synthesis and Application

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Hybrid bimetallic catalysts based on the PdRh and RhRu nanoparticles, stabilized by poly(propylene imine) (PPI) dendrimers, immobilized on the surface of the mesoporous silica, were synthesized. The hybrid support was prepared in two stages, including the modification of the dendrimer termini with silanol groups, following by the formation of the silica mesoporous structure in situ using sol-gel method. The synthesis of the bimetallic nanoparticles was carried out using a co-complexation method. Thus synthesized PdRh and RhRu catalyst were successfully tested in the hydrogenation of phenols. It was found out that both of the catalysts gave a selectivity on cyclohexanone near to 100% even at long reaction times and high catalyst loading. Using the hydrophobic anisole or phenethole instead of phenol led to the dramatic downfall in conversion and to the hydrogenolysis and deoxygenation by-products formation. Introducing the alkylic substituent into the aromatic ring of phenol also resulted in the decrease in activity in comparison with phenol. The activity of the RhRu catalyst in the alkyl-substituted phenols hydrogenation did not depend on the substrates size and geometry, whereas for PdRh decrease in activity with the substrate size increased was observed. Both of the catalyst synthesized showed high activity in the hydrogenation of polar hydroquinone and resorcinol, and poor activity for pyrocathechol with *ortho*-position for the hydroxylic groups.

II-PP145

Peroxocomplexes Contaning Rare Earth Elements as Effective Catalysts of Oxidation Reaction of Mono and Bicyclic Unsaturated Hydrocarbons with Hydrogene Peroxide

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A series of peroxotungsten and molybdenum complexes of rare earth elements (REE) (Gd, Nd, Pr, La) in the induced oxidation reaction of unsaturated hydrocarbons with cyclohexene and norbornene fragments was synthesized and studied.

II-PP146

Silver Modified MgNi/SiO_2 Catalysts for Vegetable Oil Hydrogenation

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A series of silver modified Mg-Ni materials with composition Mg/Ni = 0.1 and SiO_2/Ni = 1.15, differing in Ag content (Ag/Ni = 0.0025, 0.025 and 0.1) was prepared by precipitation-deposition on SiO_2 derived from water glass used as a silica support. The effects of silver content on the activity and the composition of the fatty acids obtained during the sunflower oil hydrogenation were studied. The catalyst with intermediate silver content (0.025AgNi) can be recommended as an appropriate for edible sunflower oil hydrogenation. This finding is based on the demonstrated high hydrogenation activity, high content of C18:1*cis* formation and low amounts of harmful for the human health C18:1*trans* and C18:0 fatty acids in the hydrogenated derivatives. The adjustment of the catalyst composition by careful changing the content of silver modifier offers a possibility to control the activity as well as the composition of the fatty acids in the hydrogenated edible oils.

II-PP147

New Insights on Active Sites of Key Catalyst Materials Using Microcalorimetry at Close to the Reaction Conditions

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Adsorption phenomena play an important role in heterogeneous catalysis because of the 1st step is the activation of the reacting molecules by adsorption. Knowledge about the heat of adsorption of reactant on the surface of a catalyst can contribute to a better understanding of complex microkinetics. Since perhaps only a minor fraction of all surface atoms form active centers, the determination of their number and strength requires a sensitive analytical method. We focus on adsorption microcalorimetry applied close to the reaction conditions.

In this work, we will demonstrate how structure-activity correlations can be established by combining microcalorimetry with electron microscopy and spectroscopic techniques, like IR and XPS. The power of these complementary methods will be illustrated by choosing the following examples:
(i) Propylene metathesis over MoOx/SBA-15 at 50°C,
(ii) Three-phase semi-hydrogenation of 1-hexyne over TiO_2-supported ceria at 80°C,
(iii) Carbon-based catalysts for oxidative dehydrogenation of propane or ethylbenzene.

With references:

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(ii) Three-phase semi-hydrogenation of 1-hexyne over TiO_2-supported ceria at 80°C
(iii) Carbon-based catalysts for oxidative dehydrogenation of propane or ethylbenzene

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II-PP148

Influence of Ruthenium Content in Co-Al Fischer-Tropsch Catalyst on Kinetics of Cobalt Reduction

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Cobalt-alumina Fischer-Tropsch catalysts prepared by DPU (deposition by precipitation during urea decomposition) method are highly active and have good C_{5+} selectivity. However the activation temperature is high for these catalysts exceeding 500^{o}C, which makes the activation procedure and equipment expensive. Introduction of tiny amount of noble metal facilitates cobalt reduction and decreases the required activation temperature. By this poster presentation we report the effect of ruthenium content on reduction behavior and kinetic parameters of Ru-promoted Co-Al catalyst as well as the catalytic activity and selectivity these catalysts in the Fischer-Tropsch synthesis. Addition of small amounts of Ru to alumina-supported cobalt catalysts significantly lowers the temperature of cobalt reduction. The promoted catalysts exhibit high catalytic activity and selectivity in the Fischer-Tropsch synthesis, which is comparable with unpromoted catalyst.

II-PP149

Novel Catalyst Supports with Lamellar and Hierarchical Porosity

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Aim of this work was to produce novel catalyst supports with different geometries (monoliths, cylinders or plates) and dimensions (up to 15 cm), with unidirectional lamellar macroporosity and fine interconnected mesoporosity by ice-templating of geopolymers. Geopolymers are mesoporous alkali-alumino-silicates, which are easily synthetized in aqueous medium, and in the ice-templating the dilution degree of the geopolymer was tailored. Ice-templated geopolymers had total porosities from 70 to 80 vol.%, lamellar pore width from 10 up to 250 µm, specific surface areas from 26 to 39 $m^2 g^{-1}$, depending on the starting dilution of the geopolymer slurries. Pore size distributions in the range 0.058-100 µm were bi-modal or tri-modal for low dilution and high dilution, respectively. Due to the alkali nature and textural features these supports may be used to prepare bifunctional catalysts and tests are in progress to assess the performances of these systems.

II-PP150

Synchrotron Based Operando Study of Structure Activity Relationships of Model Electrocatalysts for Water Splitting

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Solar hydrogen produced by (photo)electrochemical water splitting (PWS) is a promising alternative to conventional fossil energy resources. Mostly, photocatalysts are complex multicomponent semiconductor based systems. However, even the most active photocatalytic materials are not able to drive PWS without electrocatalyst due to interfacial energy losses. In order to design optimal electrocatalysts, structure-activity relationships are needed. Platinum as the best-performing and best-known H_2 evolution catalyst has thus been chosen as a model catalyst to setup a novel technique combination enabling to simultaneously track structural changes together with reaction products detection and electrochemical characterization.

II-PP151

The Problem of Correct Interpretation of Catalyst Acidity by the TPD NH_3 Curves

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The way the catalyst functions is determined by the specific genesis of the system, including formation and activation modes. Thus, the mere use of literature data on the individual components when considering the behavior of the composite in different experimental conditions can not be entirely correct. Thermal desorption of ammonia was registered (detector - TCD) after pretreatment of a granular catalyst and modeling compounds. Individual zeolites, γ-Al_2O_3, boehmite gel after acid treatment were activated similarly to the functioning catalysts. TPD curves are very similar for catalysts containing different zeolites (H-beta, mordenite, H-ZSM5, HY, Vegobond). The observed TPD curve peaks are determined not only by the desorption of ammonia, but also by the hydroxyl removal in the processes of phase transformations of aluminum oxide, formed from the binder or due to zeolite lattice destruction.

II-PP152

XPS Study of Au/C Model Samples Oxidation by NO_2

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The deposition of gold on the atomically smooth surface of HOPG results in the formation of 3D gold particles with the BE(Au $4f_{7/2}$) = 84.0 eV. The form of gold deposited on the surface activated with argon ions (HOPGA) depends on coverage Θ(Au). At low coverages, the deposition leads to the formation of isolated gold atoms. The atoms are stabilized on the graphite surface by chemical bonding with carbon with the formation of surface compounds Au-C_n. The 3D gold particles are resistant to oxidation with nitrogen dioxide at a pressure $3 \cdot 10^{-5}$ torr. The isolated atoms of gold under these conditions are oxidized to form the state Au(III) stabilized on the surface of graphite. The stabilized gold atoms may act as active sites of gold catalysts.

II-PP153

Effect of Chemical Composition on the Structural Peculiarities and Catalytic Behavior of Cu-Spinels in Water Gas Shift Reaction

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The effect of chemical composition and Fe/Cr (Fe/Al) ratio on the extent of spinel structure tetrahedral distortion and on distribution of cations between tetrahedral and octahedral positions was systematically studied. The correlation between distribution of copper ions and catalytic behavior in low temperature WGSR was experimentally confirmed.

II-PP154

Influence of Ag-CeO_2 Interfacial Interaction on Activity of Ag/CeO_2 Catalysts in Oxidative Reactions

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Catalytic activity of supported catalysts depends on both particle size of the active component and interaction between active component and support. Several strategies have been developed to control the interfacial interactions. It was shown that distribution of active component on support surface and their interaction depend on preparation method. It was shown that Ag/CeO_2 catalysts prepared by co-deposition had strong support-metal interaction expressed in epitaxy of silver on the ceria surface and more intensive simultaneous reduction of silver and cerium oxides in TPR. Weak interaction of silver clusters with ceria support was observer for catalyst prepared by impregnation method. The activity of supported small silver cluster in CO oxidation was higher in comparison with silver particles strongly bonded with ceria support.

II-PP155

Well-defined and Atomically Dispersed Supported Palladium Catalysts for Carbon-Carbon Coupling Reactions

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Surface organometallic chemistry techniques have been applied to prepare well defined palladium centres on the surface of silicon dioxide. Organometallic precursors with strongly basic alkyl ligands were reacted with a specifically pre-treated silica support. These immobilised and molecular active sites have been applied in model reactions such as catalytic carbon-carbon couplings of the Heck and Suzuki-Miyaura type. The catalysts are found to be highly active for the conversion of demanding substrates like aryl chlorides. The activity is proven to be due to palladium species dissolved into solution during the reaction. The single-site catalysts have been found to be very suitable model catalysts for the investigation of the correlation of reaction parameters, leaching phenomena and substrate conversion. The catalytic carbon-carbon coupling reaction of reasonable rate taking place at a supported molecular palladium centre can be excluded.

II-PP156

Synthesis and Redox Behavior of Oxide Supported Isolated Nickel Complexes

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Ni/SiO_2 catalysts prepared by techniques of surface organometallic chemistry exhibit unique properties due to their atomic dispersion. Single site catalysts are not only expected to be highly active in catalytic reactions, but also represent a group of ideal model catalysts. They help to gain a deeper understanding of molecular processes during catalytic reactions on the active sites. By grafting dimethyltris(trimethylphosphine)nickel on a defined silica surface, atomically dispersed nickel catalysts were obtained. The formation of isolated nickel centers was proven by means of solid state NMR, EPR and elemental analysis. Interestingly, isolated paramagnetic Ni^{I} species were found as proven by EPR and sharp NMR signals indicate the simultaneous presence of diamagnetic Ni^{II} species. Supporting experiments in solution were conducted to assess the redox properties of Ni in more detail. The apparent ability of oxidation state changes renders the grafted Ni complexes in particular a promising model for investigating the relation of the oxidation state and the catalytic activity on isolated metal centers in alkene oligomerization reactions.

II-PP157

Surface Composition of the Industrial Dehydration Alumina Catalyst

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Qualitative analysis (method – flame photometry) of the outer surface of the industrial dehydration catalysts of 1-phenylethanol to styrene showed the presence of the potassium and calcium – catalytic poisons for solid acids. Content of potassium and calcium at the surface of some catalysts samples is sufficiently high and reaches (in total) 60% of the sodium concentration.

II-PP158

Characterization of V-Al PILC Clay Surfaces after Modification by Cu-Zn Impregnation

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V-Al PILC clays, after modification by Cu-Zn impregnation, can be applied in the future for direct conversion of syngas to dimethyl ether (STD-process). V-Al PILC-supported Cu-Zn catalysts were prepared by the impregnation method using 5wt% and 10wt% of Cu and 5wt% Zn. These materials were analyzed by X-ray diffraction (XRD), energy dispersive spectroscopy (EDS), N_2 adsorption/desorption isotherms, temperature-programmed reduction (TPR) and X-ray absorption near edge structure (XANES). The acidity studies were performed using FTIR after pyridine adsorption. The 10%Cu 5%Zn V-Al PILC catalyst can be the most promising to STD-process, this is due the presence of Lewis and Brønsted acids sites and higher specific surface area and Cu^0 molar ratios.

II-PP159

Impact of the Additives on the Texture Properties of Re/γ-Al_2O_3 as Catalysts for Water-Gas Shift Reaction in the Presence of Sulphur-Containing Gases

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To our knowledge, alumina-supported Re-based catalysts have not yet been investigated in the water-gas shift (WGS) reaction conditions in the presence of S-containing gases. This promoted us to study the activity of Re/γ-Al_2O_3 system in the WGS reaction over preliminary sulphided samples, using Ni, Co and K as additives. The alkali character of K provokes a question about its effect on the pore texture of an amphoteric γ-Al_2O_3 support after addition as a second or third component. The present study provides information how the deposition of K, Ni and Co additives on Re/γ-Al_2O_3 affects the catalyst texture after the calcination procedure and after activity test in WGS reaction. Contrary to our expectations, introduction of K to calcined Re, NiRe and CoRe samples does not exert a strong impact on the primary mesopore texture of γ-Al_2O_3, and neither does addition of Co. Greatest changes in the catalyst texture are induced by Ni deposition.

II-PP160

Application of Sodium Octacarboxylate Resorcinarenes in Synthesis of Silver Nanoparticles

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In this work, we have demonstrated a method of synthesis of hybrid systems consisting of silver nanoparticles and amphiphilic resorcinarenes with alkyl ($C_{10}H_{21}$-CA), alkynyl ($C_{10}H_{19}$-CA) and ferrocene (Fc-CA) groups on the lower rim. The resorcinarenes prevent the aggregation of AgNPs and influence the size and shape of the silver nanoparticles produced. Catalytic properties of the hybride nanosystems Ag@CA were studied in the common used reaction of reduction of p-nitrophenol with sodium borohydride in water. The addition of 40 nanomole of Ag@CA rapidly accelerates the reaction, and it is finished in a few minutes.

II-PP161

A Theoretical Study on the Effect of Active Centers of SiO_2 Surface on O_2 Interaction with Small Supported Silver Clusters

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The effect of paramagnetic centers of silica surface - nonbridging oxygen (NBO) and silicon dangling bond (E) - on O_2 interaction with small Ag_n clusters (n=3,4) has been studied computationally using a density functional method and embedding of quantum-mechanical cluster in an elastic polarizable environment described by molecular mechanics. Molecular and dissociative adsorption of O_2 was analyzed. Electrostatic interaction of silver clusters with silica surface stabilizes O_2 adsorption forms. Adsorption of silver clusters at NBO defects results in their positive charging, whereas attaching to E centers keeps them neutral or slightly negative. As a consequence, activation barriers of O_2 dissociation on Ag_n/E site are notably lower. Still, the heights of activation barriers exceed O_2 desorption energies making O_2 dissociation on SiO_2 supported silver clusters, Ag_3 and Ag_4, less probable than O_2 desorption.

II-PP162

Hydroprocessing of Heavy Crude Oil

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This work explores the potential of transition metals like Co, Mo, Ni, W supported on Al_2O_3 as catalyst for the hydroprocessing of heavy oil. Four samples with different metals were incorporated into the alumina support by simultaneous impregnation and evaluated for upgrading of heavy Oil. Surface area, pore size distribution and metal contents in the catalysts were determined. The catalytic activity tests were carried out using heavy oil from Gulf of Mexico. The highest activity was observed with the CoMoNiWP /γ-Al_2O_3.

II-PP163

In-situ EPR Spectroscopy of the NH_3-SCR Mechanism of Copper Chabazite

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Selective Catalytic Reduction (SCR) using ammonia as the reducing agent is one of the most effective ways to reduce NO_x gasses emitted from combustion processes. The copper exchanged small pore zeolite; chabazite (CHA) have received increasing attention as a catalyst for this process due to its high activity and stability. Very recently a mechanism for the NH_3-SCR process catalyzed by Cu-CHA was proposed, with a key step involving the formation of a copper nitrate species. In this work *in-situ* EPR spectroscopy is used to identify steps of the NH_3-SCR mechanism. A Cu(II)-nitrate species is observed in a flow of nitrogen monoxide and oxygen, which disappears upon removal of oxygen in the flow. The EPR signal disappears in a flow of ammonia and nitrogen monoxide, which indicates an almost complete reduction of the copper, and thus loss of the EPR activity.

II-PP164

In Situ EMR / GC Study of the Conversion of Ethanol into Hydrocarbons on Fe-Zr/Al_2O_3 Catalysts

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In situ EMR under flow conditions and on-line GC analysis of gas-phase products were successfully used to study the conversion of ethanol over Fe-Zr/γ-Al2O3 catalyst. The conversion of ethanol on Fe-Zr/γ-Al2O3 catalysts leads to formation of ethane, propane, butane, pentane, hexane, benzene, toluene and xylene. The conversion of ethanol to aromatics increases as the Zr loading increases, which indicate that the active sites necessary for formation of aromatics is the Zr ion based structures. In the simultaneously recorded EMR spectra for these catalysts two different signals are observed: belong to ferromagnetic/super-paramagnetic FeOx for Fe/γ- Al2O3 (or their modified by Zr forms) catalysts with effective g-factor g=2.14-3.65 and line width ΔH=110-320 mT and paramagnetic carbon deposits with g=2.003 and ΔH= 0.5-0.7 mT. The formation of hydrocarbons is accompanied with the appearance of signals at g=2.14–2.15 in the EMR spectra. It was established that the catalytic activity of samples in ethanol to hydrocarbon conversion correlate with the concentration of magnetic particles and active catalyst are characterized with the symmetrical ESR signal, due to super-paramagnetic particles of the size 15-20nm. The Scherrer formula was used to evaluate from diffractogram the grain size of identified phases of active elements for this catalyst (35-45 nm). It is established that in the conversion of ethanol to hydrocarbons Zr active sites prefer the formation of aromatic compounds and FeOx species prefer the cracking reaction.

II-PP165

DFT Studies of Adsorbed N_2O and NH_3 on Pd(110)

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Structural, energetic and vibrational properties of N_2O and NH_3 molecules adsorbed on Pd(110)-1×2 surface has been studied by density functional theory. It was found that N_2O binds weakly to the ridge of the Pd(110)-1×2 surface in two on-top an two bridge stable forms, NH_3 adsorption occurs in two on-top forms: on the ridge and on the rows' side surface of the Pd(110)-1×2. Calculated binding energies are 0.31, 0.25, 0.23 eV for N_2O and 0.75, 0.70 eV for NH_3 adsorption. Adsorbed species are bound with the surface by terminal nitrogen atom of N_2O and nitrogen atom of NH_3.The geometry of N_2O and NH_3 is almost unchanged on adsorption.

II-PP166

Supporting Surfactant-hybridized $H_3PW_{12}O_{40}$ on TiO_2 to Obtain Highly Dispersed Entities for Acid Catalysis: the Undesired Coking Effect of Burning the Surfactant

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$H_3PW_{12}O_{40}$ was hybridized with a surfactant (dimethyldioctadecylammonium bromide – DODA) and subsequently impregnated on TiO_2 powder. According to the work of Raj *et al.* (2013) on the deposition of $H_3PW_{12}O_{40}$-DODA hybrids on HOPG surfaces, highly isolated $H_3PW_{12}O_{40}$ entities should be obtained once the surfactant is burnt. Indeed, the dispersion of $H_3PW_{12}O_{40}$ was higher within $H_3PW_{12}O_{40}/TiO_2$ samples prepared via this hybridization strategy than in the samples prepared via impregnation without a preliminary DODA-hybridization. However, the thermal treatments applied to burn the surfactant (exposure to UV/O_3, or calcination under pure O_2 at 290°C or 350°C) led to the formation of polyaromatic coke due to the superacidity of $H_3PW_{12}O_{40}$. The catalytic activity in methanol dehydration was then reduced. So, this study shows that although enhancing the dispersion thanks to a DODA-hybridization is possible, the strategy does finally not allow a better accessibility of $H_3PW_{12}O_{40}$'s acid sites because of an undesired coking effect.

II-PP167

Effect of Dopant Nature on Low-Temperature WGS Activity of Cu-Mn Spinel Oxide Catalysts Prepared by Combustion Method

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The aim of present work was to examine the effect of the nature of some doping oxides, namely, CeO_2, Fe_2O_3 and Al_2O_3 on the physicochemical properties and activity of Cu-Mn spinel oxides in the water-gas shift reaction (WGSR) at low temperature. Doped Cu-Mn-M catalysts with Cu/(Cu+Mn+M) atomic ratio of 0.30 were prepared by single-step urea-combustion method. The catalysts were characterized by N_2 physisorption, XRD, H_2-TPR and XPS. The WGS activity was evaluated in a conventional flow reactor within a temperature range of 140–240 °C. The influence of reaction gas mixture, including idealized and realistic reformate, H_2O/CO ratio and contact time on the activity were investigated. It was found that the doping of Cu-Mn spinel oxide catalysts prepared by combustion method could be an efficient approach for design of novel, highly active and stable WGS catalysts.

II-PP168

Catalytic Dehydration of Methyl Lactate to Acrylic Acid

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Calcium-phosphate-silica catalysts of methyl lactate dehydration to acrylates were investigated. The optimum ratio '$Ca\text{-}PO_x/SiO_2$' was found. Changes in the structure of the calcium phosphate component of the catalyst during operation and regeneration was studied.

II-PP169

Synthesis of Zr-BEC Zeolite Catalyst with Strong Lewis Acidity

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In past decade, use of germanium as a silicon substituent in zeolite synthesis led to a discovery of new large-pore molecular sieves structures. One of them is the polymorph C of zeolite Beta (BEC). But unfortunately, the use of such materials is strongly limited due to their low catalytic activity and poor thermal stability, because of strong tendency of Ge-O-Si bonds to hydrolyze. These drawbacks can be overcome by the replacement of Ge atoms in the framework with other atoms. This contribution is aimed to elaborate post-synthetic method to incorporate Zr in framework of BEC. Direct treatment with $ZrOCl_2$ aqueous and DMSO solutions was unsuccessful. Two-step procedure consists of following stages was more useful: 1) partial stabilization of parent structure via solvotermal treatment with TEOS; 2) incorporation of Z-heteroatom. According to XRD analysis, Zr-BEC obtained was highly crystalline, thermally stable material. According to FTIR spectra of adsorbed CO and acetonitrile-d_3, Zr-BEC possessing strong Lewis acidity, higher that traditional Zr-BEA.

II-PP170

Bimetallic Copper Catalysts Supported on Activated Carbon Fibers for Ethanol Dehydrogenation

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Ethanol is a renewable material which when dehydrogenated produces high purity hydrogen and acetaldehyde. In this work bimetal catalysts Cu-Cr and Cu-Zr supported on activated carbon fibers (ACF) were tested in the process of ethanol conversion. According SEM analysis both Cr and Zr formed a kind of oxide film on the surface of the carrier with Cu particles supported in it. The activity test results show that ethanol conversion upon Cu-Cr/ACF is higher compared with Cu/ACF, while addition of Zr leads to considerable decrease in activity.

II-PP171

Oxidative Activation of Methane over MnNaW/SiO$_2$ Catalysts: Models for Active Sites

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The oxidative coupling of methane (OCM) is a promising process for direct production of ethane and ethylene. In the present study quantum-chemical modeling of the active center of MnNaW/SiO$_2$ catalyst were performed at the B3LYP level using the LANL2TZ(F) and 6-311G basis sets for tungsten and lighter atoms, respectively. The optimization of mono- and polynuclear W and Mn species on the surface of α-cristobalite has been performed and values of barrier energy for the abstraction of hydrogen from methane were determined. The barriers of the methane dissociation at oxo-centers of closed-shell configuration provided by the W(+4) and W(+6) species on α-cristobalite are 40-70 kcal/mol. The barrier of C-H activation drops to about 5 kcal/mol for WO(OH)$_4^+$ model center where oxygen center possesses radical character. It is proposed that the true OCM active center is that associated with Mn (+5) complex having terminal oxygen ligand with a radical character.

II-PP172

The Investigation of Structure of Biocatalyst Used in the Vegetable Oils Transesterification

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In this work the biocatalysts on the base of lipase immobilized on the surface of MNPs modified by sodium citrate and aminopropyltrietoxysilane were synthesized. The comparative characterization of the synthesized biocatalysts was done using FTIR spectroscopy.

The data obtained in the work devoted to the formation of active and stable biocatalysts used in the vegetable oils transesterification reaction shows the great prospective. The pancreatic lipase immobilization on the modified surface of MNPs passes through the covalent bonds that provides high stability of biocatalysts in supercritical CO$_2$ media.

II-PP173

Enlargement of the Surface Area of Highly Porous Catalysts

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In this paper, method of polyurethane matrix replication was used for the production of highly porous cellular material. The technology involves thermal decomposition of polyurethane foam structure after its soaking in ceramic slurry. By varying the composition of slurry a new catalytic system with extended surface area can be obtained. The advantages of porous catalysts are large surface area and high permeability for gas and liquid flow, which results in high rates of mass and heat transfer.

I II-PP174

CO Oxidation on the Bimetallic Pd-Au/HOPG Catalysts: in-situ XPS and MS Investigation

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Combination of XPS and STM have been used to study the formation of Pd-Au bimetallic particles with controlled size and Au:Pd atomic ratio supported on Highly Oriented Pyrolytic Graphite. Then using the in-situ XPS and MS techniques the prepared Pd-Au/HOPG samples have been investigated in CO oxidation reaction. It has been shown that the Au/Pd atomic ratio varies together with activity in CO oxidation.

II-PP175

Reduction of Catalysts Based on Mn-Zr Oxides: In situ XPS and XRD Study

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A series of catalysts based on mixed Mn-Zr oxides have been prepared by coprecipitation of nitrates. At low Mn/Zr ratios, the catalysts are single-phase solid solutions ($Mn_yZr_{1-y}O_2$) based on a ZrO_2 structure. An increase in the Mn content leads to an increase in the number of Mn cations in the structure of the solid solutions, but a part of manganese form Mn_2O_3 and Mn_3O_4 in crystalline and amorphous states. Reduction of these catalysts with hydrogen was studied by a TPR, in situ XRD, and XPS. The reduction of the solid solutions proceeds via two stages. During the first stage, between 100 and 500°C, Mn cations incorporated into $Mn_yZr_{1-y}O_{2-\delta}$ undergo partial reduction. During the second stage, at temperatures between 500 and 700°C, Mn cations segregate on the surface of the solid solution. In the catalysts with high Mn/Zr ratios, the reduction of manganese oxide was observed: $Mn_2O_3 \rightarrow Mn_3O_4 \rightarrow MnO$.

II-PP176

Ionic Liquid Supported on Diatomic Powder as Catalist of Benzene Alkylation with 1-octene

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Texture characteristics of the ionic liquid applied to the diatomite powder were determined. It was shown that increasing the content of ioniq liquid in the initial mixture leads to decreasing the total pore volume and specific surface of the catalyst. Found that the ionic liquid applied to the diatomite powder in a weight ratio of 20:80 has the catalytic activity in the alkylation process of benzene by 1-octene.

II-PP177

Influence of Acid-Base Characteristics of the Alumina on Properties of the Supported Palladium Particles and Their Catalytic Activity

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The supported palladium catalysts are widely used in large industrial processes of hydrogenation of unsaturated hydrocarbon compounds. During of the experiment was investigated the influence of acidic characteristics of alumina support on the performances of the catalysts for the selective hydrogenation of acetylene and diene compounds. For this purpose samples of catalysts were synthesized on the different supports. Aluminum hydroxide was treated with acetic, oxalic or citric acids, and then calcined at a temperature of 550 ^{0}C. Studies showed that modification of the support by weak acids leads to changes in texture characteristics and increasing surface acidity of the alumina. This is accompanied by an increase of conversion of 1,3-butadiene and a slight decrease in selectivity to 1-butene.

II-PP178

Genesis of HDT Catalysts Prepared with the Use of Co_2Mo_{10}HPA and Cobalt Citrate: Study of Their Gas and Liquid Phase Sulfidation

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Genesis of alumina supported hydrotreating (HDT) catalysts prepared with the use of decamolybdodicobaltate heteropolyanion and cobalt citrate during their sulfidation processes and deactivation in diesel HDT has been investigated. The sulfidation stage was studied for two procedures: gas phase sulfidation by H_2S/H_2 and liquid phase treatment by a mixture of dimethyldisulfide in diesel at various temperatures and durations. Mechanisms of the active phase formation in the course of gas and liquid phase sulfidation processes have been established. It was found that gas phase sulfidation led to formation of the CoMoS active phase with higher cobalt content comparing to liquid sulfidation of the catalyst and initial activity of the gas phase treated catalysts in diesel HDT was also higher than catalysts subjected to liquid sulfidation. Catalytic examination after accelerated deactivation conditions showed that the liquid phase sulfided sample was more resistant to the deactivation.

II-PP181

Isomerization of Light Hydrocarbons over the ZSM-5 Zeolites

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The aim of this work is to investigate the catalytic activity and stability of the pentasil zeolite with the silica modulus 40 and its nickel-containing analog in the course of a hydrogen-free isomerization of C_5-C_8 n-alkanes and straight-run gasoline oil fraction. The use of different types of hydrocarbons in the course of isomerization of unmodified and nickel-containing ZSM-5 zeolites allowed to reveal the main trends in the distribution of the reaction products and to determine the optimal reaction conditions for the formation of the maximum amount of iso-alkanes and the minimum amount of coke.

II-PP182

A GGA+U DFT Investigation of Silver Atom, Trimer and Tetramer Supported by a Nanosized Particle $Ce_{21}O_{42}$

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Active sites on surface of nanosized cerium oxide particles are characterized by considering DFT GGA+U models of monomer, trimer and tetramer silver species on a $Ce_{21}O_{42}$ cluster. The effect of support on these TM species is quantified via adsorption O_2 probe molecule. On interaction with surface represented by small (111) and (100) facets as well as edge sites at their intersections Ag_n moieties are oxidized. Ag and Ag_3 adsorbates donate to the substrate particle one electron each. Ag_4 clusters in rhombus and tetrahedron configurations donate one and two electrons, respectively. Most stable $Ag_n/Ce_{21}O_{42}$ complexes are formed for adsorption on (100) facets, via interaction with O^{2c} atoms. The binding (adsorption) energies of Ag, Ag_3 and Ag_4 are calculated to 2.2, 2.9 and 3.0 eV, respectively. Binding of O_2 molecule on supported silver species are strongly dependent on the nature of supporting surface site varying in range of 0,2 - 1.5 eV.

II-PP183

Quantum-Chemical Investigation Ligand-Stabilized Gold Clusters in Oxidation Reaction

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In the past decades, metal nanoparticles with core sizes in the range of 1–100 nm have attracted a great deal of attention because of their significantly unusual properties different from those of the bulk materials and molecular compounds, as well as the diverse potential applications in nanoscale devices, catalysis, nanoelectronics, data storage, molecular imaging, biosensors and nanomedicine. Ligand-protected gold nanoclusters have been widely studied due to their interesting optical, electronic, and charging properties. However, the knowledge of ligands'structures is very limited due to the insufficient information of their single crystal structures.

We have analyzed the structural stability and electronic properties of the recently reported structurally known tetranucleargold cluster with phosphine ligands- $Au_4[P(CH_3)_2PCH_3(CH_2)_2P(CH_3)_2]_2^q$(q=+2, -2, 0), by using density functional theory. We have optimized the geometry of the cluster with different charges and we have investigated the adsorption and dissociation of oxygen on the cluster.

II-PP184

Preparation Approach to the Control of Rhodium Dispersion for TiO_2 and Al_2O_3 Supported Catalysts

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Preparation methods for size selective synthesis of supported rhodium nanoparticles were developed. It was shown that the nature of rhodium precursors, calcination temperature and support modification may significantly effect on the sizes of rhodium nanoparticles. All supported rhodium catalysts are very active in heterogeneous hydrogenation of unsaturated gaseous compounds and lead to formation of strong polarization when parahydrogen was used.

II-PP185

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The Nature of Carbon Supports Action on the Palladium Electronic State and Catalytic Properties

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The correlation of the Pd catalysts activity in CO oxidation reaction and forbidden band width of the carbon supports was determined. Catalytic activity also correlated with electron deficiency metal Pd nanoparticles. Nanoparticles with greater electron deficiency are more active.

II-PP186

Mössbauer Spectroscopy Investigation of Iron-Cerium Oxide Systems as Catalyst in the Reaction of the Methylbutene Dehydrogenation

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Samples of iron oxide and iron-cerium oxide systems as catalysts for the dehydrogenation reaction of methylbutenes are studied by Mössbauer spectroscopy method. In case of magnetite the yield of isoprene for decomposed hydrocarbons (YD) is 77%. The introduction of cerium into the magnetite composition increases the selectivity of catalyst, i.e. YD to 84%. During the catalytic reaction in oxide system conversion from α-Fe_2O_3 to Fe_3O_4 like system occurs which is attended with the changes in A and B positions populations in the spinel structure in the direction of S_A / S_B ratio increasing with respect to the initial magnetite.

II-PP187

EPR and DFT Study of the Oxygen Radicals Formation on Oxide Surfaces due to Homolytic Splitting of Water

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MgO illumination by UV light in the presence of N_2O was shown to result in the formation of spectroscopically indistinguishable O^- radicals both on electron and hole sites. Chemical properties of the O^- radicals formed on the electron and hole sites in reactions with O_2, CO and ethylene were found to be the same as well. This is possible only if these species are formed by the transfer of uncharged radical species formed from homolytic splitting of water. Our DFT simulations show that the oxygen radicals O^- obtained after UV-illumination and O^- produced due to N_2O decomposition on electron-rich site are identical in the model where surface electron and hole sites are formed due to the homolytic splitting of water. According to quantum-chemical simulations, the homolytic water dissociation on the oxide surface has the energetic barrier 2.75-3.39 eV, depending on the nature of radical stabilization sites.

II-PP188

Design of Novel Copper(I) Complexes of Pyridyl Substituted 1,5-Diaza-3,7-Diphosphacyclooctanes

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The row of novel copper(I) complexes of 1,5-diaza-3,7-diphosphacyclooctanes with pyridyl functions on the phosphorus atoms was synthesized. The ligands with pyridyl groups directly linked to phosphorus atoms demonstrate a variety of coordination modes, which depends on the sterical effects of the ligand. Aminomethylphosphines with pyridyl groups linked with phosphorus atoms by ethylene spacer form bis-P,N-chelate complexes with copper(I). All obtained complexes have additional donor and basic centers and are perspective catalysts for amination reactions.

II-PP189

SiO_2 Modified with ZrO_2 as a Complex Support for Cr-containing Catalysts for Dehydrogenation of Hydrocarbons

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The aim of this work is to study the distribution of zirconia modifier and CrO_x on the surface of silica and activity of prepared Cr-containing catalysts in the isobutane dehydrogenation. Silica with wide mesopores (10-50 nm) was used as a primary support, providing the desired porous structure of catalyst, while zirconium oxides were used as a secondary support, providing the required functional properties for active component stabilization. It was shown that complex ZrO_2/SiO_2 supports with high specific surface area and porosity may be prepared by simple impregnation technique and used as supports for Cr-containing catalyst. Elevated activity of $Cr/ZrO_2/SiO_2$ catalysts is associated with increasing of amount of Cr(VI) species stabilized by ZrO_2 surface.

II-PP190

Rh-CeO_2-Al_2O_3 Catalysts for the Partial Oxidation of Methane

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The role of Ce content on chemical-physical and catalytic properties of coprecipitated Rh-CeO_2-Al_2O_3 catalysts for the Catalytic Partial Oxidation of natural gas to syngas was investigated. A low Rh loading was used (0.25 wt.% Rh) and the amount of Ce was varied from 0, 5, 10 and 20 wt.%.

CeO_2 was dispersed in Al_2O_3 modifying the surface area, Rh dispersion, γ-Al_2O_3 stability and catalytic performances. The high dispersion of Rh in Rh-Al_2O_3 was kept by adding a 5 wt.% Ce, and an active and stable catalyst was obtained. Unlike for Rh-Al_2O_3 catalyst, neither carbon deposits nor the formation of α-Al_2O_3 occurred when Ce was added to the formulation. Contrarily, a further increase in the Ce loading decreased the Rh dispersion, catalyst surface area and hence the conversion of CH_4, syngas production and stability with time-on-stream. Moreover, after tests the sinterization and formation of well-crystallized $CeAlO_3$ were observed.

II-PP191

Stereoselective Conversion of 14-Membered to 7-Membered Cyclic Aminomethylphosphines – a New Route to Ni(II) Electrocatalysts of Hydrogen Transformation

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The condensation reaction of bis(phenylphosphino)ethane, paraformaldehyde and *iso*-propylamine leads to the formation of 14-membered cyclic aminomethylphosphine. In the solution this macrocycle undergoes nearly quantitative interconversion to 1-aza-3,6-diphosphacycloheptanes. In the acidic medium the rate of the interconversion reaction increases in several times. The reactions of the resulted 7-membered cyclic aminomethylphosphine with the Ni(II) salts give the desired bis-P,P-chelate complexes; their structures are similar to that of the most effective catalysts for the electrochemical hydrogen transformation.

II-PP192

Core/shell and Hollow Metal-Oxide Nanoparticles Supported on ZSM-5: Synthesis and Properties

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Current communication is devoted to study of oxidation processes of metal (Cu, Ni, Co) nanoparticles supported on ZSM-5 zeolite, aiming to find correlation between structures of metal-oxide particles, such as core/shell, hollow and bulk, and oxidation conditions. TPR-H_2, XRD in situ, HRTEM, XPS with sample pretreatment in high-pressure cell, UV-Vis DR, and the optical spectra modeling were used to confirm the hypothesis about structure of metal-oxide particles. CO and NO oxidation as well as NO SCR by propane were employed to examine catalytic characteristics of different metal-oxide particles.

Nanoscale Kirkendall effect was shown to be reveal at low-temperature oxidation of Cu and Ni nanoparticles and at high-temperature oxidation of Co. Hollow metal-oxide nanoparticles are formed from core/shell particles containing the 3-5 nm oxide layer on surface of 10-20 nm metal particle due to different diffusion coefficients.

The core/shell, hollow and bulk metal-oxide particles have different optical, redox and catalytic properties.

II-PP193

The Synthesis and Characterization of Co Nanoparticles Supported on Multi-Wall Carbon Nanotubes for Catalytic Applications

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Co-containing samples with different concentrations were prepared by impregnation of MWCNTs with the aqua solutions of Co (II) salts followed by calcination under an inert atmosphere and reduction in a stream of hydrogen. The obtained samples were characterized by TEM and internal field ^{59}Co NMR. It was found that the variation of the deposition condition provides the cobalt particles both inside the internal channels of the tubes and on the external surface. Co particles inside the channels of MWCNTs have an elongated and rounded shape and the average diameter of 2–3 nm. IF ^{59}Co NMR gives five different types of metallic Co particles. The increase of Co concentration leads to the decrease in the relative content of Co in a cubic stacking, resulting the increase of the HCP/FCC ratio from 1.0 to 1.7. The increase of the portion of magnetic domain walls of HCP suggests the presence of elongated particles up to 100 nm inside the MWCNTs.

II-PP194

Gallium Oxides Catalysts for Light Paraffins Conversion

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This work is devoted to the study of propane dehydrogenation in the absence and presence of CO_2 over Ga catalysts were prepared by wet impregnation of silicagel (5.0-40.0 wt.%Ga) from water solutions of gallium nitrates and direct one-pot synthesis embedding Ga species in the siliceous mesoporous framework of MCM-41(1,0-3.0 wt.%Ga). Catalysts were investigated by XRD, TPR-H_2, FTIR and BET-methods. Long-duration tests of catalysts were carried out in a flow reactor at 600°C. Unstationary phenomena were investigated using the transient response method. Results of investigations on propane dehydrogenation in the presence of CO_2 over studied catalysts showed that Ga-MCM catalysts demonstrate more high specific activity and stability in propene formation than impregnated catalysts. Besides, one-pot catalysts are characterized by low coke formation what is connected with high dispersity of active phase what decreases the possibility of oligomerization for adsorbed olefins. Data on complex investigation showed that CO_2 is adsorbed strongly and prevents with propane adsorption what results in a decrease of olefin yield. Because of, the use of CO_2 at paraffin dehydrogenation must be limited.

II-PP195

Synthesis and Catalytic Activity of the Polymer-Stabilized Palladium Nanoparticles

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In this work, we will demonstrate a new method for production hybrid nanomaterials using electroactive polymer rnanoparticles *p*(MVCA-*co*-St). Hybrid nanomaterials were obtained by the soft reduction of $PdCl_4^{2-}$ localized on the surface polymer rnanoparticles, to form of Pd^0 nanoparticles clusters (Pd@*p*(MVCA-*co*-St)). The shape, structure and stability of the hybrid clusters Pd@*p*(MVCA-*co*-St) will be discussed. Catalytic reduction of *p*-nitrophenol with $NaBH_4$, which can be easily monitored by UV–vis spectrophotometry, demonstrates that the nanoparticles are highly catalytically active. Six nanomoles of palladium in Pd@*p*(MVCA-*co*-St) is enough for the completely reduction of *p*-nitrophenol during 10-15 minutes. In the future, we plan to use this catalytic reactors in other reactions.

II-PP196

Cu(111) Chlorination on Atomic Scale: Adsorption, Diffusion, and Desorption

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In heterogeneous catalysis, 3d metals are often used as catalysts and halocarbons - as promoters. After dissociation of adsorbed halocarbon molecules, all steps of surface transformations for molecule radicals and halogens are needed to understand. In particular, halogens desorption process is rather interesting. For copper as catalyst and for chlorine as promoter, we have contradictory information about desorption process. Taking into account that chlorinated cooper surface is catalyst in 1,2-dichloroethane production as a part of industrial oxychlorination reaction, the resolution of this contradiction is important.

We have computationally studied the reaction of cooper chlorination on ideal and defective (111) surface. As a result, we obtain a consistent theoretical description of the whole reaction that allows us to make following conclusions: Cl2 dissociation occurs spontaneously; Cl atoms prefer to be adsorbed at step edges; Cl atoms easily diffuse on surface via bridge positions; CuCl molecules are desorbed species; CuCl molecules are desorbed from step edges.

II-PP197

Combustion Synthesis of Perovskites from Solid Organometallic Glycine-Based Precursors

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New organometallic glycine-based complex precursors of perovskites (ABO_3, A_2BO_4) have been synthesized and their combustion has been carried out in two regimes: the volume combustion synthesis (VCS) and the self-propagating high-temperature synthesis (SHS). Phase composition of the combustion products has been studied by a set of physicochemical methods (IR, XRD, TEM HR and etc.). It was shown that the composition of perovskite precursors and the applied combustion regime are the most significant factors determining the process of their decomposition. It was found that in the SHS regime the perovskite content in the combustion product was as high as 90% without the additional energy-consuming calcination. The observed phase homogeneity and high crystallinity degree of the resulting perovskites may indicate that a higher combustion temperature has been reached in the SHS regime.

II-PP198

The Characterization of Ziegler Type Ti-based Catalysts of Ethylene Polymerization by XPS

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Method of XPS along with other methods of research of a surface of catalytic system, naturally, at presence of the "dry" boxing combined with a spectrometer, can be useful to studying of a surface of various supports and processes of formation of the predecessor of an active component polymerization catalysts at interaction of titanium compounds with these supports, and composition and surface structure of the active centers of the catalysts, uniformity of distribution of connection of transitive metal on depth of a granule of the catalyst, and also about degree of oxidation of the supported titanium.

II-PP199

New Possibility for Investigation of Supported Pt/$MgAlO_x$ Catalysts by XPS with Use of Monochromatic AgL_α Irradiation

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The capabilities of XPS to study heterogeneous catalysts are severely restricted for supported Pt/$MgAlO_x$ catalysts. When XPS spectra from these catalysts are taken with the standard AlKα or MgKα irradiations, the Pt4f doublet line is masked by a strong Al2p line as well as by the additive lines-satellites from Mg2s line. A possible solution of this problem could be the use of AgLα irradiation with the photon energy of 2984.3 eV for excitation of $Pt3d_{5/2}$ and Al1s lines.

AgLa irradiation is an useful tool for investigation of supported Pt-alumina catalysts. The values of $Pt3d_{5/2}$ binding energy can be used for determination of the oxidation state of platinum in supported Pt/$MgAlO_x$ catalysts and other systems containing both platinum and aluminum.

II-PP200

Modeling and Optimization of Sol-Gel Process Parameters to Synthesize Nanostructured Boria-Alumina Catalyst Supports: Response Surface Methodology Approach

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Recently, nanostructured metal oxides as catalyst support materials have gained much attention for their unique physicochemical properties. Alumina-based mesoporous materials are well suited catalytic materials. Boria-alumina mixed oxides have been considered as important acid catalysts in many industrial applications. The design, synthesis and modification of binary oxide materials need to be well controlled. For this purpose, the sol-gel route seems convenient since it allows the formation of the active phase directly in the catalyst lattice.

In this study, a sol-gel process was used to prepare mesoporous B_2O_3-Al_2O_3 supports. Response surface methodology (RSM) has been studied in order to optimize the process variables. For the characterization of sol-gel prepared binary oxide supporting materials XRD, BET, FTIR, TPD, SEM and TEM techniques were used.

It was concluded that the addition of boria to the alumina support at low hydrolysis ratio was increasing total surface area by effecting the pore structure slightly.

II-PP201

Investigation of the Microstructure Features of the Solid Solutions $La_{1-x}Ca_xCoO_{3-\delta}$ in Different Gas Environment

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HRTEM and XRD methods are used to study the microstructure of $La_{1-x}Ca_xCoO_{3-\delta}$ perovskite-like oxides synthesized by pyrolysis of polymerized complex precursor in different gas environment. The XRD data show that the samples studied are single-phase solid solutions for $x \le 0.5$. In situ heating of samples up to 900°C in air does not lead to noticeable changes in the samples structure, which indicates their high thermal stability. Heating in vacuum up to 900°C leads to partial decomposition of the samples. After methane oxidation reaction the formation of planar defects and metal oxide nanoparticles on the surface of perovskite, which occurs under the reaction conditions was shown. Also formation of alternating perovskite – brownmillerite layers in reaction condition was shown by HRTEM data.

II-PP202

Deactivation Mechanism of Molybdenum Catalysts

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Molybdenum catalysts, synthesized on metal molybdenum, organic hydroperoxides and hydrogen peroxide, are studied. It is established that at temperatures close to working temperatures in the industrial reactor of epoxidation of GPEB propylene (110 ºC), there is a fast decrease in the content of the dissolved molybdenum in catalysts. Experimentally it is proved, that the deactivation of molybdenum catalysts begins with homolytic decomposition. The scheme of catalyst deactivation mechanism is offered.

II-PP203

Plasma-arc Synthesis of PdCeSnC Composites for Preparation of Highly Active Pd/CeO_2-SnO_2 Catalysts for Low-Temperature CO Oxidation

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The plasma-arc method was applied to synthesize the PdCeC and PdCeSnC composites which can be effectively used as precursors for preparation of Pd/CeO_2 and Pd/CeO_2-SnO_2 catalysts with high activity in CO oxidation reaction. The obtained Pd-ceria based catalysts modified with tin represent a very promising catalytic system, which has a unique combination of high thermal stability and activity in CO oxidation starting at low temperatures.

II-PP204

Catalytic Performance of MFI Zeolite Synthesized with Cetyltrimethylammonium Cation as SDA

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In this study it was evaluated the performance of cetiltrimethylammonium bromide surfactant ($C_{16}H_{33}N^{+}(CH_3)_3Br^{-}$) as zeolitic structure-directing agent (SDA) to obtain MFI zeolite. The X-ray diffactometry (XRD) results showed the MFI structure formation. The zeolitic materials showed catalytic activity in the transesterification reaction of ethyl acetate with metanol and the loss of catalytic activity is associated with leaching of cetiltrimethylammonium cations.

II-PP205

New High Porosity Endogas Production Catalyst on Foam Substrate for Low-Carbon Steel Heat Treatment

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This article was written by Dmitriy Fotin, PhD, Chief Process Engineer of ECAT Company. It gives an overview of production and performance tests of new high porosity endogas production catalyst on foam substrate intended for low-carbon steel heat treatment.

II-PP206

Spherical Aluminum Oxide for Synthesis of Supported Catalysts

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Spherical alumina are widely used in chemical and petrochemical industry as an adsorbent, desiccant, media and catalyst for various processes. Spherical catalyst has an optimum range in size, provides the most dense packing of grains has a maximum ratio of volume to external surface of the grain. It has a maximum surface loading. Upon receipt of spherical granules distributed way using hydrocarbon-ammonia or liquid molding processes, including chemical peptization pseudoboehmite hydrogel (PB), and the coagulation of droplets pepsirefresh PB. This technology is versatile and productive, guarantees of phase and structural uniformity of spherical granules, allows to carry out the process continuously, that is rational in heavy industries. In this work was done a method for producing spherical granules Al_2O_3 by sol-gel transition peptized pseudoboehmite alumina hydroxide, and the introduction of the active catalyst component in the step of coagulation; properties of the synthesized samples correspond to the optimum values for this type of catalysts.

II-PP207

In-situ XPS Study of Active Component of Pd/Al_2O_3 Catalysts in Total CH_4 Oxidation

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Active component of 1%Pd/Al_2IO_3 catalysts in CH_4 oxidation have been studied using *in-situ* XPS and mass-spectrometry. Samples with close particle size (4-5 nm) but different initial state of Pd (metal or oxidic) were chosen to reveal the state of active component under the reaction conditions. It was shown that mixed metal-oxide state of Pd characterized by E_b = 335.8 eV forms on the surface of samples under reaction conditions (O_2 / CH_4 = 4/1, P = 0.02 mbar, T = 430 ^{o}C) independently of the initial state of Pd in as prepared samples. Ratio between Pd^0 and PdO therein depends on both temperature and O_2 to CH_4 ratio in the reaction mixture.

II-PP208

Effect of Synthesis Method and Doping Metals (M: Pt, Ce) in Ni-M/SBA-15 Based Catalysts for Dry Reforming of Methane

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Dry reforming of methane (DRM) has become the principal source of syngas production to obtain higher alkanes and oxygenates by Fischer-Tropsch synthesis. Nickel catalysts are the most promising tools due to the balance between their catalytic performance and low price. Formation of coke is the main process involved in the decrease of the reaction stability. In order to this fact, several Ni-M/SBA-15 mono and bimetallic catalytic systems (M= Pt, Co, Cu) have been prepared in our laboratory by wetness impregnation (IM) and homogeneous precipitation (HP) method, both were slightly modified. By tuning the preparation conditions, we have obtained systems with different particle sizes and catalytic performances. Notably, we have synthesized catalytic systems with very tiny (less than 4 nm) and a homogeneous size distribution of nickel particle, that present a strong interaction with the SBA-15 support. All these properties result in an outstanding catalytic performance without meaningful carbon deposition.

II-PP209

1-Alkyne Selective Hydrogenation with Pd/AC Catalysts. Effect of Precursor Salt

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Monometallic palladium catalysts supported on activated carbon (C) were synthesized by incipient wetness impregnation. Palladium chloride and nitrate were used as precursor salts to prepare PdCl/C and PdN/C. The metal loading on the final catalysts was 0.4 wt% Pd. Catalytic behavior of both catalysts during the selective hydrogenation of 1-heptyne to 1-heptene was studied at 303 K, 150 kPa H_2 pressure and 0.75 g catalyst mass. The characterization results show that the treatment with HNO_3 during the preparation step of PdN/CNR modified the support surface. PdN/CNR showed the best performance in activity and selectivity. The best performance of PdN/CNR can be attributed to the high concentration of active species Pd° on the surface of the support catalyst. It is possible that the remaining chlorine in PdCl/CNR interacts as a poison, decreasing the total conversion.

II-PP210

Investigation of Activity of Supported Block Catalysts in Oxidation of Light Alkanes into Hydrogen-Containing Compositions

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Results of the study the activity of supported block catalysts in hydrocarbon mixtures which are close to real for obtaining hydrogen-containing compositions are presented. Optimal conditions for the preparation of block catalysts were found. Technological parameters of the reaction were optimized. It was found that CH_4 : O_2 = 2: 1 is an optimal ratio of reactants for the oxidative conversion of light hydrocarbons into hydrogen-containing compositions on 1.0% Pt-Ru (1:1)/2% Ce/(θ+α)-Al_2O_3 catalyst supported on a ceramic honeycomb block carrier. The concentration of the initial reaction gases of CH_4 and O_2 is 50% and 25%, respectively, in the temperature range 725-875^{o}C at space velocity of 5000 h^{-1}.

II-PP211

Synthesis of C/Al_2O_3 and SO_4^{2-}/Al_2O_3 Aerogels and Their Catalytic Activity in Dehydrochlorination Reactions

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Carbon-coated alumina and sulfated alumina aerogels were synthesized. The textural parameters of alumina aerogels can be effectively controlled by selection of the solvents and modifying agents. Carbon-coated Al_2O_3 with permeable carbon coating can be prepared by adding modifying agents with bulky organic groups during gelation followed calcination under vacuum. Typical dimensions of the alumina nanoparticles synthesized by this method do not exceed few nanometers. The surface areas of the sulfated alumina aerogels after calcination at 600°C usually required to make active acid catalysts were about 600 m^2/g. This value appears to the highest ever reported for sulfated alumina catalysts. The activity of high surface area nanocrystalline alumina materials in dehydrochlorination of (2-chloroethyl)ethyl sulfide (2-CEES) and 1-chlorobutane compares favorably with that of other nanocrystalline metal oxides and correlates with the concentration of weak electron-acceptor sites.

II-PP212

Hydrogen and Oxygen Interaction with Single Supported Gold Nanoparticles

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The conditions of hydrogen and oxygen adsorption on single gold nanoparticles supported on high ordered pyrolytic graphite and gold nanoparticles supported on silicon covered oxide were determined by methods of scanning tunneling microscopy and spectroscopy. Hydrogen is chemisorbed on gold nanoparticles supported on SiO_2 at room temperature as well as on gold nanoparticles supported on HOPG.Production of water molecules on gold nanoparticles was observed. It was shown that, application of semiconductor as a substrate dramatically increases the reactivity of gold nanoparticles.

II-PP214

Cu(I) and Rh(I) Complexes of Novel Pyridyl-Containing Phospholanes

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A novel pyridyl containing tertiary cyclic phosphines – 1-(pyridine-2'-yl)phospholane **1** and 1-(4'-methyl-pyridine-2'-yl)phospholane **2** were obtained in reaction of corresponding primary pyridylphosphines with 1,4-dichlorobutane in superbasic medium. Reaction of **1** and CuI led to the formation of complex **3** with "butterfly" shaped Cu_2I_2 halide core and bidentate P,N-bridge coordination of one ligand molecule and P-monodentate coordination mode of two others. The abillity of the ligand **1** to form P,N-coordinated complexes motivated us to test its coordination with rhodium, which is catalytic active metal. Thus, the reaction of **2** with $[RhCl(Cod)]_2$ led to bis-P,N-chelate complex **4**, the spectral parameters of complex **4** are similar to that of described catalyst, which makes it perspective to test **4** in hydroformylation reactions.

II-PP215

Development of Stable Catalysts for Debenzylation of Hexaazaisowurtzitane Derivatives

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A technology for the two-stage catalytic debenzylation of hexabenzylhexaazaisowurtzitane has been developed that permits the Pd catalyst consumption to be considerably decreased.

II-PP216

Molybdenum-Containing Catalyst Production for Olefins Epoxidation with Using 1,1'- Dioxydicyclohexylperoxide

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The optimum compounding and synthesis conditions of the molybdenum-containing catalyst with use 1,1 '-dioxydicyclohexylperoxide being a utilization product of the hydroperoxide-containing sewage of styrene and of propylene oxide production are developed.

II-PP217

Synthesis and Characterization of Novel Ru(II)-Diimine-Layered Double Hydroxide Nanocomposites as a Light-Responsive Water Oxidation Electrocatalyst

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In this work, developing of photo-devices with oxidation capabilities was planned. New Ru- complex as photosensitizer was prepared and directly used in composite systems, under dark and light conditions, as oxidation catalysts. Immobilization of the surface (adsorption and linkage with terephthalate anions) and the intercalation of the metal-complexes into different LDHs were investigated as a method to optimize photosensitization. Smaller organic anion (terephthalate) was used to counterweighting the positive charge of the guest cations for their intercalation. All these modifications will lead to a tunable photosensitizer device, which is easily modified at each component.

II-PP218

Barbosa A.S., Barbosa A.S., Rodrigues M.G. F.

Synthesis of Zeolite Membranes of the Type MCM-22 and Y for Use in the Separation Process Oil/Water

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Zeolite Membranes (MCM-22 and Y) were prepared on flat of α-Al2O3 by synthesis method (rubbing) to be investigated in the separation water / oil. The mateiais were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). According to the results obtained, the materials are shown quite promising for use in the separation process.

II-PP219

Barbosa A.S., Barbosa A.S., Rodrigues M.G.F.

Membrane Zeolite MCM-22/γ-Alumina Applied to the Adsorption Capacity of the Gasoline

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In this work membranes zeolite MCM-22/γ-alumina were prepared by the secondary growth method (rubbing) and investigated the adsorption capacity in gasoline. Different materials were prepared: zeolite MCM-22 with TEOS as silica source; γ-alumina ceramic zeolitic membrane supports and MCM-22/γ-alumina. The resulting samples were characterized by X-ray diffraction (XRD). Based on X-ray diffraction results, we found that the preparation method used to sow the ceramic supports, (Rubbing), was effective in obtaining the zeolite membrane. The XRD pattern showed peaks characteristic of γ-alumina and zeolite MCM-22 confirmed the formation of the zeolite MCM-22 membrane. The adsorption capacity test proved that the zeolitic membrane (MCM-22/γ-alumina) is efficient.

II-PP220

Study of Adsorption of Hydrogen and Ethane on Bimetallic Platinum and Iridium Nanoclusters Using Quantum-Chemical Calculations

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Theoretical study of the structure of nanoclusters Pt_nIr_m (n,m=1 ÷ 3) is presented using DFT methods. The dependence of the structure and energetic of the clusters on the multiplicity state is considered. The reaction of adsorption of hydrogen molecules on these nanoclusters was studied using the procedure of scanning the potential energy surface.

According to the calculation of a comparison of geometric parameters and relative energies were computed for the adsorption of hydrogen on these nanoclusters. The main trends are analyzed of the basic parameters such as the activation enthalpy and enthalpy of reaction from hydrogenolysis of ethane in bimetallic clusters $PtIr_m$ (m=2 ÷ 3).

II-PP221

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Influence of Zink on the Formation and Properties of Catalysts Pt/Mg(Zn)AlO$_x$ Obtained from the Layered Hydroxides

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The work illustrated the effect of platinum modifying by zinc when it is introduced into the structure of the support during the synthesis of the oxide support precursor, namely, layered double hydroxides (LDH). The changes in the chemical composition, morphology and sizes of supported metal particles were detected. From the EXAFS and XPS date it can be concluded that platinum in zinc-containing samples is in the Pt-Zn alloy particles with a relatively low platinum concentration. Supported platinum in catalysts Pt/Mg(Zn)AlO$_x$ was characterized by the adsorption and catalytic properties providing selective producing of olefins from light and higher alkanes.

II-PP222

Textural Properties of Iron-Based Catalysts Supported on Mesoporous Silica SBA-15 Synthesized with Different Silica Source

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SBA-15 is a new class of mesoporous silicate that has a high thermal and hydrothermal stability. The rice husk ash may be used in the synthesis of mesoporous materials because the silica is amorphous. Among various fields iron oxides are applied highlight the processes involving adsorption and catalysis, which have attracted great interest due to redox and textural properties, with promoters to ensure greater activity and selectivity. This work aims to evaluate the textural properties of the catalyst Fe/Cu/K/SBA-15RHA obtained by characterization by nitrogen adsorption. By the results from specific surface area, total pore volume there were changes in the support (SBA-15), since there was a reduction of its specific surface area, already small, and total volume of pores after impregnation.

II-PP223

Soybean Oil Transesterification Applying Iron-Based Catalysts Supported on Mesoporous Silica SBA-15

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The transesterification has emerged as the best option for obtaining biodiesel, since the process is relatively simple; combined with this technique, researchers seek to lower the biodiesel manufacturing process using reusable catalysts, developing studies on heterogeneous catalysts that are reused in the manufacture of fuel. Mesoporous materials SBA-15 type silica compounds essentially, have several properties which make them potential acid catalysts. In addition. However, to make them catalytically active by their structures are basically formed of silica, the introduction of metal is required. The catalyst Fe/Cu/K/SBA-15 was prepared and applied in Soybean oil transesterification. By results, characteristic peaks phases of the oxides of iron and copper are identified by XRD and characteristic patterns of mesoporous materials by nitrogen adsorption analysis.The transesterification reaction of soybean oil with ethanol carried out in this study had a median conversion of 65.38% with the catalyst Fe/Cu/K/SBA-15.

II-PP224

Ni-XMo(W,V)/Al$_2$O$_3$ Catalysts Comparative Investigation in Hydrotreating of Light Coker Gasoil

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A line of catalysts Ni-XMo(W,V)/Al$_2$O$_3$ (X = Si,P,V) was synthesized. Ni was introduced from organic salt, Mo and W were introduced from heteropolyacids (HPA) (SiMo$_{12}$-, PMo$_{12}$-, PVMo$_{11}$-, VMo$_{12}$-, SiW$_{12}$- and PW$_{12}$-HPA) by means of wetness impregnation method. The catalytic activity was determined in the hydrotreating process of light catalytically cracked gas oil. The maximums of PAH HYD and HDS of sulfur compounds were found for catalysts on the bases of PVMo$_{11}$ - and VMo$_{12}$ – HPA. Ni-VMo/Al$_2$O$_3$ catatalyst HYD degrees at temperatures of 340-390ºC are higher twice than Ni-AHM/Al$_2$O$_3$ ones. Ni-AHT/Al$_2$O$_3$ catatalyst HDS degrees are higher than Ni-AHM/Al$_2$O$_3$ ones. Catalysts with higher hydrogenation activities Ni-PVMo/Al$_2$O$_3$ and Ni-VMo/Al$_2$O$_3$ have a low content of coke than others. In this way, the best precursors for synthesis of high active hydrogenation Ni-XMo(W,V)/Al$_2$O$_3$ catalysts are PVMo$_{11}$ - and VMo$_{12}$ – HPA. The catalysts, which contained W, showed a better HDS and HYD activities than without W ones.

II-PP225

Influence of Morphology of Ni Surface on Emergence of Self-Sustained Oscillations in the Oxidation of Propane

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Oxidation of propane over Ni in a self-oscillating mode is studied with the focus on the reason for the appearance of the induction period. It is shown that the induction period is related with the strong reconstruction of the nickel surface. Without such reconstruction, the oscillations cannot arise because of low activity of these catalysts.

II-PP226

Study of the Catalytic Effect of Nanosilica and Polycarboxylate on Cement Hydration and Mechanical Properties of Cement Mortars

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Given that the nanosilica particles (NS) and the polycarboxylate superplasticizer (PCE) have shown respectively a great pozzolanic activity and a best fluidity for cement pastes as have been demonstrated in previous studies. Based on these results, the catalytic effect of mixture nanosilica (silica nanoparticles) and PCE-superplasticizer on hydration of different cements has been investigation in this study. The PCE addition to a cement paste can increase the flowability thus reducing the water demand and accelerated the setting time process of the different cements studied. The obtained results show that the PCE has played as a deflocculating agent of the cement particles reducing the particle size of the agglomerates through a steric hindrance mechanism. Also, Mechanical strengths of studied cements were improved by the mixture presence of NS and PCE. Indeed, it was found that the nanosilica particles have played a catalyst role of cements hydration reactions and thus causing the formation of new calcium hydrosilicates that contribute to the improvement of mechanical resistances. The optimum attained in the combined effect of the mixture (NS and PCE) that involved relevant microstructural modifications as proved by pore size distributions and SEM observations. The results indicate also the effectiveness of NS and PCE-superplasticizer in producing high bulk density and in accelerating the pozzolanic activity to produce more C-S-H gel by consuming calcium hydroxide $Ca(OH)_2$ in order to improve the mechanical properties of cement pastes. These phenomenon are highlighted by measuring the mechanical strengths of the cements studied and also, by the DTA, TGA, and XRD.

II-PP227

Functionalized Graphene-Containing Mesoporous Materials as Catalysts in Acid-Catalyzed Reactions

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A series of graphene-containing mesoporous materials with well-ordered SBA-15 structure, high surface areas (~956 $m^2\ g^{-1}$) and large pore volumes (~1.1 $cm^3\ g^{-1}$) were prepared by modified sol-gel method. Morphology, structural and textural properties of the materials were characterized by XRD, TEM, N_2 adsorption-desorption and ^{27}Al NMR methods. The functionalized graphene-containing mesoporous materials were tested in the reactions of dehydration of butanol-1 and oligomerization of n-decene-1.

II-PP228

Preparation and Characterization of MOR Catalysts, Mo- MOR Ni-MOR and for Application in the Transesterification of Soybean Oil

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The current energy production in the world comes mostly from non-renewable sources which consequently increases the environmental impact. These facts have stimulated the alternative sources for fossil fuel development. This work aims at the synthesis of heterogeneous catalysts MOR, Mo-MOR and Ni-MOR, for application in the transesterification reaction of soybean oil, aiming at the preparation of biodiesel. The transesterification reaction of soyebean oil with ethanol showed in this work presented efficient conversion of 69.70% with Ni-Zeolite MOR catalyst and 75.35% Mo-Zeolite MOR.

II-PP229

Preparation and Characterization of Mo Catalysts Supported on Clay for the Transesterification of Soybean Oil

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Biodiesel is generally produced using four different methods involving base-catalyzed transesterification, acid-catalyzed transesterification, enzyme-based transesterification and non-catalytic transesterification under supercritical alcohol conditions and transesterification of refined oils via homogeneous alkaline catalysts. The present work focuses on application of Mo catalysts supported of production biodiesel by transesterification of soybean oil. The results. The metal (Mo) present in the surface of the catalyst (Mo-HGC) showed great importance, improving the catalytic activity of the hard green clay support, providing a significant increase in conversion due to the formation of active sites generated by the presence of the metal support. The most important factor in transesterification is the reaction time. The conversion will increase the amount of reaction time, due to increased contact time with the active sites of the catalyst.

II-PP230

Structural and Textural Properties of Modified Montmorillonite Derived from an Al_{13}-Macrocation, Acid and Nickel Activations

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In this work, new materials are prepared by exchanging of sodic- montmorillonite by Al_{13}-macrocation (noted BAl_{13}), by treating of sodic-montmorillonite with sulfuric acid (noted BAc) and by intercalation of BAc by Al_{13}-macrocation (noted $BAcAl_{13}$). The materials were modified by impregnation with 1-10%W/W of nickel and characterized by XRD, SAXS (with $2\theta<8°$), TGA/DTA, X-ray fluorescence, SEM, FT-IR and specific surface area and porosity. The nitrogen adsorption/desorption isotherms showed mesoporous materials. Quantities of adsorbed N_2 vary in the order: $Ni/BAl_{13}>BAl_{13}>Ni/BAcAl_{13}$ indicating important adsorptive properties of nickel catalyst without sulfuric acid treatment. The Al_{13}-macrocation was confirmed by XRD. The interlayer distance d_{001} (Å), observed for BAc, Ni/BAc, BAl_{13}, Ni/BAl_{13}, $BAcAl_{13}$ and $Ni/BAcAl_{13}$ samples, were respectively 14.62, 11.5, 17.52, 15.7, 17.8 and 15.7. The decreasing of d_{001}, observed after Ni impregnation of support, could be attributed to the decrease of crystallinity. Catalytic activity of these materials is evaluated in degradation of organic pollutants.

II-PP231

Characterization and Activity in Dry Reforming of Methane over Alumina Supported Transition Metal Catalysts Prepared by Microemulsion and Sol-Gel Method

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Three Alumina-supported catalysts, namely Ni/Al_2O_3, Co/Al_2O_3 and Cu/Al_2O_3 (25 wt.%) were prepared by two different preparation techniques the sol-gel (SG) and the microemulsion (ME) method, and applied in CO_2 reforming of methane for synthesis gas production. BET, XRD, XPS, TPR, and TEM-EDS techniques were employed to characterize the catalysts calcined at 1173 K. Experimental results demonstrated that ME-prepared had larger specific surface area, showing higher catalytic activities and stability of catalysts. It should be noted that the better performances were recorded on the NiAl-ME catalyst.

II-PP232

Synthesis and Parameters of the Thermal Degradation of Fullerene-Containing Polymers of Norbornenes Series

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New norbornenes with the covalently bonded fullerene C_{60} have been prepared under the Grubbs catalyst as monomers for ring-opening metathesis polymerization. The thermal degradation of synthetic fullerene containing homo- and copolymers with the parent 'non-fullerene' of the norbornene series was studied.

II-PP233

Nanoheterogeneous Catalysis in Electrochemically Induced Olefin Perfluoroalkylation

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Ni-catalyzed electroreductive olefin perfluoroalkylation affords both monomeric and dimeric products depending on the reaction media. Recycling of the catalyst can be achieved by immobilization of (bpy)$NiBr_2$ complex on silica nanoparticles decorated with anchoring amino-groups. Switching the homogeneous and heterogeneous catalysts is found to be one more factor to control the products ratio. This catalytic technique is both green and atom economical and unites the advantages of nanoheterogeneous catalysis and electrocatalysis.

