

MODELING OF METAL-ORGANIC FRAMEWORKS AS TUNABLE ADSORBENTS FOR SEPARATIONS

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Metal-organic frameworks (MOFs) are an interesting 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 chemical separations, gas storage, sensing, drug delivery, and catalysis. This talk will focus on efforts to design or screen MOFs for adsorption separations. Because of the predictability of MOF synthetic routes and the nearly infinite number of possible structures, molecular modeling is an attractive tool for screening new MOFs before they are synthesized. Large databases of existing and proposed MOFs now exist and can be screened to find the top candidates for a given separation using atomistic Monte Carlo simulations. The resulting data can also provide insight into the molecular-level details that lead to observed macroscopic properties, which can, in turn, be used to design improved candidates. While molecular modeling can predict adsorption properties such as the selectivity and working capacity, process-level modeling can also play a key role in evaluating materials, and we will discuss how the interplay of molecular-level and process-level modeling can be used along with experiment to discover, develop, and ultimately design new MOFs for desired separation applications.