

## July 4

9:00 - 10:00 Third Poster Session

*Morning Session* Chairman: *Prof. Z. Latajka*

10:00 - 10:30 Manuel Ruiz-Lopez "Theoretical study of the structure of HO<sub>n</sub> and H<sub>2</sub>O<sub>n</sub> species in water"

10:30 - 11:00 Daniel Tunega "Structural, spectroscopic and magnetic properties of MeOOH minerals (Me=Al, Mn, Fe)"

11:00 - 11:30 *Coffee Break*

11:30 - 12:00 Oleg Prezhdo "Dynamics on the nanoscale: Time-domain ab initio studies of carbon nanotubes, quantum dots, and molecule-semiconductor interfaces"

12:00 - 12:30 Szczepan Roszak "Structural and thermodynamic properties of microclusters - precursors of germanium/carbon and germanium/silicon nanomaterials"

12:30 - 12:45 Ivan Yakovkin "Microscopic model of CO oxidation on Pt(111)"

12:45 - 13:00 Closing Remarks

13:00 - 15:00 *Lunch*

15:00 Excursion

### *Symposium addresses*

Hotel "Tourist": R. Okipnoi st., 2, Kyiv, 02002 (metro Livoberezhna).

Phones: +38(044) 568-40-17, 568-42-54.

Hotel "St.-Petersburg": blvd.T.Shevchenko, 4, Kyiv, 01004 (metro Teatral'na).

Phones: +38(044) 279-74-72, 279-73-64.

Student dormitory: Zabolotnogo st., 144, Kyiv, 03143. Travel: route minibus

№ 3(172) or 156 from metro Lybids'ka to "Zabolotnogo st." stop.

Additional information, including fragments of the city map, you could find at our site:

<http://xray.isc.kharkov.com/MACC-2>

### *Contacts*

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Information about the Symposium <http://xray.isc.kharkov.com/MACC-2>

# Methods and Applications of Computational Chemistry

## *Second International Symposium*



**MACC-2**

2 - 4 July 2007

Kyiv, Ukraine

*Symposium schedule*

<http://xray.isc.kharkov.com/MACC-2>

<http://ual.ccmsi.us/conference.html>

# Methods and Applications of Computational Chemistry

## Second International Symposium

### Schedule

#### July 1

8:00 - 21:00 Registration

12:00 Excursion

#### July 2

8:00 - 9:00 Registration

9:00 - 9:30 Opening Ceremony

Morning Session Chairman: *Prof. J. Leszczynski*

9:30 - 10:00 Ilya Kaplan "Principal impossibility of the developed DFT approaches to describe the spin and space degenerate states"

10:00 - 10:30 Peter Politzer "Significance and applications of local ionization energies"

10:30 - 11:00 *Coffee Break*

11:00 - 11:30 Philip Hoggan "Exponential type orbital package: strategy and applications for NMR"

11:30 - 12:00 Jacek Karwowski "Quasi-exactly solvable models of atoms and molecules"

12:00 - 12:30 Igor Zilberberg "Paired orbitals for different spins equations"

12:30 - 14:00 *Lunch*

Afternoon Session Chairman: *Prof. J. Sponer*

14:00 - 14:30 Xavier Assfeld "Enhancements of the Hybrid LSCF/MM method and its Applications to Biochemical problems"

14:30 - 15:00 Konstantin Lyssenko "Energetic crystallography: New approaches and results"

15:00 - 15:15 Stephen Wilson "Distributed Gaussian Basis Sets: Recent Progress and Future Prospects"

15:15 - 15:30 Dmytro Babyuk "Application of Quantum Trajectory Method for Multidimensional Reactive Scattering"

15:30 - 15:45 Oleg Zhikol "Analyzing Molecular Excited States within Time-Dependent Density Functional Theory"

15:45 - 16:00 Gregory Chass "Research Exchange Along the Modern Silk Road: From Electrons to Clinical Assays, China to Europe and Back"

16:00 - 16:30 *Coffee Break*

16:30 - 17:30 First Poster Session

17:30 - 21:00 *Reception (a bus from "Tourist" hotel)*

#### July 3

Morning Session Chairman: *Prof. D. Hovorun*

9:00 - 9:30 Michel Mons "Biomolecules in the gas phase: why experimentalists do need theory?"

9:30 - 10:00 Tanja van Mourik "DFT vs. MP2: which method gives the correct tyrosine-glycine structure?"

10:00 - 10:30 Jan Urban "Temporary Negative Ions - Application of Theory to Biological Molecules"

10:30 - 11:00 *Coffee Break*

11:00 - 11:30 Jerzy Leszczynski "Beyond the Ground State: Excited State Properties of DNA Components"

11:30 - 12:00 Andrzej Sokalski "Exploring physical nature of intermolecular interactions in biomolecules"

12:00 - 12:30 Oleg Shishkin "Structure and intramolecular hydrogen bonding in canonical 2'-deoxyribonucleotides"

12:30 - 14:00 *Lunch*

Afternoon Session Chairmans: *Prof. P. Politzer, Prof. P. Hoggan*

14:00 - 14:30 Jiri Sponer "Molecular Dynamics simulations as a unique tool to study functional RNAs"

14:30 - 15:00 Jaroslav Burda "Computational study on aquation of ruthenium(II) complexes and their interactions with DNA bases"

15:00 - 15:15 Olga Yevtushenko "Quantum study of antiepileptic drugs and chemoconvulsants interaction with "key" amino acids sequences of GABAA receptor"

15:15 - 15:30 Anatoly Artemenko "Analysis of the biological activity of 1,4-benzodiazepine derivatives by means of HIT QSAR System"

15:30 - 15:45 Victor Kuz'min "The comparative analysis of efficacy of hierarchical informational technology for quantitative structure-activity relationships (HIT QSAR)"

15:45 - 16:00 Vladislav Cheranovskii "Magnetic structure and low-temperature thermodynamics of transition metal compounds with magnetic sublattice of ladder type"

16:00 - 16:30 *Coffee Break*

16:30 - 17:00 Zdzislaw Latajka "Nature of chemical bonds in molecular systems containing rare gas atoms"

17:00 - 17:30 Miquel Sola "Is the H...H interaction in phenathrene responsible for its higher stability as compared to anthracene?"

17:30 - 17:45 Alexander Rozhenko "RI-DFT and RI-MP2 calculations in supramolecular chemistry: stabilities of host-guest complexes"

17:45 - 18:00 Volodymyr Khavryuchenko "Electron and spin states of conjugated carbon"

18:00 - 19:00 Second Poster Session