IAP FS2 7/05 Annual Network Meeting, UGent, September 18, 2013

Poster abstract

WP/PL n°: PL3

Title: Functionalized Metal-Organic Frameworks: MIL-47(V)+X: a computational investigation of its properties.

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Summary (max 200 words):

Metal-organic frameworks (MOFs) present the ultimate version of a porous material, and as such reside at the interface between physics and chemistry. Their tunable nature makes them of great interest for many industrial applications such as gas-storage, catalysis, etc.
Using *ab-initio* density functional theory calculations, we study the influence of functionalization of the organic linker in MIL-47(V) on the properties of the MOF. Structural optimization predicts the functionalized MIL-47(V) to collapse to a narrow-pore geometry, while a large-pore geometry is observed in experiments. By comparison to the experimental geometry, we show this discrepancy is due to thermal effects and the flat energy surface of the MOF.[1]
Hirshfeld-I atomic charges[2] are calculated, and we show these to be independent of the narrow/large-pore geometry of the MOF, furthermore we show the functionalization not to influence the charge distribution in the remainder of the MOF.[1] In conclusion, functionalization of the organic linkers in MIL-47(V) will allow for tuning of the catalytic/sorption properties without (significantly) modifying structural and electronic properties of the MOF framework.

[1] S. Biswas, *et al.*, *J. Phys. Chem. C* accepted (2013)
[2] D.E.P. Vanpoucke, *et al.*, *J. Comput. Chem.* **34** 405-417 (2013)