

# TD-DFT Computations of Photophysical Properties

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Density Functional Theory (DFT) techniques are useful tools not only to investigate molecular ground state properties like geometries, vibration frequencies, but also optical ones like electronic absorption and emission spectra and Non Linear Optical (NLO) properties, which are related to the excited states of the molecules with the help of Time Dependent DFT (TD-DFT) calculations. In all cases, DFT and TD-DFT computations could help to the design of new molecules exhibiting improved properties. Among the NLO properties, the process of simultaneous two-photon absorption (TPA) has attracted growing attention due to its potential applications, among them three-dimensional optical storage, two photon-fluorescence imaging, two-photon photodynamic therapy and optical limitation.

In this paper, the theoretical methodology used to investigate molecular photophysical properties will be presented, as well as several joint experimental and theoretical recent studies: solvent and aggregation effect on the phosphorescence spectra of platinum complexes, trans-cis photoisomerization of azo-based iminopyridine compounds (Figure1) [1] and TPA properties of octupolar molecules (example of the isocyanurate cyclotrimer core in Figure2) [2].

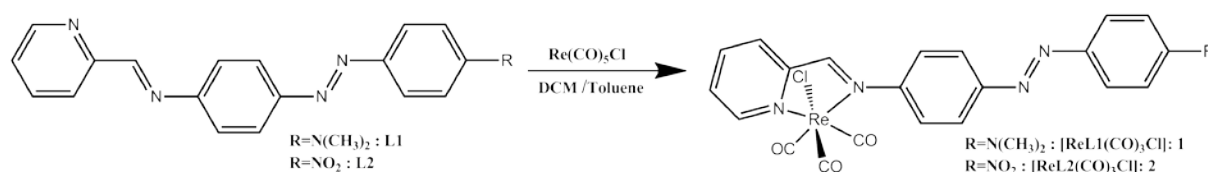


Fig. 1: Azobenzene derivatives

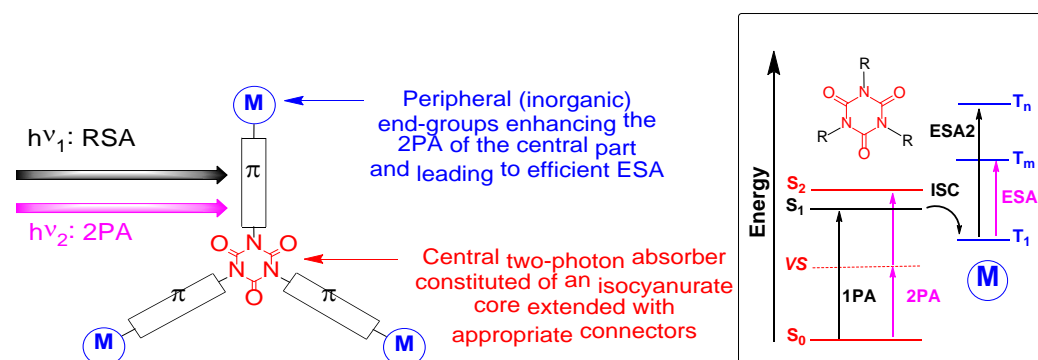


Fig. 2: TPA of the isocyanurate core

[1] M.-A. Benmensour, A. Ayadi, H. Akdas-Kilig, A. Boucekkine, J.-L. Fillaut, A. El-Ghayoury, *Azobased iminopyridine ligands and their rhenium metal complexes: Syntheses, spectroscopic, trans-cis photoisomerization and theoretical studies*. *J. Photochem. Photobiol. A* **368** (2019), 1584.

[2] A. Amar, A. Boucekkine, F. Paul, O. Mongin, *DFT study of two-photon absorption of octupolar molecules*, *Theoret. Chem. Accounts* **138** (2019), 105