Title: Minimizing Free Energy Corrugations in Electrochemical Systems

Abstract:

Electrochemistry is the science of interconversion of electrical energy and chemical energy, and therefore, occupies the driver's seat in our journey to integrate renewable energy sources into our energy ecosystem. Due to the intermittency of renewable energy there is a pressing need for storing this electron energy in chemical bonds. This can be achieved by charging long cycle life secondary batteries, or by converting abundant chemical feedstock into energy-dense fuels. Both of these processes need to be carried out near their respective thermodynamic driving forces at practical rates. The first part of this seminar will focus on a free-energy based in-silico catalyst screening methodology for small molecule electrochemical transformations. This involves the minimizing of free energy corrugations of on-path catalytic intermediates while simultaneously disfavoring off-path intermediates. Using density functional theory-based computations, it is possible to down select catalyst candidates from a large chemical space of transition metal ions and ligands, thereby accelerating an otherwise tedious catalyst design process, normally carried out through chemical intuition and/or trial-and-error based approaches in the laboratory. The latter half of the seminar will discuss the quantification of convoluted off-path electrochemical processes in high energy batteries using differential electrochemical mass spectrometry, and industrially scalable approaches to suppress these degradative pathways.