**Preliminary program of RCCT-2022**

**Sunday, 21.08.2022.**

Check in. Registration from 9.00 to 20.00

**Monday, 22.08.2022**

Registration from 8.00 to 9.00

9.00-11.00-Opening ceremony and plenary session

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| 9.00-9.20 Opening ceremony |
| 9.20-10.00 Stolyarova Valentina Leonidovna, , HIGH TEMPERATURE MASS SPECTROMETRIC STUDY OF THE MULTICOMPONENT SYSTEMS BASED ON OXIDES OF RARE EARTH ELEMENTS AND HAFNIUM |
| 10.00-10.40 Kiselev Mikhail Grigorievich, TOWARDS SCREENING OF POLYMORHISM AT SUPERCRITICAL PARAMETERS OF STATE |
| 10.40-11.20 Shchekin Alexander Kimovich, EFFECTS OF CONFINEMENT FOR SMALL AGGREGATES |

Coffee break 11.20-11.50

11.50-14.00-Section reports

1) Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation

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| **11.50-12.10****(keynote lecture)** |  | **Viktorov Alexey Ismailovich** | **Partitioning of n-octanol in mixed micellar solutions of triton with 1-methyl-3-octylimidazolium chloride: experiment and model predictions** |
| 12.10-12.30 |  | Pisarev Vasily Vyacheslavovich | Molecular dynamics study of viscosity and excess entropy of hydrocarbons |
| 12.30-12.50 |  | Mokshin Anatoly Vasilievich | Thermodynamics and statistical mechanics of alkali plasmas |
| 12.50-13.10 |  | Vishnyakov Alexey Mikhailovich | Nanoparticle interactions with lipid bilayers studied with molecular and coarse-grained modeling |
| 13.10-13.25 |  | Olkhin Andrey Sergeevich | Non-equilibrium thermodynamics of Enceladus ice shield: how Lattice-Boltzmann modeling helps us establish what’s inside |
| 13.25-13.40 |  | Akhmetshina Ekaterina Stepanovna | Homodesmotic method for determining the enthalpy of formation of free alkyl radicals |

2) Thermodynamics of Functional Materials, Interfacial and Confined Phenomena

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| **11.50-12.20 (keynote lecture)** |  | **Basova Tamara Valerievna** | **Fluorosubstituted metal phthalocyanines: physicochemical properties and thin films** |
| 12.20-12.40 |  | Malakhov Alexander Olegovich | Selectivity of gas separation membranes: an approximate predictive model |
| 12.40-13.00 |  | Okhotnikova Ekaterina Sergeevna | Study the phase composition of bitumen by calorimetry method |
| 13.00-13.20 |  | Zvereva Irina Alekseevna | Particularities of structure and thermodynamic properties of layered perovskite photocatalysts  |
| 13.20-13.40 |  | Samsonov Vladimir Mikhailovich | Nanothermodynamics: difficulties, advances and prospects |
| 13.40-13.55 |  | Davydov Nikita Anatolievich | Photocatalytic activity of layered perovskite-like oxide H2La2Ti3O10 intercalated with n-octylamine |

3) Supramolecular systems

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| 11.50-12.10 |  | Ustinov Evgeny Alexandrovich | External fields method in molecular simulation and thermodynamics of 2D crystals |
| 12.10-12.30 |  | Ziganshin Marat Akhmedovich | Self-assembly, sorption and thermal properties of short-chain oligopeptides |
| 12.30-12.50 |  | Oparin Roman Dmitrievich | Role of an intramolecular hydrogen bond in lidocaine conformer distribution and polymorph stability |
| 12.50-13.10 |  | Usacheva Tatyana Rudolfovna | Thermodynamics of molecular complexation of cyclodextrins with quercetin and routine in mixed water-organic solvents  |
| 13.10-13.25 |  | Gatiatulin Askar Kamilevich | The role of water in guest inclusion by native cyclodextrins |

13.55-15.30 Dinner

15.30-17.30 Plenary session

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| 15.30 -16.10 Navrotsky Alexandra, ORGANICS MATTER: COMMON FEATURES IN ENERGETICS OF POLYMER DERIVED CERAMICS, METAL ORGANIC FRAMEWORKS, AND OTHER HYBRID MATERIALS  |
| 16.10 -16.50 James Chickos, ESTIMATIONS OF THE LIQUID AND SOLID HEAT CAPACITY OF LARGE MOLECULES BY GROUP ADDITIVITY |
| 16.50 -17.30 Vecchio Ciprioti Stefano THERMODYNAMIC STUDY OF FORMAMIDINIUM LEAD IODIDE (CH5N2PbI3) FROM 5 TO 357 K |

17.30 - 18.30 Poster session (Participants in an alphabetical order from А to Ж)

19.30 - 22.00 Buffet

**Tuesday, 24.08.2022**.

9.00-11.00-Plenary session.

