

2nd Sino-Russian Symposium on Chemistry and Materials

29 May – 1 June 2024, Skoltech, Moscow



Skoltech



N.D. Zelinsky Institute
of Organic Chemistry



Xinjiang Technical Institute
of Physics & Chemistry

<https://events.skoltech.ru/srscm>

Chairs of the organizing committee



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2nd SINO-RUSSIAN SYMPOSIUM ON CHEMISTRY AND MATERIALS

Final Program
& Book of Abstract

Moscow, May 29 – June 1, 2024

Skolkovo Institute of Science and Technology

SRSCM is a scientific event, focused on fostering collaboration and sharing advancements in the fields of chemistry and materials science. This symposium will provide opportunities for chemists, physicists and materials scientists to share their knowledge and expertise, and also build an exchange and cooperation platform for research scientists and industrial workers.

Main topics include:

- Crystal growth
- Catalysis
- Theory of materials
- Energy materials
- Non-linear optical materials
- Photo-chemistry
- Nanomaterials

SRSCM 2024

Symposium Schedule

Wednesday, May 29

- 12:00** Registration and badge pick-up
- 13:30 – 14:00 Opening Ceremony (chair Artem R. Oganov)**
Acad. Alexander Kuleshov, President of Skoltech
Acad. Stepan Kalmykov, Vice-president of RAS
Acad. Wu Zhaohui, Vice-president of CAS
- 14:00 - 14:20** Signing of agreements (Skoltech – XTIPC)
- 14:20 - 14:30** Group photo
- 14:30 – 15:00** Tea break
- 15:00 – 16:30 Plenary session (chair Dmitry Perekalin)**
- 15:00 – 15:45 Valentine Ananikov
"Designing new catalysts with artificial Intelligence"
- 15:45 - 16:30 Haohai Yu
"Electron-phonon coupling laser crystal research"
- 16:30 – 18:00 Plenary session (chair Congwei Xie)**
- 16:30 – 17:15 Shilie Pan
"New optoelectronic functional materials"
- 17:15 – 18:00 Artem R. Oganov
"Predicting and rationalizing novel compounds"
- 19:00** Gala dinner for speakers

Thursday, May 30**10:00 – 12:15 Plenary session (chair Haohai Yu)**

10:00 – 10:45 Gang Wang
"Surface nonlinear optical effect of topological semimetal"

10:45 – 11:30 Artem Abakumov
"How advanced transmission electron microscopy can contribute to battery research?"

11:30 – 12:15 Zhihua Yang
"Design of nonlinear optical materials"

12:15 – 13:30 Lunch**13:30 – 15:00 Plenary session (chair Valentine Ananikov)**

13:30 – 14:15 Sergey Streltsov
"Orbital effects in solids: basics, recent progress and opportunities"

14:15 – 15:00 Alexander Shapeev
"Machine learning interatomic interaction and beyond"

15:00 – 15:30 Tea break**Session 1: Crystal growth I (chair Dmitry Kvashnin)**

15:30 - 15:50 Junjie Li
"In-situ atomic scale observations on crystal nucleation and growth"

15:50 - 16:10 Mikhail Medvedev
"Building a digital twin of an ICP-CVD process"

16:10 - 16:30 Yadong Xu
"Controlled crystallization of centimeter-size organic semiconductor crystals"

16:30 - 16:50 Laishun Qin
"Halide crystal growth and scintillation for neutron-gamma dual readout"

16:50 - 17:10 Min Zhang
"Structural design and optical properties of novel inorganic photoelectric functional crystals"

- 17:10 - 17:30** Shanming Li
"Growth and properties of laser crystals for high-energy repetitive pulse lasers"

Session 2: Theory of Materials (chair Sergey Streltsov)

- 15:30 - 15:50** Sergey Levchenko
"AI-assisted discovery of composition-property relationships for materials design"
- 15:50 - 16:10** Di Sun
"Construction and evolution mechanism of hierarchical silver clusters"
- 16:10 - 16:30** Junwei Hu
"Exploring solid-solid phase transition using enhanced sampling methods"
- 16:30 - 16:50** Congwei Xie
"A prediction-driven database to enable rapid discovery of novel optoelectronic materials"
- 16:50 - 17:10** Dmitry Kvashnin
"Organic/inorganic heterostructures for optoelectronic application. computational study"
- 17:10 - 17:30** Sergey Lepeshkin
"Prediction of the structure and stability of molecules and clusters"

