Challenges in Data Science Methods for Catalyst Design and Discovery

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Lecture 4:00-5:00 p.m. | NANOENGINEERING 182

Abstract

Increasing computational sophistication and resources can enable a larger and more integrated role of theory in the discovery and understanding of new materials. This process has been slower to infiltrate surface science and catalysis than the field of bulk inorganic materials due to additional scientific complexity of modeling the interface. Most catalyst studies start in a data-poor regime where the material of interest is unrelated to previous to studies (new structure, composition etc) or the computational methods are incompatible with previous studies (different exchange-correlation functionals, methods, etc). Efficient methods to quickly define, schedule, and organize necessary simulations are thus important and enable the application of online design of experiments approaches. I will discuss on-going work and software development to enable data science methods in catalysis including open datasets for the community. I will describe applications of our approach to ordered bimetallic alloy catalysts, with applications to several electrochemical catalyst discovery efforts including CO2 reduction, oxygen reduction, and water splitting chemistry. Finally, I will discuss the transition from data-poor to data-rich regimes and our experiences when data-intensive deep-learning methods become more appropriate than simpler models based on chemical intuition.

Bio

Zachary Ulissi is an Assistant Professor in Chemical Engineering at Carnegie Mellon University in Pittsburgh PA. He did his undergraduate work in Chemical Engineering and Physics at the University of Delaware, a Masters in Applied Mathematics at Churchill College, Cambridge, and his PhD in Chemical Engineering at MIT funded by the DOE CSGF fellowship. His PhD research at MIT focused on the the application of systems engineering methods to understand selective nanoscale carbon nanotube devices and sensors working with Michael Strano and Richard Braatz. Prof. Ulissi did his postdoctoral work at Stanford with Jens Nørskov where he worked on machine learning techniques to simplify complex catalyst reaction networks and discover new catalysts. Current research interests include the design of nanoscale devices and materials discovery, including high-throughput calculations for dataset generation, development of surrogate models using machine-learning and systems approaches, and all-atom classical (MD) and electronic (DFT) simulations techniques.