

The adsorption behavior of xylene isomers in MIL-47 from a theoretical perspective

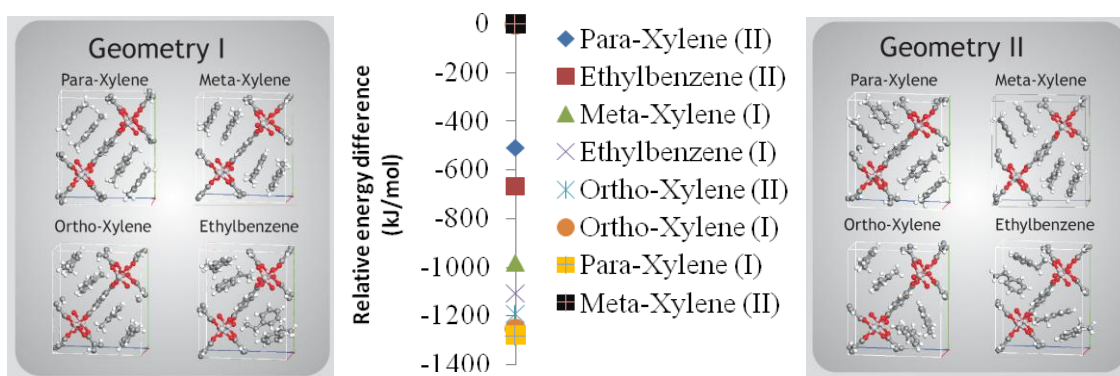
Matthias Vandichel,[†] Veronique Van Speybroeck,[†] Luc Alaerts,[‡] Dirk De Vos,[‡] Michel Waroquier[†]

[†]Center for Molecular Modeling, Ghent University, Proeftuinstraat 86, B-9000 Gent

[‡]Centre for Surface Chemistry and Catalysis, Kasteelpark Arenberg 23, B-3001 Leuven

Recently, the spectrum of nanoporous materials like zeolites and zeotype structures was further expanded through the occurrence of a new class of hybrid porous porous solids [1, 2]. Those materials are nowadays also known as metal organic frameworks or MOFs and consist of inorganic and organic moieties. Certain MOFs exhibit a very interesting adsorption and even catalytic behavior.

Our study focuses on one of them: MIL-47. MIL-47 was first synthesized by Barthelet [3], later on Alaerts [4] studied the ability of MIL-47 to separate several xylene isomers. This separation behavior of MIL-47 could be better understood with adsorption studies [4, 5]. The adsorbates were located inside the MIL-47 host by Rietveld refinements of the XRD patterns of MIL-47 samples saturated with each of the C8-isomers. The packing of each C8-pair was then discussed on the basis of the interactions between those two aromatic compounds and MIL-47 [4]. In this case, theoretical modeling could predict the relative energy difference between several possible geometries. The stability of a unit cell of MIL-47 fully loaded with four adsorbates was investigated with periodic calculations. Starting from crystallographic information (supp. info of [4]), two possible geometries were cut out for different C8-isomers: para-xylene, meta-xylene, ortho-xylene and ethylbenzene. The optimized structures are displayed in the figure below. The relative energy differences are shown relative to meta-xylene (II), the most unstable structure.



- [1] Ferey, G., *Chemical Society Reviews* 37 (2008) 191.
- [2] Tranchemontagne, D.J.L., M. O'Keeffe, Z. Ni and Yaghi O.M., *Angewandte Chemie-International Edition* 47 (2008) 5136.
- [3] Barthelet, K., Marrot, J., Riou, D. and Ferey G. *Angewandte Chemie-International Edition* 41 (2002) 281.
- [4] Alaerts, L., Kirschhock, C.E.A., Maes, M., van der Veen, M.A., Finsy, V., Depla, A., Martens, J.A., Baron, G.V., Jacobs, P.A., Denayer, J.E.M. and De Vos, D.E. *Angewandte Chemie-International Edition* 46 (2007) 4293.
- [5] Finsy, V., Verelst, H., Alaerts, L., De Vos, D., Jacobs, P.A., Baron, G.V. and Denayer J.F.M. *Journal of the American Chemical Society* 130 (2008) 7110.

E-mail: Matthias.Vandichel@Ugent.be

www: <http://molmod.ugent.be>