

**Spring Seminar Series**  
**3:30pm - 4:30pm, Wednesday March 6, 2013**  
**Johnston Hall 338, Louisiana State University**

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

by  
**Prof. Randall Q. Snurr**  
Northwestern University



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.

Randy Snurr is a Professor of Chemical and Biological Engineering at Northwestern University. He holds BSE and PhD degrees in chemical engineering from the University of Pennsylvania and the University of California, Berkeley, respectively. From 1994-95, he performed post-doctoral research at the University of Leipzig in Germany supported by a fellowship from the Alexander von Humboldt Foundation. Other honors include the 2011 Institute Award for Excellence in Industrial Gases Technology from the American Institute of Chemical Engineers, the Leibniz professorship at the University of Leipzig in 2009, and a CAREER award from the National Science Foundation. He is a Senior Editor of the *Journal of Physical Chemistry* and has served on the editorial boards of *Chemistry of Materials*, *Journal of Molecular Catalysis A*, and *Catalysis Communications*. His research interests include development of new nanoporous materials for energy and environmental applications, molecular simulation, adsorption separations, diffusion in nanoporous materials, and catalysis.

*This seminar will be broadcast at the following venues: Liberal Arts Building 234 (UNO), Qatar Pavilion Conference Room 226 (Xavier University), JB Moore Hall Room 211 (Southern University), PML 1015, Center for Instructional Technology, at the Wylly Tower (LA Tech), and via Adobe Connect at <https://connect.lsu.edu/la-sigma/>.*