II-PP234

ZrO_2-Based Oxide Supports for Pd-Containing Catalysts for Hydrodechlorination of Chlorinated Organics

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The comparison of different types of binary oxide supports for Pd -containing catalysts was made using (1) mixed or egg-shell Al_2O_3@ZrO_2, and (2) yttria or gallia stabilized ZrO_2. In order to obtain various pore size template synthesis was used. The catalysts were tested in gas and liquid phase hydrodechlorination of chlorinated benzenes.The addition of yttrium or gallium oxide to ZrO_2 used as a support for Pd catalysts leads to the improvement of catalytic efficiency (activity and stability) in liquid and gas phase hydrodechlorination of chlorobenzenes, because of the presence of both metallic and oxidized Pd. Improvement of catalytic performance in HDC of polychlorinated benzenes was achieved also by optimization of pore size both for individual and modified zirconia supports.

II-PP235

Quantum and Chemical Research of Nickel(II) Formazanates - Catalysts for Ethylene Oligomerization

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PM3 method incorporated into HyperChem has been used for quantum and chemical calculation of mononuclear nickel(II) benzothiazolylformazanates, used as catalysts for ethylene oligomerization. Energy characteristics (Highest Occupied molecular orbital energy value (HOMO), Lowest Unoccupied molecular orbital energy value (LUMO), and Energy gap value $E_{\sum}$) have been defined. The data both the energy gap and HOMO energy values for complexes are evidence of geometric configuration sustainability in these complexes. Abnormal catalytic activity of bis-1-(2-chlorophenyl)–3-butyl-5-(benzothiazol-2-yl)formazanate nickel(II) while ethylene oligomerizating resulting to butene yield can be explained by the difference in LUMO energy values.

II-PP236

Mechanism of Propane Oxidative Dehydrogenation on Surface Oxygen Radical Sites of VO_x/TiO_2 Catalysts

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The main objective of this study is to analyze the possible role of the oxygen radicals in oxidative dehydrogenation of propane to propene on VO_x/TiO_2 catalysts using periodic DFT calculations. The obtained results demonstrate that oxidative dehydrogenation of propane can proceed over oxygen radicals stabilized on the surface of VO_x/TiO_2 catalysts with low activation energies (~54 kJ/mol) matching the experimentally observed values. We believe that high temperatures are required for generation of the active radical species in sufficient concentrations. For the reaction to take place above 450°C with relatively low experimental activation energy, the concentration of the active sites should be low. These data suggest that oxygen radical species can be the active sites in this and other heterogeneous selective oxidation reactions. Further studies of reaction mechanisms with the emphasis on possible participation of such radicals in various catalytic reactions seem to be very important.

II-PP237

Fickian Spillover Models: Validation and Parameter Estimation

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The phenomenon and mechanism of spillover process is being discussed for the last two decades and accepted as an important step in understanding the dynamics of catalysts and improving their performance. Although the characterization and the theory of surface diffusion on perfect crystals has been treated to a good extent, the effect of spillover and surface diffusion on the performance of regularly synthesized supported catalysts is still vague. In this study, H_2 chemisorption involving sequential adsorption-desorption experiments was done on Pt/Al_2O_3 catalysts. The model of Kramer and Andre (J. Catal., vol. 58, pp. 287–295, 1979) is used to predict both adsorption and desorption rates from the catalysts. This Fickian description gives a good fit for both stages. Such a model is expected to predict amounts on the surface diffusion-influenced synthesis via new nanostructured catalysts. The model will be used to make predictions of hydrogenation reactions.

I-PP238

Mixed Spinel-Type Ni-Co-Mn Oxides: Synthesis, Structure and Catalytic Properties

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We have studied ESR reaction catalyzed by mixed spinel-type oxides $Co_{1.8}Mn_{1.2}O_4$, $Ni_{0.33}Co_{1.33}Mn_{1.33}O_4$ and $Ni_{0.6}Co_{1.2}Mn_{1.2}O_4$. Spinels were prepared by thermal decomposition of the mixture of corresponding metal nitrates hydrates followed by annealing at 700 °C. The samples were characterized by X-ray diffraction, X-ray absorption $L_{2,3}$-edges, BET and oxygen isotope exchange. Catalytic activity both in ESR and isotope exchange reaction rises up with Mn^{4+} content in the row $Co_{1.8}Mn_{1.2}O_4 > Ni_{0.33}Co_{1.33}Mn_{1.33}O_4 > Ni_{0.6}Co_{1.2}Mn_{1.2}O_4$.

II-PP239

Catalytic Activity of Palladium Complexes Based on Tridentate Ligands with Ancillary Sulfur Donor Groups in the Suzuki Cross-Coupling

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Novel multidentate ligands derived by the condensation of *o*-thiophosphorylaniline and amino-substituted nitrogen-containing heterocycles with mercaptobenzoic, mercaptoacetic, and mercaptopropionic acid chlorides were shown to readily form palladium(II) complexes, in all cases adopting a tridentate monoanionic coordination mode. The palladocycles based on these functionalized carboxamides were tested for the first time as (pre)catalysts for the Suzuki cross-coupling of aryl bromides with phenylboronic acid. Some interesting regularities in the structure–activity relationships were established that include the strong effect of the ligand framework flexibility and nature of the sulfur donor atom (sulfide *vs* sulfoxide).

II-PP240

Synthesis and Characterization of Spinel and Perovskite Structures with Transitions Metals

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For both $Ni_{0.1}Mg_{0.9}Al_2O_4$ and $Mn_{0.1}Mg_{0.9}Al_2O_4$ solids, we are observed by XRD the formation of spinal phase $MgAl_2O_4$, Ni or Mn is probably introduced in the spinal structure. While for the $Ni_{0.1}Mg_{0.9}Al_{0.5}La_{0.5}O_3$ material, we are noted the presence of a mixture of oxides: MgO and/or NiO and La_2O_3. Finally, the diffractogram of $Mn_{0.1}Mg_{0.9}Al_{0.5}La_{0.5}O_3$ solid revealed the presence of MgO and perovskite phase $LaAlO_3$.

Additional, themogravimetric analysis of the precursors of our catalysts are showed three main thermal events due to the elimination of free water at 100-150°C, the decomposition of ammonium nitrate between 260-290°C and the decomposition of citrate complex at 410°C. Furthermore, comparison of FT-IR spectra of various solid before and after calcination is showed a decrease of the intensity of the characteristic bands of H_2O and nitrates after heat treatment (800 °C). Likewise, characteristic bands of the metal oxides (M-O), between 450-700cm^{-1} are observed in the case of calcined solids. Otherwise, scanning electron microscopy is revealed spinal grain size of about 150 µm for the catalyst containing manganese, against about 60µm for the nickel based solids. For the perovskite structure, the grain size is estimated at about 20 µm for catalysts with manganese, and about 40 to 60µm for the solid containing nickel.

II-PP241

Photocatalysis of Hydrogen Evolution from Water by Used Thioxanthene Dyes

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The results of spectral and kinetic studies of new thioxanthene anionic dyes and kinetics of photocleavage of water into hydrogen in a homogeneous two-component photocatalytic system has been performed. It is shown that replacing the oxygen atom in xanthene moiety by a sulfur atom increases the quantum yield of triplet and photohydrogen. Replacement of the carboxyl group of the phthalic fragment on sulfonic group does not affect the photophysical and photocatalytic properties of the dye, and appears only in the nature of the interaction with the surfactant. The influence of the components of the photocatalytic system on the spectral, fluorescent, kinetic characteristics of intermediate products and photocatalytic activity has been studied. The data obtained allowed to construct a two-component photocatalytic system cleavage of water based on the tetrabromthiofluoresceine that effectively worked hundreds of hours to the initial quantum efficiency of 15%.

II-PP242

Hydrotreating of Diesel Fractions and Light Coker Gasoil Mixtures on Phosphorus Modified $Ni(Co)Mo/Al_2O_3$ Catalysts

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A line of catalysts with different amounts of phosphorus was synthesized. Modifier was introduced on the first stage of two stages synthesis by wetness impregnation method from phosphoric acid water solution. The catalytic activity of the samples was determined in a bench-scale flow reactor unit in the hydrotreating process of light catalytically cracked gas oil (LCGO) and straight-run gas oil (SRGO) mixture (1:9 by volume). Modification of carrier with P_2O_5 amounts of 2-5 wt. % get a positive effect on catalytic activities in HDS and HYD reactions. In CoMo catalysts line the maximum of activity was found for CoMo/P (2 wt.%) sample and in NiMo one – NiMo/P (5 wt. %).

II-PP243

Hydrotreating of Oil Fractions on Ni_6-$PMo_nW_{(12-n)}(S)/Al_2O_3$ Catalysts

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A line of trimetallic Ni-Mo_nW_{12-n} catalysts was synthesized and tested in hydrotreating of oil fractions. Catalyst with Mo/W = 1/1 demonstrated the highest hydrodesulphurization (HDS) activities in hydrotreating of straight run diesel fraction and light coker gasoil mixture and vacuum gasoil. Catalyst with Mo/W = 1/1 also demonstrated the highest hydrogenation (HYD) activity in hydrotreating of vacuum gasoil. Morphologies of active phases were investigated by means of HR TEM. Sulfide phase of Ni-Mo_6W_6(S) had the highest number of edge and corner Mo(W) atoms. It should be mentioned, that catalytic behavior of Ni-Mo_nW_{12-n} catalysts can't be explained in the view of active phase morphology. The Ni-Mo_nW_{12-n} catalysts are very perspective, like it was concluded from catalytic tests.

II-PP244

Crucial Role of the Graphene Edges for CNT Formation during the Preparation of Metal/Carbon Catalysts

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A detailed computational study has been carried out to study the mechanism of possible modification of the carbon surface during the preparation of Metal/Carbon catalysts. The nanotube formation process is strongly dependent on the state of the graphene edges. This result suggests a possibility to control CNT formation during the preparation of M/C catalysts.

II-PP245

MnO_2 Catalyst Prepared With Microwave Assistance

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Manganese dioxide (MnO_2) endowed crystal multiplicity with is a juicy system and dominant competitor among the materials for electrochemical energy conversion and storage. Nano-MnO_2 exhibits an electrochemical performance superior to its bulk counterpart because of its higher specific surface area. We report a strategy in microwave-hydrothermal processes that permits exquisite control over the crystal structure and morphology of MnO_2 nanostructures by temperature, time and acidity.

II-PP246

DRIFTS Studies of Support Effects on CO Adsorption and CO + O_2 Reaction over $Ce_{1-x-y}M_xCu_yO_{2-d}$ (M = Zr, Hf, Th)

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In situ DRIFTS studies of CO adsorption and oxidation are observed to be lowest over $Ce_{0.68}Zr_{0.25}Cu_{0.07}O_{2-\delta}$ among Cu substituted $Ce_{0.75}M_{0.25}Cu_{0.07}O_2$ (M = Zr, Hf and Th) catalysts. It was found that Cu^+─CO vibrational intensity increases as Zr < Ce < Th ~ Hf. With increasing effective nuclear charge (Z_{eff}) of the substituent metal (Zr<Hf<Th) in CeO_2 matrix, ionic charge on the Cu^{2+} is more localized as negative charge on oxygen gets depleted due to more polarization in the M─O bond around Cu^{2+} ion. This effect is alleviated by converting more Cu^{2+} to Cu^+ and thereby, increasing the intensity of Cu^+─CO peak. Comparison of intensities of CO_2 bands of different catalysts as a function of temperature indicates that CO oxidation activity increases in the following substitutions: CeZr < Ce < CeHf ~ CeTh. $Ce_{0.68}Th_{0.25}Cu_{0.07}O_{2-\delta}$ shows lowest temperature CO oxidation among all the catalysts due to its more electron withdrawing power.

II-PP247

Synthesis of ZSM-5 Zeolite from Fly Ash by Hydrothermal Method

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Several fly ashes from Colombian Industry were used as raw materials for ZSM-5 zeolite synthesis, by hydrothermal method. The fly ash was subjected to calcination at 700°C for 3 hours as a pretreatment, to weaken the crystallinity of the quartz phase, which is silicon oxide. To adjust the high ratio SiO_2/Al_2O_3 of the zeolite, a suspension of silicon oxide (30% LUDOX) was used and TPABr was added as the structure-directing ofZSM-5 zeolite synthesis. The synthesis through of the hydrothermal method was carried out at crystallization temperature of 190°C for 24 hours in stainless steel reactor with Teflon lining, after which the gel was left to stir for 5 hours. Finally, the material was calcined at 550°C for 5 hours to remove excess humidity and organic compounds into the structure. Characterization by DRX, atomic absorption, SEM, TGA and BET was realized for identification the structural and textural properties for the zeolite.

II-PP248

In Situ X-ray Absorption Spectroscopy and X-ray Powder Diffraction for Temperature- and Pressure- Dependent Hydride Phase Formation in Supported Pd nanocatalysts

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We performed a detailed analysis of hydride phase formation in Pd/C nanocatalysts using combined in situ x-ray absorption spectroscopy (XAS), x-ray diffraction (XRD) and volumetric measurement for the temperatures from -10 to 110 ºC in a pressure range from 0 to 10^4 mbar. The obtained results corresponding to different techniques are in a perfect agreement. We demonstrate the advantaged of X-ray based methods, XAS and XRD, in being specific to only Pd species, while volumetric measurements are also affected by hydrogen adsorption in the support. The near-edge region of absorption spectra (XANES) was fitted using theoretical simulations providing quantitative information on the amount of hydrogen absorbed in the Pd nanocatalysts.

II-PP249

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Catalytic Performance of a Polyoxometalate/Reduced Graphene Oxide Composite in Degradation of Methylene Blue

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In this study graphene oxide (GO) and reduced reduced graphene oxide GO was prepared to literature[1]. The reduced graphene oxide was dispersed and sonicated in DI water. In this step, ethylene glycol was added to the reduced graphene oxide solution to disperse POM on the graphene sheet. An aqueous solution of Silicotungstic acid was added to the rGO solution and mixed, filtered and washed with DI water and then dried[2]. Catalytic activity of rGO-POM composite was investigated by means of degradation of methlylene blue by sodium borohydride in aqueous solutions and the reaction was monitored by UV-VIS spectrometry.

I II-PP250

Porous Nickel Based Catalysts for the Dry Reforming of CH_4 to Synthesis Gas

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The reforming of CH_4 with CO_2 has attracted much attention in recent years. This process produces synthesis gas with low H_2/CO ratio which can be converted into liquid hydrocarbons in the Fisher-Tropsch reaction or in the production of methanol. Nickel is preferred metal for the catalysis the CO_2 reforming of CH_4 due to its inherent availability, low cost and high activity. For carrying out the endothermic reactions of dry reforming of CH_4 it should be used the catalysts on metallic supports for intensive heat transfer to the reaction zone. In this work the nickel catalysts based on porous nickel ribbon with MgO underlayer were prepared and characterized by XRD, low-temperature adsorption of nitrogen, SEM and TEM HR in combination with EDX microanalysis. The activity of the catalysts were studied in dry reforming of CH_4 (flow method, 750°C, 1 atm, m_{cat} = 0,40 g, reaction mixture flow rate – 25 l/h).

II-PP251

B18 Capabilities for XAS in Situ Experiments in Catalysis

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B18 beamline at Diamond Light Source have recently developed in collaboration with Industrial Liaison Group and Research Complex at Harwell sample environments which allow the in situ study of catalysts and combination of X-ray absorption spectroscopy, diffraction and other spectroscopic techniques such as IR and Raman. B18 sum up the time resolution (in the order of few seconds) provided by quick-EXAFS scanning mode with the integrated control of catalytic conditions in capillary reactor, furnaces or heated liquid cells. A gas mixing rig setup is available to allow introducing complex gas mixtures in situ and a Mass Spectrometer to monitor the reaction products.

II-PP252

Methane and Propane Oxidation Over Pd(111): Temperature Hysteresis, Induced by Oxide Formation

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During the methane and propane oxidation on Pd(111) the formation of a surface layer of PdO was found, which determined the observed temperature hysteresis in TPRS experiments. The activity of PdO in a small excess of oxygen exceeds the activity of metallic palladium, partially or completely covered by the surface oxide Pd_5O_4.

II-PP253

Copper Oxides (I, II) as Catalytic Precursor in C-S Cross-Coupling Reactions

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Nanosized CuO and Cu_2O-containing nanoparticles of different sizes and shapes were studied as precatalysts for ligand-free C-S Ullmann cross-coupling reaction. Under catalytic conditions, the morphology of starting copper oxides underwent dramatic changes, and we found that both CuO and Cu_2O played a role of precursors to Cu(I)-thiolate complex. The latter species was then responsible for the observed catalytic action.

II-PP254

Nature and Structure of Extraframework Al Species in Zeolite: NMR Study on Selective H/D Exchange between Bronsted Acid Sites and Benzene

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The effect of extraframework Al(EFAl) species on the Brønsted acid sites (BAS) in steam-calcined USY zeolite was studied by in situ H/D exchange between benzene and deuterated zeolite using NMR spectroscopy. The spectroscopic results in combination with model periodic density functional theory calculations indicate that EFAl species are preferentially stabilized in the faujasite sodalite cages in the form of multinuclear oxygenated and hydroxylated cationic Al clusters. The H/D exchange reaction involves only the zeolite (BAS), whereas the AlOH and SiOH moieties due to zeolite defects remain intact upon contacting with benzene. A much higher reactivity of BAS is observed for the EFAl-containing USY zeolite. Whereas in the absence of EFAl species (AHFSY), all BAS are equally reactive towards C_6H_6, in the case of USY zeolite, the rates of H/D exchange with the sodalite cage OH is much higher than with the accessible supercage BAS. This evidences the selective enhancement of only a fraction of zeolitic BAS neighboring the Lewis acidic extraframework Al species stabilized inside faujasite sodalite cages.

II-PP255

Catalytic Performance in Isopropanol Decomposition over $H_{3+X}PMO_{12-X}V_XO_{40}$ Heteropolyacids Supported on Mesoporous Molecular Sieve HMS

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30wt.% $H_{3+x}PMo_{12-x}V_xO_{40}$ (x=0-3) HPAs were supported on HMS by dry impregnation method. Elemental analysis, XRD, FT-IR, XPS, BET, TG-DTA and SEM were used to characterise catalysts. The catalytic performances of supported HPAs were compared to those of pure one and tested in the isopropanol decomposition reaction to propene, diisopropylether and acetone products at 75°C and atmospheric pressure.

The physico-chemical characterization of the supported HPAs showed mainly undegraded primary Keggin structure and high dispersion of heteropolyacids on the HMS surface. The BET surface area (S_{BET}) and the pore volume (Vp) of HMS decrease strongly in the presence of HPAs. The TG-DTA analysis showed that the obtained mesostructures HPA-HMS have a higher thermal stability than the HPA bulk. $H_{3+x}PMo_{12-x}V_xO_{40}$ heteropolyacids with x=0-3 supported on mesoporous HMS appear to be more active than $H_{3+x}PMo_{12-x}V_xO_{40}$ on bulk.

The substitution of molybdenum by vanadium atoms leads to higher activity especially for $H_4PMo_{11}V_1O_{40}$.

II-PP256

Speciation of Extraframework Aluminium Species in Faujasite Zeolite: a Theoretical Perspective

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The structure and stability of extraframework aluminium (EFAL) in faujasite zeolite are investigated by periodic DFT calculations. A large number of possible mononuclear as well as various bi-, tri- and tentranucelar EFAL complexes stabilized at different locations inside the faujasite structure is considered. It is demonstrated that the self-organization of mononuclear EFALs into multinuclear cationic clusters is a thermodynamically favourable process. The stable tri- and tetranuclear clusters to be preferentially formed in sodalite cages. The interconversions of different EFAL species may proceed via hydration/dehydration and protonation/deprotonation reactions. The nature of the predominant EFAL species in steam-activated zeolites is predicted by *ab initio* thermodynamic analysis. It is demonstrated that the multinuclear oxygenated and hydroxylated cationic clusters located in sodalite cage are the dominant EFAL species in steam-activated faujasite zeolites.

II-PP257

Preparation and Characterization of Sr, Ca and Mg Doped Ceria Electrolyte for Solid Oxide Fuel Cells

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Solid oxide fuel cells have received special attention because of their higher energy efficiency, rapid electrode kinetics without using expensive electrocatalysts such as Pt, relative resistance to impurities in the fuel and the possibility of processing CO, CH4 and other carbon based fuels. Most of the research efforts have focused on the development of solid oxide fuel cell materials such as yttria stabilized zirconia (YSZ) electrolytes, lanthanum or calcium doped strontium manganite (LSM) cathodes and Ni-YSZ cermet anodes. YSZ electrolytes require high operation temperatures (~1000 °C) in order to achieve sufficient ionic conductivity, placing large restrictions to candidate electrode, interconnect and housing materials. As a result, the cost of solid oxide fuel cell systems has become an important factor preventing their commercialization. To overcome these problems, electrolytes which have high ionic conductivity at intermediate temperatures are needed. According to the recent researchs, it was shown that a variety of rare earth metal doped cerium oxides can be used as electrolyte materials in order to develop solid oxide fuel cells operating in intermediate temperatures.
Hence in this study cheap, readily accessible and which may be stable at lower temperatures Mg, Sr, Ca will focus on the elements instead of the rare earth elements. This research will attend to light up the structure of electrolytes by XRD, SEM, TG/DTA anlaysis and find optimal conditions for synthesizing electrolytes by Citrate Nitrate Combustion method. Conductivity will measure by Impedance Analyzer.

II-PP258

From In Situ to Operando Mode: Experience on Synchrotron X-ray Diffraction at SSTRC

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The report describes results of first experiments on *In Situ* SR XRD applying parallel analysis of gaseous components of catalytic reactions at Siberian SR Center. The experiments demonstrated that simple attachment of gas analyzer to reactor cell does not provide *Operando* mode realization. It is suggested that *Operando* mode to be performed specific requirements to reactor cell as well as solid to gas components ratio have to be met. Actually, for each particular experimental task or class of tasks an individual reactor cell suitable for definite experimental conditions should be developed and created.

II-PP259

Mechanistic Insights into CO Oxidation and Preferential CO Oxidation over Cobalt Oxide and Promoted Cobalt Oxide Catalysts

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In the present work, operando infrared spectroscopy, in situ near ambient pressure X-ray photoelectron spectroscopy and operando X-ray absorption spectroscopy were combined to study the structural and electronic changes of cobalt oxide and promoted cobalt oxide catalysts during CO oxidation and preferential CO oxidation (PROX) with the aim to understand the promotional effect of PdO and CeO_2 on the activity of Co_3O_4 in CO oxidation and PROX, the nature of the active sites of the catalysts and the reaction pathways. Promotion of Co_3O_4 with PdO and CeO_2 improves the catalytic activity of cobalt oxide catalysts by enhancing CO adsorption and O_2 activation. A possible mechanism of CO (preferential) oxidation proceeds via CO disproportionation or carbonate formation.

Section 3. Energy-Related Catalysis

III-PP01

Kinetic Analysis of Decomposition of Ammonia over Nickel and Ruthenium Catalysts

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The decomposition of ammonia (NH_3) over Ni and Ru catalysts was investigated by using a kinetic model based on a reaction mechanism consisting of kinetically important elementary steps. Experimental results obtained over a wide range of reaction conditions were reproduced by the model. Recombinative N_2 desorption was the rate-limiting step on the Ru catalyst, whereas the overall rate of NH_3 decomposition was controlled by the NH_3 dehydrogenation step on the Ni catalyst.

III-PP02

Hybrid Membrane-catalytic Reactor for Synthesis Gas and Pure Hydrogen Co-production by Dry Reforming of Methane and Ethanol

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Original hybrid reactor consisted of Ni-Co-containing converter with integrated Pd-alloy membrane was developed. The construction allowed to carry out simultaneous processes of highly efficient dry reforming of methane (DRM) and ethanol (DRE) into syngas and in situ hydrogen separation. Removal of hydrogen decreased reaction temperature and shifted equilibrium of process.

III-PP03

Solution Combustion Synthesis of Noble Metal-loaded Ceria Catalysts and Application to Hydrogen Production and Purification for Fuel Cells

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Ceria nanopowders loaded with Pt-group metals (Pt, Pd, Ir, Rh, Ru) were prepared by one-step solution combustion synthesis and characterized by HRTEM, SEM, XRD, XPS, DRIFTS, and Raman spectroscopy. The samples, consisting of 2-6 nm metal nanoparticles strongly anchored on mesoporous ceria, were successfully employed as catalysts for the production of hydrogen from steam reforming of methane (SRM), and the purification of hydrogen through preferential oxidation of CO (PROX). Ir-doped CeO_2 exhibits the best performances in terms of activity, stability at 750 °C, and resistance to poisoning by H_2S impurities present in the SRM feed (220 ppm). While the best catalyst for H_2-free CO oxidation is Rh-CeO_2, the addition of a high hydrogen excess ($H_2/CO = 24$) decreases the Rh catalyst activity but enhances the CO oxidation rate on all other systems. Pt-CeO_2 is both the most active and selective PROX catalyst, reaching near 100% CO_2 at *ca*. 100 °C.

III-PP04

Syngas Production via Combined H_2O and CO_2 Reforming of Coke Oven Gas over La-promoted Ni/$MgAl_2O_4$ Catalyst

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La-promoted Ni/$MgAl_2O_4$ catalysts were applied for combined H_2O and CO_2 reforming of coke oven gas for syngas production. The La promotion has significant effect on the Ni dispersion and surface area after the aging treatment. La-promoted catalysts had higher Ni dispersion and Ni surface area due to the enhancement of metal dispersion and SMSI. The catalyst with 2.5 wt% La, which is optimum to achieve highly dispersed Ni particles, showed the best catalytic activity and stability in CSCR of COG.

III-PP05
Hybrid DFT Study of Fe:NiOOH O_2 Electroevolution Catalyst

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DFT calculations with an accurate hybrid functional are used to model NiOOH, a layered material of high catalytic activity (especially when Fe-doped) for the evolution of O2 in photocatalytic and electrochemical water splitting systems. Different stackings of the NiOOH layers, and different arrangements for the location of protons in them, have similar energies, which justifies the highly disordered character observed for this material. The computed bandgap of NiOOH, between ca. 1.0 and 1.4 eV, depends on the stacking and proton configuration, its edges being formed by Ni 3d levels. Insertion of Fe produces new filled levels (formed by Fe 3d orbitals) close to the NiOOH valence band edge, and in some configurations leads to electron and proton transfer from Fe to Ni sites, suggesting an easy mobility of both charge carriers which may contribute to the good electrocatalytic activity.

III-PP06
Solid Solutions for Heterogeneous Photocatalytic Hydrogen Evolution from Water - Using POM/TiO_2 Composites

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In order to respond to the rising energy demand, the interest in developing new ways of supplying solar fuel is growing. Focus is placed on the identification of new materials, composites and reaction pathways. In order to overcome the shortcomings in the photocatalytic H_2 evolution from water, it was investigated how solid solutions of polyoxometalates (POM) in the semiconductor TiO_2 can enhance the catalytic activity of TiO_2. Hence, several synthesis routes were followed to incorporate $H_3PW_{12}O_{40}$ into the framework of TiO_2 without destroying the Keggin-structure of the POM. It was found that composites of polyoxometalates $H_3PW_{12}O_{40}$ and TiO_2 exhibit a higher photocatalytic activity for hydrogen evolution in water than TiO_2 alone. Using solid state ^{31}P-MAS NMR it was proven that the Keggin structure was incorporated into TiO_2. A composite-strategy can improve the photocatalytic activity of semiconductors. Solid solutions might lead to higher photocatalytic activities due to a charge separating effect.

III-PP07
Electrophysical Properties of Cathode Materials $Pr_{2-X}Sr_XNi_{1-Y}Cu_YO_4$ for Intermediate-temperature Solid Oxide Fuel Cells

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The phase composition, thermal coefficient of linear expansions (TCLE) and electrical conductivity of $Pr_{2-Y}Sr_YNi_{1-Z}Cu_ZO_4$are investigated at air in the temperature range 100 – 1000°C.

The thermal coefficient of linear expansion of $Pr_{2-Y}Sr_YNi_{1-Z}Cu_ZO_4$ are in range of $(11.2\text{-}16{,}6)\times 10^{-6}\text{deg}^{-1}$ and depends on the size and type of addition.

One compositions are compatible on TCLE with electrolytes used in intermediate-temperature electrochemical devices. The maximum of conductivity of the most conducting compositions is in the temperature interval of 500-800°C

III-PP08
Foil of the Pd-In-Ru Alloy for the Membrane Technology of Preparing High-purity Hydrogen

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This paper presents the technological characteristics and the results of the study the specific permeability and the separation performance of a membrane unit based on a foil 28 µm thick from the Pd–6 wt.% In–0.5 wt.% Ru alloy. The specified alloy has high strength and high ductivity ($H_v = 114$ kg/mm^2, $\sigma_B = 48$ kg/mm^2, $\delta \approx 26\%$ (annealed)), sufficient specific hydrogen permeance, egual at 873 K to 2.2 m$^3\cdot$mm/(m$^2\cdot$h$\cdot$MPa$^{0.5}$), and high corrosion resistance in hydrogen-containing gas mixtures obtained by hydrocarbon fuel conversion . The hydrogen flux through the foil with the composition Pd–6 wt.% In–0.5 wt.% Ru is more than twice as large as that through the foil of the Pd–23 wt.% Ag alloy. The optimal temperature for H_2 separation from CO-containing mixtures is 773 K, since the inhibition of the separation process because of the reversible adsorption of CO molecules becomes lower, and the efficiency of the catalytic reaction on the membrane surface resulting in carbon deposits formation is insignificant.

III-PP09

Fischer–Tropsch Synthesis on Cobalt-Based Catalysts with Different Heat-conductive Additives

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The technology for producing high-quality synthetic oil from carbon-containing feedstock — XTL (X-to-liquids) technology — is attracting attention as an alternative to the use of dwindling oil reserves. Fischer–Tropsch synthesis (FTS) is the main stage of XTL technology.

The combination of FTS catalyst with zeolite in a composite material leads to formation of bifunctional catalyst producing synthetic oil in one step by eliminating hydrotreating stage. The main role of zeolite is the decrease in average molecular weight of produced hydrocarbons by cracking on acid sites. The use of metallic additives in the composition of FTS catalyst provides such advantage as intensified heat conductivity.

The purpose of this work was to study the effect of heat-conductive additives (aluminum, copper or zinc) introduction to cobalt-based catalyst.

The introduction of different heat-conductive components into catalyst influenced the main catalytic properties. Product composition and chain growth probability depend on heat-conductive component and its catalytic activity.

III-PP10

Gold Catalysts on Y-modified Ceria for CO-free Hydrogen Production Via WGSR and PROX

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Gold catalysts on Y-doped ceria supports were synthesized and characterized by XRD, HRTEM/ HAADF, XPS, TPR and Raman spectroscopy. The effect of support preparation (impregnation (IM) or co-precipitation (CP)) and dopant amount ((1, 2.5, 5 and 7.5 wt% Y_2O_3) on the catalytic properties in the water gas shift reaction (WGSR) and preferential CO oxidation in H_2 reach stream (PROX) was investigated. Addition of yttrium to ceria generally enhanced the WGS activity of the gold catalysts. However those on prepared by IM Y-doped ceria supports exhibited better WGS activity than those on supports synthesised by CP. The best CO conversion was observed over the gold catalyst on IM support containing 1% dopant. At the temperatures of interest for fuel cells (80-120°C) the PROX activity did not differ significantly over all studied samples. However, the IM method of preparation is beneficial for PROX at real conditions improving the resistance toward CO_2 deactivation.

III-PP11

Gallium-promoted Nickel/Cerium Catalysts for Hydrogen Production from Steam Reforming of Acetic Acid as a Model Compound of Bio-oil

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The aim of this work was to study the performance of nickel catalysts promoted with gallium (Ga) supported on CeO_2 to convert acetic acid into hydrogen. Acetic acid was chosen as representative compound for the steam reforming of bio-oil derived from biomass pyrolysis. Steam reforming of acetic acid was conducted in a fixed bed reactor at a temperature of 600 °C for 6 h. All catalysts showed conversion above 90% for acetic acid at 600 °C. The selectivity for H_2 for $5Ni/CeO_2$, $5Ni1Ga/CeO_2$ and $5Ni3Ga/CeO_2$ catalysts was ~3.5 mol H_2/mol $CH_3COOH_{conv.}$ at 600 °C for all catalysts. However, with addition of 3% Ga the rate of coke was 0,0098 g_c $gcat^{-1}h^{-1}$, while the rate of coke formation for $5Ni/CeO_2$ and $5Ni1Ga/CeO_2$ catalysts was 0,0295 and 0,0179 g_c g $cat^{-1}h^{-1}$, respectively. This shows that addition of Ga prevents the formation of coke on the catalyst surface.

III-PP12

Effects of Mg Content on Ni/MgO-SiO_2 Catalyst for Ethanol Steam Reforming

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Ni catalysts supported on MgO-SiO_2 (NS, N10MS, N30MS, N50MS and NM) were prepared by the wet impregnation method and characterized by energy dispersive X-ray spectroscopy (EDS), nitrogen physisorption (BET method), X-ray diffraction (XRD), thermogravimetric analysis (TGA) and temperature-programmed reduction with H_2 (TPR). XRD and TPR analysis indicated several species in the samples: SiO_2, MgO, $Mg(OH)_2$, magnesium silicate hydrate (MSH), NiO and $MgNiO_2$. The catalytic tests were performed in a fixed bed reactor containing 150mg catalyst at 600°C, with an inlet water:ethanol ratio of 6:1. These tests showed that, the deposition of carbon on the catalyst during the reaction fell steadily as the proportion of MgO in the support increased. The catalysts that showed best H_2 selectivity were N30MS and N50MS.

III-PP13
Ni/ZrO-ZnO Catalysts Applied in Ethanol Steam Reforming for H_2 Production

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Ethanol is a product derived from biomass and it can be transformed by steam reforming (ESR) in a fuel with higher value, as H_2. The goal of this study was to evaluate the effect of adding ZrO_2 in NiZnO catalysts on SRE to produce hydrogen. Catalysts containing 10 wt% Ni and 0, 10, 20 and 30 wt% ZrO_2 were prepared by coprecipitation method. These materials were characterized by temperature programmed reduction (TPR), specific surface area by the BET method and energy dispersive X-ray spectroscopy (EDX). After characterizations, the catalysts were applied on ESR. The catalyst containing 30 wt% ZrO_2 exhibited superior H_2 selectivity compared to others catalysts for SRE at 923 K.

III-PP14
Co Catalysts for the Dry Reforming of Methane: Effect of Support

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The dry reforming of methane (DRM) is an attractive reaction to obtain synthesis gas with a H_2/CO ratio close to 1 that also supposes the consumption of two greenhouse gases (CO_2 and CH_4). Among the metals able to catalyze the DRM reaction only Co and Ni are convenient from an economical point of view, but they have the drawback of a high carbon deposition during reaction. In this work, a series of cobalt catalysts has been prepared using different supports with the objective of finding a system resistant to carbon deposition.

It has been found that the support strongly influences the catalytic activity because it affects the size of the loaded Co particles and, as consequence, the number of active site on the catalyst surface and also because of its acid/basic properties. The best results have been obtained with Al_2O_3 and $MgAl_2O_4$.

III-PP16
Iron Based Catalysts Supported on KL Zeolite for Fischer-Tropsch Synthesis

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In this work iron based catalysts supported on KL zeolite were prepared by wetness incipient impregnation to be used in Fischer-Tropsch synthesis. The metal contents were 1 and 5 wt %. The samples were analysed by several techniques such as atomic absorption sprectroscopy (AAS), X-ray diffraction (XRD) and N_2 physical adsorption by BET method. The Fischer-Tropsch synthesis (FTS) performances of the catalysts were carried in a microreactor. A higher conversion was obtained for the catalyst containing 5wt % Fe and high products distribution to light fractions (C_2 –C_4) were verified for Fe catalysts proving their good performance for this purpose.

III-PP17
Highly Dispersed Ni Catalysts over Cerium Modified Mesoporous MCM-41 for Hydrogen Production by Ethanol Steam Reforming

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Mesoporous silica MCM-41 was prepared by ultrasound assisted hydrothermal synthesis in order to achieve Cerium incorporation in the silica framework. The selected Ce/Si molar ratios for the materials were 0.02, 0.04, 0.06 and 0.08. All prepared materials exhibit hexagonal structure, high surface areas (over $546 m^2/g$) and were used as catalytic support for a Nickel active phase (10% of metal loading). The catalytic activity was evaluated in the ethanol steam reforming reaction to produce hydrogen. The Ni catalyst over cerium promoted silica presented complete ethanol conversion, and H_2 selectivity ranging from 55 to 60%. Although, production distribution is slightly dependent on Cerium content, these materials did not show catalyst deactivation after 6h on stream and were selective towards H_2, CO_2, CO and CH_4 as main products. On the other hand, bare unmodified silica as catalytic support resulted in C_2H_4 and C_2H_4O, lower ethanol conversion (40%) and less hydrogen production (38%).

III-PP18

Palladium-Lead Membranes for the Separation of High-Purity Hydrogen from Hydrogen-Containing Gas Mixtures

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Palladium-based alloys, which exhibit high both the strength, plasticity, and hydrogen permeability at the expense of alloying of palladium with lead within the solid solution range (to 20 wt % Pb), have been developed. The optimum composition Pd-8 wt % Pb characterized by maximum hydrogen permeability was selected to be used for the efficient separation of high-purity hydrogen from hydrogen-containing gas mixtures. The corrosion resistance of the alloy was studied in the gas mixture 60 vol % H_2 + 31 vol % CO_2 + 9 vol % CO, which is identical to products of natural gas conversion. A foil of the alloy was used to manufacture a membrane element (diameter of membrane is 50 mm and the foil thickness is 50 μm) and its productivity in the aforementioned mixture has been estimated. At the operation parameters $P_{\text{input mix}} = 2$ MPa ($P_{\text{H2 partial.}}$=1,5 MPa), P_{output}=0,15 MPa, T = 773 K, $\eta = 0{,}8$, it is 0,25 nm^3/h and exceeds the productivity, under the same conditions, of similar membrane element with the membrane made from the industrial B1 alloy.

Membranes made from the Pd-8 wt % Pb alloy show promise for application in membrane elements for the separation of high-purity hydrogen from products of the hydrocarbon fuel conversion.

III-PP19

Structural Characterization of Nanostructured Pt-Ni Alloy Electrocatalysts for Methanol Electrooxidation

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PtNi nanoparticle catalysts supported on functionalized carbon nanotubes were prepared by polyol method using two different reduction modes, namely, heat treatment and under microwave irradiation. The influence of preparation protocol on catalyst structure and activity in methanol electrooxidation has been studied. PtNi nanoparticles are present in alloy form and are well dispersed on the supprot. Pt is in its metallic state, whereas Ni is present in metallic and oxidized form depending on the preparation conditions. The electrocatalytic activity both in terms of surface and mass specific activity is higher than that of the benchmark Pt/C (E-TEK). The enhancement of the activity is discussed with respect to PtNi alloy formation and the resulting modification of the electronic properties of Pt by Ni in the alloy structure. The microwave assisted polyol method with continuous irradiation is more effective in the preparation of PtNi electrocatalysts both in terms of reaction time and activity.

III-PP20

Effect of Pt Addition on Methane Oxidation Activity of Pd-Mn-hexaaluminate Catalysts

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Wide interest to the catalytic combustion chamber of gas turbines stimulates search of new Pd-catalysts with respect to decrease of the light-off temperature, increase of the efficiency in hydrocarbon fuels combustion and thermal stability.

Here we studied an effect of Pt to improve catalytic performance of the high-temperature Pd-Mn-hexaluminate catalysts in methane oxidation, especially in 1000 ppm SO_2 and 3 wt.% water presence, and compared them with the properties of Pd/Al_2O_3 catalysts. The Redox properties (H_2-TPR), particle morphology (HRTEM), composition and active sites (XRD, FTIR, XPS, O_2-TPR, DTA) of the initial and spent catalysts were examined in order to find a reason of high efficiency and thermal stability of the catalyst.

When Pt/Pd ratio was close to 0.25, the Pt addition modified water and SO_2 resistant of Pd-Mn-hexaaluminate without decreasing its methane oxidation activity. Such performance of the catalyst can be explained by the formation of both PdO and PtPd-alloy.

III-PP21

The Nickel Electrocatalysts $[Ni(P^R{}_2N^{R'}{}_2)_2]^{2+}$ (where R=Ph or o-Py) for Hydrogen Evolution

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The electrochemical properties of the new nickel complexes $[Ni(P^R{}_2N^{R'}{}_2)_2]^{2+}$ (where R=Ph or *o*-Py) with cyclic 1,5-diaza-3,7-diphosphacyclooctane ligands have been studied. All complexes are effective electrocatalysts for hydrogen production using $[(DMF)H]^+$ as proton source in acetonitrile. The introduction *o*-Py substituents at phosphorus as additional basic center is caused by the changing of voltage-current picture and significantly catalytic current enhancement. Presented complexes exhibit catalytic activity for the electrocatalytic hydrogen evolution reaction higher than that of complexes containing same radicals at phosphorus and aryl-, benzyl and methylbenzyl at nitrogens. So, the activity presented complexes is comparable to natural hydrogenase activity and higher than that of all known similar synthetic nickel catalysts under rigorous conditions – dry acetonitrile, acid [(DMF)H]OTf. We have found that relatively small changes in volume of the ligands achieved by introducing bulky exocyclic substituents at the nitrogen atoms lead to large changes in catalytic activity. We have also observed a unique reactivity of pyridine-substituted analogue, its effectiveness exceeding that of all known relative complexes under the selected conditions.

III-PP22

Effect of CH_4 Flow Rate and Catalyst Load on the Activity Stability of Mo/HZSM-5 in the Methane Dehydroaromatization at 1073 K in an Integral, Fixed-bed Reactor

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Case studies on Mo/HZSM-5-catalyzed non-oxidative methane dehydroaromatization have suggested this reaction should be operated at a CH_4 space velocity as high as possible to gain a performance-acceptable CH_4 conversion and benzene yield simultaneously. Since space velocity is a combined value by dividing a given CH_4 flow rate with catalyst load, there is a need to clarify either CH4 flow rate or catalyst load is more crucial for maximizing the catalyst performance. In this study a series of experiments modes were designed and conducted in multi-layer catalyst bed operation modes to clarify the effects of both variables on the activity stability of Mo/HZSM-5 catalyst. The results have shown there exists a suitable combination of CH_4 feed rate and catalyst load (bed height) for the system to reach its maximum performance.

III-PP23

Preparation and Characterization of Pt-Sn/C Electrocatalysts for Direct Methanol Fuel Cells

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INCAPE

Pt-Sn anodic catalysts supported on multiwall carbon nanotubes and Vulcan carbon were prepared using a deposition-reduction technique with sodium borohydride, characterized by different techniques and tested as anodes in a single direct methanol fuel cell at low temperatures. Characterization and CO stripping results indicate the presence of promoting effects of Sn over Pt in catalysts supported on Vulcan carbon and carbon nanotubes. This would mainly be caused both by geometric modifications induced by Sn placed in the surroundings of the active metal phase and probable electronic effects. These promoting effects make the oxidation of CO to CO2 at low potentials easier, thus improving the CO tolerance of the anodic electrocatalyst. When catalysts were tested in a DMFC, Pt-Sn catalysts supported on Vulcan carbon and carbon nanotubes gave a better power density than a commercial one mainly when working at low current densities

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III-PP24

The Use of Mixed SiW_nMo_{12-n} Heteropolyanions for Preparation of Ternary Transition Metal Sulfide Hydrotreating Catalysts

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The aim of the work was the preparation and characterization of alumina supported mixed SiW_nMo_{12-n} heteropolyanions (HPAs). For comparison purposes, catalysts based on separate $SiMo_{12}$HPA and SiW_{12}HPA were also prepared and studied. It was found that the use of mixed SiW_nMo_{12-n}HPAs as starting precursor yield high-efficient ternary transition metal sulfide HDT catalysts. This can originate from the close presence of both metals in the active sulfide phase as H_2-TPR results evidenced a modification of the metal oxides reduction.

III-PP25

Production of Palladium Filters with Using of Diffusion Welding

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For extracting high-purity hydrogen from hydrogen-containing gas mixtures design of filtration membrane element in which flat discs with a diameter of 50-150mm foil of palladium alloys with thickness of 50 to 10 microns are used as membranes is promising to create effective and reliable industrial membrane elements and modules.

The use of diffusion welding in the manufacture of such elements allowed to make a vacuum-tight full-strength connection of stainless steel frame 0.5 mm thick with foil of palladium alloys thickness 30 micron, that is to have sealed on helium wall membrane element. Chosen optimum welding conditions provided yield 85%.

III-PP26

Mn-based Water Oxidation Catalysts Supported on Tin Oxide

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In the context of growing demand for efficient energy storage solutions, PEM-electrolyzers allow for hydrogen production at high pressures through water splitting. So far, anodic electrocatalysts rely on expensive noble metals like iridium. Hence, activity and stability enhancement of earth-abundant OER-catalysts would be a major step towards making water splitting a commercially relevant energy storage solution.

We used a facile co-precipitation synthesis route followed by calcination for the preparation of Mn/Sn-based OER-catalysts. Oxygen evolution activity was assessed via detection of O_2 in an air tight sacrificial agent test setup coupled to a mass spectrometer. By combining these results with temperature programmed reduction analysis, we found that for Sn-loadings above 33% there exists a synergetic effect of Mn- and Sn-species, that stabilizes the active OER-sites of an amorphous Mn-oxyhydroxide towards thermal decomposition. First tests suggest that this synergy correlates with resilience against corrosion. Thus Mn/Sn-based OER-catalysts constitute promising candidates for OER-electrocatalysis.

III-PP27

Investigation of Co-effect of 12-tungstophosphoric Heteropolyacid, Nickel Citrate and Carbon-Coated Alumina in Preparation of NiW Catalysts for HDS, HYD and HDN Reactions

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The objective of this work was to investigate the co-effect of 12-tungstophosphoric heteropolyacid (HPA), nickel citrate and carbon-coated alumina (CCA) in preparation of NiW catalysts for HDS, HYD and HDN reactions. Comparing the active phase morphology, the $(Ni/W)_{edge}$ ratio and catalytic properties of the Ni_6-$PW_{12}S/C_x/Al_2O_3$ catalysts it was found that TOF numbers in HDS, HYD and HDN linearly increased with the decrease of both the average length of the species of the active phase and the $(Ni/W)_{edge}$ ratio. Further improvements of supported NiW catalysts may be achieved by increasing the dispersion of the active phase species and optimizing the $(Ni/W)_{edge}$ ratio.

III-PP28

Ni (II) Complex of Pyridyl Containing Eight-membered Cyclic Aminomethylphosphine – Basis for Design of Homogenous Catalysts

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The method of the synthesis of the initial 6-methyl-2-phosphinopyridine and 1,5-diaza-3,7-diphosphacyclooctane with 4-methylpyridyl substituents on phosphorus atoms was developed. The reaction of obtained 8-membered cyclic aminomethylphosphine with Ni(II) leads to the formation of bis-P,P-chelate complex with four nitrogen atoms in the second coordination sphere. Obtained complex demonstrates perfect results as a catalyst in the electrochemical hydrogen oxidation or production, which makes it one of the most perspective catalysts for the non-platinum fuel cell design.

III-PP29

Non-noble Metal Based Carbon Electro-catalysts for CO_2 Reduction to Fuels in Liquid and Gas Phase Conditions

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In this contribution, we report on the non-noble metal loaded carbon based electro-catalytic reduction of CO_2 for the production of liquid fuels under gas and liquid phase conditions. The experiments were performed in different homemade electro-catalytic (EC) cells for gas and liquid phases, designed on purpose to maximize the electro-catalytic area and reduce the volume of the aqueous solution. Initially, experiments were conducted using Cu thin film electrodes. Then, metal nano-particle based catalysts (using Fe, Cu, Co deposited on carbon-based substrates) were synthesized in order to improve the productivity and fine tune the selectivity in achieving longer chain hydrocarbon fuels. NMR analysis is performed to determine the fuel productivities. The liquid phase experimental setup CO_2 reduction yielded in higher productivity in the ratios of (25-75):1 in comparison to the gas phase, producing formic acid, acetic acid, di-methyl ether, and also trace amounts of methanol.

III-PP30

Operando X-ray Absorption Spectroscopy Studies of Co_3O_4 and CeO_2-Co_3O_4 Catalysts during Preferential CO

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In this study, we aimed to boost the understanding of preferential CO oxidation (PROX) over cobalt based oxide catalysts and shed a light on the questions: what is the electronic and geometric structure of Co and Ce during PROX, what are the active sites and reaction pathways. The operando Co K edge and Ce L_3 edge X-ray absorption near-edge spectra for Co_3O_4 and CeO_2-Co_3O_4 during PROX, CO- and H_2-temperature programmed reduction demonstrate that the reduction temperatures of CeO_2-Co_3O_4 and for Co_3O_4 in CO/He and H_2/He atmospheres are lower than in the PROX reaction mixture. Moreover, the electronic structure of Co and Ce for Co_3O_4 and CeO_2-Co_3O_4 catalysts does not change in PROX when CO oxidation is the dominant reaction. The Mars-van-Krevelen mechanism for PROX on these catalysts is rather excluded.

III-PP31

Supported Gold Nanoparticles for Formic Acid Dehydrogenation

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Supported gold nanoparticles were synthesized using sonochemical and deposition precipitation methods. Transmission electron microscopy (TEM), X-ray diffraction (XRD), UV-Vis, diffuse reflectance infrared Fourier transformed spectroscopy (DRIFTS) and steady state fixed bed reactor were used to explore the relationship between the gold catalysts and their catalytic performance in formic acid dehydrogenation. TEM reveal that sonochemical method produces small gold nanoparticles, averaging around 6 nm. Catalyst activity for formic acid dehyrogenation and selectivity to hydrogen is increasing with decreasing gold particle size.

III-PP33

Iron(II) Clathrochelates as Homogeneous Electrocatalysts of Hydrogen Production at Low pH

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Increasing energy demands of an ever-growing population calls for new energy sources, one of them being molecular hydrogen. To make hydrogen-based economics a reality, highly efficient and chemically stable catalysts for hydrogen production that do not contain precious platinum group metals need to be designed. For this purpose, we suggest to use iron(II) clathrochelate complexes with functionalizing pyridinyl substituents. The complexes obtained efficiently electrocatalyze hydrogen evolution from an acid solution in acetonitrile as well as from aqueous buffers with low pH (1 – 4). Titration of an acetonitrile solution of a clathrochelate with an acid resulted in a significant increase of the current assigned to the $Fe^{2+/+}$ pair, while the peak of the reverse process vanished. Thus, pyridinyl-functionilized iron(II) clathrochelates emerge as first homogeneous electrocatalysts of hydrogen evolution at low pH; varying their ribbed substituents allows designing electrocatalysts with better performance and stability in harsh near-industrial conditions.

III-PP34

Pt, Rh and Pt-Rh-deposited on $MgAl_2O_4$ Spinels Catalysts for Dry and Steam Reforming of CH_4

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In this work, a $MgAl_2O_4$ mixed oxide was obtained for combining the thermal stability of alumina and the basic properties of MgO. This material was used as support for the synthesis of Pt, Rh and Pt-Rh catalysts, those being tested in the dry and steam reforming of methane. The aim of this study is to analyse the interaction of the $MgAl_2O_4$ support with the active phase, and to evaluate its influence in the catalytic performances. It was found that the time and temperature of calcination of the $MgAl_2O_4$ strongly influences the interaction of the cations and the MgO segregation, affecting the catalytic activity and the metallic dispersion. The systems with Pt are the most active ones, especially under steam reforming conditions. Simulation studies demonstrated that combining steam and dry-reforming conditions allows obtaining a syngas with a H_2/CO ratio of 2, suitable for feeding the FT processes

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III-PP35

Hydrogen Storage System Based on the Catalytic Hydrogenation-dehydrogenation Reactions of Aromatic Compounds

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Evaluation of the performance of catalytic composite systems was carried out by comparing the rate of hydrogen evolution from hydrogenated condensed aromatic chemical hydrides (decalin, bicyclohexyl, perhydroterphenyl) in the dehydrogenation process. Catalytic tests have been carried out at temperatures 280–340°C and flow rates 0.5-3 h^{-1} with various catalysts based on Pt, Pd, Cr and Ni in a flow reactor. The largest amount of hydrogen released as a result of perhydro-m-terphenyl dehydrogenation to m-terphenyl is observed with the 3%Pt/Sibunit catalyst at 320°C and 1 h^{-1}. The selectivity and conversion toward complete dehydrogenation in this case is 95%. The selectivity and conversion of m-terphenyl hydrogenation to perhydro-m-terphenyl using this catalyst was higher than 99%. The high purity of hydrogen was proved by chromatography for the dehydrogenation reaction.

III-PP36

Oxidative Coupling of Methane over Li Doped MgO on a Monolithic Structure

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Abundant resources of natural gas, which is mainly methane, have motivated researchers to produce valuable products from this simple hydrocarbon. The aim of such conversion is to ease its transport and increase its value. Intensive researches have been done, and Li doped MgO showed higher performance than most other materials. Our aim is to investigate the effect of a monolithic structure on Li doped MgO prepared from different precursors and different preparation techniques. We also are investigating the effect of temperature and methane to oxygen ratio on both monolith and particulate catalyst. The methane conversion increased with increasing temperature while the C_2 selectivity increased first, and then it decreased after 800 °C. Our experiments show that oxidative coupling of methane can be performed over the monolithic structure, which are better for providing void volume for CH_3 combination reactions, and for better flow and heat management properties compared to particulate catalyst.

III-PP37

Ceria-supported Cobalt Oxide Catalysts: Synthesis, Characterization and Catalytic Combustion of Producer Gas

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The catalytic combustion of producer gas has not been much explored. Since the use of producer gas as a fuel is expected to find more interest in future, it’s important to study environmental and safety hazards associated with it, mainly due to its very high CO and hydrogen contents. This study will draw the attention and need for catalytic combustion of toxic producer gas. Co/CeO_2 as producer gas combustion catalyst was synthesized through incipient wetness impregnation and evaluated for its catalytic combustion efficiency. Our preliminary results inferred that the complete combustion of producer gas can be achieved even at moderate temperatures, commonly used for producer gas based combustion devices.

III-PP39

Cyclization of Normal Alkanes to Arenes and Cycloalkanes

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The objective of the research was to assess the current state of scientific research and the identification of promising areas in the field of cyclization of n-alkanes.During the work, we analyzed the data on the supposed mechanism of the cyclization process and the catalysts applied.

Considered literature suggests that mechanism of alkanes cyclization reactions over platinum catalysts has been studied well. It is shown that along with alumina, zeolites in the cyclization catalyst also have activity and selectivity to the cyclization of alkanes with 6 or more carbon atoms. It is established that monofunctional catalysts containing Pt as an active component deposited on a non-acidic zeolite (type L in K-form) exhibit high activity in reactions of cyclization of n-alkanes. Rhenium and analogues (iridium, palladium) can be used to improve activity of the catalyst in the target reactions, either directly by improving conditions of the reactions of hydrogenation and dehydrogenation, and by preventing deactivation of active sites. Results of the literature review on paraffin cyclization allow to determine the main directions of research to create a highly efficient catalyst for the cyclization of normal alkanes in the arenes and cycloalkanes.

III-PP40

Catalytic and Electrochemical Properties of (Cu, Ti)-YSZ for IT-Sofcs Anode

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Solid oxide fuel cells (SOFC) offer a promising way of converting chemical energy into electrical energy with great efficiency. SOFC devices need to possess simultaneously a ionic conductivity induced by the presence of oxygen vacancies and an electronic conductivity induced by the added metal together with a high porosity allowing the fuel transport through the anodic layer. The self-assembling method using Triton X100 as template was used for (Cu, Ti) –YSZ synthesis. Our proposed synthesis method favors uniformity of the crystalline network and an improvement of the ionic and electronic conductivity as well as of the catalytic activity. The XRD patterns confirm formation of cubic phase of fluorite type at 700°C and also a secondary phase with monoclinic symmetry, isostructural with tenorite (CuO) at 900°C. The composite show high methane conversion and CO selectivity in the catalytic partial oxidation of methane. Conductivity results showed a predominately n-type behaviour, highlighting a promising IT-SOFC anode.

III-PP41

Photocatalytic Acetone Vapor Oxidation over TiO_2 under Controlled Periodic Illumination. Experimental and Modeling Study

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We investigated the effect of controlled periodic illumination on photonic efficiency of photocatalytic acetone vapor oxidation. It was demonstrated that photonic efficiency increases with higher frequency of light pulses and at some point reaches its maximum value which is equal to photonic efficiency obtained under the same average photon flux. Several kinetics were applied to the experimental data and had a good fit, so we could not discriminate any of them. However the common conclusion was that there are only two kinetically distinguishable active species on TiO_2 surface with the lifetimes in 10^{-3} - 10^{1} range. Thus we demonstrated that photocatalytic oxidation proceed via not primary charge carriers but through the radical mechanism

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III-PP42

Bimetallic Catalysts Containing Palladium and Gold on Carbon Support for Hydrogen Electrooxidation: From Au Particles Coated with Submonolayers of Pd to Pd-Au Nanoalloys

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The catalytic activity and CO tolerance of the carbon-supported PdAu nanoparticles with a high dispersion and various surface compositions prepared by two different synthetic strategies were studied in hydrogen electrooxidation reaction (HOR). The PdAu/C catalysts with controlled surface composition of the bimetallic sites prepared by selective electrodeposition of Pd on pre-immobilized Au particles (*a model approach*) proved to be a valid and convenient tool for determination of the surface composition of PdAu nanoparticles providing the maximum catalyst activity in HOR and CO tolerance. The PdAu/C catalysts prepared by impregnation of the Au/C substrate with Pd(II) nitrate solution followed heat treatments for obtaining the proper Pd-Au alloying (*a pragmatic approach*) showed the significantly higher HOR current densities compared to Pd-electroplated Au catalysts with similar surface Pd:Au composition. The catalysts containing the alloy Pd-Au particles of optimal surface composition are promising for application at the anodes of polymer-electrolyte membrane fuel cells.

III-PP44

Advances in Catalyst Characterization by FTIR spectroscopy

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Variable temperature FTIR spectroscopy of adsorbed molecules, besides characterization of surface acid and basic sites provides a great deal of important information about the surface of catalysts. This is the ability of solid to enhance interaction between the adjacent sites, which can lead to the induced acidity (or superacidity) and basicity. The structure or shape of the absorption bands provide information about local arrangement of surface sites or the geometry of adsorbed layers. One more property of certain surface sites tested by variable temperature spectroscopy is their capability for linkage isomerism, when a molecule forms with surface site complexes of different geometry, such as CO bound to the cations via carbon or oxygen. To measure the surface site concentration, the factors affecting the absorbance of adsorbed probe molecules should be known. Spectroscopy with simultaneous temperature and pressure control provides information about the thermodynamics of adsorption.

III-PP45

New Nanodiamonds/TiO_2 Composite Materials for the Solar Energy Conversion into Hydrogen by Water Splitting

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The aim of this study is the control, the optimization and the characterization of Nanodiamonds/TiO_2 composite materials in order to produce hydrogen by water splitting. Different strategies of synthesis have been carried out in order to obtain the composite material. A sol gel one and another one by impregnation of nanodiamonds on TiO_2. Platinum, a co-catalyst, is used to increased the yield of production of hydrogen. Methanol, a sacrificial agent, is used for the same purpose. The efficiency of the different synthesis is study and the catalysts are compared to the industrial one TiO_2-P25. An innovative result on the production of hydrogen from Pt-free composite Nanodiamonds/TiO2 materials will be demonstrated.

III-PP46

Pt-SnO_x-TiO_2 Catalysts for Methanol Photocatalytic Reforming: Influence of Co-catalysts on the Hydrogen Production

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Photoinduced reforming of methanol on semiconducting oxides for H_2 production has been in the focus of recent research efforts. Good photocatalytic performance often requires the combination of the semiconductor with a proper co-catalyst, which can enhance the activity by orders of magnitudes. In this work tin modified TiO_2 photocatalysts were prepared by sol-gel method (SG) and by Controlled Surface Reaction (CSR) between $Sn(C_2H_5)_4$ and TiO_2 while Pt loaded by impregnation was used as co-catalyst. SG catalysts showed enhanced activity when calcination was used for activation of the co-catalyst. Tin introduction increased their photocatalytic H_2 yield, regardless if H_2 treatment or calcination was applied to evolve the co-catalyst. Sn introduction by CSR was beneficial only in the calcined case, suggesting a difference in the nature of the Sn species in the SG and CSR samples. These observations will be discussed in detail based on XPS and chemisorption results.

III-PP47

New Approaches for Solar Fuel from Suspended Photocatalysts

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It was proven in the early 1970s that water can be split photo-electrochemically. Since then, several semiconductor materials for the conversion of harvested light energy into utilizable *solar* fuels have been investigated as heterogeneous photo- or electrocatalysts. It was the aim of this work to investigate possible quantum size effects when depositing a promoter onto a semiconductor for the hydrogen evolution. Therefore, two reference semiconductors were chosen on which Co_3O_4 with different crystal sizes were deposited (TiO_2 and g-C_3N_4). While the presence of Co(II) compounds were previously shown to enhance the photocatalytic activity of semiconductors, the effect of nanoparticle size investigations have not been reported yet. In order to study the success of the particle deposition and the size of the cobalt oxide particles, the modified semiconductors were examined thoroughly. Co_3O_4 was discussed to decrease the overpotential of the water oxidation reaction and stabilize electron holes leading to a higher photocurrent.

III-PP48

Synthesis of Mesoporous SnO_2 as Anode for PEMFCs

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SnO_2 is an important n-type semiconductor material, which has been widely used in many applications that strongly depend on the material structure and morphology. Therefore special attention must be paid to the development of reproducible and cost efficient preparation methods of this material. A number of processing methods such as co-precipitation, sol-gel, chemical vapour deposition, laser ablation and thermal redox process have been developed for the preparation of SnO_2. In this study the synthesis of mesoporous SnO_2 by a hydrothermal route, using a nonionic surfactant – Triton X100 as template, is reported. Mesoporous pure tetragonal SnO_2 was obtained by hydrothermal synthesis route. Surface chemistry investigations showed that valence state of Sn is only +4. The oxygen excess found on the surface comes from OH groups and water adsorbed from environment. The preliminary results obtained in this study show that this material is a good candidate for anode in PEMFC applications.

III-PP49

Ni-based Catalysts for Methane dry Reforming: EXAFS, TEM and DRIFT Investigation on the Au/Pt/Pd Effects

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We have recently shown that trimetallic NiAuPt/Al_2O_3 catalyst, containing only 0.2wt% of Au and 0.2wt% of Pt showed improved catalytic activity and stability to carbon poisoning with respect to the monometallic Ni and to the bimetallic Ni-Au and Ni-Pt systems. Such promoting effect for the trimetallic catalyst was attributed to the formation of high active Ni-Au-Pt nanoparticles, synergistically interacting, where growth of small amount of bamboo-like carbon nanotubes occurs. In order to get more insights into the structural and surface properties of such NiAuPt/Al_2O_3 catalyst EXAFS analyses and DRIFT investigations of CO chemisorbed species were carried out. Monometallic Ni and bimetallic NiAu, NiPt and NiPd/Al_2O_3 catalysts were studied for comparison. EXAFS and DRIFT characterizations point out the occurrence of structural and geometrical effects induced by the addition of AuPt to Ni/Al_2O_3. The NiAuPt/Al_2O_3 catalyst demonstrated good catalytic stability during a 5 days long run at 750 °C

III-PP50

Catalysts (NiMg)AlO_x + CeO_2 Derived of Hydrotalcite Type Structures Applied to Dry Reforming of Biogas

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Four catalysts with different nominal nickel contents in weight (x= 5, 10, 15 and 25%) derived from hydrotalcites mixed oxides (NiMgAlO_x + CeO_2) promoted with CeO_2 and prepared by coprecipitation technique, were studied in this work. They were employed in biogas dry reforming to produce syngas (H_2+CO), which can be applied as raw material to synthesize liquid hydrocarbons similar to diesel and gasoline by means of Fischer-Tropsch processes. The main problem of the biogas reforming is formation of carbon deposits over the catalyst surface. That is why catalysts derived from hydrotalcites mixed oxides associated with CeO_2 were chosen to be employed in this reaction, once they feature basicity to ensure carbon removal. The catalysts presented here were all actives and stables, except the one derived from (NiMg)$AlO_{25\%}$ + CeO_2 mixed oxide. H_2/CO ratios obtained make the syngas produced able to be applied as raw material to Fischer-Tropsch processes.

III-PP51

Role of Rh as a Promoter on the Activity of Ni/CeO_2-ZrO_2 Catalyst for Oxidative Steam Reforming of Bio-ethanol

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The catalytic oxidative steam reforming of ethanol (OSRE) for hydrogen production was studied over two selected catalysts Ni/CeO_2-ZrO_2 and Rh-Ni/CeO_2-ZrO_2. The catalysts were prepared by impregnation-co-precipitation method and characterized by BET, XRD, TPR, TPD, TGA, SEM and TEM techniques. The effects of temperature, steam to ethanol (S/E) molar ratio, and space time on conversion and product selectivities were investigated in a tubular fixed bed reactor at atmospheric pressure with ethanol:water:oxygen molar ratio of 1:9:0.5 over a temperature range of 400 to 650°C. Conversion increased with temperature and complete conversion achieved at 600°C on 30%Ni/CeO_2-ZrO_2 with maximum hydrogen yield of 3.6 mol H_2/mol ethanol reacted. Ethanol conversion and H_2 selectivity increased with increasing contact time while CO and CH_4 selectivity decreased. Using Rh impregnated catalyst maximum 72% H_2 selectivity and 4% CO selectivity is obtained at same reaction conditions. Incorporation of Rh on Ni/CeO_2-ZrO_2 catalyst improved catalytic activity by enhancing water gas shift reaction.

III-PP52

Ethanol Steam Reforming over $Mn_xCr_{3-x}O_4$-based Spinel-type Oxide

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This work presents results of design of ethanol steam reforming (ESR) catalysts based on spinel-type oxides $Mn_xCr_{3-x}O_4$ promoted by Ru+Ni. Mixed oxides $Mn_xCr_{3-x}O_4$ (x=0.3-2.7) were prepared via modified Pechini route. Ni and Ru (2 wt.%) were supported by the incipient wetness impregnation. Structural features and microstructure of catalysts were characterized by X-ray diffraction, TEM with EDX, UV-Vis and XPS, reactivity - by H_2 and EtOH TPR. The catalytic properties of samples in ESR were studied in diluted and concentrated feeds. According to XRD and UV-Vis data, samples are comprised of several phases. A high activity was observed for catalysts containing $MnCr_2O_4$ spinel phase. Catalysts based on 2%Ru+2Ni%/$MnCr_2O_4$, both bulk and supported on Al_2O_3, showed the best results. According to *in situ* IR spectroscopy data, ESR on spinel-based catalysts proceeds via dehydrogenation route.

III-PP53
Syngas and Hydrogen Production by Dry and Steam Reforming of Methane and Fermentation Products on Porous Ceramic Membrane-Catalytic Ni-Co-containing Converters

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Original porous ceramic membrane-catalytic Ni-Co-containing converters highly efficient in dry and steam reforming of methane and fermentation products into syngas and hydrogen were developed. The structural peculiarities of these converters and their impact on processes character were studied.

III-PP54
Dry Reforming of Propane over CeO_2/Ni-foam Catalysts

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Nanocryatalline CeO_2 loaded nickel foam (NF) catalysts were investigated in order to evaluate the effect of the support structure on the catalytic activity towards C_3H_8 dry reforming. 2-4 wt.% of CeO_2 catalysts supported on Nickel Foam were prepared and tested for catalytic CO_2 reforming of propane to synthesis gas. The prepared catalysts were characterized by XRD, FESEM, TEM, EDX dot-mapping, and BET analysis. The activity measurements exhibited that the catalytic activity of 4% CeO_2 /NF was much better than those of 3 wt.% and 2wt.% CeO_2 /NF in terms of C_3H_8 and CO_2 conversion. Although Ni-based catalysts have been intensively employed in reforming reactions, they commonly suffer severe deactivation due to sintering of metal particles and carbon deposition. It was observed that CeO_2-promoted NF exhibited excellent dry reforming activity with good stability against sintering and coke formation.

III-PP55
A Catalytic Heater for an External Combustion Engine

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A catalytic heater was designed for external heat-engine applications. The heater is attached to the heat engine such as to maximise the heat transferred to its working fluid. The high heat fluxes that be attained are highly beneficial for the performance of external combustion engines. Tests reveal low emission levels, and a favorable ability to easily vary the output thermal power and temperature.

III-PP56
Ethanol Steam Reforming to Hydrogen over CoNi-based Catalysts

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The objective of present work was to explore the catalytic performance of Co, Ni and CoNi catalysts supported on $MgAl_2O_4$ in ethanol steam reforming (ESR). The effect of Co addition to Ni catalyst on the structure and surface properties was analyzed. The catalysts were characterized by XRD, XPS, EXAFS, XANES and TEM. Catalytic tests in ESR were performed in a fixed-bed quartz reactor at atmospheric pressure and temperature range of 250^0 - 700^0C. A molar ratio H_2O/C_2H_5OH of 3 was kept. It was concluded that the different behaviours of catalysts in ESR are related to the oxidation state of metallic components. A correlation between the cleavage of C-C bond, producing CO_2 and H_2, and the degree of reduction and metallic area was found for catalysts. The bimetallic CoNi catalyst was more tolerant to carbon formation, showing better ability to oxidize the carbon due to the alloy formation.

