

July 2

Morning session Chairman Prof. P. Bultinck, Prof. V. Tsirelson

9:00 – 9:30 Andrzej Sokalski "Analysis of Interactions within Catalytic Sites"

9:30 – 10:00 Frank Hagelberg "Magnetism in Novel Metallofullerenes and Ultrashort Carbon Nanotubes"

10:00 – 10:30 David Close "Problems with Delocalized Cations in Stacked Purines"

10:30 – 10:45 Pavel D'yachkov "Linear Augmented Cylindrical Wave Method for Calculating the Pristine and Chemically Modified Nanotubes"

10:45 – 11:00 Tugba Tugsuz Arifioglu "DFT Calculations of Substituent and Solvent Effects on the Electrode Potentials of Imidazole and its Derivatives"

11:00 – 11:30 *Coffee break*

11:30 - 12:00 Jerzy Leszczynski "Addressing Challenges of the First Part of the 21st Century: Merging Nano- and Bio- Chemistry"

12:00 - 12:15 Mykola Turovskyj "Molecular Modelling of Supramolecular Reactions of Organic Peroxides and Onium Salts"

12:15 - 12:30 Tatyana Shubina "Theoretical Investigations of DEA-NONOate Decomposition Pathways"

12:30 - 12:45 Iryna Doroshenko "The Kinetics of Cluster Formation during the Phase Transition Gas-Liquid in Alcohols"

12:45 - 13:00 Closing remarks

13:00 - 14:00 *Lunch*

14:30 - 17:30 *Excursion: Odesa catacombs*

Symposium addresses

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Information about the Symposium: <http://xray.isc.kharkov.com/MACC-3/>

Methods and Applications of Computational Chemistry

Third International Symposium



MACC-3

28 June – 2 July 2009

Odesa, Ukraine

<http://xray.isc.kharkov.com/MACC-3/>

Symposium schedule

June 28

8:00 – 19:00 *Registration*

15:00 – 18:00 *Excursion: Odesa city overview*

June 29

8:00 – 9:30 *Registration*

9:30 – 9:45 Brief foreword

Morning session Chairmen Prof. V. Bazilevsky, Prof. Z. Latajka

9:45 – 10:15 Alexander Bagatur'yants "Quantum Chemistry and Materials Science"

10:15 – 10:45 Ilya Kaplan "Problems in the Computational Studies of Transition-metal Clusters with 3d Electrons. Mn₂"

10:45 – 11:15 Szczepan Roszak "Theoretical Studies of Property Variations in Oligomers Precursors of Conducting Polymers"

11:15 – 11:30 Nicolay Malomuzh "To What Extent are Thermodynamic Properties of Water Argon-like?"

11:30 – 12:00 *Coffee break*

12:00 – 12:30 Frances Hill "Assessing the Environmental Impacts of High Nitrogen Explosives: A Computational Chemical Approach"

12:30 – 13:00 Eduard Matito "Extrapolation of the PES Using First and Second Derivatives"

13:00 – 13:30 Leonid Gorb "An ab initio Molecular Dynamics Study on the Initial Chemical Events in Nitramines: Mechanism and Kinetics of Thermal Decomposition of CL-20"

13:30 – 13:45 Dmytro Babyuk "Application of Quantum Trajectories to Collinear Reactive Scattering in the Hydrogen Exchange Reaction $H+ClH = HCl + H$ "
13:45 – 14:45 *Lunch*

Afternoon session Chairman *Prof. I. Kaplan*

14:45 – 15:15 Philip Hoggan "Structure Harmonics in Slater Basis Sets: Strategy and Applications for Metabolic NMR"
15:15 – 15:30 Andreas Theophilou "Minimum Principles and Asymmetry in Hartree-Fock and Density Functional Theory"
15:30 – 15:45 Vladimir Ivanov "Electronically Excited States In The Multi-reference State-Specific Coupled Cluster Theory"
15:45 – 16:00 Valery Virovoj "Deterministic Chaos in Oscillating Reactions with Three Component"
16:00 – 16:15 Vladyslav Cheranovskii "On the Energy Spectrum and Low-Temperature Thermodynamics of Model Ferrimagnet Having One-Dimensional Magnetic Sublattice of Spin Tube Type"
16:15 – 16:30 Vladimir Khavryuchenko "Spin Catalysis in the Process of H₂S Oxidation with Quinones and Quinoid Groups on the Surface of Active Carbon: A Quantum Chemical Insight"
16:30 – 17:00 *Coffee break*
17:00 – 19:00 First poster session

