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Special Guest Lectures

Computational Earth Materials for Environmental and Energy Applications**Jianwei Wang, LSU**

Department of Geology and Geophysics

Digital Media Center Theatre
September 20, 2013 - 11:30 am**Abstract:**

Knowledge of earth materials is essential to their environmental and energy applications. Because of the difficulties in direct observation of earth materials under various conditions, molecular modeling becomes indispensable in understanding their structure and properties. These simulations provide greatly increased understanding and atomistically detailed otherwise unobtainable information of the structure, dynamics, spectroscopy, and energetics. I will use a few examples to illustrate how these atomic-scale simulations can provide a bridge between theories and observations of earth materials using high performance computing facilities. In low temperature geochemistry, water exchange reaction at water-mineral surfaces is fundamentally important to the understanding of the interfacial chemistry of minerals in the environment. Molecular dynamics and rare event sampling methods are used to compute the reaction rate and to understand how the exchange rate scales from aqueous ion, nanoparticles, to mineral surfaces. For hydrogen storage materials, hydrogen clathrate hydrate is environmentally friendly because upon combustion it simply releases water. Direct calculations of the vibrational spectra of hydrogen clusters in hydrogen hydrate cages from first-principles improve the understanding of the experimental Raman spectra of the hydrogen molecules and provide a guide on the synthesis of hydrogen gas hydrate. For uranium dioxide, or a mineral called uraninite, one of the unique properties is its non-stoichiometry. First-principles molecular dynamics simulations of hyperstoichiometric uranium dioxide suggest that the well-known structural model for the oxygen defect cluster in UO_{2+x} needs a revision. The simulations show the dynamic nature of the defect cluster, which consists of three interchanging configurations, in contrast to the averaged structure established from early neutron diffraction data.

Speaker's Bio:

Dr. Wang earned his PhD from the University of Illinois at Urbana-Champaign in 2004. He has been a post-doctoral fellow and research faculty at University of California at Davis and University of Michigan from 2005-2013. He is currently an Assistant professor at the Department of Geology and Geophysics. His expertise is molecular modeling of earth materials using first-principles and molecular dynamics simulations.