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| 9.00-9.40 Verevkin Sergey Petrovich, GIBBS–HELMHOLTZ EQUATION: PRACTICAL APPLICATIONS IN THERMOCHEMISTRY  |
| 9.40-10.20 Gavrichev Konstantin Sergeevich, THERMODYNAMIC PROPERTIES OF MIXED OXIDES FOR THERMAL BARRIER COATINGS: RE ZIRCONATES, HAFNATES, TANTALATES |
| 10.20-11.00 Zherikova Ksenia Vasilievna, METAL-ORGANIC COMPOUNDS FOR GAS-PHASE DEPOSITION: HOW DO WE TINKER WITH THERMODYNAMIC AND THERMOCHEMICAL DATA POOL? |

11.00 - 11.30 Coffee break

11.30 - 13.50 Section reports

1) Thermochemistry and Databases. Organic and organometallic compounds.

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| **11.30-12.00 (keynote lecture)** |  | **Markin Alexey Vladimirovich** | **Experimental calorimetry for study of materials based on organic, organoelement and polymeric compounds** |
| 12.00-12.20 |  | Vera L.S. Freitas | Thermodynamic properties of an organic single crystal scintillator: 9-phenylcarbazole |
| 12.40-13.00 |  | Yagofarov Mikhail Iskanderovich | Temperature dependence of phase transition enthalpies of organic non-electrolytes |
| 13.00-13.20 |  | Makarenko Alexander Mikhailovich | Scandium(III) β-diketonates as MOCVD precursors: thermodynamic and “structure-property” relationships |
| 13.20-13.35 |  | Yurkshtovich Yana Nikolaevna | Experimental and theoertical thermodynamic study of 1-benzyl-4-phenyl-1H-1,2,3-triazole and 1,3-bis(1-methyl-1H-tetrazol-5-yl)propane in gaseous and condensed aggregate states |
| 13.35-13.50 |  | Karakovskaya Ksenia Igorevna | Relations between structure and thermal behavior of MOCVD precursors: iridium (I) complexes with cyclooctadiene-1,5 and beta-diketonate derivatives |

2) Modern Thermal Analysis and Calorimetry (dedicated to L.G. Berg). Fast scanning calorimetry.

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| **11.30 -12.00 (keynote lecture)** |  | **Cangialosi Daniele** | **Insights on glass dynamics from aging far below the glass transition** |
| 12.00-12.20 |  | Minakov Alexander Alexandrovich | Thermal perturbations at crystal nucleation in glasses and polymers |
| 12.20-12.40 |  | Gerasimov Alexander Vladimirovich | Crystallization kinetics and glass-forming ability of drugs from fast scanning calorimetry data |
| 12.40-12.55 |  | Andrianov Ruslan Arturovich | The stability of poly-L-lactide nuclei according to the classical nucleation theory and fast scanning calorimetry |
| 12.55-13.10 |  | Abdullin Albert Radikovich | FSC study of crystallization kinetics of cross-linked poly(butylene terephthalate) |

3) Phase Equilibria: Molecular and Ionic Compounds. Ионные жидкости

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| **11.30 -12.00 (keynote lecture)** |  | **Sedov Igor Alekseevich** | **Novel approaches for characterizing nanoheterogeneity in ionic liquids** |
| 12.00-12.20 |  | Makarov Dmitry Mikhailovich | QSPR models for phase transition and decomposition temperature of ionic liquids |
| 12.20-12.40 |  | Postnikov Evgeny Borisovich | Predicting thermodynamic properties of ionic liquids at high pressures based on the reference data at ambient pressure |
| 12.40-13.00 |  | Safonova Evgenia Alekseevna | Polymerized ionic liquids for the enhanced bioextraction |
| 13.00-13.20 |  | Kalinyuk Daria Alexandrovna | Thermodynamic functions of formation of 1-ethyl- and 1-buthyl-3-methylimidazolium clorides |
| 13.20-13.35 |  | Korchak Petr Andreevich | Liqiud-liquid equlibrium and partitioning of biocomponent in aqueous mixtures of ionic liquid of different structure and kosmotropic salt |
| 13.35-13.50 |  | Shelepova Ekaterina Alekseevna | Empty volume in ionic liquids and its connection with the solubility of gases |