III-PP57
A Study on Kinetics of Methane Oxidative Steam Reforming (OSR) over Pt-Ni/Al_2O_3 Bimetallic Catalysts

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In the current work, reliable power-law type of kinetic expression for methane OSR over Pt-Ni/Al_2O_3 catalyst is obtained as a function of temperature and partial pressures of methane, oxygen and steam. Kinetic study was performed for determining intrinsic reaction rates of methane OSR over 0.2Pt-10Ni catalyst at 375 °C. Multivariable non-linear optimization function of MATLAB^{TM} was utilized to estimate reaction orders. The proposed power-law type rate expression that is reliable in the range of $2.03 < S/C < 3.08$ and $4.0 < C/O_2 < 7.34$ feed ratios has reaction orders as 0.81, 1.60 and 0.44 in methane, oxygen and steam partial pressures, respectively. The apparent activation energy for methane OSR was calculated as 39 kJ.mol^{-1} and pre-exponential factor as 0.956 μmol.mgcat^{-1}.s^{-1}.kPa$^{-2.85}$ in the 350-400 °C interval.

III-PP58

Oxidative Steam Reforming of Logistic Fuels over a Spinel-derived Ni(17wt.%)/Al_2O_3 Catalyst

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In this work, the attention has been focused on the comparison of the reforming efficiency of various hydrocarbons such as methane, isooctane and *n*-tetradecane, selected as model compounds for natural gas, gasoline and diesel, respectively, in the oxidative steam reforming over a co-precipitated $NiAl_2O_4/Al_2O_3$ catalyst (600 ºC, 60000 cm^3 C g^{-1} h^{-1}). It was found that the high stability of OSR of CH_4 and *i*-C_8H_{18} was related to a negligible or minor coke deposition in comparison with *n*-$C_{14}H_{30}$. In this way the effect of unavoidable filamentous coke formation on the performance of heavy hydrocarbons, with a less impact on the OSR(*i*-C_8H_{18}), could be minimised with higher reforming temperatures or higher H_2O/C ratios.

III-PP59

Modifying $LaNiO_3$ Perovskite-type Oxide Catalyst with Co for the Methane CO_2 and CO_2+H_2O Reforming

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In this contribution, a series of $LaNi_{1-x}Co_xO_3$ perovskite-type oxides was well-characterized and tested in the dry and (CO_2+H_2O) mixed reforming of methane with the aim to improve the H_2 selectivity and study the catalysts stability .

The ternary oxides $LaNiCoO_3$ were synthesized via citrate method using metallic nitrate precursors. Catalysts were characterized before and after reaction by conventional methods. Steady state experiments were carried out at atmospheric pressure.

TEM images recorded before reaction confirm the presence of Ni particles together with a phase corresponding to the lanthanum oxycarbonate in the $LaNi_{1-x}Co_xO_3$ catalysts. For $LaCoO_3$ the TEM micrographs have revealed the formation of $LaCoO_3$ particles with perovskite structure and their tendency to agglomerate. After reaction some particles appear to be aggregated, the nickel particle size being comprised between 5-15 nm and as were recorded by EDAX analysis correspond to Ni^0. Additionally, it can be observed carbon nanotubes formation, where a variable carbon content between 10-20% for the serie, were registered from the elemental analysis.

CH_4-conversion and H_2-selectivity for dry and mixed reforming for $LaNi_{1-x}Co_xO_3$ catalysts showed that the conversion rates of CH_4 increased in those catalysts with highest Ni content for the CO_2 reforming of methane. While the activity in terms of CH_4 conversion was similar for those Ni/Co mixed oxide catalysts by the presence of water vapor.

Hydrogen yields depend on metal and the ratio of Ni to Co. The best performance in terms of highest hydrogen yield was achieved with the $LaNiO_3$ and $LaNi_{0.8}Co_{0.2}$ catalysts for methane dry reforming. Otherwise, the positive effect of water vapor in the selective reforming of methane was also observed in the H_2-selectivity over $LaNi_{1-x}Co_xO_3$ serie, achieving similar H_2-values above 923K; as well as a significant reduction of the coke formation performed by Co incorporation in the mixed oxides.

III-PP60

Development of Sulphur Tolerant Catalysts for the Conversion of Carbon Dioxide to Methane

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The increasing generation of electricity from renewable sources such as wind and sunlight requires the development of storage capabilities for excess energy, which cannot be taken up by the electrical grid. The synthesis of methane from hydrogen and carbon dioxide is a promising route of chemical storage. Ceria supported ruthenium catalysts were prepared and coated into microchannels for the conversion of carbon dioxide to methane with the final aim to design methanation reactors with improved heat management through integrated heat-exchange. However, carbon dioxide originating from renewable sources such as biogas plants may contain trace amounts of sulphur species which poison the catalysts. The main target of the development work was to improve the sulphur tolerance of the ruthenium catalysts through addition of other noble metals, nickel and other additives. The stability of the catalysts could be improved significantly, though further development work is required to achieve the stability required for the technical process.

III-PP61

Combined Aging Processes during Bio-Syngas Methanation for SNG Production

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This study focuses on the conversion of bio-syngas obtained from biomass gasification to synthetic natural gas (SNG). It evaluates the kinetic sensitivity of Ni based catalysts to various poisons, in parallel with metal particle sintering occurring under SNG conditions. From a combination of state-of-the-art DRIFT/SSITKA operando techniques, a rationale of these aging processes is proposed on the basis of a direct evaluation of active reacting intermediates nature and concentration. The reversible poisoning of N and Cl containing species affects essentially surface controlling steps such as hydrogenation of CH_x intermediates deriving from carbonyls decomposition, via a reversible electronic transfer from Ni to the electrophilic additives. A reverse effect would characterize the promoting effect of alkali addition. For tar-type hydrocarbons, the absence of electronic effects explain their negligible toxicity, unless surface coking and diffusion limitation. S containing molecules neutralize part of the catalytic bed without changing the reactivity of the non-poisoned metal.

III-PP62

Highly Efficient Fischer-Tropsch Synthesis over Fe and Co Catalysts on Carbon Containing Inorganic Supports

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One of the main problem of the low activity and stability of Fe and Co based catalysts during Fischer-Tropsch synthesis is strong interaction with conventional inorganic supports (alumina, silica) leading to deactivation of catalysts by formation of inactive silicates (M-O-Si), segregation and low contribution of active phase (metal, carbide). This work aims at developing of new catalytic systems for FT synthesis by addition of carbon layer between metal and silica. Metal has been in contact with the source of carbon before impregnation or has been supported on silica preliminary coated by the layer of carbon. Our results show that presence of carbon leads to significant increase of activity and stability of Fe and Co based catalysts. The main effect is due to significant increase of the dispersion of metallic nanoparticles, suppression of metal deactivation by formation of silicates and increase of the active phase (χ-Fe_5C_2) by interaction with carbon.

III-PP63

Glycerol Steam Reforming over Modified Ni/Al_2O_3 Catalysts

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The effects of B_2O_3 and La_2O_3 on the performance of Ni/Al_2O_3 catalysts for the steam reforming of glycerol are investigated. Ni content is 10 wt % in all catalysts. Physicochemical characterization includes BET, BJH, XRD, DRS TPR, HR-TEM and TPH-TPO for carbon measurement. Catalytic behavior was investigated in the temperature range 400-800 °C. The support presents a considerable activity for the dehydration reactions and influences the selectivity. The presence of a second oxide on Ni/Al_2O_3 catalyst alters the catalytic behaviour and the resistance to coking. However, this is not due to changes in the texture and/or nickel dispersion, but is related to the different metal-support interface and/or to a synergy effect.

II-PP64

The Oxygen Electroreduction Reaction Performance of Pt/C Catalysts Based on Nanostructured Carbon Supports: from the RDE to the PEMFC Studies

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In this paper, a series of Pt/C catalysts based on initial and modified nanostructured carbon supports (carbon nanotubes and carbon nanofibers) with a platinum content of 20 and 40 wt. % was synthesized. The catalysts were investigated by TEM, CO chemisorption and electrochemical methods (electrooxidation of CO, the method of impedance spectroscopy). The activity of catalysts in the oxygen electroreduction reaction (ORR) were obtained by rotating disk electrode in a 10 - 35 ^{o}C temperature range using 0.1 M $HClO_4$ electrolyte solution and in an oxygen-hydrogen fuel cell at 80 ^{o}C. It is shown that the use of the carbon nanotubes allows to improve significantly the catalyst performance in both electrochemical and fuel cells. The paper discusses the influence of pore structure and morphology of carbon supports on the properties of Pt/C catalysts and their performance in the ORR.

III-PP65

Mathematical Modelling Method Application for Catalytic Reforming Catalyst Operating Conditions Optimization in Industrial Reactors

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Catalytic reforming of naphtha is one of the most important processes for high-octane gasoline manufacture and aromatic hydrocarbons production. The naphtha reformer is used to upgrade low octane heavy naphtha that is unsuitable for motor gasoline. Nowadays mathematical modeling of industrial processes has become the universally recognized method of solving problems on increase of efficiency and creation of new technological processes and apparatuses.

In this paper the application of mathematical modeling method monitoring of catalytic reforming unit L-35-11/450K is proposed. The mathematical model-based system “Catalyst’s Control” was used for catalytic reforming installation monitoring. The mathematical model created can be used for optimization and prediction of operating parameters (octane number, reactors outlet temperature, pressure and yield) of the catalytic reforming process. It is shown, that the work on the optimal activity allows increasing product output with a constant level of production costs, and get the information about Pt-Re catalyst work efficiency.

III-PP66

Methanol Synthesis from CO_2 and H_2 on Cu/ZnO Catalysts

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We investigated Cu/ZnO catalysts in methanol synthesis, applying different Cu contents, calcination temperatures and two different synthesis methods: a modified citrate route and coprecipitation. Using the different synthetic methods it was possible to vary copper crystal size in the 12-32 nm range and to investigate its effect on the catalytic performance. Mechanical mixtures of separately prepared CuO and ZnO were also studied. The catalysts were tested for methanol synthesis in mild conditions (7 bar, 140-250°C, GHSV 40 ml/min/g_{cat}).

Results provides insight to the synthetic approach of catalysts using copper and zinc oxides and in the study of the mechanistic aspects of work of catalysts containing these oxides.

III-PP67

Active Site Analysis of Sulfided $NiMo/Al_2O_3$ Catalyst for Hydrodesulfurization of 4,6-Dimethyldibenzothiophene

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The nature and number of active sites of the sulfided phosphorus-added $NiMo/Al_2O_3$ catalyst for the hydrodesulfurization (HDS) of 4,6-dimethyldibenzothiophene (DMDBT) were estimated based on a transient study of the addition of nitrogen compounds to the HDS. The two-site mechanism is well known for the HDS on Mo containing catalysts; one site for the hydrogenation and the other site for the desulfurization. However, the simultaneous rapid desulfurization and hydrogenation of DMDBT to dimethylbicyclohexyl (DMBCH) or methylcyclohexyltoluene and of octahydrodibenzothiophene to bicyclohexyl during the dibenzothiophene HDS and the denitrogenation of *o*-propylaniline to propylcyclohexene during the quinoline hydrodenitrogenation are still debated. In this study, a new approach to the site-type analysis of the active sites for the HDS of DMDBT using the transient method proposed the presence of a third active site for the simultaneous desulfurization/hydrogenation of DMDBT to DMBCH as well as the two sites for the hydrogenation and the desulfurization.

III-PP68

Activity and Selectivity of Pt/Al_2O_3 and Metal Oxide Catalysts for NH_3 Combustion

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Catalytic activity and product selectivities of Pt/Al_2O_3 and metal oxides for NH_3 combustion have been studied. Pt/Al_2O_3 showed high catalytic activity for NH_3 combustion, but N_2O and NO_x selectivities of that catalyst were high. In case of metal oxide catalysts, MnO_2 and Co_3O_4 also exhibited the higher activity than the other metal oxides, which implied that the catalytic activity of metal oxide correlates with its oxygen bond energy. On the combustion under both excess O_2 and stoichiometric condition, Pt/Al_2O_3 and metal oxide catalysts showed the high selectivities of N_2O and NO_x. However, CuO catalyst exhibited the high N_2 selectivity on the stoichiometric reaction.

III-PP69

Amine Formation on Medium Temperature Water Gas Shift Catalyst. Role of Reaction Parameters

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H_2 is a relevant raw material and a promising fuel; SR-WGS of CH_4 is currently the main source of H_2. In the SR reactor small amounts of NH_3 forms, that in WGS one give rise to amines, that dissolve in unconverted water, recycled for economic reasons to pre-reforming reactor, where form coke. This work reports the role of the reaction parameters in presence of NH_3 on MeOH and amine formation in the WGS at Medium Temperature, i.e. in just one step to decrease the operational costs. The investigated Cu-containing catalysts reached CO conversion equilibrium values regardless of the temperature; only the thermodynamically favoured TMA was detected (>150 ppmwt). The increase of P and contact time favoured the formation of MeOH and amines, while a higher S/DG value played an opposite effect. A correlation may be hypothesized between MeOH and amine formation, suggesting that amines formed by reaction of NH_3 with MeOH surface intermediates.

III-PP70

Benefits of Hierarchization of HMFI Zeolites on the Coke Management

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The effects of the presence on HZSM-5 zeolite of macropore and/or mesopore on the coke formation are highlighted in two reactions: transformation of methylcyclohexane and ethanol conversion into hydrocarbons. The relationships between the textural properties of zeolites and the composition(s), location(s) and toxicity (ies) of coke(s) are discussed.

III-PP71

Biodiesel Production from Entirely Renewable Feedstocks

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Typically, biodiesel is produced using vegetable oil and methanol as raw materials, and sodium methoxide as catalyst, whereupon the obtained product is composed of methyl esters. However, the use of ethyl esters as biodiesel presents many advantages compared to the methyl esters, specially taking into account the renewability of the raw materials employed to their production. In this work, the transesterification with ethanol to produce ethyl esters using sodium ethoxide as catalyst was studied. It was observed that methanolysis reactions are faster than the ethanolysis and sodium methoxide catalyst is more active than the corresponding ethoxide, due to the higher steric hindrance of the ethoxi-radical and to the more intense saponification of sodium ethoxide in ethanol medium.

III-PP72

Biogas Steam Reforming for Syngas Production with Structured Catalyst

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This work describes the synthesis and structuration of a modified Ni/Al_2O_3 catalyst in order to produce syngas with a H_2/CO ratio of 2 from a mixture of CH_4, H_2O, and CO_2. The catalysts support is modified with 10%wt of MgO, and later, a simultaneous impregnation of Ni (15%wt) and Ru (0,5%wt) was performed. Catalyst slurry was prepared in order to washcoat the monolith. XRD analysis showed clear evidence of RuO_2 in the slurry sample, while no evidence of Ru species was found in the powder sample. This difference was responsible of the great variance in catalytic activity, where the slurry gets deactivated after 5h but the powder stayed stable for 50h. Although the catalyst structuration generates a "less active" catalyst, the advantages of the catalyst structuration, where mass and heat transport processes are improved, increase the stability.

III-PP73

Cadmium and Tin Magnetic Nanocatalysts Useful for Biodiesel Production

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Magnetic mixed iron/cadmium (ICdO) and iron/tin (ISnO) oxide nanoparticles were used as catalysts in relevant reactions for biodiesel production technologies. These compounds were active for hydrolysis and transesterification of soybean oil as well as esterification of soybean oil fatty acids. In the esterification assisted by ISnO high yields, ca. 84%, were achieved, after 1 h reaction at 200 ºC. The oxide was magnetically recovered and reused four times without loss in its activity, while a loss of activity was observed for ICdO catalyst. ISnO also demonstrated catalytic activity for Macauba oil, a highly acidic substrate.

III-PP74

Carbon Dioxide (CO_2) Dry Reforming of Glycerol for Hydrogen Production using Ni/La_2O_3 and Co/La_2O_3 as Catalysts

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Glycerol dry reforming is considered as a promising route to improve the economic viability of biodiesel industry. The objective of this research work is to synthesize, characterize and conduct the catalytic activity test of CO_2 glycerol dry reforming using nickel (Ni) and cobalt (Co) as active phase supported on lanthanum oxide (La_2O_3) catalyst. The catalysts were prepared by using wet impregnation method and characterized via X-ray diffraction (XRD), Scanning electron microscopy (SEM), Bruanauer-Emmett-Teller (BET) and Fourier-Transform Infrared Spectroscopy (FTIR). The catalytic activity of Ni/La_2O_3 and Co/La_2O_3 were tested using a fixed bed reactor. The characterization analysis shows an excellence physicochemical properties for Ni/LA_2O_3 as compared to Co/La_2O_3. Reaction studies demonstrated that 10 wt% Ni/La_2O_3 gives the highest hydrogen yield and glycerol conversion and this is due to excellence catalytic performance demonstrated by the Ni based catalysts.

III-PP75

Catalytic Features Controlling HZSM-5 Zeolite Performance and Deactivation during the Cracking of 1-Butene to Propylene

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Acid MFI zeolite (HZSM-5) is used in catalytic processes linked with conventional and sustainable refining concepts. The outstanding performance of MFI zeolite is attributed to its unique acid and structural features, with very attractive shape selectivity for producing light olefins, and propylene in particular. In this work we have measured the correlations between the catalytic features (acid strength and porous structure) and its intrinsic performance (conversion, selectivity and deactivation) by a sensitivity and regression analysis, during the cracking of 1-butene to propylene using catalysts based on MFI zeolites of different SiO_2/Al_2O_3 ratio and modification degree with KOH and H_3PO_4. The properties of the catalyst has been asesed by elemenal analysis, XRD, ^{29}Si and ^{27}Al NMR, N_2 adsorption-desorption, adsorption-desorption of tert-butylamine (t-BA) and TG-TPO.

III-PP76

Catalytic Upgrading of Lignin Derived Pyrolysis Vapor via HZSM-5

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Lignin, obtained as a by-product from a second generation bio-ethanol plant, is pyrolyzed in a Pyrolysis Centrifuge Reactor. The pyrolysis vapor is directly upgraded catalytically using a HZSM-5 zeolite before product condensation. It is possible to convert lignin into bio-oil at an organic yield of 25.8 wt%$_{daf}$. By direct upgrading of the pyrolysis vapor over a fixed bed of HZSM-5, the yield of organic liquid decreases significantly (<10 wt%$_{daf}$) while the production of aromatics, such as benzene and toluene, is increased. The formation of aromatics is favored at high catalyst temperature. The highest yields of olefins and aromatics are 4.3 wt% and 4.0 wt% respectively at a catalyst temperature of 600°C. At low catalyst temperature (350°C), HZSM-5 traps some of the pyrolysis vapor in the pores. The trapped reactant is still reactive at temperature >400°C. HZSM-5 rejects oxygen from the pyrolysis vapor mainly through the formation of H_2O and CO.

III-PP77

Chemical Leaching of Carbon-supported PtCu Alloy Particles –Seeking for Relations between Surface Properties and Electrochemical Activity in the Oxygen Reduction Reaction

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Carbon-supported $PtCu_x$ nanoparticles and their acidic leaching under potential cycling have been extensively studied because they are promising catalysts for oxygen reduction in PEM fuel cells. The procedure has been described to create core-shell particles with a 3-4 layer shell of pure Pt covering a largely unchanged alloy core.
We describe a study with $PtCu_{2.6}/C$ made via reductive co-deposition with ethanol and alloying at 800 °C. Chemical leaching of this catalyst (H_2SO_4, 80 °C, 36 h) was more effective than electrochemical leaching, while electrochemical leaching on top of chemical leaching produced the best result. After chemical leaching, structural characterization was made by XRD, TEM, HAADF-STEM, XAFS, XPS, and Low-energy Ion Scattering. It was found that a core strongly depleted in Cu was covered by a monolayer of Pt, which is in striking contrast to the models in literature for the state after electrochemical leaching. The consequences will be discussed.

III-PP78

CO Elimination from H_2-rich Stream Processes over Hydroxyapatite Supported Palladium Catalysts

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Calcium-hydroxyapatite loaded with different amounts of palladium (0.5-2 wt.%) were synthesized and characterized by several techniques including N_2 physisorption at -196 ºC, transmission electron microscopy, H_2-TPR, TPD-CO_2, TPD-NH_3, XRD, FTIR, UV-visible-NIR and XPS. Special attention was devoted to the dispersion of the Pd species and their influence on the textural, structural and surface chemistry properties of the prepared catalysts. The catalytic activity of the Pdx/HAp catalysts in the COPROX and WGS reactions showed that they were active and selective. Moreover their activity was compared with classical Pd catalysts used in these types of reactions. Interesting conclusions are drawn from the correlation between the distribution of Pd active species and their performance in the two investigated reactions.

III-PP79

CO_2 for the Production of Methanol and Dimethyl Ether

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CO_2 hydrogenation for the production of methanol/DME is studied over bifunctional systems comprising of a methanol synthesis and a methanol dehydration catalyst. A commercial $CuO/ZnO/Al_2O_3$ catalyst is selected for CO_2 hydrogenation to methanol and a variety of materials with acidic properties are used for methanol dehydration (γ-Al_2O_3, WO_3/Al_2O_3, Ferrerite(10) Faujasite, HZSM-5(11.5) and HZSM-5(25)). Although there are no significant variations in activity, there are differences regarding methanol and DME yields. For the catalytic configurations containing alumina, the main product is methanol, whereas zeolitic materials produce mainly DME. Differences in DME yields are observed, depending on parameters such as the micropore structure, the Si/Al ratio of the zeolite and the number, strength and nature of acid sites.

III-PP80

Comparative Study of Alumina Supported CuO-CeO_2 and CuO-ZnO Catalysts for Steam Reforming of Dimethoxymethane

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The present work reports the results of comparative study of alumina-supported bifunctional CuO-CeO_2 and CuO-ZnO catalyst in DMM SR to hydrogen-rich gas to be used for fuel cell feeding. The catalysts were characterized by BET, TPR, XRD, FTIR spectroscopy, HRTEM, EDX and HAADF-STEM techniques. Based on the data obtained, it is shown that the catalytic performance of CuO-CeO_2/γ-Al_2O_3 and CuO-ZnO/γ-Al_2O_3 in DMM SR is associated with the γ-Al_2O_3 acid sites and alumina-supported copper-cerium/zinc oxide species, which are responsible for, respectively, DMM hydration and methanol/formaldehyde SR. Bifunctional CuO-CeO_2/γ-Al_2O_3 and CuO-ZnO/γ-Al_2O_3 catalysts containing on their surface both acidic and copper-based sites are active and selective for DMM SR to hydrogen-rich gas with low (1 vol.%) CO content. These catalysts provide for 100% DMM conversion with hydrogen productivity of ~16 L $H_2/g_{cat}\cdot h$ at GHSV = 10000 h^{-1} and T = 300°C.

III-PP81

Condensed Phase Ketonization of Propanoic Acid over CeO_2-ZrO_2 Catalysts

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Bio-oils, derived from the biomass resources, contain carboxylic acids as one of the major intermediates products and its presence partly responsible for undesirable oil-properties like low pH and high oxygen content. To improve the bio-oil quality, it is required to upgrade these carboxylic acids and in this context, the conversion of carboxylic acids to a ketone would be a convenient route for lowering the acid content as well as oxygen concentration of the derived bio-oils through the removal of oxygen as CO_2 and H_2O. Many efforts have been reported in the high temperature vapour phase ketonization process; however, condensed phase conversion would be a more practical for upgrading intermediate liquid biofuels like bio-oil. Thus, the present work is focused on the study of liquid phase ketonization at lower temperature using a model bio-oil compound, propanoic acid, in presence of CeO_2 and ZrO_2 or their mixed oxide as catalysts.

III-PP82

Conversion of Methane into Methanol over Doped Mesoporous WO_3

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The conversion of methane into methanol is a good alternative to have a liquid fuel that generates less pollution than fossil ones. Since this reaction is limited, by thermodynamic factors, to high temperature and pressure conditions, unconventional techniques such as photocatalysis have been explored. In this work, a new highly active metal doped mesoporous M/WO_3 catalyst (M=Fe, Ni and Cu) was studied for the photocatalytic partial oxidation of methane to methanol with water. Among the metals, the production of methanol over Ni/WO_3 was much higher than that of pure WO_3 and the CO_2 rates was markedly diminished, resulting in the highest selectivity toward methanol. Moreover, the reaction was monitored by *in situ* DRIFTS to examine the surface chemistry involved during the photocatalytic process.

III-PP83

Cs-Promoted FER Zeolite as Ni Support in Methane Dry Reforming

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In the present work, we have investigated a lamellar zeolite (FER), still unexplored as support, and compared the performance of Cs- promoted Ni catalysts supported on both lamellar and delaminated (ITQ-6) forms in order to understand the effect of the different textural characteristics of the support in the dry reforming of methane.

The characterization of these materials by XRD, BET area, TPR, SEM-EDX and AFM has allowed to establish interesting relationships between their catalytic performance and physico-chemical properties.

The objective was to develop a catalyst able to overcome the long-standing carbon formation and thermal sintering problems.

III-PP84

Design of CO Tolerant Anode Electrocatalysts for PEM Fuel Cells

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Upon using an anchoring type Controlled Surface Reactions (CSR) we have prepared Pt-Sn alloys supported on active carbon with wide range of the Pt/Sn ratios (Pt/Sn= 0.8-12.5) and exclusive Sn-Pt interaction without tin deposition onto the support. The content and dispersion of the fcc Pt_3Sn phase within the electrocatalysts can be controlled by tuning the reaction conditions of CSR. A clear correlation between the Pt_3Sn alloy phase content and the performance in both the CO and methanol electrooxidation reactions was established.

The challenge in the preparation of novel $Ti_{0.7}W_{0.3}O_2$-C composite materials used as a support for Pt-based electrocatalysts is that the preferable properties are linked to complete incorporation of the tungsten in the +4 oxidation state into the rutile-TiO_2 crystal-lattice. Upon using composites with high degree of W incorporation better performance in the H_2-purged CO_{ads} stripping compared to the PtRu/C benchmark along with considerable stability was achieved.

III-PP86

Direct Synthesis of Dimethyl Ether from Mixture of Carbon Dioxide and Carbon Monoxide over Copper Alumina Catalysts Prepared using the Sol-gel Method

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DME direct synthesis from carbon dioxide works for CO_2 utilization and reduces of CO_2 which is one of the greenhouse effect gases. If excellent catalysts will be developed and be used widely, the problem of global warming and problem of environments such as air pollution will be solved. If the hydrogen will be produced using sustainable energies such as sun light power, window power, hydropower, and so on, the produced DME works as hydrogen carrier and energy carrier. I have developed the significant catalysts using the sol-gel method. The Cu-Ga(24-6 wt%)/Al_2O_3 catalyst prepared using the sol-gel method is excellent for DME direct synthesis from CO_2. The Cu-Zn(15-15 wt%)/Al_2O_3 catalyst prepared using the sol-gel method is excellent for DME direct synthesis from CO. These catalysts are significant catalysts for DME direct synthesis from CO_2 and CO compared with the mixed catalysts.

III-PP87

Effect of Calcination Temperature on Stability and Activity of Ni/$MgAl_2O_4$ Catalyst for Steam Reforming of Methane

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The effect of calcination temperature on the activity and stability of Ni/$MgAl_2O_4$ catalyst for methane steam reforming reaction was studied. Three catalysts were prepared in which either the precalcination temperature of the support or the final calcination temperature of the impregnated catalyst was varied. Various characterizations such as BET surface area, X-ray diffraction, temperature-programmed reduction, temperature-programmed desorption and UV-vis of the fresh, used and reduced catalysts were done. The catalyst calcined at 500°C deactivated during the activity test and the deactivation became more severe with increasing temperature and pressure. In contrast, the catalyst calcined at 850°C not only had a higher activity but also did not show any deactivation at 600°C and 5 bar for a run time of 8h. Moreover, there was no effect of precalcination on catalyst activity or stability. Most likely, the better catalyst performance was due to stronger metal-support interaction because of the increase in the calcination temperature.

III-PP88

Effect of Nickel Complexes on the Metal Dispersion and Catalyst Activity of Ni/SBA-15 Catalyst for Methane Dry reforming to Syngas

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Effect of nickel complexes $[Ni(H_2O)_6]^{2+}$, $[Ni(NH_3)_6]^{2+}$, $[Ni(en)_6]^{2+}$, and $[Ni(EDTA)]^{2-}$, respectively, on the Ni complex–support interaction and strength, dispersion as well as on the stability of Ni/SBA-15 catalysts against coking in methane dry reforming of methane was studied. Six different samples were prepared using incipient-wetness impregnation onto mesoporous silica support, SBA-15. Influence of washing excess metal complex to eliminate the counterions on the catalyst activity was also investigated. The catalysts were characterised using Fourier Transform Infrared Spectrometry (FT-IR), Scanning Electron Microscopy (SEM)/ Energy dispersive X-ray spectroscopy (EDX), X-ray Diffraction spectroscopy (XRD), Transmission Electron Microscope (TEM), N_2 adsorption-desorption at 77 K and Temperature Programmed Reduction (TPR). The results indicated that the nature of nickel complex and choosing to wash or not to wash the catalyst after impregnation had pronounced effect on the metal-support interaction, nickel particle size, dispersion, and activity and stability of the catalyst.

III-PP89

Efficient Conversion of Organic Matters Using Ionic Liquid in Hydrogenation of Coal over Mo-Based Catalyst

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Hydrocarbon compounds are very valuable chemicals as fuel and base materials in petrochemistry and can be produced by refinery and separation process of oil/petroleum. Direct coal liquefaction is an available technology to produce the liquefied hydrocarbon fuels with the combined cracking and hydrogenation of organic matters of coal under high temperature and pressure. In this study, the hydrogenation of coal using batch-type autoclave reactor was conducted under high pressure and temperature. In the reaction test, the ionic liquid was used as an additive to improve the cracking and dissolution of organic matter of coal and the reaction efficiency of the direct coal liquefaction process with catalyst. And then the effect of the ionic liquid on the catalytic effect of the cracking and dissolution of coal was investigated for the reaction characteristics. Also, the physic-chemical properties of the solid and liquid phase of reactant and product were characterized by X-ray diffraction, proximate analyzer, elemental analysis, FT-IR spectra etc. As a result, the cracking and dissolution efficiency of organic matters of coal were improved by the the ionic liquid in hydrotreating process of direct coal liquefaction over Mo-based catalyst.

III-PP90

Esterification of Levulinic Acid with Butanol over Ion-exchange Resins: a Screening Study

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Alkyl levulinates are biobased chemicals with a great variety of applications and great biofuel potential as additives to conventional diesel or gasoline. The preparation of butyl levulinate by esterification of levulinic acid with butanol requires an acid catalyst to get reasonable reaction rates. The present work focuses on the synthesis of n-butyl levulinate by esterification of levulinic acid with n-butanol using a range of acid ion-exchange resins. It has been found that selectivity is always exceptionally good. Catalyst screening has highlighted gel-type resins for their efficiency and Dowex 50Wx2 has been found to be the most efficient catalyst. Activity has been found to be inversely related to the degree of crosslinking. Elevated values for V_{sp} (swelling) correlate with high reaction rates. The more efficient acid polymeric resins have higher yields at lower temperatures than those reported for zeolites.

III-PP91

Etherification of Isobutene with C_1 to C_4 Linear Primary Alcohols in Liquid-Phase: Experimental Equilibrium and Thermodynamic Analysis

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Equilibrium and thermodynamic experimental studies are mandatory to determine innovative processes feasibility. Within novel biofuels production processes, interest in using biomass-derived reactants to produce oxygenate additives is increasing since they can be computed for the biofuel target.

Etherification reactions of isobutene with C_1 to C_4 linear primary alcohols, which can be produced through fermentation processes, give excellent oxygenate additives as methyl *tert*-butyl ether (MTBE), ethyl *tert*-butyl ether (ETBE), propyl *tert*-butyl ether (PTBE) and butyl *tert*-butyl ether (BTBE). These four reactions have been studied in two different setups and have been found to be reversible and exothermic as expected. Equilibrium conversion for PTBE and BTBE are located between those of MTBE and ETBE.

Enthalpy and entropy variations have been estimated for MTBE, ETBE, PTBE, and BTBE. MTBE and ETBE values have been compared with literature data to give reliability to the used procedures and to obtained data for PTBE and BTBE.

III-PP92

From Data to Knowledge: Analysis of Published Articles in Literature for Photo-catalytic Water Splitting

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In this work, the hydrogen production of photocatalytic water splitting (PWS) over promoted TiO_2 based semiconductors, perovskites and dye-sensitized catalysts were investigated. A comprehensive database which consists 6788 data points from 86 different papers was constructed and it consists of 32 variables. The articles on PWS have been studied from 2005 to 2014 using a number of literature databases, including Elsevier, Wiley Online Library, and ACS Publications. It was observed that annual number of publications on PWS has increased 346% in 2014 in respect to 2005. To see trends, to make predictions and to understand the effects of individual variables, the database was analyzed using several learning algorithms such as k-nearest neighbor regression, decision tree and support vector machine.

III-PP93

Further Insights into the Effect of Sulphur on the Activity and Selectivity of Cobalt–based Fischer–Tropsch Catalysts

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The objective of this work was to elucidate a currently controversial effect of S on the selectivity of Co-based Fischer-Tropsch catalysts. For that purpose, an alumina-supported cobalt catalyst was ex-situ poisoned with different S amounts. The resulting poisoned samples were tested under realistic FT conditions at the same operating CO conversion. The results showed that the presence of sulphur on the catalyst surface enhances the selectivity towards methane and reduces the selectivity to long chain hydrocarbons. This effect is more pronounced at high sulphur coverages. Further results will be discussed and compared with these obtained in previous studies.

III-PP95

Hydrocracking of FT Wax over Noble Metal / SA Catalysts: Combined Experimental and Kinetic Modelling Studies

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Hydrocracking of paraffinic wax has been carried out over platinum and palladium-based catalysts supported on silica-alumina. The catalytic tests were performed in a fixed-bed tubular reactor at: T=300 - 330 °C, P=35 bar, H_2/wax= 0.1 (wt/wt); WHSV=1-4 h^{-1}. Both noble metals result in a significant increase in the degree of isomerization. However, platinum is slightly more active than palladium and it also leads to a higher selectivity to the middle distillate fraction. The experimental data obtained has successfully been used to develop a kinetic model, based on the LHHW formalism. The influence of process parameters on conversion and selectivities can be predicted with the developed model. Further work is ongoing to improve the kinetic model and evaluate the performance of bimetallic PtPd catalysts.

III-PP96

Hydrodeoxygenation of Aliphatic Esters over Nickel Phosphide Catalysts

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Fatty acid based feedstocks such as vegetable oil, tall oil and animal fat attract much attention as renewable sources for fuel production. Hydrodeoxygenation (HDO) of these crudes leads to the mixture of hydrocarbons ("green" or "renewable" diesel). Transition metal phosphides are considered as promising catalysts for HDO processes.

The aims of the present work are the study of the Ni_2P/SiO_2 catalysts in HDO of model compounds – aliphatic methyl esters $C_{n-1}H_{2n-1}COOCH_3$ (n = 7, 12 and 16), investigation of reaction conditions and carbon chain length influence on catalytic properties.

Ni_2P/SiO_2 catalysts were synthesized by incipient wetness impregnation of SiO_2 followed by reduction *in situ* in reactor. Two parallel reaction pathways occur on the catalysts surface during HDO: decarboxylation/decarbonylation through CO_2, CO and $C_{n-1}H_{2n}$ hydrocarbons formation and direct hydrodeoxygenation through H_2O and C_nH_{2n+2} hydrocarbons formation. Hydrocarbon chain length influence on activity but almost does not effect on selectivity.

III-PP97

Hydrogen Production by Ammonia Decomposition Using Co Catalyst Supported on Mg-X(Al,Ce &La) Mixed Oxide Systems

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The effect of mixed oxide supports (MgAl, MgCe & MgLa) using cobalt as active component was studied on ammonia decomposition for the generation of CO_x free Hydrogen. The catalysts were characterized by XRD, BET surface area, TPR and TGA techniques. The MgLa mixed oxide supported Cobalt catalyst is showing better activity compared with other mixed oxide supported catalyst. An effect of the Mg/La ratio is noticed in MgLa supported catalysts and studied the catalytic activity of catalysts with varying Mg/La molar ratio on ammonia decomposition. The catalyst with Mg/La ratio of 5:1 is showing maximum performance toward ammonia decomposition, and it exhibited highest activity among the other cobalt mixed oxide supported catalysts. The eminent activity of MgLa supported Co catalyst with Mg/La ratio 5 is due to presence of high amount of moderate and strong basic sites for MLa-5 mixed oxide, high metal dispersion and easily reducible Co species which are observed from CO_2-TPD, CO chemisorptions and TPR results.

III-PP99

Hydrogen Production via Ethanol Steam Reforming over Supported Nikelates: from Powders to Structured Catalysts

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The catalysts $m\mathrm{LnNi_{0.9}Ru_{0.1}O_3}/n\mathrm{Mg\text{-}\gamma\text{-}Al_2O_3}$ (Ln = La, Pr, m=10-20%wt, n=6-15%wt) have been prepared by impregnation, characterized by XRD, BET, TEM with EDX, UV-vis, XPS, TPR-H_2, FTIRS of CO test molecule and studied in ethanol steam reforming as fractions and layers on structured ceramic and Ni-Al alloy substrates. The influence of Ln nature and Mg concentration on the structural and redox properties of the catalysts have been elucidated. High activity and coking stability of catalysts are provided by a high dispersion of metallic Ni and Ni-Ru alloy due to strong interaction with $LnO_x/MgO/\gamma\text{-}Al_2O_3$ support and suppressing support acidity by Mg/Ln cations. The optimal catalyst supported on Ni-Al foam substrate shows high and stable performance in a realistic reaction mixture during 50 hours.

III-PP100

Impact of SO_2 as Air Pollutant on Spatial PEMFC Performance

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Most PEMFCs use air as an oxidant which may contain air pollutants such as SO_2, NO_x, CO, NH_3 and some organic compounds. The air contaminants are known to cause PEMFC performance loss. In this work, the spatial performance of a fuel cell exposed to 2 ppm SO_2 and different operating conditions was studied with a segmented cell system. Sulphur dioxide was found to cause severe irreversible performance loss which is accompanied by significant current density redistribution downstream. The observed redistribution is connected with a mechanism of electrochemical SO_2 transformation and strongly depends on operating conditions. The performance can be partially recovered by reintroducing neat air and applying cyclic voltammetry at potential higher than 1.0 V, at which zero-valent sulphur species can be oxidized. A detailed analysis of the localized PEMFC behaviour under SO_2 exposure and recovery, possible SO_2 poisoning mechanisms and modelling results will be presented and discussed.

III-PP101

Insight of 1D γ-Al_2O_3 Nanorods Decoration by NiWS Nanoslabs in Ultra-deep Hydrodesulfurization Catalyst

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Novel 1D-γ-Al_2O_3 nanorods (Al-nR) were used to prepare a NiW hydrodesulfurization catalyst. HRTEM exposed homogeneously distributed active phase all-over the AlnR. Differences on the slabs stacking and length were observed. The activity for NiW/AlnR resulted higher than that for NiWP/γAl_2O_3 catalyst. Both materials showed almost same specific hydrogenation, but the main difference was the higher hydrogenolysis on the NiW/AlnR sample. Theoretical calculations showed that 1T-S-W-S cluster with Ni on the top has less metallic character than when Ni was in a corner of 2HSWS crystal. Therefore, NiWS sites on small slabs act rather as hydrogenolysis sites than as hydrogenation sites.

III-PP102

Integrated Catalytic Membrane Reactor for Hydrogen Production Using Hydrocarbon-based Fuels

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The work described in this paper is aimed at developing an innovative catalytic membrane reactor using functionalized silica membrane systems to produce pure hydrogen from a reformate stream sourced from oil based fuels. The small-scale membrane reactor will be evaluated in relation to its future economic and thermodynamic potential that could include a promising prospect of inexpensive CO_2 separation. This study will allow the development of a proof of concept catalytic membrane reactor for hydrogen production fed with a variety of liquid petroleum derivatives. The catalytic membrane reactor will be an integrated system employing innovative reforming, water gas shift and hydrogen membrane separation processes.

III-PP103

Kinetic Study of Thermoconversion of Lignocellulosic Biomass and Gasification of Charcoal in Presence of Heterogeneous Catalysts

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In this study we have investigated the kinetics of pyrolysis and gasification of spruce wood in the presence of heterogeneous catalysts (Cu_2O, CuO, ZnO, NiO, MnO, Mn_2O_3, MnO_2, Fe_2O_3, Cr_2O_3, V_2O_5, La_2O_3, MoO_2, TiO_2) by thermogravimetry method. Pyrolysis was carried out in argon, gasification – in CO_2 and water vapor. The energy of activation was defined for assessment of catalysts influence on pyrolysis by Coats-Redfern method. It was found out that all studied catalysts have impact on a pyrolysis stage and promote decomposition of heavy products of pyrolysis. It was defined that the catalysts reduce the temperature of beginning of gasification, both in the atmosphere of carbon dioxide, and in water vapors.

III-PP104

Kinetics of the Dehydration of 1-Butanol to di-n-Butyl Ether: a Next Generation Biofuel

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This work reports the kinetic study of the synthesis of a next generation biofuel, the di-n-butyl ether, from 1-butanol dehydration over the resin Amberlyst-70. The dehydration reaction was performed in a high pressure autoclave at 140 – 190 ºC in liquid phase. Three mechanistic models, with various assumptions on rate determining steps and quasi-steady state for surface species have been considered: a Langmuir-Hinselwood- Hougen-Watson (LHHW) formalism; an Eley-Rideal (ER) formalism in which the formed DNBE molecule remains adsorbed; an ER formalism in which the formed water remains adsorbed. The rate expression based on water desorption as the rate limiting step in the LHHW elementary mechanism has been found to be statistically the most reliable representation, with physicochemical meaning, of the experimental data. The activation energy was found to be 121±3 kJ/mol, in good line with literature data for such reaction.

III-PP105

Knowledge Extraction for Fischer-Tropsch Synthesis from Published Data in the Literature

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In this work, Fischer-Tropsch Synthesis (FTS) performance was investigated over various catalysts, with different catalyst preparation methods, and under diverse reaction conditions. A database containing 2404 instances and 22 variables was constructed from 223 research papers published in the platforms such as Elsevier, Wiley Online Library, and ACS Publications between 2005 and 2014. All instances have three main outputs, namely CO conversion, H_2 conversion, and selectivity to hydrocarbon chains and carbon dioxide. A support vector machine model was successfully implemented to model the outputs of the Fischer-Tropsch synthesis from the input variables.

III-PP107

Low Temperature Decomposition of Hydrogen Sulfide the Metal Catalysts under Layer of Solvent to Produce Hydrogen and Diatomic Sulfur

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The catalytic decomposition of hydrogen sulfide into hydrogen and diatomic sulfur {$2\ H_2S \leftrightarrow 2\ H_2 + S_2^{(gas)}$} occurs on metal catalysts at ambient conditions with H_2S conversion about 15 %. The paper demonstrates the principal feasibility to shift equilibrium of the reaction to the right, so that H_2S conversion can be considerably (up to 100 %) upgraded, on passing H_2S at room temperature through the metal catalyst being immersed into the solvent capable of dissolving sulfur produced. These experimental data seem to offer new challenges and very promising opportunities to produce hydrogen from renewable inexhaustible resources, at the same time very toxic H_2S is utilized. Main regularities of hydrogen production and sulfur recovery from the solutions are been discussed. The S_2 electronic state and the reaction thermodynamics are considered.

III-PP108

Material Performance of CoO_x, CeO_2 and Co-Ce Mixed Oxide on Oxygen Storage for Solar Thermal Hydrogen Production

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Solar thermal hydrogen production is an emerging technology for clean energy production. Ceria as proper candidate has high oxygen transport capacity. The high temperature step required for thermal decomposition of ceria limits the overall process efficiency. Redox ability of cobalt oxide is better than ceria at low temperatures. In this study, the synergy between the unique properties of cobalt and cerium was investigated. Temperature programmed reduction, oxidation, thermal decomposition experiments were performed for oxygen transfer mechanisms of Co, Ce, and Ce-Co mixed oxide samples up to 800ºC. The oxygen storage capacity of ceria is calculated after oxidation of reduced ceria. This capacity is dramatically reduced after thermal decomposition. The oxygen capacity of cobalt oxide is almost same over repetitive cycle between 400 and 800ºC. For the mixed oxide materials, oxygen capacity increases depending on the cobalt content whereas the minimum temperature for oxidation depends on ceria content.

III-PP110

New Carbon Supports for Pt/C Oxygen Electroreduction Reaction Catalysts

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A sharp increase in the cathode potential (up to 1.4 V. vs. RHE) due to the simultaneous presence of oxygen (air) and hydrogen in the anode side is the main degradation cause of Pt/C catalysts for polymer electrolyte fuel cells (PEMFC) using as a power source for cars. This potential is much higher than the carbon oxidation potential, so the corrosion resistance of a carbon support is an important parameters of the PEMFC effective operation.

In this paper, the stability of carbon support was improved by modifying the surface under different conditions. Modification of commercial carbon black KetjenBlack DJ-600 by pyrocarbon and nitrogen was carried out in order to investigate the influence of these additives on the support corrosion resistance. It was shown that the modification of the carbon blacks with both nitrogen and pyrocarbon improves the corrosion stability of the composite materials.

III-PP111

Ni/Al_2O_3 Catalysts for Heavy Molecules Steam Reforming: Effect of Modifiers on Catalysts Structure and Activity

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A complete study on the effect of modifiers on Ni/Al_2O_3 catalysts in terms of activity and structure was undertaken. Different modifiers such as SiO_2, B, Mg and La were added to the conventional formulation and they were fully characterized using XRD, FE-SEM, UV-vis, IR and H_2-TPR. Experiments of steam reforming of phenol/ethanol mixtures show that the silica-free alumina support does not produce a better catalyst than the silica-containing support, while the addition of lantana promotes the catalyst activity and reduces coke deposition. The addition of Lanthanum (20%La_2O_3) to the formulation of 20%NiO/Al_2O_3 does not prevent a huge interaction between Ni and alumina with $NiAl_2O_4$ formation. Naphthalene steam reforming was also compared with phenol steam reforming.

III-PP112

Nickel Carbonyl Formation under Low Temperature Methanation Conditions. The Importance of Intraparticle Heat and Mass Transfer Effects

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Ni-based catalysts (Ce-Ni-O, Ni-Mg-Al-O) were successfully prepared by coprecipitation method for the efficient and sustainable syngas production from methane and carbon dioxide. The influence of different parameters was studied, such as the Ni loading, the concentration of the reactants, the reaction temperature (600°C-800°C) and the pretreatment temperature. An almost linear increase between the metal loading and the conversion of the reactants is obtained, however, an optimized system can be proposed with high activity and selectivity. At the mild temperature of 600°C high conversions i.e. 58% for CH_4 and 66% for CO_2 are obtained at the stable state on Ni-Mg-Al-O compound (10 mg) with a high selectivity (H_2/CO ratio of 0.81) with reactants concentration at 20 %. The catalysts were characterized to find correlations between catalytic activity and physico-chemical properties. All the catalysts correspond to nanomaterials with small average particles size and well dispersion of Ni species.

III-PP115

Praseodymium Nickelate-cobaltite Based Functionally Graded Cathodes for Intermediate Temperature Solid Oxide Fuel Cells

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State-of-the-art SOFC cathode materials based upon Sr-doped perovskites (LSFN, LSM etc.) deteriorate in the intermediate temperature (IT) range due to carbonation, while Sr-free $PrNi_{1-x}Co_xO_{3-\delta}$ provides a stable performance. In this work nanocrystalline $PrNi_{1-x}Co_xO_{3-\delta}$ (PNC, $x = 0 \div 0.6$) and $Ce_{0.9}Y_{0.1}O_{2-\delta}$ (YDC) oxides were synthesized by Pechini route, and PNC – YDC nanocomposites were prepared via ultrasonic dispersion. All samples were characterized by XRD and TEM, their oxygen mobility and reactivity –by O_2 TPD and oxygen isotope heteroexchange including CO_2 SSITKA. Disordering of PNC and YDC domains in nanocomposites due to Pr redistribution provides very fast diffusion of up to 80% of bulk oxygen with $D_{fast} \sim 10^{-6}$ $cm^2 \cdot s^{-1}$ at 700 °C exceeding by 2-3 orders of magnitude that for LSCF – GDC nanocomposite. Anode-supported SOFCs with PNC – YDC nanocomposite cathodes demonstrated power density ~ 420 mW/cm^2 at 700 °C which exceeds that for traditional cathode materials.

III-PP116

Production of Hydrogen Enriched Gas by Biogas Reforming over the Multicomponent Co-containing Catalysts

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This paper deals with the development of the new Co-containing catalysts modified with noble and rare earth metals for production of hydrogen enriched gas by dry and steam biogas conversion.
A model biogas with a ratio of $CH_4/CO_2=1$ was used. The processes were carried under P=0.1MPa, GHSV=1000 hr^{-1} and temperature varied from 300 to 800°C.
The effect of the amount of the rare earth metal, temperature, and steam on biogas conversion was examined.
The catalysts have shown the high stable activity in both dry and steam reforming of biogas. No loss of the $5\%(Co\text{-}M_1)\text{-}5\%M_5/Al_2O_3$ activity was occurred during 150 hours of its continuous exploitation.
The new multicomponent catalysts based on Co with additives of noble and rare earth metals and supported on alumina perform the high activity, stability and resistance to coke formation in production of hydrogen enriched gas by steam biogas conversion.

III-PP117

Reuse of Low Value By-Products of a Biodiesel Industry. Esterification/Transesterification over Acid Catalysts

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The use of biomass is viewed as the most interesting alternative to produce energy with low environmental impacts. Biodiesel produced by alcoholysis of vegetable oils is pointed out as a feasible renewable fuel. The use of low value by-products as raw-materials for biofuels production can contribute with higher reduction of GHG, being one of the major advantages for sustainability of biofuels. High acidity and low value by-products from a biodiesel industry were converted into biodiesel using heterogeneous acid vanadyl phosphate catalysts The new sol-gel like technique used revealed to be a simply route to synthetize such catalysts. The calcination temperature displays an important role on the catalytic performances of the prepared VPO materials. Deactivated catalysts were easily reactivated by thermal treatment in oxidant atmosphere.

III-PP118

Selective CO Methanation over Ceria-supported Ni, Co and Fe Catalysts

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The selective CO methanation in hydrogen-rich gas mixtures in the presence of CO_2 is a promising way for deep CO removal designed for low-temperature proton-exchanged membrane fuel cell feeding applications, as well as a challenging fundamental problem of substrate-selective hydrogenation. Catalytic properties of Ni-, Co- and Fe/CeO_2 catalysts, prepared from nitrate and chloride precursors, in the selective CO methanation were studied. The $Ni(Cl)/CeO_2$ catalyst, prepared from $NiCl_2$ precursor, was the most efficient, being less active than Ni/CeO_2 and Co/CeO_2, but considerably more selective. This phenomenon could be explained by ceria surface blocking by chlorine species and appropriate inhibition of CO_2 hydrogenation activity.

III-PP119

Steady State and Dynamic Performance Analysis of OSR and Serial OSR-PROX Reactors

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In the current study, steady state and dynamic performances of individual propane oxidative steam reforming (OSR) reactor and serially combined OSR and preferential oxidation (PROX) reactors, utilizing novel $Pt\text{-}Ni/\delta\text{-}Al_2O_3$ and Pt-Sn/AC catalysts, respectively, were analyzed in a lab scale fuel processor prototype. The experiments have been conducted for different OSR feed compositions and reactor temperature combinations, which were determined by experimental design, and for the presence and absence of additional O_2 stream fed to the PROX reactor. Owing to the HT-WGS activity of the OSR catalyst, CO concentrations as low as 1% at the exit of OSR and 0.1% at the exit of the serial OSR-PROX system were achieved when C_3H_8 conversion in the OSR reactor was a 100%. Results confirmed the beneficial effect of O_2 addition to the PROX reactor on selectivity.

III-PP120

Steam Reforming of Methane on Ni-based Catalysts Characterized by Innovative Structured Carriers

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In this paper the performances of highly thermal conductive nickel based structured catalysts were investigated for the methane steam reforming reaction. The study focused on the effect of the flux geometry role in the reaction kinetics, by using both flow-through and wall-flow honeycomb monoliths. In the latter, the process stream was forced to cross the catalyst porous walls, so optimizing the solid-gas contact. This condition was demonstrated to led a marked improvement in the catalytic performances, more evident in the more severe operating conditions (low contact time, low operating temperature). Moreover, the role of a ceria-based washcoat deposition on the structured support was investigated. Experimental tests highlighted the crucial role of the ceria on the catalytic system performances, since the well note oxygen storage capacity ascribed to the ceria in one hand enhanced the reforming reaction, in the other improved catalyst stability.

III-PP121

Structured Pt(2%)/CeO_2/Al_2O_3 WGS Catalyst Design: Introduction of Buffer Layer

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This study is focused in the development of a structured platinum ceria based catalytic system for the WGS reaction. The new concept introduced is the presence of a pre-catalytic layer formed by the catalyst support aiming to increase the number of participating sites in the reaction. Its performance appears to be strongly dependent by the stream composition showing a highly beneficial effect in the reductive atmospheres. The improved catalytic behavior achieved appears to be related with the higher oxygen vacancies concentration incorporated being those directly related with the activation of the water species. The enhanced performance exhibited by this bilayer structured catalyst could be associated to higher resistances towards deactivation keeping up the oxygen vacancies capacity to dissociate water molecules. This concept provides an innovative strategy for a structured catalyst development as a function of the reaction variables.

III-PP122

Synthesis and Characterization of CuO-ZnO-Al_2O_3 with Protonated Beta or Y-Typed Zeolite Supporter for Dimethyl Ester Production

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Carbon dioxide is one of the green house gases (GHGs) that have caused climate change significantly. To reduce the affect of GHGs on the climate, conversion of CO_2 is the most favorite method, because it can create profit by using CO_2 as a feedback to produce various valuable hydrocarbon fuels, e.g. dimethyl ester, DME. Due to the thermodynamic barriers of CO_2, it needs catalysts to decrease the activation energy and then accelerate the reaction rate during the conversion of CO_2 to other chemicals. The copper-based catalysts (e.g. CuO-ZnO-Al_2O_3, CZA) are the most popular commercial catalyst for the conversion of CO_2 to DME by reason of its cheap price and unique redox property. In this study, protonated beta (HBZ) and Y-Type zeolites (HYZ) were adopted as catalytic supporters to offer well-defined structure, and maximize the contact between methanol synthesis/dehydration sites in CZA catalyst. Introduce of zeolitic supporters leads copper well-dispersed in nanocatalysts that can overcome the barriers in DME production. Beta/Y-type zeolites as supporters were the great options for the enhancement of commercial copper-based catalyst.

III-PP123

Tar Elimination in Pyrolysis of Sewage Sludge using HighlyStable Ni/SBA-15 Catalyst

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A research project was carried-out to develop a catalytic hot gas clean-up unit to convert tar to non-condensable gases to increase the gas fraction and eliminate tar from pyrolysis of sewage sludge. The first stage of the project was the synthesis and characterisation of a cheap but highly stable Ni/SBA-15 catalyst using a novel synthetic route. The second stage was testing the catalyst for tar elimination via cracking and dry reforming reactions. The catalyst was found to be highly active and resistant to deactivation from carbon deposition for more than 72 hours with optimum reaction temperature as low as 500 °C. This work will be a major contribution towards the cost effective and efficient commercialisation of the process to feed the upgraded gas into gas turbine for electricity or other useful applications.

III-PP124

The Chemical-loop Bio-alcohol Reforming for Hydrogen Production

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In order to produce hydrogen with inherent C-containing products separation, a thermochemical cycle using ethanol as reducing agent and ferrites as looping material has been developed. The main principle of the cycle is: the material first reduced by ethanol stream at 450°C, and then reoxidized with water, in order to produce hydrogen and restore the original oxidation state of the loop-material. The current experiments has been carried out with ferrites – $CoFe_2O_4$, $MnFe_2O_4$, $Co_{0,5}Mn_{0,5}Fe_2O_4$, $Cu_{0,5}Mn_{0,5}Fe_2O_4$ and $CuFe_2O_4$, as electrons and O^{2-} vectors, prepared by co-precipitation method. Characterization technics used for studying are: BET, XRD, TEM and EDX analysis, Raman Spectroscopy, XPS and in-situ DRIFT-MS, in order to investigate oxides modification, occurring during the redox cycles. The reactivity tests performed on a laboratory-scale plant and products analyzed by on-line micro-GC.

III-PP125

The Effect of Zeolite Addition into Cobalt-based Fischer–Tropsch Catalysts

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Fischer–Tropsch synthesis (FTS) is the main stage of the technology of synthetic oil and high-quality fuel production from carbon containing feedstock (XTL), for example from natural gas or biomass. The products produced by FTS are clean burning, almost odorless and biodegradable – qualities that make them environmentally attractive.

Since recently zeolite-containing catalysts are considered as promising prototypes for commercial Fischer–Tropsch catalysts because they allow producing synthetic oil or fuel that does not contain sulfur, nitrogen and aromatics in the "short-track" XTL.

The purpose of this work was to study the effect of Beta zeolite addition into composite skeleton cobalt-based Fischer–Tropsch catalysts.

It has been found that the introduction of H-form zeolite into a composite catalyst on skeleton Co basis has a positive effect both on the process parameters and on the composition of FTS products. This is probably due to secondary reactions occurring at acid sites of zeolite.

III-PP126

The Investigation of the ORR of the Pt/C Catalyst Produced by the Coaxial Pulsed Arc Plasma Deposition

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This is a kind of dry catalyst manufacturing method where the target platinum is ionized through vacuum pulse arc discharge and is then caused to collide against the carrier. First, platinum corpuscles only several nanometers across can be formed and evenly distributed across the carrier. Also, the process is extremely easy to perform. The catalyst material can be easily changed and it is also possible to synthesize a catalyst material. we investigate the electrocatalytic activity for oxygen reduction reaction of our PtC-5% catalyst which is prepared using CAPD, For compression, commercially available PtC-20% and commercially available PtC-5% are also tested. The half-wave potential of our catalyst is higher than those of the others. The currents of four catalysts at 0.80 V, normalized by Pt mass (mass activity) and Pt electrochemically active surface area (ECSA), are also investigated.

III-PP127

The Use of Heteropolyanions and Chelating Agents for Designing TMS Catalysts for Hydroprocessing of Oil Cuts and Residues

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The report presents the results of the research and development of new hydrotreating catalysts for hydroprocessing of various hydrocarbon raw feeds using heteropolyacids and chelating agents. New approaches for creating TMS catalysts were developed. Simultaneous use of Co_2Mo_{10}HPA and chelating agents allows to change significantly the promotion ratio and morphology of CoMoS active phase type II and, thereby, catalyst properties in HDS and HYD reactions. New catalysts for (i) deep diesel hydrotreating, (ii) selective hydrotreating of FCC gasoline with saving octane number, and (ii) deep VGO hydrotreating were developed.

III-PP128

Nickel-Cobalt Based Catalysts for Ethanol Steam Reforming

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Catalysts based on Nickel, Cobalt and Nickel-Cobalt bimetallic formulations on Ceria Zirconia (CZ) support have been completely characterized and tested in Ethanol Steam Reforming. The bimetallic formulation actually shows an improved ethanol conversion as well as hydrogen yield (above 80% from 600°C). TPR data and FT IR spectroscopy data from adsorbed probe molecules CO and methanol suggest that this effect can be due to a synergic effect between the two metals leading to a good reducibility of the catalyst, possibly also enhanced by the ceria-based support. On the other side, the CZ support, mainly characterized by the ceria basic character, limits the formation of dehydration products such as ethene, in comparison to similar catalyst formulations over different supports.

III-PP129

Highly Reducible and Carburizable Precipitated Iron-Based Catalysts for Fischer-Tropsch Synthesis

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Fischer-Tropsch synthesis (FTS) was carried out over as-prepared precipitated iron-based catalysts at 275 °C and 1.5 MPa. Interestingly, the as-prepared catalysts displayed a CO conversion higher than 60% at the beginning of reaction, which implies that the catalysts prepared in this study can be spontaneously activated during the FTS. Furthermore, the spontaneously activated catalysts showed high catalytic performance in terms of C_{5+} hydrocarbon productivity, which is even higher than that of pre-activated catalysts.

Section 4. Catalysis and Chemicals

IV-PP01

Production of Liquid Hydrocarbons from Syngas over the Co-containing Supported Catalysts Modified with Rare Earth Metal

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The new multicomponent Co-based catalysts promoted by additives of VIII Group metal and rare earth element and supported on alumina have been synthesized and tested in Fischer-Tropsh synthesis.

The effect of the amount of the rare earth metal and the process conditions (pressure, temperature and space velocity) on the 5%(Co-M$_1$)-M$_6$/Al$_2$O$_3$ catalyst performance in syngas conversion have been studied.

The developed multicomponent Co-containing catalysts are active, stable, and selective in producing the narrow hydrocarbon fraction from syngas.

The highest yield of liquefied hydrocarbons is equal to 79.7% was produced over the 5%(Co-M$_1$)-0.5%M$_6$/Al$_2$O$_3$ catalyst (P=1.0 MPa, t=230ºC, GHSV=1500 hr^{-1}).

The catalyst was continuously tested more than 50 hours and showed no decrease in activity and selectivity in the production of gasoline-kerosene fraction of hydrocarbons.

IV-PP02

Metalcomplex Catalysis on Oil Metalloporphyrins

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Our studies revealed that catalytic properties of oil metalporphyrins have been studied and found that synthesized complexes fasilitate the selective reaction of olefins oxyqeneting at low temperatures. The study of complexformation influence on ligand reactionability it has been ditermined that redistribution of electron density causes the changes by reaction ability when oxygen molecules transform from free state info coordinated.

Synthesized oxygen adducts of metalporphyrine complexes are oxygen carriers and provide oxygenizating reactions in mild condition with high output.

IV-PP03

Metal-Free Polymer Catalyst for Selective Semihydrogenation of Alkynes

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Hydrogenation of carbon–carbon multiple bonds is one of the most important processes widely used in chemical industry. Currently, this type of reaction is carried out on a very large scale, using noble metals such as platinum, palladium and the first row transition metals such as chrome, cobalt and nickel. We have demonstrated for the first time that polymeric carbon nitrides can be successfully used as solid catalyst for the selective partial hydrogenation of alkynes in the absence of any metal and metal oxides. It was established that the polymeric carbon nitride samples possess high catalytic activity in partial hydrogenation of phenylacetylene to styrene providing excellent conversion with remarkable selectivity (up to 95- 97%). The developed method is more advantageous due to effective catalyst recyclability on the metal-free polymeric carbon nitrides and prevents the consumption of precious metals.

IV-PP04

Effect of Support on Co$_x$ Free Hydrogen and Carbon Nanofibers Production from Methane over Fe Catalysts

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The production of pure hydrogen is essential for industry in general and particularly for fuel cell applications. Catalytic methane decomposition is viable process since it produces valuable carbon and pure hydrogen free from oxides of carbon. In this work, performance of iron based catalysts supported over γ-Al$_2$O$_3$, MgO, SiO$_2$, La$_2$O$_3$ and TiO$_2$-P25 for production of hydrogen and nano-structured carbon from Catalytic methane decomposition was explored. The catalysts were prepared by wet impregnation technique fixing the iron loading to 20 wt %. Subsequently catalysts were calcined at 500ºC and tested in affixed bed reactor at 700ºC. The result revealed the formation of carbon nanofibers as shown by SEM and TEM and the superiority of alumina supported catalysts over the other catalysts. About 60% yield of hydrogen was obtained using 20%Fe/Al$_2$O$_3$ catalyst.

IV-PP05

Novel Class of Natural Zeolite for the Catalytic Acetalization of Carbonyl Compounds and Diols

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This project deals with the preliminary evaluation and improvement of Clinoptilolite and Mordenite as naturals zeolites for use as catalytic material in petrochemical process. Catalyst design will be achieved by tailoring properties taking into account key factors as structural origin, composition, stability, porosity and acidity as key parameter determining catalytic performance. Catalysts will be characterized by appropriate physico-chemical method including new type of solid state NMR measurements. Catalytic performance regarding to application will be checked using appropriate catalytic test reactions with model molecules in order to determine and control catalytic properties.

IV-PP06

Novel Nickel(II) Complexes with 2-iminopyridyl Ligands Containing Electron-Withdrawing Groups: Ethylene Polymerization and Oligomerization Behaviour

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A series of novel 2-[(arylimino)alkyl]pyridine derivatives containing electron withdrawing groups (F, Cl, Br, CF_3, NO_2) in aryl rings have been synthesized and fully characterized by ^{1}H, ^{13}C and ^{19}F NMR spectroscopy. The corresponding bidentate nickel(II) complexes have been prepared in good yields. The structure of the complexes obtained was proved by elemental analysis, X-ray diffraction studies and ^{1}H NMR spectroscopy of paramagnetic compounds. These complexes, activated with methylalumoxane (MAO), have been found highly active catalysts of oligomerization and polymerization of ethylene (up to $9.58 \cdot 10^{6}$ g (mol of cat.)$^{-1}$ h^{-1} bar^{-1}), yielding highly branched polyethylene or mixtures of low-molecular-weight oligomers, with butenes and hexenes predominanting. The content and ratio of ethylene oligomers as well as the polymer properties (molecular weight, degree of branching) strongly depend on the nature of the substituents at the aryl(imino) and pyridine rings.

IV-PP07

Thiazolium-based Catalysts for the Etherification of Benzylic Alcohols under Solvent-free Conditions

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In this work, thiazolium and imidazolium hybrid materials (SBA-15-Thia and SBA-15-Imi) were prepared by grafting the bis-vinylthiazolium or imidazolium salts onto thiol functionalized SBA-15 mesostructured silica. The catalytic activity was tested for the etherification of 1-phenylethanol, in heterogeneous conditions.

The reactions were performed under different gas phases and reaction times. The SBA-15-Thia displayed an excellent catalytic performance, also with others benzyl alcohols. This material was successfully used in seven consecutive runs. Further studies were carried out in homogenous conditions. The results obtained allow proving that oxygen play an active role in the reaction probably regenerating the catalysts. This study represents the first use of thiazolium-based compounds as catalysts for the etherification reaction of alcohols.

IV-PP08

Propylene Oligomerization over Meso/Microporous Zeolites Modified with Chromium

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The main advantages of synthetic zeolites are that they can be engineered with a wide variety of chemical properties and pore sizes. Although the use of zeolites as catalysts are well establish and there are a large increase of zeolite types and application of theoretical approaches for prospective zeolite structures, the synthesis and modification of the commercial zeolites to avoid drawbacks associated with steric and diffusion limitations of zeolite is perhaps now the new trend in catalysis by zeolites. Herein we evaluated the effects on the catalytic activity after incorporate mesoporosity by templating method in the conventional zeolite Beta

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IV-PP10
Fischer-Tropsch Synthsis on Nanosized Metal-polymer Composite Catalysts in Slurry Reactor

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In this paper the effect of polymer additives on the catalytic suspensions properties in Fischer-Tropsch synthesis in slurry reactor was studied. It was shown that the structure of polymer molecule had a significant influence on the selectivity of the catalyst toward target products. A polymer folding into coils of different geometry as a result of polymer molecules interaction with the dispersion medium was established by molecular modeling methods. Analysis of the folding process revealed the most favorable conformation of the polymer to form a complex structure of the metal-containing particle-polymer, leading to the formation of the composite system with high activity in the Fischer-Tropsch synthesis.

IV-PP11
Gas-phase Carbonylation of Dimethoxymethane to Methylmethoxyacetate over $Cs_xH_{3-x}PW_{12}O_{40}$ Catalysts

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Gas-phase carbonylation of dimethoxymethane (DMM) to methylmethoxyacetate (MMAc) over cesium salts of 12-tungstophosphoric acid ($Cs_xH_{3-x}PW_{12}O_{40}$) was studied for the first time. Among the studied catalysts, $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ showed the best performance: the MMAc yield and productivity amounted to 40 % and 2.4 mmol g^{-1} ·h^{-1}, respectively at mild conditions: T = 110 °C, P = 10 atm, GHSV = 6000 h^{-1} and DMM/CO = 4/76 mol/mol. Catalysts were characterized by BET, XRD, TEM, FTIR techniques. Based on the data obtained, the nature of the active centers, origin of the observed catalytic activity order and probable mechanism of DMM carbonylation over $Cs_xH_{3-x}PW_{12}O_{40}$ were discussed.

IV-PP12
Transfer Hydrogenation of Acetophenone in the Presence Bis-imine Rhodium(I) Complexes

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The testing of rhodium complex with three structurally similar N,N,N,N-bis-imine ligands in transfer hydrogenation of acetophenone, and establishing the composition and structure of rhodium complex with N,N'- (1R,2R)-cyclohexane-1,2-diyl)bis(1-(pyridin-2-yl)methanimine.

Hydride transfer from 2-propanol to acetophenone in the presence system [Rh(cod)Cl]$_2$ + L], where L- bis-aldimine ligands, synthesized by condensation of (*R,R*)-1,2-cyclohexandiamine and pyridin- (**1**), quinolin- (**2**) and thiophencarboxaldehyde (**3**). Enantioselectivity of the catalytic reaction increases in series of ligands: **2** < **3** < **1**, the activity is approximately equal for catalysts with ligands **1** and **2**.

To establish the structure of this complexes we studied interaction of a solution [Rh(COD)Cl]$_2$ in *i*-PrOH with ligand **1**using ^{1}H and ^{13}C NMR spectroscopy method.

