

DEPARTMENT OF **CHEMICAL & ENVIRONMENTAL ENGINEERING**

2011 - 2012 **SEMINAR SERIES**



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FRIDAY NOV 18, 2011

9:30 - 10:30 AM

WCH 205/206

ENHANCING AND UNDERSTANDING HETEROGENEOUS CATALYSIS USING ORGANIC-INORGANIC INTERFACES

Enzymes control catalysis by tuning microenvironments within the active site. An open question that my research group aims to address is: what minimal degree of complexity needs to be incorporated into synthetic systems in order to be able to accomplish this? Three subquestions related to this are: (i) what are the requirements for a tethered functional group (A) to interact with another functional group (B) in its immediate surroundings on the surface, in order to facilitate cooperative heterogeneous catalysis, (ii) can the isolation of a grafted metal cation and its surrounding environment be programmed for catalysis using an organic ligand, and (iii) can metal cluster active sites be made stable and accessible simultaneously, while providing for the possibility of electronic tuning, with the use of an organic ligand? The latter subquestion is inspired by enzymes consisting of metal clusters at the active site. Results within area (i) are discussed by understanding the role of organically-modified surface in heterogeneous aminocatalysis, and applying these results for the hydrolysis of linkages relevant to the depolymerization of cellulose, the main component of biomass. In area (ii), grafted Al(III) calixarenes are used as oxo ligands for Al(III) grafted sites. The calixarene scaffold enforces site isolation as shown via ^{27}Al MAS solid-state NMR spectroscopy, and control of steric and electronic effects surrounding the active on a highly refined level. This approach has led to the design and synthesis of the most enantioselective catalyst reported for MPV reaction, using an Al(III)-calixarene active site. A heterogeneous variant of the calixarene-containing MPV catalyst provides valuable information into the open/closed connectivity requirements for heterogeneous catalysis, and this is demonstrated with new mechanistic information in related heterogeneous olefin epoxidation catalysis using organic hydroperoxides as oxidant. Finally, in area (iii), organically-modified metal clusters are used because the organic portion of these materials makes the electronic structure of the metal near the surface readily tunable via synthesis, and useful as a building block for heterogeneous catalysis. When using calixarenes as surface ligands for metal clusters, this passivation decreases the ubiquitous tendency of metal clusters to aggregate during catalysis, and enables programming of the electronic and steric environment on the metal surface. Corroborative data for programming electronic environment on the metal surface via ligand effects is provided by FTIR Spectroscopy, X-ray photoelectron spectroscopy (XPS) and single-crystal X-ray diffraction in comparative studies of iridium and gold clusters bound with calixarene phosphine ligands.

Alexander Katz was born in Minsk, Belarus and immigrated to the United States at age four with his family. Alex and his parents moved to Minnesota, where he grew up in and attended public schools. Alex graduated University of Minnesota with highest honors as a Bachelor of Chemical Engineering in 1992 and a research M.S. in Chemical Engineering with Prof. Michael D. Ward as advisor. It is at that time that he first became inspired by chemical engineering on the molecular level and controlling properties of functional materials via synthesis. He was awarded a Fannie and John Hertz Foundation Fellowship for doctoral studies in catalyst synthesis with Prof. Mark Davis at California Institute of Technology in 1994, and later, in 1998, undertook postdoctoral studies in supramolecular chemistry at Institut Le Bel in Strasbourg, France, with Prof. Wais Hosseini, as a NSF International Awards Postdoctoral Fellow. It is there that Alex learned about calixarene macrocycles and their synthesis. Alex began a multidisciplinary research program as Assistant Professor of Chemical Engineering at UC Berkeley in 2000, and has been promoted to Associate Professor. He was a Technion-Fulbright Fellow visiting professor at the Wolfson Department of Chemical Engineering in Haifa, Israel in 2008-2009. His current research interests are focused on understanding catalysis by using comparative structure-function relations and synthesis as a tool. Much of his efforts are geared at defining new paradigms of synthesizing hybrid organic-inorganic interfaces, and applying them to gain new insight into binding and catalysis involving surfaces. He is on the editorial board of *Chemistry of Materials*, and received a Young Scientist Prize from IACS in 2004 for his contribution of grafted calixarenes as hybrid organic-inorganic scaffolds for catalytic structures.