Minicolloque n° MMB15 ☑ **Oral** ☐ **Poster**

Mechanical Pressure Effect on Hexane Isomers Separation in MOFs Materials by Flexible Force Field Simulation

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A series of MOFs was studied intensively in order to investigate their ability to separate hexane isomers[1]. We focus here especially on MIL140-B and MIL-140C. Both computational and experimental method confirmed that the elution order is same to the boiling point of the compounds nC6 > 2MP > 3MP > 23DMB > 22DMB. It is notable that this material enables separation of hexane isomers by class, linear > mono-branched > di-branched. Experimentally the selectivity reaches to 10 at 343K for ambient pressure. We have shown the importance to consider the tilting of linkers in such tiny, triangle form MOFs[1]. To the best of our knowledge, there are only three computational studies on MIL140 series MOFs[1,2,3], but the structure is considered as rigid. In this work, hybrid Osmotic Monte Carlo (HOMC) simulations were performed in order to gain more insight into the separation mechanisms, which highlight the crucial role of tiny tilting of the organic linkers in order to capture the experimental observations.

The figure below highlights the selectivity of hexane isomers in MIL-140B under the influence of the mechanical pressure. We obtain the enhancement of the selectivity of 22% by using the mechanical pressure.

[1] Hexane isomers separation on an isoreticular series of microporous Zr carboxylate metal organic frameworks. *J. Mater. Chem. A*, 2020, 8, 17780-17789
[2] Computer-Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. *Angew. Chem., Int. Ed.*, 2012, 51, 11867–11871
[3] Separation of Hexane Isomers in a Metal-Organic Framework with Triangular Channels. *Science*, 2013, 340, 960–964
[4] A Series of Isoreticular, Highly Stable, Porous Zirconium Oxide Based Metal–Organic Frameworks. *Angew. Chem., Int. Ed.*, 2012, 51, 9267-9271

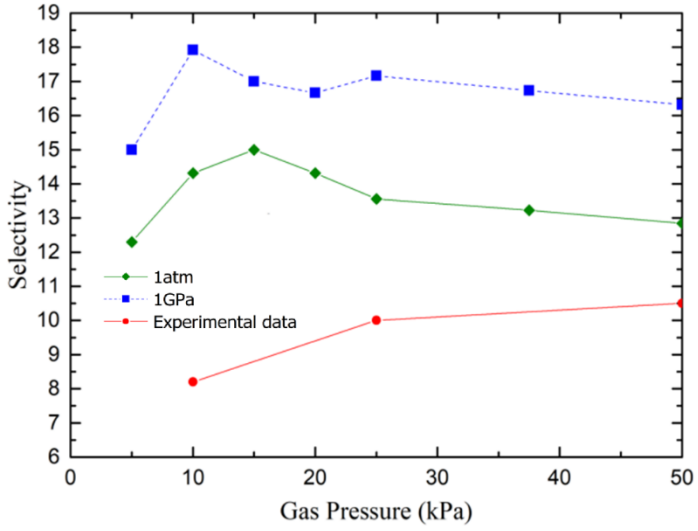

Figure 1 : Selectivity of hexane quinary isomers adsorption in fucntion of mechanical pressure.