DFT calculated geometry proves asymmetric coordination of C$_2$-symmetry ligand **1**.

It was found that after hydrogenation of cyclooctadien, Rh(cod)(1)Cl complex transforms into C$_2$-symmetry five-coordinated hydride rhodium complex, which is active in hydrogen transfer from 2-propanol to ketones.

IV-PP13
Kinetic of the Formation of the 5,7-dichloro-4,6-dinitrobenzophyroxan Complex in Hexagonal Mesophase Formed in Water by Neonol

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In this study we investigated the effect of the hexagonal mesophase formed in water by the ethoxylated alkylphenol (NPh 9-n) on the chemical behavior of the 5,7-dichloro-4,6-dinitrobenzophuroxan (DChDNBPh) substrate. In the micellar environment DHDNBFO has the absorption bands at 323 nm and at 407 nm. When concentration of the NPh 9-12 reaches 30%, hexagonal mesophase is formed. Injection of the DChDNBPh substrate in E-phase stimulates the reaction leading to the shift of the absorption band from 407 nm to 450 nm, what may be caused by the formation of σ-complex. The first-order reaction of DChDNBPh was observed. This study reveals the formation of the σ-complex in the hexagonal mesophase of the NPh 9-12+ H_2O+ DChDNBPh system, whereas this complex has not been observed in the micellar pseudophase.

IV-PP14

Oxidation of Heavy Oil in the Presence of Supercritical Water

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In this paper studied the influence of the supercritical water on the process of heavy crude oil conversion. Shown unique results of this process: the viscosity of product decreased and the amount of asphaltene and resins decreased too.

IV-PP15

Bimetallic Au-Cu/Al_2O_3 Catalysts in Selective Aerobic Oxidation of Glucose and Benzyl Alcohol

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AuCu/Al_2O_3 (Au/Cu=1/1 atomic ratio) catalysts derived from bimetallic colloids prepared by co- and consecutive reduction of precursor ions, presented clear synergetic activity increase in selective oxidation of benzyl alcohol as compared to the monometallic analogous, while in glucose oxidation the Cu addition decreased the activity of Au/Al_2O_3. Catalytic activities were correlated with the structural results obtained by UV-vis spectroscopy, HRTEM, XPS and CO chemisorption followed by FTIR. In both reactions Au&Cu/Al_2O_3 with alloyed core (Au/Cu≈1/9) and possible less Cu-oxide decoration was the most active bimetallic sample.

IV-PP16

Comparative Analysis of the Thermal Stability of Unmodified and SiO_x-modiefed Chromia-alumina Dehydrogenation Catalysts

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The activity in the isobutane dehydrogenation reaction of unmodified and SiO_x-modified chromia-alumina catalyst calcined at temperatures 900-1100°C were determined. Treatment at 900-1000°C increased the activity of a catalyst with 9.0 wt.% Cr_2O_3 by 2-3% due to the formation of Cr_2O_3 clusters. Similar treatment of SiO_x-modified catalysts results in a decrease of the dehydrogenation activity of 1-7 % due to the combination of Cr_2O_3 clusters into larger crystallites. During treatment at 1100°C activity of the modified catalysts is less reduced compared to unmodified samples, due to the smaller amount of chromium incorporated to the support.

IV-PP17

Study of Bimetallic Catalyst Pd-Ni for Styrene Hydrogenation

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Gasoline and BTX (Benzene, toluene and xylenes) streams coming from the cracking of petroleum must be purified in order to minimize the concentration of diolefins, responsible of gums formations. The widespread method of purification is the selective hydrogenation of vinyllic bond, keeping the aromatic rings unaltered. These streams can have up to 1000 ppm of sulfur compounds, among them thiophene is one of the most common ones, being these sulfur compounds the main cause of the loss of activity of metal catalysts in several refinery processes. The objective of this work is to evaluate the influence of the order of impregnation of Pd and Ni in bimetallic catalysts on the activity and sulfur resistance during styrene partial hydrogenation.

IV-PP18

Metathesis Homopolymerization of New Fullerene-containing Norbornenes by Catalyst Grubbs 1’st Generation

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New norbornenes with the covalently bonded fullerene C_{60} have been prepared as monomers for ringopening metathesis polymerization. Under the Grubbs 1’st generation catalyst these monomers smoothly enter homopolymerization reactions with the formation polymers insoluble in typical organic solvents.

IV-PP19

Catalytic Systems Based on Iron and Nickel in the Synthesis of Graft Copolymers

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The synthesis of polymers with well-defined compositions, architectures and functionalities is the primary field of polymer chemistry. We have developed a method for producing the graft copolymers on the basis of brominated polystyrene in the presence catalytic systems based on zerovalent iron and nickel. Many graft copolymers based on different nature monomers (methyl acrylate (**MA**), methyl methacrylate (**MMA**), butyl acrylate (**BA**), tret.-butyl methacrylate (**t.-BMA**), octyl methacrylate (**OMA**), vinyl acetate (**VA**), acrylonitrile (**AN**))was produced using these catalytic systems by the method of «grafting from» in the temperature range 25-80°C. The structures of the copolymers obtained were proved with the help spectroscopic methods: IR and H^1-NMR spectroscopy. The glass transition temperature was defined for these graft polymers. The proposed technique for obtaining graft copolymers is more effective as compared with the conventional method for producing graft copolymers based on systems polymer - monomer - radical initiator.

IV-PP20

The First Example of Catalytic Tandem Interaction N-allyl-N-arylamines with Diazocompounds: Aza-Claisen Rearrangement – Carbenation

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Aza-Claisen rearrangement by reacting N-allyl-N-methylaniline with diazocarbonyl compounds in the presence of yttrium triflate was found.

IV-PP21

Hydrotalcite Supported Co Catalyst with Bimodal Structure for Fischer-Tropsch Synthesis (FTS)

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The stranded gas fields have received much attention as attractive resources to produce the liquid fuels by GTL-FPSO process due the high oil prices and limited petroleum reservoirs. Many researchers have reported that the cobalt based catalysts are more effective in CO hydrogenation for LTFT due to the high conversion, long lifetime and selectivity towards higher hydrocarbons. The support with bimodal structure has taken advantages for FTS with presence of meso-pore and macro pore.The objective of this work is to propose the hydrotalcite(HT)-like compound which posses bimodal structure as a new kind of supports. This work also includes the effect of bimodal pore structed with different pore size on the hydrocarbons selectivity for FTS. The outcomes of these investigations were confirmed through N_2 physisorption, FT-IR, XRD, SEM, TPR and TPD. It was suggested that the bimodal structure of support maintained the surface area of meso-pore and enhanced the porosity from macro-pore, which provided facile mass-transfer of heavy hydrocarbons.

IV-PP22

Deactivation Studies on Non-Oxidative Methane Conversion to Aromatics over Molybdenum Modified HZSM-5 Catalyst

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Pre-treatment of the catalyst show the remarkable effect on activity and coke deposition in non-oxidative methane dehydro-aromatization over bi-functional MoO_3-HZSM-5 catalyst. Catalyst pre-treated with 90% CH_4+H_2 leads to formation of less coke higher methane conversion, and product selectivity. Coke deposits formed on the catalyst were characterized by TG/DTA, TPO and TEM Techniques. Performance of the catalyst decreased with molybdenum loading. Two combustion temperature regions were observed at higher (6-8%) molybdenum loading. Combustion at lower temperature (300-450ºC) was attributed to Mo_2C and molybdenum associated carbonaceous species, which are located on the external surface of the catalyst. The combustion at high temperature (450-600ºC) was due to coke deposition on the Bronsted acid sites. Kinetic analysis of the TG profiles were done by assuming that the oxidation of the coke is a first order reaction. The activation energy of the catalyst pre-treated with CH_4+H_2 is found to be lower than the N_2 and H_2 pre-treated catalyst. HRTEM images of the coked catalyst show that there is a formation of graphite layer on the Mo_2C active sites, and surrounded by the amorphous carbon on the catalyst surface. Graphite layer formation on the catalytic active site and aromatic coke formed on the Bronsted acid sites are main cause for the deactivation of the catalyst.

IV-PP23

Development of Unusual Oxidation State Metal Catalysts for C(sp2)-H Bond Functionalization Electrochemically Induced

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Achievements of electrosynthesis mediated by nickel and palladium complexes in unusual oxidation states will be demonstrated. Important advances are associated with the development of synthetic approaches to the C = C, C-Hal, P-Cl, P-P and C-H bonds functionalization in one-step mild conditions. The reactivity of key intermediates, such as Ni(I)L, Pd (III)L(dimer or monomer complexes), was investigated. The key trends and the potential of this field of organic chemistry are considered.

IV-PP25

Direct Catalytic Oxidation of Lower Alkanes

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Homogeneous catalytic systems for the partial alkanes oxidation by dioxygen were designed and studied. The systems consist of rhodium complexes and redox catalysts - iodine, copper or iron compounds. The necessary requirement for the systems operating is the use of the reducing agent – carbon monoxide. Based on the experimental data and DFT calculations the schemes for mechanisms of alkanes oxidation were proposed.

IV-PP26

Preparation of Substituted Methylenebisphenol Using Heterogeneous Acid Catalyst

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This research is aimed at finding an effective catalyst for the preparation of substituted methylenebisphenol by reacting of 2,4- or 2,6-di-tert-butylphenol with formaldehyde and its derivatives: trioxane and 1,3-dioxolane. In the reaction of electrophilic substitution 2,2'-methylene-bis(4,6-di-tert-butylphenol) and 4,4'-methylene-bis(2,6-di-tert-butylphenol) are formed.

As the catalysts a number of heterogeneous acid catalysts are studied: Purolite Ct 151, Amberlist 35, KY-2. By varying of the temperature (90° ÷ 105°C), reaction time (2 ÷ 6 h), the reactant ratio (2:0.33 ÷ 2:0.43 for reaction with trioxane and 2:0.5 ÷ 2:3 for reaction with 1,3-dioxolane) the most optimal reaction conditions are identifyed. That led to the main product yeld up to 81% mass. for 2,2'-methylene-bis(4,6-di-tert-butylphenol) and up to 68% mass. for 4,4'-methylene-bis(2,6-di-tert-butylphenol).

IV-PP27

Kinetics of Glyceric Acid Obtaining

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This work is devoted to the study of the formation of glyceric acid by oxidizing glycerol with oxygen in presence of 1.5%Au/TiO_2 catalyst. The following process parameters were varied during the experiments: glycerol initial concentration (0.1-0.3 mol/L), oxygen partial pressure (1-10 atm), amount of the catalyst (by varying glycerol to gold molar ratio from 1000 to 10000 mol/mol), base concentration (by varying base to glycerol molar ratio from 0.5 to 5 mol/mol) and temperature (55-70 ^{o}C). The kinetic model of the reaction is proposed. Reaction rate constants are calculated and the reaction activation energy value is found to be 145 kJ/moL. A possible glycerol oxidation reaction kinetic mechanism is proposed. The optimal parameters for selective glycerol to glyceric acid oxidation are identified for full glycerol conversion.

IV-PP28

Magnetic Nanocomposites: Design, Synthesis and Application in Biochemicals Synthesis

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One of the big challenges of nowadays is the development of cleaner catalytic processes to convert biomass to multiple platform molecules as strategic precursors for valuable products. These cleaner catalytic processes may involve the development of new, highly selective catalysts, to guarantee the cost-effectiveness of the process. Further, the stability, durability, and costs are other conditions that should be accomplished for their widespread usage in industry. In this context, the main objective of this work was the design and development of Nb-based magnetic nanocomposites (Nb@MNP) suitable for the glucose conversion into biochemicals. The obtained catalytic results are very promising for the development of novel magnetic nanocomposites highly active and selective in the synthesis of biochemicals from real biomass.

IV-PP29

Levulinic Acid Intercalated into LDH - a Novel Heterogeneous Organocatalyst for the Trans-Cinnamic Ester Epoxidation

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The epoxidation represents one of the most useful synthetic transformations in organic chemistry, since the epoxide ring may be opened in several ways allowing building complicated organic structures. Although several epoxidation methods of alkenes have been developed in the recent past, the epoxidation of cinnamic ester is not so common. In this context, here we report the development of a novel LA@LDH heterogeneous organocatalyst for the epoxidation of *trans*-methylcinnamate. Although levulinic acid (LA) not generates enantiomerically pure phenyl glycidate but rather racemic mixtures several advantages like the easy catalyst preparation from cheap and renewable raw materials, the use of a heterogeneous organocatalyst, the use of H_2O_2 and the absence of any inorganic soluble base recommend the present system as a "green" candidate for such reaction. All these green elements can successfully compensate any costs related to the separation of enantiomers from the obtained racemic mixture.

IV-PP30

Heteronuclear Coordination Compounds in the Catalysis of Low-temperature Dissociation of Urethane Groups

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Polyurethanes are the polymers for creating a material with a wide range of operational parameters - high hardness, high elastic modulus, high elasticity, resistance to abrasion, solvents, oils and high strength. It was shown that copper coordination compounds (CCCs), produced using N,N'-diethylhydroxylamine (DEHA) and (γ-aminopropyl)triethoxysilane exhibit catalytic activity in reactions of low-temperature dissociation of urethane groups and are capable of interacting with isocyanate groups with the subsequent formation of azoaromatic derivatives. A specific feature of how these complex compounds are formed is that a larger part of copper(II) is converted to copper(I). Transition metal coordination compounds (TMCCs) based on copper and cobalt is a more effective, compared with CCC, catalyst for the reaction of dissociation of urethane groups, accompanied by the release of TDI (and, accordingly, by an increase in the concentration of NCO groups). For example, a third of urethane groups of the prepolymer undergo dissociation with CCC, whereas in the case of TMCC, nearly all urethane groups may dissociate

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IV-PP31

Palladium-Catalysed Synthesis of Markovnikov Vinyl Sulphides with Aliphatic and Aromatic Thiols

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The present study is dedicated to the development of the universal catalytic system for Markovnikov-selective hydrothiolation of variety of terminal alkynes by aliphatic, benzylic, and aromatic thiols. Detailed study of the catalytic system and optimization of the conditions for the synthetic procedure will be presented and discussed.

IV-PP32

Carbon Nanotube-supported Pt Nanoparticles as Efficient Catalysts for Base-free Aerobic Oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic Acid

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Pt/CNT was a highly efficient catalyst for the selective oxidation of HMF to FDCA under O_2 in water without addition of any bases. An FDCA yield of 98% could be attained over this catalyst at 368 K. Pt nanoparticles and the oxygen-containing functional groups on CNTs played key roles in the selective oxidation of HMF. Pt nanoparticles were proposed to activate O_2 and HMF, while the oxygen-containing groups such as C=O enhanced the adsorption of HMF and the intermediates, i.e., DEF and FFCA onto catalyst surfaces. Our kinetic studies suggest that the reaction mechanism over the Pt/CNT is different from that proposed for the catalytic systems with a strong base additive.

IV-PP33

Transformation of Glycerol to Acrolein over Isomorphously Substituted Iron Zeolites

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Research on sustainable energy and transformation are part of alternative current challenges to the use of fossil fuels for a more sustainable future. Glycerol from biomass is becoming more abundant. It is a by-product of the transesterification of biodielsel and can turn into a variety of value-added product like acrolein. Acrolein is an important petrochemical intermediate formed by dehydration of glycerol, it serves among other things to make the acrylic acid for the manufacture of paints, adhesives or plastics. Acrolein can also be produced by oxidation of propene from fossil fuel over bismuth molybdate, the yield of acrolein achieve almost 82% on this catalysts. Zeolites are among the most used acid catalysts for this process with high yields. Nonetheless, the problem of these materials is the rapid deactivation by coke over time on stream. Recent studies have shown that the addition of a metal in the zeolite and the work in oxidative medium may reduce this deactivation. The aim of this study is to compare two iron zeolites (Fe-MFI and Fe-BEA) prepared by post-synthetic isomorphic substitution from mothers commercial zeolites MFI (Zeolyst, CBV15014) and BEA (Clariant, HCZB 150.5) with the same Si / Al ratio of 60 for the dehydration of glycerol to acrolein.

The preparation consists in an NH_4F aqueous attack of the zeolite framework which involves the removal of aluminum lattice and the substitution by iron introduced as FeF_3, $3H_2O$ for 3 hours at 75 °C. After, the samples were filtered, washed and dried in the oven à 100°C for 24H. Finally, the zeolites were calcinated at 500°C on air (150 $ml.min^{-1}$) to obtain the protonic form of the iron zeolites. The isomorphous substitution stabilizes iron in the framework of zeolite in order to modulate acidity and create redox site over the materials. Reaction was carried out at 320°C in vertical furnace. The feed was a 10 mol% aqueous solution of glycerol introduced with a syringe pump (0.1$ml.min^{-1}$) at atmospheric pressure in the reactor. 300 mg of catalyst (GHSV= 2770 h^{-1}) were used in N_2 or air (15 $ml.min^{-1}$) as a carried gas. Different characterization techniques (IR, BET, MALDI-TOF, GC-MS) coupled with the method of analysis of "coke" developed at IC2MP allow to shed light on the nature and type of coke formed on each catalyst to explain its influence on the catalytic properties and better understand the role of iron in zeolites.

X-ray diffraction and nitrogen adsorption at 77K show that the physical and textural properties (table 1) of zeolites are conserved after preparation. In the first time, the reaction was carried out over H-BEA on air (15 ml/min) but the catalyst was rapidly deactivated (fig.1). The addition of 0,6wt% of iron (measured by ICP) on zeolite BEA (Fe-BEA(0,6%)) improves the catalytic performances. H-MFI is better than BEA catalysts. Fe-MFI(0,6%) is clearly the best catalyst with acrolein yield reaching 95% at the beginning of the reaction for total glycerol conversion and still 75% after 8h of the reaction.

The post synthesis isomorphous substitution is easy to implement and allows the insertion of iron in the framework of zeolite with conservation of physical and textural properties. The BEA zeolite deactivates faster than MFI zeolite for the dehydration of glycerol to acrolein. Iron in BEA and MFI zeolites increases the catalytic performances with important reduction of deactivation. Fe-MFI (0,6%) give the best result for dehydration of glycerol to acrolein over zeolite.

IV-PP34

Selective Oxidation of Glycerol with H_2O_2 Catalyzed by Fe/SiO_2

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The transformation of glycerol into value-added chemicals by catalytic oxidation was performed using the H_2O_2-Fe system in aqueous solution at mild operating conditions (50-90 ºC, 1 atm). The use of a homogeneous catalyst resulted in a high transformation of glycerol and H_2O_2 accompanied by a heterogeneous mixture of oxygenated compounds, whereas the Fe/SiO_2 catalyst performed an interesting role on the reaction selectivity. At 50 ºC the glycerol oxidation yielded dihydroxyacetone, glyceraldehyde and formic acid, while an increase of the reaction temperature was associated with a high selectivity to formic acid and an increase of the mineralization grade. No iron leaching was detected until the H_2O_2 conversion was approximately 100 %, remaining the catalyst stable along the reaction. Assuming an apparent first order dependence on glycerol oxidation, the apparent activation energy for glycerol transformation was determined and a value of 80 kJ/mol was obtained.

IV-PP35

Stages of Hydrogen Oxidation Reaction on Silver

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The hydrogen oxidation reaction on polycrystalline silver was studied. It has been shown that only adsorbed at the surface oxygen species interact with hydrogen. Oxygen atoms located into the metallic silver bulk not participate in the reaction. The interaction of hydrogen with surface oxygen occurs in two stages: the fast one and the slow one. The rate-determining step of the reaction is revealed, which is the interaction of a hydrogen molecule with a surface hydroxyl group giving a water molecule and adsorbed hydrogen atom. The adsorbed hydrogen atom rapidly interacts with the second surface hydroxyl group according to the following equation. The results obtained in this study show a mechanistic similarity between the catalytic oxidation of hydrogen on silver and the branched chain reaction of hydrogen combustion.

IV-PP36

Catalytic Carbonylation of Olefins, Alcohols and Benzyl Halides in Ionic Liquids

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Transition metal-catalyzed carbonylation of unsaturated hydrocarbons, alcohols and halides is a direct one-step route to carboxylic acids and esters. In presented work we systematically studied application of some ionic liquids such as molten tetrabutylammonium and 1-butyl-3-methylimidazolium derivatives as a media for these reactions. The most striking result is higher activity of phosphine-free palladium catalyst than that of “traditional” Pd-phosphine complexes. Bromide-containing ionic liquids stabilize palladium in the form of nano-sized suspension, as demonstrated by TEM. For unsymmetrical olefinic substrates, regioselectivity depends on anion nature in ionic liquid. In particular, chloride improves selectivity to 2-phenylpropanoic acid in carbonylation of styrene. Due to high solubility of catalyst in molten salt, it can be used repeatedly by simple extraction of products from reaction mixture with diethyl ether. Hydroxycarbonylation of benzyl halides in ionic liquids proceeds fast in the absence of base.

IV-PP37

Rhodium-catalyzed Reductive Carbonylation of Iodobenzene

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Rhodium-phosphine complexes are efficient catalysts for reductive carbonylation of iodobenzene into benzaldehyde. Rhodium phosphine complexes such as $HRh(CO)(PPh_3)_3$ and $RhCl(CO)(PPh_3)_2$ surpass $PdCl_2(PPh_3)_2$ in respect to activity and selectivity to benzaldehyde. Aromatic solvents such as toluene and o-xylene seems to be the most suitable medium. Reaction is highly sensitive to the nature of the base. Triethylamine is the base of choice. Replacing NEt_3 with NBu_3 resulted in almost threefold reduction in benzaldehyde yield. The best catalyst formulation found: 0.5% $RhCl(CO)(PPh_3)_2$, 150% NEt_3, toluene. At 110°C and 1.5 MPa ($CO/H_2 = 1/1$) iodobenzene is totally converted within 2 hours giving benzaldehyde with the yield of 88%.

IV-PP38

Chemical and Structural Transformation of Ni(111) Upon Propene Decomposition and Gold Intercalation: Monocrystalline Quasi Free-standing Graphene Synthesis

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In the wake of impressive experiments performed at ‘the Manchester group’ on a single atomic sheet of graphite transferred on silicon oxide by means of ‘Scotch Tape technology’, the academic community has struggled to create an intelligent technique for graphene layers production on a solid state surface. This issue has not been appropriately addressed so far. Both methods viewed as most promising - high-temperature annealing of hexagonal silicon carbide and cracking of hydrocarbons on surfaces of some metals (Ni, Ru, Re, etc.) – require gold intercalation under graphene to create a quasi free-standing graphene layer (the Dirac point being at the Fermi level). Also, the graphene electronic structure (the Dirac cone energy position, the formation of an energy band gap, etc.) varies depending on the intercalated metal (Ag, Cu, Si, Cs, etc.). The conditions under which metal intercalation under graphene is possible have been found empirically, while the intercalate atomic structure and the process explaining how alien atoms settle under a graphene layer have remained unknown.

This paper presents the results of a study of synthesis of graphene during propene adsorption at 300°C/ annealing at 500°C cycle with following gold intercalation process under the graphene monolayer on Ni(111).

1. New precise temperature programmed method for graphene synthesis on Ni(111) has been proposed and tested. As a result, monocrystalline graphene monolayer of size 6×6 mm has been grown on Ni(111).

2. Mechanism of Gr synthesis includes the following steps:

1. hydrocarbon molecules dehydrogenation on terraces and complete dissociation on step edges
2. carbon atomic chains formation on terraces
3. carbon atoms diffusion under surface through step edges and their accumulation between nickel atomic layers in subsurface area
4. at annealing, carbon atom segregation on surface with Ni_2C formation and then transformation into graphene

3. As a result of gold intercalation at 450 °C, graphene monolayer on Ni(111) is detached from nickel without any damage. Network of dislocation loops Ni(111)-9.5×9.5-Au is real indication of gold intercalation under graphene monolayer.

IV-PP39

Photooxidation of Aniline and its Derivatives in the Presence of Heterogenized Substituted Zinc Phthalocyanines

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It is shown for the first time that photooxidation of anilines leads to products of *p*- hydroxylation in the presence of the heterogenized sensitizers on the basis of the substituted zinc phthalocyanines adsorbed on Amb. or NH_2-SiO_2, or in sulfochlorid form covalent attached to NH_2-SiO_2. Selectivity of *p*-aminophenol formation is more 70%. The most effective heterogenized sensitizers, namely, adsorbed (3-$PhSO_2$-5-*t*-Bu)$_4$PcZn on Amb. and attached (3-$PhSO_2$)$_4$-(SO_2Cl)$_n$-PcZn to NH_2-SiO_2 can be used in several times. Thus the total of photocatalysts turnovers number is more than 4000.

IV-PP40

A New Type of Catalyst for Hydrolytic Hydrogenation of Cellulose

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In this paper a new type of Ru-containing catalysts based on non-functionalized and functionalized hypercrosslinked polystyrene (HPS) is proposed for cellulose hydrolytic hydrogenation. HPS is characterized by ultra-high porosity and excellent sorption properties and was successfully used as a support for nanocomposite catalysts.

IV-PP41

Micro- and Mesoporous Aluminosilicates – New Efficient Catalysts for the Synthesis of Pyridines

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The synthesis of pyridines has been performed by a multi-component reaction of ethanol, formaldehyde, and ammonia in the presence of microporous zeolites (HY, H-Beta, H-ZSM-12, H-ZSM-5), a micro-meso-macroporous zeolite HY-MMM and amorphous mesoporous aluminosilicates ASM.

Catalysts based on zeolites with a combined micro-meso-macroporous structure and mesoporous aluminosilicates showed high activity in the synthesis of pyridine and picolines (conversion of ethanol reaches 90% and 70%, respectively).

The selectivity of the pyridine formation reaches its maximum over microporous zeolites (49%) at 200-300°C and 7 h^{-1}. The most selective formation of 3-picoline over micro-meso-macroporous zeolite H-Y-MMM and mesoporous aluminosilicate ASM (60%) at 300°C, 7 h^{-1}.

IV-PP42

Optimization of Raw Materials and Process Parameters Dehydrogenation Higher Alkanes

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The main stage of linear alkylbenzenes production (LAB) is dehydrogenation process of n-paraffins C_{10} – C_{13}. The formation of byproducts occurs in this stage and it contributes to formation of coke on the dehydrogenation catalyst surface. Composition of raw materials has significant effect on the yield and quality of the LAB and accumulation rate of coke on the catalyst. Using the mathematical model developed dehydrogenation process, the optimal modes of water feed to the dehydrogenation reactor at a molar ratio of reducing hydrogen / feedstock: decreasing the molar ratio of hydrogen / feedstock to 7/1 to 6/1 to compensate for the high rate of catalyst deactivation can be achieved by increasing the flow rate of water. It is shown that a change in the type of catalyst is necessary to adjust the recommendation of water flow in the dehydrogenation reactor, as it is determined by the rate of coke formation reactions, which is different for different catalysts.

IV-PP43

Photocatalytic Conversion of Glucose in TiO_2 Aqueous Suspensions

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Glucose, a major component of biomass, can be used as a model compound for the sustainable production of high value chemicals. To this aim photocatalysis can be considered as an alternative particularly because it is performed at ambient pressure and room temperature. TiO_2 Commercial (Evonik P25, Merck and BDH) and home prepared TiO_2 powders have been used as photocatalysts for the glucose oxidation in aqueous suspension. Different conversion extent and distribution of intermediate products were observed, depending on the photocatalyst used. The main glucose oxidation product was gluconic acid in the presence of the commercial TiO_2 Merck and BDH samples, whereas with Evonik P25 and all of the home prepared materials mainly arabinose was obtained along with eritrose, glyceraldehyde and formic acid. The isomerization of glucose into fructose was also observed.

IV-PP44

Study of Zeolite Ni-Al-Si-th Catalyst of Hydrocracking Vacuum Distillate by EM, DTA and Radiography

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Based on the previously synthesized zeolite Ni-Al-Si- th catalyst, the highly efficient wide-porous catalyst was developed for the process of heavy feed stocks light hydrocracking .

It was established that the modification of the porous structure of the zeolite-containing Ni-Al-Si- catalyst increases the dispersibility of the nickel and therefore allows to get the light hydrocracking catalyst, keeping the stable activity after prolonged use.

IV-PP45

Methylation and Carboxymethylation of Alcohols, Diols, Phenols and Acids with Green Reagents Dimethyl Carbonate under the Influence of Homogeneous Tungsten, Cobalt, and Manganese-containing Catalysts

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Methylation and carboxymethylation of alcohols, diols, phenols and acids with green reagent dimethyl carbonate under the influence of homogeneous tungsten, cobalt, and manganese-containing catalysts

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IV-PP46

Photocatalytic Oxidation of Propane: Designing Catalysts for Selectivity Tuning

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Using a TUD-1 matrix, a high degree of control over the size of TiO_2 particles in the range of 3 to 8 nm was achieved at identical Ti loading, which allowed unique experiments leading to improved understanding of the effect of nanoparticle size in mesoporous materials on photocatalytic activity. Due to enhanced luminescence, the initial reaction rate in photo-catalytic oxidation of propane under ultraviolet irradiation (335 nm, selectively activating the nano-particles), was found to be smaller for the 3.5 nm particles, while ultimately the larger total available surface area lead to a higher propane consumption with higher photochemical selectivity toward acetone (as opposed to carboxylates), as compared to the 8 nm particles.

IV-PP47

Production of Substituted Anthraquinones via Diene Synthesis in the Presence of Solution of Mo-V-P Heteropoly Acid as Bifunctional Catalyst

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9,10-Anthraquinone and its derivatives are the valuable products of organic synthesis. We developed one-pot processes for the preparation of substituted anthraquinones via diene synthesis in the presence of heteropoly acid $H_{17}P_3Mo_{16}V_{10}O_{89}$ (HPA-10) solution as a bifunctional catalyst, i.e., acidic catalyst for diene synthesis and catalyst for the oxidation of the obtained adduct. In the present study, experimental data were obtained for two one-pot processes:
1) 2-methylanthraquinone (2-MAQ) synthesis from naphthoquinone (NQ) and isoprene;
2) 2,3-dimethylanthraquinone (2,3-ДMAQ) synthesis from NQ and 2,3-dimethyl-butadiene.

We investigated the possibility of multicycle catalyst performance. After the desired reaction, the HPA-10 solution was rapidly regenerated in separate stage and reused. Various methods for regeneration of the catalyst were alternated.

IV-PP48

Development of Bifunctional Catalysts Containing Ru and CsHPA for One-Pot Conversion of Polysaccharides to Polyols

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Cs salts of HPAs with different HPA structures and Cs content as well as Ru catalysts supported on carbon and CsHPAs were prepared. All the catalysts were characterized by the different analytical methods and tested for the stability in the hydrothermal conditions. The synthesized bifunctional Ru/CsHPA catalysts (where HPA was $Cs_2HPW_{12}O_{40}$ and $Cs_3HSiW_{12}O_{40}$) showed very high stability, activity and selectivity in the one-pot hydrolitic hydrogenation of polysaccharides (cellulose and xylan). High yields of sorbitol or xylitol up to 60 and 70% respectively were archived.

IV-PP49

Conversion of Cellulose into 5-Hydroxymethylfurfural over Solid Acid Catalysts Based on Sibunit Carbon Material

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The availability of 5-HMF and glucose production from cellulose with quite high yields using one-pot catalytic process of hydrolysis-dehydration over sulfonated and oxidized samples of graphite-like carabon Sibunit was shown. The sample of carbon treated by fuming H_2SO_4 at 200 °C seems to be very promising one. The kinetic study allowed to evaluate rate limiting stapes and suggest reaction pathways and the mechanism of catalytic action.

IV-PP50

Macroinitiators in the Polyaddition Reaction of 2,4-toluene Diisocyanate

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The influence of reaction conditions on the mechanism of 2,4-toluene diisocyanate (TDI) polyaddition to anionic macroinitiator, which is a block copolymer of propylene oxide and ethylene (PPEG), part of the hydroxyl groups substituted on potassium alcoholate, was studied,. The relevance of this work is the fact that this reaction is the basis of obtaining polymer film nanoporous materials.

In this research was used octaglycidyl polyhedral oligosilsesquioxane (gl-POSS). The role of POSS as stabilizers of active terminal polyisocyanate units which formed during the opening N=C bond and the formation of the linear N-substituted polyisocyanates (N-polyisocyanates) was studied. This effect was specified for wide range of epoxy-POSS concentration.

IV-PP52

The Effect of Dealumination with HCl on MFI and FER Type Zeolites on the Dehydration of n-butanol

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The increasing commercial production of bio-butanol makes it an interesting and emerging bio-based building block in view of the depletion and increasing costs of fossil feedstocks for the synthesis of butenes (through dehydration) that are widely used in polymers, oxygenated additives and rubbers... The dehydration of alcohols can be catalysed by acid sites, of which zeolites are the most promising. Shape selective effects of zeolites can give rise to high yields of butene isomers compared to other types of catalysts and differences in selectivity are found with the use of various zeolites. The assessment of the catalysts was performed in a high throughput setup equipped with 2 tubular reactors. Typical Space time curves are measured to determine effects of the zeolite treatment and lattice structure.

IV-PP53

Features of the Zeolite Containing Catalysts of Oxidative Catalytic Cracking by Thermal Analysis

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Our studies revealed distinct nature of CP, formed in the course of the traditional non-oxidative and oxidative catalytic cracking. Oxidative cracking of vacuum gas oil for 45 minutes formed two distinct phases surface CP: deposition of an amorphous type with a high hydrogen content and low coke density. Deleting the CP data observed in the temperature range 574 ... 675°C, which is lower than the regeneration temperature range of the traditional catalysts for catalytic cracking and shows promising oxycracking. It was also found that increasing the catalyst mileage oxycracking 60 minutes resulting in the formation of highly surface and graphitized structures, over which the burning temperature of 800°C, far exceeding the stability limit temperature of zeolite catalysts.

IV-PP54

Effect of the Physico-Chemical Characteristics of the Various Mn-Based Oxide Catalysts on the Catalytic H_2O_2 Decomposition

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Hydrogen peroxide has been utilized as an oxidizing agent in the waste water disposal facilities for the environmental remediation such as the bleaching and deodorization in industry. The steam, oxygen and heat energy, which can be utilized in industry and other field and the reactant is a non-toxic and an environment-friendly, can be generated by the decomposition of H_2O_2. For these merits, the catalytic decomposition of H_2O_2 has been researched in view of the effect of the various oxide-based catalysts on the performance. The various metal oxide catalysts were prepared for the catalytic H_2O_2 decomposition and the effect of their characteristics on the performance was investigated in this study. The performance test of the various prepared catalyst was conducted using both fixed and batch type reactor. The catalytic activity was compared through the variation of the temperature, pressure and reaction duration time during the catalytic H_2O_2 decomposition.

IV-PP55

Investigation of the Thermocatalytic Conversion Process of Catalytic Cracking Heavy Gasoil and its Mixture with Cotton Oil by Using the Mix Catalytic System

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During the recent years the role of the catalytic cracking process assumes importance in the trend of obtaining the main feedstock to the polypropylene industry. The investigations are carried out in most of the countries for increasing the yields of low molecular olefins, especially ethylene and propylene in the conducted deep catalytic cracking.

IV-PP56

Au-Cu^+ Synergy in $MgCuCr_2O_4$-spinel Supported Gold Nanoparticles for Selective Oxidation of Alcohols and Olefins

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Gold nanoparticles supported on a $MgCuCr_2O_4$-spinel are highly active and selective for the aerobic oxidation of ethanol to acetaldehyde and propylene to acrolein. The good performance of Au/$MgCuCr_2O_4$ in these two selective oxidation reactions is due to the strong synergy between metallic Au and surface Cu^+ sites. Density functional theory calculations provide a molecular level insight to the reaction mechanism and unravel the importance of Au-Cu synergy in both reactions. For the ethanol selective oxidation, dissociative adsorption of ethanol is facilitated by cooperative action of the interfacial gold atom and a basic oxygen atom of the support. The most difficult step is the recombinative desorption of water from the surface, in which Cu plays key role. For the propylene selective oxidation, adsorbed O_2 oxidizes the allylic C-H bonds of adsorbed propylene. The role of Cu in the support is to decrease the desorption energy of acrolein.

IV-PP57

Effects of Promotion Techniques on ZSM-5 activity in Conversion of Alcohols to Fuel Range Hydrocarbons

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Fermentation broth is a potential source of alcohols. The effect of zsm-5 promotion technique on the product distribution of alcohols conversion has been investigated. ZSM-5 zeolites were synthesized and promoted using different techniques. The catalyst activities and selectivity were assessed by converting ethanol, isopropanol and butanol in a fixed bed reactor. All synthesized catalysts were very crystalline and with average particle sizes not more than 2 μm as confirmed by XRD and SEM analyses. It is seen that both gasoline and diesel range hydrocarbons can be produced from alcohols at different ratios depending on the catalyst promotion as well as the promoter type. The promoted catalysts showed different selectivity towards gasoline and diesel range hydrocarbons. Loading with 5% nickel oxide by IWI showed the highest selectivity to gasoline range hydrocarbons.

IV-PP58

Fischer-Tropsch Synthesis in Presence of Composite Materials Based on Pyrolyzed Polymers of Different Structure

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Nanocomposite materials based on pyrolyzed polymers were synthesized. High activity of systems in Fischer-Tropsch synthesis was showed. Synthesized materials were characterized by magnetometric *in situ* methods and XRD. The assumption of influence of polymeric matrix structure on activity of materials in Fischer-Tropsch synthesis was made.

IV-PP59

Conceptual Design of the Catalytic H_2O_2 Decomposition Process for the Production of Dry Oxidizing Agent Used in the NO Oxidation

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NOx is a major air pollutant produced by the combustion of fossil fuel. Many technologies of the NOx treatment have been conducted and the NO oxidation using the various wet and dry oxidants was investigated to improve the NOx removal efficiency. The dry oxidant can be produced by the H2O2 decomposition and then iron, zirconium and some other transition metal-based oxide were used for the catalytic H_2O_2 decomposition. In this study, the catalytic process for H2O2 decomposition was investigated for the production of the dry oxidizing agent to use for the NO oxidation. The catalytic H_2O_2 decomposition over the various catalysts for the dry oxidant production and the combination with NO oxidation process using dry oxidant produced were investigated under the various reaction conditions (e.g., temperature, amount of catalysts, gas composition and space velocity).

IV-PP60

Gas Phase Glycerol Acetylation to Fuel Additive over Solid Acid Catalysts

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In the recent years, biodiesel has gained significant attention as renewable transportation fuel. Glycerol is inevitably produced by 10 wt% in total biodiesel production which resulted in a large surplus of low value glycerol in the market. Glycerol esterification with acetic acid (acetylation) is one of the processes to valorize glycerol to useful chemicals such as monoacetin (MAG) and diacetin (DAG) have applications in cryogenics and polymers. Triacetin (TAG) can act as cold flow improver and viscosity reducer for biodiesel [1]. Glycerol acetylation is usually performed in batch operation using homogeneous catalysts like H_2SO_4, p-toluenesulfonic acid or heterogeneous acidic catalysts such as heteropolyacids [2], resins like Amberlysts [3], etc. Surprisingly, very few reports are currently available on continuous flow glycerol acetylation [4]. In the present work, several silica-based catalysts (SiO_2-MO_x in molar ratio of 30:1) were prepared, characterized and evaluated in the gas phase glycerol acetylation for their catalytic activity.

IV-PP61

A Novel Coupling of Cyclohexanol Dehydrogenation and Cinnamaldehyde Hydrogenation Using In-Situ Liberated H_2 in One Reactor under Identical Conditions

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A novel catalytic coupling process that combines two industrially important reactions (i.e. cyclohexanol dehydrogenation and cinnamaldehyde hydrogenation) was studied for the first time over Cu/Al_2O_3 catalysts in gas phase. This approach avoids external supply of H_2 and utilises the in-situ liberated H_2 from the dehydrogenation step of first reactant for the hydrogenation reaction of second reactant. A catalyst series consisting of four Cu/Al_2O_3 solids with varying Cu loadings (2.5 - 10 wt%) were prepared, and characterized by BET, ICP, XRD, TPR, XPS, TEM etc. Among the series, 7.5 wt% Cu/Al_2O_3 catalyst exhibited the best performance with nearly 100% conversion of cinnamaldehyde and 80% cyclohexanol conversion into cyclohexanone and hydrocinnamaldehyde. Furthermore, significantly higher space time yields of 500 $g/kg_{cat}\cdot h$ (cyclohexanone) and 370 $g/kg_{cat}\cdot h$ (hydrocinnamaldehyde) could be achieved successfully.

IV-PP62

Black Oil Macromolecular Structuring Technology in the Process of its Oxidation for Obtaining the Bituminous Isolation Materials

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One of the effective ways to improve the properties of special bitumens are their chemical and physical modification. Considering oxidative polymerization is connected with radical-chain reactions, oxidizing process of residual oil was carried out with the use of modifiers, which are able to take part in this process, subjecting the segments of paraffin chains to chemical structuring with further formation of polycyclic naphthene-aromatic fragments, promoting the intense resin formation and preventing from the formation of the asphaltene crystalline phase. Bituminous insulating materials (BIM), based on acidified flux oil, showed the ambiguity of their assessment, i.e. at identical speeds of fuel-oil residues oxidation processes, there are differences in strength properties of coverings. The properties of air-blown asphaltic bitumen are regulated by resizing of the core and solvation shell of the complex structural unit by injection of multicomponent bifunctional modifier, promoting the reduction of oxidation duration and the improvement of physical-mechanical and insulation properties of BIM.

IV-PP63

Intensification of Chemical-Technological Oil Refining Processes by the Use of Wave Technologies

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Traditional methods of intensification of chemical and technological processes of oil refining are energy intensive and often reached effect's value does not cover the costs. In this regard, there is the task to use modern high technologies, ensuring the achievement of the required effect without the high material and energy costs, among which most promising and effective are the wave technologies. The aim of the study was to investigate the effect of wave impacts on the speed and depth of chemical processes. The technologies which use wave methods of impacting oil refining chemical-technological processes are applied for enhancement of physical-chemical properties and fractional composition of oil and oil products are discussed. The increase in the light hydrocarbon molecules oscillation amplitude during oil fraction distillation, contributes to weakening of intermolecular interactions, separation of these molecules from supermolecular structure solvation shells and transfer to a vapor phase, which results in increase in the yield of light fractions.

IV-PP64

Bitumen Isolation Materials Producing Technology Based on Macromolecular Structuring of Naphtha Crude Residues during Their Oxidation

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One of effective methods to improve the properties of special bitumen is their chemical and physical modification. Oxidative polymerization related to chain-radical reactions is suggested. The modifiers which able to participate in the oxidation of crude naphtha residues, by chemical structuring of the segments of paraffinic chains followed by the formation of polycyclic naphtheno-aromatic fragments that contribute to gumming and preventing the crystalline phase of asphaltene formation are required. Bituminous insulating material (BIM) obtained from oxidized tars showed the ambiguity of their assessment, i.e. the differences in the strength properties of the coatings (C) were observed at similar velocities of naphtha residue oxidation. Modification of the properties of oxidized bitumen occurs by alteration of the nucleus size and the solvate shell of a structurally complex unit (CSU), the introduction of a multi-component bifunctional modifier (MBM) that reduces the oxidation duration and improves the physical, mechanical and insulating properties of BIM.

IV-PP65

Ways of Regeneration of Highly Effective Catalysts Based on Mo-V-P Heteropoly Acid Solutions

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In oxidative processes involving homogeneous catalysts based on aqueous solutions of Mo-V-phosphoric heteropoly acids with Keggin composition $H_{3+x}PMo_{12-x}V_xO_{40}$ (HPA-x), the catalyst regeneration step (oxidation of the reduced HPA-x form) usually is the key reaction. It determines the processability of the catalyst, i.e. the possibility to implement an effective two-stage catalytic process of substrate oxidation with oxygen. The work discusses various ways of regeneration of the HPA-x solutions: 1) by O_2 at temperatures 150−170 °C and $PO_2 = 3-4$ atm; 2) by the 30 % H_2O_2 solution and 3) by oxygen air under atmospheric pressure with the addition of nitric acid.

IV-PP66

Synthesis of a Novel Anthracene Based Schiff Base-copper(II) Complex as a Potential Catalyst

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Many Schiff base complexes shows the catalytic activity in a large number of homogeneous and heterogeneous reactions such as oxidation, epoxidation, hydroxylation, aldol condensation, polymerization and hydrogenation reactions. Considering wide catalytic properties of Schiff base complexes, we have designed a simple methyl anthracenylimine benzoate (MAB) derivative, which has the ability to form self-assembled anthracenyl excimer species with a specific metal ion. Its complexing ability for a wide range of metal ions has been explored. **MAB** exhibits high selectivity and sensitivity for Cu^{2+} in the presence of various metal ions with a significant emission enhancement via unique copper(II)-directed static excimer formation. The present study is a good example of a receptor in which the rational conversion of excimer species to monomers can be monitored distinctly. The copper complex of **MAB** will be further explored as catalyst in some organic reactions.

IV-PP67

Determination of Pt-catalyst Efficiency of Reforming Process for Different Industrial Plants

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It is shown that the use of computer modeling system taking into account the physical and chemical nature of the reforming process allows evaluating the effectiveness of catalyst replacement. Solving the inverse kinetic problem, the relative rates of chemical reactions are found for Pt-catalysts. Using computer modeling system it is shown that technological parameters of the unit LCh-35-11/1000 provided low activity of the catalyst in spite of this, it possible to obtain the yield in the range of 89-90% by weight.

IV-PP68

New Chiral Catalysts of Nitroaldol Condensation

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The work presented in the paper is devoted to the development of the synthesis of the new chiral copper catalysts for nitroaldol condensation containing tetradentate ligands derived from natural terpenes. Novel chiral copper complexes with nitrogen-containing ligands catalyze the reaction of nitromethane with aldehydes to give nitroalcohol in yields of 45-99% and optical purity of 60% ee.

IV-PP69

Green n-octanol Oxidation on Promoted Silver Catalysts

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Green catalytic processes for alcohols selective oxidation are needed to substitute conventional methods that use stoichiometric oxidants and cause environmental problems. Platinum group metals and nanosized Au are useful catalysts for this, but very costly. We investigate here silver as a cheaper alternative for catalysts for alcohols selective oxidation, using octanol, a model molecule of the less reactive alcohol types, to assess its feasibility. We found that the relatively low activity of Ag/TiO$_2$ catalyst can be boosted by modifying the support with transition metals (Ce, Fe, La). These modifications does not affect the metal content or the surface area, but change the average particle size and the electronic properties of silver. Besides, Ce-modification causes decoration of Ag particles with CeO$_2$. Based on CO adsorption FTIR and XPS data, charged metal clusters $Ag_n^{\delta+}$ are found to be the most probable active sites.

IV-PP70

Highly Active and Recyclable Metal Oxide Catalysts for Prins Condensation of Bio-renewable Feedstocks

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Metal oxides such as Nb$_2$O$_5$, Cr$_2$O$_3$ and especially Zn(II)-Cr(III) mixed oxide are demonstrated to be highly active and recyclable heterogeneous catalysts for Prins condensation providing a clean, high-yielding route for the synthesis of nopol by the condensation of bio-renewable β-pinene with paraformaldehyde. Zn-Cr mixed oxide with an optimum Zn/Cr atomic ratio of 1:6 gave 100% nopol selectivity at 97% β-pinene conversion, with the catalyst easily recovered and recycled. The acid properties of Nb$_2$O$_5$ and Zn-Cr mixed oxide were characterised by DRIFT spectroscopy of adsorbed pyridine and ammonia adsorption microcalorimetry. An appropriate combination of acid-base properties of the Zn-Cr oxide is thought to be responsible for its efficiency.

IV-PP71

A One-step Technique for in situ Synthesis of the Aerogels of the Multi-walled Carbon Nanotubes

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A new cost-efficient technique for one-step in situ MWCNT aerogel production under conditions close to industrial nanotube synthesis was developed. Preformed catalyst employing provides stabilization for MWCNT aerogel structure. The aerogels produced possess as low density as 0.03-0.08 g/cm^3.Such properties of the aerogels as S_{BET}, pore size distribution, density, conductivity and shape can be varied in a wide range. In situ produced MWCNT aerogels demonstrate high electrical conductivity (several S/cm), remain stable in different solvents and hold more than 2500 their weight. Any shape of MWCNT aerogels is possible to obtain by using different geometry of preformed catalyst (balls, cylinders etc.)Due to high polarizability, MWCNT can be employed as low weight reflecting coatings. Macroporous and rigid structure combined with high surface area allow MWCNT aerogel to be promising support material for a different compounds including biological and supramolecular species.

IV-PP72

Carbon Nanomaterials in 1,2-dichloroethane Dechlorination and Aliphatic Alcohols Conversion. The Role of Surface Chemistry and Carbon Matrix Structure

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The carbon nanomatherials: nanotubes (CNTs), nanodiamond (ND) and nanoflakes (CNF) were employed as catalysts in the 1,2-dichloroethane dechlorination and the C_2-C_4-alcohols conversion. Catalytic activity in 1.2-dichloroethane conversion was exhibited only by ND, and the selectivity to ethylene was almost 100%. The key role in catalysis plays a "diamond" structure of ND and hydrogen groups on its surface. It was established that oxygen-containing Lewis sites and unsaturated surface C=C bonds on CNTs play a key role in the conversion of alcohols while just the basic oxygen-containing centers on the ND surface responsible for the catalysis on it. UNFs-N, containing 10% nitrogen, exhibit catalytic activity only in conversion of primary alcohols, that allows to judge about the participation only of nucleophilic nitrogen-containing groups in conversion of alcohols.

IV-PP73

Synthesis of CO and H_2 Conversion Nanoheterogeneous Catalysts in Disperse Systems

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Results of last period researches on synthesis of ultrafine and nanosized particles of CO and H_2 conversion catalysts suspended in liquid hydrocarbon medium or distributed in solid organic matrix are given in report.

IV-PP74

Titanium (+4) Complexes Containing 2-(hydroxymethyl)phenol Derivatives as Pre-catalysts for the Polymerization of Ethylene

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The polymerization of olefins by single-site catalysts has experienced a phenomenal growth in the last decades. Numerous highly active single-site homogeneous catalysts based on metals across the transition series have been reported. Among them metal complexes with OO-type ligands (especially where ligand structure contain both phenol and alcohol hydroxyls) are indeed unique. In recent studies, we have found the ability of lithium and magnesium compounds to promote the catalytic process due to the products of secondary coordination.

Herein, we report the synthesis of tetranuclear titanium complexes, stabilized by saligenin-type ligand - 4-bromo-2-(hydroxymethyl)-6-methoxy-phenol and their utility as polymerization catalysts.

IV-PP75

Catalytic Conversion of Mechanically Activated Aspen Wood in Supercritical Ethanol in the Presence of Zeolites with Different Si/Al Ratio

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Thermal conversion of mechanically activated aspen wood in sub- and supercritical ethanol in the presence of high silica zeolites in H- form with different Si/Al ratio was investigated.
It was shown that the increase of pressure of mechanically activated aspen wood conversion from 4.0 to 20.8 MPa significantly increases of the conversion degree (up to 95.5 and 76.0 wt.% at temperatures of 350 °C and 270 °C, respectively).
The use of zeolites catalysts increased the yield of liquid fraction boiling up to 180 °C by 1.7–2.2 times and reduced the yield of the fraction boiling above 180 °C by 3.2 - 6.3 times at process temperature of 350 °C and pressure of 18.0 MPa.

IV-PP76

Bio-inspired "Buckyball-shaped" Photocatalytic Architectures

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In the current study, bio-inspired buckball-shaped TiO_2 structures were synthesized using a simple sol-gel method. We showed that the crystal structure and surface composition of the buckyball-like TiO_2 overlayer could be fine-tuned by altering the calcination temperature as well as the titanium (IV) isopropoxide:ethanol volume by volume (v/v) ratio during the synthesis process. It was also illustrated that the unique surface morphology and the pore structure of the LC biotemplate could be successfully transferred to the inorganic TiO_2 overlayer, followed by the effective removal of the biological scaffold. Moreover, we demonstrated the photocatalytic functionality of micron-sized buckyball-like TiO_2 architectures in the photocatalytic degradation of Rhodamine B dye.

IV-PP77

KMo Alumina Supported Catalysts for the Synthesis of Methylmercaptan from Syngas and H_2S: New Insight into the Nature of the Active Phase

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Methylmercaptan (CH_3SH) is an industrially chemical of major importance and is currently manufactured at industrial scale by the reaction of methanol with hydrogen sulfide. The development of a new route using a simple feedstock (syngas/hydrogen sulfide) is then increasingly attractive. In this study, K-Mo based catalysts supported on alumina have been prepared, fully characterized and their catalytic performances have been evaluated in the synthesis of CH_3SH from syngas and H_2S. From careful analysis of XPS results, the presence of an intercalated K_xMoS_2 is proposed for the first time in supported KMo sulfide catalysts. By correlating the amount of this phase with the catalytic performances, intercalated K_xMoS_2 is assumed to be the active phase in the reaction of thiolation of syngas. Catalytic performances can be improved by changing the support and increasing the Mo loading.

IV-PP78

Investigation of Palladium Catalysts Supported on Highly Porous Cellular Metal Carriers

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The influence of morphological, tekstrure and acid characteristics composite of aluminum oxide and nickel-containing highly porous cellular material (HPCM) on the electronic and geometric properties of the activity in the selective hydrogenation of acetylenic hydrocarbons inflicted on him palladium particles. Found that compared with conventional catalysts having a support just as γ-Al_2O_3, the carrier γ-Al_2O_3/ Ni-HPCM provides for more uniform formation of the charge distribution of the active component - the particles of palladium to the surface atoms having higher electron density on the valence orbitals . Such a state of active component determines the higher selectivity of the catalyst Pd /γ-Al_2O_3/ Ni-HPCM in the selective hydrogenation of acetylenic hydrocarbons.

IV-PP79

Aqueous Phase Hydro-deoxygenation of Glycerol towards One-step Production of "Green" Propene

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Aqueous glycerol hydro-deoxygenation (HDO) towards propene formation is a novel and environmentally-friendly chemical process, promising significant contribution into meeting the increasing demand for propene, worldwide. Catalytic results of this study validate that this innovative method can lead to propylene production, using biomass-derived feedstock. Green propene can be selectively formed via one-step glycerol HDO reaction, in the liquid phase, over Mo-based catalysts. Specifically, the latter selectively catalyze C-O bond scission and generate a C=C bond, resulting in complete removal of oxygen from the glycerol molecule. Reaction product distribution indicates that propene is the main product, exhibiting, at 300oC, 67% yield and 100% selectivity in the gas phase. Propene is primarily produced through the acrolein-2-propenol route, via sequential dehydration/ hydrogenation steps; glycerol is converted into acrolein and then to 2-propenol, which is subsequently hydro-deoxygenated to propene.

IV-PP81

Development of Chemical Conversion for Methanol/Carbon Dioxide to Dimethyl Carbonate by V_2O_5 Catalysts

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CO_2 is the main global warming potential (GWP) greenhouse gas. Direct influence on environmental and green-house effects has been an important issue for environmental protection all over the world. The direct synthesis of dimethyl carbonate (DMC) from CH_3OH and CO_2 is one of the good choices to mitigate the CO_2 problem and has attracted considerable attention. DMC has been used as a green chemical and an alternative to corrosive and toxic reagent. Therefore, the direct synthesis of DMC is an effective way to solve environmental pollution. Due to its high mixing octane number (105), excellent compatibility with hydro carbonates and high amount of O_2 in the molecule (3 times than methyl-tert-butyl ether), it can reduce the emission of off-gas after adding it to gasoline/petroleum. It is also considered as an ideal additive for transportation fuels due to its higher oxygen content (53.3%) and good mixing properties with octane. Additionally, DMC is also considered as a promising alternative to the use of ketones and ester acetates in the field of paints and adhesives due to a strong solvation power. DMC becomes an important additive of gasoline/fuel oil due to its many advantages nowadays. In this study, Cu-Ni/AC and V-Cu-Ni/AC catalysts were synthesized by hydrothermal. Furthermore, V_2O_5 was added for the efficiencies of DMC conversions, selectivity, yields, and production technologies from methanol and carbon dioxide. Correlations between catalyst structures and DMC production efficiencies were also investigated via the characterization of catalysts in this study.

IV-PP82

Effect of Microemulsion-synthesized Support in the Aqueous Phase Reforming Reaction of Glycerol

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The Aqueous Phase Reforming reaction (APR) represents a valuable pathway to transform glycerol into hydrogen or liquid valuable products by tuning the reaction conditions and the type of catalyst. In this field, the application of microemulsion TiO_2 synthesis to APR reaction appears to be interesting for the good results obtained in preliminary reactions with H_2 productivity data comparable to the literature and yields higher than commercial supports. This is due to the enhanced control of the parameters of reaction for microemulsion synthesis that allows the obtainment of a better control of pore dimension and dispersion of the Pt particles. Extended studies on the reaction conditions allow the hypothesis of two reaction pathways: dehydrogenation that leads to ethylene glycol and lactic acid as primary products and dehydration that gives first hydroxyacetone and then propylen glycol and propanol as main product of reaction.

IV-PP83

Obtaining (Z)-3-hexene with Ni Catalysts Supported on Alumina Modified with Magnesium Precursor

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The selective hydrogenation of internal alkynes for Z-alkene stereoisomers is applicable in the petrochemical and pharmaceutical industry. This paper evaluates the activity and selectivity of a Ni 1% catalyst in the selective hydrogenation of 3-hexyne modifying the alumina support with a 5 and 10% magnesium precursor with excellent results in conversion values for the reaction time considered. The binding energies for the monometallic nickel catalysts reduced at 673 K can be assigned to electro-deficient nickel species (Ni^{n+}, with n close to 2), probably interacting with alumina. The higher values of conversions are obtained at higher reaction temperature. At 303 K, Ni1 % catalyst modified with 5% MgO on alumina presented the highest 3-hexyne total conversions (ca. 100%) and moderate selectivity (≅70%). Besides this prepared catalyst is inexpensive compared to the Lindlar catalyst (5 wt % of Pd) or others mentioned in the literature.

IV-PP84

Catalytic Carbonylation as a Component of Alternative Route for GTL Processes

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Traditional manufactury of GTL products (synthetic liquid fuels, lubricant, waxes etc.) is extremely expensive and consists of three steps, which are costly themselves, especially the step of syngas production. An alternative two-stage route for GTL processes based on direct partial oxidation of natural or associated petroleum gases into methanol and CO and/or olefins and CO with subsequent catalytic carbonylation of oxidation products is suggested. This approach allows developing an integrated new GTL process without expensive and complicated stage of syngas formation. Exactly carbonylation opens up possibilities for production of such high value-added marketable products as diethylketone, methylacetate, dimethylcarbonate, methylpropanoate, ethylidenediacetate, oligoketones, polyketones etc. At present many carbonylation processes operate industrially in large-scale production. The most active and selective in carbonylation are catalysts based on platinum group metals. Suggested new type GTL processes based on oxidative conversion can be successfully used for the monetization of stranded natural and associated petroleum gases.

IV-PP85

Isomerization of Verbenol Oxide to a Diol with Paramenthenic Structure Exhibiting Anti-Parkinson Activity

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Development of new pharmaceuticals, especially from natural compounds, is currently of high interest. Catalytic isomerization of biomass derived verbenol oxide into a chiral paramenthenic diol is a route for synthesis of a potential anti-Parkinson drug. The latter can be an alternative to Levodopa, the main contemporary drug for the Parkinson desease, known for severe side effects. Selective verbenol oxide isomerization into the desired product is, however, challenging. Verbenol oxide isomerization was, therefore, systematically investigated over different zeolites by varying their structure and SiO_2/Al_2O_3 ratio. The isomerization reaction was performed typically in dimethylacetamide 140°C using the initial concentration of VO 0.016 mol/l and 75 mg catalyst. The results showed that a large pore zeolite H-Y with a mild acidity was active and selective towards the desired product. In the final work the reaction mechanism will be proposed.

IV-PP86

Exploring New Synthetic Ways for Cyanopyridines

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3-cyanopyridine is an intermediate in niacin production; it can be synthesized starting from 2-methylglutaronitrile (2MGN), via hydrogenation and cyclisation with loss of ammonia to produce 5-methyl-2,3,4,5-tetrahydropyridine, which is then dehydrogenated to β-picoline and finally ammoxidised to 3-cyanopyridine. We investigated the direct cyclisation of 2MGN as a possible alternative route, while avoiding the loss of the ammonia molecule, with bifunctional catalysts containing a metal (Pt, Pd or Ru) supported over basic or acid/basic supports. The predominant products were short-chain nitriles with negligible formation of cyanopyridines or methylpyridines. Moreover, C deposits accumulated on the catalyst surface; tests with co-feeding of oxygen/water led only to minor improvements. As an alternative route, we studied the condensation of acetaldehyde and acetonitrile to picoline using acidic, basic, or bifunctional catalysts. The reaction led to the formation of several products with low yield to picolines, mainly due to the lower reactivity of acetonitrile compared to acetaldehyde.

IV-PP87

Highly Selective Pd-Cu Supported Catalyst for Liquid-Phase Semihydrogenation of Substituted Alkynes

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As a result of highly homogeneous bimetallic particles formation, Pd-Cu catalysts synthesized via acetate heterobimetallic complexes demonstrate excellent selectivity to stilbene and high stereoselectivity in terms of *Z-/E*-olefin formation. From the practical viewpoint this result is of great interest, since it was found that the Pd-Cu catalyst demonstrates superior activity and selectivity in comparison with commercial Lindlar catalyst ($Pd/PbO/CaCO_3$). It should be noted that this performance is achieved at a substantially lower content of noble metal (1% instead of 5% Pd). Furthermore, the absence of toxic Pb components makes Pd-Cu catalyst promising for usage in pharmaceutical and food industries.

IV-PP88

Catalytic Conversion of Cellulose to C_2-C_3 glycols by a Dual Combination of a Homogeneous Metallic Salt and a Perovskite-Based Heterogeneous Catalyst

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The conversion of cellulose to C_2-C_3 glycols is usually achieved under hydrothermal - above 100°C and 1 bar- and reducing conditions via a cascade pathway including depolymerization of cellulose to glucose, subsequent retro-aldol reactions and hydrogenation of the resulting glycolaldehyde and glyceraldehyde molecules.[1] Multifunctional catalytic systems are thus necessary to achieve a selective formation of C_2-C_3 glycols. Original dual catalytic systems combining a homogeneous metallic salt and a heterogeneous transition metal catalyst for the conversion of cellulose into C_2-C_3 glycols are presented. A sharp analysis of reaction pathways led us to identify an optimal combination of cerium chloride and a barium zirconate-based platinum catalyst for the production of ethylene glycol and propylene glycol with good selectivities (>40%). Remarkably, the platinum catalyst supported on a barium zirconate perovskite exhibited enhanced hydrothermal stability.

IV-PP89

MoCrGa Catalysts Supported on Natural Clays for the Process of Oxidative Conversion of Propane-butane Mixture

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Oxidative conversion of propane-butane mixture by air to oxygen-containing compounds at T=573-873K and space velocity 330-15000$ч^{-1}$ on polyoxide catalysts containing 1-, 5- and 10% Mo, Ga, Cr of different composition and ratio supported on natural Torgai clays (TC), Sary-Ozek, Chankanai, IK-30 and IR-301 zeolites. The influence of reaction temperature, contact time, composition and percentage of the active component of catalyst were determined.

The important petrochemical products - acetone (823K), acetaldehyde (723K), methyl ethyl ketone (723K), ethylene (723K), benzene (823K) were the main liquid products of reaction on natural Kazakhstan's clays and also on clays modified by Mo, Bi, Cr, Ga ions.

IV-PP90

Magnetically Recoverable Biocatalyst for 2,3,6-trimethylphenol Oxidation

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In this paper the activity of the enzyme peroxidase (EC 1.11.07, HRP) immobilized on magnetic nanoparticles Fe_3O_4 was studied. The syntesized biocatalyst was studied in the oxidation reaction of 2,3,6-trimethylphenol (TMP) with hydrogen peroxide to 2,3,5-trimethylhydroquinone (TMHQ), the precursor of vitamin E.

IV-PP91

Catalytic Oxidation of Veratryl Alcohol – a β-O-4 Lignin Model Compound - to Veratraldehyde

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The oxidation of veratryl alcohol to veratraldehyde is a benzylic oxidation representing the valorization of one of the β-O-4 model compounds of lignin. Since the product veratraldehyde is a useful flavorant and odorant the transformation has been comprehensively studied by both enzymatic and homogeneous catalyst systems.

In the present work we have prepared, characterized and examined the performance of heterogeneous catalysts with ruthenium or other transitions metals supported on □-alumina for the conversion of veratryl alcohol to veratraldehyde by aerobic oxidation in water.

IV-PP92

Pd-Ce Nanoparticles on Functional Fe-MIL-101: An Efficient Catalyst for Glycerol Oxidation

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Glycerol is a by-product of biodiesel. Due to the increased demand of biodisel, glycerol production is continually increased [1]. Therefore, selective oxidations of glycerol into more value added chemicals are of great interest in current biomass research. Dihydroxyacetone (DHA), a simple oxidation product of glycerol, is currently the most popularly used sunless tanners, which is the only active ingredient approved by the US Food and Drug Administration (FDA) for sunless tanning [2]. Currently, DHA is mainly produced from an atom-inefficient fermentation process [2]. Transition-metal nanoclusters with particle size around 5nm own big surface area, and demonstrate physical and chemical properties which are significantly different from their bulk counterparts [3,4]. In the presentation, we report the synthetic methods and catalytic performances the Pd-Ce NPs/functional Fe-MIL-101 for the selective oxidations of biomass-based alcohols of glycerol, ethanol, etc. to corresponding aldehyde and ketone products.

IV-PP93

Oxidative Dehydrogenation of Ethane on MoVTeNbO Catalysts

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Mo/V/Te/Nb mixed metal oxide catalysts, prepared by hydrothermal synthesis, are active and highly selective (up to 98%) in the oxidative dehydrogenation of ethane. Conversion achieves 37% at temperature 400 °C; however, selectivity to ethylene decreases to 85%. Under such conditions the catalyst is irreversible deactivates in connection with tellurium reduction. In this case, the catalyst deactivated in reaction of the ODH of ethane shows lower conversion and selectivity to ethylene which are similar to the data received for Mo/V/Nb mixed oxide catalysts which aren't containing tellurium. In the most optimum process parameters conversion of ethane reaches 18%, oxygen - 50%, selectivity to ethylene - 92% at 360 °C.

IV-PP94

Oxidative Catalytic Upgrading of Biomass-derived Glycolaldehyde to Glycolics

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Lignocellulosic biomass is a potential renewable carbon-source for industrial production of important chemical compounds.
5-hydroxymethylfurfural (HMF) and furfural are products obtained from acid catalyzed depolymerization of cellulose or hemicellulose to glucose or xylose, followed by dehydration. Both of these chemicals can be transformed into a range of de- or re-functionalized "furanic" compounds, with varied carbon content, thus serving as valuable platform chemicals. A number of chemicals derived from HMF have already proven useful as alternatives or substitutes to fossil based fuels and polymer components. Lignocellulose can also be transformed into smaller building blocks by partial pyrolysis. A major byproduct obtained from pyrolysis is the C2 chemical, glycolaldehyde. Noticeably, glycolaldehyde contains, like HMF, both an aldehyde and an alcohol moiety which potentially makes glycolaldehyde prone for re-functionalization into value-added "glycolic" chemicals. The focus of this project is the catalytic aerobic oxidation of glycolaldehyde to glycolic acid under mild conditions.

IV-PP95

Mathematical Analysis Options to Upgrade Plants of Dehydrogenation Isoamylenes to Isoprene and Conduct Pilot Tests

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Mathematical modeling of the various areas of engineering optimization process of dehydrogenation of isoamylenes to isoprene. Namely, the proposed three options: 1) a single reactor with an additional introduction of superheated steam into the catalyst bed; 2) two reactors in series with intermediate heating of the contact heat exchanger in the gas; 3) two consecutive reactors with intermediate addition of superheated steam into the gas pin. After analyzing the results, optimal in terms of energy efficiency was selected last optimization method. For the successful implementation of the above scheme in the industrial practice of petrochemical plants carried out tests in a pilot plant, in industrial environments.

IV-PP96

Hypercrosslinked Polystyrene-supported Palladium Catalysts for Suzuki Cross-coupling Reaction

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In this work we investigated the hypercrosslinked polystyrene (HPS)-supported palladium catalysts in Suzuki cross-coupling of 4-bromoanisole and phenylboronic acid. Pd/HPS catalysts with different metal loadings and precursors were synthesized via conventional wet-impregnation method. The reaction was carried out at ambient pressure at variation of solvent nature and composition, temperature, nature and concentration of base, substrate-to-catalyst ratio and stirring rate. HPS-supported palladium catalysts were found to be promising (active, selective and stable during four runs) for the Suzuki cross-coupling reaction of 4-bromoanisole and phenylboronic acid in order to produce the corresponding biaryl with high yield (more than 93%) at mild reaction conditions in environmentally favourable solvents.

IV-PP97

Enantioselective Hydrogenation of Prochiral Arylketones and Keto Acid Ethers Catalyzed by Pd(acac)$_2$- Chiral Base

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Enantioselective hydrogenation of ketone and keto acid ethers by molecular hydrogen over colloidal palladium, which have been formed in system Pd(acac)$_2$ - chiral base - H$_2$ was studied. As a chiral bases we used natural alkaloid (-)cinchonidine (Cin) and its N- and N,N'-protonated derivatives: Cin*HCl and Cin*2HCl, they were preliminary synthesized and characterized by physical and chemical methods.
We found that reaction rate of hydrogenation of acetophenone at p_{H2} = 5 bar decreases with increasing ratio of Cin/Pd in ratio range 0.5 - 1.0 – 1.5 (2.31; 1.17; 0.73 mmol/l*h. The highest hydrogenation rate is observing in hydrogenation of ethylbenzoylformate (up to 180 mol Sub/g-atom Pd*h). In hydrogenation of methylpyruvate we found abrupt decreasing of reaction enantioselectivity (from 86% to 55%) during the reaction time.

