IONEL HUMELNICU

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Theoretical and Physical Chemistry

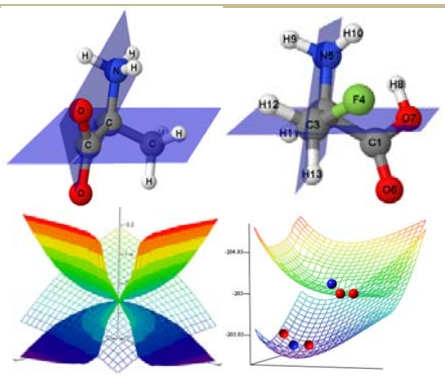
Computational Chemistry

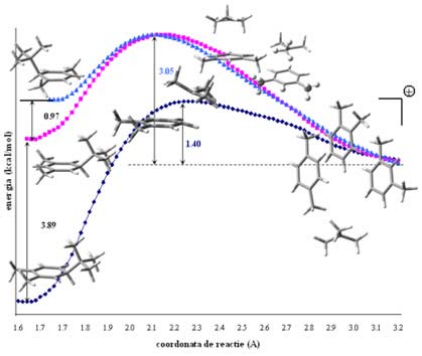
Research Areas/Interest

- Study of structure and reactivity of molecular systems
- Study of intermolecular interactions and the influence of the solvent on the structure, spectroscopic properties and reactivity of molecular systems
- Conformational study and properties of molecular systems with biological activity using the methods of theoretical chemistry
- Determination of potential energy surfaces, dynamics and mechanism of chemical reactions

Investigation of the spatial structure and determination of the reactivity descriptors that characterize the chemical systems. Study of intra-and intermolecular interactions and investigation the influence of the solvent nature on the spatial structure, electronic and spectroscopic properties and the reaction capacity of molecular systems. Spectroscopic characterization and study of transitions between energy levels that characterize the investigated systems in the ground and excited state. Molecular modeling. Theoretical approach of the complex systems containing transition metals.

Study of the conformational structure and spatial distribution of the electron density of the molecular systems with properties, or of interest, in the biological field. Correlation between structural parameters and biological reactivity properties of the studied molecular systems. Study of the reaction dynamics using the computational chemistry investigation methods. The determination of the reaction mechanisms based on the potential energy surface that characterizes the reaction system.





PhD studies
„Alexandru Ioan Cuza" University of Iaşi, 2000

Postdoc Scholarship
Westfälische Wilhelms University of Münster, Germany, 2001-2002

Publications (selection)

Humelnicu, I., Würthwein, E-U., Haufe, G., The Conformers of 3-Fluoroalanine. A Theoretical Study Influence of a Fluorine Substituent on the Physicochemical Properties and Chemical Reactivity of Fluorinated Amino Acids. Part 1, *Organic & Biomolecular Chemistry*, 10 (10), 2084-2093, **2012**.

Oprea, C., Panait, P., Cimpoeşu, F., **Humelnicu, I.**, Ferbinţeanu, M., Gîrţu, M., Broken symmetry DFT calculations of exchange coupling constants for manganese-porphyrin quasi-one-dimensional molecular magnets, *Theoretical Chemistry Accounts*: *Theory, Computation, and Modeling* (Theoretica Chimica Acta), *Theor Chem Acc* 131 (7) 1249-1261, **2012**.

Maftei, D., Zbancioc, Gh., **Humelnicu, I.**, Mangalagiu, I., Conformational Effects on the Lowest Excited States of Benzoyl-Pyrrolopyridazine. Insights from PCM Time- Dependent DFT, *The Journal of Physical ChemistryA*, 117 (15), 3165–3175, **2013**.

Weinberg, J., Cimpoesu, F., Lerner, D., **Humelnicu, I.**, The Association of Dehydro-Epiandrosterone and Adenosine Triphosphate Acid. A DFT Study of Interactions between Prototypic Biologically Active Molecules, *Journal of Molecular Structure*: THEOCHEM, 912 (1-3), 32-37, **2009**.

Nadejde, C., Creanga, D.E., **Humelnicu, I.**, Filip, E., Dorohoi, D.O., Study on the Intermolecular Interactions in Rifampicin Ternary Solutions – Calculation of Microscopic Parameters of Rifampicin Molecules, *Journal of Molecular Liquids*; 150 (1-3) 51-55, **2009**.