INTERNATIONAL SCHOOL AND CONFERENCE "CURRENT CHALLENGES IN CHEMICAL PHYSICS AND THEORETICAL CHEMISTRY"

CHALLENGES 2024

SCHOOL & CONFERENCE

PROGRAMME



Session codes

- QT Quantum Theory
- TC Computational and Theoretical Chemistry
- ML Machine Learning and High-Performance Computing
- MS Molecular Spectroscopy and Physics of Planetary Atmospheres
- CM Radiative Aspects of Climate Modeling and Remote Sensing
- PP Photoinduced Processes in Molecules

Round-table discussion topics

- A Classical and Quantum Dynamics in Molecular Spectroscopy
- B Modern Software for Modeling Electronic Structure and Properties of Molecular Systems
- C Photoinduced Nonadiabatic Molecular Dynamics
- D Science and Industry Collaboration

Hyperlink to the book of abstracts



https://lk.challenges2024.ru/Book_of_abstracts.pdf

Visit the School & Conference website: https://www.challenges2024.ru

School & Conference Programme

Monday, July 1

9:00-11:45	Registration							
11:45-12:00		Opening Ceremony						
Invited Session A (Chairperson: K. Kazakov)								
12:00-12:45	ML	D. Kononchuk RT-Techpriemka, Moscow	K Machine learning methods to reducing the influence of the human factor and minimizing equipment failures in aviation					
12:45-13:30	QT	D. Naumov Joint Institute for Nuclear Research, Dubna	Vibrating quantum fields — the foundation of the universe					
13:30-15:00			Lunch					
			Invited Session B (Chairperson: A. Mitin)					
15:00-15:45	TC	D. Sabirov Institute of Petrochemistry and Catalysis, Ufa	The information-entropy concepts in chemistry					
15:45-16:30	QT	A. Titov Petersburg Nuclear Physics Institute	Modern problems of quantum theory of materials contain- ing elements of the lower half of Mendeleev periodic table					
16:30-17:00	16:30-17:00 Coffee Break							
Invited Session C (Chairperson: V. Bochenkov)								
17:00-17:45	ML	M. Zabezhailo FRC Computer Science and Control, Moscow	Zabezhailo Computer Science Control, MoscowOn the experience of using AI-tools to represent experimen- tal data in the form of partial empirical theories					
17:45-18:15	ML	D. Shadrin Skoltech, Moscow	Computer vision methods for multimodal data processing and solving remote sensing tasks					
18:15-18:45	ML	A. Moskovsky RSC Group, Moscow	Microelectronic technology trends and numerical simula- tion tools					
18:45-19:00	0 Coffee Break							
19:00-21:00	Poster Session							
21:00-23:00	Welcome Party							

Tuesday, July 2

Invited Session D (Chairperson: L. Surin)									
9:30-10:15	MS	A. Vigasin Institute of Atmospheric Physics, Moscow	Vigasin Institute of spheric Physics, MoscowWeakly interacting molecular pairs in planetary atmo- spheres						
10:15-11:00	MS	A. Fedorova Space Research Institute, Moscow	High resolution infrared spectroscopy as a tool to study the Mars' and Venus' atmospheres						
11:00-11:30			Coffee Break						
		In	vited Session E (Chairperson: A. Zaitsevskii)						
11:30-12:15	QT	V. Shabaev Saint Petersburg State University	Quantum electrodynamics effects in heavy atomic systems						
12:15-13:00	тс	V. Stegailov Joint Institute for High Temperatures, Moscow	First-principles molecular dynamics models of electronic excitations in dense media						
13:00-14:30	13:00-14:30								
Invited Session F (Chairperson: V. Stegailov)									
14:30-15:15	тс	Zh. Lyutova Petersburg Nuclear Physics Institute The possibility and expediency of using multiscale modelin to predict and describe the structure and properties of ne carbon nanocomposite materials based on polylactic ac for medical purposes							
15:15-16:00	PP	A. Borisenkova Petersburg Nuclear Physics Institute Physics Institute Radiolabeled carbon-based nanostructures for targete livery to tumor cells							
Invited Session G (Chairperson: V. Shabaev)									
14:30-15:15	QT	A. Petrov Petersburg Nuclear Physics Institute	Search for new physics in molecules						
15:15-16:00	QT	L. Skripnikov Petersburg Nuclear Physics Institute	Studying the magnetic properties of nuclei using atoms and molecules						
16:00-16:30 Coffee Break									
16:30–18:15 Round Table A (K. Kazakov) & Round Table B (A. Oleynichenko)									
18:15-19:00	QT	S. Petrov Lomonosov Moscow State University	Evening lecture: Uniqueness of spin 1/2						
19:00-20:00	Dinner								

