Texas Tech University
Department of Chemical Engineering
Seminar Series

Joseph Gauthier
Stanford University

Theoretical Investigations in Electrocatalysis for Sustainable Energy Conversion and Storage

Abstract
Commercial implementation of technologies for electrochemical conversion and storage of inherently intermittent renewable energy sources such as solar and wind is largely hindered by poor electrocatalysts, which struggle with activity, selectivity, and stability. In the past 15 years, computational simulations have proven to be of tremendous value in the search for improved catalyst materials and morphologies. However, one of the major open challenges in *ab initio* simulations of the electrochemical interface is the determination of electrochemical reaction energetics under a constant driving force. Existing methods to do so include extrapolation techniques based on fully explicit treatments of the electrolyte, as well as implicit solvent models which allow for a continuous variation in electrolyte charge. Emerging hybrid continuum models have the potential to revolutionize the field, since they account for the electrolyte with little computational cost while retaining some explicit electrolyte, representing a "best of both worlds" method. Here, we present a unified approach to determine reaction energetics from both fully explicit, implicit, and hybrid treatments of the electrolyte based on a new multi-capacitor model of the electrochemical interface. A given electrode potential can be achieved by a variety of interfacial structures; a crucial insight from this work is that the *effective* surface charge gives the true driving force of electrochemical processes. In contrast, we show that the traditionally considered work function gives rise to multi-valued functions depending on the simulation cell size. Finally, we demonstrate this approach by developing a microkinetic model for metal doped graphene electrodes used for electrochemically reducing CO2.

Bio
Joe Gauthier holds a Bachelor's of Science from Ohio State University in Chemical Engineering (2015), and is a Ph.D. Candidate in Chemical Engineering at Stanford University. His Ph.D. work with Prof. Jens Nørskov has focused on understanding the role of solvation in electrocatalysis. From 2018-2019, he was a visiting Ph.D. student at the Technical University of Denmark, where he worked with Prof. Jens Nørskov and Prof. Karen Chan to develop an energetic model of the electrochemical interface using polarizable continuum models.

Seminar

Wed, Jan 15th
3:00 pm
Livermore 101