ChE SEMINAR

Reaction Mechanisms and the Design of Heterogeneous Catalysts for Sustainable Energy

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ABSTRACT

Diminishing fossil fuels and increase in demand of energy worldwide has led to the development of innovative technologies for sustainable energy supply. Some of the key technologies which can play a major role are: the conversion of biomass into fuels and chemicals, and the development of fuel cells for the efficient conversion of chemical energy into electrical energy. In most cases, underneath the development of these technologies lies the molecular level design and development of a catalyst material which can carry out the desired reaction with high conversions and selectivities. Catalyst design at the molecular level is carried out by conducting experiments augmented with *ab initio* theoretical modeling and study of the reaction mechanism.

In order to elucidate the molecular level design of a catalyst material, three specific cases are discussed. In the first case, the ring opening and decarboxylation of a pyrone molecule derived from biomass was carried out in aqueous phase to produce valuable industrial chemicals. In the second case, mechanism of oxygen reduction reaction on a fabricated thin-film electrode of solid oxide fuel cell (SOFC) was studied. Detail understanding of the reaction mechanism leads to a better design of the catalyst. As the third case, a bimetallic catalyst was designed for the conversion of syngas to ethanol with enhanced activity and selectivity.

ABOUT THE SPEAKER

M. Ali Haider has completed his Ph.D. in Chemical Engineering from the University of Virginia in 2011 and B.Tech in Biotechnology from Indian Institute of Technology Guwahati in 2006. Currently, he is working as postdoctoral research associate at the University of Virginia. His research interests include experimental heterogeneous catalysis, computational catalysis, reaction engineering, electrocatalysis, alternative energy, SOFC, biofuels and biorenewable chemicals.