Wednesday, July 3

Invited Session H (Chairperson: A. Titov)								
09:30-10:15	QT	A. Trofimov Irkutsk State University	Propagator methods in the ADC approximation: Theory, development and current state					
10:15-11:00	QT	A. Zaitsevskii Petersburg Nuclear Physics Institute	Multipartitioning perturbation theory in quantum chem- istry					
11:00-11:30			Coffee Break					
		I	nvited Session I (Chairperson: A. Vigasin)					
11:30-12:15	QT	A. Stolyarov Lomonosov Moscow State University	Analytical capabilities of the diatomic quantum defect the- ory					
12:15-13:00	MS	A. Kouzov Saint Petersburg State University	Raman spectra induced by binary collisions: retrospective and the current status of research					
13:00-14:30 Lunch								
	Invited Session J (Chairperson: A. Tchougreeff)							
14:30-15:15	тс	V. Kiselev Institute of Chemical Kinetics and Combustion, Novosibirsk	Modern predictive quantum chemical calculations for ther- mochemistry and kinetics: procedures and limitations					
15:15-16:00	тс	P. Dyachkov Institute of General and Inorganic Chemistry, Moscow	Electronic cylindrical waves in nanotubes					
	1	In	vited Session K (Chairperson: D. Chistikov)					
14:30-14:50	QT	N. Mosyagin Petersburg Nuclear Physics Institute	Tiny-core generalized relativistic pseudopotentials for ex- tremely accurate electronic structure calculations					
14:50-15:10	тс	Y. Lomachuk Petersburg Nuclear Physics Institute	Compound-tunable embedding potential method to model local electronic excitations on f-element ions in solids: Study of Ce and Th impurities in yttrium orthophosphate, YPO $_4$					
15:10-15:30	тс	I. Odud Petersburg Nuclear Physics Institute	The pilot application of the CCSD method for calculating the structural parameters of perovskites using the Compound-tunable Embedding Potential method					

15:30-15:50	тс	A. Mysovsky Institute of Geochemistry, Irkutsk	Seamless multilayer (SML) formulation of hybrid QM/MM approach and its application to inorganic oxide compounds					
15:50-16:10	ML	S. Konyukhov RSC Group, Moscow	Assessing containerisation overhead for running Firefly quantum chemistry program					
16:10-16:30		Coffee Break						
Invited Session L (Chairperson: D. Shalashilin)								
16:30-17:15	PP	V. Nadtochenko Federal Research Center for Chemical Physics, Moscow Femtosecond laser spectroscopy of primary ever charge separation in photosynthetic centers						
17:15-17:45	PP	E. Stepanov Lomonosov Moscow State University	Time-resolved broadband two-dimensional spectroscopy with ultrashort pulses in the visible and mid-infrared					
17:45-18:15	PP	T. Domracheva	Applications of quantum chemistry for mapping electron transfer pathways in photoinduced DNA repair					
18:30-19:30	Dinner							
19:30-21:00	Round Table C (A. Bochenkova)							

