

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	REGISTRATION (<i>Science Faculty Hall</i>)
10 00–14 00	Master Class on OLEX2 (<i>Computer Class</i>) "A complete structure solution and analysis program" <i>Ilia A. Guzei</i> University of Wisconsin-Madison (USA)
14 00–15 00	Lunch
15 00–18 00	Round Table (<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)

	Workshop Opening
9 30–9 40	Vladimir M. Filippov (Conference Chair)
9 40–9 45	Igor L. Eremenko (Co-Chair of Program Committee)
9 45–9 50	Mikhail V. Kovalchuk (Co-Chair of Program Committee)
9 50–9 55	Tatiana V. Timofeeva (Member of Program Committee)
9 55–10 00	Leonid A. Aslanov (Co-Chair of Organizing Committee)
Session A	Session Chairs: Alexander V. Virovets (Russia), Tatiana V. Timofeeva (USA)
10 00–10 45	Plenary <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	Plenary <i>The Struchkov Group and Crystallographic Instrumentation Development</i> <i>Susan Byram</i> Bruker (USA)
11 30–12 00	Coffee Break
12 00–12 45	Plenary <i>Effect of wax crystallinity on oil production</i> <i>Olga E. Lindeman</i> Ecolab, Energy Services Department (USA)
12 45–13 30	Plenary <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	Lunch
Session B	Session Chairs: Igor A. Litvinov (Russia), Olga E. Lindeman (USA)
14 30–15 15	Plenary <i>Click reactions + ultrasound = a new aurora of chitosan chemistry</i> <i>Andreii S. Kritchenkov</i> Institute of Technical Acoustics, National Academy of Sciences of Belarus (Belarus)

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

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

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

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

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

	Struchkov Prize Session
	Session Chairs: Leonid A. Aslanov (Russia), Arkady M. Ellern (USA)
10 00–10 30	Invited <i>Giant supramolecules at atomic resolution: how far away is the horizon?</i> Alexander V. Virovets, The First Struchkov Prize Laureate of 1997 University of Regensburg (Germany), Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk, Russia)
10 30–11 00	Invited <i>Giant pentaphosphaferrrocene-based supramolecules</i> Eugenia V. Peresypkina, The 2008 Struchkov Prize Laureate University of Regensburg (Germany), Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk, Russia)
11 00–11 30	Invited <i>Hydrocerussite-related minerals and materials: structural principles</i> Oleg I. Siidra, The 2010 Struchkov Prize Laureate Saint-Petersburg State University (Russia)
11 30–12 00	Coffee Break
12 00–12 30	Invited <i>Evolution of structural and topological complexity in uranyl sulfates and selenates</i> Vladislav V. Gurzhiy, The 2015 Struchkov Prize Laureate Saint-Petersburg State University (Russia)
12 30–12 50	Oral <i>Protonic metal-based ionic liquids: DEAHFeCl₄, (DEAH)₂CoCl₄, DEAHMnCl₃</i> Maksim A. Zakharov, The 2001 Struchkov Prize Laureate Lomonosov Moscow State University (Russia)
12 50–13 10	Oral <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> Dmitriy A. Yatsenko, The 2013 Struchkov Prize Laureate Boreskov Institute of Catalysis SB RAS (Novosibirsk, Russia) Novosibirsk State University (Russia)
13 10–13 30	Oral <i>Serial crystallography studies of 7-TM membrane proteins</i> Valentin I. Borschchevskiy, The 2015 Struchkov Prize Laureate Moscow Institute for Physics and Technology (Russia)

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

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

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