**14 - Understanding framework flexibility by Monte Carlo simulation**

***An Ghysels*, Veronique Van Speybroeck, Michel Waroquier, Berend Smit. Center for Molecular Modeling, Ghent University, Gent, \, Belgium; Department of Chemical Engineering, University of California - Berkeley, Berkeley, California, United States**

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. Well-known structures showing volume changes of over 50% are MIL-53 and Cu(CBT). 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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Materials (08:30 AM - 10:30 AM)
**Location: Anaheim Convention Center**
**Room: 212 B**

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