



# 2<sup>nd</sup> INTERNATIONAL SYMPOSIUM

"NONCOVALENT INTERACTIONS IN SYNTHESIS, CATALYSIS, AND CRYSTAL ENGINEERING"

(NCI-2022)

Moscow, 14-16 November 2022

# PROGRAM

## **TECHNICAL SUPPORT**



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In the framework of the Russian Academy of Sciences initiative  
“Towards the 300th anniversary of the Russian Academy  
of Sciences”

## ORGANIZERS

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Tomsk Polytechnic University  
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Shubina E.S.

### Academic secretaries

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# Monday, November 14

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	<b>Main hall, Chair Elena Shubina</b>
10:00	OPENING CEREMONY
10:15-10:55	<b>PL1 Valentine Ananikov</b> Hierarchical structure of catalytic systems studied with artificial intelligence algorithms
10:55-11:25	<b>KL1 Alexey Timoshkin</b> Donor-acceptor origin of Noncovalent Interactions
11:25-11:55	COFFEE BREAK
	Parallel sessions <b>Main hall, Chair Alexey Timoshkin</b>
11:55-12:15	<b>IL1 Alexander Martynov</b> Structure, optical and magnetic properties of sandwich lanthanide phthalocyaninates as a function of solvation
12:15-12:35	<b>IL3 Sergey Ketkov</b> The role of non-covalent interactions in the stability and spectroscopic properties of organoelement compounds: From phenylated pnictogen derivatives to sandwich complexes of 3d metals
12:35-12:50	<b>OC1 Andrei Churakov</b> Peroxo-solvates of biologically active compounds
12:50-13:05	<b>OC3 Pavel Petunin</b> Stable radicals as tectones in design of magnetic materials
13:05-13:15	<b>SC1 Matvey Shurikov</b> Noncovalent interactions as the driving force for building of molecular magnets based on nitronyl-nitroxide radicals
13:15-13:25	<b>SC3 Marina Volostnykh</b> Supramolecular Hybrids Based on Ru(II) Porphyrin and Isonicotinate end-Decorated Octahedral Mo(II) Iodide Cluster
13:25-13:35	<b>SC5 Leila Zargarova</b> Noncovalent interactions in fluorinated bis(benzofuro) benzenes and their influence on the physical properties

<b><i>Library, Chair Sergey Konchenko</i></b>	
11:55-12:15	<b>IL2 Elena Grachova</b> Non-covalent interactions in the design of luminophores based on transition metal complexes
12:15-12:35	<b>IL4 Pavel Panchenko</b> Novel fluorescent chemosensors for the detection of metal ions in aqueous solutions and in living cells
12:35-12:50	<b>OC2 Ivan Fedyanin</b> Supramolecular organization and electronic structure of 4H [1,2,3]Triazolo[4,5-c][1,2,5]oxadiazole 5-oxide and its salts
12:50-13:05	<b>OC4 Nikolay Semenov</b> 1,2,5-chalcogenadiazoles – donors of chalcogen bonding for molecular recognition and sensorics
13:05-13:15	<b>SC2 Anna Shchukina</b> Study of the complexing properties of ligands with picolinate chelating groups
13:15-13:25	<b>SC4 Sergey Kovalenko</b> Tricarbonyl manganese(I) hydrides as donors of proton or hydride ion
13:25-13:35	<b>SC6 Alsu Nugmanova</b> Self-Assembly of Hybrid Photocatalysts Based on Porphyrin SURMOFs and Graphene Oxide
13:35-15:00	LUNCH
<b><i>Main hall, Chair Petr Tolstoy</i></b>	
15:00-15:30	<b>KL2 Julia Kostina</b> Non-covalent interactions polymer-solvent: from a “small nuisance” to structural-molecular plasticization
15:30-16:00	<b>KL3 Andrey Karasik</b> Molecular Recognition via Chemo- and Biosensing of Novel Luminescent Complexes Based on Cyclic Phosphines
16:00-16:30	<b>KL4 Pavel Abramov</b> Self-assembly patterns of non-metalloid silver thiolates
16:30-17:00	COFFEE BREAK