Thursday, July 4

Invited Session M (Chairperson: A. Bochenkova)									
9:30-10:15	PP	Zh. Lan South China Normal University, Guangzhou, China	Nonadiabatic Dynamics, Time-Resolved Spectra and Ma- chine Learning						
10:15-11:00	РР	D. Shalashilin University of Leeds, United Kingdom	 An overview of trajectory guided coherent state basis sets methods of quantum dynamics with examples of applications in photochemistry and in physics 						
11:00-11:30		1	Coffee Break						
		Inv	rited Session N (Chairperson: M. Tretyakov)						
11:30-12:15	СМ	E. Loskutov Institute of Applied Physics, Nizhny Novgorod	skutov of Applied s, Nizhny gorod						
12:15-13:00	СМ	M. Gorbunov Institute of Atmospheric Physics, Moscow	Fractional Fourier Transform and distributions in the phase space						
13:00-14:30		Lunch							
		Ir	nvited Session O (Chairperson: D. Sabirov)						
14:30-15:15	тс	A. Mitin Moscow Institute of Physics and Technology Chemical bonding in biomolecules							
15:15-16:00	тс	A. Tchougreeff Institute of Physical Chemistry and Electrochemistry, Moscow Cartesius fort - object fortran library for chemistry and ma- terials science. Recent developments							
16:00-16:30	Coffee Break								
16:30-18:00	Round Table D (D. Kononchuk)								
18:30-20:00		Evening Cultural Programme: Piano Concert							
20:00-23:59	Conference Dinner								

Friday, July 5

Invited Session P (Chairperson: A. Trofimov)							
9:30-10:00	QT	D. Bezrukov Lomonosov Moscow State University	Current state of the coupled cluster method in quantum chemistry: present situation, objectives, and challenges				
10:00-10:30	QT	A. Oleynichenko Petersburg Nuclear Physics Institute	Recent advances in relativistic coupled cluster methods for open shell states				
10:30-11:00	PP	A. Skitnevskaya Irkutsk State University	Intermolecular Coulombic decay – an ultrafast intermolec- ular energy transfer mechanism. The case of biologically relevant systems				
11:00-11:30 Coffee Break							
Invited Session Q (Chairperson: A. Finenko)							
11:30-12:00	РР	C. Xu South China Normal University, Guangzhou, China The Development of the QM/MM Interface and Its Applica- tion for the on-the-fly QM/MM Nonadiabatic Dynamics in JADE Package: Theory, Implementation and Applications					
12:00-12:30	PP	D. Makhov University of Leeds, United Kingdom	Direct simulations of ultrafast chemical dynamics with <i>ab initio</i> multiple cloning approach				
12:30-13:00	тс	V. Bataev Lomonosov Moscow State University	How true are our estimates of PES based on experimental data: A theorist's view of internal rotation barriers?				
13:00-13:30	Closing Ceremony						
13:30-15:00	Lunch						

- P1. Theoretical insight into lithiation of N-doped molybdenum disulfide <u>V. Alekseev</u>, L. Bulusheva, Nikolaev Institute of Inorganic Chemistry of SB RAS, Novosibirsk, Russian Federation
- P2. Theoretical modeling of the adsorption, desorption and migration of heavy and superheavy atoms on a metal surface: beyond a mobile adsorption model

<u>A.A. Astakhov</u>, G.A. Bozhikov, N.V. Aksenov, Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, Dubna, Russia

P3. MCSCF approach to many-electron Pauli equation

<u>A.A. Bodunov</u>, G.K. Ozerov, D.S. Bezrukov, Chemistry Department, Lomonosov Moscow State University, Moscow, Russia

P4. Quantum chemical study of 1,3-cyclopentadiene trimerization mechanism

N.A. Dontsenko, R.S. Shamsiev, Physical Chemistry Department, Lomonosov Institute of Fine Chemical Technologies, MIREA – Russian Technological University, Moscow, Russia

P5. Multilevel calculation schemes as a new approach to molecular docking calculations

<u>A.V. Zhilenkov</u>, O.A. Kraevaya, L.G. Gutsev, P.A. Troshin, Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia; Institute for Micromanufacturing, Louisiana Tech University, Ruston, LA, USA; Zhengzhou Research Institute, Harbin Institute of Technology, Zhengzhou, China

P6. Multiscale modeling of heterogeneous oxygen loss in plasma conditions

I. Ziganshin, A. Rakhimov, D. Lopaev, Physics Department, Lomonosov Moscow State University, Moscow, Russia; Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia

