

# International Workshop on Chemical Crystallography and Structural Biology “The Second Struchkov Meeting”

## Scientific Program

<https://struchkovprizeassociation.org/2nd-struchkov-readings/>

**Monday November 12, 2018** (Ordzhonikidze Street, 3)

9 00–18 00	<b>REGISTRATION</b> ( <i>Science Faculty Hall</i> )
10 00–14 00	<b>Master Class on OLEX2</b> ( <i>Computer Class</i> ) “A complete structure solution and analysis program” <i>Iliia A. Guzei</i> University of Wisconsin-Madison (USA)
14 00–15 00	<b>Lunch</b>
15 00–18 00	<b>Round Table</b> ( <i>Room 102</i> ) “Advances in the modern X-ray structural analysis” <i>Sergey V. Lindeman</i> Marquette University (USA)

**Tuesday November 13, 2018** (Miklukho-Maklay Street, 6)

	<b>Workshop Opening</b>
9 30–9 40	<i>Vladimir M. Filippov</i> (Conference Chair)
9 40–9 45	<i>Igor L. Eremenko</i> (Co-Chair of Program Committee)
9 45–9 50	<i>Mikhail V. Kovalchuk</i> (Co-Chair of Program Committee)
9 50–9 55	<i>Tatiana V. Timofeeva</i> (Member of Program Committee)
9 55–10 00	<i>Leonid A. Aslanov</i> (Co-Chair of Organizing Committee)
<b>Session A</b>	<b>Session Chairs: Alexander V. Virovets (Russia), Tatiana V. Timofeeva (USA)</b>
10 00–10 45	<b>Plenary</b> <i>Yu. T. Struchkov and his role in the development of organic crystallochemistry in the territory of the former Soviet Union</i> <i>Igor A. Litvinov</i> Arbuzov Institute of Organic and Physical Chemistry RAS (Kazan, Russia)
10 45–11 30	<b>Plenary</b> <i>The Struchkov Group and Crystallographic Instrumentation Development</i> <i>Susan Byram</i> Bruker (USA)
11 30–12 00	<b>Coffee Break</b>
12 00–12 45	<b>Plenary</b> <i>Effect of wax crystallinity on oil production</i> <i>Olga E. Lindeman</i> Ecolab, Energy Services Department (USA)
12 45–13 30	<b>Plenary</b> <i>Tenses of Service Crystallography. Past – Perfect. Present – Continuous. Future – Indefinite?</i> <i>Arkady M. Ellern</i> Iowa State University (USA)
13 30–14 30	<b>Lunch</b>
<b>Session B</b>	<b>Session Chairs: Igor A. Litvinov (Russia), Olga E. Lindeman (USA)</b>
14 30–15 15	<b>Plenary</b> <i>Click reactions + ultrasound = a new aurora of chitosan chemistry</i> <i>Andrei S. Kritchenkov</i> Institute of Technical Acoustics, National Academy of Sciences of Belarus (Belarus)

15 15–16 00	<b>Plenary</b> <i>Editorial advice for authors</i> <b>Ganna B. Lyashenko</b> Chemistry – A European Journal, Wiley-VCH (Germany)
16 00–16 30	<b>Coffee Break</b>
16 30–17 15	<b>Plenary</b> <i>Model study of the structure of supramolecular complexes of glycyrrhizic acid and its monoammonium salt (glycyram)</i> <b>Bolot K. Sadybakasov</b> Kyrgyz-Russian Slavonic University (Kyrgyzstan)
17 15–18 00	<b>Plenary</b> <i>Crystal structure of some iron(II,III) sulfate solid solutions and forbidden by symmetry X-ray reflections</i> <b>Vakhob K. Sabirov</b> Auezov South-Kazakhstan State University (Kazakhstan)
18 30–20 30	<b>Welcome Cocktail</b>

**Wednesday November 14, 2018** (Ordzhonikidze Street, 3, Science Faculty Club)

<b>Session C</b>	<b>Session Chairs: Igor S. Antipin (Russia), Bolot K. Sadybakasov (Kyrgyzstan)</b>
10 00–10 45	<b>Plenary</b> <i>Structural chemistry of cyanoximes and their metal complexes</i> <b>Nikolay N. Gerasimchuk</b> Missouri State University (USA)
10 45–11 30	<b>Plenary</b> <i>How conformational dynamics can relate structure and function in biomolecular systems</i> <b>Petra Imhof</b> Freie Universitaet Berlin (Germany)
11 30–12 00	<b>Coffee Break</b>
12 00–12 45	<b>Plenary</b> <i>“A graveyard of experimental errors”? What lies behind thermal ellipsoids</i> <b>Sergey V. Lindeman</b> Marquette University (USA)
12 45–13 30	<b>Plenary</b> <i>A step to predictive structural biochemistry: QM/MM &amp; QTAIM approach</i> <b>Maria G. Khrenova</b> Federal Research Center of Biotechnology RAS (Moscow, Russia)
13 30–14 30	<b>Lunch</b>
<b>Session D</b>	<b>Session Chairs: Vladimir G. Tsirelson (Russia), Nikolay N. Gerasimchuk (USA)</b>
14 30–15 15	<b>Plenary</b> <i>Coordination chemistry of diazenium diolates. Structure-spectral overview</i> <b>Olga V. Kovalchukova</b> RUDN University (Moscow, Russia)
15 15–15 45	<b>Invited</b> <i>Electron density distribution in catecholate, amidophenolate and acrylate complexes of triphenylantimony</i> <b>Georgy K. Fukin</b> Razuvaev Institute of Organometallic Chemistry RAS (Nizhny Novgorod, Russia)
15 45–16 00	<b>Oral</b> <i>Structures and properties of new push-pull molecules</i> <b>Georgii V. Bogdanov</b> New Mexico Highlands University (USA)
16 00–16 30	<b>Coffee Break</b>

