MIT Chemical Engineering

Fall 2023 Seminar Series

Has the Reaction Prediction Problem Been Solved?

Brett Savoie

The Charles and Nancy Davidson
Associate Professor of Chemical Engineering
Purdue University

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2:45pm Reception

The reaction prediction problem consists of predicting the transition states(s) and product(s) of all experimentally observable reactions involving a set of reactants under given conditions. Decades of research have produced practical algorithms for very efficiently finding transition states and predicting the relative kinetics of competing reaction pathways. While these approaches historically often relied on manual fine-tuning or were restricted to specific classes of chemical reactions, they are increasingly general and automatic. In this talk I will describe our group's work in this area using several case studies to illustrate the opportunities for reaction network elucidation and reaction discovery created by the rapid routinization of reaction prediction. The second half of the talk will discuss the intersections between physics-based and machine learning approaches to reaction prediction and the closely related problem of AI interpretation of reaction outcomes.

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