Session 3: Catalysis and Chemistry (chair Artem Abakumov)

- 15:30 - 15:50** Sergei Ponomarenko
"Organic semiconducting molecules as artificial retina pigments"
- 15:50 - 16:10** Xiao Dong
"High pressure induced of H₄O₂⁺ ion"
- 16:10 - 16:30** Dmitry Perekalin
"Asymmetric catalytic reactions using racemic rhodium complexes"
- 16:30 - 16:50** Xiang-Feng Zhou
"Hard copper boride with exceptional conductivity"

- 16:50 - 17:10** Vitaly Korepanov
"Synthetic approaches to 2D polymeric phthalocyanines"
- 17:10 - 17:30** Konstantin Bryliakov
"Biomimetic chemistry toolbox for direct C(sp³)-H
heterofunctionalizations"
- 17:30 - 19:00** **Poster session**
- 19:00 – 21:00** Fourchette dinner for all participants

Friday, May 31

10:30 – 12:00 Plenary session (chair Artem Oganov)

10:30 – 11:15 Vladimir Fedin

"Chemical design and functional properties of porous coordination polymers"

11:15 – 12:00 Haiyang Niu

"Investigation of material phase transition based on deep learning advanced molecular dynamics"

12:00 – 13:00 Lunch

13:00 - 20:00 Visits of Moscow (Moscow State University, Kremlin and Red Square, VDNKh) and of Skoltech and Skolkovo Innovation Center

Saturday, June 1**10:30 – 11:15 Plenary session (chair Haiyang Niu)**

10:30 – 11:15 Albert Nasibulin

"SWCNT transparent conducting films: towards the theoretical limit"

11:15 – 12:00 Vladimir Pudalov

"Progress, problems and prospects of room-temperature superconductivity"

12:00 – 13:30 Lunch**Session 4: Energy materials (chair Alexander Kvashnin)**

13:30 - 13:50 Tao Fan

"Machine learning and DFT for the search for thermoelectric materials"

13:50 - 14:10 Alexey Lukoyanov

"Novel magnetocaloric materials GdTX for energy applications"

14:10 - 14:30 Zhengyang Zhou

"Determination of controversial structures in thermoelectric materials through 3D electron diffraction"

14:30 - 14:50 Victor Abruks

"Neural networks for development of advanced solid rocket propellant in the framework of materials genome initiative conception"

Session 5: Non-linear optical materials (chair Larisa Shvanskaya)

13:30 - 13:50 Miriding Mutailipu

"Hydroxyfluorooxoborates: a fresh opportunity for borate chemistry"

13:50 - 14:10 Qi Wu

"Exploration of semi-organic nonlinear optical crystal materials"

14:10 - 14:30 Ivan Kruglov

"AI-guided screening of novel nonlinear optical materials"

14:30 - 14:50 Mingxia Xu

"Progress on DKDP crystals for high power laser system application"

Session 6: Chemistry and photochemistry (chair Vladimir Fedin)

- 13:30 - 13:50** Alexey Tarasov
"Perovskite chemistry and engineering at the Faculty of Materials Science of Moscow State University"
- 13:50 - 14:10** Mariia Fedyaeva
"Boron-containing "magic" clusters"
- 14:10 - 14:30** Huan Ye
"Photochemistry and geologic significance of elemental sulfur"
- 14:30 - 14:50** Alexander Dilman
"Synthetic methods: from fluorine chemistry to photocatalysis"
- 14:50 - 15:20** Tea break

Session 7: Hot Topics I (chair Alexey Emeline)

- 15:20 – 15:40** Yuntao Wu
"Low-Dimensional all-inorganic Cu(I) halide single crystals as efficient X- and gamma-ray scintillators"
- 15:40 – 16:00** Alexander Korsunsky
"Rational experimental-computational correlation (RECC)"
- 16:00 – 16:20** Dmitry Krasnikov
"Multi-level organization of carbon nanotubes for advanced THz optics"

Session 8: Crystal growth and crystallography II (chair Miriding Mutalipu)

- 15:20 – 15:40** Xiuhong Pan
"Progress of crystal growth under microgravity in China"
- 15:40 – 16:00** Tao Wang
"Growth and applications of Cd-Zn telluride single crystals in advanced radiation detector technologies"
- 16:00 – 16:20** Elena Belokoneva
"Topology-symmetry analysis of inorganic crystals: structures and properties prediction"

