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Understanding framework flexibility of periodic structures by Monte Carlo simulation AN GHYSELS, University of California - Berkeley, VERONIQUE VAN SPEYBROECK, MICHEL WAROQUIER, Center for Molecular Modeling, BEREND SMIT, University of California - Berkeley — Metal Organic Frameworks (MOFs) are a new class of porous materials synthesized from metal clusters connected by organic linkers. Most crystalline solids are fairly rigid, and undergo small changes in volume when stress is applied. Although most MOFs are rigid, some have an unexpectedly high flexibility, and swell under pressure, temperature or adsorption changes. A well-known structure showing volume changes of over 50% is MIL-53. A better understanding of the process will allow to design materials with improved properties for carbon capture, i.e. the framework captures CO2 from fuel gasses. In this presentation, we explore framework flexibility effects induced by gas adsorption using Monte Carlo techniques. For instance, when MIL-53 is brought into contact with a gas at increasing pressure, the framework's pores constrict, while at even higher pressures, the pores return to their original geometry. To study this phenomenon, it is essential to incorporate framework flexibility into the Monte Carlo free energy calculation.

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