IV-PP98

Cumene Hydroperoxide Decomposition in the Presence of Organic Group II Metal Salts

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Cumene hydroperoxide decomposition in chlorobenzene in the presence of magnesium, calcium, zinc, cadmium, or mercury 2-ethylhexanoate has been investigated. It has been established and kinetically proved that the decomposition reaction is preceded by the formation of a hydroperoxide–catalyst complex. Thermodynamic parameters of this complexation have been determined. The catalytic activity of the salts correlates with the ionization potentials of the metals.

IV-PP99

Selective Hydrogenation of Furfural Using SiO$_2$ Based Catalysts: Impact of Reaction Conditions and Metals Employed

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The production of furfuryl alcohol from furfural by liquid phase hydrogenation using precious metals supported on silica was studied. From the metals studied, platinum was found to be the metal which is most selective to furfuryl alcohol while 2%Pt/SiO$_2$ was the superior catalyst of those investigated. The solvent used in the reaction was found to have a significant influence on the selectivity of the reaction to furfuryl alcohol as the use of an alcohol as solvent resulted in the formation of undesirable products involving both the reactant and desired product furfuryl alcohol. Temperature studies conducted found the selectivity was independent of temperature as the conversion which was influenced by both solvent and catalyst selection. These factors concluded this fragment of the research with further work focused on the impact of bimetallic platinum based catalysts on the hydrogenation reaction.

IV-PP100

Selective Hydrogenation of 2-methyl-3-butyne-2-ol Catalyzed by Embedded Polymer-protected PdZn Nanoparticles

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PdZn stabilized nanoparticles were prepared by polyol method and introduced into the matrix by addition into TiO$_2$ sol in the presence of a template Pluronic F127. The prepared catalyst have been tested in the selective hydrogenation of 2-methyl-3-butyn-2-ol, and the results have been compared with catalysts prepared by conventional impregnation. Nanoparticles stabilized with polyvinylpyrrolidone exhibited good activity (1.1 to 1.8 molMBY/molPd/s^{-1}) and high selectivity to 2-methyl-3-buten-2-ol (81.5-88.9% at 95% conversion). The influence of the kind of the stabilizer, the stabilizer/metal molar ratio and activation conditions on the catalytic behavior of the samples was analyzed. It is shown that the particle size does not significantly affect the catalytic properties in the range of 4.4 to 6.5 nm. The kind and amount of stabilizer seems to be crucial to prepare efficient catalyst

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IV-PP101

Capillary Microreactor with PdZn(Ti,Ce)O_2 Coating for Selective Hydrogenation of 2-methyl-3-butyne-2-ol

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The performance of a capillary microreactor coated with mesoporous Pd/(Ti,Ce)O_2 and $Pd_{80}Zn_{20}$/(Ti, Ce)O_2 thin films has been tested in the selective hydrogenation of alkyne alcohol. Catalytic coatings were prepared by dip-coating method of the inner wall of a fused silica capillary with an internal diameter of 250 µm using nanoparticles-based precursor solution. The capillary microreactors were tested in the hydrogenation of 2-methyl-3-butyne-2-ol (0.05-0.3M solution with methanol as a solvent) in 313-323 K temperature range and at the hydrogen partial pressure ranging from 0.3 to 1.0. The highest selectivity of 94% to 2-methyl-3-butene-2-ol was obtained at 99.8% conversion on the $Pd_{80}Zn_{20}$/(Ti,Ce)O_2 coating

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IV-PP102

New Catalysts for Lignin Depolymerisation

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The complex structure of lignin offers various possibilities of exploitation involving the efficient cleavage of etheric- and C-C bonds. To achieve this, this study proposes to combine the lignin hydrogenolysis with the reductive depolymerization using magnetically separable heterogeneous nano-catalysts. The catalytic results revealed that each catalyst component play a separate role in this complex reaction: the reductive depolymerisation is catalysed by cobalt nano-particles, nano-shells of niobia confers necessary acidity for hydrolysis of the β-O-4’ bounds, while magnetic properties of magnetite/maghemite nanoparticles ensure the easy separation and recycling. Combining these entities it was possible to control both the catalysts activity and selectivity to dimer, trimer and tetramer building blocks. While the conversion reached a maximum of 53%, the maximum in selectivity to dimers was of 49% for Co-Nb_2O_5-Fe_3O_4 catalyst.

IV-PP103

Deactivation of Mixed Oxides as Catalysts for Ethanol Condensation: in situ DRIFT Spectroscopy Studies

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The deactivation of Mg-Al and Mg-Zr mixed oxides catalysts with different distribution of acid and basic sites for gas-phase ethanol condensation (being butanol and butadiene the target products) is studied in this work. Deactivation studies were conducted at different temperatures (523-573 K) at ambient pressure. Two different strategies were followed for characterising this deactivation: characterisation (BET, TPO; XRD, etc.) of samples of catalysts used at different reaction temperatures and times on stream and “*in situ*” characterisation of the catalysts under reaction conditions using Diffuse Reflectance Infrared Fourier Transform (DRIFT) spectroscopy. Obtained results demonstrate that these materials are stable at temperatures under 700 K whereas, at higher temperatures important deactivation is observed, caused by the strong adsorption of unsaturated oligomers on the surface.

IV-PP104

Modification of Skeletal Nickel Surface on Effects of Hydrogenation for Adsorption Behavior of p–nitrotoluene

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We studied the kinetics of *p*-nitrotoluene hydrogenation on skeletal and modified skeletal Nickel catalyst in aqueous solutions of 2-propanol and find out that some condition can turn the effect of poison catalyst into promoter [1, 2]. This fact is possible to explain by the formation of new active centers of surface or by shifting the surface balance between individual adsorption forms of hydrogen toward the most active one in the investigated process [2, 3]. This enhance of the catalyst stability is explained by elimination of the most unstable-working surface active centers of the reaction space and by the stabilization of the remaining ones [4, 5].

All the experiments were carried out in a batch laboratory scale tank reactor with stirring frequency of the reaction mixture about 3600 rpm. Physicochemical analysis of quantitative and qualitative composition of reaction samples was performed by liquid chromatography. RC syringe microfilter in alcoholic media of the research system was successfully tested.

Hydrogen chemisorption and *p*-nitrotoluene adsorption behavior have been examined by means of in-situ FTIR spectroscopy. In this case, the hydrogen and 4-nitrotoluene are adsorbed on the different active centers, "metallic" and "organometallic" respectively. α-form molecular hydrogen, H_2 or $H_2^{\delta+}$ associated with one or two surface atoms, γ-form - unionized form atomic hydrogen H or $H^{\delta+}$ with binding energy less than β-form but higher than the α-form are associated with the nickel surface [6, 7].

We now reported that kinetic curves in a wide range of solvent 2-propanol-water don’t depend on the solvent concentration and well describe by the Langmuir-Hinshelwood model with independent adsorption of hydrogen and organic compounds.

IV-PP105
Fischer-Tropsch Synthesis over the Multicomponent Fe-based Catalysts Modified with Additives of Rare Earth Metals

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The Fe-containing catalysis promoted by the transition metals, modified by additives of the rare earth metals VIII Group metals and supported on alumina have been tested in Fischer-Tropsch synthesis.
The process was carried out in a stainless steel reactor under pressure varied from 0.5 to 1.5 MPa, temperature region of 250-340ºC, and gas hourly space velocity (GHSV) of 1000-4000 h-1 with using 6 mL of the catalyst.
The physico-chemical properties of the catalyst were studied by BET, TEM, X-Ray and TPR-methods.
The effect of nature of the rare earth metal and process conditions (pressure, temperature and gas hourly space velocity) on the behavior of the Fe-based catalysts in syngas conversion has been studied.
The results obtained show that the synthesized nano-sized iron-based catalysts have the high activity and selectivity on liquid hydrocarbon in the FTS.

IV-PP106
Selective Oxidation of Toluene Using Noble Metals under Mild Condition

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The aim of this study was to investigate the selective oxidation of toluene using TBHP at 80 °C with supported noble metal nanoparticle catalysts prepared by sol-immobilisation techniques. Au, Pd and Pt have been used to form mono, bi and trimetallic catalysts of different morphology supported on C and TiO_2. These catalysts have been tested for toluene oxidation and show a high selectivity towards benzoic acid. AuPdPt/ C catalyst shows the best activity and has been used for further investigation such as reuse test.

IV-PP107
Mechanistic Understanding on MoO_3 Catalyzed Transesterification between Phenol and Dimethyl Carbonate

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Supported MoO_3 catalysts have been explored as highly selective and active catalyst for the transesterification of DMC and phenol under mild reaction conditions. Combined spectroscopy and reactivity data showed that orthorhombic microcrystalline MoO_3 is the important phase for this reaction. A catalytic cycle for the most critical step in the transient DPC formation has been proposed. The competitive adsorption of DMC and phenol on the coordinative unsaturated active sites of MoO_3 results in the formation of stable asymmetric surface carbonate species, from which target molecule is formed.

IV-PP108
MP/C (M: Ni, Mo, W) Catalysts Hydrodenitrogenation of Aminocaprolactam: Effect of the H_2 Pressure

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The systems based on 10 wt. % monometallic phosphide (Ni, Mo and W) supported on carbon, have been prepared by impregnation under vacuum for the reaction of hydrodenitrogenation (HDN) of the heterocycle alpha-amino-epsilon-caprolactam (ACL). The aim of this reaction is the production of caprolactam (CL) due to its application as precursor in the Nylon 6 production. In this context we have developed this reaction under different values of H_2 pressures to evaluate how it affects in caprolactam production. A better selectivity for CL was detected for moderate hydrogen pressure (10-30 bar) and for the molybdenum containing catalyst.

IV-PP109
Conversion of Heavy Hydrocarbons into Light Oils Using Nanoparticles and Complexes of Transition Elements

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Influence of particles of transition elements on the conversion of bituminous oil is considered in this paper. Studies on a bituminous oil conversion were conducted in a batch reactor at different temperature and pressure conditions.

IV-PP110

Ethanol Conversion to Useful Products: Ethylene, Diethyl Ether, Higher Hydrocarbons, Acetaldehyde and Acetone

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Ethanol conversion was investigated over different acido-basic catalysts in flow reactor in the temperature range 373-873 K, and TPSR as well as in IR experiments. Characterization of catalysts was performed by TEM, XRD, UV-vis, TG-DTA, XRD, NH_3-TPD, Raman spectroscopy and IR spectroscopy. Ethanol is a very versatile intermediate that can be converted with high selectivity/yield in a number of useful products over heterogeneous catalysts. High or very high selectivities or yield have been obtained in ethylene, diethyl ether, acetaldehyde, acetone, propene, butenes and aromatics, depending on catalyst composition.

IV-PP111

Synthesis of Platform Molecules from Cellulose over Bifunctional Magnetic Nanocatalysts

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The purpose of this work was to prepare a series of new magnetic bifunctional catalysts for one-pot conversion of cellulose to different platform molecules. This target was successfully attained using carbon nanotubes as stable catalytic support, niobic acid for the acidic function and ruthenium as active species. Additionally, magnetic nanoparticles were inserted inside the carbon nanotubes offering more functionality for the catalyst recovery. Among different parameters of catalyst preparation, the calcination temperature seems to have significant influence on the product distribution, the lower calcination temperature was leading to the formation of levulinic acid. A synergic effect of niobia and ruthenium led to a high cellulose conversion resulting in different platform molecules as lactic, glycolic and levulinic acids. Using glucose as reaction substrate resulted in very different distribution of products, hydroxymethylfurfural beeing the main product. Introducing oxygen in the system gave a good selectivity to succinic acid.

IV-PP112

"Green" Propylene Glycol: Kinetic Determination for the Valorization of Biodiesel Side Stream

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In triglyceride transesterification to fatty acid methyl esters, 10 wt% of glycerol byproduct is formed. This provides an opportunity for the synthesis of 'green' chemicals instead of their petroleum based route. Among other alternatives, glycerol hydrogenolysis towards propylene glycol is a relevant and attractive valorization route.

Glycerol hydrogenolysis over copper catalyst was tested in a high throughput kinetic set-up with the objective of developing an intrinsic kinetic model for the hydrogenolysis reaction to propylene glycol, aiming at a better understanding of the catalytic chemistry and opening up perspectives for rational catalyst design. The effect of temperature, pressure and space time on the conversion of glycerol and the selectivity towards different hydrogenolysis products have been investigated experimentally. Experimental results show increase in selectivity towards the acetol intermediate with increasing temperature signifying that the activation energy for acetol formation significantly exceeds the one for its further conversion into propylene glycol.

IV-PP113

Research of Hydrogenation of the Nitrobenzene in Supercritical Carbon Dioxide with Use Ru/HPS Catalysts

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Carbon dioxide is perspective solvent for carrying out organic synthesis, including hydrogenation of organic nitrocompounds. On the example of process of catalytic hydrogenation of a nitrobenzene with use of the Ru-containing catalysts positive influence of $CO_{2(sc)}$ is shown. Decrease of influence of a matrix by activity of heterogeneous catalysts that testifies to increase in availability of the fissile Ru-centers to the reacting substratum in the environment of supercritical carbon dioxide is established.

IV-PP114

Catalytic Transformation of Glycerol to Lactic Acid over Au-Pt Supported Catalysts Prepared by Redox-method

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Glycerol (Gly) is as a large-scale by-product in biodiesel production and a versatile feedstock for the synthesis of a wide range of different chemicals. One of the challenging task is to obtain lactic acid (LA), a monomer to a biodegradable polymer, through the catalytic Gly oxidation. In this work, we aimed at evaluation of the activity of Au-Pt catalysts supported on active oxides (TiO_2, CeO_2, $CeZrO_x$) in the Gly aerobic oxidation to LA. The catalysts were prepared by facile redox-method ensuring the formation of close contact between the Au and Pt responsible for the synergetic effect in the catalysts activity. The highest activity and selectivity were obtained for the low-loaded catalysts with atomic ratio Au:Pt=0.025:1.

IV-PP115

Peculiarities of Obtaining Alkyl-Substituted 1,4-benzoquinones in Two-Phase Systems in the Presence of Mo-V-P Heteropoly Acid Solutions

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In the present study, aqueous solutions of Mo-V-phosphoric heteropoly acids $H_{3+x}PMo_{12-x}V_xO_{40}$ with high and low vanadium content were applied as homogeneous catalysts for oxidation of 2,3,6-trimethylphenol and 2,6-dimethylphenol into corresponding 1,4-benzoquinones. The reaction was performed in two-phase system. Different reaction parameters such as substrate concentration, organic solvent, temperature, catalyst composition etc. were analysed in terms of product selectivity. The quinone yield was found to depend strongly on the catalyst redox potential which determines the rate of electron transfer. The results obtained enabled to establish the optimal reaction conditions and to prepare 2,3,5-trimethyl-1,4-benzoquinone and 2,6-dimethyl-1,4-benzoquinone with selectivities of 99 and 85%, respectively. The catalyst used is rapidly regenerated in separate stage under oxygen pressure and reused.

IV-PP116

Efficient Metal-Free Pathway to Vinyl Thioesters with Calcium Carbide as the Acetylene Source

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Calcium carbide was used to synthesize useful vinyl thioesters in accordance with a simple procedure. The reaction proceeded in a mild, metal-free conditions using regular laboratory setup. Due to our mechanistic investigations vinyl thioesters formation occurred *via* gaseous acetylene that was immediately attacked with thiolate-nucleophile. Optimized reaction conditions allowed the selective synthesis of the vinyl thioesters with high yields and the reaction conditions could be scaled up to the synthesis of grams of sulfides from inexpensive calcium carbide.

IV-PP117

Liquid-phase Methanol Synthesis Using Polymerstabilized Catalysts Based on Zinc

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In this paper the results of the study of the kinetics and modeling of methanol synthesis process on polymer-stabilized catalysts – Zn on hypercrosslinked polystyrene are presented. Methanol maximal yield was achieved at a temperature of 170˚C and a gaseous flow rate 270 mL/min.

IV-PP118

High Catalytic Activity of Nanoheterogeneous Systems Based on Aqueous Solutions of Cationic Surfactants of Low Concentrations in Hydrolysis of Phosphorus Acid Esters

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Self-organization and catalytic activity of a highly diluted aqueous solutions (10^{-2}-10^{-16} M) of cationic surfactants in the hydrolysis of 4-nitrophenyl esters of phosphorus acids (substrate) were studied by a complex of physicochemical methods (DLS, electrophoresis, NTA, UV, ^{31}P NMR and ESR). The properties of solutions prepared by successive serial dilutions and kinetics of the hydrolysis were investigated under natural conditions (laboratory bench) and in absence of external physical fields (permalloy container). The solutions of surfactants are dispersed systems in which micelles, domains and nanoassociates are formed in various concentration ranges (10^{-2}-10^{-3}, 10^{-4}-10^{-5}, 10^{-6}-10^{-16} M respectively). The formation of domains and mixed domains was also observed in water-ethanol (10 %v. ethanol) solution of substrates and mixed system surfactant+substrate. The correlation between nonmonotonic concentration dependence of the size of nanoassociates and mixed domains and observed rate constant (k_{obs}) of the reaction was established. It was shown that in nanoheterogeneous systems based on aqueous solutions of cationic surfactants of low concentrations highly reactivity nanoreactors (mixed domains surfactant+substrate) are formed. For example in solutions of CTAB at $1 \cdot 10^{-9}$ M where mixed domains with extreme size are formed k_{obs} is higher than k_{obs} in the micellar solution (10^{-2} M) and k_{obs} of alkaline hydrolysis of substrate at pH 8.0 approximately two and five orders respectively.

IV-PP119

Differential Selectivity Measurements as Effective Means for Mechanistic Studies of Catalytic Reactions

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The differential selectivity of a catalyst is rarely considered in kinetic investigation. However, differential selectivity measurements have a number of advantages in comparison with catalytic activity measurements. When complex catalytic processes accompanied by intensive catalyst transformations occur outside the catalytic cycle (formation, deactivation and/or poisoning of the active species) the differential selectivity can be the sole tool to clarify the nature of the active species and kinetics of the elementary steps in the catalytic cycle. We attempted to briefly review the basic principles and practices of mechanistic studies based on differential selectivity measurements, including the use of artificially created competitive reactions.

IV-PP120

Some Aspects of Kinetics and Mechanism of the Heterogeneous Iso-butane/butene Alkylation over Solid ZrO_2-Al_2O_3/HY Catalyst

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The paper studies some aspects of iso-butane/butene alkylation over solid ZrO_2-Al_2O_3/HY catalyst. The aim of this work was to examine the rates of different alkylation reaction based on experimental results. The experimental data was obtained using a laboratory scale plug-flow reactor operated in continuous mode. The abstract describes the determined activation energy and pre-exponential factors for 4 reactions steps. The kinetics parameters were calculated using reactor model which is fitted to the experimental data. The results obtained are used for development of alkylation process based on solid catalyst to minimize the rates of trimethylpentane undesirable secondary reactions.

IV-PP121

Alkylation of Phenol Using Ionic Liquid Catalyst: A Mechanistic Study

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The Alkylation of Phenols using Ionic Liquid catalyst (N-(1,4-sulfonic acid) butyl triethylammonium hydrogen sulphate) has been investigated by performing Quantum chemistry calculations to understand the tert-butylation reaction mechanism qualitatively at molecular level and obtain relative rates, reaction barriers, effect of solvents, and product selectivity. All gas phase and liquid phase geometries of reactants, products, intermediates and transition states were fully optimized using a semiempirical PM6 method, in MOPAC'09. In order to identify transition state (TS), SADDLE calculations in MOPAC package were successfully applied, to generate trial geometries for unknown transition state complexes.

IV-PP122

Preferential Hydrogenation of Carbon Monoxide to Olefins over Catalysts of Perovskite-type Ferrites

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Catalytic properties of advanced materials - perovskite-type ferrites ($A_{n+1}B_nO_{3n+1}$, n=1,2,3…∞, A=Gd, Sr, B=Fe) were investigated in the carbon monoxide hydrogenation at atmospheric pressure. It was found correlation between the catalytic activity, selectivity to olefins and methods synthesis of complex oxides, the number of perovskite layers, crystallite size, cationic composition and iron valence state.

IV-PP123

Hydrodearomatization Processes in Dispersion Systems: Unsupported Ni-W-S Catalysts Synthesized in situ

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In situ preparation method of sulfide catalysts based on tungsten and nickel in ionic liquids and in the hydrocarbon solution of substrate for the hydrogenation of polyaromatic hydrocarbons was developed. To obtain the catalysts *in situ* in the ionic liquid, thermostable ionic liquid [BMPip][CF_3SO_3] as the solvent for the precursor has been selected. The complex nickel-tiotungstate 1-butyl-1-methylpiperidinium was used as a precursor. Also, the possibility of *in situ* preparation of nanosized catalysts in hydrocarbon solution of substrate through reverse microemultion has been demonstrated.
Synthesized catalysts were characterized by HRTEM, FTIR-spectroscopy and XPS. Obtained catalysts showed high activity and selectivity in the hydrogenation of aromatic compound at the hydrogen pressure of 5 MPa and the temperature 350^{o}C. The possibility of light cycle oil hydrotreating using obtained catalysts has been shown.

IV-PP124

In Situ Synthesis of Unsupported Transition Metal Sulfide Catalysts for Hydrodearomatization Processes

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The preparation method of sulfide catalysts *in situ* in the hydrocarbon solution of substrate for the hydrogenation of polyaromatic hydrocarbons was developed. Used precursors were oil-soluble salts: tungsten carbonyl $W(CO)_6$, ruthenium carbonyl $Ru_3(CO)_{12}$ and molybdenum carbonyl $Mo(CO)_6$. The influence of nickel addition on catalytic activity was studied. Added nickel was in oil-soluble salts form (nickel(II) 2-ethylhexanoate $Ni(C_7H_{15}COO)_2$). Synthesized catalysts were characterized by HRTEM, FTIR-spectroscopy and XPS. Obtained catalysts showed high activity and selectivity in the hydrogenation of naphthalene under a hydrogen pressure of 5-7 MPa at the temperature 350^{o}C. Catalytic activity obtained catalysts increases in the case of nickel addition and optimal M/Ni ratio was found (M = Ru, W, Mo), for tungsten W/Ni ratio was 1/2, for molybdenum Mo/Ni ratio was 1/2 and for ruthenium Ru/Ni ratio was 1/3.

IV-PP125

Selective Oxidation of Alkylarenes with H_2O_2 Catalyzed by γ-Keggin Divanadium-substituted Polyoxometalate

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The possibility of application of $[\gamma\text{-}PW_{10}V_2O_{40}]^{5-}$ polyoxometalate as catalyst for the selective oxidation of pseudocumene (PC) and 2-methylnaphthalene (2-MN) with H_2O_2 in MeCN/tBuOH solvent (1:1 v/v) in the presence of mineral acid was explored .The reaction mechanism was studied by experimental and theoretical methods. Unusually high chemo- and regioselectivity towards 2,3,5-trimethylphenol (TMP) was found in PC oxidation. Atypical regioselectivity was found in the oxidation of 2-MN where 6-methyl-1,4-naphthoquinone predominates over 2-methyl-1,4-naphthoquinone.
DFT studies revealed that the formation of 2,3,5-TMP in PC oxidation is, most likely, due to peroxo complex $[\gamma\text{-}PW_{10}O_{38}V_2(O_2)]^{3-}$ (**I**), which may arise from dehydration of hydroperoxo complex $[\gamma\text{-}PW_{10}O_{38}V_2(OH)(OOH)]^{3-}$ formed upon interaction of the $H_2[\gamma\text{-}PW_{10}V_2O_{40}]^{3-}$ with H_2O_2. The kinetic regularities and estimated rate constants acquired from the kinetic study on PC oxidation with H_2O_2 are in good agreement with the theoretically predicted reaction mechanism where **I** is the main active species responsible for the aromatic ring hydroxylation.

IV-PP126

Strong Synergetic Effect of Ceria and Alumina in Aerobic Oxidative Esterification of Benzyl Alcohol and Benzaldehyde over Gold Nanoparticles Supported on Nanostructured Ce-Al-O Mixed Oxides

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Gold nanoparticles (NPs) are considered to be promising catalysts for the aerobic oxidation of alcohols, which involve O_2 as an oxidant, due to their high activity and stability. In the present work, the performance of AuNPs supported on nanostructured unitary Al_2O_3 and CeO_2 and binary Ce-Al-O oxides was studied in the liquid-phase aerobic oxidation of benzyl alcohol and benzaldehyde in methanol solutions under neutral conditions. AuNPs supported on Ce-Al-O mixed oxides prepared by sol-gel route demonstrates higher activity in the liquid-phase aerobic oxidative esterification of benzyl alcohol and benzaldehyde than gold supported on unitary ceria and alumina. The thermal pre-treatment in oxygen resulted in more active catalysts than pre-treatment in hydrogen. The order of activity is as following: $Au/Al_2O_3 < Au/CeO_2 < Au/Ce(10)\text{-}Al < Au/Ce(30)\text{-}Al$.

IV-PP127

Synthesis, Characterisation and Activity Testing of Titanium-Containing Zeolite Systems of the MFI-type

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The successful design of titanium silicalite, TS-1, by Enichem as an oxidation catalyst for environmentally benign industrial oxidation reactions with hydrogen peroxide, comprises one of the most important innovations in heterogeneous catalysis over the last thirty years. The unique performance of this MFI-type zeolite catalyst, which is isomorphous with the ZSM-5 zeolite and silicalite-1, is attributable to the specific features of isolated Ti^{4+} active sites incorporated in the silica structure of the zeolite framework.

This paper, describes the synthesis, characterization and activity-testing of a series of Ti-silicalite catalysts (TS-1) using the hydroxylation of phenol as the test reaction. In addition, high-silica ZSM-5 zeolites and silicalite-1, comprising isomorphous zeolite systems were also produced and characterized and their textural and structural properties were compared with those of the TS-1 zeolite. For characterization, the zeolite nano catalysts were analyzed with XRD, SEM, TEM, FTIR, and UV-vis. The spatial distribution of the titanium and silicon in the TS-1 micro particles was studied with EDS. The rate of Si:Ti in the TS-1 was 24. Finally, N_2-adsorption isotherms were obtained, in order to determine the textural properties of the nano catalysts. The TS-1 catalysts designed and tested by our team demonstrated significant catalytic activity and high selectivity for the hydroxylation reaction of phenol to hydroquinone and catechol. The selectivities obtained were dependent on the solvent used.

IV-PP128

Ch-Phosphorylation of Aromatic Substrates Involving Redox-activated Co, Ag, Mn, Fe, Ni and Their Complexes

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The aim of this work is to find new reactions capable to activate and transform catalytically inert C-H bonds in organic molecules to carbon-phosphorus functional groups using redox -activated metals Co, Mn, Fe, Ni and their complexes.

Within this work it was shown that the electrochemical activation of metal complex to M (III) oxidation state (apart from Ag) allows to add the dialkylphosphite to the aromatic substrates (benzene, pyridine, coumarine) successfully. Silver nitrate yields to monoalkylphosphonate in th same electrochemical conditions.

IV-PP129

Metalcomplex Catalysis in Synthesis of Biological Active Esters of the Isovaleric Acid

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Hydroalkoxycarbonylation of isobutylene with carbon monoxide and alcohols in the presence of catalytic systems based on Palladium Phosphin Complexes was applied for preparing of biological active isovaleric acid esters: l-menthylisovalerate (main active component of the spasmolytic medicine “Novovalidolum”), ethylisovalerate (intermediate product for obtaining sedative and spasmolytic medicines “Ethyl ether of α-bromisoveleric acid” (EEBIA) and “Corvololum-K”), cyclohexylisovalerate (bactericide and antifungus activity), benzylisovalerate (bactericide activity) and monoglyceryde of isovaleric acid (bactericide and antifungus activity).

Hydroalkoxycarbonylation reaction of isobutulene with carbon monoxide and alcohols (ethanol, cyclohexanol, l-menthol, benzyl alcohol, glycerol) in the presence Palladium Phosphin Complexes carried out at conditions: temperature 100^0C; CO pressure 2,0 MPa; reaction time 4 h. [1-3]. The yields of the products were 57,0-96,0%. The selectivity in linear reaction products was 100%. Such a high regioselectivity is apparently provided both by the structure of the starting alkene (isobutylene) and by the reaction mechanism. The most probable is a hydride mechanism.

New efficient technologies for preparation of drugs (Novovalidolum, EEBIA and Corvalolum-K) are based on isovaleric acid esters were worked out. Due to the more advanced technology of production the Medicines will have better qualitative characteristics. The cost of production of the Medicines with the use of new technologies is 2-3 times lower as compared to the medicines produced by existing at the present traditional technologies.

IV-PP130

Selective Hydrogenation of Hexanoic Acid to Hexanol under Mild Conditions over Titania-based Pt-Re Catalyst

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The Pt-ReO_x species ($x \leq 1$) of atomic dispersion were formed and stabilized on the titania surface. Their size, charge and chemical composition were characterized by means of HRTEM/STEM with EDX mapping, XPS, FTIR. It was shown these centers with Re:Pt = 2 are highly active and selective in hydrogenation of carboxylic acid to alcohol under very mild conditions (T = 110°C, P = 50 bar). The reaction rate constant for hydrogenation of hexanoic acid increased linearly with Pt content. As for *Ru-NPy* pair in homogeneous pincer-type complexes, the neighboring *Pt-O* atoms form a similar pair capable to dissociate H_2 heterolytically with generation of Pt hydride to hydrogenate the carbonyl group of acid. Indeed, the TOF (40 h^{-1}) and selectivity (99%) are approaching those of homogeneous catalyst. The first order kinetic model described well the kinetic data obtained in a wide range of reaction conditions.

IV-PP131

Effect of Technological Parameters on the Process of Epichlorohydrin Synthesis

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Quantitative information was obtained on how technological parameters affect the fundamental aspects of the liquid-phase epoxidation of allyl chloride to epichlorohydrin with an aqueous-methanolic solution of hydrogen peroxide in the presence of a titanium-containing zeolite in a batch reactor. The effect of the amount of a solvent, reagents ratio, and temperature was studied. The optimal conditions of epichlorohydrin synthesis were found.

IV-PP132

Lactulose Isomerisation over Magnetic Nanoparticles Incorporated with Borate Ions

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A series of borate modified catalysts based on magnetic nanoparticles (III) were synthesized. The catalysts activity strongly depends on surface concentration of borate ions. The catalytic properties of the synthesized catalysts have been examined under a wide variety of reaction conditions in lactose isomerization process. The most active catalyst providing the highest lactulose yield was found to be Fe_3O_4-6-BO_3.

IV-PP133

Selective Synthesis of Butadiene from Ethanol over ZrBEA Catalysts

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In the present study, the activity of ZrBEA catalysts promoted with silver was studied in the reaction of selective ethanol transformation into butadiene. The natures of activity of the ZrBEA zeolite catalyst in the reaction of the transformation of ethanol into butadiene have been studied. Our results suggest that the Zr(IV) Lewis acid sites in such catalyst are represented by isolated Zr atoms in tetrahedral positions of the zeolite crystalline structure linked with four (closed site) and three (open site) silicon atoms. Combination of the results of the FTIR and the DFT calculations allowed us to show that the open sites of ZrBEA are the most efficient in the reaction of butadiene synthesis form ethanol, which can be rationalized in terms of higher acid strength and better steric accessibility of such sites.

IV-PP134

Gamogen-catalytic Vinylation of Aromatic Acetylene Alcohols

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Vinylation reaction with aromatic acetylenic alcohol (AAA) gamogeneous methods. The influence of the nature and amount of catalyst, the molar ratio of the starting materials during the reaction temperature on the yield of the product. Definitely purity, structure, elemental composition and physical constants and quantum chemical calculations of the synthesized compounds. The optimal conditions for the synthesis of a product with a high yield.

It can be explained the coming out of AAA vinyl ethers (VE) with higher yield in the presence of DMFA than DMSO. DMFA is considered as a solution in average solidity. Positive charge in the nitrogen atom allows DMFA reacting as a weak proton acid. Owing to the presence of autoprotolysis in DMFA, it can't create convenient homogeneous medium for the process of reaction, as a result product is synthesized with partly low yield. And DMSO possesses two nucleophil consisting of solid-oxygen and soft sulphur atoms. Because of relatively strong protonation of hydrogen atoms in it, having been drawn with the help of alkalis, catalytic active interval complexes are formed. It causes the rise of product yield, at the same time creating convenient medium for the acetylene connection.

IV-PP135

The Gold Particle Catalysed Mechanism for the Oxidation of Hydroxymethylfurfural to 2,5-Furandicarboxylic Acid: A DFT Study

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Hydroxymethylfurfural (HMF), (figure 1) is obtained from dehydration of sugars such as glucose, fructose and xylose[1]. This biomass derived molecule is the subject of great interest as it can be used as a platform to replace traditional chemical feedstocks used within industrial processes. This versatility has seen HMF labelled a "top 10" molecule by the United States department of energy[2]. One such molecule obtained from HMF is 2,5-furandicarboxlyic acid (FDCA), (figure 1), which is obtained via an oxidation reaction. FDCA being a dicarboxylic acid can undergo polymerization to form polymers suitable for usage within the packaging industry, therefore replacing crude oil derived terephthalic acid. It is reported this oxidation to FDCA can be performed using heterogeneous gold nanoparticles as catalysts under mild reaction conditions[3]. There is some debate within the literature regarding the oxidation route and therefore computational modelling is required to shed light on this reaction.
Here a detailed computational (DFT) study is presented discussing the interaction of HMF with gold clusters various sizes (Figure 2). The effect of alloying gold particles with palladium is presented along with the influence of the following particle supports: Fe_2O_3, and TiO_2. Dispersion interactions have been included within calculations and the importance of accounting for dispersion within mechanistic studies will be presented.

IV-PP136

REALCAT: A New High-throughput Platform Dedicated to the R&D in Catalysis for Biorefineries

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In this lecture the REALCAT project will be described and its first results will be presented. REALCAT is a unique in the world highly integrated platform devoted to the acceleration of innovation in the emergent field of catalytic processes for biorefineries. REALCAT represents a top-level HTT workflow including (i) robots for the automated synthesis of catalysts, (ii) rapid characterization tools and (iii) parallel reactors combined with ultra-fast analytical tools. Three laboratories of the University of Lille have gathered their forces in this challenging project: UCCS, specialized in chemo-catalysis; Institut Viollette (ProBioGEM team), specialized in bio-catalysis and CRIStAL, specialized in computer engineering and data treatment. This integrated combination of skills is a key point of the project.

IV-PP137

Pd-catalyzed Selective Hydrogenolysis of γ-ketoamides as a New Approach to the Synthesis of 5-alkylpyrrolidin-2-ones or Linear Carboxylic Acid Amides

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Possibility of using available γ-ketoamides in the open form as convenient starting substrates for synthesis of 5-alkyl- and 5-arylpyrrolidin-2-ones is first demonstrated.

IV-PP138

Insights on the Mechanism for the Transformation of Ethanol on Basic Oxides (Lebedev and Guerbet Reactions)

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A new mechanism for the transformation of ethanol into C_4 compounds over MgO is proposed. The results made clear that the formation of acetaldol by aldolic condensation supposedly favoured by the basicity properties of the catalysts was not the key reaction to explain the products distribution as it has been stated in the literature. Instead, the reaction pathway proposed, made it possible to draw a unifying picture of the different routes leading to either 1-butanol (Guerbet reaction), butadiene (Lebedev process), or ethylene. The study was motivated by the increasing interest in upgrading bioalcohols and the lack of an agreement in role played by the basic properties of the catalysts during the ethanol transformation.

IV-PP139

Catalysis by the Noble Metals in the Process of Obtaining New Biologically Active Compounds

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A new way of obtaining oxygen containing products based on dicyclopentadiene (for example, 3-oxotricyclo[5.2.1.$0^{2.6}$]decane and 3,4-dioxotricyclo[5.2.1.$0^{2.6}$]decane) for pharmaceutical synthesis are proposed and studied. The direction includes selective process of catalytic hydrogenation of dicyclopentadiene to dicyclopentene using the noble metals as the catalyst, which provides high purity of products.

IV-PP140

The Conversion of Propane into Aromatic Hydrocarbons over Ga-containing Zeolite Catalysts

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Ga-containing zeolite catalysts are produced and their physico-chemical and catalytic properties in the course of conversion of propane into aromatic hydrocarbons are investigated. The features in distribution and state of gallium in the aluminosilicate crystal framework of zeolite depending on the method of its introduction into the catalyst are established. It is shown that the highest activity and selectivity in the course of propane aromatization are exhibited by Ga-containing catalyst, prepared by impregnation of zeolite.

IV-PP141

Dehydration of Biodiesel-derived Crude Glycerol into Acrolein over HPW Supported on Cs-modified SBA-15

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Our previous work showed that acrolein was produced from pure glycerol with a high yield. However, the glycerol purification is very costly. The present work explored the feasibility of using crude glycerol as feedback for the acrolein production by dehydration reactions. Among the impurities commonly contained in crude glycerol, only the alkli metal ions caused catalyst deactivation and decrease in acrolein selectivity. The reason was that alkli metal ions deposited on the HPW/Cs-SBA catalyst surface to form alkaline salts of HPW by neutrilization and decreased the effective medium Brønsted acid sites. This problem was solved by glycerol desalination, and a stable acrolein yield of 85% was obtained in 60 h of reaction, which was as good as that with pure glycerol. In addition, the HPW/Cs-SBA catalyst showed good thermal stability and regeneration ability after the reaction with desalted crude glycerol.

IV-PP142

Modified Nickel Catalysts for Oxidation of Methane

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Nickel catalyst supported on γ-Al_2O_3 has been investigated for the partial oxidation of methane. The addition of a modifier (Co, Ce, or La) to the Ni/γ-Al_2O_3 catalyst increased the selectivity to H_2 and CO with the decreasing selectivity to CO_2, and the highest selectivity to H_2 was obtained by the NiLa/γ-Al_2O_3.

IV-PP143

Catalytic Hydrogenation of Dienone for Getting Vitamins and Odorous Substances

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The hydrogenation β-ionone was studied over metals VIII of group in 96% ethanol at 2,0 MPa and temperature 303 K. Determined, that the nature of metal has essential effect on row saturation of unsaturated bonds in the molecule β-ionone. The nickel, ruthenium and palladium can be used as selective catalysts for hydrogenation β-ionone in dihydro-β- ionone by the continuous process.

IV-PP144

The Spectral Analysis of Hydrocarbons in the Oil from the Well1311 of Surakhani Field

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Oil wells No. 1311 in Surakhani field separated by -liquid chromatography method to the component structures. The obtained I, II, III, IV group of aromatic fractions has been studied by the method of the IR and UV-spectroscopy analysis .As the result of the analysis it has become clear that the outcome of the aromatic fractions containing 1, 2, 3, multilink aromatic hydrocarbons is dominated over 4.5 multilink aromatic hydrocarbons.

IV-PP145

Oligopeptide Modified Mesoporous Silica Catalyts for Direc Aldor Reaction

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Mesoporous silicas have been regarded as potential support materials for catalysts and adsorbents. However, its applicability is still limited because their inner surfaces are covered with silanol groups, which are rather inert to promote reactions while it can act as effective hydrogen boding donors/acceptors. Oligopeptide is one of the nice candidates for investing with asymmetric catalytic activity to mesoporous silicas, because immobilization of oligopeptide on solid surfaces is an established technique as the solid phase peptide synthesis. In this work, the Pro-Pro-Asp tripeptide molecules (PPA), which are reportedly effective homogeneous catalyst for direct aldol reaction, were immobilized on the surfaces of various mesoporous silica supports. In comparison with microporous silica and resin supported PPA catalysts, the mesoporous silica catalysts exhibited superior catalytic activity to the direct aldol reaction of 4-nitrobenzaldehyde and acetone. Wide surface area and mesoporous structure may facilitate diffusion of reactants and products from catalytically active sites.

IV-PP146

The Method of Dealumination of Zeolite Ferrierite with Ammonium Hexafluorosilicate

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The obtained samples (SiO_2/Al_2O_3 = 64, 74) were investigated by TPD of ammonia, low temperature nitrogen adsorption, ^{29}Si, ^{27}Al NMR, X-ray analysis, IR spectroscopy. Optimal samples of has the following catalytic performance: conversion – 40 %, selectivity – 87 % (at the temperature 450 ºC).

IV-PP147

Paramagnetic Nickel Complexes in the Catalytic Carbon-Carbon Bond Formation Reactions

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Paramagnetic complexes of nickel in the catalytic reactions dimerization of norbornadiene and homocoupling of aryl halides were detected by the ESR method. It was shown, that paramagnetic complexes of nickel can be found among the reaction products. The obtained results do not conclusively establish the role of the paramagnetic nickel complexes in catalysis. However, on the basis of kinetic, spectroscopic and calculated quantum-chemical data the consistent mechanisms of norbornadien dimerization and aryl halides homocoupling in the presence of nickel(I) complexes was proposed.

IV-PP148

Microwave Assisted Heterogeneous Vapor-Phase Oxidation of 3-picoline to Nicotinic Acid over Vanadium–titanium Oxide Catalytic System

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A comparison of heterogeneous vapor-phase oxidation of 3-picoline over V-Ti-O system by using both sources of energy, conventional and microwave was performed. Application of microwave energy as a remote heating source to the heterogeneous vapor-phase oxidation of 3-picoline has several new advantages. This method consumes less energy and creates an optimal temperature profile in vanadium-containing catalyst particles making a positive contribution to the selectivity and capacity of the green method of nicotinic acid synthesis.

IV-PP149

Pt Based Bimetallic Catalysts Prepared by Conventional Impregnation and Deposition and Reduction in Liquid Phase Methods for Selective Hydrogenation of Citral

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Pt-based bimetallic catalysts supported on carbon nanotubes were prepared by two methods and evaluated in the selective hydrogenation of citral. The conventional impregnation CI-method consisted in depositing H_2PtCl_6 and the corresponding precursor of the second metal (Fe, Sn,Ga, In) followed by a reduction step under H_2-flow at high temperature. The method RLP consisted in the deposition of the metals followed of a reduction in liquid phase using $NaBH_4$ at low temperature. Additionally a thermal treatment with N_2 was carried out on the catalysts. It was found that the addition of a second metal significantly increase the selectivity to unsaturated alcohols in all the bimetallic catalysts prepared by CI, while only PtFe catalyst prepared by RLP showed a high selectivity to UA. The thermal treatment applied in catalysts prepared by RLP only improved the selectivity to UA in PtSn catalysts. The results were explained taken into account the more adequqted interaction achieved between the metals according to the promoter nature, the application of the N_2-thermal treatment and the catalyst preparation method.

IV-PP150

Study of the Reaction Network of Fischer-Tropsch Synthesis by Multicomponent Steady-State Isotopic Transient Kinetic Analysis

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A detailed mapping of the kinetic parameters involved in the reaction pathway has been provided over a Co-Re/CNT catalyst in the Fischer-Tropsch synthesis. The site coverage of the different products calculated from the multicomponent analysis of their isotopic distribution allowed the study of its effect in chain growth, as well as in olefin and paraffin formation. The evaluation of the different reaction steps at different H_2 partial pressures demonstrated the presence of two mechanisms which depends on carbon number. Hydroxycarbene like intermediates have been identified for intermediates up to C_3 and alkylene like intermediates have been identified for C_4 intermediates. This methodology provides a valuable tool to determine easily the reaction network and allows the study of the effect of catalytic properties, such as promotion, particle size or support characteristics in the reaction mechanism.

IV-PP151

The Characteristics of Phosphoric Acid Modified Niobia Catalysts in the Gas Phase Glycerol Dehydration

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We conducted gas phase glycerol dehydration reactions using nanosized PO_4/Nb_2O_5 catalysts. The catalysts were synthesized by incipient wetness impregnation method using niobium oxide and various amounts of phosphoric acid. The highest glycerol conversion, after 3 h using 20 wt% PO_4/Nb_2O_5 as catalyst, was 89% and the acrolein selectivity was 43%. In all the results, the acrolein selectivity was not affected by the amount of phosphoric acid. The physical and chemical properties of the catalysts were determined by X-ray diffraction, X-ray photoelectron spectroscopy, and transmission electron microscopy.

IV-PP152

Fischer-Tropsch Synthesis (FTS) Reaction over Co- Based Catalyst Supported on Al-SBA-15

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In this work we synthesized Al-SBA-15 materials for adjusting to Fischer-Tropsch Synthesis (FTS) reaction which is regarded as a promising technology to produce clean energy from syngas. The diffrent amounts of alumina (Si/Al = 0,5,7,10) were used for manufacturing the support to find out the effect of acid site on FTS reaction. Cobalt was used as a active metal by impregnation method after the Al-SBA-15 supports were made. It was found that with the increase of the Si/Al ratio, the interaction between cobalt metal and support was increased and it affects to the catalyst reducibility. Indeed, by adding the alumina to SBA-15, the weak acid site was also increased and the isomerization during the reaction was activated. Therefore it showed relatively middle range hydrocarbon distribution compared with the catalyst which uses SBA-15 as a support.

IV-PP153

Kinetics for Hydrogen Production from Glycerol Steam Reforming Reaction Using Ni-Fe-Ce/Al_2O_3

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Glycerol steam reforming for hydrogen production is one of the best methods for the utilization of the surplus amounts of biodiesel's crude glycerol. In this work, we focused on kinetics of glycerol steam reforming for hydrogen production over Ni-based catalyst. Glycerol steam reforming has been investigated in a 6mm ID fixed-bed reactor under atmospheric pressure, glycerol concentration, 12-30 wt.%, and temperatures between 723K and 823K. Kinetic parameters were obtained under conditions free from heat and mass transfer limitations. Kinetics study was carried out using the power law equation. The activation energy and the frequency factor were calculated using Arrehenius equation.

IV-PP154

Heterogeneous Lipase-Active Biocatalysts for Oil Triglycerides' Hydrolysis and Interesterification

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Heterogeneous biocatalysts with activity of the thermostable lipase were prepared by entrapment of the fully destroyed microorganisms (cells' lysates) inside {nanocarbon-in-silica} composites. Properties of the biocatalysts such as enzymatic activity and operational stability were studied in the reactions of triglycerides' interesterification in vegetable oil-fat blends, as well as in reactions with participation of methyl- or ethyl-acetate for production of the esters of fatty acids (biodiesel). It was found that the prepared multicomponent biocatalysts operate in the periodic process of interesterification of sun flower oil by ethyl-acetate into biodiesel for more than 1000 h at 40°C.

IV-PP155

Highly Selective Catalysts for Synthesis of Alkylaromatic Hydroperoxides and Prospects of their Industrial Application

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In the present work a comparative results of kinetic studies of catalytic oxidation of ethylbenzene and i-propylbenzene into the corresponding hydroperoxides are shown both with and without catalyst. The results of model tests of hydrocarbons oxidation in conditions close to industrial process are shown. High conversion of the feed per single run was reached in the presence of phtalimide derivatives as catalysts, in particular, N-hydroxyphtalimide. 40% i-propylbenzene conversion was achieved at 130 °C per 1 h, which is two times higher compared to industrial process. It is noteworthy that selectivity towards i-propylbenzene remains above 90%. If i-propylbenzene oxidation is carried out with 17-20 % conversion (typical for industrial process), selectivity reaches 94-96 %. Mathematical models of the processes have been developed taking into account the parameters of industrial instrumentation.

Section 5. Catalysis and Environmental Protection

V-PP01

Structured Cartridges with Glass-fiber Catalysts: New Trend in the Design of Catalytic Reactors for Pollution Control

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The presentation is dedicated to development of the catalytic structured cartridges with glass-fiber catalysts, characterized with low pressure drop and, simultaneously, with high heat and mass transfer efficiency. It was shown that such structured cartridges provide the best compromise between high mass exchange and low pressure drop than any other forms of existing catalysts, thus highlighting their superb engineering potential. The optimal design of reactors with such cartridges is discussed.

V-PP02

Catalysts on the Base of Ceramic Highly-porous Block-cellular Carriers

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Small volume catalytic systems based on ceramic highly-porous cellular materials developed in Russian Mendeleev University of Chemical Technology are used in various liquid-phase catalytic processes and in gas-phase environmental catalysis for the conversion of toxic products of burnout of motor fuels and localization of volatile radionuclides in exhaust of special manufactures.

Characteristics and structure of highly-porous block-cellular catalyst with the deposited palladium active layer for the oxidation of hydrogen isotopes, as well as catalytically active compositions on the base of rare-earth metals, containing nano-dispersed multi-component solid solution $Pr_{0,1}Zr_{0,18}Ce_{0,72}O_2$ for oxidation of hydrocarbons and carbon monoxide in the exhaust gases of vehicles are presented.

V-PP03

The Synthesis Charcterization and Catalytic Performances of Three-dimensionally Ordered Macroporous x-CeO_2/Al_2O_3 Catalysts for Diesel Soot Combustion

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Diesel engine vehicles are a promising power source for light vehicles owing to good power performance and high fuel efficiency. However, the emission of soot particle matter (PM) can cause human carcinogen. Thus, it is crucial to reduce emissions of particulate matter before the wide utilization. The combination of traps and oxidation catalysts in the continuously regenerating particulate trap (CRT) appears to be one of the most efficient and economic after-treatment techniques for diesel engines. This key challenge is to find effective catalysts for soot combustion that operates at low temperature. In our work, we successfully fabricated 3DOM CeO_2/Al_2O_3 catalysts by micropores-diffused precipitation (MDP) method using ammonia solution as the precipitation agent There exists a synergistic effect between CeO_2 and Al_2O_3, leading to the formation of Al-Ce-O solid solutions. The synergistic effect is crucial to enhancing the catalytic performance.

V-PP04

Are Perovskite Materials Efficient for Tree Way Catalysis? A Theoretical Study of $LaFeO_3$

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We have carried out a first principle study of NO reduction over $LaFeO_3$ perovskite catalyst surface. The relevant surfaces for LFO were identified prior to the description of the active site. The most stable surfaces are the (100) and the (112) ones with surface formation energy values of 0.94 J.m-2 and 0.86 $J.m^{-2}$, respectively. A mechanism involving as first step the formation of an oxygen vacancy upon CO oxidation which is further regenerated along NO reduction was proposed. The corresponding computed energy barrier of 135 $kJ.mol^{-1}$ is consistent with the usual reacting conditions of three way catalysis. The above-mentioned mechanism is derived from a Mars Van Krevelen mechanism involving network oxygen, which is quite typical of several oxide catalysts.

V-PP06

Soot Oxidation on Manganese Oxide Catalysts in Diesel and Gasoline Exhaust

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This paper deals with the catalytic soot oxidation for regeneration of particulate filters of diesel engines and gasoline engines with direct fuel injection. We evaluated a series of bare manganese oxide catalysts, whereas the catalyst prepared by flame spray pyrolysis (FSP) showed highest activity in diesel as well as gasoline model exhaust. The correlation of the physical-chemical properties and the soot oxidation activity of the catalysts showed that high amount of surface oxygen vacancies and small particle sizes are crucial for the oxidation of soot. These findings coincide with the mechanistic studies of FSP-Mn_3O_4/soot suggesting that the supply of oxygen occurs from the gas-phase and catalyst bulk via the surface of the catalyst to the contact points of the soot. The contribution of the bulk is very pronounced indicating strong mobility of inner oxygen, particularly when comparing with other catalysts, e.g. iron oxides. Moreover, tests of laboratory-scaled particulate filters coated with FSP-Mn_3O_4 indicated high soot oxidation as well.

V-PP07

Development of MnOx-based Catalysts for the Catalytic Wet Air Oxidation (CWAO) of Organic Pollutants

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The Catalytic Wet Air Oxidation (CWAO) of organic compounds represents to date the most reliable technique for the abatement of pollutants from wastewater streams. Systematic studies conducted on manganese-based catalysts indicate the basic requirements of the optimum CWAO catalyst. In particular, the mineralization of phenol proceed through the fast adsorption of the substrate and the subsequent slowly oxidization to CO_2. The enhancement of catalyst surface exposure and redox properties are the key features to improve CWAO catalysts. New "redox" synthesis route allows to obtain novel $MnCeO_x$ system with high surface area exposure, amorphous structure, greater active phase surface dispersion, stabilization of the manganese at high oxidation number, improved redox features and strong ability to restore the initial redox features. Catalytic tests confirm the higher activity towards various organic compounds at mild conditions, showing better performances than co-precipitated ones at any Mn/Ce atomic ratio, worthy of potential industrial exploitation.

V-PP08

Attractive Route for New Hydroxyapatite Supported Calcium-manganese Oxides for Total Oxidation of Toluene

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The research of new catalytic materials requires available cheap and non-toxic components. Phyllomanganates are amongst the strongest known natural oxidants and Mn is an easily reducible/oxidable element. Among them well dispersed CaMn oxides have not been studied so far. In the present work an attractive route for new hydroxyapatite supported calcium-manganese oxides has been explored. This study takes advantages of the fact that Ca^{2+} ions are easily expelled from the flexible HAP structure. Dispersion of Mn over the HAP is performed by wet impregnation and calcination at 400°C allows to get the catalyst Mn-HAP. Indeed Tof-SIMS study of Mn-HAP reveals $CaMnO_x$ phases whose Raman features resemble those found in birnessite-pristine/birnessite oxides. This catalyst performs better than a reference MnO_2 oxide dispersed on Al_2O_3 in toluene total oxidation. The best activity achieved on Mn-HAP can be rationalized by the formation of a well dispersed/amorphous CaMn layered type oxide with high-valence Mn.

V-PP09

Unravelling the Complexity of CO Oxidation Catalysis on Au Nanoclusters

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The CO oxidation reaction is crucial in the development of catalytic converters for emissions control. Gold has attracted significant attention in this context since the 80's, after experimental evidence by Haruta and co-workers suggested that Au, while inert in bulk, is highly active at the nanoscale. Despite the intense research on Au-catalysed CO oxidation during the past 30 years, the reaction mechanisms are still debated, and effects such as the experimentally observed magic number activity of Au nanoclusters remain elusive. Motivated by these challenges, we employ first-principles-based kinetic modelling of MgO-supported Au_6, Au_8 and Au_{10} nanoclusters to understand what determines their CO oxidation activity. We unravel a variety of influencing factors: charge transfer, size/shape effects, reconstruction, adsorbate binding configurations, and poisoning by carbonate. We further reproduce and rationalise the experimental activity patterns, showing that computational approaches can significantly advance our understanding and lead to better catalysts and processes.

V-PP10

Effect of Au and Ag on the Performance in CO and VOCs Oxidation of Alumina Supported Cu-Mn Catalysts

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The aim of this work was the development of cost-effective and catalytically efficient formulations by promotion of alumina supported Cu-Mn mixed oxides with Au or Ag. The role of Au or Ag on the structural and catalytic properties of Cu-Mn/Al_2O_3 catalysts for simultaneous elimination of different type air pollutants – CH_3OH, $(CH_3)_2O$ and CO in waste gases from formaldehyde production, as well benzene as representative of aromatic hydrocarbons, was examined in detail. The deposition of Au over Cu-Mn with ratio 2:1 caused significant improvement of catalytic activity toward oxidation of CO and MeOH, whereas addition of Ag affected beneficially MeOH oxidation activity, slightly CO oxidation and negatively $(CH_3)_2O$ oxidation. A slight improvement of complete benzene oxidation over Au/Cu-Mn and Ag/Cu-Mn samples was achieved. In-depth analysis of XRD, TEM, H_2-TPR and EPR data was performed in order to clarify the relationship between enhanced catalytic behavior and structural features.

V-PP11

Change in the Chemical Composition of an LNT as a Result of its Ageing in Diesel Exhaust Gases: Physical and Chemical Analysis

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The work was focused on investigating a nature of the compounds formed in LNT catalyst during its ageing in exhaust of the diesel engine operating under realistic NOx aftertreatment protocol.

Samples of fresh and aged LNT catalyst were cut from the frontal area of corresponding monolith catalyst.

It was found that during the LNT catalyst ageing under real diesel exhaust conditions, accumulating of the oil- and fuel-derived impurities such as S, P, Ca and Zn is taking place. Sulfur is being distributed over the whole thickness of the wash-coat layer, while phosphorus, calcium and zinc are being concentrated in the thin sub-surface layer of the wash-coat. Sulfur was found to be bonded into barium sulfate, while phosphorus – into cerium phosphate.

V-PP12

The Process of H_2S Selective Catalytic Oxidation for On-site Purification of Hydrocarbon Gaseous Feedstock. Technology Demonstration at Bavly Oil Field in Republic of Tatarstan

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In the Laboratory of Environmental Catalysis of the Boreskov Institute of Catalysis, new processes based on direct catalytic oxidation of hydrogen sulfide were developed. The technology was successfully tested in pilot scale on the largest sour gas fields, refineries and gas processing plants in Russia. In 2011 full scale industrial installation was set into continuous operation at the Bavly oil-field (OJSC "Tatneft" – company-operator).

The efficiency of hydrogen sulfide removal was proved to exceed 99%.

During two years of continuous operation:

- 120 10^6 m^3 of commercial gas were produced;
- 1200 tons of hydrogen sulfide were recovered as elemental sulfur;
- emission of more than 2300 tons of sulfur dioxide and sulfuric acid to the atmosphere was prevented;
- pollution damage for the amount of $ 10 million was averted.

Characteristics of the produced sulfur surpass those specified by Russian National Standard #127.1-93 (commercial grade sulfur 9990).

V-PP13

Pd Catalysts Supported on Metal Organic Coordinated Structures in Chlorobenzene Hydrodechlorination and CO Oxidation

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Pd/MOF-5-type sample prepared by co-precipitation of MOF-5 together with Pd nitrate with subsequent vacuum thermal treatment is active both in CO oxidation and in chlorobenzene hydrodechlorination, in contrast to the similar catalyst produced by supporting of Pd from nitrate after MOF-5 preparation with subsequent reduction with hydrazine. On the base of preliminary data such difference could be caused not only by the different nature of active Pd sites situated in the framework of MOF or on the surface, but also by the use of thermal vacuum treatment to clean MOF structure from the absorbed solvent, and by the difference in crystal structure and MOF-5 content in the samples.

V-PP14

A New, Active Iron-complex Catalyst for Converting CO_2 into Cyclic Carbonates and Cross-linked Polycarbonates with Enhanced Properties

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The finite availability of fossil resources is stimulating the production of chemicals from alternative and sustainable carbon resources, among which CO_2 is a readily available, inexpensive and renewable C_1-feedstock. The atom-efficient reaction of CO_2 with epoxides can generate two valuable products: cyclic carbonates and polycarbonates, both having current and potential applications. Here, we present iron(III) pyridylamino-bis(phenolate) complexes as new, highly active homogeneous catalysts for the reaction of different epoxide substrates with CO_2. The selectivity of the reaction could be switched between the cyclic or polymeric carbonate by tuning the reaction conditions and catalyst to co-catalyst ratio. Among the studied epoxide substrates, 1,2-epoxy-4-vinylcyclohexane could be converted with nearly complete selectivity to the polycarbonate. The obtained polymer presents pending vinyl groups, which allow post-synthetic cross-linking. The cross-linked polycarbonate displays a substantial increase in the T_g and chemical resistance, thus opening new opportunities for the application of these green polymers.

V-PP15

Design of Catalysts of Carbon Dioxide Conversion of Methane

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The catalytic activity of polyoxide catalytic system (MgO, CoO, NiO) on the basis of fiberglass KT-11-TO-30K was carried out in dry reforming of methane. The activity of catalysts was tested on-line with using of gas chromatographic analysis method on device «HROMOS -1000», is equipped with software (SW), and data recording to the computer. Synthesized samples are examined by XRF, SEM, TEM methods as well as thermo-programmed reduction by hydrogen. The influence of temperature, bulk composition and volume velocity of the catalytic activity of catalysts polyoxide were carried out. The optimal process temperature is the temperature in the range of 850-900 ^{0}C. It is shown that optimum characteristics are samples with a content of magnesium oxide in them - 2 nickel - 1.4, and cobalt - 1.6%. It was established that in the range of 3200-9600 h^{-1} conversion of the starting components is 98-99%, the yield of H_2 - 42-43% and yield of CO - 52-53%.

V-PP16

Modified Ni-Al Layered Double Hydroxides as Catalyst Precursors for Utilization of Carbon Dioxide

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The effect of the Mg and Cr addition to the co-precipitated Ni-Al layered double hydroxides on the activity in CO_2 removal from hydrogen-rich gas streams through the methanation reaction was studied by variation of the reduction and reaction temperature as well as the space velocity. The dominated methanation activity of NiMgAl catalyst especially after reduction above 500^{o}C is related to both the highest Ni^0 specific surface area and highest Ni^0 dispersion because of the retarding the effect of the Mg on the Ni^0 sintering via Ni^0 particle migration.

The studied catalytic compositions are found to be promising catalyst precursors for utilization of CO_2 through the methanation reaction, depending on the technological regime of the catalyst activation: (i) NiCrAl and NiAl catalysts – at low and medium reduction temperatures and (ii) NiMgAl catalyst – at higher reduction temperatures.

V-PP17

Two-dimensional $SrNb_2O_6$ as an Efficient Photocatalyst for the Preferential Reduction of Carbon Dioxide in the Presence of Water

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We successfully synthesized $SrNb_2O_6$ with nanoplate morphology by a facile hydrothermal method. The $SrNb_2O_6$ nanoplate exhibited promising photocatalytic performance for the preferential reduction of CO_2 to CO and CH_4 in the presence of H_2O vapour due to its high electron-hole separation and high CO_2 chemisorption abilities.

V-PP18

Design and Development of Efficient AC-based Adsorbents for CO_2 Removal

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Thermal power plants fed by fossil fuels, which generate CO_2 as a by-product, accounts for 40% of total CO_2 emissions. Since reducing CO_2 emissions is crucial for environmental concerns, there is a growing interest on CO_2 capture technologies. In order to be used in pre-combustion and post-combustion technology applications, selective adsorption has attracted great interest. In the current study, activated carbon (AC) based adsorbents, which have large surface area and suitable porosity, were investigated for their CO_2 capturing ability. Structural and chemical modification of AC are important parameters affecting CO_2 adsorption properties. Different oxidation procedures and alkali impregnation, such as NaOH and KOH impregnation, were applied. Selective adsorption of CO_2 from CO_2-CH_4 mixtures was studied on AC-based adsorbents and the effects of temperature, pressure, and adsorbate gas composition were investigated. Alkali impregnated ACs were found to be promising adsorbents as they have high adsorption capacity and selectivity towards CO_2 adsorption.

V-PP19

Preperation and Characterization of Ni-based Catalysts for Oxy-CO_2 Reforming of Methane by Using Wet Impregnation Method

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Consuming two major greenhouse gases, carbon dioxide (CO_2) and methane (CH_4), to produce synthesis gas, which is a mixture of carbon monoxide (CO) and hydrogen (H_2), carbondioxide reforming of methane shows significant environmental and economic benefits. Nickel (Ni)-based catalyst became commercially more attractive for the methane reforming processes due to it is reasonable catalytic activity, availability and affordable price compared to noble metal-based catalysts. Ni /Al_2O_3, Ni/MgO, Ni/ZrO_2, Ni/$MgAl_2O_4$, Ni/SiO_2, Ni/TiO_2 and Ni/CeO_2 catalysts were prepared by incipient wetness impregnation using nitrate precursor and tested with a reaction of combination of CO_2 reforming and partial oxidation of methane to produce syngas (H_2/CO). The effect of support on NiO catalysts was investigated. They were characterized by Brunauer–Emmett–Teller (BET) Surface Area, X-ray Diffraction (XRD), High Resolution Transmission Electron Microscopy (HRTEM), Scanning Electron Microscopy (SEM), X-ray Photoelectron Spectroscopy (XPS), thermally programmed reduction/oxidation/desorption (TPR/TPO/TPD).

It was found that the co-precipitated Ni/Al_2O_3 catalyst exhibited the best activity and stability at 800ºC during the reaction. The conversions of CH_4 and CO_2 maintained at 92% and 89.6% respectively after 8 h of reaction.

V-PP20

A Honeycomb-Type Ni/CeO_2 Catalyst for CO_2 Methanation to Transform Greenhouse Gas into Useful Resources

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For constructing the structured methanation system, first, we investigated the performance of methanation of some nickel-based catalyst loaded on various support. Secondly, a structured catalyst with Ni/CeO_2 component having the highest methanation ability was prepared by wash-coat method on an aluminum honeycomb-fin and was measured its methanation property and durability performances. As a result, the honeycomb-fin type catalyst prepared by wash-coating of Ni/CeO_2 showed a relatively high activity. The durability performance of the Ni/CeO_2-honeycomb catalyst showed a high and stable performance for methanation.

V-PP21

CO_2 Capture by Hierarchical Mesoporous Chabazite Type Zeolites

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Zeolites have numerous advantageous properties as an adsorbent for CO_2 capture when compared with their alternatives such as their high thermal stability and tuneable pore sizes. In industrial gas separations, low silica zeolites such as faujasite and LTA type zeolites (A, Y, 13X) are used extensively. In this study we have investigated the use of mesoporous SSZ-13 as a sorbent for CO_2 capture. Introducing mesoporosity could provide fast adsorption/desorption rates alongside the desirable properties of zeolites such as the ability to work at flue gas temperatures. Mesoporous SSZ-13 zeolites were synthesised by dual templating methods employing microporous template (trimethyl adamantyl ammonium hydroxide) and a mesopore generating template (octadecyl-(3-trimethoxysilylpropyl)-ammonium chloride) together. Mesoporous SSZ-13 has an adsorption rate of 0.070 $mmol \cdot min^{-1}$, which was higher than that of zeolite Y. Over a long period of time, no decrease in CO_2 capacity proved the stability of the mesoporous materials.

V-PP22

Autocatalytic Fixation of Carbon Dioxide

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Theoretical concepts of autocatalytic coupled cycles of CO_2 fixation (including the need for the development of reaction reversibility conditions) will make it possible the activation of thermodynamically stable CO_2 by organocatalysts (dicarboxylic, keto- and hydoxy acids, including phosphorylates compounds) and also organocomplexes of transition metals in various redox states.

V-PP23

Surface Oxidation Mechanism of Pb-based Materials by Utilization of CO_2 as an Oxidant

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CO_2 sequestration is the key challenge of the 21st century. The potential of CO as chemical and energy production is the ultimate goal for carbon neutral technologies. In this study, CO_2 reduction by Pb-based materials was investigated in a home bench setup. The magnitude of the CO formation shows different steps during oxidation of Pb. CO formation increases rapidly up 720°C. Mars and van Krevelen mechanism was proposed for the surface reaction between CO_2 and Pb. A strong diffusion barrier was observed as the lead oxide thickness increases. Activation energy was calculated as 120.9kJ/mol by assuming shrinking core model. After the experiment, sample from the surface of oxidized material was taken. The performed SEM/EDX analysis showed the coke formation which is the clue of Boudard reaction.

V-PP24

Catalytic Activity of Supramolecular Systems Based on Mono- and Dicationic Surfactants with Aromatic or Heterocyclic Moieties

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In this work a comparative study of the aggregation behavior and catalytic effect on the rate of transfer of the phosphoryl and acyl group in different organized media based on cationic surfactant was carried out. To optimize the relationship between a structure and catalytic activity, it was investigated amphiphiles of varying nature, particularly mono- and dicationic surfactants with aromatic or heterocyclic moieties and different length of alkyl chain and spacer.

V-PP25

Supramolecular Catalytic System Based on Amphiphilic Triphenylphosphonium Bromide for the Hydrolysis of Phosphorus Acid Esters

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The biomimetic nature of micellar catalysis permits to achieve significant enhancement of reaction rate under mild conditions. The quantitative assessment of these parameters will shed light on the mechanism of the reaction. The most studied cationic surfactants in this context are alkyltrimethylammonium and alkylpyridinium halides. However, the change of the atom of the charged center and transition to surfactant with highly hindered head groups might have a significant impact on the catalytic effect. The aim of this work is the investigation of alkyltriphenylphosphonium bromides (TPPB) properties such as the solubilizing activity to the hydrophobic substrates and catalytic effect on the alkaline hydrolysis of phosphorus acid esters.

V-PP26

Modified by Lanthanum Cerium - containing Catalysts for Converting Bio-Ethanol into Ethylene

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The influence of lanthanum oxide as modifying additives to structure Ce/γ-Al2O3 catalyst was investigated. The catalysts were prepared by incipient wetness impregnation of the support. Physical-chemical characteristics of the catalysts were studied by electron microscopy and BET. Doping Ce/γ-Al2O3 with lanthanum increases the dispersion of the catalyst, but some aggregates of fine (2 nm) particles are observed in the aggregates, along with particles 10 nm in size.

V-PP27

An in-situ FTIR-DRIFTS Study on Carbon Dioxide Reforming of Methane on Pt-Ni/Al_2O_3

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Carbon dioxide reforming of methane (CDRM) is an important reaction for the utilization of the two major greenhouse gasses, namely methane and carbon dioxide. The aim of this work is to understand the routes and mechanistic steps of the CDRM reaction on the active sites of the Pt-Ni/Al_2O_3 bimetallic catalysts with different Ni:Pt ratios, i.e. 0.2Pt-15Ni/Al_2O_3 and 0.3Pt-10Ni/Al_2O_3, which had been designed by our group and shown to have high activity and selectivity in CDRM reaction. The results obtained from the *in-situ* FTIR-DRIFTS analysis revealed that Pt has a significant role on the structure of the active sites as well as on course of the reaction by both affecting the surface carbonate formation and CO adsorption mechanisms. FTIR-DRIFT results indicate that CO_2 activation/utilization is directly affected by the Ni:Pt ratio of the bimetallic catalysts.