	Parallel sessions
	<b>Main hall, Chair Andrey Karasik</b>
17:00-17:15	<b>OC5 Maksim Shmelev</b> Influence of noncovalent interactions on the structure and luminescent properties of Cd(II) and Ln(III) fluorobenzoate complexes.
17:15-17:30	<b>OC7 Dmitry Lyubov</b> The first examples of acetylene complexes of Ca and Ln(II) based on 1,8-bis(ethynyl)carbazoles
17:30-17:40	<b>SC7 Maksim Sokolov</b> Self-assembly of porphyrin-based metal-organic framework in layered europium hydroxide: a symbiotic hybrid material
17:40-17:50	<b>SC9 Grigory Zhigulin</b> Noncovalent interactions in the aminohydroximate metallamacrocycles bearing alkali and rare earth ions
17:50-18:00	<b>SC11 Anton Rozhkov</b> Non-covalent interactions of cyclometallated diketonate platinum(II) complexes with anticrown
	<b>Library, Chair Pavel Abramov</b>
17:00-17:15	<b>OC6 Ruslan Asfin</b> Self-association of Dimethylarsinic Acid: Optical, NMR, and Calculation Study of Solid State and Solutions
17:15-17:30	<b>OC8 Elena Tupikina</b> Non-covalent interactions in the active center of the antioxidant enzyme glutathione peroxidase
17:30-17:40	<b>SC8 Aleksandra Puzyk</b> Structure of hydrogen-bonded complexes of compounds containing As=O group
17:40-17:50	<b>SC10 Mger Navasardyan</b> Hydrazinosolvates: unusual isomorphism and isomorphous substitution
17:50-18:00	<b>SC12 Mikhail Kostin</b> Estimation of the strength and geometry of hydrogen bonds in complexes with phosphine oxides by IR and NMR spectroscopy
18:00-20:00	Welcome reception

# Tuesday, November 15

	<b>Main hall, Chair Oleg Filippov</b>
10:00-10:30	<b>KL5 Sergey Adonin</b> Supramolecular polyhalogen-halometalates
10:30-11:00	<b>KL6 Maria Kalinina</b> Noncovalent self-assembly of supramolecular hybrids
11:00-11:40	<b>PL2 Jean-Pierre Djukic (remote lecture)</b> Correlation of Noncovalent Interactions with Reactivity, a «Game Changer» for Catalyst Engineering?
11:40-12:10	COFFEE BREAK
	Parallel sessions <b>Main hall, Chair Sergey Adonin</b>
12:10-12:40	<b>KL7 Leyong Wang (remote lecture)</b> The Orthogonal Self-Assembly of Supramolecular Materials
12:40-13:00	<b>IL5 Dmitrii Bolotin</b> Homogeneous Organocatalysis Provided by the $\sigma$ -Hole Donors
13:00-13:20	<b>IL7 Vladimir Larionov</b> Chiral Non-Classical Metal-Templated Hydrogen Bond Donor Catalysts
13:20-13:35	<b>OC9 Olga Syzgantseva</b> Theoretical insights on non-covalent interactions in functional materials
	Parallel sessions <b>Library, Chair Maria Kalinina</b>
12:40-13:00	<b>IL6 Sergey Konchenko</b> Functionalised Chalcogenadiazoles and their Coordination Compounds: Intermolecular Contacts in the Crystals
13:00-13:20	<b>IL8 Daniil Ivanov</b> Metal iodide as I-centered Lewis acid