June 30

Morning session Chairmen *Prof. D. Close, Prof. A. Sokalsky*

9:00 – 9:30 Zdzislaw Latajka "Quantum Chemical Topology Description of the Nature of Chemical Bonds and Chemical Reactions"
9:30 – 10:00 Vladimir Tsirelson "Looking for the Bonding Descriptors Based on Electron Density"
10:00 – 10:30 Oleg Shishkin "Intermolecular Interactions with Participation of π -System in Supramolecular Complexes and Molecular Crystals"
10:30 – 11:00 Konstantin Lyssenko "Bond Energy Estimation via XRD: from H-EH Interactions to Metal-Ligand Bonds"
11:00 – 11:30 *Coffee break*
11:30 – 12:00 Michal Cyranski "Energetic Aspects of Cyclic π -Electron Delocalization"
12:00 – 12:30 Remi Chauvin "Shaping the Key to Aromaticity"
12:30 – 13:00 Gerbert Kamalov "Crown Ethers Complexes with Chromium(VI) Compounds. Supramolecular Aspects of Structure and Reactivity"
13:00 – 13:30 Xavier Assfeld "From Simple Molecules to Biomolecules: a Hierarchy of Complexity. Some Applications on the Electron Addition on Dichalcogen Bond"
13:30 – 14:30 *Lunch*

Afternoon session Chairman *Prof. R. Chauvin*

14:30 – 15:00 Jiande Gu "Low-Energy Electron attachment to DNA fragments"
15:00 – 15:30 Tanja van Mourik "Explicit Hydration of Nucleic Acid Bases"
15:30 – 16:00 Mikhail Basilevsky "The Implicit Electrostatic Solvent Model with Continuous Dielectric Permittivity Function"

16:00 – 16:15 Igor Zhiganyuk "Nature of the Positive and Negative Hydration for Single Charged Ions of Alkali Metals in Water Solutions"
16:15 – 16:30 Oleksandr Slobodyanyuk "Abnormal Shifts in Raman Spectra of Deuterated Cytidine and 6-Azacytidine: Experimental and Calculated"
17:30 – 19:30 *Reception*

July 1

Morning session Chairmen *Prof. T. Clark, Prof. J. Leszczynski*

9:00 – 9:30 Alex Tropsha "Prediction of Animal Toxicity Endpoints Using a Combination of Chemical and Biological in vitro Descriptors of Molecules"
9:30 – 10:00 Vladimir Palyulin "Molecular Design of Neuroprotectors"
10:00 – 10:30 Patrick Bultinck "The Promise (or not) of Quantum Chemistry in QSAR"
10:30 – 11:00 Serge Tratch "Computer-Assisted Search for New Types of Organic Reactions: an Application of the ARGENT-1 Program"
11:00 – 11:30 *Coffee break*
11:30 – 12:00 Victor Kuz'min "Properties of Compounds Mixtures - Challenge for QSAR/QSPR Analysis"
12:00 – 12:15 Anatoliy Artemenko "QSAR Analysis of the Antiherpetic Activity of Macrocyclic Compounds and Its Structural Analogs"
12:15 – 12:30 Pavel Polishchuk "Application and Efficacy of Random Forest Method for QSAR Analysis"
12:30 – 12:45 Eugene Muratov "Trust, but Verify: Principles of Dataset Curation for Cheminformatics Research"
12:45 – 13:00 Alexey Lagunin "Creation and External Validation of QSAR Models for Cyclooxygenase/Lipoxygenase Inhibitors"
13:00 – 13:15 Alexey Zakharov "QSAR Modelling of Rodent Acute Toxicity"
13:15 – 13:30 Andriy Golub "Computer-Aided Design Of Novel Protein Kinase CK2 Inhibitors"
13:30 – 14:30 *Lunch*

Afternoon session Chairman *Prof. V. Palyulin*

14:30 – 14:45 Nina Kharchevnikova "Quantum Chemical Simulation of Metabolism, Toxicity, Carcinogenic Potency, and Biodegradation of Benzene Derivatives"
14:45 – 15:15 Tim Clark "Molecular Dynamics and Signal Transduction"
15:15 – 15:45 Leonid Sukhodub "Intermolecular Interactions of DNA Bases and the Bases with Water Molecules: Mass Spectrometric Studies"
15:45 – 16:00 Inta Liepina "Amyloid Formation of Two Abl-SH3 Domain Peptides"
16:00 – 16:15 Dmytro Hovorun "Comprehensive Conformational Analysis of Canonical and Modified Nucleosides: Structure-Activity Relationship. Ab initio DFT and MP2 Study"
16:15 – 16:30 Yuri Rubin "Modeling of Electronic and Molecular Structures of M-DNA Fragments: from Monomer to Stacking Oligomers"
16:30 – 17:00 *Coffee break*
17:00 – 19:00 Second poster session