V-PP28

An Experimental Study on Characterization and Mixed Reforming Performance of Co-Based Bimetallic Catalysts

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The aim of this study was to investigate the mixed reforming performance of Co-Ce supported on ZrO_2 in a detailed fashion. In this context, CH_4:CO_2 ratio in the feed, the presence and amount of H_2O or O_2 in the feed stream and reaction temperature were considered as the experimental parameters. The effects of type and amount of additional oxygen source in mixed reforming on the oxidation states of the active phases, Co and Ce, were studied by XPS. The results showed that H_2/CO product ratio can be controlled, and the addition of steam or oxygen improved overall performance and stability in mixed reforming compared to those in individual CDRM. In CDRM + POX mixed reforming, the H_2/CO product selectivity was much closer to unity than that in CDRM + SR mixed reforming.

V-PP29

DR UV-Vis Study of Copper(II) Oxo/Peroxocomplexes in Cu-substituted ZSM-5

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Elucidation of the oxygen activation pathways are very important for the understanding the mechanism of oxidative action of monooxygenase type enzymes. The Cu-containing zeolites are of interest for the biomimetic approach due to the square-plain coordination of Cu(II) ions in copper oxide/hydroxide clusters and nanoparticles, easy transformation Cu(I) – Cu(II), and formation of α–like site.

Here the DR UV-Vis spectroscopy was used to reveal condition where a peroxo/oxo complexes copper (II) are formed in CuZSM-5 catalysts.

Cu-ZSM-5 possess the capability to stabilize copper(II) pero/oxocomplexes at treatment by hydrogen peroxide in alkaline solution as well as high-temperature calcination in O_2-containing atmosphere. Peroxocomplexes copper(II) with terminal OOH-group are formed in H_2O_2 solution and characterized by CTB L-M 21500 and 35500 cm^{-1}. They contain two copper ions located near and long distance, respectively. Oxocomplexes dicopper(II) with bridged OO-group (CTB L-M 26500 – 28000 cm^{-1}) are formed at activation in H_2O_2 and in O_2.

V-PP30

Structured Glass-fiber Catalysts for Selective Oxidation of H_2S

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This work is dedicated to the glass-fiber catalysts for selective oxidation of hydrogen sulfide by oxygen into sulfur. The samples of glass-fiber catalysts were prepared by means of impulse surface thermo-synthesis method. The preparation included the supporting of the thin layer of porous SiO_2 at the external surface of glass micro-fibers with following impregnation of this layer with solution of the active component (V_2O_5, Fe_2O_3 and $CuCrO_4$) precursor and fuel additive. Vanadia and iron oxide samples showed high oxidation activity, significantly exceeding that for conventional catalyst. These catalysts may be recommended for practical application.

V-PP31

Photocatalytic Oxidation of CO over TiO_2 Modified by Noble Metals

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Three series of M/TiO_2 (M = Pt, Pd or Au) photocatalysts with metal content varied from 0.01 to 4.0 wt. % were synthesized by deposition and subsequent chemical reduction of metal precursor compounds. Modified TiO_2 samples were tested in the reaction of CO oxidation in a static reactor at ambient conditions with or without UV irradiation. The rate of CO oxidation under UV irradiation was 1.5-5 times greater than the rate of oxidation without lighting if we compare the different metals used for modification. It was demonstrated that in the case of Pt/TiO_2 and Pd/TiO_2 samples CO photooxidation rate increased with increase in the metal content up to an optimum level. The rate of CO oxidation for the most active sample in each series increases in the following sequence: $Au/TiO_2<Pd/TiO_2<Pt/TiO_2$, wherein Pt-containing sample in 6-fold more active compared to other samples.

V-PP32

Characterization of the Automotive Exhaust Gas Aftertreatment Catalysts with Flow Chemisorption Methods

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Applications of the chemisorption methods (pulse chemisorption, Temperature-programmed desorption (TPD), reduction (TPR) and oxidation (TPO)) to characterization of the thermal aging of the automotive exhaust catalysts, was described.

Pulse chemisorption and TPR were applied to study deactivation of the LNT catalyst. Relatively safe rich operation temperature for LNT was found to be ca. 800°C. Above this temperature, rapid irreversible deactivation due to PGM and support sintering were taking place.

For evaluated NH_3 SCR catalyst, ammonia TPD study helped to determine not-to-exceed temperature of ca. 900°C. Above this temperature, there is a high probability that zeolite will undergo destruction, so all NH_3 SCR reaction related properties will be irreversibly lost.

For the sample of the in-field failed three-way catalyst, temperature of the exposure was deducted based on the characterization of the catalyst with CO pulse chemisorption and TPR.

V-PP33

Kinetic and Mechanistic Studies of Dehydrogenation of Propane and Isobutane Assisted by High-Throughput Tools

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Non-oxidative dehydrogenation (DH) of propane and isobutane over VO_x/SiO_2-Al_2O_3 catalysts was studied with the aim to investigate the influence of VO_x species structure and acidity of the catalysts on their ability to form carbon. With aid of high-throughput and in situ methods, it was found that polymerized VO_x species are substantially more active in coke formation than highly dispersed ones. For isobutane DH, it was demonstrated that isomerization of isobutene into n-butenes opens a fast route to coke, most likely through n-butenes DH into butadiene and its further conversion into high molecular products. It is also hypothesized that active sites for DH and coke formation are the same in case of propane but for isobutane there exist additional sites responsible for coke formation from butadiene. Then, catalyst optimization shall encompass suppression of sites active for isomerization that are presumably surface acidic sites.

V-PP35

Catalytic Neutralization of Toxic Emissions of Furnaces of Oil Heating

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In Kazakhstan daily throw out about 3 million tons of industrial and transport harmful pollution, such as CO, NOx, hydrocarbons, etc. Level of air pollution of industrial cities exceeds existing standard limits more, than 6-10 times because of emissions of motor transport, boiler-houses and plants. The most effective way neutralization of harmful emissions is deep catalytic oxidation of organic substances to carbon dioxide and water.

17 metal block catalysts with the honey comb structure of channels were developed and prepared for 8 furnaces of heating of oil and carried out skilled - industrial tests of catalysts on real waste gases of furnaces of JSC "Embamunai-gas" for the purpose of decrease in toxic emissions.

Catalytic filters on metal blocks installed on furnaces work effectively and reduce the content of poisonous gases: CO - 100 %, NO - 7,7 %, NO_x - 7.7 %, on SO_2 - 57.1 %.

V-PP36

Study of the Interaction of Chloroform and Hydrogen with the Metallic Species in Precious Metals Supported Catalysts for the Hydrodechlorination of Chloroform

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The aim of the study is to analyze the effect of the oxidation state of the metal on Pd, Pt, Rh and Ru supported catalysts, in their interaction with chloroform and hydrogen for the hydrodechlorination of chloroform. The experiments were conducted in a quartz fixed bed reactor coupled to a gas-chromatograph with a FID detector to analyze the reaction products. Catalysts of the former metals were prepared using CeO_2-Sm_2O_3 support and characterized by XPS. A density functional theory (DFT) analysis was performed to study the activation of hydrogen and chloroform by metal clusters by analyzing their adsorption energies. Pd and Pt catalysts resulted more active than Rh and Ru ones, probably due to their higher dissociative adsorption energies of H_2. Pd/CS showed by far the best stability which can be attributed to the lower strength of adsorption of chloroform on zero-valent metal clusters when compared to the other metals.

V-PP37

Mineralization of Aniline and Reactive Dye Blue 5 Solutions by Photocatalytic Ozonation

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This work targets at the degradation of aniline (ANL) and C. I. Reactive Dye Blue 5 (RDB) by photocatalytic ozonation in the presence of P25. In order to verify the presence of synergetic effects, photocatalysis (Light/P25) and catalytic ozonation (O_3/P25) were also carried out, as well as, photo-ozonation. With the exception of photocatalysis alone, all tested oxidation processes easily degraded both model compounds. This result was expected since O_3 by itself attacks selectively aromatic moieties and unsaturated bonds, such as ANL and RDB. On the other hand, in terms of TOC removal, photocatalytic ozonation was the most efficiency process achieving a mineralization higher than 80%. In addition to model compounds, O_3 with light and P25 removed a considerable amount of oxidation by-products. Photo-ozonation also presented a good performance during RDB degradation, leading to mineralization level of 65% after 1 h of reaction.

V-PP39

Preferential Oxidation of Carbon Monoxide over NiO/CeO_2 and NiO-CuO/CeO_2 in Hydrogen-rich Streams: Effect of Copper

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Preferential oxidation of CO (CO-PROX) with an appropriate catalyst is one of the most economically and technologically promising methods for remove CO from H_2-rich gas streams, as compared to other processes [1]. The crucial requirements for the PROX reaction are high CO oxidation rate and high selectivity to CO_2. Selectivity is crucial considering the competing H_2 oxidation that may lead to a decrease in the overall fuel cell efficiency. Besides oxidation of both CO and H_2, methanation and WGS reactions can also take place simultaneously [2]. Several catalyst formulations have been reported in open literature and tested for this purpose. Particularly, copper-containing catalysts have been the object of numerous publications in the environmental catalysis field, due to their catalytic properties for CO oxidation applications [3]. Some works reported in literature suggesting that copper oxide catalysts are actives and selective as the platinum-group catalysts when operating at a lower reaction temperature [4]. However, the debate about what copper species are most beneficial in the preferential oxidation of CO is still open in literature and not well understood. In the present study, we investigated the effect of addition of CuO oxides species on supported NiO. We have prepared and characterized monometallic (NiO/CeO_2) and bimetallic (NiO-CuO/CeO_2) system and tested for CO-PROX reaction.

NiO/CeO_2 and NiO-CuO/CeO_2 supports were prepared by incipient wet impregnation method [5]. The nominal loading amount of NiO and CuO were 20 and 5 wt. %, respectively. The catalysts were characterized by X-ray diffraction measurements and fluorescence (XDR, XFR), reduction in thermal programmed reduction (TPR), high-resolution transmission electron microscopy (HRTEM) and textural analysis. The catalytic tests were carried out in a continuous-flow and fixe-bed microreactor, using 150 mg of catalyst and operating at atmospheric pressure. The reaction was performed at different temperatures from 50 to 200 °C, in steps of 25 °C and kept for 30 minutes at each temperature. The feed composition consisted in 1 vol.% CO, 1 vol.% O_2, 60 vol.% H_2 and He balance at a flow rate of 150 cm^3 min^{-1}.

As expected, the insertion of NiO led to a decrease in the specific surface area (from 48 to 33 m^2 g^{-1}) and pore volume (from 0.205 to 0.154 cm^3 g^{-1}) of ceria. On the other hand, the addition of CuO on NiO/CeO_2 increased the specific surface area (from 33 to 39 m^2 g^{-1}) and a decreased the pore volumes (from 0.154 to 0.116 cm^3 g^{-1}), as shown in Table 1. The CO and O_2 conversion and selectivity to CO_2 for the samples are shown in Fig. 1. Note that all samples exhibited CO conversion increases with temperature, with a maximum at 125 °C for the promoted Cu sample and at 170 °C for the unpromoted sample. For higher temperature, the conversion decreases competing with the oxidation of H_2 affecting the CO_2 selectivity. The CO_2 selectivity of the NiO-CuO/CeO_2 catalyst was 100% up to 150 °C. Then, the CO_2 selectivity decreased significantly ($T = 200$ °C, $S_{CO2} = 53\%$).

The NiO/CeO_2 and NiO-CuO/CeO_2 were active and selective to CO-PROX reaction until 200 °C and also showed good stability during time on stream. These materials are promising catalysts for CO-PROX reaction presenting more resistant to methanation than platinum-group catalysts reported in the literature.

V-PP40

Photocatalytic Reduction of Nitrate to Nitrogen in Water under Visible Light Irradiation in the Presence of $Pt/SrTiO_3$:Rh Photocatalyst and $SnPd/Al_2O_3$ Non-photocatalyst

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Photocatalytic reduction of nitrate in water in the co-presence of $Pt/SrTiO_3$:Rh and $SnPd/Al_2O_3$ under visible light irradiation ($\lambda > 420$ nm) was investigated. This reaction system efficiently and selectively promoted the photocatalytic reduction of nitrate to nitrogen, whereas $Pt/SrTiO_3$:Rh or $SnPd/Al_2O_3$ alone showed little activity under the reaction conditions. The selectivity to N_2 was 94% under the optimum reaction conditions, where the amounts of $Pt/SrTiO_3$:Rh and $SnPd/Al_2O_3$ loaded in the reaction system were 500 and 150 mg, respectively. Furthermore, this reaction system was superior in the decomposition rate of nitrate and selectivity to nitrogen to $SrTiO_3$:Rh directly-modified with SnPd bimetal. From the reaction mechanism analysis, hydrogen formed by photoreduction of water over $Pt/SrTiO_3$:Rh acted as the reductant for non-photocatalytic nitrate conversion reaction over $SnPd/Al_2O_3$. Moreover, hydrogen as well as the products (formaldehyde and formic acid) formed by photo-oxidation of methanol over $Pt/SrTiO_3$:Rh acted as a reductant for nitrate over $SnPd/Al_2O_3$.

V-PP41

Co, La and Ce Modified Pd-Al_2O_3 - Catalysts for Methane Combustion

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The single-component (Pd/Al_2O_3 and Co/Al_2O_3) and multi-component ($Pd+Co/Al_2O_3$, $Pd+Co/LaAl_2O_3$, $Pd+Co/LaCeAl_2O_3$) samples were prepared by impregnation of γ-Al_2O_3 with aqua solution of nitrates. The as prepared samples were tested in the reaction of complete methane oxidation. The alumina-supported palladium catalysts, modified with cobalt demonstrate highest activity and stability. The activities of the catalysts, modified with La and Ce drop after ageing, most probably due to sintering of palladium.

V-PP42

Deep Ethanol Oxidation over Nanosized Co-Mn-Al Mixed Oxides Supported on Pelletized Magnesia-alumina

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Preparation of supported catalysts for VOC oxidation with low concentration of active Co and Mncomponents placed exclusively in the outer shell of the support pellets was studied. Impregnation of magnesia-alumina support having basic properties with acidic solution of Co and Mn nitrates was applied and to achieve limited penetration of the metalcations into the support (about 45 % of the pellet radius). The prepared catalysts showed similar catalytic activity like the commercial catalyst with uniform Co and Mn distribution. The most active supported catalyst containing about 15 wt. % of Co+Mn was even more active than the commercial Co-Mn-Al mixed oxidecatalyst with nearly five times higher Co+Mncontent.

V-PP43

Synthesis of Macro-porous Cu-Sn-Zr Catalyst for SO_2 Reduction

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SO_2 is produced in the regeneration process of hot gas desulphurization process. Macro-porous Cu-Sn-Zr catalyst for SO_2 catalytic reduction was synthesized in order to enhance the catalytic activity. The surface area of Cu-Sn-Zr catalyst was measured by nitrogen adsorption method was approximately 80 m^2/g and non-porous Cu-Sn-Zr catalyst surface area was 40 m^2/g. The activity of macro-porous Cu-Sn-Zr catalyst was tested under regenerator-off gas contained with steam (20 mol%), oxygen(4 vol%) and SO_2(4 vol%). The conversion of SO_2 was 95 %, sulfur yield was 93 % at 400 ^oC and SO_2 conversion of non-porous Cu-Sn-Zr catalyst was 78 %, sulfur yield was 75 % at 400 ^oC. Macro-porous Cu-Sn-Zr catalyst has a high surface area than non-porous Cu-Sn-Zr catalyst and the catalytic activity of macro-porous Cu-Sn-Zr catalyst was higher than that of the non-porous Cu-Sn-Zr catalyst. Therefore, it was concluded that the formation of a macro-pores in Cu-Sn-Zr catalyst enhance the catalytic activity for direct sulphur recovery process.

V-PP44

Degradation of Paracetamol by Homogeneous Catalytic Photo-Fenton Process in an Open Channel Reactor

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The conventional wastewater treatment plants do not warranty the degradation of emergent persistent organic pollutants (POPs), among them the pharmaceuticals. Advanced Oxidation Processes, like photodegradation using artificial ultraviolet radiation or solar radiation, are proposed as an alternative for the treatment of contaminated water with POPs. In the present work, the hydrodynamic characterization and evaluation of an open channel reactor for ultraviolet degradation of paracetamol by homogeneous catalytic photo-Fenton are presented. The hydrodynamic characterization of the reactor was performed through the analysis of the residence time distribution (RTD) using a radioactive ^{99m}Tc tracer. The results of the degradation of paracetamol by photolysis and photolysis with H_2O_2 at different values of pH and different concentration of H_2O_2 show that the increase of hydrogen peroxide at pH = 3 favor drug degradation. The best results were obtained for photo-Fenton process, when the pharmaceutical was completed destroyed at 15 minutes with mineralization of 85 % at 6 hours.

V-PP45

Catalytic Oxidation of Polycyclic Aromatic Hydrocarbons (PAH) over Zeolite Type Catalysts: Effect of Si/Al Ratio, Structure and Acidity

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The presence of PAH in the environment is harmful to humans and also to ecosystems. For instance, benzo(a)pyrene is classified as carcinogenic by IARC. Catalytic oxidation is one of the most promising technologies to reduce the emissions of air pollutants[1]. Acid zeolites (protonic forms) have been considered as effective cheap alternative catalysts to metal oxides for hydrocarbons oxidation[2]. In this work, the removal of 1-methylnaphtalene(1-MN), a model compound representative of PAH, by catalytic combustion in the presence of steam is investigated.

The behavior of various acidic zeolites towards the gas-phase catalytic oxidation of 1-MN is investigated. The effect of some parameters on 1-MN oxidation is studied: the structure of the zeolite, Lewis and Bronsted acidity and Si/Al ratio. The performance of these zeolites is compared to 0.97 wt% Pt/Al2O3 which is one of the most active catalysts in complete oxidation of naphthalene[3].

V-PP47

Photocatalytic and Ozone Combined UV Treatment for VOCs Abatement at Trace Concentrations

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This work investigates the efficiency of a treatment with UV light coupled with a photocatalyst to degrade trace concentrations of VOCs in air emissions with a low UV power. At first, the VOC degradation due to UV light only and UV light + ozone is investigated. Then, different catalysts will be implemented to compare the effect of catalytic oxidation vs. oxidation due UV +ozone. The catalysts will be commercial catalysts as well as specifically synthesized with different techniques (e.g. sol-gel or microemulsion) and different dopants.

The experimental results show an increased VOC conversion for higher residence times and a linear correlation between the conversion and the inlet concentration.

V-PP48

Direct Synthesis of Cyclic Carbonates by Oxidative Carboxylation of Styrenes over Ti-containing Catalysts

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The mesoporous titanium-silicate Ti-MMM-E prepared by the simple and affordable evaporation-induced self-assembly methodology demonstrated superior catalytic performance in terms of substrate conversion and carbonate selectivity in the oxidative carboxylation of styrenes with the environmentally benign oxidant, *tert*-butyl hydroperoxide, in the presence of tetrabutylammonium bromide cocatalyst at mild reaction conditions (50-70 °C, 8 bar CO_2). Ti-MMM-E showed superior catalytic performance as compared to other types of mesoporous and microporous Ti-containing catalysts, including the metal-organic framework MIL-125. Under green solvent-free conditions, the selectivity towards styrene carbonate reached 68 and 70 % at 72 and 92 % substrate conversion at 50 and 70 °C, respectively. The volume yield of styrene carbonate as high as 0.3 kg per L of the reaction mixture could be achieved. Importantly, no titanium leaching into solution occurred and the Ti-MMM-E catalyst could be easily recycled and used repeatedly with maintenance of the catalytic properties.

V-PP49

Hydrogenation of Terpineol to Dihydroterpineol over Various Catalysts

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Natural or synthetic α-terpineol is one of the most important and demanded substances, utilized in perfumery and cosmetics to give to remedies the smell of lilac. Dihydro-α-terpineol is also actively used as component of fragrances, perfume compositions and odorants.

In present work the technique of dihydro-α-terpineol obtaining was enclosed in heterogeneous catalytic hydrogenation of terpineol. As a result of terpineol hydrogenation data analysis in all of the investigated reactions dihydro-α-terpineol was obtained with high yield (84-94%) for 1-3 hours at 70°C. There were shown that the most active catalysts are block-structured palladium catalysts.

V-PP50

Catalyst for Complete Oxidation of Nitrogen Containing Samples

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The complete oxidation of nitrogen containing samples has special importance for environmental concerns for NO_x abatement. In this study, the catalytic activities of three different catalyst samples, CuO/ Al_2O_3, CuO-CeO_2 / Al_2O_3 and Pt/ Al_2O_3, for total oxidation of nitrogen containing compounds were analyzed. The catalyst samples were prepared to obtain a loading of 10% Cu, 3%Cu-7%Ce, 1% Pt over the Al_2O_3 as a suppport by impregnation method. Characterization of the catalyst samples was performed by X-ray powder diffraction (XRD) and BET. EDTA, urea, potassium nitrate, ammonium chloride, thiourea, pyridine, glycine, yeast extract, metylamine were selected as model components representing various nitrogen functional groups. The oxidation reaction was performed in a quartz tubular reactor between temperatures 700-850 °C with the air flow rate of 50 ml/min. The catalytic activities of the samples were investigated with mass spectrometry by analyzing combustion products.

V-PP51

Oxidative Desulfurization of Light Oil Distillates Using Ozone

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The work is devoted to the development of a new method of oxidative desulfurization of light petroleum distillates using ozone. The new type of catalysts allows to combine the availability of ozone as an oxidant and safety of the entire process due to the absence of direct contact of ozone and fuel. Using this method allows to obtain the degree of desulfurization of gasoline and diesel fractions 74 and 60%, respectively.

V-PP52

Investigation of Commercial Catalyst for Methane Oxidation after Real Operation Condition

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Monolith catalyst have been investigated after 13000 km run within a bus with lean CNG-engine. Catalyst loses its activity in methane oxidation. The main object was define of causes of palladium catalysts deactivation under life tests. Active layer Pd(2.5%)-Pt(0.6%)/(Al_2O_3+$Ce_{0.5}Zr_{0.5}O_2$) was investigated by BET, XRD, TEM-EDX, TGA-MS. The results indicate that essential amount of sulfur stored in the alumina structure (1,5-4%) and palladium particles decorated by carbon. Catalyst activity may be partially recovered by treatment in the medium enriched by methane. During the process sulfur compounds desorbing takes place. The findings allow to develop the strategy of periodic catalyst regeneration in operation condition.

V-PP53

EPR Spectroscopic Study of the Active Species of Iron-Catalyzed Enantioselective Epoxidation

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The extremely unstable iron-oxygen intermediates formed in bioinspired catalyst systems based on dinuclear ferric complexes with aminopyridine ligands containing electron-donating substituents, H_2O_2 and acetic acid have been detected by EPR spectroscopy for the first time. The detected intermediates are highly reactive and selective towards electron-rich alkene epoxidation even at −85 °C. They exhibit rhombic EPR spectra with the main values of *g*-tensor close to those of known oxoiron(V) complexes. On the basis of this similarity and reactivity data, we have assigned the observed intermediates to the oxoiron(V) $[(L)Fe^{V}{=}O(OC(O)CH_3)]^{2+}$ active species of selective alkene epoxidation by the catalyst systems studied herein.

V-PP54

Analysis of Performance of a Bimodal Cu-CHA as SCR Catalyst Coupled in a NSR-SCR Dual System

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The reduction of NO_x emission in diesel vehicles and new biofueled engines to achieve zero emission is an important environmental issue. In recent times, the combination of after-treatment systems (NSR-SCR) emerges as a promising solution. Decoupled fixed-bed catalysts have been studied individually to confirm that exist an improvement in the NOx elimination with these catalyst formulations. All catalysts were synthesized and well-characterized by different techniques. The Pt-Ba-K/Al_2O_3 formulation presents a high adsorbed NO_x conversion and almost complete N_2 selectivity values. The copper-chabazite with a bimodal porous distribution synthesized in one step, allows to obtain complete NO-conversion values in the SCR whole range, being mainly Cu^{2+} species involved in the DeNOx-SCR process. It has been tested that the combination of after-treatment systems, consisting of a LNT catalyst (Pt-Ba-K/Al_2O_3) with minimum NH_3 emission and a Cu-CHA, highly selective to N_2, acts as an effective NO_x removal process.

V-PP55

$(Gd,Sr\ )_{n+1}Fe_nO_{3n+1}$ Catalysts Applied in Dry (Carbon Dioxide) Methane Reforming

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The perovskite-type ferrites $(Gd,Sr)_{n+1}Fe_nO_{3n+1}$ (n=1, 2, ∞) were studied. Obtained catalytic properties in carbon dioxide methane reforming. It is shown that samples synthesized by ceramic technology are present in microcrystalline state and oxides prepared by sol-gel technology are in nanodispersed state. Heterovalent state of iron atoms (Fe^{3+}, Fe^{4+}) with oxygen vacancies has been found in perovskite-type ferrites prepared using sol-gel technology. It is reflected in the increase in the total number of electron-seeking surface centers and activity of CH_4 and CO_2 conversion.
Was shown the role of the structure of perovskite-type ferrites in the catalytic methane conversion.

V-PP56

Mechanistic Kinetic Modeling of NO Oxidation over a Commercial Cu-Zeolite Catalyst for Diesel Exhaust Aftertreatment

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We present a mechanistic kinetic model for NO oxidation to NO_2 over Cu–zeolite catalysts based on a Redox mechanism which assumes copper dimers $(Cu\text{-}O\text{-}Cu)^{+2}$ as active sites. The first step is the oxidative activation of NO on the Cu sites, forming nitrites as surface intermediates (Cu^{+2}-ONO). In the next step, nitrites decompose releasing gaseous NO_2, which leaves reduced Cu sites (Cu^{+1}). This step is believed to be the Rate Determining Step (RDS) of the NO oxidation mechanism at low T. The effects of several operating variables on NO oxidation were investigated, including temperature, NO, O_2, H_2O, NO_2 feed concentrations, and space velocity. The experimental and calculated results are in a good accordance. This mechanistic model seems therefore a step forward towards a better understanding of the SCR-deNO_x activity of Cu-zeolite catalysts.

V-PP57

Modelling Hydrocarbon Deactivation of SCR Zeolite Catalysts

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Hydrocarbon poisoning is a key issue in the low-T operation of NH_3-SCR converters. The aim of the present work is to develop a reliable numerical simulation tool of the HC poisoning process, useful for the design of effective SCR systems. As proposed in literature, the deactivation process is modeled according to a dual site approach, including: i) a redox site (S1), where NO and O_2 are activated and HC poisoning occurs due to partial oxidation, intermediate adsorption and coke formation; ii) an acid site (S2), responsible for ammonia adsorption. This approach, based on lumped HC molecules, correctly accounts for the transient and long term deactivation effects reported in literature. The kinetic model is validated against literature results and fitted to experimental data collected on a Cu-zeolite commercial catalyst with good agreement.

V-PP58

Green Synthesis of Ruthenium Nanoparticles on Magnetic Carbon Nanostructures and their Use for the Selective Hydrogenation of Nitroaromatics

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Carbon nanostructures find a wide range of applications in different industrial and technological fields. In particular their promising electrical, chemical and physical properties could improve the catalytic activity of metal nanoparticles attached on their surface. The aim of this work is to propose a new sustainable and eco-friendly procedure for the preparation of magnetic recoverable nanocatalysts. In particular we prepared ruthenium and/or magnetite nanoparticles supported on multiwall carbon nanotube (CNT) and graphene oxide (GO) following a new microwave-assisted approach. This new green method is characterized by the use of an alcohol as solvent, monomodal microwave as heating source, in the absence of hazardous reducing and stabilizing agents. All the synthesized nanocatalysts were employed in the selective hydrogenation of 4-chloronitrobenene to 4-chloroaniline under mild reaction conditions obtaining promising results. The ruthenium on magnetic graphene oxide ($Ru@(Fe_3O_4\text{-}GO)$) nanocatalyst shows the highest catalytic activity and it is efficiently magnetically recoverable and recyclable.

V-PP59

Catalytic Wet Oxidation of Organic Wastewater over TiO_2 Supported Ru-Pt Bimetallic Catalysts

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In this study, Ru-Pt/TiO_2 bimetallic catalysts with total metal loading of 1wt% were synthesized by impregnation method. These catalysts were characterized by XRD, N_2 physical adsorption, H_2-TPR and TEM, and applied to catalytic wet oxidation (CWO) of organic wastewater. In CWO of acrylic acid, succinic acid and PEG-1000 wastewater, 0.4%Ru-0.6%Pt/TiO_2 catalyst shows higher catalytic activity than 1%Ru/TiO_2 or 1%Pt/TiO_2 catalyst. The synergic effect between Ru and Pt is the main reason that high CWO efficiency was achieved.

V-PP60

Decomposition of N_2O by Ruthenium Catalysts: Influence of the Support

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As a reaction of high environmental relevance, the catalytic abatement of N_2O by ruthenium was studied on different oxide (MgO, SiO_2, CeO_2, Al_2O_3, TiO_2) and carbon-based supports (activated carbon, SiC). The activities of Ru catalysts were determined in the presence and absence of O_2. They were found to be significantly affected by the support material used. Ru particles of similar sizes were highly active when supported on oxides, with Ru/TiO_2 exhibiting the best performance. Ru catalysts, supported on activated carbon and silicon carbide were clearly less active and acted as stoichiometric reducing agents. The oxidation of the carbon and SiC supports was found to be strongly enhanced by the presence of Ru. TEM and XRD measurements suggest that the catalytic activity does not correlate to the particle size of Ru. H_2-TPR and O_2-desorption experiments revealed that the redox properties of the Ru catalysts are a key parameter for the interpretation of the catalytic activity and the role of the support.

V-PP61

Catalytic Effect of Carbon Nanotubes in the Electrochemical Reduction of Nalidixic Acid

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The catalytic effect of carbon nanotubes (CNTs) on the electrochemical abatement of nalidixic acid (NAL) is analysed in this work. The reaction was studied by differential pulse voltammetry (DPV), using glassy carbon electrode (GCE) modified with CNTs. Three different CNTs have been used, multiwall carbon nanotubes (MWCNTs) and two functionalized: MWCNT-NH_2 and MWCNT-COOH. A constant potential was applied before DPV in order to deposit the NAL under the electrode surface, increasing the amount of reduced NAL. Several parameters were optimized: pH, stirring, scan rate and deposition time. It was observed that the modified GCE exhibited catalytic activity since a higher peak current than the bare GCE was obtained. MWCNT presents the best results, so different DPV cycles were carried out with this electrode in order to remove the NAL. With a constant total volume of 5 mL, the maximum removal achieved was 80 %, obtaining a complete removal when the total volume was reduced until 1.5 mL.

V-PP62

Perturbing the Surface Polarity of Cellulose to Improve its Catalytic Conversion to Glucose

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Cellulose (MC) conversion into useful chemicals has become a major research goal, but its highly ordered molecular structure inhibits its depolymerisation and hence reduces its reactivity.

In order to take advantage of this raw material, efforts have been made to convert cellulosic materials into valuable chemicals and renewable fuels.

This work intends to perturb the hydrogen bond network of MC grafting different combinations of amino acids onto its surface and then, depolymerise the material in the presence of acid catalysts. As a model of MC, cellobiose (Cb) was also perturbed and catalytically hydrolyzed to produce glucose.

Amino acid grafting is not enough to damage the primary structure of the cellulosic materials, but it does causes significant modifications at superficial level on Cb as well as on MC.

Surface modification experienced by Cb and MC, as a result of the grafting of amino acids, is sufficient to increase their reactivity.

V-PP63

Co Catalysts for the Dry Reforming of Biogas

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The dry reforming of methane (DRM) produces synthesis gas with a desirable H_2/CO ratio, contributes to the removal of two greenhouse gases and offers a solution for the valorization of biogas. Cobalt catalysts supported on Al_2O_3 are very suitable for DRM and they have shown also to be good catalysts for biogas reforming. The study reported in this work deals with catalysts containing a 9 wt.% nominal Co content prepared considering two variables: support (Al_2O_3 and $MgAl_2O_4$) and presence of K as promoter. They have been tested in the DRM reaction using a oxygen containing gas mixture resembling the composition of biogas. Catalysts Co/Al_2O_3 and Co/$MgAl_2O_4$ have shown to be very active for biogas reforming, with high CO yield and low carbon deposits; while the addition of K as a promoter has been found not to bring any advantage.

V-PP64

Pd Nanoparticles via Water in Oil Microemulsion as Catalyst for Nitrite Reduction

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The catalytic reduction of nitrite in aqueous phase has been studied as an intermediate and critical step in the reduction of nitrate using non supported Pd nanoparticles (NPs). Pd NPs with different particle sizes (6.2, 7.7 and 11.6 nm) were prepared using water/AOT/isooctane microemulsions and were evaluated in nitrite hydrogenation. Moreover, pH effect was also considered. The particle size showed a significant role in the nitrite reduction, large particles led to a higher catalytic activity. The pH was also found as a key parameter in nitrite reduction, since higher nitrite conversions and much lower or null selectivites towards NH_4^+ were achieved when reaction was buffered with CO_2.

V-PP65

$CaO/CoFe_2O_4$ Synthesized by Citrate Precursor Method for Transesterification Reaction

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In this study was evaluated the $CaO/CoFe_2O_4$ for transesterification reaction. The CaO catalyst supported on $CoFe_2O_4$ (prepared by citrate precursor method) were obtained by calcination at 650°C for 1 hour. These materials were characterized by different methods. The catalytic activity was evaluated through of transesterification between methyl acetate/ethanol and soybean oil/ethanol. The catalytic performance of this catalyst in the methyl acetate transesterification showed conversion level above 85%, reaching the equilibrium after 120 minutes. The ester yield in tests with soybean oil/ethanol showed that varying the reaction time and the ethanol/oil ratio resulted in a gradual increase in the esters conversion. The results confirmed that the $CaO/CoFe_2O_4$ can be considered a promising heterogeneous catalyst, can be easily separated from reaction due to the magnetic characteristic of cobalt ferrite and be reused for successive batches, showing no contribution of homogeneous activity

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V-PP66

EXAFS Study in Operando Conditions of Au/Co-doped CeO_2 Catalysts for Methanol Oxidation Reaction

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The aim of this work was an accurate EXAFS study on the nature of the active sites exposed at the surface of highly dispersed gold catalysts supported on ceria modified by Co_3O_4. The catalysts exhibited very high oxidation activity - 100% CH_3OH conversion degrees at 40 °C. The methanol oxidation reaction was investigated in-operando conditions. Research efforts were focused to achieve information on the local structure of the active sites in terms of position of cobalt atoms in respect to the gold metallic phase. The correlation of the catalytic activity with the findings, provided by EXAFS study allows to bridge the gap of experimental data previously obtained by HRTEM, XRD FTIR, TPR and to clarify the precise nature of the synergy between the gold phase and the Co-doped ceria support, which resulted in an excellent CH_3OH oxidation activity.

V-PP67

Effect Promoter of Cobalt on the Catalyst Ni-Mg-Al Obtained via Hydrotalcites for the Dry Reforming of the Methane

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The Catalysts materials Ni-Mg-Al and Ni-Co-Mg-Al were synthetized by classical method of coprecipeation at basic pH.We studied the effect of cobalt on the previous catalyst for the reaction of dry reforming.
The catalysts were characterized by a number of technical physicochemical:XRD,ICP, H_2-TPR,BET and SEM.
The diffraction X-ray analysis showed HDL structure for all the catalysts before calcination. The catalytic tests on CH4 / CO_2 reaction showed a good conversion of methane and Carbon dioxide and good stability of catalysts. The addition of cobalt improves the conversion of methane and carbon dioxide.

V-PP68

On the Correlations between Redox Properties and Catalytic Performances of $Ce_xPr_{1-x}O_{2-\delta}$ Catalysts Towards Environmentally Relevant Oxidation Reactions

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A series of $Ce_xPr_{1-x}O_{2-\delta}$ catalysts was prepared by co-precipitation method in alkali media. These catalysts were characterized by N_2 isotherms at -196°C, XRD, Raman spectroscopy, XPS, H_2-TPR and CO-TPR. Catalytic tests were performed for NO oxidation to NO_2 (from 25 to 750ºC) and for the preferential oxidation of CO in H_2 rich stream (CO-PROX reaction) in the range of 150-500ºC. The trends in order of catalytic activities towards NO oxidation and CO-PROX (correlated with the redox properties of the catalysts) were analyzed.

$Ce_xPr_{1-x}O_{2-\delta}$ mixed oxides present very different catalytic behaviors towards NO oxidation and CO-PROX reactions. Reasonable hypothesis to explain these experimental trends are: the different temperature range where both reactions occur, and/or the acid character of the NO and CO molecules, which interact differently with ceria-praseodimia. The understanding of the features that govern the activity towards these environmentally relevant oxidation reactions is important in the designing of effective catalysts.

V-PP69

Identifying the Nature of the Copper Entities over Ceria-based Supports to Promote Diesel Soot Combustion: Synergistic Effects

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The aim of this research is to synthesize catalysts exhibiting a wide range of degrees of copper incorporation/distribution/contact on ceria-zirconia mixed oxide by preparing catalysts with a high degree of copper incorporation, well-dispersed copper on the porosity and different degrees of physical interaction. Their catalytic activities towards diesel soot combustion and NO oxidation to NO_2 were analyzed with the purpose to identify the nature of the copper entities over ceria-based supports to promote soot combustion.

The catalysts were characterized by physico-chemical techniques and activity tests were performed towards NO oxidation (from 25ºC to 700ºC) and diesel soot combustion in NOx/O_2, under ramp mode (25ºC- 700ºC) and isothermal conditions (450°C).

Results reveal that copper in close contact with ceria greatly promotes its reducibility at lower temperatures. Mainly, 2%Cu/ceria-zirconia catalyst prepared by impregnation shows the highest activity towards soot combustion at low temperatures ($\leq$ 450ºC), due to the observed synergistic interactions copper-ceria.

V-PP70

Catalytic Performance of 2%$CuO/Ce_{0.8}Zr_{0.2}O_2$ Loaded over SiC-DPF in NOx-assisted Combustion of Diesel Soot

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This work presents a comparative study between the catalytic performance of 2%CuO/ceria-zirconia powder catalyst and the same catalyst supported on silicon carbide DPF (Diesel Particulate Filter) towards NO oxidation and soot combustion reactions.

Ceria-zirconia catalyst was prepared by co-precipitation method and copper was incorporated by incipient wetness impregnation method. The catalyst incorporation onto the ceramic support was achieved by simple dipping of the DPF in a catalyst aqueous solution. The catalytic coating morphology was evaluated by SEM and its mechanical stability by an adherence test. Both catalysts configuration were tested for NO oxidation and soot combustion reactions under NOx/O_2.

Results revealed a successful incorporation of the catalyst onto a SiC-DPF. Furthermore, a satisfactory catalytic performance of the catalytic-coated filter was reached towards the NO oxidation and soot combustion reactions. Otherwise, it was proved that a coated-DPF can be reused in several NO oxidation cycles as the catalytic coating is stable.

V-PP71

Pd-Cu Nanostructured Catalysts for Water Phase Reduction of Nitrates. Influence of the Support and of the pH

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Liquid-phase catalytic reduction of the nitrates seems to be an adequate technique for the removal of nitrate from natural water. In order to obtain greater activity and selectivity to nitrogen, different catalysts have been designed. Pd-Cu nanoparticles were synthesized by alkaline polyol method and further supported on alumina or titania. The nanoparticles show a crystalline Pd core and a shell reach in amorphous cooper as was put in evidence by complex characterization methods (X ray diffraction, X ray photoelectron spectroscopy, transmission electron microscopy, and CO chemisorption). The performances of as prepared catalysts in the water phase reduction of nitrate were assessed in comparison with catalysts obtained by impregnation. The supported nanoparticles catalysts have a smaller Pd crystallite size and more important coverage of the palladium surface with copper in comparison with the catalyst obtained by impregnation method. It was assumed that these specific characteristics of the nanostructured catalysts led to their superior activity in the reduction of nitrate. Nevertheless, the choice of the support appeared to be an important aspect. Pd-Cu nanoparticles on titania (PCT-np) are the most active, selective and stable bimetallic catalyst among those investigated. Also, the influence of pH conditions on the PCT-np catalyst performances was emphasized.

V-PP72

Red Mud Catalysts for Sulphide Oxidation in Wastewater

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This contribution investigates an alternative route for the valorisation of red mud (RM) industrial waste by utilizing it as raw material in the manufacture of catalysts for the oxidation of sulphide ions from wastewaters to elementary sulphur using air as oxidation agent. The preparation method proposed for the obtaining of the catalysts involves the functionalization of trivalent iron sites from RM waste by treatment with polycarboxylic acids.The catalysts were characterized by DRIFT, DR-UV-Vis, XRD, surface area and porous structure determinations. Besides the formation of Fe(III) complexes on the surface of the RM and RMN solids, the preparation method allows also the re-adsorption of the complexes formed in the solution following the dissolution of iron by the complexation agents. The catalysts obtained by functionalization present catalytic activity for sulfide oxidation under mild reaction conditions even at room temperature and avoid the formation of Fe(II)S in treated wastewater.

V-PP73

Photocatalytic Activity in the Degradation of Phenol over Zn^{2+}:Al^{3+}:W^{6+} Layered Double Hydroxide Prepared by Coprecipitation

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Zn^{2+}:Al^{3+} and Zn^{2+}:Al^{3+}:W^{6+} layer double hydroxide (ZnAl and ZnAlW LDH) were prepared by the co-precipitation method. The ZnAl and ZnAlW LDH were characterized by N2 physisorption, XRD, UV and Raman spectroscopy. The LDH were tested in photodegradation of phenol in aqueous medium using UV light as irradiation source. The presence of W^{6+} produced a significant increment of S_{BET} and VP_T of the LDH at any treatment temperature. ZnAl LDH contain aggregates of plate-like particles or slit-shape pores which are enlarged with doping with W^{6+}. There are loss of crystallinity and structural changes in both ZnAl and ZnAlW treated at 573 K. The photocatalytic activity of ZnAl is improved both with treatment temperature and doping with W^{6+}. In the last case the photoconversion is significantly increased obtaining 75% for ZnAlW treated at 373 K and 92% for ZnAlW treated at 573 K after 4h of UV irradiation.

V-PP74

Photodegradation of Phenol over Al_2O_3-Nd_2O_3 Nanomaterials Doped with Fe, Mg, and Zn Oxide

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Al_2O_3-Nd_2O_3-M_xO_y (M = Fe, Mg, Zn) nanomaterials (Al-Nd-M) with 5 wt% of Nd_2O_3 and 1 wt% of metal oxide were prepared by a combined method of dissolution of organic precursors at high temperature and the conventional sol-gel route. The nanomaterials were characterized N_2 physisorption, X-ray diffraction, UV-Vis and Raman spectrocopy. Al_2O_3-Nd_2O_3 nanomaterials doped with 1.0 wt% of Mg or Zn oxide exhibited high specific surface area (> 300.0 m^2g^{-1}) and high specific pore volume (~1.1 cm^3g^{-1}). The photodegradation of phenol over Al-Nd was improved by doping with 1 wt% of Zn or Mg oxide obtaining phenol photoconversions of 84 and 91% respectively after 5h of UV irradiation. In contrast, doping with 1 wt% of Fe oxide was in detriment of the specific surface area and phenol photoconversion.

V-PP75

Polyisobutylene Oligomer-bound Polyoxometalates as Efficient and Recyclable Catalysts for Biphasic Oxidations with Hydrogen Peroxide

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Polyisobutylene (PIB) oligomer-bound amines render Keggin polyoxometalates (POM) heptane soluble, making them efficient and recyclable catalysts for environmentally benign biphasic oxidations with hydrogen peroxide. This is illustrated using both oxidative desulfurization and alkene epoxidation reactions that can be efficiently carried out in a heptane-water two-phase system occurring through facile phase transfer of POM by the amine terminated PIB oligomer.

V-PP76

Catalytic Combustion of Toluene over MnO_x-CeO_2 Mixed Oxides

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MnO_x-CeO_2 catalysts (molar ratio Mn/Ce = 1) were prepared using two methods: carbonate and redox coprecipitation routes. The prepared solids were calcined at 500°C, and characterized by XRD, nitrogen adsorption-desorption technique, H_2 temperature-programmed reduction (H_2-TPR) and SEM, they were, then, tested in the toluene combustion reaction. The catalytic performances of the prepared solids were evaluated in the temperature range 150-400° C. The XRD analysis of the two solids showed that the only crystalline phase detected is cerium oxide. BET surface area measurements showed that the incorporation of manganese led to an increase in the specific surface area of ceria, the solid prepared by the co-precipitation method led to the highest specific surface area (156 m^2/g). The solids showed good performances in the toluene combustion reaction that depend strongly on the preparation method. The best catalytic activity was obtained for the catalyst prepared by the redox method.

V-PP77

Effect of Preparation Method on Catalytic Properties of Co-Mn-Al Mixed Oxide for N_2O Decomposition

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The present article is dealing with comprehensive analysis of the effect of preparation method performance of Co-Mn-Al mixed oxide catalyst on the N_2O decomposition. Co-Mn-Al mixed oxides were prepared by three different methods: (i) from hydrotalcite-like precursors (Co-Mn-Al-HT-ex), (ii) by calcination of corresponding nitrates (Co-Mn-Al-nitr) and (iii) by mechanochemical reaction of Co, Mn, Al nitrates with NH_4HCO_3 (Co-Mn-Al-carb). The Co:Mn:Al molar ratio of 4:1:1 was kept constant in all catalysts. The catalysts were charakterization by AAS, XRD, Raman, FTIR, H_2-TPR, TPD of CO_2 and NH_3 and tested for N_2O decomposition in inert gas and simulated waste gas from HNO_3 production. The highest catalytic activity was achieved on the calcined precursors having carbonates in their molecules (Co–Mn–Al-carb and Co–Mn–Al-HT-ex), the lowest one on the calcined Co–Mn–Al nitrates due to the lower surface area, less advantageous porous structure and worse reducibility.

V-PP78

K/Co_4MnAlO_x Catalyst for N_2O Abatement from Nitric Acid Plant Waste Gases – Results of Pilot Plant-scale Testing

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The K-doped Co-Mn-Al mixed oxide deN_2O catalyst was prepared by calcination of the Co-Mn-Al layered double hydroxide, impregnated with KNO_3, pelletized into 5 x 5 mm tablets, and again heated at 500 °C. The catalytic N_2O decomposition was tested in a pilot plant-scale fixed bed stainless steel reactor (0.31 m i.d.) in the temperature range from 300 to 450 °C and inlet pressure of 0.6 MPa. The reactor inlet was connected to the bypassed tail gas from the nitric production plant downstream the SCR NO_x/NH_3 catalyst. Feed to the reactor varied between 300 and 600 kg h^{-1} and contained typically 400-700 ppm N_2O together with oxygen, water vapor and low concentration of NO, NO_2 and NH_3. High output in N_2O removal for 112 days without any deactivation was observed. The kinetic parameters of N_2O decomposition over the catalyst tablets in the pilot plant reactor were evaluated and used for the reactor scale-up calculations. The developed deN_2O K/Co_4MnAlO_x catalyst can be considered as very promising for commercial application.

V-PP79

DFT Studies on the Mechanisms of Nickel-Catalyzed Reductive Carboxylation of Styrenes Using CO_2 as the Building Block

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As an abundant renewable carbon source, carbon dioxide is an attractive C1 building block in synthetic organic chemistry. Here, we studied the detailed mechanisms for the nickel-catalyzed reductive carboxylation of styrenes using CO_2 with the aid of DFT calculations. Two possible mechanisms, oxidative-coupling mechanism and nickel-hydride mechanism, were calculated and compared. Our calculation results show that, for the oxidative-coupling mechanism, a metallacycle thermodynamic sink is generated, which should be avoided in order for smooth reductive carboxylation. For the nickel-hydride mechanism, a nickel-hydride species is the active species. Calculations show that either the olefin insertion or the reductive elimination step can be the rate-determining step, and both the transition states are only slightly more stable than the oxidative coupling transition state leading to the thermodynamic sink. Because of the competitive nature between the two mechanisms, the reaction conditions and other factors (substituent, pressure and ligand) affect significantly the reaction outcome.

V-PP80

Catalytic Decomposition of NF_3 Exhausted in Semiconductor Manufacturing Process over γ-Al_2O_3 Catalyst with H_2O or without H_2O

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It is required to remove the wasted NF_3 by safe and low cost method because NF_3 has an enormously large global warming potential of 17,000 times than that of CO_2 and long lifetime for the decomposition in atmospheric condition. The catalytic reaction can be very useful for commercialization of NF_3 decomposition process. In this study, γ-Al_2O_3 catalyst was prepared for the decomposition of NF_3. NF_3 of 5000 ppm and the excessive H_2O were used as the reactant for hydrolysis. The catalytic activity tests were carried out at 400℃ and space velocity of 15000ml/g cat·h for 35 h, and were performed with or without H_2O in order to investigate the effect of hydrolysis. The characterisation of catalyst surface was carried out with XRD, BET. In case of reaction without H_2O, the conversion of NF_3 gradually decreased during the activity test for NF3 decomposition. While, the conversion of NF_3 on catalytic hydrolysis was maintained at about 40% for 35 hours. Catalytic hydrolysis was more effective NF_3 decomposition process than gas-solid reaction without H_2O in the long term tests.

V-PP81

"Bifunctional" [Mn-Ce/Fe-zeolite] Catalysts for Selective Catalytic Reduction of NO_x by NH_3 at Low Temperature

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In this study we attempted to increase the catalytic activity of the Mn-Fe-Beta catalyst at low temperatures by promoting with Ce. NH_3-$DeNO_x$ activity of the Mn/Beta at 150-300ºC can be significantly enhanced by additional modification with Ce. Modification with Ce leads to enhanced oxidation activity of Mn-Ce species thus promoting "bi-functional" SCR mechanism comprising two reactions: (1) oxidation of NO to NO_2 over Mn-Ce oxide species followed by (**2**) fast-SCR over zeolite component. Our data indicate that the "bi-functional" pathway predominates over MnO_x-CeO_2/Beta, and a contribution of the standard-SCR activity of zeolite component is negligible.

V-PP82

Increase of CO Photocatalytic Oxidation Rate on Titania under Moderate H_2O Coverages

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Photocatalytic oxidation method is commonly used for removing volatile organic compounds from air, but for CO this method is usually considered as ineffective mainly due to competition for adsorption sites between H_2O and CO. Obtained results demonstrate that the role of water is more complex than just a competitive adsorbent, and the adsorbed water at moderate coverages increase the rate of photocatalytic CO oxidation on undoped TiO_2. This effect doesn't appear for some other types of photocatalysts. In contrast of organic substances, the role of H_2O cannot be reduced to deblocking active sites and most likely that water contributes light-induced transformation of molecular oxygen into more active forms.

V-PP83

Supported Polymer-Metal Comlexes for n-Octane Oxidation by Hydrogen Peroxide under Mild Conditions

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In this paper we present the results of the development of bimetallic nickel-iron polymer-containing catalysts supported on sorbents and their use as catalysts for oxidation of n-octane by hydrogen peroxide under mild conditions.

Chromatographic analysis of the reaction products indicates the formation of alcohols and ketones. The highest degree of conversion of the substrate is observed in the presence of 1% Co-Fe (1:3)-PHMG/Al_2O_3 catalyst (12.2%). The lowest activity showed 1%Co-Fe(1:3)-PHMG /ZnO.

The developed cobalt-iron catalyst was studied by TEM. According to TEM images, the metal particles of 10 nm are evenly spread in the polymers which are fixed on the surface of Al_2O_3 (Figure 1).

Thus, the developed heterogenized catalysts based on polymer-metal complexes fixed on inorganic sorbents are active in both decomposition of H_2O_2, and the reaction of n-octane oxidation under mild conditions.

V-PP84

Sorption of Sulfur-containing Molecules on CuZnAl-O Catalysts from Model and Straight-run Diesel Fuel

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One of new perspective method for diesel fuels desulfurization is selective oxidation of their sulfur-containing compounds over catalysts with oxygen (ODS). Therein during this process the sulfide and heterocyclic sulfur-compound are transformed to sulfur dioxide, and the hydrocarbon fragment is oxidized to carbon dioxide and water. According to the literature CuZnAl-O catalysts can be promising for ODS. The goal of this work is to study sulfur adsorption capacity of CuZnAl-O in a model (dibenzothiophene in toluene) and a straight-run diesel fuel. It has been shown that CuZnAl-O catalysts actually possess sorption capacity. The trend of an increase of the sorption capacity with respect to sulfur at the transition from DBT derivatives to simpler sulfur containing molecules has been observed. DTA-TG-MS analysis has shown that the sulfur on the catalyst surface is represented by sulfides/polysulfides and sulfate of metals. Carbon deposits on the surface are products of the hydrocarbon condensation.

V-PP85

Role of Electron-Acceptor Sites during Destructive Sorption of CF_2Cl_2 over MgO and VO_x/MgO Aerogels

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It was found that addition of vanadium had a catalytic effect on the interaction of nanocrystalline MgO aerogels with halocarbons, accelerating the formation of the active sites on the surface of the nanoparticles. The electron-acceptor sites on the surface of initial samples of MgO and VOx/MgO were not observed. Their concentration gradually increased during the induction period, reaching a clearly defined maximum in the active state when the rapid topochemical destructive sorption reaction occurred. A good correlation was observed between the rate of the halocarbon destructive sorption and the concentration of weak electron-acceptor sites characterized using anthracene or perylene as spin probes. The concentration of electron-donor sites decreased during reaction with CF_2Cl_2 and did not correlate with reactivity. These results clearly demonstrate that weak electron-acceptor sites are accumulated on the MgO surface during the induction period of its reaction with CF_2Cl_2.

V-PP86

The Synergistic Effect for [RedOx + Zeolite] CombiCat in NH_3-SCR: Contributions of Different Pathways to the Overall Mechanism

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Recently we have observed the pronounced synergistic effect for combined catalysts [CeO_2-ZrO_2 + FeBeta] and [Mn/CeO_2-ZrO_2 + FeBeta] in NH_3-SCR: the catalytic activity of the composite systems significantly exceeds activity of the individual components. It was suggested that the synergistic effect over CombiCats stems from the "bifunctional pathway" comprising NO oxidation over RedOx component followed by Fast SCR on FeBeta. However, the "bifunctional pathway" operates in parallel with the Standard SCR over Mn/CeO_2-ZrO_2 and FeBeta. In this study we attempted to discriminate semi-quantitatively "bifunctional pathway" and Standard SCR contributions to the overall mechanism of NH_3-SCR over CombiCat. Quantitative analysis of NO_x conversion data allowed us to distinguish contributions of three main pathways. It was shown, that Fast SCR activity of zeolite component is a prerequisite of synergistic effect, while Standard SCR activity plays a minor role in the overall performance of CombiCats.

V-PP87

Conversion of Lignin Catalyzed with Sub- and Supercritical Water

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Conversion of sodium lignosulphonate (LS) is studied in sub- and supercritical water in the temperature range 200-430°C at 220 atm and the residence times 2.5-10 min. The influence of the parameters of the process (temperature, reaction time) on the yield of monomeric products was determined. Varying the temperature and reaction time makes it possible to adjust the rate and extent of LS depolymerization. In the subcritical region, the conversion proceeds through hydrolysis. In the supercritical region, it is dominated by free radical processes.

V-PP88

Aqueous Phase Hydrodeoxygenation of Phenol on Bifunctional Catalyst Systems: Ru/C and Acids

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The hydrodeoxygenation of phenol, the model compound of bio-oil, was carried out in a fixed-bed flow reactor. Phenol conversion was performed at 150–250°C and 7.5 MPa in an aqueous solution with a concentration of 1 wt % (0.106 M). Using bifunctional catalyst systems (Ru/C and acid), phenol was converted to cyclohexane and fully hydrogenated hydrocarbons. Addition acid function as mineral acid (phosphoric acid) or solid acid (Nafion) to the ruthenium catalyst leads to increasing of cyclohexane selectivity at a complete conversion of phenol. It indicates the acidity of the catalyst system is the determinative factor for cyclohexane formation from phenol in an aqueous medium.

V-PP89

Kinetics and Mechanism of the Total Oxidation of CO and p-Xylene and their Mixtures on Supported Copper Catalysts

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One of effective and economic ways for the removal of toxic impurities of chemical plants is their total catalytic oxidation. Supported copper catalysts are active ones in total oxidation of CO and aromatic hydrocarbons. Their activity can be increased at addition of small amounts of noble metals. This work is devoted to the study of kinetics and mechanism of separate and mutual CO and p-xylene oxidation on Cu/CeO_2 catalysts without and with Pt. The catalysts were investigated by TPR, XRD, TEM, BET, EDS-methods. Optimal contents of Cu and Pt were 7.5 and 0.1 % (wt.), respectively. Pt resulted in the increase of the dispersity of Cu and its reduction degree. The rates of CO and xylene oxidation were described by power-ration equations with the inhibition of reaction products. The rate of CO oxidation is considerably more than the rate of xylene oxidation. Xylene had a big influence on CO oxidation but CO little affected on xylene. At mutual oxidation new formed intermediate compounds were oxidized with low rate in comparison with the separate oxidation. This resulted in a change of process kinetics. Data of unstationary investigations showed that the introduction of Pt resulted in the increase of bond strength of all reaction components. The lattice oxygen made a little contribution in the reactions. The step-schemes of CO and xylene oxidation were proposed.

V-PP90

Catalytic Flow Syntheses of Oligopeptides in the Glycine – Trimetaphosphate – Imidazole System

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One of the most important and unsolved problems of modern science is prebiotic peptide synthesis. Despite of numerous research efforts, the optimal conditions, kinetic parameters and mechanisms of peptide synthesis in early stages of biochemical evolution are still not established. To develop the prebiotic peptide synthesis problem the oligopeptides formation kinetics in the glycine – sodium trimetaphosphate – imidazole system in water has been investigated in flow conditions at different temperatures and pH values. The syntheses have been performed using Syrris ASIA-330 flow chemistry system. The kinetics of the processes has been monitored by the Knauer Smartline HPLC system and ^{1}H and ^{31}P NMR spectra recorded on a Bruker Avance III 400 NMR spectrometer. The synthesis conditions were optimized. The reaction mechanism was proposed and grounded on the basis of quantum-chemical computation results with GAMESS program. The system investigated may be used as a good model for peptide synthesis in prebiotic conditions.

V-PP91

A Study of Glycolysis of Polyethylene Terephthalate Waste in the Presence of Catalyst for the Production of bis(2-hydroxyethyl)terephthalate

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The aim of our investigation is to obtain a monomer bis(2-hydroxyethyl) terephthalate (BHET) by degradation of PET wastes for the synthesis polyurethanes, biodegradable polymers for medical purposes, etc.
Investigation of dosage of catalyst showed that increasing the concentration of the catalyst leads to decrease in time of destruction of polymer. Increasing the temperature leads to the same.
The resulting product was studied by IR spectroscopy ; key functional groups are identified. The infrared spectrum of product was compared with the spectrum of bis(2-hydroxyethyl) terephthalate: they are almost identical.

V-PP92

The Aluminum Oxide Active Catalyst's Regeneration Using Supercritical Carbon Dioxide

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Results of catalyst regeneration using pure and modified with polar additive (2 wt.% DMSO) supercritical carbon dioxide gives.

V-PP93

The Composite Rubberized Material with Coated Photocatalytic Layer

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Protective clothing made from rubberized material provides protection from toxic, corrosive chemicals and flame. After infection by toxic chemicals protective clothing requires decontamination by special solutions, which makes certain load on the environment - pollution from wastewater. A photocatalytic decomposition of these substances adsorbed on the surface of rubberized material is an alternative to this method of decontamination of chemical clothing.The composite rubberized protective material is developed.

V-PP94

Electromagnetic Catalytic Reactor of Water Treating from Oils and Hydrocarbons

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The problem of clearing of water resources from oil pollution is rather actual now. The clearing process of water environments from oil pollution and dangerous hydrocarbons aromatic and olefinic the lines, based on use is developed and tested in industrial scale as basic reactionary unit of the device of electromagnetic processing water environments. The general distinctive characteristics of installation: High efficiency; Stability to a high level of pollution of communications (a rust, sand, fine stones); Standardization of a design with an opportunity of fast replacement of elements (a grid, a pipe, nozzles and so forth); Absence of a problem of deterioration in case of use the plastic case of a reactor; Installation has passed industrial tests in a zone of the Caspian pool.

V-PP95

Optimization of Catalytic Gas-To-Liquid Technology for better Carbon Efficiency

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The prospects of industrial application of Gas-to-Liquid technologies (GTL) depend strongly on the overall carbon efficiency of this complex combination of catalytic processes.
The GTL technology includes two main stages: conversion of methane into syngas and Fischer-Tropsch synthesis (FT) to produce liquid hydrocarbons from the syngas. The syngas production technology is the most capital-intensive stage. Selection of technological solutions for the production of syngas is usually determined by the required H_2/CO molar ratio.
The purpose of this work is to study the effect of different methods of natural gas-to-syngas conversion with different circulation loops of FT tail gas on the GTL efficiency.
The results of simulation suggest that the highest carbon efficiency can be reached with ATR- or POX-based GTL. However, it is reasonable to suggest that a better way of producing syngas in GTL technology is combined steam and dry reforming (SDR) due to much lower power consumption.

V-PP96

Catalytic Performance of Ni-based Catalysts Supported on λ-Al_2O_3-ZrO_2-TiO_2-CeO_2 Composite Oxide for CO_2 Methanation

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Carbon dioxide methanation fits the current topic of reducing the greenhouse gases emissions and is advantageous from the thermodynamics point of view. In this work, the CO_2 methanation has been studied over a series of composite oxide supported Ni-based catalysts. The effect of composite oxides (ZrO_2-TiO_2-CeO_2) loading in different percentage (5-10-15% for each one) on γ-Al_2O_3 support was investigated. In particular, 10% loading was found to be the optimal ratio with the highest CO_2 conversion level at relatively low temperatures (300°C). It influences the Ni-support interactions, inhibiting the incorporation of metal species into the γ-Al_2O_3lattice, as proved by TPR measurements.

V-PP98

Preparation of Cobalt Titanate Nanoparticles and the Study of Their Photocatalytic Behaviors

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Water gets polluted by harmful chemicals, dyes, oils. All the wastewater that contains harmful chemicals is drained into nearby water bodies. This causes water pollution and will lead to various health problems to flora and fauna. Among the pollutants of water, dyes play a major role. Most of the dyes released from the pharma and textile industries are mutagenic, toxic and teratogenic that can cause serious health hazards to humans and live stock. This work reports on the preparation of cobalt titanate by the co-precipitation method, using solutions of titanium tetrachloride ($TiCl_4$) as titanium source, $CoCl_2$ as cobalt source and KOH as a precipitating agent. The aim of our investigations was the use of cobalt titanate as photocatalyst for the degradation of organic pollutants.

V-PP99

CO_2 Hydrogenation to Light Olefins on a High Surface Area K-promoted Iron Catalyst

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The one-pot hydrogenation of CO_2 to light olefins is an interesting process which would allow a significant reduction of CO_2 emission and the concomitant production of added-value products. In this work, a simple K-promoted iron based-catalyst was prepared by a carefully controlled thermal decomposition of an iron glycolate complex, followed by impregnation with potassium. The obtained material is active for CO_2 hydrogenation and the C_2-C_4 olefins are the most abundant species. The small crystallites size and the spinel structure of the prepared material facilitates the in-situ carburization of the Fe_xO_y precursor so that the activity of the activated catalyst is higher than those of K-promoted reference materials obtained from commercial Fe_2O_3 and Fe_3O_4.

V-PP100

The Analysis of Carbon Dioxide Reforming of Methane (CDRM) Performance of Co-Ce/ZrO_2 System

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The aim of this study is to establish a link between Co:Ce loading ratio and CDRM performance of the catalyst, and to confirm the roles of Co, Ce and ZrO_2 in Co-Ce/ZrO_2 system. The favorable combination(s) of catalyst and reaction condition for stable performance were investigated through following an experimental design involving Co and Ce loadings, reaction temperature and CH_4/CO_2 feed ratio as parameters. All freshly reduced and selected spent samples were characterized by XPS, SEM-EDX and HRTEM-EDX. The Co:Ce loading ratio affects the mechanisms of carbon and oxygen forming reactions and changes their relative extent. Cobalt is dominantly responsible for CH_4 dehydrogenation, and both Co loading and Co:Ce loading ratio change product distribution. Ceria limits coke deposition by enhancing surface oxygen transfer, and its activity is limited by CO_2 concentration in the feed. The characterization test results were in accordance with that of performance tests.

V-PP101

Novel Imidazolium Based Catalyst for the Chemical Fixation of Carbon Dioxide

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In this work, the synthesis of a novel imidazolium-based polyhedral oligomeric silsesquioxane (POSS-mim-Cl) material is presented. The new nanometer-size organosilica based compound was employed as catalyst for chemical fixation of CO_2 into epoxide under homogeneous conditions.

Styrene oxide was chosen as reference substrate. In addition, different parameters (solvent, temperature, pressure of CO_2, and mass of the catalyst) were modified to find the best condition for CO_2 conversion. The POSS-mim-Cl displayed good catalytic performances, the best results being obtained at 40 bar, 150°C, with 110 mg of catalyst and using anhydrous ethanol as co-solvent. It is worth to mention that POSS-mim-Cl displayed better catalytic performance than the corresponding 1-butyl-3-methyl imidazolium chloride. As far as we know this study represents the first use of imidazolium-based POSS as catalysts for the chemical fixation of CO_2.

V-PP102

Real-time in situ Atomic-scale Study of the Surface Termination of Ceria Nanoparticles under Vacuum, O_2 and CO_2 Pressures by Environmental Transmission Electron Microscopy

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The advent of Cs-corrected transmission electron microscopes has brought a new impulse to environmental transmission electron microscopy (ETEM) studies. This is particularly true in the field of catalysis in which high resolution imaging of the catalyst surface is required to assess structural/chemical evolutions in presence of controlled gaseous environments. Here we present a study on the adsorption of both O_2 and CO_2 on ceria nanoparticles at room temperature. These preliminary steps are part of a global approach aimed at gaining fundamental insights at reactions used for the valorization of CO_2 and the related global warming issues.

This high spatial resolution study (structural/chemical) of ceria nanoparticles by environmental TEM not only clearly shows the capability of observing/measuring real-time atom mobility at the surface of nanoparticles and chemical evolution (reduction) but also enables the indirect detection of surface adsorbates (here carbonates due to CO_2 adsorption) by monitoring the surface termination structural evolution.

V-PP104

Synthesis of Organic Carbonates Using Catalyst Containing K Metal from Waste Source

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Over the years production of glycerol as a crude waste from biodiesel making industries has been largely increasing. For every 100 kg of biodiesel produced, 10 kg of glycerol is produced as a by-product which corresponds to 10 weight percentage of biodiesel. It is estimated that by the year 2016, the production of crude glycerol will reach 4 billion gallons.[1] Thus, in order to make this waste a useful substance for future use, the conversion of glycerol to other value added product is suggested.[2] Glycerol carbonate is one of the value added product of glycerol which is important to many industries. Glycerol carbonate has low toxicity, noble biodegradability and high boiling point.[3] There are various methods to produce glycerol carbonate using different sources of starting material. However the method used in this study is the most prominent method of near to a green synthesis approach whereby it uses bio-renewable feedstock. Besides, glycerol and urea are relatively cheaper and readily available.[3,4] On the other hand introducing waste material from local palm oil industry in Malaysia which is boiler ash has certainly raised the benchmark to the synthesis of organic carbonate to another level. This does not only propose a cheaper and economical route of transforming polyols into carbonates but also support proper disposal of waste for the betterment of our environment.

V-PP105

Simultaneous Removal of o-dichlorobenzene and NO_x over TiO_2-Al_2O_3 Supported Vanadium Catalysts

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The present investigation concerns the modification of alumina by titania loading close to the theoretical monolayer, obtained by calcinations at 600 ºC, and its use as support for vanadium catalysts. The TiO_2-Al_2O_3 supported vanadium catalysts were prepared and characterized by N_2 adsorption at -196 ºC, XRD, FTIR, UV-Visible, NH_3-TPD, CO_2-TPD and TEM techniques. By combining the information obtained from all these studies, a detailed description of their texture, structure, VO_x and titania distribution, and chemical properties could be gained.
The prepared catalysts were successfully assayed in simultaneous removal of o-DCB and NO process. Their behaviors were discussed with reference to that expected for the use of pure alumina as support. We concluded that the dispersion of titania on high surface area oxide (alumina) as support of VO_x species represents an advantageous catalytic properties.

V-PP106

Effect of the Nature and Location of Cu Species in Cu-BETA Catalysts for NH_3-SCR of NO_x

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Cu/BETA catalysts for NH_3-SCR have been synthetized by copper ion exchange over H^+- or NH_4^+-BETA zeolite, including for some preparations an intermediate ion exchange with Na^+ ions before Cu ion exchange. The prepared catalysts were characterized in terms of XRF, N_2 adsorption-desorption, EPR, H_2-TPR, TEM and FT-IR of NO and CO adsorption. Among the prepared catalysts NH_4^+/Na/Cu, presented a superior NH_3-SCR activity in the whole temperature range (150-550 °C), with a maximum NO_x conversion of 87% around 350 °C. H_2-TPR revealed that Cu ions were much more easily reducible in NH_4^+/Na/Cu catalyst compared with its counterparts, which was related with copper ions located in more accessible sites of the zeolite framework. Besides, combining FT-IR of NO and EPR techniques, it was possible to detect that copper ions in NH_4^+/Na/Cu catalyst coexist in the form of Cu^{2+} (80%) and Cu^+ (20%) which seems to benefit the NH_3-SCR activity.

