



**International Workshop
on Chemical Crystallography and Structural Biology
“*The Third Struchkov Meeting*”**

dedicated to the 95th Birth Anniversary of Yuri T. Struchkov

Moscow • November 15-19, 2021

**Scientific Program
(*online*)**

<https://struchkovprizeassociation.org/2021-struchkov-society-meeting/>

Moscow Time • JCT+6 • CST+5 • GMT+3 • IST+2.30 • CET+1 • EST-8

JCT – Japan; CST – China; GMT – Portugal; IST – India; CET – France; EST – New York

Monday • November 15, 2021

/ Moscow – 10:00 / London – 07:00 / New York – 02:00 / Tokyo – 16:00 /

10 00–11 00	Workshop Opening • Moscow Time
10 00–10 20	Victor N. Khrustalev (Conference Chair)
10 20–10 30	Igor L. Eremenko (Chair of Program Committee)
10 30–10 40	Leonid G. Voskressensky (Dean of Faculty of Science, RUDN University)
10 40–10 50	Tatiana V. Timofeeva (Member of Program Committee)
10 50–11 00	Leonid A. Aslanov (Member of <i>Struchkov Prize</i> Association)
Session A	Chair: Victor N. Khrustalev; Working language – <i>Russian/English • Moscow Time</i>
11 00–11 45	Plenary – Commemorative <i>Yuri Timofeevich Struchkov: Commemorating 95th Birthday</i> Yuri L. Slovokhотов Institute of Control Science RAS (Moscow, Russia)
11 45–12 30	Plenary <i>Fluoride-phosphates with the KTP-type structure as perspective cathode materials for metal-ion batteries</i> Evgeny V. Antipov Lomonosov Moscow State University (Moscow, Russia)
12 30–13 15	Plenary <i>Pushing the Limits: Orbital-Free Quantum Crystallography</i> Vladimir G. Tsirelson Mendeleev University of Chemical Technology (Moscow, Russia)
13 15–14 00	Plenary <i>Proton transfer in 3d metal carboxylates</i> Sergei E. Nefedov Kurnakov Institute of General and Inorganic Chemistry RAS (Moscow, Russia)
14 00–15 00	LUNCH
Session B	Chair: Igor A. Litvinov; Working language – <i>Russian/English • Moscow Time</i>
<i>Struchkov Prize-2020 Session</i>	
15 00–15 30	Keynote <i>X-ray diffraction study of structural organization of the unsubstituted and substituted phthalocyanine thin films</i> Alexander S. Sukhikh Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk, Russia)
15 30–16 00	Keynote <i>(Thia)calix[4]arenes and their functional derivatives as versatile molecular building blocks for rational design of crystalline materials</i> Alexander S. Ovsyannikov Arbuzov Institute of Organic and Physical Chemistry RAS (Kazan, Russia)
16 00–16 30	Keynote <i>Structural diversity of rhenium(I) complexes: approaches to fine-tuning photophysical behavior</i> Kristina S. Kisel Saint Petersburg State University (Saint Petersburg, Russia)
16 30–17 00	Keynote <i>Synthesis of Novel Cationic 1,2,4-Selenadiazoles via Addition of 2-Pyridylselenyl Halides to Unactivated Nitriles</i> Alexander G. Tskhovrebov RUDN University (Moscow, Russia)
17 00–19 00	Round Table “Advances in the Modern X-Ray Structural Analysis” dedicated to the 70th Birth Anniversary of Mikhail Yu. Antipin Anna V. Vologzhanina Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)

