

# The solvent and nitrogen geometry effect on the absorption spectra of a ferrocene-naphthalimide derivative

Christina-Eleftheria Tzeliou<sup>a</sup>, Demeter Tzeli<sup>a, b</sup>

<sup>a</sup> *Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens, 157 84, Greece*

<sup>b</sup> *Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens, 116 35, Greece*

*e-mail: [ctzeliou@chem.uoa.gr](mailto:ctzeliou@chem.uoa.gr)*

The ability of molecules to process information similar to electronic systems was proposed in 1993. [1] Molecules respond to changes in their environment resulting in alteration of the absorption spectra. [2] These types of molecules are designed according to the principles of photoinduced electron transfer systems. Recently, we studied theoretically the photophysical properties of a 3-input AND molecular logic gate (MLG) [3], which had been synthesized by Magri et al. [4], and presented an enhanced fluorescence spectrum. The fluorophore is the 4-amino-1,8-naphthalimide, the terminal fragment is a piperazine unit which easily is protonated and acts as a proton receptor and a crown ether group. Here, we are focusing on the truncated molecule of this 3-input AND MLG, without the crown ether. The inclusion of two different solvents explicitly and implicitly was studied via DFT/TD-DFT calculations. The N atom of piperazine towards ferrocene presents a crucial role, and its geometry affects the absorption spectrum of the molecule. The effect of the geometry of the N was studied.

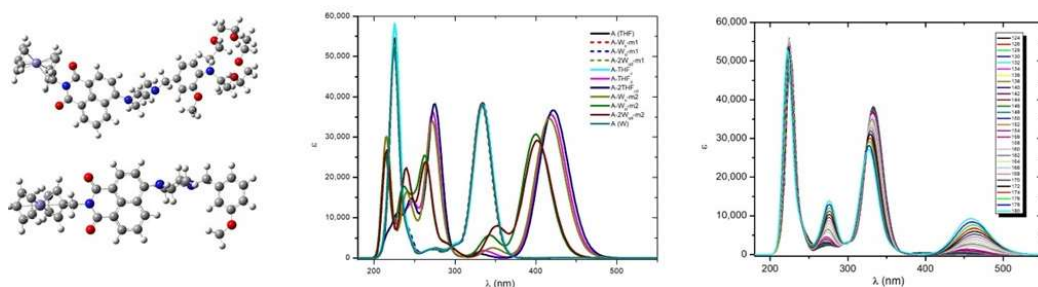


Figure 1: Calculated minimum structure of the initial (*top left*) and truncated MLG (*bottom left*), absorption spectrum in THF and water (*middle*) and absorption spectrum of the structure upon changing N dihedral angles in THF at PBE0/6-31G(d,p) (*right*).

**Acknowledgements:** The author acknowledges the Hellenic Foundation for Research and Innovation for the financial support of this project under the 5th Call for HFRI PhD Fellowships (Fellowship Number: 21006).

## References:

- [1] A. P. de Silva, H. Q. N. Gunaratne, C. P. McCoy, *Nature* 364 (1993) 42-44.
- [2] S. Erbas-Cakmak, S. Kolemen, et al., *Chem. Soc. Rev.* 47 (2018) 2228-2248.
- [3] C. E. Tzeliou, D. Tzeli, *J. Chem. Inf. Model.* 62 (2022) 6436-6448.
- [4] G. J. Scerri, J. C. Spiteri, C. J. Mallia, D. C. Magri, *Chem. Comm.* 55 (2019) 4961-4964.