V-PP107

Separation and Recycling of $NiFe_2O_4$ Nanocatalyst for CO_2 Decomposition with CH_4 Recovery from Steel Industrial Flyash

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Recently, over 0.2 million tons per year of flyash hazardous wastes are produced from steel industries in Taiwan and they cause potential environment pollution. The flyashes are ultrafine particles with toxic metals that can be leached out, bioaccumulated, and intaked into body having high risk for human beings or environment. In stainless steel/carbon steel manufacturing plants, the $ZnFe_2O_4$ is major components and can be easily separated/purified using magnetic separation method after ball mill process. The $NiFe_2O_4$/$ZnFe_2O_4$/$MnFe_2O_4$ nanocatalysts are used for CO_2 reductive decomposition. The structural characterization of these nanocatalysts and CO_2 decomposition efficiencies of $NiFe_2O_4$/$ZnFe_2O_4$ separated from flyash were studied and compared with as-synthesized ferrites in the present study. The catalysts prepared from hydrothermal method showed better CO_2 decomposition performance compared to the catalysts separated from the steel industries flyash. Moreover, the yields of CH_4 from synthesized catalysts were more than 90% while only 6% for flyash catalyst.

V-PP108

Regeneration of the Hydrogenation Catalysts by Supercritical Fliud Extraction

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The aim of the present work was to explore the possibility of regeneration of spent catalyst from the enterprise of "Nizhnekamskneftekhim" (nickel-on-kieselguhr, palladium catalyst LD- 265) in a supercritical carbon dioxide (SC-CO_2) medium. Regeneration of coked catalysts was carried out at 423 K and pressures 20, 30 MPa by pure and modified supercritical CO_2. Methanol, dimethylsulfoxide, chloroform and acetone were used as modifiers (co-solvents) of supercritical CO_2.
The activity of the nickel-on-kieselguhr catalyst was estimated from the extent of hydrogenation of ethylene to ethane. Evaluation of the activity of samples of aluminum-palladium catalyst was carried out on residual value of diene and bromine numbers in the hydrogenation product.

V-PP109

CO_2 Adsorption Kinetics on Chemically Modified Activated Carbon

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CO_2 adsorption capacities of a commercial activated carbon subjected to different treatments such as HNO_3 oxidation, air oxidation, alkali impregnation and heat treatment under helium gas atmosphere were determined by gravimetric analyses for 298-473 K temperature and 0-20 bar pressure range. Pseudo-first and pseudo-second order kinetic models as well as the intra-particle diffusion model were applied to the experimental kinetic data on the CO_2 adsorbent samples studied for the 1 bar CO_2 pressure. Pseudo-first and pseudo-second order kinetics explain adsorption for the kinetic region for most of the samples. When the whole adsorption data range is considered, the adsorption cannot be explained by any model due to complex nature of the adsorbents, but the adsorption behavior fits rather well to pseudo-first order kinetics at 120°C for the alkali impregnated samples, and at 25°C for non-impregnated samples and the adsorbents subjected to high temperature helium treatment as well.

V-PP110

Epoxidation of Fatty Acid Methyl Esters of Vegetable Oils by Air

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Kinetic laws of oxidation and epoxidation of fatty acid methyl esters of vegetable oils by atmospheric oxygen were explored. Two possible mechanisms of the formation of epoxy compounds, as well as adequate kinetic model were presented.

V-PP111

Perovskite-based Catalysts as Alternative to Commercial Three-Way-Catalysts? – Impact of Cu and Ca Doping and Optimisation of Surface Properties

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Three-way catalysis (TWC) is an expensive technology due to extensive use of precious metals (Platinum group metal PGM). Previously, perovskite-type materials were developed for three-way applications especially to stabilize PGM from thermal sintering. This strategy led to interesting outcomes with lower PGM contents. In this study, low cost Fe-based perovskites being non-toxic and thermally stable were investigated. However, the main drawback lies in the surface reconstruction and a usual lanthanum enrichment which affects their catalytic properties [2]. A better optimisation of the surface proprieties can be obtained through partial substitution of A- and B-site ($LaFe_{1-x}Cu_xO_3$ and $La_{1-x}Ca_xFe_{1-x}Cu_xO_3$). It was also found that none stoichiometric perovskite especially lanthanum-deficient perovskites leads to significant enhancement of the catalytic performances.

V-PP112

Effect of Desilication of HY Zeolite in Pt/HY Catalysts for Polystyrene Hydrocracking

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An important aspect in catalytic hydrocracking of plastic wastes to liquid fuels is related to the accessibility of the polymer molecules to the active sites, polymers size preventing their access to the internal pores of the catalyst. In order to overcome this problem, we have desilicated, to different extents, an HY zeolite and, after preparing the corresponding Pt/HY catalysts, we have studied their performance in catalytic hydrocracking of polystyrene in the kinetic regime. Desilication improves external area, metal dispersion and accessibility to the active sites, thus increasing PS hydrocracking rate and selectivity to products in the diesel range. However, TOF values are higher for the untreated sample, what can be related to the loss of acid strength upon desilication.

V-PP113

Study of Supported Pt/TiO$_2$ Catalysts with Enhanced Activity in CO Oxidation

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The improvement of the catalytic activity of Pt/TiO$_2$ catalyst in low-temperature CO oxidation could be achieved by modification of a small amount of iron. The relationship between Pt/TiO$_2$ and Pt,Fe/TiO$_2$ behaviour depends on the chemical composition and real structure. The introduction of iron additives in Pt/TiO$_2$ catalyst results in the formation of nanocrystaline structure of support. It leads to increase in platinum dispersion and change in the electronic state. For the optimum amount of Fe in the catalyst 1 wt.% Pt, 0.28 wt.% Fe/TiO$_2$ the Pt$^{\delta+}$/Pt^0 ratio arises to maximum value of 1.55. It is due to the changes in the interaction of platinum with support because the iron stabilized in nanocrystalline structure of TiO$_2$. This provide the high catalytic activity Pt,Fe/TiO$_2$ catalysts in low-temperature CO oxidation.

V-PP114

Composite Carbon /Zeolite Adsorbent-catalysts for Organic Containing Wastewater Purification Using Wet Peroxide Oxidation

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The aim of this study was the development of preparation mode of the composite adsorbent-catalysts and the testing of the prepared adsorbent-catalysts in a purification of solutions of model organic substrates. The carbon/zeolites composite absorbent-catalysts were prepared by two preparation modes (mechanical mixing of the zeolite H-ZSM-5 with the mesoporous graphite carbon Sibunit and pyrolysis of carbon compounds supported on the zeolite) and tested in CWPO of phenol and formic acid. The obtained results testify that the combination of carbon and the zeolite can improve the adsorption capacity as well as the catalytic activity in the CWPO of organic substrates. However, the catalytic activity depends on the substrate nature and the mechanism of its interaction with the surface of the solid catalyst.

V-PP115

Effect of SO$_2$ on N$_2$O Decomposition over Ir Catalysts Supported on CeO$_2$-Modified Al$_2$O$_3$

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Nitrous oxide (N$_2$O) has recently attracted great attention, due to its deleterious environmental impact. Catalytic decomposition of N$_2$O to N$_2$ seems to represent the most promising approach in de-N$_2$O, especially with modified noble metal-based catalysts. Other components that typically exist in flue gas are O$_2$, SO$_2$, H$_2$O, etc. Therefore, the objective of this work is to gain insight into the effect of SO$_2$ and/or O$_2$ on the activity of Ir catalysts, supported either on bare alumina (Al$_2$O$_3$) or CeO$_2$-modified alumina (AlCe), during the N$_2$O decomposition. The results revealed that under oxygen excess conditions, CeO$_2$-promoted catalyst achieved N$_2$O conversion value as high as 96.9%. However, the co-presence of O$_2$ and SO$_2$ in the feed stream resulted in a decrease of catalyst's N$_2$O conversion to 39.2%. On the other hand, it is worth mentioning that the performance of Ir/Al$_2$O$_3$ catalyst was notably enhanced upon sulfidation (from 66.4% to 78.2% N$_2$O conversion).

V-PP116

Highly Active Nanocatalysts by Ion Beam Surface Modification

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Ion irradiation is proven to be an effective and innovative method for the controlled surface modification of several solid catalytic materials which microstructure can be tailored to significantly enhance their catalytic activity and durability. The feasibility of this method has been deeply investigated on Ce$_{0.7}$Zr$_{0.3}$O$_2$ and Pt/Ce$_{0.7}$Zr$_{0.3}$O$_2$ catalysts with different techniques (IR operando spctroscopy, HRTEM and XPS). The ion bombardment treatment induces a remarkable change in the nanoparticle morphology such as the formation of atom vacancies and incomplete terraces which lead to a higher oxygen mobility on the catalyst surface. The microstructural modification observed results in a higher reducibility and a significant enhancement in catalytic activity evaluated in representative pollutants combustion measurements.

V-PP117

Effect of Metal Loading in Pt/Hβ Catalysts for PS Hydrocracking

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Catalytic hydrocracking of plastic wastes to liquid fuels can be an alternative in plastic recycling. Bifunctional Pt/Hβ catalysts have been found to be suitable for this process, the presence of the metallic function being necessary to reduce the aromatic content of the product. In this work, the effect of platinum content in the range 0.1 - 1 wt.% has been studied, using polystyrene as a model compound, in the kinetic regime. The catalyst with the lowest Pt content has been found to produce the highest TOF, with little variation in the selectivity to the desired products, what points to it as a good candidate with lower cost. This behavior has been related to the higher accessibility of the big reactant molecule to the active sites in the catalyst.

V-PP118

Insights into the Elementary Kinetics of the Low-temperature NO_x Reduction by H_2 on $Pt/WO_3/ZrO_2$ under Lean Conditions

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This work addresses the elementary kinetic mean field modelling of the NO_x reduction by H_2 on $Pt/WO_3/ZrO_2$ under oxygen-rich conditions. $Pt/WO_3/ZrO_2$ was recently shown to reveal substantial low-temperature $deNO_x$ activity with enhanced N_2 selectivity referred to traditional Pt catalysts. The model was developed based on a postulated reaction mechanism as well as kinetic examinations and implied a network of 48 reaction steps described by Arrhenius-based rate expressions. Kinetic parameters were taken from literature and by fitting calculations, while pre-exponential factors of adsorption were estimated from kinetic gas theory. For validation, experiments were simulated and thermodynamic consistency was proven by checking the Gibbs free enthalpy of the catalytic surface reactions. As a result of the kinetic model, the formation of OH surface species was identified as the rate determining step of H_2 oxidation, while the reduction of NO predominately occurs by dissociation of chemisorbed NO.

V-PP119

$VO_x/TiO_2/ZSM5$ Catalysts Activity for the Simultaneous Abatement of NO_x and PCDDs for MWI Plants

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The simultaneous removal of NO_x and dioxins by the catalytic abatement in the municipal solid waste incineration plants is studied as alternative to current non destructive methods. The addition of TiO_2 to H-ZSM5 is analyzed in order to increase the surface area of commercial $VO_x/WO_3/TiO_2$ catalyst. It has been found that $VO_x/TiO_2/ZSM5$ catalyst is valid for the simultaneous removal of NO and o-DCB. The addition of TiO_2 to H-ZSM5 zeolite improves significantly its catalytic performance by shifting the light-off curves to lower temperatures. More than 14 wt. % of TiO_2 is necessary to avoid the formation of small V_2O_5 crystallites and thus obtain similar catalytic activity to VO_x/TiO_2 catalyst. Furthermore, zeolite based catalyst show higher NO conversion (>90%) in the range of temperature between 200 and 300 ºC due to their high surface acidity, in comparison to the 70% conversion obtained by the VO_x/TiO_2 catalyst.

V-PP120

Selective Oxidation and Hydrogenation of CO over Precious Metal Catalysts for Fuel Cell Applications

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Production of CO free hydrogen for fuel cell applications following the water-gas shift reaction can be obtained by either preferentially oxidizing CO to CO_2 or hydrogenating it to CH_4. Both reactions have to be carefully maintained to avoid usurping the hydrogen in the feed. Therefore the design and method of synthesis for a selective catalyst for these reactions are important. Noble metals are known to adsorb CO very strongly, but desorption of CO is also critical as this is the main concern leading to CO poisoning on the active metal.

Pt supported on two reducible oxides (TiO_2 and ZrO_2) have been synthesized by two different methods and characterized by various physical and chemical techniques. These materials were tested for the various reactions for the final stage hydrogen clean-up. The catalytic activities of these materials were compared, and various chemisorption studies were also conducted to determine the properties leading to the difference in performance of these materials.

V-PP121

Enhanced-SCR Reaction over a Commercial Fe-Zeolite Catalyst: Activity and Mechanism

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Diesel vehicles with reduced fuel consumption result in lower mean exhausts temperatures, thus novel more efficient exhausts aftertreatment technologies are under development. In this context it was shown that the addition of an aqueous solution of NH_4NO_3 (AN) to a NO–NH_3 containing feed results in the "Enhanced SCR" (E-SCR) reaction over a commercial Fe-zeolite catalyst. In order to assess the potential and elucidate the mechanistic implications of AN injection, both steady state and transient E-SCR runs have been carried out in a wide range of temperatures (180-500°C) and GHSVs. The results clearly demonstrate that AN greatly boosts the DeNOx performances, particularly in the low temperature region. The improvement is consistent with the evidence of in-situ generation of NO2 by AN oxidation of NO. On this basis, a simple kinetic model has been successfully fitted to all the experimental data. Furthermore, simulations of EAT systems in standard test cycles (both cold and hot WHTC) confirm significant reduction of NOx emissions due to AN dosing.

V-PP122

Magnetic Carbon Xerogels for the Catalytic Wet Peroxide Oxidation of 4-Nitrophenol Solutions

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Nanostructured hybrid composites containing iron magnetic species and carbon xerogels materials were synthesized and tested as catalysts in the CPWO of highly concentrated 4-nitrophenol solutions ($5\ g\ L^{-1}$). In this way, the synergistic effects that can arise from the combination of the high catalytic activity of iron oxide species with the flexibility for tuning the textural properties of carbon-based materials are explored. In addition, *in-situ* magnetic separation of the catalysts at the end of the process is a further advantage.

4-NP removals up to 77% were obtained in CWPO runs performed during 24 h considering pH = 3, T = 50 ºC, catalyst load = $2.5\ g\ L^{-1}$, and the stoichiometric amount of H_2O_2. In addition, a 4-NP removal of 45% was obtained when the initial pH was not adjusted. Further improvements on the synthesis of magnetic carbon xerogels are now envisaged in order to maximize catalyst activity and stability.

V-PP123

Acceleration of Catalytic Ozonation of Ammonium Ion in Water over Cobalt Oxide Catalyst by Repeated Use

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Oxidative decomposition of ammonium ion (NH_4^+) in water over Co_3O_4 by repeated use was studied. The conversion of NH_4^+ for Co_3O_4 was increased by the repeated use with slight change in the high selectivity to gaseous compounds. Ammonium ion was completely decomposed after the second reuse of Co_3O_4. High concentration of NH_4^+ was applied to investigate how far the catalytic activity of Co_3O_4 was accelerated by repeated use over Co_3O_4. The conversion was increased from 31% for fresh catalyst to 81% for 9 times-reused catalyst. The acceleration effect did not occur for other oxide catalysts. Crystalline structure and degradation of surface area of spent catalyst were not the reason for acceleration. The formation of acid sites by oxidation of Co_3O_4 surface with O_3 may lead to the enhancement of the catalytic activity.

V-PP124

Novel Hybrid Perovskite Catalysts for DeNOx Applications

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In the current work, a novel synthesis strategy has been utilized in order to design novel hybrid perovskite structures that can combine unique functional characteristics of different conventional perovskite structures (i.e. $LaCoO_3$ and $LaMnO_3$) within a single hybrid catalytic architecture (i.e. $LaCo_xMn_{1-x}O_3$). Our results indicate that through this novel approach, NOx/SOx oxidation, adsorption, storage and release properties of hybrid perovskite architectures can be fine-tuned in an attempt to obtain next generation Pt-free DeNOx catalysts not only revealing superior activity but also possessing enhanced stability.

V-PP125

NH_3-SCR and NH_3 Oxidation over V-based Catalysts: Design of "High-Efficiency" NH_3-SCR Reactor for Stationary Applications

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In this work, the kinetics of the $NH_3/NO/O_2$ reacting system over V_2O_5-WO_3/TiO_2 catalysts was studied under conditions of NH_3/NO ratio ≥ 1 and temperature up to 400°C, where some ammonia oxidation is expected. NH_3-SCR and NH_3-oxidation tests were performed over powdered catalysts, at varying V-loads. Experimental data highlighted the occurrence of an unselective NH_3-oxidation route, giving rise to some NO production; a quantitative analysis of data showed that the observed product distribution is fully in line with an indirect-consecutive reaction scheme from NH_3 to N_2, wherein NO is formed by NH_3 oxidation and is then rapidly converted to N_2 via NH_3-SCR. Preliminary evaluations suggest that the impact of NH_3-oxidation on the integral performance of monolith reactors (operating at NH_3/NO ratios close to 1) is non negligible, so that the correct identification of the reaction stoichiometry is crucial.

V-PP126

Synthesis and Properties of Silver-containing Photocatalytic Systems on the Base of Titania

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Photocatalytic processes have become quite actual in the recent time due to the increased interest in energy-saving technologies and effective oxidation of organic pollutants. Titania is considered the most popular material for photocatalysts due to its high stability, relatively cheap price and noticeably higher photoactivity. Besides, the addition of small-sized silver particles to titania surface has been found to improve the photocatalytic properties of samples due to the formation of Schottky barrier, influence on the band gap characteristics and general affinity of silver to oxidation processes. The silver particles dispersed on the surface of both pure titania and titania/silica grafted systems do increase the photocatalytic activity of the samples, and the grafting technique responsible for the preparation of titania/silica systems also seems to increase the photocatalytic activity of the samples in the model reaction. The best photoactivity is shown by 0.5 % Ag / 6% TiO_2 / SiO_2 catalyst.

V-PP127

Epoxidation of Fatty Acid Methyl Esters of Plant Oils with Hydrogen Peroxide

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The reactivity peracetic acid epoxidation of the methyl esters of fatty acids generated ex-situ and in-situ is considered. The advantages of partition processes of obtaining peracid and its use in the epoxidation reaction, as well as simplifying their mathematical description are presented.

V-PP128

Mesoporous Nanomaterials Based on Ceria: Synthesis and Catalytic Application

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The catalysts based on ceria are of interest because they have a large oxygen storage capacity and high mobility of oxygen, which will provide their high catalytic activity. Solid solutions based on ceria ($Gd_xZr_yTi_zCe_{1-x-y-z}O_2$) were obtained. It was shown that these composites are highly efficient catalysts for the oxidation of CO and preferential oxidation of CO.

V-PP129

Catalysts for Selective Hydrogenation of Benzene in the Presence of Other Aromatic Compounds

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Previously, we have developed rhodium catalysts on carriers with high specific surface area, such as sibunite, BAU and CAU. This report presents the results of the development of ruthenium catalysts. Ruthenium has been applied to the activated carbon BAU (birch activated carbon), with a surface area up to 1000 m^2/g. Experiments in the autoclave equipped with a turbine agitator in the isobaric-isothermal conditions in the pressure range 10-100 atm. of hydrogen, temperature 40-120°C. The design allows selecting the samples from the autoclave during the reaction. 3% Ru/ULA is exceptional hydrogenation of benzene and toluene, p-xylene and cumene are not hydrogenated, whereas 1% Ru/ULA toluene hydrogenation occurs at speeds three times lower than that of benzene. Xylene and cumene under these conditions are hardly hydrogenated. The selectivity of the hydrogenation of benzene at 3% Ru/98% BAC. It has been determined the order of the reaction by reacting components and other kinetic parameters. Catalysts are verified by physical methods.

V-PP130

Utilizing Water as the Oxygen Atom Source: Catalytic Formation of Lactams from Amines

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Utilizing water as an inexpensive and "green" reagent and solvent is of high practical importance for developing new environmentally friendly transformations in organic synthesis. We were able to develop a fundamentally new type of lactam formation reaction directly from cyclic amines in water with liberation of hydrogen gas, with water serving as oxygen-atom source in the amide group. This reaction is catalyzed by an acridine-based Ru pincer complex under oxidant-free conditions. We will present mechanistic investigation of this reaction through a combined experimental and DFT study. In particular, we were able to identify a catalytically active species responsible for the observed reactivity. The proposed pathway through the intermediacy of imines and hemiaminals was consistent with experimental findings. Insights into the reaction mechanism from a DFT study will also be discussed.

V-PP131

Effects of La and Ce Promotion on CDRM Performance of Co-Ni/ZrO_2 Catalysts

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The aim of this study was to design and develop effective Co-La bimetallic, and Co-Ni-La and Co-Ni-Ce trimetallic CDRM catalysts supported on ZrO_2. The performance tests consisting of 27 experiments were conducted for the temperature interval of 873-973 K with CH_4/CO_2 feed ratios of 1/1, 2/1, 1/2, and space velocities of 20000 and 60000 mL/h g-catalyst. For all catalysts, Co- and promoter-loadings were fixed at 5wt% and 2wt%, respectively. Ni-loading was changed between 3 and 5wt%. Higher reaction temperatures were found beneficial for increased activity and obtaining H_2/CO product ratio values close to 1. La and Ce were proven to be suitable promoters for enhancing the stability of Co-Ni/ZrO_2 CDRM catalysts. For optimum activity and stability, even small amounts of Ni addition was found sufficient. Co-Ni-Ce trimetallic system was shown to be the most active and stable catalyst at all reaction conditions.

V-PP132

Photocatalytic Oxidation of Diethyl Sulfide Vapor over TiO_2 Deposited on Porous Supports

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Composite TiO_2/activated carbon (TiO_2/AC) and TiO_2/SiO_2 photocatalysts with TiO_2 contents in the 10 to 80 wt. % range were synthesized by the $TiOSO_4$ thermal hydrolysis method. All TiO_2 samples were in the anatase form, with a primary crystallite size of about 11 nm. The photocatalytic activities of samples synthesized were tested in the gas-phase photocatalytic oxidation (PCO) reaction of diethyl sulfide (DES) vapor in a static reactor by the FT-IR in situ method. The influence of the support on the kinetics of DES PCO and on the TiO_2/AC and TiO_2/SiO_2 samples' stability during three long-term DES PCO cycles was investigated. The highest PCO rate was observed for TiO_2/SiO_2 photocatalysts. To evaluate the activity of photocatalysts the turnover frequency values (TOF) were calculated for the same amount of DES mineralized. It was demonstrated that the TOF value for composite TiO_2/SiO_2 photocatalysts was 3.5 times higher than for pure TiO_2.

V-PP133

High Temperature N_2O Decomposition over Massive and Supported Mixed Oxides: Principles of Activity Regulation

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Correlation between activity of massive and supported La(-Sr)-Fe and CeO_2 based mixed oxides in the reaction of high-temperature N_2O decomposition and their capability to supply oxygen from the near subsurface layers to adsorbed species formed after N_2O decomposition on the active surface sites was analyzed. Formation of heterostructured interfaces on the surface of intergrown composites or mixed solutions enriched by oxygen vacancies was shown to promote oxygen exchange in the surface and near subsurface layers thus hastening O_2 desorption.

V-PP134

Development of the Methods for Fast Catalytic Air Purification from CWAs

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In today's world there is a high probability of terrorist attacks and technological disasters. The result is a deadly emission of dangerous organic vapors and aerosols. It is especially dangerous if it happens in the places of the people congestion. In our study, we propose the method of fast air and surfaces decontamination based on the fast adsorption with subsequent degradation of adsorbed CWA by the Fenton system. The butyl-β-chloroethylsulfide (BCES), dimethyl methylphosphonate (DMMP) and O, O-diethyl-O-3,4,5- trichlorophenylphosphate (DETCPP) have been chosen as the conventional imitators of mustard and organophosphorus CWAs. Adsorption experiments were conducted on the following adsorbents: TiO_2, AlOOH, SiO_2, MgO, Fe_2O_3. Purification of the surfaces from the CWA's simulants takes less than 30 minutes with using of the heterogeneous Fenton system on Fe-ZSM-5 zeolite.

V-PP135

Stabilization Effect of Pd–Rh Alloyed Nanoparticles in Three-way Catalysts

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Three-way catalysts are well known systems used for neutralization of gasoline automotive emissions. As a rule they contain palladium and rhodium as active components providing the conversion of pollutants via a number of oxidation and reduction reactions. The catalysts with atomically dispersed or sub-nanometer sized ionic clusters of precious metals have been recently shown to have the highest activity in these reactions. In our previous study, we have observed that alumina donor sites play defining role in stabilization of atomically dispersed forms of supported Pd. The present study is focused on the activity and stability of bimetallic Pd–Rh catalysts obtained from heterometallic complexes and supported on γ-Al_2O_3. The total precious metal loading in the synthesized samples was as low as 0.2 wt. % that complicated the use of the most of conventional physical and chemical methods of characterization.

V-PP136

Synthesis Effect on CH_4 Partial Oxidation over Ni-CeO_2 Catalysts

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Ni-CeO_2 catalysts were prepared by conventional co-precipitation (CP), by wet impregnation (WI), by microwave assisted CP and WI (mw-CP) and (mw-WI) and by hydrothermal (HT) procedures. The effect of the different syntheses on the catalyst structural properties was investigated by XRD, TPR, TGA, TEM and XPS. The catalytic behavior of the catalysts was tested in the methane partial oxidation reaction carried out at 1 atm in a temperature range of 400 °C – 800 °C using He diluted feed gas mixture with $CH_4/O_2 = 2$, WHSV=60000 $mLg^{-1}h^{-1}$. On stream stability tests were also performed. The performance of the Ni-CeO_2 catalysts in terms of activity and on stream stability was in fact affected by the syntheses. Moreover, the deactivation was largely due to the nickel particle sintering likely related to the Ni-support interaction modulated by the synthesis.

V-PP137

Improved Diesel Soot Oxidation Performance of Manganese-substituted Strontium Ferrite

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The pure perovskite phase of $SrFeO_{2.83}$ and $SrFe_{1-x}Mn_xO_{2.83}$ (x = 5, 10) was synthesized through co-precipitation method followed by step-wise calcination at 900 ºC. The catalysts were characterized by using XRD, SEM, TEM, TPD, TPR investigations to study their structure, morphology and redox properties. The soot oxidation activity was evaluated by using a steady state fixed bed evaluation assembly as well as therogravimetry. Both $SrFeO_{2.83}$ and $SrFe_{1-x}Mn_xO_{2.83}$ showed the catalytic activity for the oxidation of soot and Mn-substitution enhances the catalytic activity significantly. The maximum catalytic oxidation temperature of soot decreased for 10 % of Mn-substitution in $SrFeO_{2.83}$ by 125 ºC. Present strontium ferrite type diesel soot oxidation catalysts are of significance considering commonly available abundant precursors of Fe and Mn and their relative environmental safety.

V-PP138

Selective Elecrochemical Reduction of NOx

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Removal of NOx from diesel trucks and cars are of major importance. Traditionally the removal of NOx is done using the selective catalytic reduction (SCR) of NOx. An alternative solution is to use an all solid state electrochemical reactor. The major obstacle of this approach is high power consumption. Here the selectivity is a problem. One way to solve the selectivity problem is to add a NOx storage compound, in the form of potassium or barium nitrate. This can be done in two ways; either by adding the nitrates in a separate layer on the top of the electrode or by getting the nitrates into the structure, by wet infiltration. It has been shown that a ceramic cell can be used to remove NOx from gasses containing oxygen. Current efficiencies of up to 6.4% have been obtained. Removal of NOx at temperatures down to 300 °C has been shown possible.

V-PP139

Hydrogenation of 2,4,6-trinitrobenzoic Acid on Pd/Sibunit Catalysts

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The catalytic hydrogenation of trinitroaromatic compounds is of practical importance for utilization of explosives and synthesis of various commercial products. The study examined the effect of 2,4,6-trinitrobenzoic acid (TNBA) hydrogenation parameters (temperature, pressure, concentration of reactant, and nature of solvent) as well as conditions of the catalyst synthesis and pretreatment on the process rate and selectivity. The mesoporous carbon material Sibunit was chosen as a support for the palladium catalysts. The catalyst having the highest dispersion of palladium particles showed the maximum activity in the target reaction of TNBA hydrogenation to 2,4,6-triaminobenzene (TAB) (with a selectivity above 90%) under the specified conditions (a temperature of 50 °C, a pressure of 0.5 MPa, 170 g TNBA / 1 g Pd ratio). The NMR analysis of the products was used to suggest a scheme of the transformations occurring in the presence of Pd/C catalysts.

V-PP140

Biocatalytic Generation of Oil-Displacing Systems in Low-Temperature Reservoirs of Viscosity Oil

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The enzymatic hydrolysis of carbamide contained in an oil-displacing composition by the action of plant urease has been studied. Optimal ratios of carbamide to natural urease-containing sources have been determined for the intense hydrolysis accompanied by the release of CO_2, which reduces the viscosity of crude oil, and ammonia, which forms an alkaline buffer system, thereby increasing the detergent properties of the composition. The effect of hydrolysis products on the rheological characteristics of heavy crude from the Usinskoye oil-field has been examined. The recovery of viscous crude oil from a model reservoir using the oil-displacing composition and urease has been investigated.

V-PP141

The Rehydration of Centrifugal Thermal Activation Products of Gibbsite – the Industrial Waste of Catalyst KDM

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Consistent patterns of rehydration a small fraction from carrier of the waste - the products of centrifugal thermal activation (CTA) from gibbsite in production of microspherical chromium oxide/alumina catalyst KDM for fluidized-bed isobutane dehydrogenation was researched. The degree of rehydration of the CTA product in bayerite or pseudoboehmite depends in many ways on the method of production and physical and chemical properties of the starting gibbsite.

V-PP142

Iron –Containing Catalysts from By-Products of Underground Water Ozonation

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In this research, we present the ecologically safe way of processing of ferriferous slimes, produced as by-products of underground water ozonation, as raw materials in the synthesis of the catalysts suitable for destruction of residual amounts of ozone in dry air-gas streams. it is proved that this technology is in good agreement with the principles of green chemistry. For this purpose wet wastes were mixed with cement- talume binder, granulated, subjected to hydrothermal treatment at 90°C, and calcinated at 400°C. Mechanical properties and catalytic efficiency in ozone decomposition of the optimized catalyst comprising 60 wt.% of the ferriferous raw material and 35 wt.% of cement talume binder are comparable with those of industrial catalyst Goptalum GTT.

V-PP143

Sol-Gel Synthesis of Robust Silica Monoliths by Interfacial Solution/Precipitation Reactions: Application in the Preferential Oxidation of Carbon Monoxide

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In this study, we report a new synthetic route to completely avoid the silica shrinkage during the formation of the structure, by incorporating a mesoporous silica thin film over the inner walls of the capillary prior to the SiO_2 filling synthesis. These novel materials have been loaded with Pt nanoparticles and tested as microreactors in PrOxCO reaction.

A novel methodology has been developed to anchor silica monoliths inside capillary tubes, depositing a mesoporous silica thin-film prior to the synthesis of the monolith. This technique has been successfully used to prepare Pt-loaded microreactors with a very good performance in the PrOxCO reaction.

V-PP144

Photocatalytic Removal of NO under Visible Light Irradiation over Sol-Gel Synthesized $PbTiO_3$ Nanoparticles

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$PbTiO_3$ perovskite type oxide nanoparticles was prepared by sol-gel method. XRD indicated pure crystalline structure of the perovskite. The band gap of the synthesized material was measured by UV-Vis DRS as 2.7 eV indicating visible light absorption capacity of $PbTiO_3$. ISO-22197:2007(E) method was used to determine the photocatalytic activity of the sample for NO oxidation under ambient visible light for the first time. The $PbTiO_3$ exhibited very high and sustainable activity towards NO oxidation under visible light irradiation. The catalyst is sensitive to humidity: decreasing of photocatalytic activity is investigated by changing of color and the bandgap is increased close to pure TiO_2. The crystal structure, band gap energy changing and oxidation state changing of the catalyst is monitored by XRD, UV-DRS and TPR.

V-PP146

Coherent Synchronized Monooxidation of Ethylene by Hydrogen Peroxide on a Biomimetic Catalyst

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Heterogeneous biomimetic catalysts synthesized on the basis of iron porphyrin complexes been the analogs of a ferment of cytochrome P-450, carry out efficiently the processes of gas-phase monooxidation, epoxidation and hydrooxilation of hydrocarbons. Biomimetic catalyst- iron(III) perfluorotetraphenylporphyrin, drawn on aluminium oxide (per-FTPhPFe(III)/Al_2O_3) displayed high activity and selectivity in the processes of oxidizing a great series of hydrocarbons. Using of immobilized biomimetic catalyst, per-FTPhPFe(III)/Al_2O_3 and ecologically pure hydrogen peroxide as oxidizer ("green oxidizer") the high selective process of ethylene oxidation was realized.

V-PP147

Hydrogen Production from Olive Mill Wastewater through Steam Reforming. Catalyst Development

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In this work ceramic monoliths were functionalized with different lanthanum-stabilized ceria supports and impregnated with Pt (0,5-2% w/w based on catalytic support weight). These monolithic catalysts were tested under steam reforming of Olive Mill Wastewater (OMW), acetic acid, and 2-phenylethanol. This process provides a reduction of organic content in OMW, and thus, a reduction of the environmental contamination, while producing a valuable product. Catalytic performance was evaluated by means of chromatographic analyses of effluent dry gas and post-reaction condensate liquid. Total Organic Carbon (TOC) and Chemical Oxygen Demand (COD) of reactants and post-reaction condensate were also used to evaluate the reaction extension.

Characterization of supports was conducted by means of X-Ray photoelectron spectroscopy (XPS) analyses, X-Ray diffraction (XRD), Temperature Programmed Reduction (TPR), and Temperature Programmed Desorption of NH_3 (TPD-NH_3). Characterization results have been related to the catalytic behavior.

V-PP148

Bulk Mixed Al-transition Metal Oxide Catalysts for Enhanced Oxidation of 1,2-dichloroethane

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Mesoporous powders of composites of γ-alumina containing different transition metal ions with relatively high surface areas and large pore volumes were prepared. Besides different other preparative conditions, the gel formation and the textural properties of the calcined powders were dependent on the type of metal ion dopant and its concentration. The type of precursor also played a role in the textural properties of the final product. The presence of transition metal ions resulted also in noticeable enhancement of the surface acidic and redox properties. Cu- and Cr-doped catalysts showed enhanced capability for the oxidation of 1,2-dichloroethane resulting. On the contrary, V(III)-containing catalysts showed a considerably lower catalytic activity. While vinyl chloride was the major Cl-containing hydrocarbon product from reactions over Al-V-3 and Al-Cr-3, it formed only in negligible amounts over Al-Cu-3 catalyst where the deep oxidation product, CO_2, was the major product.

V-PP149

Green Alternative for Guideline Monoterpenoids to Value-added Products – Tailored the Biocatalytic Transformation of α-pinene

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Green transformation of α-pinene mediated by lipase designed as heterogeneous catalyst was study in this work. The general goal of the study was to concentrate the conversion of the substrate into only one reaction product, knowing that α-pinene oxidation is famous for how many reaction products are usually obtained.

The experimental data point out that the enzyme immobilization approach (e.g. adsorption, entrapment, covalent attachment and cross-linking) affected substantial the catalytic capacity of the system to convert α-pinene to oxidized derivatives. Indeed, enzyme immobilization using the entrapment approach allowed to improve the α-pinene conversion and moreover to concentrate the selectivity of the biocatalytic process onto verbenol production. The other biocatalyst configurations behaved similar between them in term of selectivity leading to α-pinene oxide as dominant product next to verbenol, camphene, campholenal in varied proportions.

XI European Workshop on Innovation in Selective Oxidation (ISO ‘15) "Selectivity in Oxidation: Key to new resources valorization"

Keynote Lectures

ISO-KN1

Liquid-Phase Selective Oxidation Catalysis with Metal-Organic Frameworks

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Metal-organic frameworks (MOFs) possess crystalline open structures, extremely high surface areas, tunable pore size and functionality, as well as high content of uniform metal sites. In the past decade, a large scientific effort has been directed to evaluation of their potential as heterogeneous catalysts for organic synthesis. Here, we give an overview of catalytic applications of MOFs of the MIL family in environmentally benign liquid-phase selective oxidations. The impact of the transition metal nature on the reaction selectivity and mechanistic features of the oxidation catalysis by MOFs are addressed. Peculiarities of adsorption of organic compounds on MOFs and their consequences for catalysis are discussed. Special attention is paid to the nature of catalysis and catalysts stability and reusability. A comparison of MOFs with conventional single-site catalysts (zeolites, aluminophosphates and mesoporous silicates) is provided, and the scope and limitations of the MOF catalysts are discussed.

ISO-KN2

Microstructured Reactors as Efficient Tool for the Operation of Selective Oxidation Reactions

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Selective oxidation reactions are re-considered currently to improve the efficiency and ultimately the sustainability of the processes under operation. The performance of the catalysts applied for these reactions highly depends on the operating conditions which are in turn determined by the reactor technology.

The exothermic character of selective oxidation reactions creates a challenging task for the heat management of the chemical reactor hosting them. Microchannel plate heat-exchanger technology offers unique opportunities of integrated heat removal by the introduction of energy consuming processes into the reactor, such as endothermic reactions or, closer to conventional solutions, evaporation of liquids. The plate heat-exchanger reactor, which is coated with thin layers of catalyst allows improved heat and mass transfer in the catalyst and therefore avoids hot-spot formation and related problems. The current contribution provides an overview of the research activities in the field of selective, partial and preferential oxidation reactions in mocroreactors.

Oral Presentations

ISO-OP01

V-, Nb-, and Ti-promoted Hexagonal Tungsten Bronzes as Selective Catalysts in the Transformation of Glycerol and Methanol in Aerobic Conditions

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In this paper we present the synthesis, characterization and catalytic performance for the aerobic conversion of glycerol and methanol of Nb-, Ti- and V- promoted tungsten oxide with hexagonal tungsten bronze (HTB) structures. They have been prepared hydrothermally at 175ºC and heat-treated in N2 atmosphere in the 400-600ºC temperature range. They have been also studied as catalyst in the selective aerobic transformation of glycerol and methanol.

ISO-OP02

Metal-free Heterogeneous Catalysts for the Epoxidation of Alkenes with H_2O_2

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The epoxidation of alkenes with H_2O_2 is an industrially relevant route to produce epoxides, which are valuable and versatile compounds. Many heterogeneous catalysts in which the active site is a metal centre have been developed for this reaction (*e.g.* TS-1, Ti-MCM-41, Ga_2O_3). Here, we show for the first time that epoxidation reactions can be catalysed also by metal-free heterogeneous catalysts obtained by straightforward functionalisation of carbon materials. The active sites are phenol and carboxylic acid groups, which can be generated by acid treatment of activated carbon, as demonstrated by TPD analysis. The most active catalyst among a series of functionalised activated carbons could achieve high epoxide yields. The selectivity varied according to the type of alkene employed: complete selectivity towards the epoxide was observed with cyclooctene, whereas both epoxide and diol products were obtained from limonene. The catalysts are truly heterogeneous (no leaching) and they retain their activity upon recycling.

ISO-OP03

Tuning the Selectivity in Pd Catalyzed Liquid-phase Oxidation of Benzyl Alcohol: an in situ ATR-IR Study

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In order to clarify the role of the metal and the support in determining the selectivity of the benzyl alcohol oxidation, Au, Pd and AuPd catalysts were prepared by immobilizing polyvinyl alcohol (PVA) protected metal nanoparticles on different supports (TiO_2, NiO, Al_2O_3). Catalytic tests have been followed from both point of views, the substrate (by measuring product evolution), and the support (by using using *operando* attenuated total reflection infrared (ATR-IR) spectroscopy). The *operando* ATR-IR spectroscopy evidenced that the addition of Au to Pd drastically limited irreversible adsorption thus decreasing the deactivation and partially modifying the selectivity of the reaction. Not only the metal participates in determining this beneficial effect but also the support and the protective agent used for generating the metal nanoparticles can be used to tune the reaction pathway.

ISO-OP04

Ethanol Selective Oxidation into Syngas over Pt-promoted Fluorite-like Oxide: SSITKA and Pulse Microcalorimetry Study

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Catalysts based on oxides with a high lattice oxygen mobility and reactivity are known to be able to efficiently transform ethanol into syngas by selective oxidation. Mechanism of this reaction over Pt/ $Pr_{0.15}Sm_{0.15}Ce_{0.35}Zr_{0.35}O_2$ catalyst was studied by using SSITKA and pulse microcalorimetry. The rate–determining step is C-C bond rupture in ethanol/acetaldehyde molecules, while C-H bond breaking in the ethanol dehydrogenation step proceeds easily. The mechanism is described by step-wise red–ox scheme including ethanol oxidative decomposition on Pt sites with participation of bridging oxygen species (with the heat of adsorption ~ 550 kJ/mol O_2) located at Pt-oxide interface followed by fast reoxidation of reduced support sites by O_2. Rapid oxygen migration from oxide sites to Pt provides conjugation between these steps, thus suppressing coking.

ISO-OP05

Selectivity Control in Oxidation of 1-tetradecanol on Supported Nano Au Catalysts

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Selective oxidation of tetradecanol, a representative higher fatty alcohol, has received little attention despite the great industrial interest of its products, myristaldehyde (tetradecanal) and myristyl myristate (tetradecyl tetradecanoate). We investigate here the effect of operation conditions (temperature, run time and alcohol/metal (A/M) ratio) on the catalytic performance of Au/CeO_2-Al_2O_3 catalyst to assess the factors that control selectivity. The results confirm the previous hypothesis that the acid formation only starts when the produced water saturates the hydrophilic surface of the support and becomes available as reactant. This makes A/M a critical factor to control selectivity to aldehyde and acid. Nevertheless, by proper selection of operation parameters, high yields to either aldehyde or acid can be reached with high selectivity. Selectivity to the ester is less sensible to operation parameters.

ISO-OP06

Promoted Au and Ag Catalysts for Liquid Phase Selective Oxidation of Octanol

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Selective oxidation (SO) of fatty alcohols (C8+) is commercially attractive as a source of fine chemicals. One of them, octanol, is often used as alkanol model molecule for comparative studies of alcohols reactivity on Au nanoparticles catalysts. Replacing Au for Ag for its SO is interesting due the metals' price difference, but few works report it on Ag catalysts in vapor phase. We compare here the catalytic performance of TiO_2-supported Au and Ag for the title reaction, investigating the effect of support modification and of catalyst reducing and oxidizing pretreatments. Ag catalysts are less active than Au ones, but more selective to octanal. Reducing preteatment boosts Au catalysts activity but not that of Ag. Partly charged metal clusters $Au_n^{\delta+}$ and $Ag_n^{\delta+}$ are probable active sites. Ag catalysts activity may be boosted by the appropriate support modification, making them a promising alternative system for *n*-octanol oxidation.

ISO-OP07

Selective Epoxidation of Propylene to Propylene Oxide on Gold-based Catalysts: a Theoretical Study

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Propylene oxide (PO) is an important bulk chemical used for synthesis of many added value products. Currently there is a surge of interest in finding a simple and "green" process for PO production. Promising results in terms of activity and selectivity have been achieved for propylene oxidation on supported gold catalysts with a mixture of O_2 and H_2 or with molecular O_2 alone as an oxidant. In this work a detailed transformation network of competitive reaction pathways following the initial steps of oxidation has been studied theoretically using density functional theory. The results of calculations question some of the earlier assumptions regarding the mechanism of PO formation. Peroxo species (HOO) formed *in situ* are shown to be responsible for the high selectivity of propylene epoxidation with O_2 on gold-based catalysts using hydrogen or water as co-reactants.

ISO-OP08

Oxidant-free Formal Oxidation of Alcohol Substrates towards Higher Value Added Products

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Previous work on the transformation of alcohols to carboxylic acid salts without the use of an oxidant with water as the only reagent and selective deuteration of alcohols in the α carbon position will be discussed. In addition, current work focused on intercepting the putative intermediate aldehyde with a view to creating value added products, will also be discussed.

ISO-OP09

Metal-Support Interaction – A Key Reason for Ag Catalyst Activity in Low-Temperature Oxidation

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The metal-support interaction in supported catalysts is very important for understanding of both nature of catalytic action and mechanisms of oxidative reactions. The aim of the present work is to reveal the role of ultrasmall silver particles – oxide support interaction in low-temperature oxidation. The Ag-"inert" support (Ag/SiO_2 catalysts) and Ag-"active" support (Ag/CeO_2 catalysts) interfaces were studied in details. It was shown that weak interaction of ultrasmall silver particles with both "inert" (silica) and "active" (ceria) supports is a compulsory condition for high activity in low-temperature CO oxidation. In $Ag/CeO_2/SiO_2$ catalysts the oxidation of CO even at temperatures below 0 °C takes place only in the presence of $Ag\text{-}SiO_2$ interaction, while the enhanced $Ag\text{-}CeO_2$ interface is a reason for elevated activity in deep oxidation of formaldehyde and dehydrogenation of ethanol to acetaldehyde.

ISO-OP10

Study of a New Process for the Synthesis of Adipic Acid: the Oxidative Cleavage of trans-1,2-cyclohexanediol

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We report about a study of the second step of a more sustainable and economically affordable two-step process for Adipic Acid (AA) synthesis from cyclohexene: the oxidative cleavage of 1,2-cyclohexanediol with oxygen. Different catalysts were used: homogeneous $H_5PMo_{10}V_2O_{40}$ was very selective, because there were no side reactions occurring under the acid pH at which the catalyst is active. However, an additional step of hydrolysis was necessary to obtain the pure product, and the separation of the catalyst was quite troublesome. $Ru(OH)_3/Al_2O_3$ catalyst was active under strongly basic conditions, but the reaction showed poor selectivity; the intermediate compound of the reaction was 1,2-cyclohexanedione. Catalysts based on supported Au nanoparticles were more selective because the oxidation of 1,2-cyclohexanediol took place in less basic conditions than for the Ru-based catalyst, and gave rise to the formation of 2-hydroxycyclohexanone as the key intermediate compound; the latter was rapidly oxidized into AA with good selectivity.

ISO-OP11

Influence of the Ionic Liquid Presence on the Selective Oxidation of Glucose over Molybdenum Based Catalysts

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The use of biomass as carbon source to obtain valuable compounds, known as platform chemicals, is of great importance and it is current topic of interest in Chemistry. Within the glucose platform chemicals, D-gluconic acid is an important intermediate, widely used in pharmaceutical and food industries, which can be obtained by selective oxidation of glucose. In the last years, ionic liquids (ILs) have shown a great potential in carbohydrate chemistry, as solvents or catalyst. Although many studies have reported the conversion of glucose into valuable compounds in ILs, the use of the IL as an integral part of the catalyst is scarcely studied. In this way, the main goal of this work is to study the influence of the IL on the catalytic performance of Mo based catalysts, when is used as a part of the catalyst or as solvent, in the selective liquid-phase oxidation of glucose by H_2O_2 under mild conditions.

ISO-OP12

Morphology-dependent Nanocatalysts: Rod-shaped Metal Oxides

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Nanocatalysis is characterized with the unique and nanoscale properties that originate from the highly reduced dimension of the catalyst particle. Extensive studies in the past decades have readily demonstrated the size effect of catalyst particles whereas the shape effect is less studied. We found the particle morphology has profound impact on the catalytic performance as well. The redox and acidic-basic properties of rod-shaped metal oxides such as Co_3O_4, Fe_2O_3, CeO_2, TiO_2 and La_2O_3 were examined in terms of the dominantly exposed crystal facets. The catalytic activities of these rod-shaped oxides are correlated with the atomic configurations on the crystal planes. Moreover, the exposed planes of these rod-shaped oxides mediated the manner and strength of metal-support interaction in the integrated metal-oxide catalysts like Au/CeO_2 and Cu/La_2O_3.

ISO-OP13

On the Mechanisms of Selective Bioinspired Oxidations Catalyzed by Aminopyridine Manganese Complexes

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Insights into the mechanisms of (1) selective epoxidations and (2) C-H oxidations mediated by aminopyridine manganese complexes have been achieved on the basis of kinetic (Hammett plot analysis, *KIE* measuments) and isotopic (^{18}O) labelling studies. For the first time, the incorporation of labelled oxygen into the products of oxidation catalyzed by aminopyridine manganese complexes in the presence of $H_2{}^{18}O$ was observed. The data obtained bear evidence in favour of the key role of Mn^V-oxo species, the most likely catalytically active sites of both processes.

ISO-OP14

Catalytic Upgrading of Furfural by Oxidative Methylation over Au NPs-based Catalysts

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Methyl 2-furoate (2-MF), a compound that may widely be used in the industrial field of flavourings and fragrances, was synthesized by oxidative esterification of furfural with methanol by using Au-based catalysts. In the aim of enhancing selectivity to 2-MF, we prepared CeO_2 and ZrO_2 supports by chemical precipitation method and subsequently deposited size-controlled Au nanoparticles onto their surface. Particularly, we investigated two different Au deposition techniques: i) deposition-precipitation and ii) photo-deposition. The main purpose was to optimize the methodology of synthesis identifying a method capable to modulate size and dispersion of the Au nanoparticles, which represent the actual active phase controlling the catalytic performances. Results showed that Au/ZrO_2 catalyst (with Au deposited by deposition-precipitation) was the best catalyst tested in terms of high conversion and 2-MF selectivity, due to the small size of Au particles (<5 nm), opening new perspectives in the selective oxidative production of fine chemicals.

ISO-OP15

Selective Oxidation of 5-HMF to 2,3-diformylfuran on Intercalated VPO Catalysts

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The selective oxidation of *5*-hydroxymethylfurfural to *2,5*-diformylfuran was successfully achieved using intercalated vanadium phosphate oxides (VPOs) as heterogeneous catalysts in the liquid phase under mild conditions (1 atm of oxygen, 110 °C). The maximum yield was 83% over $C_{14}VOPO_4$ and $C_{14}VOHPO_4$ after 6 h of reaction. While the desired oxidation reaction indeed proceeded over the catalyst, the formation of by-products was linked to the presence and reactivity of free radicals in solution.

ISO-OP16

Oxidation of 5-Hydroxymethyl Furfural to 2,5-diformylfuran in Aqueous Media over Heterogeneous Manganese Based Materials

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2,5-Diformylfuran (DFF) is one of the oxidation products of HMF which has multiple application (fluorescent materials, precursor for drugs, antifungal agents or ligands). Oxidation of HMF can conduct to various other products, thus the selectivity to DFF remains an issue to be overcome in mild conditions. Herein, we report manganese-copper material able to perform oxidation of HMF to DFF under mild aqueous conditions. The effect of amount of catalyst, pressure of oxygen, reaction temperature and reaction time were studied in the synthesis of DFF starting from HMF. Higher amount of catalysts and oxygen pressure resulted in higher conversion and selectivity to DFF, while increasing the reaction temperature over 90 °C and of reaction time resulted in a decrease of selectivity in DFF. In conclusion, manganese-copper material is highly effective heterogeneous catalysts for the selective oxidation of HMF to DFF (87%) in the presence of molecular oxygen in water.

ISO-OP17

Key Parameters Controlling Selectivity and Conversion in OCM: from Experiments and Modelling, towards an Optimised Reactor Design

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The present work focuses on the engineering descriptor Volume-to-Surface (V/S) ratio required for designing an Oxidative coupling of Methane (OCM) reactor. This parameter is analysed against catalytic performance (activity, C_2 selectivity and ethylene-to-ethane ratio) for two Sr-La/CaO and Mn/Na/WSiO_2 OCM catalysts. In parallel, changes of that parameter are calculated from a micro-kinetic model and the convergence between experiments and calculations is analysed. From this analysis, guide-lines are proposed for further reactor design.

ISO-OP18

Oxygen Availability and Catalytic Performance of NaWMn/SiO_2 Mixed Oxide and Its Components in Oxidative Coupling of Methane

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Structural features and catalytic performance in oxidative coupling of methane (OCM) of mixed NaWMn/SiO_2 oxide are studied. Differential scanning calorimetry and thermogravimetry are employed to characterize the properties of reactive lattice oxygen. The results indicate that the alkali component (Na) is required for the formation of appropriate crystalline phase (mainly α-cristobalite) in which W and Mn interact in an optimal way to form the structures containing exchangable oxygen that is responsible for light alkane activation in the conditions of steady-state OCM reaction. Almost total reversible reduction of transition metals (W and Mn) accompanied with the formation of gaseous products typical for OCM (C_2-hydrocarbons, carbon oxides) may occur if this system interacts with methane in the absence of gaseous oxygen.

ISO-OP19

Alkaline-earth Promoted $SrTiO_3$ and Sr_2TiO_4 in Oxidative Methane Coupling: Role of Microstructure and Surface Composition on Activity, Kinetics and Oxygen Exchange

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The aim of this work was to take a close look in catalytic performance of alkaline-earth promoted strontium titanates, being the active catalysts of oxidative methane coupling reaction (OCM), and to find the correspondence between the microstructure, catalytic activity, kinetics of OCM and oxygen exchange properties. We have found that under OCM conditions surface composition and microstructure of alkaline-earth promoted $SrTi_{0.9}A_{0.1}O_3$ and $Sr_2Ti_{0.9}A_{0.1}O_4$ (A = Mg, Ca, Ba) may undergone a change revealing (Sr,A)O mixed oxide on the surface of the particles, which strongly increases both catalytic properties of titanates and the rate of the oxygen exchange between surface and bulk. Detailed kinetic analysis, together with electron microscopy, XPS, XRD and IR methods, allowed us to establish the quantitative relationships between the rate of methane conversion, selectivity, oxygen exchange characteristics and surface concentration of (Sr,A)O mixed oxide.

ISO-OP20

Redox Treatment of Orthorhombic $Mo_{29}V_{11}O_{112}$ and Relationships between the Crystal Structure, Microporosity and Catalytic Performance for the Selective Oxidation of Ethane

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Redox treatments of an orthorhombic $Mo_{29}V_{11}O_{112}$ catalyst (MoVO) were conducted and their crystal structure, microporosity, and catalytic activity were investigated. TPR and TG revealed that MoVO evolved two kinds of lattice oxygen (α-oxygen and β-oxygen) from the structure by reduction treatment. In the early stage of the reduction, the α-oxygen was evolved from the structure, which caused an expansion of the micropore channel. For the further reduction, the atoms in the pentagonal $[Mo_6O_{21}]^{6-}$ unit moved toward the micropore channel, resulting in the decrease in the micropore size. The expansion of the micropore drastically increased a catalytic activity for the selective oxidation of ethane, however, the activity dropped by the decrease in the micropore channel size. Strong relationships between the crystal structure, the microporosity, and the catalytic activity for the selective oxidation of ethane were found.

ISO-OP21

The Selective Oxidation of Polysaccharides to Formic Acid at the Presence of P-Mo-V Heteropoly Acid Catalysts. The Mechanism of Reaction

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The kinetics of one-pot oxidative hydrolysis of cellulose, arabino-galactan and xylan were studied in the presence P-Mo-V heteropoly acids as catalysts. The main reaction products fro all substrates appeared to be formic acid and formaldehyde. The observed results allowed us to suppose that one-pot oxidative-hydrolysis in the presence of P-Mo-V heteropoly acids proceeded by a mechanism similar to the periodate oxidation. Vanadium species can connect to hydroxide groups of sugars and broke C-C bond to give formic acid and shorted sugar. Finally such oxidation of C6-aldose leads to formation of 5 molecules of formic acid a 1 formaldehyde molecule. Moreover connection of vanadium to polysaccharides molecules facilitating hydrolysis is also possible.

ISO-OP22

Study of M-doped NiO (M = Li, Mg, Al, Ga, Ti, Nb) Catalysts by in situ Electrical Conductivity Measurements in Correlation with their Catalytic Performances in Ethane Oxydehydrogenation

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Electronic and redox properties of doped NiO, catalysts for ethane oxydehydrogenation, were investigated by *in situ* electrical conductivity measurements. Thus, electrical conductivity of two series of doped NiO, i.e. M-NiO (M = Li, Mg, Al, Ga, Ti, Nb) and Nb(x)NiO (x = Nb at. %), was studied as a function of temperature and oxygen partial pressure and temporal responses during sequential exposures to air, ethane – air mixture (reaction mixture) and pure ethane in conditions similar to those of catalysis were analyzed. Comparisons between the different catalysts and correlations between their redox and semiconductive properties and their catalytic performance in ethane oxydehydrogenation have been established. These correlations highlighted the role of non-stoichiometric oxygen species for ethane oxydehydrogenation over doped NiO based catalysts and provide a clear and direct evidence for a heterogeneous redox mechanism involving surface lattice O^- species.

ISO-OP23

In-situ XPS and XAS Studies of a New Phenomenon of Kinetic Hysteresis in Selective Methane Oxidation over Platinum

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Recently, we discovered a new phenomenon of kinetic hysteresis in selective methane oxidation over platinum catalysts. To establish the causes of this phenomenon, we studied changes in the oxidation state of active component in real $Pt/\gamma\text{-}Al_2O_3$ catalysts by *in-situ* X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS). *In-situ* XPS experiments revealed the presence of kinetic hysteresis even at low pressures (~ 0.01 mbar). Analysis of the *in-situ* XPS spectra showed that the catalyst activation was associated with partial reduction of the supported platinum. The XAS data also implied that the activation was accompanied by predominant formation of the metallic platinum, while oxidation of the platinum surface led to deactivation.

ISO-OP24

Quasicatalytic and Catalytic Oxidation of Methane to Methanol by Nitrous Oxide over FeZSM-5 Zeolite

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Methane oxidation by N_2O at 200°C and below was shown to proceed in a quasicatalytic mode resulting in product accumulation on FeZSM-5 surface. Methanol that formed via methane oxidation by α-oxygen, $CH_4 + (Fe^{III}\text{-}O^{\bullet-})_\alpha$, migrated from α-sites, initiating new reaction cycles. At 200°C, a 4-h run provided turnover number close to 7. Methanol and dimethyl ether (DME) were the products extracted from the surface.

At above 200°C, the reaction moved to conventional catalytic mode with product desorption into gas phase. Water strongly increased methanol selectivity, which attained 62% at 275°C (accounting coke). Contrary to expectations, DME was not detected among the gas-phase products being converted to coke.

Comparison of quasicatalytic and catalytic data can provide new information on the reaction mechanism including a possibility of identifying potential intermediates invisible under catalytic conditions. Mechanistic scheme presenting main steps of both reaction modes was suggested.

Poster Presentations

ISO-PP01

Trinuclear Copper Oxo-clusters in ZSM-5 Zeolite for Selective Methane Oxidation to Methanol

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A periodic DFT study complemented by *ab initio* thermodynamic analysis was performed to predict the structure of the active sites for selective oxidation of methane to methanol in Cu/ZSM-5 and investigate the associated reaction mechanism. It is shown that in addition to binuclear $[Cu(\mu\text{-}O)Cu]^{2+}$ species, trinuclear hydroxylated $[Cu_3(\mu\text{-}OH)_2(\mu\text{-}O)]^{2+}$ and oxygenated $[Cu_3(\mu\text{-}O)_3]^{2+}$ clusters can be stabilized in the zeolite micropores. The latter represents the most stable extra-framework Cu species in Cu/ZSM-5 catalysts activated in O_2-rich atmosphere. Methane activation by the binuclear sites is limited to a stoichiometric reaction yielding a number of strongly bound methoxy species in the zeolite micropores. In contrast, the newly proposed trinuclear clusters favor the transformation of CH_4 towards methanol coordinated to the partially reduced Cu complexes. These theoretical insights are supported by complementary experimental studies.

ISO-PP02

Remarkable Enhancement of O_2 Activation on YSZ Surface in a Dual-Bed for Catalytic Partial Oxidation of CH_4

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Methane conversion to synthesis gas is a promising way to yield more easily transportable liquid fuels or chemicals. In this study, it was demonstrated by oxygen isotope exchange that a remarkable oxygen activation and mobility is possible on YSZ at moderate temperature (698 K) when $LaMnO_3$ perovskite is placed upstream in a dual catalyst bed. This quicker activation step is proposed to be linked to the generation of an active singlet oxygen species on $LaMnO_3$ bed. This phenomenon is shown to improve the catalytic activity of the $LaMnO_3$-Pd/YSZ system for the partial oxidation of methane.

ISO-PP03

A Qualitative Kinetic Analysis of Steady-State Selective Oxidation Process: Role of Water and Oxygen

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Acrylic acid is a valuable large-scale product in the chemical industry. The currently applied two-step process starts with propene as reactant, forming acrolein as major intermediate, which is then further oxidised. A one-step process, starting from propane, has been the subject of intensive research for more than two decades, however not yet transferred into production.

A steady-state approach was chosen to investigate in detail the role of water and oxygen, and its representation in the reaction network for the selective oxidation of propane to acrylic acid. Several two-route mechanisms were considered. A qualitative description of the experimentally determined kinetic trends for the consumption rates of propane and oxygen was achieved by applying a two-route mechanism containing two independent active sites. Water activates as a buffer the first catalytic centre for propane consumption. Oxygen was a participant and a ‘poison’ in selective oxidation (on the second catalytic centre).

ISO-PP04

Nanomaterial Based Catalysts for Low-temperature Oxidation of Carbon Monoxide

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In the present work we have studied CO catalysts containing platinum and palladium nanoclusters on the TiN, TiC ,TiC_xN_y and TiO_2 particles. TiN, TiC and TiC_xN_y particles of 10 60 nm size prepared by us by plasma chemical method and industrial titanium dioxide crystallites of 5-9 nm size were used as supports. Catalytic oxidation of CO was studied at room temperature at low concentration (less than 200 ppm) characteristic of homes and offices.

ISO-PP05

Gold Supported on Fe-doped Ceria Supports Prepared through the Microemulsion Method for the PROX Reaction

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The present work proposes the synthesis of gold catalysts using Fe-doped ceria mixed oxides (previously synthesized by the microemulsion method) for the PROX reaction. In these catalysts, the abilities of gold for adsorbing and to dissociate CO are combined with the oxygen mobility abilities of the Fe-doped ceria solids for supplying structural oxygen. The nanoparticles of gold cooperate with the Fe-doped supports for the enhancement of the activation of the O_2 and CO molecules during the oxidation reaction by means of the strong interaction between the noble metal and the oxygen vacancies of the supports. Higher the amount of oxygen vacancies higher the amount of gold deposited. Concerning the catalytic activity, the presence of noble metal greatly increases the CO conversion at lower temperatures of the Fe-doped supports in all cases. However, a superior catalytic activity is showed by the gold catalyst whose support presented the highest oxygen vacancies population.

ISO-PP06

Silica-supported Silver-containing OMS-2 Catalysts for Ethanol Oxidative Dehydrogenation

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The Ag/OMS-2/SiO_2 and OMS-2/SiO_2 catalysts were synthesized and tested in ethanol oxidation. It was stated that silver addition increases the reducibility and reoxidation ability of OMS-2, as a consequence catalytic activity increases. Catalytic properties of Ag/OMS-2/SiO_2 catalysts may be controlled by variation of Mn/Ag molar ratio and preparation method. When molar ratio Mn/Ag increases, deep oxidation activity increases.

ISO-PP07

A Heterogeneous Single-site Organocatalyst for Alkene Epoxidation

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In this work we aimed to develop catalyst with immobilized trifluoroacethophenone organocatalyst for the epoxidation of alkenes. For this purpose at first step we synthesized SBA-15. After that, modification of support through phenylation was performed. Third step was the acylation of immobilized phenyl groups by trifluoroacetic anhydride. Nitrogen adsorption measurements for both as-synthesized SBA-15 support and materials modified by phenylation and then acylation showed the noticeable decrease of surface area and mean pore size which suggests the anchoring of TFAP catalytic species to the pore walls. The TFAP surface centers were successfully quantified by using ^{19}F NMR technique. The hybrid catalyst prepared by such way allows, for propene epoxidation with H_2O_2 at ambient temperature, to produce propylene oxide with selectivity of 100% and peroxide efficiency of 20%.

ISO-PP08

Selective Photo-Oxidation of α-pinene with dioxo-Mo(VI) complex /TiO_2 with Different Textural Properties

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The dioxomolybdenum(VI) complexes covalently anchored on the surface of TiO_2 exhibited attractive oxidative properties for the selective photo-oxidation of aryl alkanes and olefins with UV-Vis radiation and molecular oxygen. TiO_2 functionalization is carried out through the hydroxyl groups on the surface which can change substantially according to the preparation method. However, concentration, distribution, accessibility and type of titanol groups influence the chemical reactivity of the support. So far, determination of hydroxyl groups has been performed by IR, thermogravimetric analysis (TGA) and chemical methods such as titration with hexamethyldisilazane (HMDS). In the present work, was performed anchor of a dioxo-dichloro-(4,4'-dicarboxylic acid-2,2'-bipyridine) Mo (IV) complex on three TiO_2 (commercial Degussa P-25, Aldrich nanopowder and nanotubular structure) in order to increase the amount of functionalized hydroxyl groups on the surface. Photo-assisted oxygen transfer to α-pinene was evaluated with molecular oxygen and UV light in a long term reaction at room temperature.

ISO-PP09

Study on Kinetics of Liquid Phase Photocatalytic Oxidation of Dibutyl Sulfide Over Fullerenes

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The influence of several parameters on the rate and selectivity of dibutyl sulfide (DBS) photooxidation on C70 under visible light is investigated. Spectrum of light was measured with spectroradiometer ILT950. Products were identified with GC-MS (CP-3800 + Saturn 2000). Quantitative analyses of reaction mixture were carried on with gas chromatography (Hewlett Packard 5890, capillary column CP-Sil 8 CB and flame ionization detector). Intensity of irradiation affects on the rate and selectivity. Fullerene C70 has equal activity in whole visible light range.

ISO-PP10

Liquid Phase Oxidation of L-sorbose over Metallic and Bimetallic Particles Stabilized in Polymer Matrix

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The unique features of HPS facilitate incorporation of various compounds into the nanostructured HPS matrix and, thus, nanoparticle formation. Such hybrid materials give the opportunity to prevent the agglomeration of nanoparticles and do not require ligands for stabilizing, that makes nanoparticles more active in catalytic processes. It can be stated that in this limited experimental series the highest selectivity achieved for the target compound, 2-keto-L-gulonic acid was 41 % at 88 % of L-sorbose conversion over 3%Pt –2%Au/ HPS in water with NaOH as alkaline agent at 70°C. The reaction network is complex and further studies are required to optimize the formation of the target product

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ISO-PP11

Propylene Glycol Oxidation over Cr-MIL-101 with Tert-butyl Hydroperoxide

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Propylene glycol can be produced from glycerol, which is a low-cost by-product in transesterification of triglycerides for biodiesel production. A number of valuable products that find application in the production of fine chemicals and pharmaceutics can be obtained through oxidation of 1,2-propylene glycol. The potential of the chromium terephthalate Cr-MIL-101 in the selective oxidation of propylene glycol under mild conditions (50-70°C) using *tert*-butyl hydroperoxide as oxidant was explored. The effects of reaction conditions (temperature, concentrations, solvent nature) on this reaction were evaluated. Hydroxyacetone was shown to be the predominant product. C-C cleavage, which is typical of PG oxidation, did not take place in the catalytic system studied. However, the oxidation products (for example, methyl glyoxal) could undergo non-oxidative transformations under the reaction conditions. Further work is in progress to clarify this matter.

ISO-PP12

Influence of Pre-treatment on the Oxidative Coupling of Methane over MgO Catalysts

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The pre-treatment of a nanostructured MgO catalyst with N_2, CO_2, O_2, H_2 and H_2O and the analysis of the changes in reactivity helped to interpret the deactivation mechanism of MgO in OCM. CO_2, O_2, H_2 or H_2O are either reactive gases or formed during the OCM reaction. Analysis of their influence on the catalyst is of main importance to understand the deactivation mechanism in OCM over alkaline earth oxides and to develop alternative strategies and stabilization concepts. CO_2 and O_2, have no (or minor) effects on the OCM reactivity. H_2O has a detrimental influence due to sintering of the primary particles, while H_2 pre-treatment increases the concentration of active sites for CH_4 adsorption and activation.

ISO-PP13

New Insights in the Catalytic Oxidation of Levulinic Acid to Succinic Acid

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Nowadays, due to the increasing environmental concerns, many efforts have been made to develop oxidation systems using environmentally-benign molecular oxygen as a sole oxidant. Ru-based oxidation catalysis was rapidly developed being envisaged to play a major role in the renewable sources capitalization. Not long ago we developed a Ru(III)/functionalized silica-coated magnetic nanoparticles catalyst which was proven to be a highly active, selective and easily recoverable catalyst for the oxidation of levulinic acid (LA) to succinic acid (SA) under green conditions. Encouraged by these initially promising results, here we report the optimization of the former MNP-NH_2/Ru^{III} catalyst in order to further improve its catalytic performances in the LA oxidation to SA. Moreover, to extent the catalyst utility, LA was replaced with glucose as raw material. The best results (1wt.% Ru) were: C_{LA} = 59%, S_{SA} = 98.3%; $C_{glucose}$ = 100%, S_{SA} = 62.7%.

