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Modeling Complex Chemical Systems: Insights in Catalytic Activity of Sn-Beta Zeolite and Thermophysical Property Prediction

– Neeraj Rai, Mississippi State University

SEMINAR
WEDNESDAY
MAY 6
211 NETHKEN HALL
LA TECH
3:30 PM

Computational science is now widely recognized as the third pillar of scientific enquiry. Algorithmic improvements coupled with advances in computer hardware allow us to investigate more complex systems with greater detail. In this talk, I will present an application of electronic structure calculations to explore catalytic activity of Sn-Beta zeolite for isomerization and epimerization of glucose. Glucose to fructose isomerization is a key step in the conversion of biomass to chemicals. A better understanding of zeolitic activity for this reaction can allow us to develop more efficient catalyst for biomass conversion. In the second half of the talk, I will discuss Monte Carlo algorithmic improvements that allowed us to compute vapor liquid equilibria of ionic liquids using atomistic force fields, and discuss the suitability of dispersion corrected density functionals in predicting the phase equilibria of hydrofluoromethanes.

Neeraj Rai obtained bachelor's degree in Chemical Engineering from Karnataka Regional Engineering College, Surathkal, India in 2000. After short industrial stint in a fertilizer plant (Ammonia/Urea complex), he pursued his research interests first at Indian Institute of Science, Bangalore and later at the University of Minnesota, where he obtained PhD degree in Chemical Physics in 2009. Subsequently, he performed postdoctoral work at the University of Notre Dame and the University of Delaware. In August 2013, he started as an Assistant Professor in the Dave C. Swalm School of Chemical Engineering at Mississippi State University. His research interests are in the areas of force field and algorithm development, catalysis, and self-assembly of organic molecular systems. http://railab.che.msstate.edu/