P7. Information entropy changes in elementary and complex chemical reactions

<u>A.D. Zimina</u>, A.A. Tukhbatullina, I.S. Shepelevich, D. Sh. Sabirov, *Institute of Petrochemistry* and Catalysis UFRC RAS, Ufa, Russia

P8. Investigation of the structure and stability of boron-carbon clusters using the DFT method

M.A. Fedyaeva, S.V. Lepeshkin, A.R. Oganov, Skolkovo Institute of Science and Technology, Moscow, Russia; Vernadsky Institute of Geochemistry and Analytical Chemistry RAS, Moscow, Russia P9. Calculation of the kinetic isotope effect for the dissociation of polyglycine dimers as a model system for protein denaturation

<u>A.O. Yanshin</u>, V.G. Kiselev, A.V. Baklanov, Novosibirsk Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk, Russia; Novosibirsk State University, Novosibirsk, Russia

P10. Possible room-temperature superconductivity in Ca-Y-H system at high pressure

<u>M.A. Grebeniuk</u>, G.M. Shutov, D.O. Poletaev, A.R. Oganov, *Skolkovo Institute of Science and Technology*, *Moscow*, *Russia*

P11. Molecular parameter of spatially-odd nuclear-electron interactions in the ²⁹Si¹⁶O⁺ cation

<u>P.D. Turchenko</u>, L.V. Skripnikov, Advanced Development Division, Petersburg Nuclear Physics Institute, Gatchina, Russia; St Petersburg University, St Petersburg, Russia

P12. Band alignment transformations in heterostructures by applying external stimuli: a first principal investigation

<u>E.V. Sukhanova</u>, Z.I. Popov, Emanuel Institute of Biochemical Physics RAS, 119334, 4 Kosigin st., Moscow, Russia

P13. Quantum chemical modeling of the electronic structure of ytterbium halides by the coupled cluster method

<u>P.A. Khadeeva</u>, V.M. Shakhova, Y.V. Lomachuk, N.S. Mosyagin, L.V. Skripnikov, A.V. Titov, RC «Kurchatov Institute» - PNPI, Gatchina, Russia; Saint-Petersburg State University, Saint Petersburg, Russia

P14. Theoretical modeling of the structural and spectral properties of a magnesium atom in a methane matrix

<u>N.N. Kleshchina</u>, B.B. Kamorzin, G.K. Ozerov, B.V. Rutskoy, D.S. Bezrukov, Chemistry department, Lomonosov Moscow State University, Moscow, Russia; National Research Centre "Kurchatov Institute"; National Research Nuclear University "MEPhI", Moscow, Russia

P15. Predicting emulsion type in octane- $C_{10}E_4$ -water systems using dissipative particle dynamics simulation

N.S. Sopova, V.E. Bochenkov, Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

P16. Ab initio study of dioxidine dimers as a tool to predict polymorphs formation

<u>A.V. Soloviev</u>, A.Y. Ermilov, T.I. Shabatina, *Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia*

P17. Calculation of higher-order correlation effects in highly charged ions

<u>Y.S. Kozhedub</u>, M.Y. Kaygorodov, A.V. Malyshev, V.M. Shabaev, I.I. Tupitsyn, A.V. Volotka, *Department of Physics, St. Petersburg State University, 199034 St. Petersburg, Russia; National Research Centre "Kurchatov Institute" B. P. Konstantinov Petersburg Nuclear Physics Institute, Gatchina, Russia; School of Physics and Engineering, ITMO University, St. Petersburg, Russia*

P18. Investigation of the structure and properties of the ThF⁺ molecule using relativistic coupled-cluster method

<u>I.G. Kozhevnikov</u>, A.V. Oleynichenko, A.V. Zaitsevskii, Petersburg Nuclear Physics Institute named by B.P. Konstantinov of NRC "Kurchatov Institute", Gatchina, Russia; Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Russia; Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

- P19. Molecular modeling of reagents potentially active against sulfide minerals <u>I. Kunilova</u>, P. Solozhenkin, A. Lavrinenko, Institute of Comprehensive Exploitation of Mineral Resources Russian Academy of Sciences, Moscow, Russia
- P20. Cryochemical synthesis and quantum chemical modeling of the IR spectrum of magnetic iron oxide nanoparticles and their hybrid systems with chloramphenicol

