Department of Electrical and Computer Engineering
Materials Engineering Program
Texas Center for Superconductivity at Univ. of Houston
Center for Integrated Bio and Nano Systems
10:00 a.m., April 1, 2022
Join Zoom Meeting
https://zoom.us/j/845619943?pwd=QlZvYUV6M2dxNDkvNWxBd3F2YzdJZz09

Meeting ID: 845 619 943
Password: 016104

How Things Fall Apart: Discovering New Chemistry with Automated Reaction Prediction

Brett M. Savoie

Charles Davidson Assistant Professor
Department of Chemical Engineering
Purdue University

Abstract:

Advances in both experimental and computational methods have dramatically accelerated the prediction, optimization, and validation of organic chemical and materials properties. Despite this progress, chemical stability, which is central to analyzing the life-performance and feasibility of novel organic materials, remains beyond our current capability to predict. This capability gap has resulted in many computational design efforts yielding libraries of conceptually interesting organic molecules and materials that nevertheless often fail to connect with real applications. Moreover, chemical stability prediction faces the challenge that degradation chemistry is poorly represented in reaction databases, and as such cannot use domain heuristics that have been successful in other reaction prediction contexts. In this talk, I'll discuss how recent developments in automated reaction prediction, by our group and others, have created an opportunity to bring chemical stability into the realm of routine predictability. In particular, we have recently been able to reduce the cost of predicting reactions involving generic organic molecules over 100-fold while also improving the accuracy of transition states and increasing the scope of kinetically relevant pathways. This method has been used to elucidate several reaction networks governing thermal degradation. Each of these networks constitutes the most comprehensive exploration to date and all have been generated without using reaction templates or other domain knowledge implements that are commonly used in network construction. On the horizon, the throughput enabled by these and similar efforts will generate valuable data sources for nascent machine learning efforts in this space, which will ultimately allow us to routinely predict how things fall apart.

Short Bio:
Brett Savoie graduated with degrees in chemistry and physics from Texas A&M University in 2008 and obtained his Ph.D. in theoretical chemistry from Northwestern University in 2014. From 2014-2017 Brett was a postdoc with Thomas Miller at Caltech where he developed new simulation methods for polymer electrolytes. In 2017, Brett joined the faculty of the Davidson School of Chemical Engineering at Purdue University, where his research group develops physics-based and machine learning methods to characterize and discover new organic materials. Brett is the recipient of the ACS PRF, NSF CAREER, Dreyfus Machine Learning in the Chemical Sciences, and ONR YIP awards. In 2020 he was named the Charles and Nancy Davidson Assistant Professor of Chemical Engineering. His group's research has been highlighted in Science and Nature, and contributed to the development of a polymer named as one of the "Molecules of the Year" by C&E News in 2018.

Please contact Dr. Yan Yao <yyao4@uh.edu> if you want to meet with the speaker.