

Publication list : 2018-present

Project related publications:

- 1 A.-A. Farcaș T. A. Beu and A. Bende: "*The influence of the metal-to-ligand charge transfer on the strength of the spin-orbit coupling in Ni(II)-based metal-ligand complexes*", International Journal of Quantum Chemistry, (2019) - to be submitted.
- 2 A.-A. Farcaș and A. Bende: "*DFT study of adiabatic singlet-triplet energy gaps in Ni(II)-based macrocyclic-ligand supramolecular complexes.*", AIP Conference Proceedings, **2206**, 030001 (2020).
- 3 A.-A. Farcaș and A. Bende: "*Improving the Light-Induced Spin Transition Efficiency in Ni(II)-Based Macrocyclic-Ligand Complexes.*", **Molecules**, **24**(23), 4249 (2019).
- 4 A.-A. Farcaș, T. A. Beu and A. Bende: "*Mapping the light-induced intersystem crossings in Ni(II)-based macrocyclic-ligand complexes: A DFT study.*", **Journal of Photochemistry and Photobiology A: Chemistry**, **376**, 316–323 (2019).

Conference participation:

- 1 International Conference on "Processes in Isotopes and Molecules" (PIM 2019); 25 – 27 September **2019** in Cluj Napoca, Romania; **Oral presentation:** A. Bende and A.-A. Farcaș: "*Structural stability of Ni (II)-based macrocyclic-ligand complexes with square-pyramidal and octahedral coordination configuration.*"
- 2 17th Central European Symposium on Theoretical Chemistry (CESTC 2019); 9 – 12 September **2019** in Burg Schlaining, Austria; **Poster presentation:** A.-A. Farcaș, T. A. Beu and A. Bende: "*The influence of the metal-ligand charge transfer effects on the structural stability and the strength of the spin-orbit coupling in Ni(II)-based metal-ligand complexes.*"
- 3 18th International Conference on Density-Functional Theory and its Application (DFT 2019); 22 – 26 July **2019** in Alicante, Spain; **Poster presentation:** A.-A. Farcaș, T. A. Beu and A. Bende: "*Light induced singlet-triplet transition in Ni(II)-based macrocyclic-ligand complexes.*"
- 4 10th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP 2019); 11 – 17 July **2019** in Tromsø, Norway; **Poster presentation:** A.-A. Farcaș, T. A. Beu and A. Bende: "*The influence of the metal-ligand charge transfer effects on the structural stability and the strength of the spin-orbit coupling in Ni(II)-based metal-ligand complexes.*"
- 5 9th Conference on Molecular Modeling in Chemistry and Biochemistry (MOLMOD2018); 28 – 30 October **2018** in Cluj Napoca, Romania; **Poster presentation:** A.-A. Farcaș and A. Bende: "*Intersystem crossing in metalligand coordination complexes with pyramidal-planar and octahedral coordination configurations*"
- 6 12th Joint Conference on Mathematics and Computer Science (MaCS 2018); 14 – 17 June **2018** in Cluj-Napoca, Romania; **Oral presentation:** A.-A. Farcaș and A. Bende: "*Modeling laser-induced spin crossover transitions using time-dependent density functional theory.*"
- 7 Central European Conference on Photochemistry (CECP 2018); 4 – 8 February **2018** in Bad Hofgastein, Austria; **Poster presentation:** A.-A. Farcaș and A. Bende: "*Structural stability*"

and laser induced singlet-triplet transition in Ni(II) macrocyclic ligand complex: A TD-DFT study."

Workshops:

1. A.-A. Farcaş: ZCAM School on New Computational Methods for Attosecond Molecular Processes, 21 – 25 May **2018** in Zaragoza, Spain;