16 30–16 50	<b>Oral</b> <i>Relationship "structure-conductivity-activity" in alcohol conversions over solid electrolyte catalysts</i> <b>Irina I. Mikhailenko</b> RUDN University (Moscow, Russia)
16 50–17 05	<b>Oral</b> <i>Non-covalent interactions in the reactions of catalytic olefination</i> <b>Gulnar T. Suleymanova</b> Baky State University (Azerbaijan)
17 05–17 20	<b>Oral</b> <i>On morphotropic transition in apatite-structured compounds</i> <b>Evgeny N. Bulanov</b> , <i>The 2014 Struchkov Prize Laureate</i> Lobachevsky State University (Nizhny Novgorod, Russia)
17 20–17 35	<b>Oral</b> <i>New uranyl compounds with microporous frameworks</i> <b>Evgeny V. Nazarchuk</b> , <i>The 2014 Struchkov Prize Laureate</i> Saint-Petersburg State University (Russia)

**Thursday November 15, 2018** (Ordzhonikidze Street, 3, Science Faculty Club)

	<b>Struchkov Prize Session</b>
	<b>Session Chairs: Leonid A. Aslanov (Russia), Arkady M. Ellern (USA)</b>
10 00–10 30	<b>Invited</b> <i>Giant supramolecules at atomic resolution: how far away is the horizon?</i> <b>Alexander V. Virovets</b> , <i>The First Struchkov Prize Laureate of 1997</i> University of Regensburg (Germany), Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk, Russia)
10 30–11 00	<b>Invited</b> <i>Giant pentaphosphaferrocene-based supramolecules</i> <b>Eugenia V. Peresykina</b> , <i>The 2008 Struchkov Prize Laureate</i> University of Regensburg (Germany), Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk, Russia)
11 00–11 30	<b>Invited</b> <i>Hydrocerussite-related minerals and materials: structural principles</i> <b>Oleg I. Siidra</b> , <i>The 2010 Struchkov Prize Laureate</i> Saint-Petersburg State University (Russia)
11 30–12 00	<b>Coffee Break</b>
12 00–12 30	<b>Invited</b> <i>Evolution of structural and topological complexity in uranyl sulfates and selenates</i> <b>Vladislav V. Gurzhiy</b> , <i>The 2015 Struchkov Prize Laureate</i> Saint-Petersburg State University (Russia)
12 30–12 50	<b>Oral</b> <i>Protonic metal-based ionic liquids: DEAHFeCl<sub>4</sub>, (DEAH)<sub>2</sub>CoCl<sub>4</sub>, DEAHMnCl<sub>3</sub></i> <b>Maksim A. Zakharov</b> , <i>The 2001 Struchkov Prize Laureate</i> Lomonosov Moscow State University (Russia)
12 50–13 10	<b>Oral</b> <i>Development and application of the Debye scattering equation method for a full-profile analysis of X-ray diffraction patterns for the structural diagnostics of powder nanomaterials</i> <b>Dmitriy A. Yatsenko</b> , <i>The 2013 Struchkov Prize Laureate</i> Boreskov Institute of Catalysis SB RAS (Novosibirsk, Russia) Novosibirsk State University (Russia)
13 10–13 30	<b>Oral</b> <i>Serial crystallography studies of 7-TM membrane proteins</i> <b>Valentin I. Borshchevskiy</b> , <i>The 2015 Struchkov Prize Laureate</i> Moscow Institute for Physics and Technology (Russia)

