

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

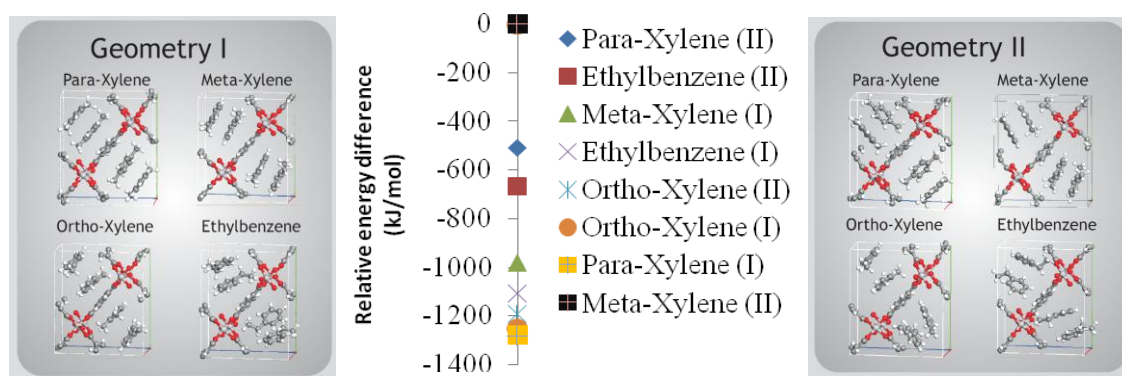
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Recently, the spectrum of nanoporous materials like zeolites and zeotype structures was further expanded through the occurrence of a new class of hybrid porous porous solids [1, 2]. Those materials are nowadays also known as metal organic frameworks 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.



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- [2] Tranchemontagne, D.J.L., M. O'Keeffe, Z. Ni and Yaghi O.M., *Angewandte Chemie-International Edition* 47 (2008) 5136.
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