Session 9: Theory of materials II (chair Alexander Shapeev)

- 15:20 – 15:40** Elizaveta Vaneeva

"Prediction of the stability and abundance of organic molecules"

Ludmila Bereznikova

"Application of graph neural networks to search for new deep-ultraviolet nonlinear optical materials"

15:40 – 16:00 Nikita Rybin

"Calculating thermophysical properties of liquid electrolytes using moment tensor potential"

Alexey Maltsev

"Prediction of new materials for battery applications"

16:00 – 16:20 Yu Xie

"Machine-learning aided material simulation software ARES and its applications"

16:20 – 16:50 Tea break

S10: Magnetic materials (chair Dmitry Krasnikov)

16:50 – 17:10 Mojtaba Alaei

"Benchmarking DFT on the prediction of antiferromagnetic transition temperatures"

17:10 – 17:20 Larisa Shvanskaya

"How the archetypes of minerals inspire us to create new magnetic materials"

17:20 – 17:50 Anhua Wu

"Preparation and spin reorientation transition of mixed rare-earth composite orthoferrite $\text{Sm}_x\text{R}_{1-x}\text{FeO}_3$ crystals"

S11: Breakthrough materials (chair Mikhail Medvedev)

16:50 – 17:10 Alexey Emeline "Effects of intrinsic defects on optical behavior of halide perovskites"

17:10 – 17:20 Alexander Kvashnin "Higher tungsten boride and its application in catalysis"

17:20 – 17:50 Elena Obratsova "One-dimensional graphene nanomaterials for laser physics"

17:50 – 18:10 **Closing ceremony. Best poster awards.**

List of Posters

Thursday, May 30**Poster session**

- P1 Abduragimov Bayram**
"Growth of single crystals of $\text{CoSiF}_6 \times 6\text{H}_2\text{O}$ and $\text{NiSiF}_6 \times 6\text{H}_2\text{O}$ from aqueous solutions and study of some of their properties"
- P2 Akhmadeev Albert**
"Influence of the molybdenum on the transport and mechanical properties of the perovskite-like lanthanum nickelates doped with cobalt and iron"
- P3 Arakelyan Liana**
"Towards a Comprehensive Database: Exploring the Cytotoxicity of Ionic Liquids"
- P4 Bahrami Faezeh**
"A study of crystal structure prediction: A pharmaceutical compound"
- P5 Bashirov Igor**
"Biased molecular dynamics based on diffraction patterns difference"
- P6 Basov Bogdan**
"Plasma Polarization of Polyvinylidene Fluoride Films"
- P7 Bespalov Ivan**
"Bayesian optimization for conformational search"
- P8 Burov Arseniy**
"Validation of machine-learning potentials for diffusion modeling in systems with metal/insulator interfaces"
- P9 Buryanskaya Evgeniya**
"The effect of electric aging on vinylidene fluoride copolymers for ferroelectric memory"
- P10 Chen Luyi**
"Synthesis of new hybrid halocuprates for X-Ray scintillation detectors"
- P11 Chepkasov Ilya**
"Structure-driven tuning of O and CO adsorption on AuCu nanoparticles: A density functional theory study"
- P12 Cherepanova Vera**
"Study of the dynamics of nanoscale systems on the surface of carbon materials under conditions of catalytic cross-coupling processes"

- P13 Chernyshev Victor**
"Improving the stability and activity of Pd/NHC catalytic systems with a new NHC ligand design"
- P14 Davydov Nikita**
"Impact of high symmetry grain boundaries on oxygen stability in LiNiO₂"
- P15 Dembitskiy Artem**
"Stability, electrochemical window, and Na-ion conductivity of NaGaPO₄F solid electrolyte"
- P16 Erokhin Kirill**
"Analysis of the materials used for additive technologies in agriculture"
- P17 Erzunov Dmitrii**
"Novel High-Efficient Catalysts and Photocatalysts Based on Metal Phthalocyanines for Medical Purposes"
- P18 Fedyaeva Maria**
"Investigation of the structure and stability of boron-carbon clusters"
- P19 Gavryushkin Pavel**
"Carbonates with sp³-hybridised carbon atoms stable at pressure above 5 GPa"
- P20 Geondzhian Andrey**
"Electronic structure of cathode material LiNiO₂"
- P21 Gordeev Evgeniy**
"Theoretical study of reductive elimination reactions in palladium(II) complexes leading to carbon-carbon and carbon-heteroatom bond formation"
- P22 Grebeniuk Maksim**
"High-temperature superconductivity in Ca–Y–H system"
- P23 Grudova Mariya**
"Comparison of dynamic transformations and catalytic activity of copper (I) and gold (I) complexes"
- P24 Gudymenko Alexey**
"Crystals of complex cobalt chlorides with CoCl₄²⁻ anions in structure"
- P25 Iosimovska Anastasiia**
"Thermodynamic Stability and Ionic Conductivity in Lithium-Germanium Binary System"

