2014 Spring Departmental Research Seminar

Title: Multiscale modeling of chemical systems: insights in the activity of zeolitic material and thermodynamic property prediction

Time: March 6, Thursday 11:00~11:50 am.

Place: AIME 110 (coffee and snacks will be provided)

Speaker:

Neeraj Rai
Assistant Professor
Dave C. Swalm School of Chemical Engineering
Mississippi State University

Abstract: 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. In the second half of the talk, I will discuss force field development for actinide elements, and Monte Carlo algorithmic improvements that allowed us to compute vapor liquid equilibria of ionic liquids using atomistic force fields.

Biography: 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 biological systems.