13:00 - 13:30 Muratov E. "Predictive QSAR models of skin sensitization and skin permeability and their application to identifying potentially hazardous chemicals"
13:30 - 14:30 *Lunch*
Session 11. Chairman: Istvan Mayer
14:30 - 15:00 Chauvin R. "The fundamental equation of aromaticity: from mathematics to chemistry"
15:00 - 15:30 Lepetit C. "Carbo-chromophores for two-photon absorption"
15:30 - 16:00 Hagelberg F. "Novel materials based on carbon nano-structures"
16:00 - 16:15 Khavryuchenko O. "Impact of the half-metallicity of carbon on chemical reactions: a computational (CASSCF) investigation"
16:15 - 16:30 Azizoglu A. "Substituent effects on the ring-opening mechanism of silacyclopropylidenoids to silallenes: A computational study"
16:30 - 18:30 *Poster session II (pp. 98-143 of the Book of Abstracts)*

5 July
Session 12. Chairman: Alexey Arbuznikov
9:00 - 9:30 Kalugin O. "Control of carbon nanotube electronic properties and operational chirality by lithium intercalation"
9:30 - 10:00 Yudanov I. "Catalytic activity of metal nanocrystallites: DFT studies of structure sensitivity and particle size effects"
10:00 - 10:15 Ijagbuji A. "The new pathway of nitric acid preparation - reproduction of HNO_3"
10:15 - 10:45 *Coffee break*
10:45 - 11:15 Cheranovskii V. "The energy spectrum and magnetic properties of spin models for quasi-one-dimensional bimetallic magnets"
11:15 - 11:30 Grechnev G. "Electronic structure and physical properties of layered magnetic superconductors"
11:30 - 11:45 Rozhenko A. "Perfluoroalkylamino carbenes: structure, stability and an intermediate formation in the desulfurization reaction"
11:45 - 12:00 Zakharov A. "Linear and non-linear optic characteristics of π-conjugated polymers in a new local semiempirical coupled-cluster approach"
12:00 - 12:15 *Closing ceremony*

Symposium addresses:
Institute of Single Crystals – Lenin ave. 60; phone +38(057)341-02-73
"Mir" hotel – Lenin ave. 27a; phone +38(057)720-55-43
"National" hotel – Lenin ave. 21; phone +38(057)702-16-24
"Hotel12" hotel – Otakar Yarosh lane, 4; phone +380(57)340-31-03
"Kharkov" hotel – Svobody sq. 7; phone +38(057)758-00-08

MACC-5 Symposium (1-5 July, Kharkiv, Ukraine) Schedule

30 June
14:00 - 20:00 *Registration (Institute of Single Crystals)*

1 July
9:00 - 11:30 *Registration (Institute of Single Crystals)*
11:30 - 11:45 *Opening ceremony*
Session 1. Chairman: Jerzy Leszczynski
11:45 - 12:15 Kaplan I. "Modern state of the Pauli Exclusion Principle. Can it be proved?"
12:15 - 12:45 Mayer I. "Extracting chemical information from molecular wave functions"
12:45 - 13:15 Arbuznikov A. "Local hybrid exchange-correlation functionals: advances and challenges"
13:15 - 14:30 *Lunch*
Session 2. Chairman: Zdzislaw Latajka
14:30 - 15:00 Prezhdo O. "Quantum dots - artificial atoms, large molecules or small pieces of bulk? Insights from time-domain ab initio studies"
15:00 - 15:30 Pendas A.M. "Towards a real space description of the insulating or metallic character of a material: A quantum chemical topology point of view"
15:30 - 16:00 Tunega D. "Assessment of DFT methods in predicting structures and properties of phyllosilicates: importance of dispersion corrections"
16:00 - 16:30 Fil D. "Electron-hole pairing in double-layer graphene and graphyne"
16:30 - 18:30 *Poster session I (pp. 57-97 of the Book of Abstracts)*

2 July
Session 3. Chairman: Oleg Prezhdo
9:00 - 9:30 Rivail J.-L. "Hybrid quantum mechanical/molecular mechanical methods for modeling large molecular systems"
9:30 - 10:00 Assfeld X. "Electronic excited states of biomolecules"
10:00 - 10:30 Krylov A. "Towards first-principle calculations of redox potentials: Theory and applications to green fluorescent protein"
10:30 - 10:45 Etienne T. "Coupling molecular dynamics with hybrid QM/MM methods: Dynamic effects on the photophysical properties of a chromophore"
10:45 - 11:00 Loboda O. "Linear scaling modelling of biomolecules with electron delocalization networks"
11:00 - 11:30 *Coffee break*
Session 4. Chairman: Remi Chauvin
11:30 - 12:00 Latajka Z. "Xenon compounds - theoretical studies of molecular complexes"