ISO-PP14

Vanadium-Based Catalyst for Ethanol Transformation: Relation Between Structure and Catalytic Activity

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Fe/V and Cu/V oxides were tested as catalysts for ethanol transformation under both aerobic and anaerobic conditions, and characterized before and after catalytic tests by XRD and SEM. Moreover, catalytic behaviour was followed by operando DRIFT/MS. When ethanol only was fed, both catalysts were progressively reduced until a stable phase was developed. With both catalysts ethanol was transformed mainly to ethylene and acetaldehyde, produced in different proportions depending on the reduction degree of the catalyst. The extent of reduction was found to be directly related to the in-situ generation of acid sites, which led to an enhanced ethylene selectivity to the detriment of acetaldehyde. This behaviour was more relevant with Fe/V/O than with Cu/V/O; in fact, the latter system maintained higher acetaldehyde selectivity also in its reduced form because of the segregation of Cu^0. Oxygen co-feeding with ethanol showed the main effect of preventing catalysts reduction, increasing acetaldehyde and CO_x selectivity to the detriment of ethylene.

ISO-PP15

Structure and Reactivity of Nanostructured MnO_x Catalysts in the Liquid Phase Selective Oxidation of Benzyl Alcohol with Oxygen

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The use of special and expensive precursors and reagents for selective oxidation of alcohols raises significant environmental and economic concerns. Then, the discovery of eco-friendly catalytic technologies for their selective oxidation with oxygen has been recently designated as a major Green Chemistry topic. Various catalysts drive the oxidation of many alcoholic substrates, but high cost, deactivation phenomena and safety issues hinder their industrial applications. Systematic analysis of activity data using Mn–based catalysts in the aerobic liquid phase oxidation of benzyl alcohol to benzaldehyde sheds lights onto the factors controlling the functionality of MnO_x catalysts, while a simple kinetic model allows predicting their activity-stability pattern over a wide range of experimental conditions. The reactivity of promoted systems lowers with the Mn/Ce ratio, despite a fairly constant MnO_x rate rules out significant electronic effects. Remarkable deactivation phenomena disguise 0^{th}-order reaction kinetics, while the activity-stability pattern is determined by strong adsorption phenomena.

ISO-PP16

Structural Peculiarities and Catalytic Properties of Supported Vanadium Oxide Catalysts for Oxidative Dehydrogenation

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The oxidative dehydrogenation (ODH) was suggested as an alternative way to produce propylene and styrene, with catalysts based on supported vanadium oxide showing promising results for the ODH of hydrocarbons. In this work the structural peculiarities and catalytic properties of vanadium species on the surface of different support were considered in ODH reactions. The interaction of vanadium oxide with the support to form polymerized surface vanadium oxide species was shown to result in increase of catalyst activity. The selectivity was shown to depend on the strength and electron density change of V-O-support bond in the formed surface vanadium oxide species.

ISO-PP17

Silica Supported Vanadia Catalysts for Selective Methane Oxidation: Impact of Morphology and Heteroatom Doping on Catalyst Performance

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Ti-doped and Ti-free silica supported vanadia catalysts of varying pore size distributions were prepared and employed in selective oxidation of methane to formaldehyde. Maximum achieved space-time-yield was 3.6 kg/kg$_{cat}$h (686 °C, 360,000 L/kg$_{cat}$h) over V/Ti-SBA-15 compared to 3.2 kg/kg$_{cat}$h over V/SBA-15 (665 °C, 360,000 L/kg$_{cat}$h). Catalytic tests showed S_{HCHO} = 50% at 1% methane conversion (X_{CH4}) over 0.2 wt% Ti containing V/Ti-SBA-15 (d_{pore} 6 nm), while S_{HCHO} of V/SBA-15 (d_{pore} < 5 nm) was significantly lower (between 40 and 50%) at comparable conversion. Over the range of conversion observed, samples containing larger pores exhibit higher selectivity of formaldehyde formation. Influence of titanium doping and pore size distribution of V/SiO$_2$ catalysts is put in perspective.

ISO-PP18

Selective Oxidation of Cyclic-alkane, Catalyzed by Nano Size SWNTs Supported Pt and Pd Complexes Catalysts

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The *NH$_2$*-functionalized magnetic carbon nanotubes have been used as novel support for pincer Pd$^{(II)}$ and Pt$^{(II)}$ complexes immobilization as magnetic nano-catalysts. These magnetic single-walled carbon nanotubes (SWNTs) with Ni/Co have been synthesised by arc discharge technique using Ni/Co carbon composite rod in inert atmosphere and surface modified by the 3-aminophenyl trimethoxysilane. These magnetic nano-catalysts have been tested industrially important cyclohexane (*Cy-hx*) oxidation with O$_2$ and achieved significantly high TONs 1678 to 1946 under solvent free and relatively mild condition. The SWANTs/Pd catalyst has performed best conversion 22.7 % but SWANTs/Pt system has also provided good conversion 20.7 % result. Morphology of catalysts has been characterized by IR, EPR, SEM, TGA, TEM, XRD, AAS and EDS analysis.

ISO-PP19

Catalytic Synthesis of 2-methyl-1,4-naphthoquinone in 1%Au/HPS Presence

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The 2-methylnaphthalene oxidation stage has a low selectivity, and consequently a small target product yield. At oxidation 2-methylnaphthalene such products, as 2-methyl-1,4-naphthquinone, isomerous 6-methyl-1,4-naphthquinone, methyl groups oxidation products, dinaphthquinone, epoxiquinone and other products of deep oxidation are formed. It necessary to find the way of selective synthesis of menadione. We decided to use the based on HPS catalyst, because of its properties. The yield of the non-catalytic process attained 43%. The yield of the catalytic process attained 72%.

ISO-PP20

Mo-incorporated KIT-6 Mesoporous Silica Catalysts with High Performance for the Selective Oxidation of Propane to Acrolein

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A kind of framework-incorporated Mo-KIT-6 mesoporous molecular sieve catalysts with different Mo contents were successfully synthesized by one-spot co-assembly method. The structures of the catalysts were characterized by means of XRD, TEM, N$_2$ adsorption-desorption and UV-Raman, and their catalytic performance for the oxidation of propane was studied. It was found that the catalyst maintained highly ordered mesoporous structures with large surface and was effective for the oxidative conversion of propane to acrolein. The one-spot co-assembly method achieved that molybdenum was substituted into the silica matrix of KIT-6, which contributed to restraining the aggregation of molybdate ions compared with the impregnation method. Detailed characterizations and catalytic behavior showed that highly dispersed MoO$_x$ species were predominant in the catalysts and the high concentrations of highly dispersed active sites are favorable for improving the activity of selective oxidation of propane to acrolein.

ISO-PP21

Oxidative Dehydrogenation of Ethane on NiO supported on Pillared Clays

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At the present work, the use of a silica with a pillared structure as a support for nickel oxide has been studied for the oxidative dehydrogenation of ethane and its performance compared to that of conventional silica. Pillared clays, especially if columns are SiO_2/TiO_2-made, have demonstrated to be excellent supports for NiO, achieving remarkably higher selectivity towards ethylene than if conventional silica is used. Selective Ni-species with low reducibility are likely involved in the high ethylene formation.

ISO-PP22

Gas Phase Hydroxylation of Benzene to Phenol over M (Co, Ni, Cu, Zn)/ZSM-5 using Nitrous Oxide

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The gas phase catalytic hydroxylation of benzene to phenol over M (Co, Ni, Cu, Zn) supported on ZSM-5 (Si/Al=25) was carried out at atmospheric pressure and in the temperature range from 290 to 450 °C. The catalysts were prepared by wet impregnation technique and calcined at 500 °C for 6 h in air. The content of Co, Ni, Cu, and Zn in the catalyst is 1wt%. These samples were characterized by ICP, XRD, N_2 adsorption etc. Nitrous oxide was used as an oxidizing agent. Among all, Zn/ZSM-5 catalyst exhibits the best performance while the Cu/ZSM-5 displays relatively poor performance. Zn/ZSM-5 gave nearly 9 % yield of phenol at 410 °C. Coking is the major constraint of this reaction due to which the catalysts are observed to deactivate during time-on-stream.

ISO-PP23

DFT Study of the Interaction of CO and $O_2$with Gold-Copper Tetrahedral Bimetallic Clusters

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The CO and O_2 adsorption on neutral, positively and negatively charged isolated $Au_{20-x}Cu_x$ clusters have been investigated by density functional theory calculations. Three isomers of $Au_{19}Cu$ and $Cu_{19}Au$ having a heteroatom on the top, an edge, and a facet are considered. An Cu-doping in gold clusters improves CO or O_2 adsorption on $Au_{20-x}Cu_x$ cluster. The neutral Au_{20} and $Au_{20-x}Cu_x$ clusters exhibit relatively poor reactivity for CO and O_2 adsorption. Compared to the neutral clusters, the charging of $Au_{20-x}Cu_x$ can improve not only O_2 adsorption, but also CO adsorption. The Cu-doped Au nanoparticles are comparable with Au nanoparticles.

ISO-PP24

Selective Isopropyl Alcohol Oxidation on Palladium and Ruthenium Catalysts Supported on Amphiphilic Hybrid Carbon Nanotubes

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In this study, amphiphilic hybrid carbon nanotubes (CNTs) are synthesized and used as supports of (2% w/w) ruthenium and palladium supported catalysts, and evaluated for the reaction of decomposition of isopropyl alcohol as probe reaction. These hybrids CNTs interact very well with aqueous media due to the hydrophilic nitrogen doped section, while the undoped hydrophobic part has strong affinity for organic molecules. The presence of nitrogen functionalities on the nitrogen doped support induces a high metal dispersion. Decomposition of isopropyl alcohol on the CNT supports, leads to acetone by dehydrogenation and propene by dehydration. Thus, on hybrid N-CNT, at 210°C as reaction temperature, and in the presence of air as carrier gas, the conversion was higher on the hybrid CNT than on the simple CNT and nitrogen doped CNT samples. From 90°C, Pd over hybrid CNT catalysts was 100% selective towards acetone for a conversion of 100%, whereas Ru catalysts lead to dehydration and dehydrogenation products. The nitrogen doping induces the appearance of redox properties, which appear when oxygen is present in the reaction mixture.

ISO-PP25

Ethanol Transformation over Cu-containing Zirconium Phosphate

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4 - Novosibirsk State University, Novosibirsk, Russia

The study of structure, phase composition and catalytic properties of Cu-containing zirconium phosphate and zirconium phosphate was carried out in ethanol transformation both in the presence and in the absence of oxygen. Catalysts were characterized by XRD, HRTEM, TPR and TGA. High-temperature treatment of Cu-containing zirconium phosphate led to formation of Cu^0 particles with sizes in the range from 2 nm to ~1 µm. Ethanol conversion reached 100% for both samples. The absence of oxygen in the feed gas favored for dehydrogenation of ethanol to form acetaldehyde over Cu-containing zirconium phosphate: acetaldehyde yield was 75%. Dense distribution of copper particles on the surface of zirconium phosphate prevented formation of dehydration products. Zirconium phosphate demonstrated typical acidic activity to yield ethylene and diethyl ether in the absence of oxygen. Acetaldehyde yield about 40 % was reached for zirconium phosphate in oxygen-containing atmosphere.

ISO-PP26

Kinetic Conjugation Effects during C_1-C_2-hydrocarbon Oxidation in the Conditions of Methane Oxidative Coupling

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C_1-C_2-hydrocarbon oxidation has been studied in conditions of methane oxidative coupling. It is demonstrated that gas phase oxidation of ethane and ethylene proceeds with a high rates at typical OCM temperatures. $NaWMn/SiO_2$ catalyst acts as an efficient inhibitor of gas phase oxidation of C_2-hydrocarbons and substantially changes their reaction pathways. A complex reciprocal influence of C_1-C_2 hydrocarbons during their simultaneous oxidation is demonstrated. Unlike the process in the gas phase, methane and ethane strongly increase the reactivity of each other while oxidized over the OCM catalyst.

ISO-PP27

Metal-catalyzed Electrochemical Oxidative Phosphonation of Azoles

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The metal-catalyzed electrochemical oxidation (phosphonation) of heteroarylazoles (benzoxazoles, benzothiazole and other) with dialkylphosphite was developed. Palladium and nickel complexes were tested as catalysts. Electrocatalitic C-H phosphonation of heteroarylazoles affords the desired *ortho* C-H substitution product, 2-substituted azoles.

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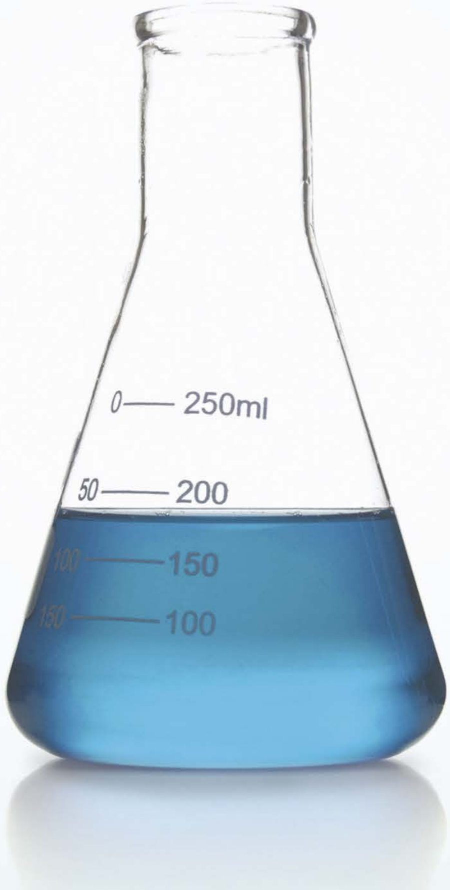
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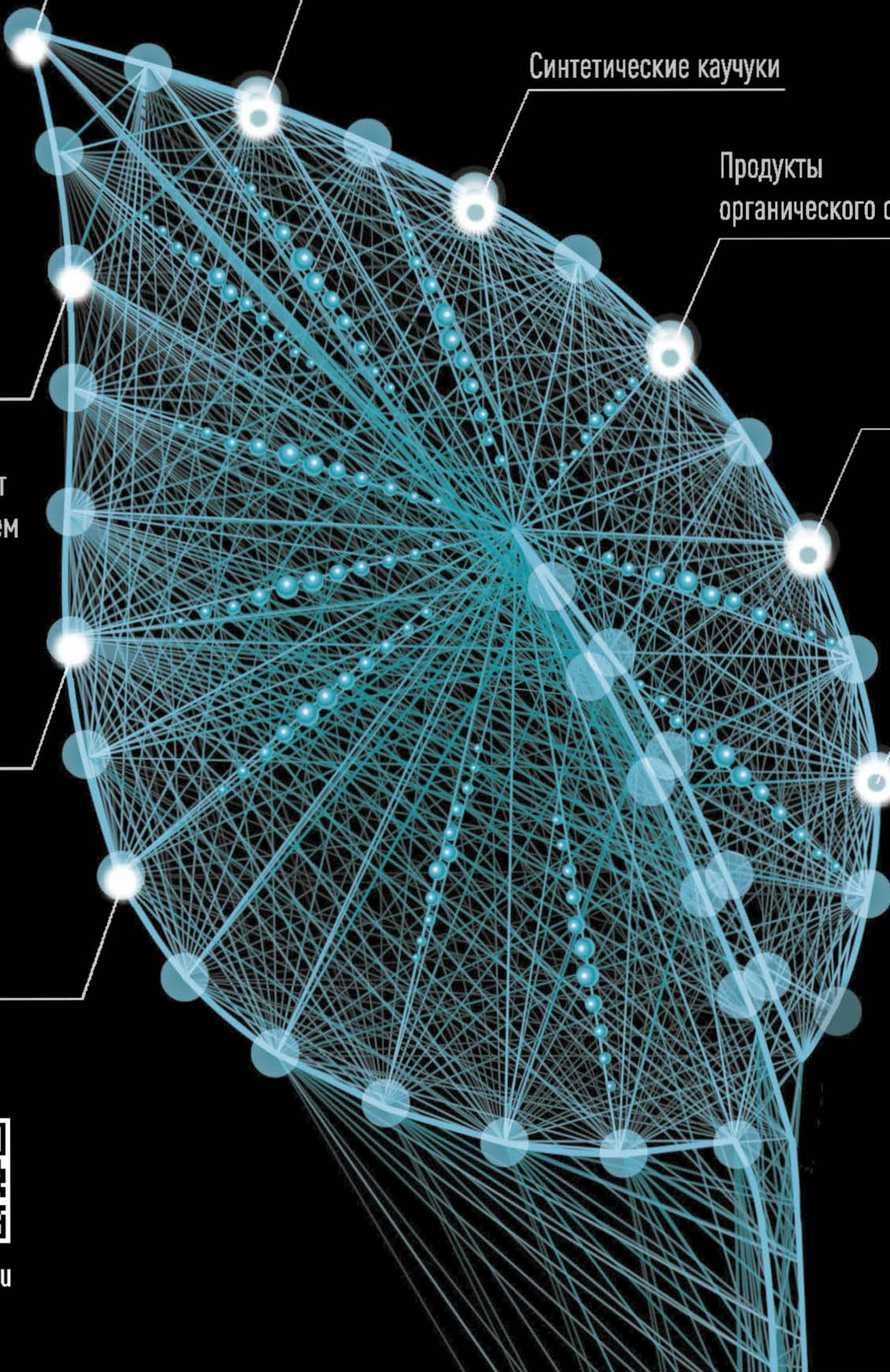

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- размещение до 3-4 устройств ввода в любом сочетании
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- одновременный анализ паро-газовой смеси - постоянные газы (H_2,O_2,N_2,CO,CO_2) и C_1-C_{15}

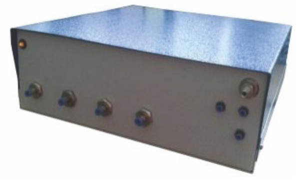
Вспомогательное оборудование и комплектующие:

- генераторы водорода, воздуха, азота; системы очистки
- фазы, носители, сорбенты, насадочные колонки
- капиллярные колонки ведущих мировых производителей и Российские
- септы, ферулы, шприцы и микрошприцы, виалы, ГСО, ПГС

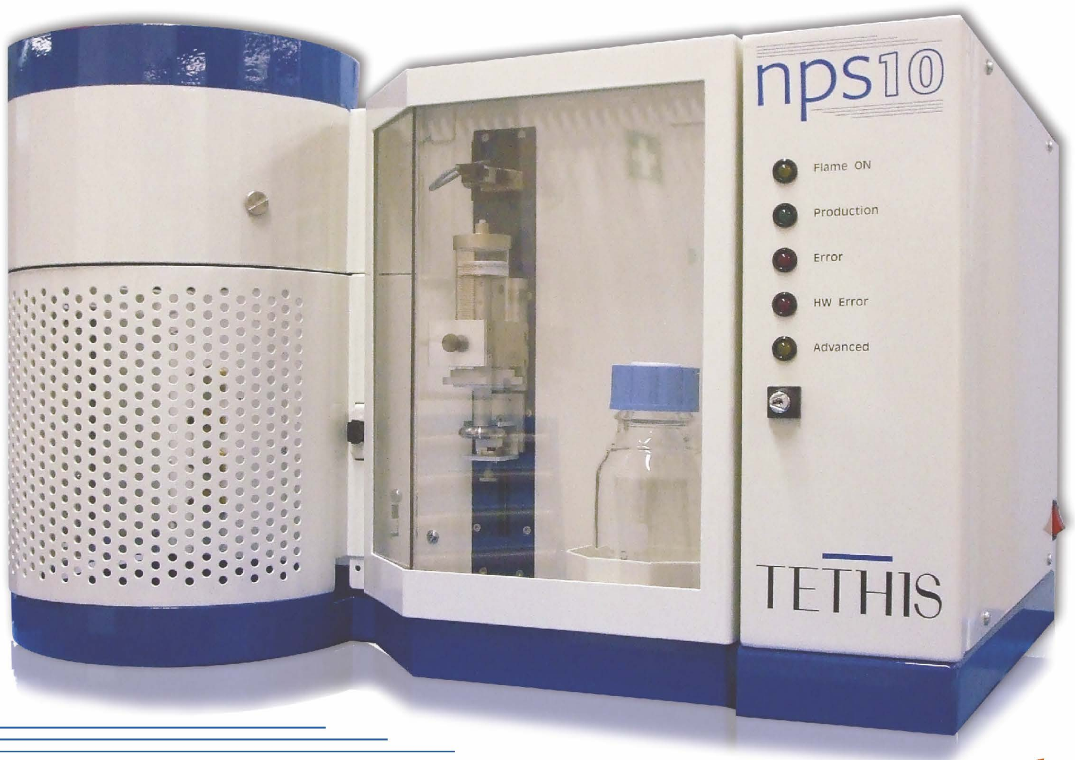
И тысячи других наименований для ГХ/ВЭЖХ от Agilent, SGE, Restek, VICI, Supelco !

ТЕХНОЛОГИЧЕСКОЕ ОБОРУДОВАНИЕ

- каталитические установки низкого и высокого давления: проточные и проточно-циркуляционная
- установка определения общей поверхности и пористости твердых тел *«МУЛЬТИСОРБ»*
- установка определения активной поверхности нанесенных металлов *«ХЕМОСОРБ»*
- формирователь/калибратор и измерители газовых потоков



644050, г. Омск, ул. Химиков 25
т/ф. (3812)67-23-35, 90-60-33, 51-60-98
mail@chromosib.ru, www.chromosib.ru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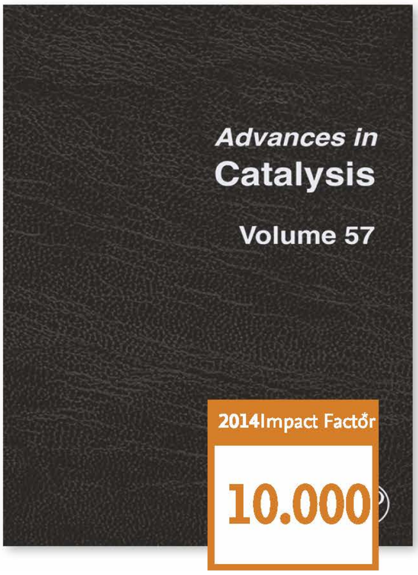
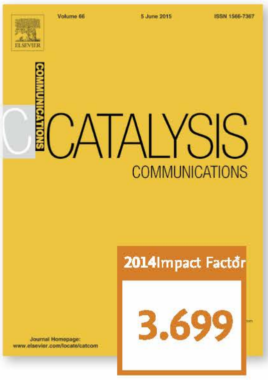
Advanced
TETHIS


JOURNAL OF CATALYSIS
2014 Impact Factor
6.921


Advances in Catalysis
Volume 57
2014 Impact Factor
10.000


APPLIED CATALYSIS B: ENVIRONMENTAL
2014 Impact Factor
7.435


APPLIED CATALYSIS A: GENERAL
2014 Impact Factor
3.942


CATALYSIS COMMUNICATIONS
2014 Impact Factor
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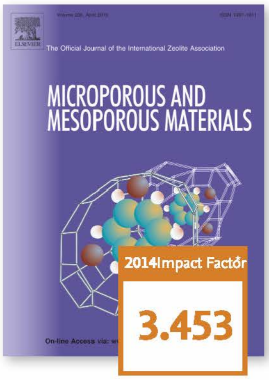
CATALYSIS TODAY
2014 Impact Factor
3.893


JOURNAL OF MOLECULAR CATALYSIS A: CHEMICAL
2014 Impact Factor
3.615


JOURNAL OF MOLECULAR CATALYSIS B: ENZYMATIC
2014 Impact Factor
2.128


MICROPOROUS AND MESOPOROUS MATERIALS
2014 Impact Factor
3.453

ЛАБТЕСТ

LABTEST

ЛАБТЕСТ

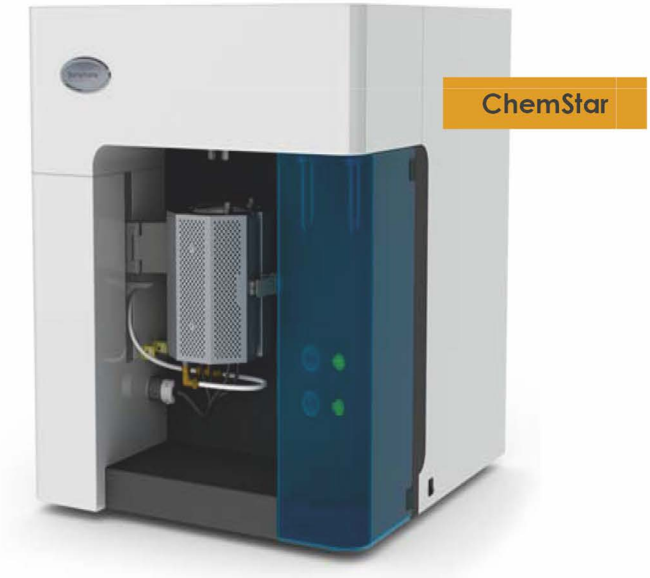
Quantachrome

INSTRUMENTS

www.lab-test.ru

+7 (495) 605-3507; info@lab-test.ru

С НАМИ НАДЁЖНО



Оборудование для исследования каталитических свойств материалов

ChemBET

ChemStar

Autosorb-iQ-C

Линейка приборов компании Quantachrome охватывает все аспекты исследования катализаторов: определение размеров активной поверхности катализатора, дисперсии, среднего размера зерна, энергии активации, оптимальной температуры реакции, определение удельной поверхности и размеров пор на подложке и т.д.

ChemStar и ChemBET Pulsar осуществляют исследование динамической хемосорбции, проведение температурно программируемых реакций и автоматического импульсного титрования, детектор – устойчивый к окислению и аммиаку катарометр либо масс-спектрометр. ChemStar работает под давлением до 100 атмосфер и даже может быть превращен в мини-реактор.

Autosorb-iQ-C – непревзойденный прибор серии, может работать в режимах как статической физи- и хемосорбции, так и осуществлять все динамические методы исследования катализаторов с дополнительной приставкой.

Quantachrome Instruments - мировой лидеро в производстве оборудования для исследования катализаторов и пористых материалов. Помимо представленных приборов компания выпускает ртутные и жидкостные анализаторы размеров пор, пикнометры, приборы для исследования сорбции паров воды, газовой сорбции под давлением и т.д.

ООО «НКЦ «ЛАБТЕСТ», является официальным дилером Quantachrome, США.
Адрес: Москва, Б.Тишинский пер. д.38
www.lab-test.ru, info@lab-test.ru, +7-(495)-605-3507

Boreskov
Institute of Catalysis

ИК
СО РАН

IS THE LARGEST
RESEARCH CENTER IN RUSSIA
SPECIALIZED IN THE AREA
OF CATALYSIS

www.catalysis.ru

Our mission

To make the Russian chemical complex effective, energy saving and ecologically sound.
For many decades, the Institute cooperates with Russian research institutions and industrial enterprises to improve the existing and to develop and put into practice new catalysts, materials and technologies for Russian industries.

Our research potential

410 research scientists including 5 members of the Russian Academy of Sciences, 66 Drs.Sci., more than 250 PhDs.

Our partners

Largest Russian corporations, among which are Gazprom, Gazpromneft, Rosneft, Tatneft, Sibur, as well as companies and research centers of the USA, Great Britain, German, China, France, Corea, The Netherland etc.

Contact information

Boreskov Institute of Catalysis
Pr. Ak. Lavrentieva 5,
Novosibirsk 630090, Russia

E-mail: bic@catalysis.ru
http://www.catalysis.ru

Our priorities

Catalysts and catalytic processes:

- Conversion of light hydrocarbons and natural gas
- Oil processing
- The most important processes of chemical industry
- Processing of natural gas (desulfurization etc.)
- Pharmaceutics
- Agrochemistry
- Olefin polymerization
- Porous oxides
- Zeolites
- Environmental protection
- Non-traditional energy, utilization and conversion of renewable raw materials and coal

Adsorbents and composite materials with controlled properties:

- Selective sorbents of water, carbon dioxide, etc.
- Carbon materials and technical carbon
- Filling agents based on disperse materials

N.D. Zelinsky Institute of Organic Chemistry
Russian Academy of Sciences

Our team

350 research fellows,and 320 engineers and other services, including 85 Ds.Sci., 6 Full Members and 4 Associate Members of RAS among them, and more than 230 PhDs.

Science and education centers

From high school to a PhD degree

- Moscow Chemical Lyceum
- Higher Chemical College of RAS
- PhD courses

Environmental Catalytic Technologies,
Photocatalysis, and Green Chemistry,
Organic Photonics

Contact information

N.D. Zelinsky Institute of Organic Chemistry

Leninsky Prospect, 47,
Moscow 119991, Russia

E-mail: secretary@ioc.ac.ru
http://zioc.ru/

Research areas

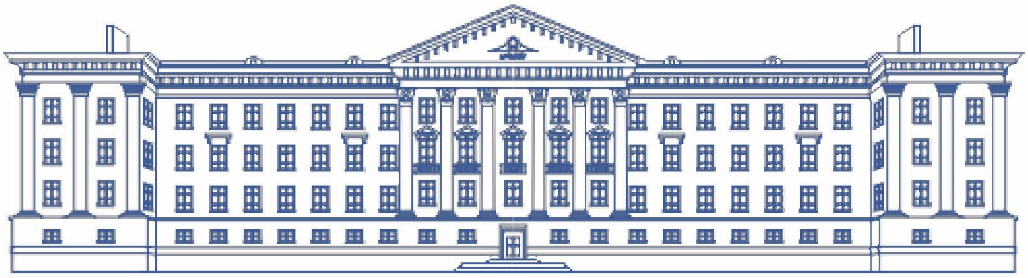
- studying the structure and reactivity of organic and organoelement compounds, mechanisms and intermediates of chemical reactions, and developing physical methods for the molecular structure research;

- identifying general regularities of the organocatalysis and mechanisms of catalytic reactions, developing catalytic systems for production of motor fuels, envieromental protection, materials for hydrogen energy and valuable chemical products from natural and alternative carbon-containing sources;

- developing the methodological basis of the organic synthesis and creating scientific backgrounds for ecofriendly and resource-saving processes focusing on the preparation of organic compounds and materials, including polymeric, high energy and nanomaterials with valuable properties for various engineering, biological, medical, and agricultural applications;

- exploring chemistry of natural compounds and their analogs and designing new pharmaceuticals and materials for medicine and researching living systems;

- predicting the structure and properties of new molecules, materials, and chemical process parameters by computational methods; using state-of-the-art information and communication technologies.



World Research Institutions Ranking: BBB+

The Department of Chemistry of M.V.Lomonosov Moscow State University

is a world-known center for Chemistry science and education

The Department of Chemistry includes 15 chairs, 83 laboratories, as well as 7 branches in the neighboring countries. 1048 students and 283 postgraduates study at the Department. 12 Full Members of Russian Academy of Sciences, 9 Corresponding Members, more than 250 Doctors of Science and about 800 PhDs perform teaching and scientific researches and preparing students to become high class specialists in modern Chemistry.

Department of Chemistry is a world-known center for scientific research in nearly all fields of chemistry, including catalysis for oil refining and petrochemistry, environmental catalysis and medicine chemistry, green chemistry, new inorganic, organic and composite materials, medicine chemistry, polymers, radiochemistry, biotechnology etc. Scientists of the Chemistry Department made great contributions to the development of modern theory of catalysis, photochemistry, electrochemistry and chemistry of high dispersion systems. High theoretical level and practical skills of teachers, as well as implementation with modern high-technological scientific equipment make possible to couple education with research activity to prepare universally educated specialists.

The Department of Chemistry closely collaborates in researches and personnel training with leading Russian and foreign universities, all chemical institutions of Russian Academy of Science, National Research Centre "Kurchatov Institute", Rosatom, Rospromstroy, Rosenergo, all fertilizers producing companies of Russia, Lukoil, Sibur, Gasprom, Rosneft, Gaspromneft and many other companies.

Dean of the Chemistry Department
Full Member of Russian Academy of Sciences Professor
Valery Lunin is known for his works in the field of catalysis, ozone chemistry, supercritical fluids etc.

Postal address:
Chemistry Department
M.V.Lomonosov Moscow State University
Leninskie Gory 1 stroenie 3
119991 Moscow
Russia

Phone: 7(495) 939-3571
Fax: 7(495) 939-0067
http://chem.msu.ru

ИОФХ
им. Арбузова

A.E.Arbuzov Institute of Organic and Physical Chemistry (IOPC)

IOPC – unique scientific and research center on synthesis, analysis and manufacturing of novel medical substances. International Scientific and Innovative Center of Neurochemistry and Pharmacology was created in 2015 on the basis of the Institute to provide qualitative breakthrough in the field of creation of new generation of innovation drugs.

IOPC – a world recognized scientific center of chemistry of phosphorus and its organic and organoelement compounds as the basis for the development of new substances, materials and technologies.

IOPC – center of research and engineering of novel composition and nanomaterials based on modern advances in organometallic and supramolecular chemistry.

IOPC – center of competence in the field of output, transportation and refining of extremely viscous oil and native bitums.

Contact Information
A.E.Arbuzov Institute of Organic and
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Russian Federation
tel: (007) 843 273 93 65
fax: (007) 843 273 22 53
e-mail: arbuzov@iopc.r

Director Oleg Sinyashin,
academician of RAS, Doctor of Science,
Professor


Казань
Нижнекамск
Альметьевск

MONOMAX PCO

Professional Conference Organizer

Monomax PCO offers full expertise in meeting management since 1991. The professionals of Monomax have a vast experience in different aspects of the MICE industry. They are always eager to manage events with their greatest personal care to guarantee the highest standards of service.

Why contact *Monomax PCO* when planning your congress, etc.?

TIME is a valuable asset. You get a remarkable **time cost reduction** by handing over technical tasks of **congress management** to our team.

COSTS SAVING - The rates for services offered by our company can be lower than the rates negotiated by you as an independent party. We have already got a large network of proven suppliers so why not benefit from our resources?

PROFESSIONAL BUDGETING AND FINANCIAL MANAGEMENT – We provide qualified assistance in draft budget planning and registration fee estimation, account management and payments handling, liaison with vendors and many other aspects of financial planning and management.

ADVANCED TECHNOLOGIES – Company's in-house integrated congress management software – Alternative Events – is the modern instrument of any size event administration. It offers mechanisms of delegate on-line registration, abstract handling and Internet payment processing. For congress secretariat it is a useful tool for event Web site support, customized reports generation and cash flow management.

QUALIFIED SECRETARIAT MANAGEMENT - Company's experienced personnel with excellent English language skills is able to accomplish all the tasks and duties of professional congress Secretariat with maximum efficiency and accuracy.

ON-SITE MANAGEMENT – Our team will provide professional on-site coordination throughout the congress to control all services and to resolve any possible emergencies. Our personnel speak good English and we supply all the necessary equipment for registration as well as the information desk.

PROFESSIONAL TRAVEL SERVICES – Being experts in logistics handling we guarantee efficient organization of social aspects of your conference – visa support for the delegates, cultural and social program, hotel accommodation, and transportation.

EXPERIENCE AND QUALITY – Our managers have experience in managing dozens of congresses, they know how to organize an event on a step-by-step basis and how to cope with underlying potential problems in the process of organization. We work as a team with constant exchange of knowledge and experience. We work only with proven and most qualified services vendors – they know our needs and are flexible to deal with.

Monomax PCO is proud to be a member of ***International Congress & Convention Association (ICCA),*** the Netherlands, in MEETINGS MANAGEMENT category.

EUROPACAT EXHIBITION

CATALOGUE

EXHIBITION of compact installations and advertising materials will take place in the framework of the EuropaCat XII Congress in the hotel Korston Kazan on August 31 – September 4, 2015.

Companies and their regional representatives will exhibit scientific equipments and devices for control of chemical and phase composition of materials, analytical devices, facilities for spectral analysis, catalysts testing (including combinatorial studies), as well as high-end equipment for the investigation of catalytic reaction mechanisms at the atomic and molecular scale.

Of particular interest are analytical devices, including those coupled with catalytic units, as well as equipment for the control of the catalyst state in the course of catalytic reaction, and those allowing the analysis (including isotopic) of the reaction products with high resolution.

We also welcome devices for the control of environmental pollution, analysis of contaminants in heavy oils, setups and instruments for the analytical control of electrocatalytic processes.

ВЫСТАВКА малогабаритных научных приборов и рекламных материалов состоится в рамках Конгресса EuropaCat-XII в отеле «Корстон-Казань» с 31 августа по 4 сентября 2015 г.

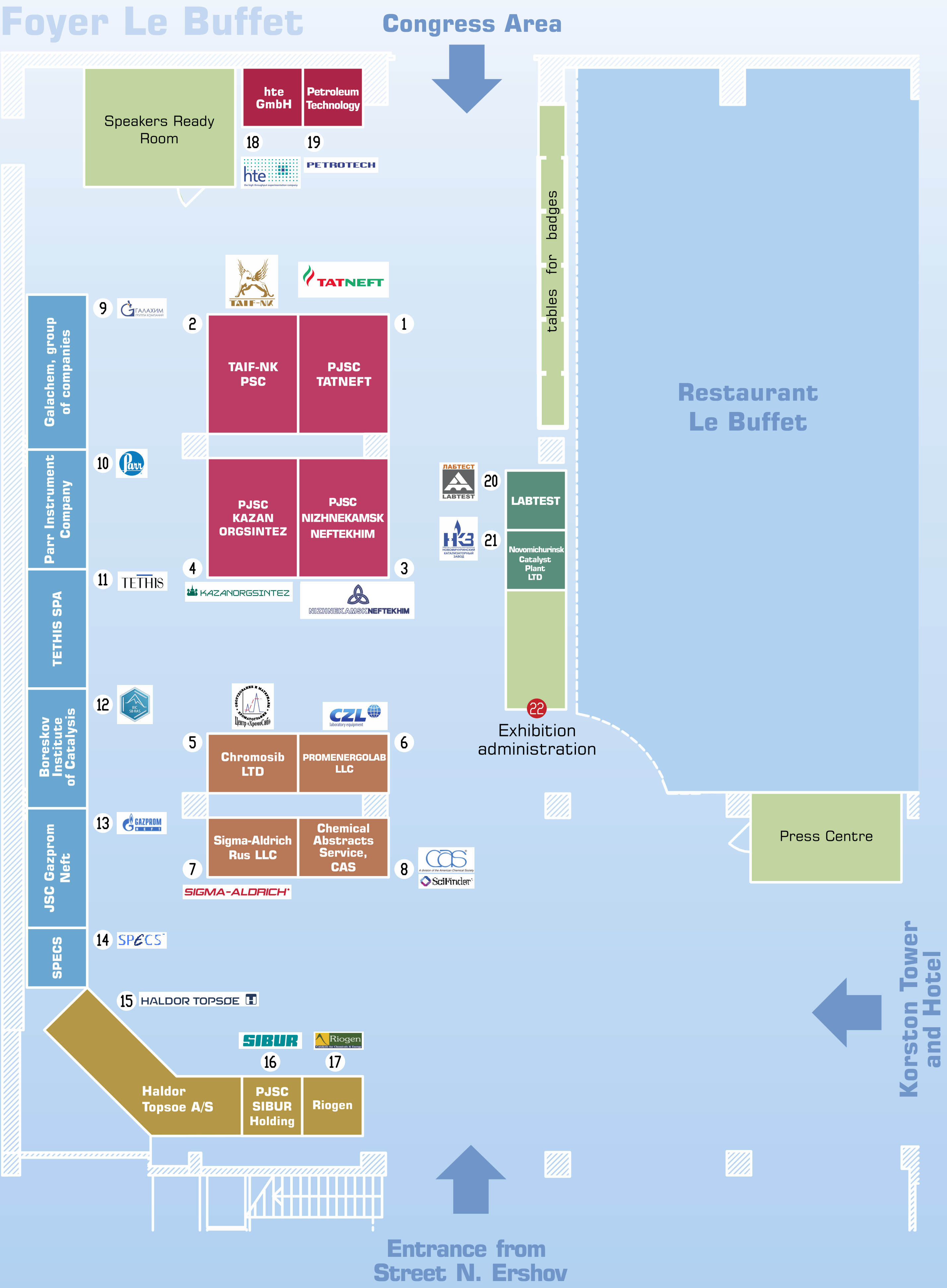
К участию в выставке приглашены организации и компании, их региональные представители, заинтересованные в презентации научно-технологического оборудования для контроля химического и фазового состава различных материалов, аналитического оборудования, приборов для спектрального анализа и тестирования катализаторов (в том числе устройства для комбинаторных исследований катализаторов), а также высокотехнологичного оборудования для исследования механизмов каталитических реакций на атомном и молекулярном уровне.

Особый интерес для участников Конгресса будет представлять аналитическое оборудование для исследований *in situ*, в том числе сопряженное с каталитическими установками, а также приборы, позволяющие определять состояние катализатора в ходе реакции, осуществлять анализ (включая изотопный) продуктов реакции с высоким разрешением.

В выставке примут участие производители и дистрибьюторы приборов для контроля загрязнения окружающей среды, анализа примесей в тяжелой нефти, установок и приборов аналитического контроля для электрокаталитических процессов.

EUROPACAT XII

EUROPACAT EXHIBITION



Stand № 1

PJSC TATNEFT

Address	Tel/Fax	E-mail	Add Information
75, Lenin Str., Almetyevsk, 423450, Republic of Tatarstan, Russia	+7 (8553) 307800	tnr@tatneft.ru	http://www.tatneft.ru

TATNEFT is one of the largest Russian oil companies, which is an internationally recognized vertically integrated holding company. The operation complex of the Company is steadily developing including crude oil and gas production, crude oil refining, petrochemicals production, tire manufacturing complex, network of filling stations and a block of service structures.

Stand № 2

TAIF-NK PSC

Address	Tel/Fax	E-mail	Add Information
423570, Industrial Aria, Nizhnekamsk, Republic of Tatarstan, Russia	+7(8555)-38-16-16 +7(8555)-38-17-17	referent@taifnk.ru	www.taifnk.ru

TAIF-NK PSC is a modern conventional oil refining complex comprising all integral components and the combination of process units and facilities. The company's overall throughput capacity is 7,3 mln tpa of crude oil plus 1 mln tpa of gas condensate, with the refining depth over 74 %. The company's core business lines are oil refining, sales and marketing of petroleum products and derivatives, construction and operation of petrochemical facilities. TAIF-NK production divisions include the refining plant and the motor gasoline plant. The processing capacity utilization currently reaches 100%.

TAIF-NK Product Lines:

Motor Gasoline Regular-92 and Premium Euro-95, meeting Euro-4 quality requirements, Diesel Fuel Euro-5, Jet Fuel RT Grade, Fuel Oil M-100, Bitumen 60/90 and 90/130, Granulated Sulfur.

Stand № 3

PJSC NIZHNEKAMSKNEFTEKHIM

Address	Tel/Fax	E-mail	Add Information
423574, Republic of Tatarstan, Nizhnekamsk, PJSC "Nizhnekamskneftekhim»	+7 (8555) 37-58-29 (-70-09) +7 (8555) 37-93-09	nknh@nknh.ru	http:// www.nknh.ru

PJSC «Nizhnekamskneftekhim» is the largest petrochemical company and it holds leading positions among Russian producers of synthetic rubber, plastics and ethylene. It makes part of TAIF Group. The Company was established in 1967, the main production facilities are located in Nizhnekamsk, Tatarstan Republic. The Company products are exported to more than 50 countries of Europe, America, South-East Asia. Export share in the total amount of products makes about 50%.

Stand № 4

PJSC Kazanorgsintez

Address	Tel/Fax	E-mail	Add Information
101, Belomorskaya st., Kazan, 420051, Russia	+7 843 533 98 09 +7 843 533 97 04	kos@kos.ru	www.kazanorgsintez.ru

PJSC Kazanorgsintez is one of the largest enterprises of the Russian Federation, being of strategic importance for the economic development of the Republic of Tatarstan. The company was established in 1958 and in 1963 launched its first products: phenol and acetone. Currently PJSC Kazanorgsintez belongs to TAIF Group of Companies.

The company is the producer of over 47% of the Russian polyethylene and is the only producer of polycarbonates.

At present, the Company produces ethylene, polyethylene, polycarbonate, polyethylene pipes, bisphenol, phenol, acetone, ethylene glycols, ethanolamines, and other organic synthesis products. The whole range of products includes over 170 items with the output of 1.6 million tonnes. The products comply with the international quality standards and are exported to 23 countries worldwide.

Stand № 5

Chromosib LTD

Address	Tel/Fax	E-mail	Add Information
25, Chimikov str., Omsk, 644050, Russia	+7 (3812) 672335	mail@chromosib.ru	http://www.chromosib.ru

Chromosib is a Regional sales representative and certified Service center for chromatographic equipment generation series "CHROMOS". It is Development of hardware and analytical schemes of chromatograph (regular and multifunctional models), commissioning, training, warranty, service and information service of gas chromatographs. Manufacture: capillary column with a phase WCOT (100% Dimethyl Polysiloxane; 5-15% Phenyl Polysiloxane; 15% Cyanopropyl Polysilixane; 25% Trifluoropropyl Polysiloxane; Carbowax)/PLOT (polymer sorbent;

Stand № 6

PROMENERGOLAB LLC

Address	Tel/Fax	E-mail	Add Information
7, Prostornaya Str.,Moscow, 107392, Russia	+7 (495) 22-11-208	info@czl.ru	http://www.czl.ru

Promenergolab LLC is a Russian company, specializing in complex equipping of laboratories with a wide range of equipment. Priority orientations: • spectroscopic, analytical instruments and lasers; • equipment porous materials' studying; • system for contact angle determining; • optical components; • equipment laboratory for catalysts' testing; • spectrophotometers; • microscopes; • alumina ceramics; • general laboratory equipment.

Stand № 7

Sigma-Aldrich Rus LLC

Address	Tel/Fax	E-mail	Add Information
2/21 Ul. Makarenko, Bld. 1, Office 22, Moscow, 105062, Russia	8-800-100-7425	ruorder@sial.com	http://www.sigmaaldrich.com

Sigma-Aldrich company is a supplier of chemical, biochemical reagents and expendable materials for science and industry. Company products are released under brand names of Sigma, Aldrich, Fluka and Supelco.

Stand № 8

Chemical Abstracts Service, CAS

Address	Tel/Fax	E-mail	Add Information
2540 Olentangy River Road Columbus, OH 43202, U.S.A.	+1-614-447-3700 +1-614-447-3751	help@cas.org	http://www.cas.org

Chemical Abstracts Service (CAS), a division of the American Chemical Society, is the world's authority for chemical information. CAS is the only organization in the world whose objective is to find, collect and organize all publicly disclosed chemical substance information. A team of scientists worldwide curates and controls the quality of our databases, which are recognized as the most comprehensive and authoritative by chemical and pharmaceutical companies, universities, government organizations and patent offices around the world. By combining these databases with advanced search and analysis technologies (SciFinder® and STN®), CAS delivers the most current, complete, secure and interlinked digital information environment for scientific discovery.

SciFinder® is a research discovery application that provides unlimited access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences. SciFinder is the leading research tool for chemists and researchers which offers instant access to the most comprehensive collection of chemical substance and reaction information, including CAS REGISTRY — the gold standard of chemical substance collections. Fortune 500 corporations, more than 2,220 universities, and major government agencies around the world rely on SciFinder to fuel R&D initiatives and foster innovation. And now **PatentPak™**, a robust new patent workflow solution, offers instant access to hard-to-find chemistry in full-text patents directly in SciFinder.

STN® - The choice of patent experts. STN is the premier single source for the world's disclosed scientific and technical research, intellectual property professionals and patent examiners at the world's major patent offices and research organizations rely on STN to answer business critical questions and make informed decisions. STN provides an information advantage. Only STN offers access to the world's scientific information on one integrated platform, including the authoritative chemistry content from CAS and patent content from Thomson Reuters' Derwent World Patents Index®.

Stand № 9

Galachem, group of companies

Address	Tel/Fax	E-mail	Add Information
14\3, Malenkovskaya street, 107113, Moscow, Russia	+7 (495) 984-42-44	galachem@galachem.ru	www.galachem.ru

Full range of laboratory equipment and reagents: • analytical devices (LC/MS, LC/MS/MS, GC/MS systems, chromatographs, spectrophotometers, spectrofluorometers): Hitachi, Waters, InterChim, Agilent; • all for microbiology; • chemical reagents, reagents for biochemistry of the world's leading manufacturers: Sigma, Aldrich, Fluka, Merck, ABCR, Serva, Bio-Rad, Invitrogen, Millipore; • pharmaceutical reference standards: USP, BP, EP, MicroMol (LGC); • analytical standards for chemistry.

Stand № 10

Parr Instrument Company

Address	Tel/Fax	E-mail	Add Information
61265-1770, USA, IL, Moline, 211 53rd Street	+1-309-762-7716 +1-309-762-9453	parr@parrinst.com	http://www.parrinst.com

Parr Instrument Company designs and manufactures Laboratory Reactors and Pressure Vessels, stirred and unstirred, used at elevated temperatures and pressures in the catalytic hydrogenation, organic synthesis and the polymerization processes. Parr also specializes in providing complete systems for batch, semi-batch and continuous-flow applications. Parr's manufactures Oxygen Combustion Calorimeters for determination of the heat of combustion in solid, liquid and refuse derived fuels.

Stand № 11

TETHIS SPA

Address	Tel/Fax	E-mail	Add Information
VIA RUSSOLI 3, 20143 MILANO, ITALY	+39-02-36568349 +39-02-36569183	info@tethis-lab.com	http://www.tethis-lab.com

Tethis S.p.A. is one of the leading nanotechnology company within Europe specialized in the design and manufacture of laboratory-scale equipments for the synthesis of nanoparticles and the deposition of porous coatings. Its main activities are:

- *Manufacture and sale* of lab equipments for the production of nanopowders and nanoparticle coating based on a flame-synthesis process.

- *high quality R&D* for the integration of functional material into innovative devices. Tethis' joint efforts focus on the realization of proof-of-concept devices based on the synergetic contribution of nano-, bio-, and microfabrication technologies.

Stand № 12

Boreskov Institute of Catalysis

Address	Tel/Fax	E-mail	Add Information
Prospekt Akademika Lavrentieva, 5, Novosibirsk 630090, Russia	+7 (383) 330 67 71 +7 (383) 330 80 56	bic@catalysis.ru	http://www.catalysis.ru

Boreskov Institute of Catalysis is a large research center engaged in development of catalysts and catalytic technologies for oil processing, oil chemistry, chemistry, synthesis of polymers, manufacturing of complex organic products, neutralization of anthropogenic waste, processing of plant feedstock, energy generation.

Stand № 13

JSC Gazprom Neft

Address	Tel/Fax	E-mail	Add Information
3–5, Pochtamtskaya St., St. Petersburg,190000, Russia	+7 (812) 363 3152; 8 (800) 700 3152 (toll-free calls throughout Russia)	info@gazprom-neft.ru	http://www.gazprom-neft.ru

Gazprom Neft is a vertically integrated oil company, primarily engaged in oil and gas exploration and production, oil refining, and the production and sale of petroleum products.

The company is among the top three companies in Russia in terms of refining volumes, and the fourth most significant by volume of oil produced.

The company refines approximately 80 percent of all oil produced – among the best production–refining ratios in the Russian oil industry.

Stand № 14

SPECS Surface Nano Analysis GmbH

Address	Tel/Fax	E-mail	Add Information
Voltastrasse 5, 13355 Berlin, Germany	+49 30 4678240 +49 30 4678240	info@specs.com	www.specs.com

SPECS Surface Nano Analysis GmbH - A Story of Constant Innovation
SPECS has more than 150 employees at its headquarters in Berlin and its subsidiaries in the USA and Switzerland. The company also has sales offices and international sales channels in more than sixteen countries. A team of scientists and engineers are involved in developing and producing scientific instruments for surface analysis, material science and nanotechnology. By constant innovation new techniques, components or system concepts are launched every year since more than 30 years, revolutionizing the field of surface analysis. Contact SPECS Surface Nano Analysis GmbH (www.specs.com) for further information.

Stand № 15

Haldor Topsoe A/S

Address	Tel/Fax	E-mail	Add Information
Haldor Topsø esAllé 1 DK-2800 Kgs. Lyngby, Denmark	+45 45 27 20 00	topsoe@topsoe.dk	http://www.topsoe.com

Haldor Topsoe is a global market leader with 75 years of experience in heterogeneous catalysis. Our activities encompass R&D, process and plant design, catalyst production, sales and global supply, all backed by fundamental surface science, continual innovation and state-of-the-art support tools.

Stand № 16

PJSC SIBUR Holding

Address	Tel/Fax	E-mail	Add Information
16/1, Krzhizhanovskogo Str. Moscow, GSP-7, 117997, Russia	+7 (495) 777 5500	info@sibur.ru	http://sibur.com

SIBUR is a uniquely positioned gas processing and petrochemicals company with a business model focused on the integrated operation of its two core segments.

Stand № 17

Riogen

Address	Tel/Fax	E-mail	Add Information
107 Gilbreth Parkway, Suite 103, South Jersey Technology Park, Mullica Hill, NJ 08062	609-606-2012 609-228-8285	info@riogeninc.com	www.riogeninc.com

Riogen provides a range of supported noble and transition metal catalysts having high surface area and performance using carbon, alumina, silica, silica-alumina, titania, zirconia, ceria and zeolite supports in different forms. In addition to various ion-exchanged zeolites, we also supply catalyst or packed columns. Product quality is monitored regularly.

Stand № 18

hte GmbH – the high throughput experimentation company

Address	Tel/Fax	E-mail	Add Information
104, Kurpfalzring, Heidelberg, 69123, Germany	+49 (0) 62 21.74 97 - 0 +49 (0) 62 21.74 97 - 137	info@hte-company.de	http://www.hte-company.com

hte is a leading provider of high throughput technology and services for enhancing R&D productivity. Working with clients in the oil, chemical and petrochemical industry hte offers:

- R&D Solutions – research cooperations at hte's state-of-the-art laboratories in Heidelberg, Germany, and
- Technology Solutions – construction of customized high throughput reactor systems, installed and ready for use on site at the customer's premises.

Stand № 19

Petroleum Technology

Address	Tel/Fax	E-mail	Add Information
4-1A Leninskiy prospekt, Moscow, 119049 Russia	+7 (495) 232-26-82 +7 (495) 232-26-81	info@petro-technology.ru	http://www.petrotech.ru

Petroleum Technology is an integrated supplier of analytical equipment and turn-key laboratories for enterprises of oil refining and gas processing industries, oil producing industry, transport enterprises, scientific-research laboratories and metrology centers in CIS countries.

A range of available equipment includes the following: equipment for determining the quality of crude oil, petroleum and gas processing products; general purpose laboratory equipment; laboratory and office furniture; mobile laboratories for inspection control; modular complete laboratories. These laboratories are separate buildings equipped by internal plumbing installations, laboratory testing equipment, glassware and accessories for chemical analyses.

Stand № 20

RCC LABTEST, LLC

Address	Tel/Fax	E-mail	Add Information
38, Bolshoy Tishinskiy pereulok, Moscow, 123557, Russia	+7 (495) 605-35-07 +7 (495) 605-36-10	info@lab-test.ru	http://lab-test.ru

RCC LABTEST is an official dealer of QUANTACHROME and CILAS in Russia. Our products: Surface Area & Pore Size analyzers, High Pressure Gas Sorption instruments, Chemisorption, TPR/TPD instruments, Vapor Sorption analyzers, Liquid and Hg Pore Size analyzers, Pycnometers, Particle Size Laser Analyzers and other research instrumentation.

Stand № 21

Novomichurinsk Catalyst Plant LTD

Address	Tel/Fax	E-mail	Add Information
1, Promyshlennaya str., Novomichurinsk, 391160 Russia	+7 (49141) 4-11-35 +7 (49141) 2-23-31	mail@nkz-ooo.ru	http://www.nkz-ooo.ru

Novomichurinsk Catalyst Plant LTD is the actively developing company in the field of industrial production of chemicals.

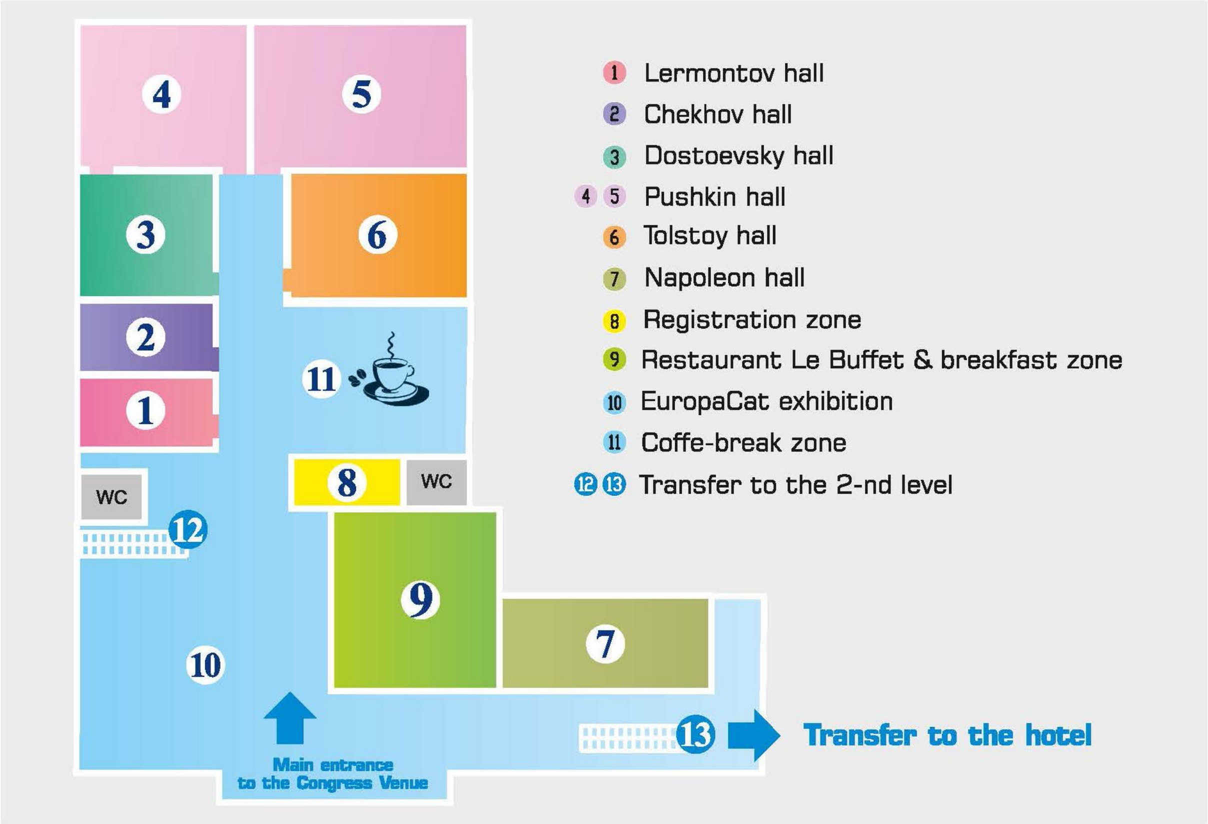
The main company activity is manufacture of catalysts for purification of gas from sulfur compounds based on aluminum oxide for chemical and petrochemical industry.

BRUKER LTD

Address	Tel/Fax	E-mail	Add Information
50/2 bld., Pyatnitskaya Str., Moscow, 1119017, Russia	+7 495 517-9284 (-85) +7 495 517-9286	ir@bruker.ru	http://www.bruker.com

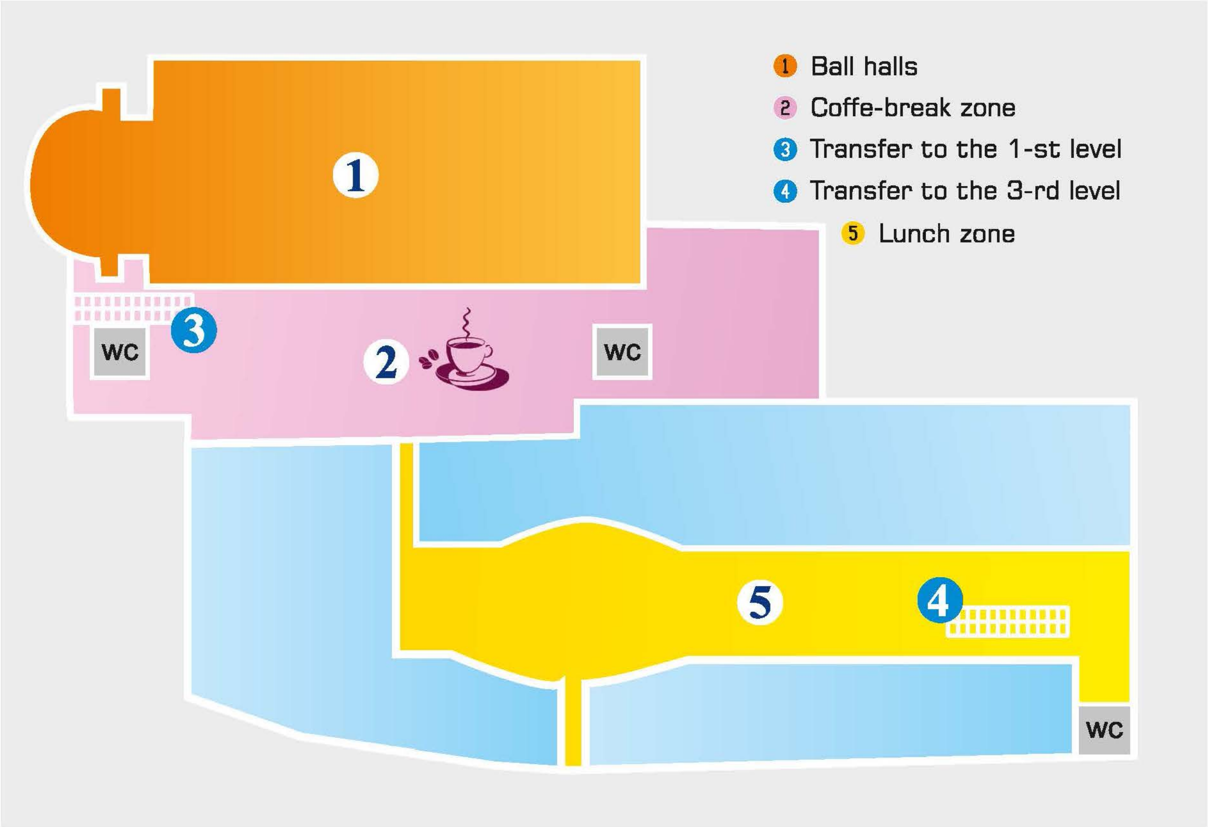
Bruker is a worldwide company which analytical systems cover a broad spectrum of applications in all fields of research and development and are used in all industrial production processes for the purpose of ensuring quality and process reliability.

1-st LEVEL OF THE CONGRESS VENUE



①	Lermontov hall
②	Chekhov hall
③	Dostoevsky hall
④ ⑤	Pushkin hall
⑥	Tolstoy hall
⑦	Napoleon hall
⑧	Registration zone
⑨	Restaurant Le Buffet & breakfast zone
⑩	EuropaCat exhibition
⑪	Coffe-break zone
⑫ ⑬	Transfer to the 2-nd level

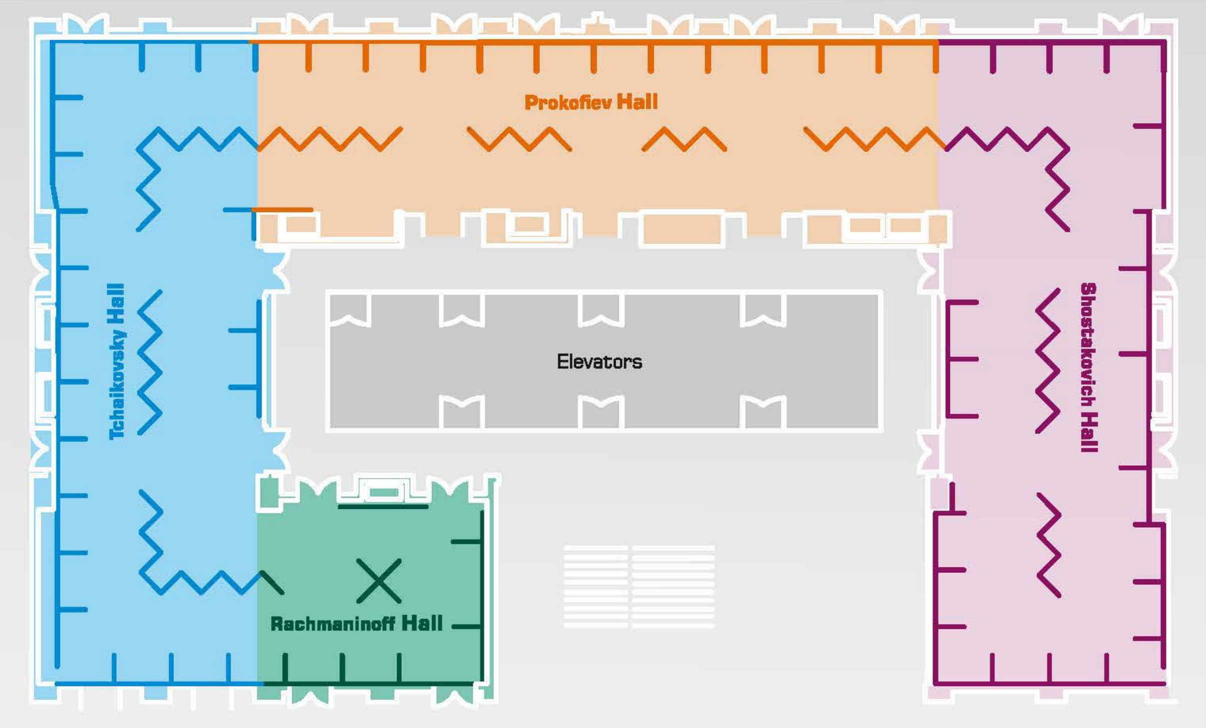
2-nd LEVEL OF THE CONGRESS VENUE



①	Ball halls
②	Coffe-break zone
③	Transfer to the 1-st level
④	Transfer to the 3-rd level
⑤	Lunch zone

POSTER SESSION

2-nd level of the Korston Tower

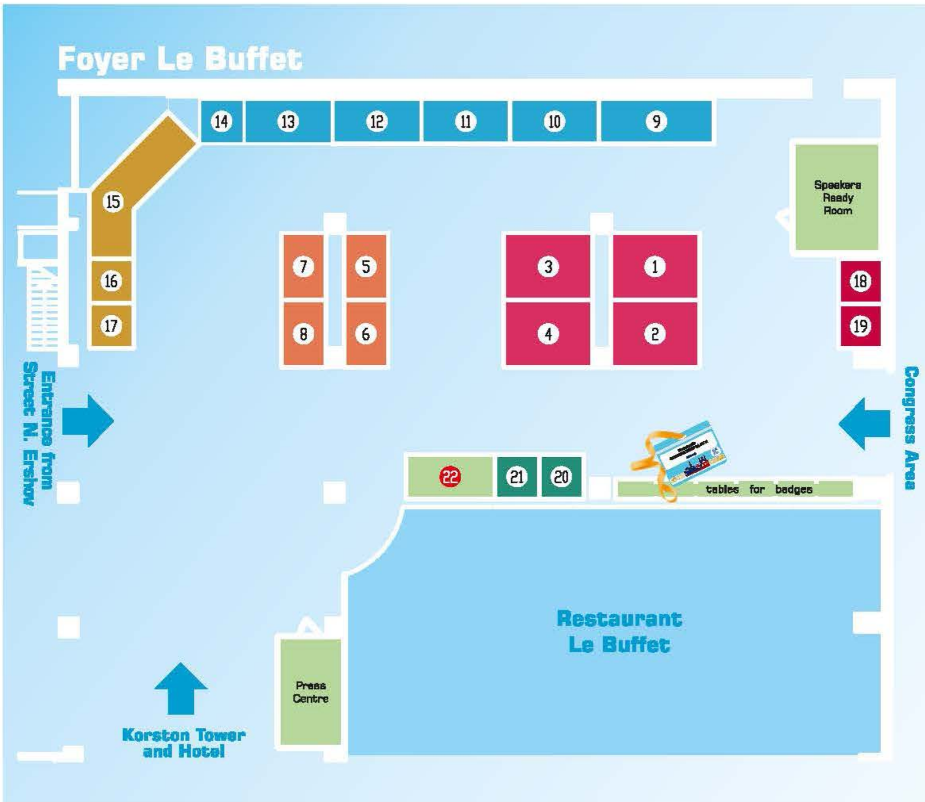


Poster Session-I (September 1) includes the presentations:
I-PP01 – I-PP114, III-PP01 – III-PP130,
IV-PP01 – IV-PP155, ISO-PP01 – ISO-PP30

Poster Session-II (September 2) includes the presentations:
II-PP01 – II-PP260, V-PP01 – V-PP150

EUROPACAT EXHIBITION

1-st level of the Congress Venue



① PJSC TATNEFT
② TAIF Group of Companies
③ PJSC NIZHNEKAMSKNEFTEKHIM
④ PJSC KAZANORGSINTEZ
⑤ Chromosib LTD
⑥ PROMENERGOLAB LLC
⑦ Sigma-Aldrich Rus LLC
⑧ Chemical Abstracts Service,CAS
⑨ Gelachem, group of companies
⑩ Parr Instrument Company
⑪ TETHIS SPA
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⑯ PJSC SIBUR Holding
⑰ Riogen
⑱ hte GmbH
⑲ Petroleum Technology
⑳ LABTEST
㉑ Novomichurinsk Catalyst Plant LTD
㉒ Exhibition administration