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Thursday, February 16, 2017
Seminar Presentation: 11:00am – 12:00pm
Cymer Conference Center, SME 248

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Librational Entropy and Quantum Effects Inform Stability at the Nanoscale

Abstract:
The relative Gibbs "free" energy of molecules at interfaces underlies the macroscopic observables and ultimately material properties and function. For example, the contact angle of water and the relative "hydrophicity" of solid surfaces is a manifestation of the tension between microscopic surface energies. Understanding the fundamental forces in these systems, such as entropy, hydrogen bonding in water, dipolar screening etc., is critical, not only for developing an appreciation of the nanoscale physics and chemistries that inform the intrinsic stability, but also for predictive design strategies for engineering solutions to some of our biggest challenges. To this end, we have advanced several methods aimed at efficiently evaluating the absolute entropy and quantum corrections to the enthalpy of condensed phase systems at equilibrium. In this talk, we elucidate the delicate balance between these fundamental molecular forces in a variety of nanoscale systems, including 1) water at hydrophobic interfaces, relevant for nanofluidics and desalination, 2) melt impregnation of microporous carbon with liquid sulfur, used as advanced cathode materials for lithium sulfur batteries and 3) the interfacial structure of aqueous gold electrodes. Our ultimate goal is to predict electronic structure changes that can be exploited to both resolve the underlying physical morphologies and reveal molecular scale details of function. Thus in all of the above examples, we present the associated spectroscopic fingerprints, probed by high-energy electrons and photons and subsequently validated by experiments.

Biosketch:
Tod A Pascal is a project scientist at the Theory facility of the Molecular Foundry, a national nanoscience center at Lawrence Berkeley National Laboratory (LBNL), Berkley CA, USA. He is a chemical physicist with interest in the structure and dynamics of electro-chemical systems, disorder in condensed phase systems and spectroscopy at molecular interfaces. He has taught courses on nanotechnology, statistical mechanics, thermodynamics and computer simulations of materials. He received his undergraduate degree in chemistry from Lincoln University, PA, USA in 2003 and his PhD degree in Chemistry from the California Institute of Technology (Caltech) in 2009, where he did research on developing and applying methods to quantify disorder in nanostructures. He won a US Department of Energy Computational Science Fellowship during graduate school and an EEWS international postdoctoral fellowship from Korea Advanced Institute of Science and Technology. Currently, as a US DOE BMR fellow at LBNL, his research focuses on predicting speciation, spectra and thermodynamics of lithium sulfur batteries from first principles simulations.