Glenn T. Seaborg Center Seminar

First-principles simulations of X-ray Absorption Spectroscopy in Complex Materials

David Prendergast

The Molecular Foundry, Materials Sciences Division
Lawrence Berkeley National Laboratory, Berkeley, CA

Wednesday, June 6, 2012
4:00 - 5:00 pm
Building 70A, Room 3377

X-ray absorption spectroscopy (XAS) enables us to probe the local electronic structure of materials with elemental and chemical specificity. However, interpretation of such spectra relies heavily on detailed understanding of their electronic structure and the ability to accurately model the resonant core excitations induced by x-ray absorption. We have developed a first-principles approach to accurately simulate and interpret XAS. In addition we have explored the sensitivity of such spectra to dynamical degrees of freedom and included them in our simulations through molecular dynamics sampling. Such studies have revealed new electronic transitions, visible in measured XAS, which are only present due to broken symmetry induced by structural variation or change in chemical state. Such detailed interpretations of spectral features enhance the utility of XAS measurements on complex materials. We provide examples from our work on nanomaterials, aqueous solutions, and the solid state.

Host: David Shuh (510) 486-6937 DKShuh@lbl.gov Admin. Asst: Catherine Mendez (510) 486-5587
Ernest Orlando Lawrence Berkeley National Laboratory
One Cyclotron Road, Berkeley, California 94720 Tel: 510.486.4000