

PhD. student Dragoş Lucian ISAC

Research Assistant: 2017– “Petru Poni” Institute of Macromolecular Chemistry (ICMPP);

Education: 2014-present: Doctoral studies, position PhD student;

Project experience: Professional experience in theoretical studies (QM, QM/MM, MD, docking)-employed as team member (research assistant) in 3 national projects and 1 international project.

International and national conferences/symposia: 17+ presentations

Winter/Summer Schools & workshops: – "Molecular Modeling: Real Applications and New Approaches", 29th July- 2nd Aug. (2019) - at the Technology Park of Sardinia, Italy –Joint innovative training and teaching/learning program in enhancing development and transfer knowledge of application of ionizing radiation in materials processing, Sept. 7-17 (2015) in Warsaw, Poland, and Sept.28-Oct. 2, (2015) in Palermo, Italy–LLP Erasmus mobility, March 3 – June 9, (2014), Krakow, Poland.

Expertise fields: Exploring the ground and excited states of molecular systems, transition states structure, reaction processes, biological investigations, theoretical spectroscopy, study of inter- and intramolecular interactions, multi-scale modeling.

Scientific achievements: Theoretical study of amphiphilic silicone-bridged bis-triazoles as effective, selective metal ligands and biologically active agents in lipophilic environment; on the charge-transfer excitations in azobenzene maleimide compounds (a theoretical study), density functional study of bond dissociation energies in highly brominated diphenyl ethers; trends in bond dissociation energies of brominated flame retardants from density functional theory, solvatochromic analysis and DFT computational study of an azomaleimide derivative; steady state and time resolved fluorescence studies of new indolizine derivatives with phenanthroline skeleton, a new pathway for the synthesis of a new class of blue fluorescent benzofuran derivatives, thermal degradation study of decabromodiphenyl ether (translating thermo-analytical results into optimal chromatographic conditions). 7 publications in ISI indexed journals and 1 BDI article, h-index (Google Scholar Citations): 2, i10 index: 0, Number of citations 8.