

**PROGRAMME - MOLMOD 2018**

**MOLECULAR MODELING IN CHEMISTRY AND BIOCHEMISTRY**

**28-30 October, Cluj-Napoca, Romania**

**The Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University**

**SUN 28 OCT (54, Plopilor str., Universitas Complex of the Babes-Bolyai University)**

**12.00-22.00 Registration, social events**

**MON 29 OCT – room 88 (at 11, Arany Janos str., Faculty of Chemistry and Chemical Engineering)**

***08.30-09.00 Registration, poster set-up***

***09.00-09.10 Opening remarks***

**09.10-09.50 Paul Mezey, Memorial University of Newfoundland, Canada – Symmorphism of molecular shapes, a generalization of symmetry groups**

**09.50-10.30 Mihail V. Vener, Mendeleev University of Chemical Technology, Russia – Inhibiting low-frequency vibrations explains exceptionally high electron mobility in 2,5-Difluoro-7,7,8,8-tetracyanoquinodimethane (F2-TCNQ) single crystals**

***10.30-10.50 Coffee break, poster viewing***

**10.50-11.30 Snezana Zaric, University of Belgrade, Serbia & Texas A&M University at Qatar – Stacking interactions of metal-chelate rings and hydrogen-bridged rings**

**11.30-12.00 Attila Bende, National Institute for Research and Development of Isotopic and Molecular Technologies, Romania – DFT modeling of singlet-triplet spin transitions in Ni(II)-based macrocyclic-ligand supramolecular complexes**

**12.00-12.40 Valera Veryazov, Lund University, Sweden – Symmetric or antisymmetric? Electronic structure of dimers with even and odd numbers of electrons**

***12.40-14.30 Lunch***

**14.30-15.10 Fanca Cimpoesu, Institute of Physical Chemistry, Bucharest, Romania – Bond. Chemical Bond! Spying the secrets of molecular structure with state-of-the-art and revisited computation method**

**15.10-15.40 Mihai V. Putz, West University of Timisoara, Romania – Bondonic theory of chemical interactions. Applications on graphenic systems**

15.40-15.55 Andrei Neamtu, Iasi University of Medicine and Pharmacy, Romania – Antibody structure prediction and epitope mapping by molecular dynamics simulations

15.55-16.10 Szilard Fejer, Ab Initio Research Services Ltd & Provitam Foundation, Romania – Coarse-grained models for self-assembling hollow shells from colloidal building blocks

16.10-16.25 Dragos Isac, Petru Poni Institute of Macromolecular Chemistry, Romania – A new pathway of azobenzene interconversion assisted by DFT and ab initio methods

*16.25-16.50 Poster Session / coffee*

16.50-17.05 Mihai Medeleanu, Polytechnical University of Timisoara, Romania – Novel staffane-like structures, topological and quantum chemical characterization

17.05-17.20 Lorentz Jantschi, Technical University of Cluj-Napoca, Romania – The eigenproblem for alignment of molecules

17.20-17.35 Janos Szoverfi, Provitam Foundation, Romania – Molecular dynamics studies of CCMV capsid protein oligomers

17.35-17.50 Adrian Branzanic, Babes-Bolyai University, Romania – Role of siroheme and the Fe<sub>4</sub>S<sub>4</sub> cluster in the active site of sulfite reductase

17.50-18.05 Octav Caldararu, Lund University, Sweden – Quantum refinement of X-ray and neutron protein crystal structures

18.05-18.35 Power-poster presentations

*19.00 Conference cocktail/dinner (Universitas complex of the Babes-Bolyai University)*

**TUE 30 OCT – room 88**

09.00-09.40 Peter Szalay, Eotvos Lorand University, Hungary – Characterization of the excited states of DNA building blocks: a coupled cluster computational study

09.40-10.20 Andreas Savin, CNRS & Sorbonne University, France – On choosing the “best” density functional...or any computational method in chemistry. Probabilistic estimators

10.20-10.35 Alexandru Lupan, Babes-Bolyai University, Romania – Density functional theory investigation of carbalane polyhedra

*10.35-11.00 Coffee break*

11.00-11.30 Paul Nicu, Lucian Blaga University of Sibiu, Romania – Implications of the generalized coupled oscillator mechanism for the interpretation and calculation of Vibrational Circular Dichroism spectra

11.30-12.10 Dragos Horvath, Louis Pasteur University, France – The mapping of conformational space

12.10-12.50 Henning Henschel, University of Oulu, Finland – Water and proton dynamics from semi-empirical QM/MM Simulations

12.50-14.30 Lunch

14.30-15.10 Marilena Ferbinteanu, University of Bucharest, Romania – On the use of time-dependent density functional methods in the account of ligand field-type spectra of the coordination compounds

15.10-15.25 Claude Millot, Université de Lorraine, France – Modeling electric properties of hexahalobenzenes

15.25-15.40 Istvan Horvath, Ab Initio Research Services Ltd, Romania - A modified adjustable density matrix Assembler approach for fast computation of ab initio quality electron densities of complete proteins

15.40-16.10 Titus Beu, Babes-Bolyai University, Romania – Coarse-grained modeling of polyethyleneimine