13:20-13:35	<b>OC10 Alina Sonina</b> Crystal Structure Control of Perylene Single Crystals by Additive-Assisted Crystallization
13:35-15:00	LUNCH
	<b>Main hall, Chair Petr Prikhodchenko</b>
15:00-15:40	<b>PL3 Igor Alabugin (remote lecture)</b> Non-Covalent Interactions with Neutral Radicals: Control of Selectivity of Bond Formation and Bond Breaking in Radical Cyclization/Fragmentation Cascades of Alkynes
15:40-16:10	<b>FLASH POSTER PRESENTATIONS</b>
	<b>FP1 Aleksandra Antonova</b> Structure and properties of hydrazide-chelate of the Hoveyda-Grubbs type catalysts
	<b>FP2 Sergey Baykov</b> Stacking interactions: a supramolecular approach to upgrade weak halogen bond donors
	<b>FP3 Vladimir Burmistrov</b> Synthesis of supramolecular complexes of beta-cyclodextrin with adamantane ureas - new series of encapsulated soluble epoxide hydrolase inhibitors
	<b>FP4 Ekaterina Radiush</b> Chalcogen-bonded donor-acceptor complexes of 1,2,5-selenadiazoles with halide ions
	<b>FP5 Daria Sedlova</b> Characterization of novel bimetallic complexes ( <sup>t</sup> BuPXCYP)Pd( $\mu$ -OC)M(CO) <sub>2</sub> L and their reactivity toward HCOOH
	<b>FP6 Gleb Taranenko</b> Alkoxide ligand environment for stabilization of reactive complexes of rare- and alkaline-earth metals
	<b>FP7 Hamza Zakaria</b> Alkali metal complexes with 1,8-bis(ethynyl)carbazolyl ligands
16:10-16:40	COFFEE BREAK



	Parallel sessions
	<b><i>Main hall, Chair Vladimir Larionov</i></b>
16:40-16:55	<b>OC11 Aleksandra Zvyagina</b> One-Step Self-assembly of Graphene Oxide and Organic Chromophores into Multicomponent ultrathin films for Organic Electronics
16:55-17:10	<b>OC13 Alexander Voronin</b> Application of lattice sums of non-covalent interaction energies in pharmaceutical crystal engineering
17:10-17:20	<b>SC13 Alexander Volodin</b> Various Approaches to Studying the Phase Transition in an Octamethylcyclotetrasiloxane Crystal: From X-Ray Structural Analysis to Metadynamics
17:20-17:30	<b>SC15 Roman Guliaev</b> Preparation of PET@UiO-66 Functional Materials for Selective Binding of Chlorobenzenes Via Halogen Bonding: From Design to Application
17:30-17:40	<b>SC17 Edem Chakalov</b> The distance between minima of electron density and electrostatic potential as a measure of halogen bond strength
17:40-17:50	<b>SC19 Natalia Kulikovskaya</b> Electrophoretic NMR is a tool for studying ionic compounds
	<b><i>Library, Chair Pavel Panchenko</i></b>
16:40-16:55	<b>OC12 Svetlana Kuznetsova</b> Three-dimensional Crystalline Organic Framework Linked by Hydrogen bonds and Additionally Stabilized by the Opposite Charges of the Components as Heterogeneous Acid Catalyst and a Media Stabilizing Metal Nanoparticles
16:55-17:05	<b>SC23 Alena Naumova</b> Plasmon resonance-enhanced absorption of visible light in ultrathin films of organic dyes and gold nanoparticles

17:10-17:20	<b>SC14 Maria Ustimova</b> Noncovalent DNA/RNA labeling with asymmetric bis(styryl) dyes
17:20-17:30	<b>SC16 Alina Saifutiarova</b> Study of the interaction of benzo[d]thiazolo[3,2-a]quinolin-10-ium derivatives with DNA and antitumor activity in vitro
17:30-17:40	<b>SC18 Anastasiya Eliseeva</b> Metal-involving Noncovalent Interactions in Dithiocarbamate and Dithiocarbonate Pt(II) and Pd(II) Complexes
17:40-17:50	<b>SC20 Evgeniia Ondar</b> Hydrosilylation reaction catalyzed by platinum on carbon support: heterogeneous or dynamic?
17:50	Poster session