12:00 - 12:30 Millot C. "Endeavour to improve an ab initio potential for water"
12:30 - 13:00 Nerukh D. "Modelling liquid solutions at atomistic and continuum representation at the same time: hybrid MD/hydrodynamics implementation of two dimensional water model"
13:00 - 13:15 Belyaeva E. "Quantum-chemical approach in calculations of thermodynamic and structural parameters of fatty acids Clusterization at the air/water interface"
13:15 - 13:30 Fomina E. "Quantum chemical analysis of the thermodynamics of 2D film formation of homochiral β-hydroxycarboxylic acids at the air/water interface"
13:30 - 14:30 *Lunch*

Session 5. Chairman: Tanja van Mourik

14:30 - 15:00 Leszczynski J. "Latest suggestions for prebiotic reactions revealed by computational studies"
15:00 - 15:30 Mons M. "Gas phase isolated peptides: structure, flexibility and excited state dynamics"
15:30 - 16:00 Poater A. "Computational insights in olefin metathesis"
16:00 - 16:30 Gu J. "Electron through DNA: A theoretical exploration"
16:30 - 17:00 *Transfer to the Conference Picnic*
17:00 - 20:00 *Picnic (presence of a bathing costume is recommended)*
20:00 - 20:30 *Transfer to the hotels*

3 July

Session 6. Chairman: Michel Mons

9:00 - 9:30 Gorb L. "Quantum-chemical modeling of DNA properties: from single DNA bases to DNA double strands"
9:30 - 10:00 van Mourik T. "The mutagenic action of 5-bromouracil: Static and dynamic DFT calculations on uracil and 5-bromouracil in nanodroplets"
10:00 - 10:30 Kuramshina G. "Correction of molecular force fields in Cartesian coordinates"
10:30 - 10:45 Rubin Yu. "Modeling of physical properties of nucleic acid fragments"
10:45 - 11:15 *Coffee break*

Session 7. Chairman: Szczepan Roszak

11:15 - 11:45 Boese A.D. "Intermolecular interactions: approaching chemical accuracy for surfaces and molecular solids"
11:45 - 12:15 Shishkin O. "Role of different intermolecular interactions in the formation of supramolecular architecture of molecular crystals"
12:15 - 12:45 Merz K. "Deuterium and fluorine substituents disturbe the aggregation of molecules"
12:45 - 13:00 Bartashevich E. "Characterizing noncovalent interactions in N,S-heterocycle complexes with iodine"
13:00 - 13:15 Tsendra O. "Periodic and cluster models in quantum chemical study of adsorption of nitro compounds on the α-quartz surfaces"
13:15 - 14:30 *Lunch*

Session 8. Chairman: Anna Krylov

14:30 - 15:00 Basilevsky M. "Kinetics of transfer reactions in condensed phase. The distributions of energy fluctuations for a local mode within the Fermi golden rule approximation"
15:00 - 15:30 Roszak S. "The properties of C-B, Si-B, and C-Be bonds - elements of functionalized materials"
15:30 - 16:00 Bagatur'yants A. "Multiscale atomistic modeling of the structure and electronic properties of functional layers used in OLED stacks"
16:00 - 16:15 Sushko M. "Finding the parameters of the interphase layers in fine dispersions with dielectric spectroscopy studies near the electrical percolation threshold"
16:15 - 16:30 Efremenko I. "Counterions in quantum chemical modeling: Thermochemistry and reactivity of polyoxometalates"
16:30 - 17:00 *Coffee break*
17:00 - 20:00 *City excursion*

4 July

Session 9. Chairman: Viktor Kuz'min

9:00 - 9:30 Cronin M. " Structure-based methods to estimate toxicity: The role of computational chemistry to make better predictions"
9:30 - 10:00 Vassiliev P. "Complex consensus approach to in silico search for novel drugs"
10:00 - 10:30 Polischuk P. "Structural interpretation of QSAR models - universal approach"
10:30 - 10:45 Devinyak O. "Statistical misconceptions in QSAR"
10:45 - 11:00 Richarz A. "Novel computational approaches to predict repeat dose toxicity from chemistry"
11:00 - 11:30 *Coffee break*

Session 10. Chairman: Mark Cronin

11:30 - 12:00 Poroikov V. "Prediction of activity spectra for substances: twenty years of the development"
12:00 - 12:15 Palafox M.A. "Structure-activity relationships/tendencies in stavudine, 2'-deoxyuridine and Nikavir antiviral derivatives"
12:15 - 12:30 Mokshyna E. "Study of second virial coefficient: new challenge for QSPR"
12:30 - 12:45 Klimenko K. "Two-layer QSPR model for prediction of organic compounds a queous solubility at various temperatures"
12:45 - 13:00 Novoselska N. "Nanoparticles: unusual QSAR for unusual structures"