- P26 Iskhakova Elvina**
"Stands for Measuring Piezoelectric Coefficients of PVDF Films"
- P27 Jalolov Faridun**
"Mechanical properties of single and polycrystalline solids from machine learning"
- P28 Kharitonov Vladimir**
"Diphenylcyclopentadienyl rhodium complexes as highly active catalysts for the formation of naturally occurring scaffolds via C-H activation"
- P29 Kharkova Anna**
"Bionanocomposite for phenol measurement"
- P30 Khrizanforov Mikhail**
"Ferrocene based ligands for the creation of redox-switchable catalysts. Synthesis, structure, properties"
- P31 Komornikov Vladimir**
"Crystal growth of Nickel&Cobalt Chlorides and its spectral characteristics"
- P32 Korabelnikova Victoria**
"Catalytic reaction of transfer hydrogenation in the flow system of FFF-reactors"
- P33 Kotelevskaya Ekaterina**
"Assessment of the ability of the twin boundary in fluorite to capture rare earth elements. Quantum-chemical modeling"
- P34 Koval Olga**
"Self-catalyzed GaPN nanowire array into PDMS-based platform: optical studies"
- P35 Kovaleva Olga**
"Investigation of polaron conductivity in cathode materials for Na- and K-ion batteries"
- P36 Kozlov Kirill**
"Synthesis of wyerone compounds from 5-(hydroxymethyl)furfural"
- P37 Kozlova Natalya**
"Growth specifics of GUHP single crystal for terahertz applications"
- P38 Kravtsov Konstantin**
"Ab Initio Raman spectra for vdw materials"

- P39 Kulikova Olga**
"Self-assembly of AgInS/ZnS core/shell quantum dots with tetrapyrrole-type photosensitizers: biomedical applications"
- P40 Kulishov Artem**
"Trans-stilbene single crystals: growth from solution and scintillation properties"
- P41 Li Yang**
"Several defects in KDP crystal which related to its laser damage performance: hybrid density functional theory calculations"
- P42 Lubimova Anastasia**
"Photosensitive Memristive Behavior in Hybrid Metal-Organic Framework/Perovskite structure"
- P43 Lukanov Mikhail**
"Phase distribution in high-entropy alloys of TiNbZrTaTiC₅ obtained in terms of graph representation approach"
- P44 Matveeva Diana**
"Double chlorides Rb₂MCl₄·2H₂O (M = Co²⁺, Ni²⁺): growth, structure and optical properties"
- P45 Mikhailova Anastasiia**
"Reaction barriers for CO oxidation in Cu–Au nanoclusters"
- P46 Miryashkin Timofey**
"Learning Phase Diagrams from Thermodynamic Data with Uncertainty Propagation"
- P47 Mirzaeva Sabina**
"DiZyme Assistant as an example using ML in nanozyme experiments design"
- P48 Momenzadeh Abardeh Zahrasadat**
"Co-crystal Structure Prediction of N-Halide Phthalimides with 35DMP"
- P49 Nelkenbaum Konstantin**
"Development of additives that improve the lubricating and oxidizing properties of diesel fuel"
- P50 Nematov Dilshod**
"Thermodynamic properties and phase transitions of CsSnI₃: implementation of the SCAN exchange-correlation functional"