13.50-15.00 –Dinner

15.00-17.00-Section reports

1) Thermochemistry and Databases. Inorganic compounds.

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| **15.00-15.30 (keynote lecture)** |  | **Khvan Alexandra Vyacheslavovna** | **Experimental and theoretical investigation and critical assessment of thermodynamic data for pure in, cu and some binary systems from 0K** |
| 15.30-15.50 |  | Blokhin Andrey Viktorovich | Heat capacity in the interval 80-370 K and parameters of phase transitions of barium dopped strontium ferromolybdate |
| 15.50-16.10 |  | Shtenberg Mikhail Vladimirovich | Calculation of temperature dependences of heat capacity of alkaline borates |
| 16.10-16.30 |  | Ostroushko Alexander Alexandrovich | Complex thermal analysis of oxide materials synthesis processes via combustion reactions taking into account charge generation |
| 16.30-16.45 |  | Tolmacheva Nelli Nikolaevna | Thermodynamic properties of the Na2O-BaO-B2O3 system |
| 16.45-17.00 |  | Osipenko Anastasia Alexandrovna | Thermodynamic behaviour of palladium in LiCl–KCl–CsCl eutectic melt |

2) Phase Equilibria: Molecular and Ionic Compounds

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| **15.00-15.30 (keynote lecture)** |  | **Toikka Alexander Matveevich** | **Liquid phase splitting and critical states in quaternary systems with chemical reactions: new experimental data**  |
| 15.30-15.50 |  | Pestov Sergey Mikhailovich | Thermodynamic modelling of systems containing liquid crystals |
| 15.50-16.05 |  | Kuzovchikov Semyon Valerievich | Phase stability and thermodynamic modelling of alloys based on the Co-Cr-Mn system |
| 16.05-16.20 |  | Brezhnev Nikolai Yurievich | Phase diagram for the In-Se system according to the data of the thermal, structural and vapor-pressure investigations |

3) Modern Thermal Analysis and Calorimetry (dedicated to L.G. Berg). Fast scanning calorimetry.

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| **15.00-15.30 (keynote lecture)** |  | **Zhuravlev Evgeny Alexandrovich** | **Polymer and metal powders for additive manufacturing guided by differential fast scanning calorimetry** |
| 15.30-15.50 |  | Tropin Timur Vasilievich | Modeling of DSC curves of polystyrene during glass transition: from conventional to fast cooling rates |
| 15.50-16.10 |  | Buzyurov Alexey Vladimirovich | New approach for vapor pressure determination by means of fast scanning calorimetry |
| 16.10-16.25 |  | Bolmatenkov Dmitry Nikolaevich | Vaporization enthalpy of organic non-electrolytes in a wide temperature range: pencil and paper vs experimental measurements |
| 16.25-16.40 |  | Larionov Radik Anatolievich | Thermal and supramolecular properties of oligopeptides  |

17.00-18.30 Poster session (Participants in an alphabetical order from З to П)

**Wednesday, 24.08.2022**

 9.00-11.00 - Plenary session.

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| 9.00-9.40 Solomonov Boris Nikolaevich,THE DISSOLUTION THERMODYNAMICS AS THE KEY TO UNDERSTANDING VARIOUS PHYSICOCHEMICAL PHENOMENA |
| 9.40-10.20 Mukhametzyanov Timur Anvarovich, FAST SCANNING CALORIMETRY: NEW OPPORTUNIES FOR CHEMICAL THERMODYNAMICS |
| 10.20-11.00 Varfolomeev Mikhail Alekseevich, THERMOCHEMISTRY OF NATURAL GAS STORAGE AND OF HEAVY OIL RECOVERY  |

