Adsorption in Nanoporous Metal-Organic Frameworks: Hysteresis and Effects of Framework Flexibility

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Metal-organic frameworks (MOFs) are a versatile class of nanoporous materials synthesized in a "building-block" approach from inorganic nodes and organic linkers. By selecting appropriate building blocks, the structural and chemical properties of the resulting materials can be finely tuned, and this makes MOFs promising materials for applications such as gas storage, chemical separations, sensing, drug delivery, and catalysis. Much recent interest has focused on the application of MOFs in atmospheric water harvesting and carbon capture, where adsorption of water plays an important role. Adsorption isotherms for water often display hysteresis, in which the adsorption and desorption branches of the isotherm do not trace one another. Adsorption of water can also be sensitive to adsorbent flexibility, either local or global (as in framework phase transitions). This talk will discuss on how molecular simulation can provide new insights into adsorption hysteresis and the effects of framework flexibility on adsorption of water and other species in MOFs and related materials.