Johns Hopkins University

Department of
Chemical & Biomolecular Engineering

Spring 2023 Seminar Series

Professor Randall Snurr
Northwestern University
Date: Thursday, April 20, 2023
Time: 10:30 a.m.
Shaffer Hall 3
Zoom Meeting ID: 919 5918 2879
Passcode: 270887

Title: Designing Metal-Organic Frameworks with Optimal Surface Area and Catalytic Properties

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 in gas storage, chemical separations, sensing, drug delivery, and catalysis. In the early days of MOFs, remarkably high surface areas were reported, leading to questions about the applicability of the traditional method for determining surface areas due to Brunauer, Emmett, and Teller (BET). The talk will describe how molecular-level modeling provided new insights into these questions and how molecular simulation played a role in designing MOFs with ever-higher surface areas as well as optimized properties for gas storage and separation. In addition, the role of quantum chemical modeling to design and better understand MOF catalysts will be presented, focusing on selective oxidation of alkanes.

Bio: Randy Snurr is the John G. Searle Professor and Department Chair 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. 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 Institute Award for Excellence in Industrial Gases Technology from the American Institute of Chemical Engineers, the Ernest W. Thiele Award from the Chicago Section of AIChE, and election as a corresponding member of the Saxon Academy of Sciences. He has been named a Highly Cited Researcher by Clarivate Analytics from 2014 to 2022. He served as a Senior Editor for the Journal of Physical Chemistry and is currently on the advisory boards of several journals. His research interests include development of new nanoporous materials for energy and environmental applications, molecular simulation, machine learning, adsorption separations, diffusion in nanoporous materials, and catalysis.