

Insights on the adsorption behavior of aromatics in MIL-47 and MIL-53 from a theoretical perspective

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

Within this contribution, we will mainly focus on adsorption and separation of aromatic species in MIL-47 and MIL-53 [3, 4, 5]. Some of the presenting authors reported for first time on the successful use of MOFs as selective adsorbents for the extremely difficult and industrially relevant separations of para-xylene versus meta-xylene and para-xylene versus ethylbenzene [3]. Their study focuses on the MIL-47, which was first synthesized by Barthelet [4]. This separation behavior of MIL-47 could be better understood with adsorption studies [3, 5]. The packing of each C8-pair will be discussed on the basis of the interactions between those two aromatic compounds and MIL-47 [3]. In order to unravel the interaction between the guest molecules and the lattice, periodic Density Functional Theory calculations have been conducted. The DFT calculations were corrected for dispersion interaction [6] to include the long-range attractive forces. It seems that pi-pi stacking energies between pairs of aromatics but also with the walls of the MOF are crucial for the packing behavior in the pores.

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