

CHEMICAL AND BIOLOGICAL ENGINEERING DEPARTMENT SEMINAR SERIES

## ***Catalysis and Electrochemistry on Transition Metal Nanoclusters***

Presented by: Jeffrey P. Greeley, Center for Nanoscale Materials, Argonne National Laboratory

Time: Wednesday, October 7; 3:15 – 4:30 pm

Location: Perlstein Hall Auditorium

### **Abstract**

Catalysis is the study and control of chemical transformations; a good catalyst will permit a given chemical reaction to proceed at high rates at modest temperatures (“activity”) and will, at the same time, prevent the formation of unwanted byproducts (“selectivity”). Typical catalysts are composed of either metal alloy or metal oxide nanoparticles and have been developed primarily by trial and error-based approaches. To fully optimize their properties, however, it is essential to develop fundamental understanding of the molecular-level properties that govern their operation. DFT analyses play an essential role in developing such understanding and will, ultimately, also facilitate the design and discovery of novel catalytic materials.

In this talk, I will describe recent work in our group in both computational heterogeneous catalysis and computational electrochemistry. The former studies focus on the chemical properties of subnanometer metal clusters for selective alkane dehydrogenation reactions, with a view to elucidating the fundamental structural features that give subnanometer clusters significantly different catalytic properties from those of larger nanoparticles. The latter studies focus on the development of descriptor-based models to rapidly estimate the electrocatalytic properties of transition metal alloys for various reactions of importance in low-temperature fuel cell operation. I will focus primarily on the Oxygen Reduction Reaction and will demonstrate how computational approaches have reached the stage where they can be used to find promising catalytic materials not previously identified by experiment.

### **Biography**

Dr. Jeffrey Greeley obtained his PhD from the University of Wisconsin-Madison in 2004. He then postdoc'd with Jens Nørskov at the Technical University of Denmark and developed methods to rapidly screen transition metal alloys for promising catalytic properties. Since 2007, he has been a staff scientist at Argonne's Center for Nanoscale Materials where he is developing a research program in computational nanocatalysis and electrochemistry.