<u>A.S. Shumilkin</u>, O.I. Vernaya, T.I. Shabatina, *Lomonosov Moscow State University*, *Chemistry Department*, Moscow, Russia; Bauman Moscow State Technical University, Moscow, Russia

P21. Ground state of the light relativistic atoms in intermediate and strong magnetic fields

F.A. Petryaykin, O.N. Mazaleva, A.A. Bodunov, D.S. Bezrukov, G.K. Ozerov, Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

P22. Branching in internal conversion of the methylene iminium cation

D.S. Popov, A.V. Bochenkova, Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

P23. From humorous post to detailed quantum-chemical study: Isocyanate synthesis revisited

<u>I.V. Prolomov</u>, Mendeleev University of Chemical Technology, Moscow, Russia; N.D. Zelinsky Institute of Organic Chemistry, Moscow, Russia; Center NTI, Bauman Moscow State Technical University, Moscow, Russia

P24. Search for T, P-violating axionlike-particle-mediated interactions in HfF⁺ molecular cation

S.D. Prosnyak, L.V. Skripnikov, Advanced development division, NRC "Kurchatov Institute" - PNPI, Gatchina, Russia; Physics Department, Saint Petersburg State University, Saint Petersburg, Russia

P25. Quantum chemical simulation of the effect of silica gel substrate on luminescent systems with charge transfer

A. Samolyga, Federal Research Center "Crystallography and Photonics", NRC "Kurchatov Institute", Moscow, Russia; Moscow Institute of Physics and Technology, Moscow, Russia

P26. Tensor decomposition methods for high-precision relativistic modeling of electronic structure

<u>A.S. Rumiantsev</u>, A.V. Oleynichenko, A.V. Zaitsevskii, NRC «Kurchatov Institute» - PNPI, Gatchina; SPbU, Saint-Petersburg; MIPT, Dolgoprudny; Lomonosov MSU, Moscow, Russia

P27. Speed-dependent broadening and shifting of water lines in the subTHz range

<u>I.N. Vilkov</u>, G.Yu. Golubiatnikov, M.A. Koshelev, A.I. Chernova, I.I. Leonov, M.Yu. Tretyakov, A.V. Gaponov-Grekhov Institute of Applied Physics of the Russian Academy of Sciences, Nizhny Novgorod, Russia

P28. High-precision measurements of the J = 1 - 0 rotational transitions of the jet-cooled rare CO isotopologues

I.V. Tarabukin, V.A. Panfilov, L.A. Surin, Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow, Russia

P29. Physically based water-related continuum modelling in the SubTHz range for atmospheric applications

T.A. Galanina, <u>A.O. Koroleva</u>, D.S. Makarov, M.Yu. Tretyakov, A.V. Gaponov-Grekhov Institute of Applied Physics of the Russian Academy of Sciences, Nizhny Novgorod, Russia

P30. SubTHz molecular laboratory spectroscopy: experimental methods and results

<u>M.A. Koshelev</u>, M.Yu. Tretyakov, S.P. Belov, G.Yu. Golubiatnikov, V.V. Parshin, I.N. Vilkov, T.A. Galanina, E.A. Serov, I.I. Leonov, A.I. Chernova, A.F. Krupnov, A.V. Gaponov-Grekhov Institute of Applied Physics of the Russian Academy of Sciences, Nizhny Novgorod, Russia

P31. Parametric broadening of the electronic-vibrational spectrum of a molecule caused by zero-point vibrations and thermal fluctuations of interatomic bonds

P. Lebedev-Stepanov, NRC "Kurchatov Institute", Moscow, Russia; NRNU MEPhI, Moscow, Russia

P32. Bimolecular absorption in nitrogen

<u>A.Yu. Sekacheva</u>, T.A. Galanina, A.O. Koroleva, I.S. Amerkhanov, E.A. Serov, M.A. Koshelev, M.Yu. Tretyakov, D.N. Chistikov, A.A. Finenko, A.A. Vigasin, A.V. Gaponov-Grekhov Institute of Applied Physics RAS, Nizhny Novgorod, Russia; A.M. Obukhov Institute of Atmospheric Physics, RAS, Moscow, Russia; Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia; Institute of Quantum Physics, Irkutsk National Research Technical University, Irkutsk, Russia

