PROGRAM - MOLMOD 2014
MOLECULAR MODELING IN CHEMISTRY AND BIOCHEMISTRY

Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University

THU 13 NOV – ROOM 97

08:30-09:00 Registration, Faculty of Chemistry and Chemical Engineering, 1st floor

09:00-09:10 Opening remarks by the organizers

09:10-09:50 TBA on behalf of Paul Mezey, Fuzzy Electron Density Fragments in Macromolecular Quantum Chemistry, Combinatorial Quantum Chemistry, Functional Group Analysis, and Shape-Activity Relations

09:50-10:30 Mircea Diudea, Fullerene aggregation

10:30-11:00 *Coffee break/poster session*

11:00-11:30 Mariusz Mitoraj, From Bonding To Catalysis - An Insight Based on the Combined Charge and Energy Decomposition Scheme (ETS-NOCV)

11:30-12:10 Attila Bende, Higher Level Singlet-Triplet Excited State Relaxation Dynamic Pathways for Acetophenone and Benzophenone Molecular Systems

12:10-12:40 Teobald Kupka, Molecular Modeling of Structure and Spectroscopic Parameters for Small and Large Molecules

12:40-14:30 *Lunch*

14:30-15:10 Fănică Cimpoeșu, Back to the Basis! Revisiting Some Methodological Issues of Computational Chemistry

15:10-15:25 Adrian Brânzanic, Density Functional Theory Study on Hydrogen-Rich Metallaboranes

15:25-15:40 Matei-Maria Uță, Manganese-Centered Ten-Vertex Germanium Clusters: In Search of the Missing Link

15:40-16:10 Lorentz Jäntschi, Monovalent Ions Dissolved in Water

16:10-16:50 *Coffee break/poster session*

16:50-17:05 Francisco Carrascoza, Exploring the Reactivity of Globins beyond Reversible Binding of Molecular Oxygen

17:05-17:20 Alexandru Lupan, From Closo to Isocloso Polyhedra and Beyond in Metallaborane Chemistry

17:20-17:35 Mihai Surducan, DFT Revision of DNA Reactions with Metallo-Bleomycins: Hydroperoxo or Oxo?

17:35-17:50 Sorana D. Bolboacă, The Influence of the Atom Type on High-Symmetry Structures

19:30 *Conference cocktail*

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09:00-09:40 Zoltan Néda, Kinetic Monte Carlo Study of Pt clusters on Pt (111) Surfaces

09:40-10:20 Romuald Poteau, First-Principles Modeling Of Organometallic Nanoparticles. The Ruthenium Case

10:20-10:50 *Coffee break*

10:50-11:30 Dragoș Horvath, S4MPLE – Sampler for Multiple Protein-Ligand Entities: Simultaneous Docking of Several Entities

11:30-12:10 Titus Beu, Tight-binding Vibrational Analysis of Single-Wall Carbon Nanotubes

12:10-14:00 *Lunch*

14:00-14:30 Vasile Chiș, Modeling Non-Covalent Interactions and Molecular Excited States by DFT Methods

14:30-15:10 Marilena Ferbințeanu, Discovering the Poles of the Molecular Magnets

15:10-15:25 Ahmet Atac, The Spectroscopic (FT-IR, FT-Raman, NMR, And UV-Vis) and Quantum Chemical Studies (DFT Approach) of 3,4-Difluoroaniline

15:25-15:40 Marina Alexandra Tudoran, Bondonic Effects on Topo-Reactivity of Nano-organics

15:40-15:55 Adel Abbas El-Azhary, Conformational and Vibrational Analysis of Dibenzo-18-crown-6

15:55-16:30 *Coffee break and poster session*

16:30-16:45 Mustafa Ali Cipiloglu, Spectroscopic and Molecular Structure Investigation of Neutral, Dimer and Anion Forms of 3,4-Pyridinedicarboxylic Acid: A Combined Experimental (FT-IR, FT-Raman, NMR, UV Spectra) and Theoretical Study

16:45-17:00 Attila Kun, A Quantum-Chemical Approach to Calculation of Structural Parameters of Theophylline Containing Transition Metal Complexes

17:00-17:30 Radu Silaghi-Dumitrescu, Exploring Unusual Ligands at Biological Metal Centers: From Molecular Nitrogen to Peroxochlorate

17:30 Closing remarks

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