PennState College of Engineering | CHEMICAL ENGINEERING

Faculty Candidate Seminar

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9:30 -10:30 am
102 Chemistry

Understanding catalysts from first-principles: Tackling challenges in modeling catalysts

Abstract

An atomically detailed understanding of catalysts would assist their development for sustainable chemical production and pollution abatement applications. In this talk, a few examples will be presented that demonstrate how first-principles modeling can facilitate an in-depth understanding of heterogeneous and homogeneous catalytic processes. Although there has been success in modeling crystalline catalysts such as zeolites and metal surfaces, approaches for modeling amorphous catalytic materials lag far behind due to their intrinsic disorder. Here a systematic method for modeling isolated catalyst sites on amorphous supports is introduced. This method uses a sequential quadratic programming framework that helps relate chemical properties, such as the activation energy, to active site structure. In contrast to amorphous catalysts, homogeneous catalysts are structurally well-defined and are more amenable to experimental characterization; however, accurate modeling of the kinetics and the role of solvent remains challenging. In the second part of this talk, it is shown how first-principles modeling combined with kinetics experiments can enable a deep understanding of methyltrioxorhenium (CH_3ReO_3)-catalyzed olefin epoxidation by H_2O_2. The kinetics of this process are fully characterized, and the important role of water is elucidated. Lastly, recent efforts to extract structure-property descriptors of materials using data-mining will be shown.

Biography

Bryan Goldsmith's research uses electronic-structure theory and molecular simulation, as well as data analytics, to understand catalysts and materials under realistic conditions, and to help generate a platform for their design and use in chemical synthesis and pollution reduction. He obtained his BS in Chemical Engineering at the UC Riverside (2010) and earned his PhD degree in Chemical Engineering at the UC Santa Barbara (2015) in the group of Baron Peters. His doctoral research was awarded the Schlinger Fellowship for Excellence in Chemical Engineering Research and a National Science Foundation PIRE-ECCI Fellowship. Bryan is currently a Humboldt Postdoctoral Fellow at the Fritz Haber Institute of the Max Planck Society in Berlin, Germany.