11.00 - 11.30 Coffee break

11.30 - 13.00 Section reports

1) Applied Thermodynamics and Biothermodynamics (dedicated to A.A. Pimerzin)

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| **11.30 -12.00 (keynote lecture)** |  | **Bykov Alexey Gennadievich** | **Proteins, polyelectrolytes and copolymers for pulmonary surfactants**  |
| 12.00-12.20 |  | Maksimov Evgeniy Georgievich | Control of hydrogen bonding in photoactive orange carotenoid protein by noncanonical amino acid substitutions of tyrosine-201 |
| 12.20-12.40 |  | Manin Alexey Nikolaevich | Study of the cocrystallization effect on the carbamazepine thermal stability  |
| 12.40-13.00 |  | Portnova Svetlana Valerievna | Influence of the structure of esters of natural hydroxycarboxylic acids on thermodynamic and thermophysical property |

2) Thermochemistry and Databases. Organic and organometallic compounds.

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| **11.30 -12.00 (keynote lecture)** |  | **Smirnova Natalia Nikolaevna** | **The dependence of thermodynamic properties of polyphenylenes on their structure** |
| 12.00-12.20 |  | Dávalos Juan Z | Thermochemical and structural properties of the new sulphur-containing compounds with relevance on atmospheric chemistry |
| 12.20-12.40 |  | Samarov Artemy Andreevich | Alkyl-substituted biphenyls as potential candidates for liquid organic hydrogen carriers |
| 12.40-12.55 |  | Sarmini Yulia Alexandrovna | Study of the thermodynamic properties of organosilicon dendrimers and their corresponding nanogels with different nature terminal groups |

3) Thermodynamics of solutions

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| **11.30 -12.00 (keynote lecture)** |  | **Kustov Andrey Vladimirovich** | **Solvophobic and solvophilic effects in urea and tetramethylurea solutions**  |
| 12.00-12.20 |  | Kononova Elena | Research of the systems amino-alcohol - water |
| 12.20-12.40 |  | Germanovna | Thermodynamic models for aqueous, organic and electrolyte solutions |
| 12.40-13.00 |  | Kovalenko Nikita Andreevich | Dependence of formal electrode potential on ionic strength |

13.00-14.00 Dinner

14.00-18.00 Excursion.

19.00-22.00 Banquet.

**Thursday, 25.08.2022**

9.00-11.00 Plenary session.

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| 9.00-9.40 Budkov Yury Alekseevich, MEAN-FIELD THEORY OF MACROSCOPIC FORCES IN INHOMOGENEOUS IONIC FLUIDS |
| 9.40-10.20 Fedorov Pavel Pavlovich, APPLICATION OF THE THIRD LAW OF THERMODYNAMICS TO THE STUDY OF PHASE DIAGRAMS |
| 10.20-11.00 Baidakov Vladimir Georgievich, LIMITS OF STABILITY OF METASTABLE PHASES AND METASTABLE PHASE EQUILIBRIA IN SIMPLE ONE-COMPONENT SYSTEM |

11.00 - 11.30 Coffee break

11.30 - 13.50 Section reports

1) Amphiphilic compounds: thermodynamics of self-organization, physicochemical properties and practical application.

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| **11.30-12.00 (keynote lecture)** |  | **Derkach Svetlana Rostislavovna** | **Gelatin as a stabilizer for emulsions: molecular modification** |
| 12.00-12.20 |  | Gainanova Gulnara Akhatovna | Ammonium-phosphonium-isothiuronium amphiphiles: CMC, solubilizing capability and catalytic effect |
| 12.20-12.40 |  | Burilov Vladimir Alexandrovich | New macrocyclic amphiphiles for sensing and green micellar&metal/photocatalysis |
| 12.40-12.55 |  | Pavlov Rais Valerievich | Aggregation of carbamate gemini surfactants and their potential as liposome modifiers |
| 12.55-13.10 |  | Radaev Dmitry Denisovich | Amphiphilic NHC precursors based on imidazole-4,5-dicarboxylic acid: synthesis and aggregation in aqueous media. |
| 13.10-13.25 |  | Faria Bruna Franciele | Simulation of surfactant adsorption at liquid-liquid interface |
| 13.25-13.40 |  | Oselskaya Victoria Yurievna | Hydration effect on encapsulation of indometacin by solid cyclodextrins |
| 13.40-13.55 |  | Chirkov Nikolai Sergeevich | Formation of mixed DNA/polyelectrolyte layers at the water–air interface |