13 30–14 30	<b>Lunch</b>
14 30–15 00	<b>Invited</b> <i>Crucial role of water in the reactivity of a chiral NNO type copper(II) coordination polymers in the asymmetric Henry reaction</i> <b>Vladimir A. Larionov</b> Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia) RUDN University (Moscow, Russia)
15 00–15 20	<b>Oral</b> <i>Relationships between crystal structure and electrochemical properties in fluoride-phosphate-based cathode materials for rechargeable batteries</i> <b>Stanislav S. Fedotov</b> , <i>The 2017 Struchkov Prize Laureate</i> Skolkovo Institute of Science and Technology (Moscow, Russia) Lomonosov Moscow State University (Russia)
15 20–15 40	<b>Oral</b> <i>In situ XRD study of mixed Mn-containing oxide catalysts</i> <b>Olga A. Bulavchenko</b> , <i>The 2016 Struchkov Prize Laureate</i> Boreskov Institute of Catalysis SB RAS (Novosibirsk, Russia)
15 40–15 55	<b>Oral</b> <i>Rotation of molecules in crystals: the influence of crystallographic symmetry</i> <b>Daut R. Islamov</b> , <i>The 2016 Struchkov Prize Laureate</i> Butlerov Chemistry Institute, Kazan Federal University (Russia)
15 55–16 10	<b>Oral</b> <i>Combined experimental and theoretical studies of non-covalent interactions using X-ray diffraction analysis and quantum chemical calculations</i> <b>Alexander S. Novikov</b> , <i>The 2017 Struchkov Prize Laureate</i> Saint-Petersburg State University (Russia)
16 10–16 40	<b>Coffee Break</b>
16 40–17 00	<b>Oral</b> <i>Intermolecular complexes of macrocyclic copper(I) and silver(I) pyrazolates with Lewis bases: comparison of structures in the solution and in the crystal</i> <b>Alexey A. Titov</b> Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
17 00–17 15	<b>Oral</b> <i>Dehydrogenation of propane on catalytic systems based vanadium salts</i> <b>Ekaterina B. Markova</b> RUDN University (Moscow, Russia)
17 15–17 30	<b>Oral</b> <i>Substituents effect on the crystal packing and solid state transformations of phosphorylated acetothiosemicarbazides</i> <b>Aida I. Samigullina</b> Arbuzov Institute of Organic and Physical Chemistry RAS (Kazan, Russia)
17 30–17 45	<b>Oral</b> <i>The effect of Fe<sup>3+</sup> and Zr<sup>4+</sup> on the structural and catalytic properties of BIMEVOX</i> <b>Elena I. Knyazeva</b> RUDN University (Moscow, Russia)
17 45–18 00	<b>Oral</b> <i>New approaches for the reductive formation of C-N bond</i> <b>Alexey A. Tsygankov</b> Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
18 00–18 30	<b>Struchkov Prize 2018 Award Ceremony</b>
19 00–22 00	<b>Banquet</b>

**Friday November 16, 2018** (Ordzhonikidze Street, 3, Science Faculty Club)

<b>Session E</b>	<b>Session Chairs: Vitaly K. Belsky (Russia), Sergey V. Lindeman (USA)</b>
10 00–10 45	<b>Plenary</b> <i>Observing mechanisms of nanochemistry through a keyhole of molecular models</i> <b>Vadim Kessler</b> Swedish University of Agricultural Sciences (Sweden)
10 45–11 30	<b>Plenary</b> <i>Crystal chemistry of functionally substituted cyclic phosphines</i> <b>Igor A. Litvinov</b> Arbuzov Institute of Organic and Physical Chemistry RAS (Kazan, Russia)
11 30–12 00	<b>Coffee Break</b>
12 00–12 45	<b>Plenary</b> <i>Structural chemistry of organometallosiloxanes at INEOS RAS. History and prospects</i> <b>Alexander A. Korlyukov</b> Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
12 45–13 30	<b>Plenary</b> <i>Substituents effect on structure and properties of pincer-ligated (PXCXP)IrH(Cl) complexes</i> <b>Natalia V. Belkova</b> Nesmeyanov Institute of Organoelement Compounds RAS (Moscow, Russia)
13 30–14 30	<b>Lunch</b>
<b>Session F</b>	<b>Session Chairs: Andrey V. Shevelkov (Russia), Vadim Kessler (Sweden)</b>
14 30–15 15	<b>Plenary</b> <i>3,7-Diazabicyclo[3.3.1]nonanes as unique platform for studying the supramolecular interactions and as a building block for organic synthesis</i> <b>Sergey Z. Vatsadze</b> Lomonosov Moscow State University (Russia)
15 15–15 35	<b>Oral</b> <i>Quantum chemical investigations of <math>Cr_2O_n</math> and <math>Cr_2O_n^-</math> series (<math>n = 1-14</math>)</i> <b>Konstantin V. Bozhenko</b> Institute of Problems of Chemical Physics RAS (Chernogolovka, Russia) RUDN University (Moscow, Russia)
15 35–15 50	<b>Oral</b> <i>The evaluation of nanostructured Perovskite-type oxides <math>SrFeO_{(3-\delta)}</math>, <math>GdFeO_3</math>, <math>GdSrFeO_4</math> and <math>Gd_{2-x}Sr_{1+x}Fe_2O_7</math> in catalytic processes</i> <b>Tatiana F. Sheshko</b> RUDN University (Moscow, Russia)
15 50–16 05	<b>Oral</b> <i>Co(Ni)–Zr-Phosphates modified by plasma treatments: physico-chemical properties and catalytic activity</i> <b>Anna I. Pylina</b> RUDN University (Moscow, Russia)
16 05–17 00	<b>Awarding the Winners for the best presentation from the Chemistry – A European Journal</b> <b>Concluding remarks of the Rector of RUDN University, Chairmen and Members of the Program and Organizing Committees</b> <b>Workshop Closing</b>