Practical Information

All Fields are compulsory

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Understanding Light-Absorption in MOFs: Combined Experimental and Theoretical Study of UiO-66 Type Frameworks

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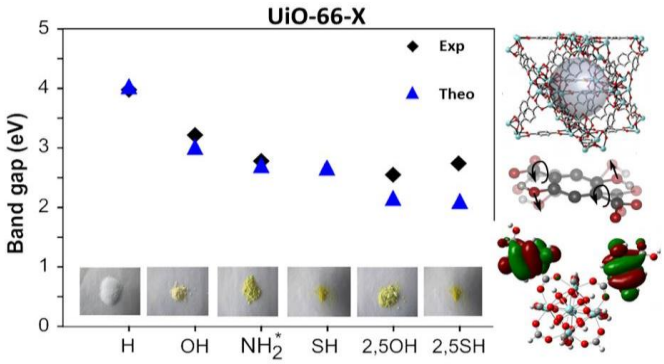
The importance of renewable energy sources has become more and more stringent with the increasing environmental concerns, and much research focuses on the use of sunlight for photochemical, catalytic transformations. To produce a useful photocatalyst, the system has to efficiently harvest (solar) energy and combine high activity with recyclability and stability. Hybrid materials, e.g. Metal-Organic Frameworks (MOFs) have already shown interesting potential for photo-catalytic applications. The large band gap of most MOFs normally limits their use to the UV region of the spectrum. However, (post-) functionalizing the organic linkers allows to shift this absorption towards the visible region. [1,2]



This contribution will discuss the absorption properties of the UiO-66 framework and isoreticular analogues. Via a combination of experimental measurements and theoretical calculations, we try to provide more insight in how the different functional groups influence the electronic structure of the frameworks. First, a series of simple model systems is constructed, ranging from the isolated linkers to a cluster model comprising a full zirconium node with two linkers. This deconstruction of the framework proved very handy to gain insight in the changing properties of the functionalized linkers and to study the proposed energy transfer occurring in the system. Thereafter, we looked into detail to the periodic structure. High level HSE calculations gave very accurate values for the band gaps. Furthermore a detailed analysis of the vibrational fingerprint [3] of the different systems gave additional information on how different vibrational modes influenced the excitation energies of the linkers. Large differences were observed between free linkers and linkers in the frameworks. This combined study gives some important additional insights, opening perspectives for more tailor-made materials.

[1] Hendrickx, K., Vanpoucke, D.E.P., Leus, K., Lejaeghere, K., Van Yperen-De Deyne, A., Van Speybroeck, V., Van der Voort, P. and Hemelsoet, K., Inorg. Chem. 54 (2015) 10701-10710
[2] Nasalevich, M.A. , van der Veen, M. and Gascon, J., CrystEngComm. 16 (2014) 4919
[3] Van Yperen-De Deyne, A., Hendrickx, K., Vanduyfhuys, L., Sastre, G., Van der Voort, P., Van Speybroeck, V. and Hemelsoet, K., Theor. Chem. Acc. 135 (2016) 102

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