

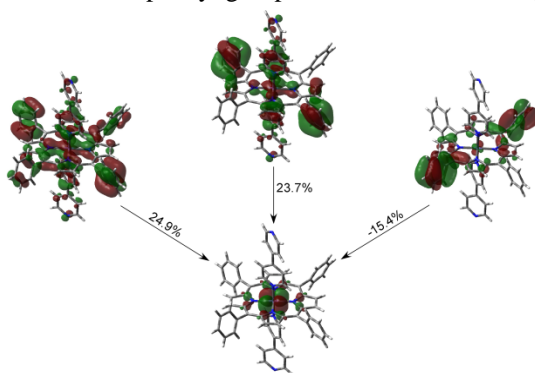
Theoretical and experimental absorption spectra study of $[(\text{FeTPPbipy})]_n$ provided by TD-DFT calculations

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Iron metalloporphyrins are paradigmatic examples of nanodevices used by natural systems like haemoglobin or cytochromes in oxygen transport, electron transfer and catalysis [1]. Therefore, they can be thought to be developed as MOFs for several applications. UV-Vis spectra of metalloporphyrins exhibit typical Soret and Q bands, that are very useful to understand their electronic behaviour. In this work, we have characterised the UV-Vis spectrum of $[(\text{FeTPPbipy})]_n$ (TPP= *meso*-tetraphenylporphyrin, bipy= 4,4'-bipyridine) from both experimental and theoretical points of view. The later has been carried out by means of TD-DFT calculations (TD-DFT is Time Dependent-Density Functional Theory) [2]. The interest of this compound lies on the presence of an unpaired electron per metallic centre that is delocalised on the phenyl groups of TPP. The results lead to the conclusion that an important charge transfer takes place between the phenyl groups and the metal centre (see figure).



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