

Tuning the absorption spectra of Nickel and Zinc Complexes of N-confused Tetraphenyl Porphyrin

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Porphyrins are heterocyclic organic compounds, containing four modified pyrrole subunits. Based on that and adding four phenyl rings tetraphenyl porphyrin (TPP) is formed. Our target is to create a sensor by linking tetraphenyl porphyrin on a MoS₂ nanosheet. Molybdenum disulfide (MoS₂) is a layered transition-metal dichalcogenide and its structure descriptively consists of an atomic layer of Mo sandwiched between two layers of sulphide. It's an established¹ fact that there is a ping-pong energy transfer between porphyrin and the MoS₂ layer under the influence of external factors.

N-confused porphyrin (NCP) or inverted porphyrin possesses a "confused pyrrole", where the positions of pyrrolic NH and β-CH are switched. As a result, NCP contains an NNNC core and an outward pointing N atom which serves as a hydrogen bonding donor/acceptor as well as a metal coordination site.²

We study theoretically Ni and Zn complexes of TPP and NCTPP and of substituted NCTPP. Our aim is to show how the molecular structure of substituted NCTPP affect the absorption spectra of these porphyrins and influence their selective detection of cations.

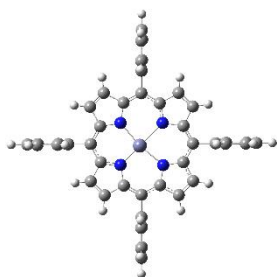


Figure 1: Simple Porphyrin-Zn

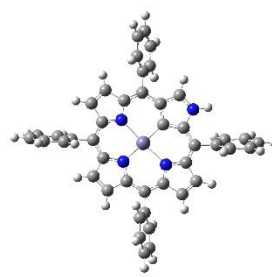


Figure 2: N-Confused Porphyrin-Zn

References:

1. R. Canton-Vitoria, T. Schar, A. Stergiou, A. Cadrane, R. Arena, D. M. Guldi, N. Tagmatarchis, *Angew. Chem. Int. Ed.* **59**, 3976 (2020)
2. H. Furuta, H. Maeda, A. Osuka, *Chem. Commun.* **102**, 1795 (2002)