16.10-16.25 Ionut-Tudor Moraru, Babes-Bolyai University, Romania – On the possible presence of carbides in the Fischer-Tropsch process catalyzed by ruthenium nanoparticles: a DFT study

16.25-16.40 Dennis Dinu, Institute of General, Inorganic and Theoretical Chemistry, LFU Innsbruck, Austria – Anharmonic Vibrational Spectroscopy of Small Organic Compounds

16.40-17.00 Radu Silaghi-Dumitrescu, Babes-Bolyai University, Romania – TBA

17.00- Closing remarks

#### POSTER PRESENTATIONS:

1. Reka-Anita Domokos, Babes-Bolyai University, Romania – Adsorption of the two isomers of resveratrol on Graphene
2. Luana Radu, Babes-Bolyai University, Romania – Reversible complexation of ammonia by breaking a manganese-manganese bond in a manganese carbonyl ethylenedithiolate complex
3. Alina Matei, Babes-Bolyai University, Romania – The high affinity of small-molecule antioxidants for hemoglobin and myoglobin
4. Adrian Branzanic, Babes-Bolyai University, Romania – DFT benchmarking for the correct description of spin states in bioinorganic centers. Heme vs. siroheme models of the sulfite reductase active site
5. Raluca Septelean, Babes-Bolyai University, Romania – Density functional theory investigation of hypoelectronic eight-vertex metallaboranes
6. Adrian Branzanic, Babes-Bolyai University, Romania – Dimetallaborane Analogues of the Octaboranes: Structural Variations with Changes in the Skeletal Electron Count
7. Alex-Adrian Farcas, NIRDIMT and Babes-Bolyai University, Romania – Intersystem crossing in metal-ligand coordination complexes with pyramidal-planar and octahedral coordination configurations
8. Hussein Unver, Ankara University, Turkey – DFT Calculations, Green synthesis and biological applications of methanesulfonamide functionalized graphene quantum dots
9. Donatella Balint, Babes-Bolyai University, Romania – Comparison of geometry optimization methods on amino acid structures
10. Teodor-Lucian Biter, INCDTIM Cluj-Napoca, Romania – Theoretical study of phenylene- and biphenyl-linked porphyrin layers

11. Tudor Vasiliu, Petru Poni Institute of Macromolecular Chemistry, Romania – Functionalized  $\beta$ -cyclodextrin as trans-membrane channel
12. Cristina Maria Buta, Institute of Physical Chemistry Bucharest, Romania – Through-space and Through-solvent Interactions between Nitroxide-based Stable Radicals
13. Alice Mischie, Institute of Physical Chemistry Bucharest, Romania – Hybrids and Bond Angles in Small Prototypic Hydrocarbon Molecules
14. Ana-Maria Toader, Institute of Physical Chemistry Bucharest, Romania – Reshaping the principles and techniques of Gaussian-type basis sets in computational chemistry
15. Larisa-Milena Timbolas, Babes-Bolyai University, Romania – Photophysical properties of perylene derivatives
16. Florin Teleanu, Babes-Bolyai University, Romania – Antiaromaticity comes in six: A HOMA/NICS study of [n]helicenes (n = 6 - 24)
17. Artiom Gaina Gardiuta, Babes-Bolyai University, Romania – Linkage isomerism in complexes of cobalamin with cysteine sulfenic, sulfinic and sulfonic acids
18. Roxana Pasca, Babes-Bolyai University, Romania – Thermodynamic properties of ethylenimine and ethylene glycol polymers
19. Mircea Nasui, Technical University of Cluj-Napoca, Romania – Challenges in designing nanoceria for antioxidant therapy
20. Dragos Isac, Petru Poni Institute of Macromolecular Chemistry, Romania – Computational studies of silicon-containing benzoic acid derivatives: 4-((Trimethylsilyl)methoxy) and 4-(3-(trimethylsilyl)propoxy)benzoic acid
21. Szabolcs Jako, Babes-Bolyai University, Romania – Data processing: dull or fun task?
22. Ionut-Tudor Moraru, Babes-Bolyai University, Romania – Towards a unitary description of E-O and E-N bonds (E = Si, Ge, Sn); from inorganic ethers to amines and isoelectronic species
23. Amr A.A. Attia – Nickel-substituted iron dependent cysteine dioxygenase: implications for the dioxygenation activity of nickel model compounds
24. Augustin Mot – Chemometric methods applied in questing phytooglobins roles in plant stress conditions

#### Other participants

1. Svetlana Pevzner, Nuclear Research Center – Negev at Beer Sheva, Israel
2. Israel Zilbermann, Nuclear Research Center – Negev at Beer Sheva, Israel
3. Gabriela Nemes, Babes-Bolyai University, Romania
4. Cornelia Majdik, Babes-Bolyai University, Romania
5. Luminita Silaghi-Dumitrescu, Babes-Bolyai University, Romania
6. Ionel Haiduc, Babes-Bolyai University, Romania
7. Oleg Rudenco, Babes-Bolyai University, Romania
8. Cosmin Balaiu, Babes-Bolyai University, Romania
9. Matei Uta, Babes-Bolyai University, Romania
10. Attila Kun, Babes-Bolyai University, Romania
11. Cristina Bischin, Babes-Bolyai University, Romania
12. Lavinia Buta, Babes-Bolyai University, Romania