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**Molecular Modeling of Metal-Organic Frameworks for  
Energy and Environmental Applications**

September 2, 2015  
3:25 p.m.  
202 Gavett Hall

Metal-organic frameworks (MOFs) are a new class of nanoporous materials synthesized in a “building-block” approach from inorganic nodes and organic linkers. Some of the most intensively studied applications are related to solving energy and environmental problems, including hydrogen and natural gas storage for cleaner vehicles, capture of CO<sub>2</sub> from power plant exhaust, and energy efficient 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. Modeling can also provide insight into the molecular-level details that lead to observed macroscopic properties. This talk will illustrate how a combined modeling and experimental approach can be used to discover, develop, and ultimately design new MOFs for desired gas adsorption applications.