Tuesday • November 16, 2021

/ Moscow – 10:00 / London – 07:00 / New York – 02:00 / Tokyo – 16:00 /

Session C	<u>Chair: Yan V. Zubavichus</u> ; Working language – English • Moscow Time
10 00–10 45	Plenary <i>Crystal Engineering in Chemistry and Society</i> Gautam R. Desiraju Indian Institute of Science (India)
10 45–11 30	Plenary <i>Silver Nanoclusters</i> Di Sun Shandong University (China)
11 30–12 15	Plenary <i>Iron oxide nanoparticles and nanocomposites: their biosafety and applications</i> Yannick Guari University of Montpellier (France)
12 15–13 00	Plenary <i>Metal Coordination Catalysis of Selected Small Molecules towards Sustainability</i> Armando J. L. Pombeiro University of Lisbon (Portugal)
13 00–13 45	Plenary <i>Receptor Tyrosine Kinase KIT: A New Look for an Old Receptor</i> Luba Tchertanov Centre Borelli, CNRS – ENS Paris-Saclay (France)
13 45–14 15	Keynote <i>Titanium phenoxides and phosphonates as molecular models and molecular precursors of hybrid oxide materials</i> Vadim G. Kessler Swedish University of Agricultural Sciences (Sweden)
14 15–15 15	LUNCH
Session D	<u>Chair: Alexander G. Tskhovrebov</u> ; Working language – English • Moscow Time
15 15–16 00	Plenary <i>Synthetic Chemistry with Laughing Gas</i> Kay Severin Ecole Polytechnique Fédérale de Lausanne – EPFL (Switzerland)
16 00–16 45	Plenary <i>Supramolecular crystallography</i> Kari Rissanen University of Jyväskylä (Finland)
16 45–17 30	Plenary <i>Accessing micro- and macroscopic pictures of gas adsorption by <i>in situ</i> powder diffraction</i> Yaroslav Filinchuk Université catholique de Louvain (Belgium)
17 30–18 00	Keynote <i>Some examples of Co(II), Zn(II), Cd(II) and Cu(I) coordination polymers with inclusion and luminescent properties</i> Marina S. Fonari Institute of Applied Physics (Moldova)
18 00–18 30	Keynote <i>Back to the Roots – Dress Chemistry in Green</i> Adam Slabon Stockholm University (Sweden)
18 30–19 00	Keynote <i>Structural Chemistry of Azulenes</i> Nick Gerasimchuk Missouri State University (USA)

Wednesday • November 17, 2021

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Session E	<u>Chair: Andrey S. Kritchenkov</u> ; Working language – English • Moscow Time
10 00–10 45	Plenary <i>Prussian blue type nano-objects: new opportunities for old materials</i> Joulia Larionova University of Montpellier (France)
10 45–11 30	Plenary <i>Well-defined silsesquioxanes with novel structures</i> Masafumi Unno Gunma University (Japan)
11 30–12 15	Plenary <i>4th Generation Synchrotron Radiation Facility SKIF: New Prospects for Small-Molecule and Macromolecular Crystallography in Russia</i> Yan V. Zubavichus Boreskov Institute of Catalysis SB RAS (Novosibirsk, Russia)
12 15–13 00	Plenary <i>Functional Metal-Organic Architectures: from Self-Assembly in Water to Applications</i> Alexander M. Kirillov University of Lisbon (Portugal)
13 00–13 45	Plenary <i>Many Faces of a Cubooctahedron: A Journey of an Intermetallic Fragment from Simple structures to Complex Arrangements</i> Alexey N. Kuznetsov Lomonosov Moscow State University (Moscow, Russia)
13 45–14 30	Plenary <i>Structural chemistry of polynuclear complexes of transition metals</i> Dmytro S. Nesterov University of Lisbon (Portugal)
14 30–15 30	LUNCH
Session F	<u>Chair: Igor S. Antipin</u> ; Working language – Russian/English • Moscow Time
15 30–16 15	Plenary <i>Structure and reactivity of transition metal tetrahydroborates and their dihydrogen bonded complexes</i> Natalia V. Belkova Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
16 15–17 00	Plenary <i>Supramolecular Interactions in the Condensed State on the Example of Bispidines</i> Sergey Z. Vatsadze Zelinsky Institute of Organic Chemistry RAS (Moscow, Russia)
17 00–17 45	Plenary <i>Statistical and local structure of large-sized multifunctional single crystals</i> Galina M. Kuzmicheva MIREA – Russian Technological University (Moscow, Russia)
17 45–18 30	Plenary <i>Charge density distribution of APIs in crystals and ligand-receptor complexes</i> Alexander A. Korlyukov Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
18 30–19 00	Keynote <i>Molecular and supramolecular design of cagelike metallacompounds based on sil- and germsesquioxane ligands. Synthesis, structure, properties</i> Alexey N. Bilyachenko Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)