# Wednesday, November 16

<b>Main hall, Chair Pavel Postnikov</b>	
10:00-10:40	<b>PL4 Giuseppe Resnati</b> Anion...anion Self-assembly via unconventional interactions
10:40-11:20	<b>KL8 Ekaterina Bartashevich</b> Can we merge the covalent and tetrel bonds (TtB)?
11:20-11:40	<b>KL9 Olga Kataeva</b> Noncovalent Interactions in Crystal Engineering of Charge-transfer Complexes of Polyaromatic Donors and Quinone-type Acceptors
11:40-12:10	COFFEE BREAK
	Parallel sessions
<b>Main hall, Chair Ekaterina Bartashevich</b>	
12:10-12:40	<b>KL10 Di Sun (remote lecture)</b> Silver Nanoclusters
12:40-13:00	<b>IL9 Mikhail Kinzhalov</b> Metal-Involving Noncovalent Interaction in Palladium(II) and Platinum(II) Isocyanide Complexes
13:00-13:20	<b>IL11 Petr Prikhodchenko</b> Structure-directing Role of Hydrogen Bonds of Hydroperoxo Groups in Crystalline Adducts of Organic and Inorganic Hydroperoxides
13:20-13:35	<b>OC15 Alexander Goloveshkin</b> Noncovalent interaction-driven stabilization of octahedral coordination in molybdenum disulfide sheets alternating with organic interlayers
<b>Library, Chair Olga Kataeva</b>	
12:40-13:00	<b>IL10 Maxim Sokolov</b> Phosphorescent complexes of $\{\text{Mo}_6\text{I}_8\}^{4+}$ and $\{\text{W}_6\text{I}_8\}^{4+}$ with perfluorinated aryl thiolates featuring unusual molecular structures
13:00-13:20	<b>IL12 Aleksei Trofimov</b> Photonics in Superbasic Environment

13:20-13:35	<b>OC16 Marina Gorshkova</b> New self-cross-linkable hydrogels based on natural and synthetic polyacids.
13:35-15:00	LUNCH
	<b><i>Main hall, Chair Sergey Ketkov</i></b>
15:00-15:20	<b>IL13 Natalia Soldatova</b> Diaryliodonium sulfonates as tecton for crystal engineering
15:20-15:35	<b>OC17 Anna Vologzhanina</b> Voronoi molecular surface for analysis of noncovalent interactions
15:35-15:50	<b>OC19 Mikhail Vener</b> Calculations of the energy of non-covalent interactions in organic crystals. Comparison of periodic and non-periodic models
15:50-16:05	<b>OC21 Ivan Ananyev</b> Inhomogeneity of electron density in a central potential: more insights into the localization phenomenon
16:05-16:20	<b>OC23 Alexander Medvedev</b> Noncovalent interactions in crystalline hydroperoxo complexes of p-block elements
16:20-16:30	<b>SC21 Anastasia Danshina</b> Crystallization cocktails for X-ray diffraction analysis of liquids
	<b><i>Library, Chair Mikhail Kinzhalov</i></b>
15:00-15:20	<b>IL14 Aleksei Titov</b> Role of Intermolecular Interactions in the Chemistry of Cyclic d <sup>10</sup> Metal Pyrazolates
15:20-15:35	<b>OC18 Anastasia Solomatina</b> Aggregation-induced emission of non-symmetric C <sup>N</sup> *N <sup>C</sup> -cyclometallated platinum(II) complexes
15:35-15:50	<b>OC20 Alexander Antonov</b> Steric Effects in The Synthesis, Structure and Reactivity of Lithioanilines

15:50-16:05	<b>OC22 Elena Osipova</b> Bimetallic ionic pairs ( <sup>tBu</sup> PXCYP)Pd(μ-OC)M(CO) <sub>2</sub> L in catalytic dehydrogenation
16:05-16:20	<b>OC24 Lev Zelenkov</b> The case of cocrystals of group 10 metal dithiocarbamates with electrondeficient arenes: the first example of Ni(II) reverse sandwich structure
16:20-16:30	<b>SC22 Roman Pankov</b> Study of the effect of the electron-withdrawing substituents on the catalytic capabilities of Pd/NHC complexes
16:30-17:00	COFFEE BREAK
	<b><i>Main hall Chair Natalia Belkova</i></b>
17:00-17:30	<b>KL11 Oleg Filippov</b> The intriguing world of noncovalent interactions
17:30-18:00	<b>KL12 Petr Tolstoy</b> NMR study of hydrogen and halogen bonds with P=O and POOH groups
18:00	<b>Closing ceremony</b>

