



BOUNDARY-SPANNING SEMINAR SERIES

Development of Tools for Computational Discovery of Metal-Organic Framework Materials

Dr. Randall Q. Snurr, Northwestern University



Abstract: 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, drug delivery, and catalysis. 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, and methods from data science are finding increasing application in this field. This talk will discuss the development of tools to accelerate the computational discovery of new MOFs for particular applications, emphasizing tools from data science and machine learning.

**9:00 a.m.
Tuesday
November 23, 2021**

Join us by Zoom:
<https://kansas.zoom.us/j/93403833438>
Passcode: 0802

cebc@ku.edu
cebc.ku.edu
nrt.ku.edu

Bio: Randy Snurr is the John G. Searle Professor of Chemical and Biological Engineering at Northwestern University. His research interests include development of new nanoporous materials for energy and environmental applications, molecular simulation, adsorption separations, and catalysis. He is a corresponding member of the Saxon Academy of Sciences and received the AIChE Institute Award for Excellence in Industrial Gases Technology.

Randall Q. Snurr

Department of Chemical & Biological Engineering
Northwestern University, Evanston, IL
e-mail: snurr@northwestern.edu
<http://zeolites.cqe.northwestern.edu>

Seminar overview: this seminar series nurtures learning across academic boundaries. Expect rich conversations, spanning machine learning to catalysts, from lab bench to smokestack, with an eye toward protecting nature. Sponsoring units include: KU's Center for Environmentally Beneficial Catalysis (CEBC), the Internet of Catalysis National Science Foundation Research Traineeship (NRT), Information and Telecommunication Technology Center (ITTC), and the Departments of Chemistry, Chemical and Petroleum Engineering, and Electrical Engineering and Computer Science.

You belong here!

We invite everyone from the KU community to join us for this inclusive seminar