Computational Catalysis Workshop

2:30PM – 5:30PM **Sunday, March 17th** **Location: Regal Suite**

Organizers: Matthew Neurock (U of Virginia), Lars Grabow (U of Houston)

Summary: Aimed at fostering the use of advanced computational tools including density functional theory (DFT) and multi-scale modeling of surface catalytic phenomena for realizing fundamental breakthroughs in catalyst design, this workshop will feature scientific and technical presentations highlighting the potential impact of computational catalysis tools by two academic experts (Dr. Lars Grabow, University of Houston and Dr. Matthew Neurock, University of Virginia), followed by hands-on demonstrations provided by Accelrys (San Diego, CA).

Schedule

I. Introduction to Computational Catalysis: Benefits and Challenges (2:30 – 3:00 PM)
Matthew Neurock and Lars Grabow

Overview of the capabilities and limitations of Computational Catalysis with focus on realistic expectations of the accuracy, types of problems that can be studied, and time frames necessary to obtain meaningful results. The role of Computational Catalysis in today's industry landscape is also discussed.

II. Computational Methods (3:00 – 3:45 PM)
Matthew Neurock and Lars Grabow

A brief introduction to the underlying methods, approximations and algorithms used in multiscale modeling of catalytic reactions: Quantum Mechanical and Wave-Function Methods, Density Functional Theory, Monte Carlo, (*Ab-initio*) Molecular Dynamics, Descriptor-based catalyst screening.

III. Tutorial 1: Adsorption on Metal Surfaces (3:45– 4:30 PM)
Accelrys

IV. Tutorial 2: Reactions on Metal Surfaces (4:30PM – 5:15 PM)
Accelrys

Tutorials will be presented by Accelrys, demonstrating the use of DFT techniques to gain fundamental insight into surface phenomena in heterogeneous catalytic reactions. Accelrys is a leading provider of scientific software with over 1,300 customers world-wide including 4 of the top 5 chemicals companies.

V. Open Discussion and Questions (5:15 – 5:30 PM)
Matthew Neurock and Lars Grabow