2) Applied Thermodynamics and Biothermodynamics (dedicated to A.A. Pimerzin). Biothermodynamics

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| **11.30-12.00 (keynote lecture)** |  | **Noskov Boris Anatolievich** | **Protein microgel layers at the liquid-gas interface** |
| 12.00-12.20 |  | Milyaeva Olga Yurievna | The impact of thrombine on dynamic surface properties of fibrinogen solutions |
| 12.20-12.40 |  | Magsumov Timur Ilnurovich | Influence of organic solvents on thermal stability and denaturation mechanism of lysozyme |
| 12.40-13.00 |  | Akentiev Alexander Vladimirovich | Films of lysozyme fibrillar aggregates on the water surface |
| 13.00-13.20 |  | Bazhin Nikolai Mikhailovich | Helmholtz energy: is it energy or not? |
| 13.20-13.35 |  | Khaibrakhmanova Dilyara Raisovna | Evaluation of the binding properties of drugs to albumin from DSC thermograms |
| 13.35-13.50 |  | Fatkhutdinova Alisa Amirovna | Step-scan differential scanning calorimetry for investigation of protein denaturation |

3) Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation. Quantum Chemical Methods.

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| **11.30-12.00 (keynote lecture)** |  | **Khursan Sergey Leonidovich** | **Homodesmotic method for studying the molecular energetics of organic compounds** |
| 12.00-12.30 |  | Medvedev Nikolai Nikolaevich | Voronoi-Delaunay method. Applications to solutions |
| 12.30-12.50 |  | Ageenko Vera Nikolaevna | Monoethanolamine hydration as seen by dielectric relaxation spectroscopy and quantum chemical calculations |
| 12.50-13.10 |  | Rychkov Denis Alexandrovich | Comparison of different computational techniques for evaluation of quercitin conformers |
| 13.10-13.30 |  | Chuev Gennady Nikolaevich | A new approach to the calculation of solvation effects in biomolecular solutions in the framework of the classical density functional theory |
| 13.30-13.45 |  | Maltsev Maxim Alexandrovich | Quantum chemical study of the interatomic interaction of diatomic argides  |

4) Phase Equilibria: Molecular and Ionic Compounds

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| **11.30-12.00 (keynote lecture)** |  | **Gorbatchuk Valery Vilenovich** | **Thermodynamics of molecular recognition and polymorphism** |
| 12.00-12.20 |  | Almeida Ana Rita Rocha Pinheiro | Pressure-temperature phase diagrams near the triple point of four benzaldehydes |
| 12.20-12.40 |  | Golikova Alexandra Dmitrievna | Heat effects of phase and chemical processes in a multicomponent system with chemical interaction |
| 12.40-13.00 |  | Kabanova Elizaveta Genrikhovna | Experimental study and CALPHAD modeling of the Ag-In-Pd ternary |
| 13.00-13.20 |  | Guskov Vladimir Yurievich | Thermodynamic features of enantiomer adsorption on the surfaces with supramolecular chirality |
| 13.20-13.35 |  | Lyubichev Dmitry Alekseevich | Separation of azeotropic mixtures: novel approaches of using choline chloride based deep eutectic solvents |
| 13.35-13.50 |  | Smirnov Alexander Alekseevich | Investigation of the efficiency of the ethanol-ethyl formate system separation by various DESS based on choline chloride |

13.50-15.00 Dinner

15.00-16.40 Section reports

1) Amphiphilic compounds: thermodynamics of self-organization, physicochemical properties and practical application.

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| **15.00-15.30 (keynote lecture)** |  | **Zakharova Lucia Yarullovna** | **Structural factor controlling self-assembly behavior and functional activity of surfactant systems** |
| 15.30-15.50 |  | Ziganshina Albina Yulduzovna | Stimuli-responsive nanocarriers for substrate binding and release |
| 15.50-16.10 |  | Volkov Nikolai Alexandrovich | Modelling micelles in polar and non-polar solvents: from single aggregate to aggregates size distribution |
| 16.10-16.25 |  | Belov Roman Nikolaevich | Reductive cleavage of C-O bonds in p-tert-butylcalix[4]arene derivatives in the presence of hydrazine. |
| 16.25-16.40 |  | Makarov Egor Grigorievich | Novel tetra-azide and triazole derivatives of thia- and calix[4]arene with free phenolic hydroxyls |

2) Thermochemistry and Databases. Inorganic compounds.