**POSTER SESSION**

FP1	<i>Aleksandra Antonova</i>	Structure and properties of hydrazide-chelate of the Hoveyda-Grubbs type catalysts
FP2	<i>Sergey Baykov</i>	Stacking interactions: a supramolecular approach to upgrade weak halogen bond donors
FP3	<i>Vladimir Burmistrov</i>	Synthesis of supramolecular complexes of beta-cyclodextrin with adamantane ureas - new series of encapsulated soluble epoxide hydrolase inhibitors
FP4	<i>Ekaterina Radiush</i>	Chalcogen-bonded donor-acceptor complexes of 1,2,5-selenadiazoles with halide ions
FP5	<i>Daria Sedlova</i>	Characterization of novel bimetallic complexes ( <sup>t</sup> BuPXCYP)Pd( $\mu$ -OC)M(CO) <sub>2</sub> L and their reactivity toward HCOOH
FP6	<i>Gleb Taranenko</i>	Alkoxide ligand environment for stabilization of reactive complexes of rare- and alkaline-earth metals
FP7	<i>Hamza Zakaria</i>	Alkali metal complexes with 1,8-bis(ethynyl) carbazolyl ligands
P8	<i>Ruslan Asfin</i>	Application of the Morse Approximation for the Study of Noncovalent Interactions
P9	<i>Gleb Averochkin</i>	Bioderived C <sub>6</sub> furanics in cycloaddition reactions
P10	<i>Anna Cheranyova</i>	Tin(IV) iodide as a halogen bond donor
P11	<i>Anton Fedonin</i>	Molecular interactions in racemic and enantiopure thioureas
P12	<i>Grigory Chernov</i>	Nucleophilic Ring Opening of Donor-Acceptor Cyclopropanes Catalyzed by Iodonium Salts
P13	<i>Veronika Gak</i>	Diaryliodonium iodides and polyiodides
P14	<i>Anna Efimova</i>	Styryl dyes for noncovalent labeling
P15	<i>Darya Gerasimova</i>	Relationship between the configuration lability of nitrogen and sulfur atoms of sulfonamides of the thiazine series during the formation of crystal-forming motifs
P16	<i>Eugene Katlenok</i>	Supramolecular Assembly Of Binuclear Metal Complexes Via Metal-Involving Chalcogen Bonds

P17	<i>Sergei Legkov</i>	Study of the structural features of aqueous solutions of monoethanolamine of various compositions by experimental and theoretical methods of vibrational spectroscopy
P18	<i>Olga Lodochnikova</i>	Forming Stereochemically Challenging $Z' > 1$ Motifs in Organic Crystals through Various Non-Covalent Interactions
P19	<i>Darina Nasyrova</i>	Short contacts in nitroxide radicals' crystals with adamantyl and perfluorophenyl substituents
P20	<i>Ekaterina Patil</i>	Quantification of Pd/NHC evolution products in the Heck, Sonogashira, and transfer hydrogenation reactions
P21	<i>Pavel Pirozhkov</i>	Analysis of Noncovalent Interactions in the Polymorphic Structures of N-(3-Chloro-2-methylphenyl)anthranilic Acid
P22	<i>Liliya Sahharova</i>	Re-thinking the Role of Dimeric Species in Catalysis
P23	<i>Irina Sterkhova</i>	Noncovalent Interactions in New Derivatives of Triflamide
P24	<i>Ruslan Shaydullin</i>	XAS study of palladium catalyst changes in the Heck reaction
P25	<i>Polina Verbitskaya</i>	Crystal Structure Control of Organic $\pi$ -Conjugated molecules by Additive-Assisted Crystallization
P26	<i>Anna Vorobyova</i>	Crystal engineering and magnetic properties of coordination polymers based on transition metal nitrate complexes with singly charged cations
P27	<i>Julia Voronina</i>	Non-covalent interactions in organic precursors as a driving factor of coordination compounds structure
P28	<i>Dmitriy Zakharychev</i>	Stable reproducibility of a stereochemically complex three-dimensional motif of hydrogen bonds in various crystalline forms of 15-en-steviol and dihydrosteviol
P29	<i>Daria Zapravdina</i>	Application of Zn carboxylates in the synthesis of symmetrical nitrogen-containing derivatives of camphor

