Clarkson University
Department of Chemical and Biomolecular Engineering
SEMINAR

Atomistic Modeling and Data-Driven Approaches to Understand Heterogeneous Catalysts for Sustainable Chemical Conversion

Bryan R. Goldsmith
Department of Chemical Engineering
University of Michigan, Ann Arbor

The world is facing an increasing global energy demand, lack of clean water, and rising greenhouse gas emissions, all the while people strive to improve their standard of living. Computational modeling of catalysts, and making use of its synergy with experiments, aids the process to design new catalytic systems to address these major societal challenges. Here I will discuss two on-going research efforts in our lab: (1) Understanding electrocatalysts for the conversion of aqueous nitrate, a pervasive water pollutant, to ammonia, and (2) Advancing data-driven approaches using machine learning to extract knowledge from catalyst and materials data.

Nitrate ions (NO_3^-) are a highly distributed nitrogen source in industrial wastewater and polluted groundwater. Electrochemically converting nitrate ions into ammonia (NH_3) represents a route for wastewater remediation and sustainable ammonia generation. Ammonia is a foundational compound for society because of its broad use in chemical synthesis and fertilizers. I will discuss our atomistic modeling efforts to understand and design catalysts for the electrocatalytic nitrate reduction reaction (NO3RR). Based on computational predictions, a series of platinum-ruthenium (PtxRuy/C) catalysts were synthesized, characterized, and tested, all of which show superior performance to Pt, one of the best pure metal electrocatalysts for nitrate reduction. These findings demonstrate how electrocatalyst performance is tunable by changing the adsorption strength of reacting species through alloying and provide a blueprint to rationally select alloy compositions for NO3RR.

Combining atomistic modeling with machine learning has been demonstrated as a powerful approach to accelerate catalyst predictions. However, extracting meaningful physical insights from these machine learning models has often proven challenging. Here I will discuss interpretable machine learning approaches that can overcome some of these challenges, with some cases studies highlighted. These case studies show that data-driven approaches with interpretable machine learning can help extract physical insights to aid catalyst and materials understanding.

Wednesday, September 14th, 2022 at 3:00 pm
https://clarkson.zoom.us/j/95178712834

Bryan R. Goldsmith is the Dow Corning Assistant Professor of Chemical Engineering at the University of Michigan, Ann Arbor. He joined Michigan in 2017 after completing a Humboldt Postdoctoral Fellowship at the Fritz Haber Institute of the Max Planck Society in Berlin, Germany. He received his PhD in Chemical Engineering from the University of California Santa Barbara in 2015 from Baron Peter's group. Goldsmith's research lab specializes in atomistic modeling and machine learning to understand and design catalysts for chemical conversion, pollution reduction, and energy generation and storage. He was a recipient of the AIChE 35 under 35 Award and the ACS OpenEye Outstanding Junior Faculty Award.