MSE SEMINAR

Materials Science and Engineering
Michigan Technological University

Tuesday, March 19, 2013
11:00 am – 12:00 pm
Room 610, M&M Building

Catalyst Design Strategies for Chemicals and Fuels

John & Virginia Towers Distinguished Lecture Series

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Abstract

A major challenge in heterogeneous catalysis has been to design better catalysts from a molecular-level understanding of surface reaction mechanisms and site requirements. It has been a dream for decades to be able to specify the composition and structure of matter to effect a desired catalytic transformation with desired and predicted rate and selectivity. The combination of surface science techniques and powerful, computationally efficient theoretical methods has shown promise, not just for identifying catalytic intermediates and reaction pathways accessible to experiments, but of providing quantitative predictions of energetics for elementary reaction processes not easily accessed experimentally. However, prediction without demonstrating performance is of limited value, and there are critical steps in between. One must be able not only to construct the design, but to demonstrate its survival, if not its detailed function, under operating conditions, in order to claim successful "design."

This presentation will consider examples of catalyst design utilizing new chemical insights from first principles studies, as well as the introduction of well-known catalytic functions into new environments. Regardless of the starting point, whether DFT calculations of the chemistry of individual sites or the assembly of new catalysts from molecular building blocks, issues of synthesis, stability and the working environment of the catalyst are common to all. The catalyst design strategies illustrated here will, it is hoped, be applicable to the development of new routes to fuels and chemicals from a feedstock base growing beyond fossil resources.

Biography: Mark A. Barteau is the new Director of the University of Michigan Energy Institute and the inaugural DTE Energy Professor of Advanced Energy Research. He previously served as the Senior Vice Provost for Research and Strategic Initiatives at the University of Delaware, where he held appointments as the Robert L. Pigford Endowed Chair of Chemical Engineering and Professor of Chemistry & Biochemistry. He was elected to the National Academy of Engineering in 2006. He was one 17 members of the National Research Council committee that authored the report *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering*, in 2003. He has served as the co-chair of the Chemical Sciences Roundtable of the NRC and the chair of the Council of Chemical Sciences for the DOE Office of Science. He currently serves on science advisory boards for the Environmental Molecular Sciences Laboratory at Pacific Northwest National Lab and for the National Institute of Clean and Low-Carbon Energy (NICE) China. Dr. Barteau was named in 2008 as one of the "100 Engineers of the Modern Era" by the American Institute of Chemical Engineers. He is the recipient of numerous awards from AIChE, ACS, and national and international catalysis societies.

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