P33. Model-based reinforcement learning for Iterative Prisoner's Dilemma in a Multi-agent environment

M. Chistikov, A. Shuranova, HSE University, Moscow, Russia

P34. Prediction of proton conductivity of metal-organic frameworks using a multimodal transformer

<u>I. Dudakov</u>, V. Korolev, MSU Institute for Artificial Intelligence, Lomonosov Moscow State University, Moscow, Russia

P35. Dataset formation for refolding of the GLP-1 agonist precursor protein <u>A. Kazakova</u>, S. Ishchuk, R&D center, GEROPHARM, Saint Petersburg, Russia

P36. Effective collaboration between science and industry in biotechnology

<u>A. Sibiriakova</u>, Moscow Institute of Physics and Technology, Russia; Russian Quantum Center, Russia

P37. Machine learning approaches for fuel design

<u>O. Mazaleva</u>, A. Pupeza, F. Petryaykin, I. Romashin, *Chemistry Department*, *Lomonosov Moscow State University*, *Moscow*, *Russia*

P38. Development of sustainable technologies for flotation plants

<u>Y. Shimkunas</u>, A. Lavrinenko, Institute of Comprehensive Exploitation of Mineral Resources Russian Academy of Sciences, Moscow, Russia

P39. Transferable ML-based variational Monte Carlo

A.K. Pupeza, D.S. Bezrukov, Chemisrty Department, Lomonosov Moscow State University, Moscow, Russia

P40. Effect of quantum entanglement on two-photon absorption probabilities in fluorescent proteins

V.R. Aslopovsky, A.V. Scherbinin, A.V. Bochenkova, Chemisrty Department, Lomonosov Moscow State University, Moscow, Russia

P41. Impact of intramolecular hydrogen bonding on the photophysics of the modified GFP chromophore anion

<u>O.B. Beletsan</u>, L.H. Andersen, A.V. Bochenkova, *Department of Chemistry*, *Lomonosov Moscow State University*, *Moscow*, *Russia*; *Department of Physics and Astronomy*, *Aarhus University*, *Aarhus*, *Denmark*

P42. Unsupervised Machine Learning in the Nonadiabatic Surface Hopping Dynamics

Y. Zhu, Zh. Lan, South China Normal University, Guangzhou, China

P43. Multiscale quantum chemical calculations of highly efficient narrowband deep-blue fluorophores

<u>N. Dubinets</u>, A. Sosorev, Institute of Synthetic Polymer Materials RAS, Moscow, Russia; NRC "Kurchatov Institute", Moscow, Russia; National Research Nuclear University "MEPhl", Moscow, Russia

P44. Influence of Mode-specific Excitation on the Nonadiabatic Dynamics of Methyl Nitrate (CH₃ONO₂)

J. Zhang, Zh. Lan, South China Normal University, Guangzhou, China

P45. Development of descriptors for assessing maximum resistance to the principles of independence and reverse thermal isomerization time in computerassisted screening of photopharmacological methods

<u>A. Gorislav</u>, M. Ryazantsev, St Petersburg State University, St Petersburg, Russia; St Petersburg Academic University, St Petersburg, Russia