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| **15.00-15.30 (keynote lecture)** |  | **Kurapova Olga Yurievna** | **The use of the thermodynamic approach for advanced ceramics development** |
| 15.30-15.50 |  | Semerikova Anna Nikolaevna | Thermodynamic characteristics of cesium dimolybdate and lithium monomolybdate doping by 10% cesium |
| 15.50-16.10 |  | Silyukov Oleg Igorevich | Inorganic-organic derivatives of layered perovskite-like oxides thermal stability and photocatalytic activity |
| 16.10-16.25 |  | Kutuzova Valeria Evgenievna | Study of Al2O3 - ZrO2 -Yb2O3 precursors by the differential scanning calorimetry  |
| 16.25-16.40 |  | Vorozhtsov Viktor Alekseevich | Mass spectrometric study and modeling of the thermodynamic properties of the Al2O3-SiO2-ZrO2 system |

3) Термохимия и базы данных. Органические и металлоорганические соединения.

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| 15.00-15.20 |  | Ribeiro da Silva Maria Dores Melo Cruz | An experimental insight on the thermochemistry of naphthalene diols |
| 15.20-15.40 |  | Nagrimanov Ruslan Nailievich | New relationship between enthalpies of vaporization and solution for molecular and ionic liquids |
| 15.40-16.00 |  | Chernyaykin Ivan Sergeevich | Heat capacity and thermodynamic functions of crystalline copper(II) dipivaloylmethanate from 0 to 430 K |
| 16.20-16.40 |  | Miroshnichenko Evgeny Alexandrovich | The rearrangement energy of frame radicals |

4) Thermodynamics of solutions

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| 15.00-15.20 |  | Tkachev Nikolai Konstantinovich | Thermodynamic perturbation theory for molten alkali halides |
| 15.20-15.40 |  | Khodov Ilya Anatolievich | Conformational preferences of fenamates in supercritical state parameters of the solvent based on NOESY data |
| 15.40-16.00 |  | Anashkin Ivan Petrovich | Molecular simulation of the pervaporation process |
| 16.20-16.40 |  | Kadtsyn Evgeny Dmitrievich | Volumetric properties of aqueous alcohol solutions: a Voronoi analysis |

16.40-18.10 Poster session (Participants in an alphabetical order from Р to Я)

**Friday, 26.08.2022**.

 9.00-10.40 Oral presentations

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| 9.00-9.20 Sun Li-Xian, ENERGY STORAGE MATERIALS AND SENSORS |
| 9.20-9.40 Sineva Svetlana Igorevna HIGH-TEMPERATURE PHASE EQUILIBRIA IN THE Fe-Sn-S SYSTEM |
| 9.40-10.00 Lőrinczy Dénes Márton, APPLICATION OF DSC FOR STUDYING THE DOSE DEPENDENT EFFECT OF CYCLOPHOSPHAMIDE TREATMENT ON ACTIN |
| 10.00-10.20 Meier Robert GROUP CONTRIBUTION REVISITED: THE ENTHALPY OF FORMATION OF ORGANIC COMPOUNDS WITH “CHEMICAL ACCURACY” |
| 10.20-10.40 Malyshev Vladimir Mikhailovich COMPUTERIZED MEASURING DEVICES IN ADIABATIC CALORIMETRY |

10.40-11.20 Coffee break.

11.20-12.40 Plenary session

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| 11.20-12.00 Turovtsev Vladimir Vladimirovich APPLICABILITY OF POPULAR FUNCTIONALS IN CALCULATIONS OF THE ENERGY, THERMODYNAMIC AND SPECTROSCOPIC PROPERTIES OF SUBSTANCES |
| 12.00-12.40 Tovbin Yuri Konstantinovich EQUILIBRIUM DROPS: A DIFFERENCE BETWEEN THERMODYNAMICS BY CLAUSIUS AND GIBBS IN TASKS OF THE PHASE EQUILIBRIUM  |

12.40 Closing ceremony.