DAN MAFTEI

(b. 1980)

Research themes:

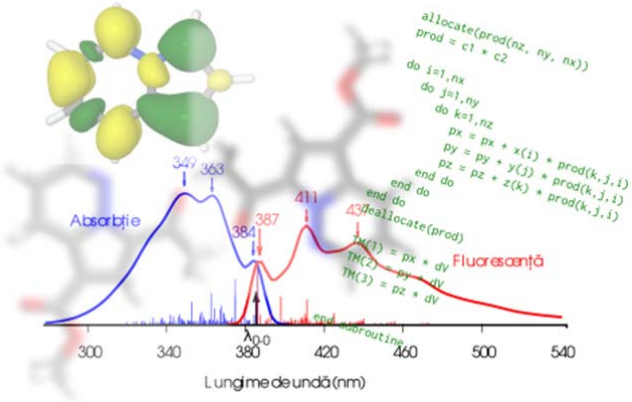
- **Electronic structure of molecules:** theory, algorithms and implementations;
- **Computational spectroscopy:** theoretical computation of optical spectral properties of molecules;
- **Dynamics and intermolecular interactions:** atomistic modeling of intermolecular interactions and molecular dynamics of biological systems

Molecular electronic structure: computing and interpreting the electronic structure of molecular systems; molecular properties derived from electronic structure computations; use, computer implementation and assessment of electronic structure methods în reproducing molecular properties

Computational spectroscopy: modeling optical spectral properties of molecular systems; interpreting electronic absorption and fluorescence spectra with application în raţional design of highly emissive fluorescent materials;

Dynamics and intermolecular interactions: molecular geometry and dynamics of biomolecules în solution; modeling receptor-ligand interactions;

Keywords: electronic structure, computational chemistry, *ab initio*, density functional theory, electronic spectra, molecular dynamics.



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Physical and Theoretical Chemistry

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Publications (selection)

Moldoveanu, C., Zbancioc, G., Mantu, D., **Maftei**, **D.** and Mangalagiu, I.I., The Cycloaddition of the Benzimidazolium Ylides with Alkynes: New Mechanistic Insights, *PLoS One*, 11 (5), e0156129, **2016**.

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Odochian, L., Moldoveanu, C. and **Maftei**, **D.**, TG–FTIR study on thermal degradation mechanism of PTFE under nitrogen atmosphere and in air. Influence of the grain size, *Thermochim. Acta*, 598, 28–35, **2014**.

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Mantu, D., **Maftei**, **D.**, Iurea, D., Ursu, C. and Bejan, V., Synthesis, structure, and in vitro anticancer activity of new polycyclic 1,2-diazines, *Med. Chem. Res.*, 23 (6), 2909-2915, **2013**.

Fifere, A., Marangoci, N., Maier, S., Coroaba, A., **Maftei**, **D.** and Pinteala, M., Theoretical study on β-cyclodextrin inclusion complexes with propiconazole and protonated propiconazole., *Beilstein J. Org. Chem.*, 8, 2191-2201, **2012**.

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