- P46. Photoionization of γ-pyrone: Nonadiabatic nuclear dynamics in the lowlying electronic states of the γ-pyrone radical cation <u>E.K. lakimova</u>, A.D. Skitnevskaya, A.B. Trofimov, Laboratory of quantum chemical modeling of molecular systems, Irkutsk State University, Russia
- P47. Prediction of photophysical properties of organometallic compounds using machine learning algorithms E.A. Ilin, Science Center, SkyLab AG, Lausanne, Switzerland
- P48. Modeling kinetics of the photoinduced retinal fragmentation <u>R.G. Kuliev</u>, O.B. Beletsan, A.V. Bochenkova, Chemistry Department, Lomonosov Moscow State University, Moscow, Russia
- P49. Role of the protein environment and structural heterogeneity in the mechanisms of photochromic reactions of microbial and animal rhodopsins <u>P.A. Kusochek</u>, V.V. Belov, Chemistry Department, Lomonosov Moscow State University, Moscow, Russia
- P50. Modeling photoabsorption spectra of conformationally flexible calcium indicators in solution upon one- and two-photon excitation <u>V.I. Nazarova</u>, O.N. Voldaeva, A.V. Bochenkova, Chemistry Department, Lomonosov Moscow State University, Moscow, Russia
- P51. Non-adiabatic excited-state dynamics simulations based on highly accurate quantum chemistry and neural network interatomic potentials P.M. Radzikovitsky, D.N. Chistikov, V.V. Korolev, D.A. Firsov, V.E. Bochenkov, A.V. Bochenkova, Chemistry Department, Lomonosov Moscow State University, Moscow, Russia
- **P52. Polarizability in computational astrochemistry of fullerenes and PAHs** <u>D.Sh. Sabirov</u>, A.A. Tukhbatullina, I.S. Shepelevich, *Institute of Petrochemistry and Catalysis UFRC RAS*, *Ufa*, *Russia*
- P53. Experimental and theoretical study of intermolecular interactions in wateracetonitrile system

<u>D.A. Firsov</u>, V.P. Chertkova, A.I. Abramovich, T.V. Bogdan, *Chemistry Department*, *Lomonosov Moscow State University, Moscow, Russia*

- **P54.** Modeling of P-O bond cleavage mechanism of nucleoside phosphates <u>A. Kulakova</u>, T. Mulashkina, M. Khrenova, Chemistry Department, Lomonosov Moscow State University, Moscow, Russia; Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, Russia
- P55. Nonadiabatic electronic exitations as a trigger mechanism of plasma phase transition in dense fluid H₂ and N₂ <u>I.D. Fedorov</u>, V.V. Stegailov, Moscow Institute of Physics and Technology, National Research University Moscow Pussian Joint Institute for High Temperatures of the Pussian Academy of

<u>1.D. Fedorov</u>, v.v. Steganov, Moscow Institute of Physics and Technology, National Research University, Moscow, Russia; Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia; HSE University, Moscow, Russia

School & Conference Timetable

Monday, July 1		Tuesday, July 2		Wednesday, July 3		Thursday, July 4		Friday, July 5		
Time	Activity	Time	Activity	Time	Activity	Time	Activity	Time	Activity	
9:00- 11:45	Registration	9:30- 11:00	Session D	9:30- 11:00	Session H	9:30- 11:00	Session M	9:30- 11:00	Session P	
11:45- 12:00	Opening ceremony	11:00- 11:30	Coffee	11:00- 11:30	Coffee	11:00- 11:30	Coffee	11:00- 11:30	Coffee	
12:00- 13:30	Session A	11:30- 13:00	Session E	11:30- 13:00	Session I	11:30- 13:00	Session N	11:30- 13:00	Session Q	
13:30- 15:00	Lunch	13:00- 14:30	Lunch	13:00- 14:30	Lunch	13:00- 14:30	Lunch	13:00- 13:30	Closing ceremony	
15:00- 16:30	Session B	14:30- 16:00	Sessions F&G	14:30- 16:10	Sessions J&K	14:30- 16:00	Session O	13:30- 15:00	Lunch	
16:30- 17:00	Coffee	16:00- 16:30	Coffee	16:10- 16:30	Coffee	16:00- 16:30	Coffee			
17:00- 18:45	Session C	16:30- 18:15	Round tables A&B	16:30- 18:15	Session L	16:30- 18:00	Round table D		R	
18:45- 19:00	Coffee	18:15- 19:00	Evening lecture	18:30- 19:30	Dinner	18:30- 20:00	Piano concert	ARTUI		
19:00- 21:00	Poster session	19:00- 20:00	Dinner	19:30- 21:00	Round table C	20:00-	Caladianau		DEP	
21:00- 23:00	Welcome party	21:00- 23:59	Disco party	21:00- 23:00	Discussion time	23:59	Gaia dinner			