- P51 Pasechnik Liliya**
"Crystallization of coordination sulfates of scandium and alkali metals or ammonium and their functional properties"
- P52 Poletaev Daniil**
"SSCHA-based evolutionary crystal structure prediction at finite temperatures with account for quantum nuclear motion"
- P53 Popov Zakhar**
"Noncarbon 2D materials for solar hydrogen production"
- P54 Popova Elena**
"Structure and properties of Mg - containing solid solutions based on Y₂FeTaO₇"
- P55 Prilipko Sergei**
"Sintering mechanisms of α - and γ - Al₂O₃ nanopowders with the addition of Bi₂O₃"
- P56 Prolomov Ilya**
"From humorous post to detailed quantum-chemical study: isocyanate synthesis revisited"
- P57 Provotorova Daria**
"Tuning surface morphology of polymeric materials for the purpose of biofouling control"
- P58 Radina Aleksandra**
"Embrittlement of lead telluride from a chemical bonding point of view"
- P59 Raskildina Gulnara**
"Synthesis of polyfunctional compounds by low-temperature ozonation of linear and cyclic compounds"
- P60 Razlivina Julia**
"AI-based Prediction of Multiple Catalytic Activities"
- P61 Rezaei Nafiseh**
"ESpinS: A program for classical Monte-Carlo simulations of spin systems"
- P62 Rudakovskaya Polina**
"Engineering of ultrasound microbubbles by tuning the structure"
- P63 Rudneva Tatiana**
"Polymeric phthalocyanines synthesized in high boiling solvent"

- P64 Rybkovskiy Dmitry**
"Structure and stability of Li-P nanoclusters"
- P65 Samatov Mikhail**
"Studies of the influence of grain boundary dynamics on the properties of CsPbBr₃ perovskite"
- P66 Savchenko Artem**
"Light promoted functionalization of alkenes enabled by polyfluoroaryl group transfer"
- P67 Selivanov Nikita**
"Synthesis of single crystals and study of the optical properties of NH₄Pb₂Br₅, a perspective material for application in photonics and optoelectronics"
- P68 Setkova Tatiana**
"Ga,Ge-analogues of minerals as advanced materials"
- P69 Shaydullin Ruslan**
"High-temperature method of carrying out organic reactions with a high energy barrier"
- P70 Shekhovtsova Anna**
"Self-assembly of silver nanoparticles at the liquid-liquid interface as scaffold for new generation of Raman sensors"
- P71 Shepovalov Kirill**
"Spiroconjugated molecules: structural, electronic, topological and optical properties"
- P72 Sidnov Kirill**
"Novel deep learning approach for a crystal structure prediction"
- P73 Sokolov Petr**
"Utilizing digital light processing 3D printing for compacting in the production of transparent GYAGG:Ce ceramics"
- P74 Sokov Sergey**
"Functional derivatives of 1,3-Dioxacyclohexanes as starting materials for acid corrosion inhibitors"
- P75 Sukhanova Ekaterina**
"Reversible band alignment transformations in heterostructures for novel biomimetic devices"
- P76 Surzhikova Iana**

"A novel photoactive palladium N-heterocyclic carbene complex and its application in the photocatalytic reaction"

P77 Tamboura Mamadou

"Impact of ultraviolet radiation on graphene structure"

P78 Tarakanovskaya Darya

"Modeling the properties of multi-resonance thermally activated delayed fluorescence materials based on B,N-heteroarenes using quantum chemical calculation and neural networks"

P79 Tedzhetov Valentin

"Structural Metastability and Specific Magnetic State of FeTiB Films"

P80 Timakov Ivan

"Crystal growth of $\text{Cs}_6(\text{SO}_4)_3(\text{H}_3\text{PO}_4)_4$ and preparation of functional materials based on it"

P81 Trukhan Elena

"Application of Deep reinforcement learning to accelerate ionic optimization in structure relaxation"

P82 Ustinova Irina

"Synthesis and dielectric properties of new complex oxide $\text{La}_{1.7}\text{Sr}_{0.3}\text{Ni}_{0.8}\text{Cu}_{0.2}\text{O}_4$ "

P83 Vavilina Regina

"Formation of new structures based on single-walled carbon nanotubes with superacids"

P84 Vildanova Aliya

"Novel approach of obtaining nickel nanowires inside carbon nanotubes"

P85 Yu Yaochen

"The Nucleation of Metastable Ice in Silver Iodide Dipole Field"

P86 Yurasik Georgy

"Improving the electrical properties of thin crystalline pentacene films by annealing them in an inert atmosphere"

P87 Yzhikova Karina

"Programmed synthesis of Co_3O_4 -ZnO heterostructures"

P88 Zaytsev Roman

"Machine learning models in analyzing particle placement on a multilayer surface"