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Session G	<u>Chair: Vladimir A. Larionov</u> ; Working language – <i>Russian/English • Moscow Time</i>
Young scientist Session	
10 00–10 20	Oral <i>The tetrานuclear lanthanide-based silsesquioxanes: synthesis, structure and properties</i> Alena N. Kulakova RUDN University (Moscow, Russia)
10 20–10 40	Oral <i>High-resolution powder diffraction with the scanning 2D detector at the «XSA» beamline of Kurchatov synchrotron radiation source</i> Roman D. Svetogorov National Research Centre “Kurchatov Institute” (Moscow, Russia)
10 40–11 00	Oral <i>Crystal structure of low-melting organoelement compounds</i> Alexander D. Volodin Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
11 00–11 15	Oral <i>Salts of nucleobases and alkali metals: preparation and structural study at broad range of T, P</i> Anna A. Gaydamaka Novosibirsk State University (Novosibirsk, Russia)
11 15–11 30	Oral <i>The influence of experimental setup on the thermal expansion of glycinium phosphite</i> Nikita E. Bogdanov Boreskov Institute of Catalysis SB RAS (Novosibirsk, Russia)
11 30–11 45	Oral <i>The crystal structure elucidation of a tetrapeptide analogue of somatostatin DOTA-Phe-D-Trp-Lys-Thr-OMe</i> Sabina E. Diusenova Boreskov Institute of Catalysis SB RAS (Novosibirsk, Russia)
11 45–12 00	Oral <i>Structure investigation of bismuth-containing binary apatite system</i> Evgeny N. Bulanov Lobachevsky University (Nizhny Novgorod, Russia)
12 00–12 15	Oral <i>Distribution of electron density in luminescent and magnetic coordination compounds. Molecular and crystal invariom approaches</i> Roman V. Rumyantsev Razuvaev Institute of Organometallic Chemistry RAS (Nizhny Novgorod, Russia)
12 15–12 30	Oral <i>Computer Modeling in Chemistry: Reactivity and Non-Covalent Interactions</i> Alexander S. Novikov Saint Petersburg State University (Saint Petersburg, Russia)
12 30–12 45	Oral <i>Novel heterocyclic chitosan derivatives and their derived nanoparticles</i> Niyaz Z. Yagafarov RUDN University (Moscow, Russia)
12 45–13 00	Oral <i>Structural studies of chitosan and its composites with iron (II) hydroxide and sulfate</i> Yana V. Sultanova RUDN University (Moscow, Russia)

13 00–13 15	Oral <i>Synthesis and structural investigation of new aryl- and heteroaryl gold(I) isocyanide complexes</i> Maria V. Grudova RUDN University (Moscow, Russia)
13 15–13 30	Oral <i>Features of supramolecular organization in the crystals of benzimidazolone derivatives</i> Aida I. Samigullina Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
13 30–14 30	LUNCH
Session H	Chair: Yuri L. Slovokhotov ; Working language – English • Moscow Time
14 30–15 00	Keynote <i>Chiral metal-templated Co(III) complexes as a powerful class of catalysts</i> Vladimir A. Larionov Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
15 00–15 30	Keynote <i>Structure-driven possibilities and challenges: from heterogeneous catalysis to extracellular matrix glycation</i> Alexey V. Kletskov RUDN University (Moscow, Russia)
15 30–15 45	Oral <i>Palladium-based reagents for protein bioconjugation</i> Ivan V. Buslov RUDN University (Moscow, Russia)
15 45–16 00	Oral <i>Ultrasound-mediated synthesis of Co/Al layered double hydroxide</i> Nbutsu D. Sikaona Shared with RUDN University (Zambia)
16 00–19 00	Master Class on OLEX2 “A complete structure solution and analysis program” Ilia A. Guzei University of Wisconsin-Madison (USA)

Friday • November 19, 2021

/ Moscow – 10:00 / London – 07:00 / New York – 02:00 / Tokyo – 16:00 /

Session I	<u>Chair: Vitaly K. Belsky</u> ; Working language – <i>Russian/English • Moscow Time</i>
10 00–10 30	Keynote <i>High-pressure X-ray diffraction experiments and data reduction: the difference from ambient pressure studies and factors influencing the data quality</i> Boris A. Zakharov Boreskov Institute of Catalysis SB RAS (Novosibirsk, Russia)
10 30–11 00	Keynote <i>Ultrasound-mediated polymer-analogous reactions in the chitin and chitosan chemistry</i> Andrei S. Kritchenkov Institute of Technical Acoustics NASB (Belarus)
11 00–11 30	Keynote <i>Platinum and palladium-based heterometallic carboxylic complexes. New approaches to the synthesis and X-ray synchrotron radiation crystallography studies</i> Ilia A. Yakushev Kurnakov Institute of General and Inorganic Chemistry RAS (Moscow, Russia)
11 30–11 50	Oral <i>Synthesis and crystal structure of the zinc complex of cildenafil citrate (Viagra®)</i> Vakhab Kh. Sabirov Tashkent State Technical University (Uzbekistan)
11 50–12 10	Oral <i>NMR spectroscopy and X-Ray crystallography at the investigations of conformationally non-rigid molecules</i> Ibrahim G. Mamedov Baku State University (Azerbaijan)
12 10–12 30	Oral <i>Fuzzy sets in chemical crystallography</i> Yuri L. Slovokhotov Institute of Control Science RAS (Moscow, Russia)
12 30–13 30	Workshop Closing • Moscow Time
	Concluding remarks of Chairmen and Members of the Program and Organizing Committees