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Wednesday, January 15th, 2025
Location and final seminar start time TBD

Prof. Brandon Bukowski

Chemical Engineering, Johns Hopkins University

Leveraging advances in atomistic simulations and machine learning to design nanoporous microenvironments for sustainable chemical transformations

There is a critical societal need to develop new selective heterogeneous catalysts that enable large-scale decarbonization of the transportation and chemical industries. One specific application is the synthesis of sustainable aviation fuel (SAF) from bioethanol. Catalytic valorization processes that utilize biomass derived from agricultural waste are typically selectivity-limited which limits their commercial viability. One exemplar catalyst family includes crystalline nanoporous solids such as zeolites which are employed in a wide range of chemical processes due in part to their tunable shape selectivity and framework-substituted cations. Reaction kinetics at internal zeolite acid sites can be modified by changing pore size, pore architecture, polarity, or acid site identity. These active site microenvironments impart shape-selectivity that preferentially stabilizes transition states and unique water matrices that in turn influence the stability of reactive intermediates. The large design space of zeolite catalysts including their pore architecture, polarity, and active site identity complicates comprehensive kinetic studies to predict new selective catalysts. Computational modeling of kinetic mechanisms in heterogeneous

catalysis has emerged over the last few decades as a tool to predict both the structure and function of active sites to accelerate catalyst design. Here we will discuss how synergistic combinations of density functional theory (DFT), molecular dynamics, and machine learning techniques can provide design principles to design new selective zeolite catalysts for fuels and fine chemicals.

Speaker Bio

Brandon Bukowski is an Assistant Professor in the department of Chemical and Biomolecular Engineering and associate researcher in the Ralph O'Connor Sustainable Energy Institute at Johns Hopkins University. He holds BS and PhD degrees in chemical engineering from Worcester Polytechnic Institute and Purdue University, respectively. At Purdue he was advised by Jeffrey Greeley, received the Faculty Lectureship Award, and was supported in part by a Dick Reitz fellowship from the Center for the Innovative and Strategic Transformation of Alkane Resources NSF ERC. He performed post-doctoral research at Northwestern University under the supervision of Randall Snurr. Bukowski started at Johns Hopkins University in July of 2021. He has received a Ralph E. Powe award from Oak Ridge Associated Universities a Doctoral New Investigator grant from the ACS Petroleum Research Fund, and an Amazon Research Award. He is a member of the Catalysis division board of the American Chemical Society, and program co-chair of the Catalysis Club of Philadelphia and Northeast Corridor Zeolite Association.

Schedule TBD

Meeting Fees

Professional Members	$40
Non-members	$50
Students	$25 (Student Members = $10)
Retired/Post-Doc/Unemp.	$40 (Members = $30)

Deadline for reservations is **5:00PM Friday, January 10th, 2025**

Please RSVP online using the online form.

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