## SCHOOL OF CHEMICAL, BIOLOGICAL & MATERIALS ENGINEERING

And

## UNIVERSITY OF OKLAHOMA BIOENGINEERING CENTER

100 E. Boyd, Sarkeys Energy Center, T-335 405-325-5811 The University of Oklahoma Norman, Oklahoma 2010 – 2011 Seminar Series

## DR. ALEXANDER KATZ

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DEPARTMENT OF CHEMICAL AND BIOMOLECULAR ENGINEERING
UNIVERSITY OF CALIFORNIA, BERKELEY
BERKELEY, CALIFORNIA

Will present a seminar on

## "DESIGN OF BIOINSPIRED HETEROGENEOUS CATALYST: SYNTHESIS, CHARACTERIZATION, AND PERFORMANCE"

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 in hybrid organic-inorganic synthetic heterogeneous catalysts in order to be able to accomplish this? We describe our efforts along these lines in two areas: (i) grafted metal complexes and (ii) organically-modified metal clusters. In the former area, we use Ti(IV) and Al(III) calixarene complexes as active sites for olefin epoxidation and MPV reduction catalysis. Ti K-edge XANES demonstrates that the calixarene can be used to control d-orbital occupancy in the catalyst resting state, and our results in turn demonstrate that this directly affects site productivies for olefin epoxidation in the catalyst working state by over 20-fold. Using the calixarene as template for coordination environment surrounding the metal center, we gain further insight into open coordination site requirements at the metal center for Lewis acid catalysis involving these reactions, and furthermore show that heterogeneous catalysts based on chiral calixarene ligands can be synthesized to be just as enantioselective as similar homogeneous catalysts in solution. In the area of organically-modified metal clusters, the organic portion of these materials makes the electronic structure of the metal near the surface easily 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, akin to using residues in a metalloprotein. Corroborative data for programming electronic environment on the metal surface via ligand effects is provided by Fourier Transform Infrared (FTIR) Spectroscopy, X-ray photoelectron spectroscopy (XPS) and single-crystal X-ray diffraction in comparative studies of Ir4 and gold clusters bound with calixarene phosphine ligands.

THURSDAY, MAY 6, 2011
COOKIES AND COFFEE -- 2:45 P.M.
SEMINAR -- 3:00 P.M.
SARKEYS ENERGY CENTER, ROOM M-204

THIS IS A REQUIRED SEMINAR FOR CHE 5971

Accommodations on the basis of disability are available by contacting the office above three days before the event.