**Metal-Organic Frameworks as Tunable Platforms for Gas Storage and Chemical Separations**

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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. This talk will focus on efforts to design or screen MOFs for storage of gaseous fuels, such as hydrogen and natural gas, and for separating mixtures of small molecules, including $CO_2$ capture. 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. Modeling can also provide insight into the molecular-level details that lead to observed macroscopic properties. This talk will illustrate how a combination of molecular modeling, machine learning, and experiments can be used to discover, develop, and ultimately design new MOFs for desired separation and storage applications.