Glenn T. Seaborg Center Seminar

Computational studies of bonding, spectra, and coordination of actinide species in the natural environment

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Wednesday, February 16, 2011
4:00 - 5:00 pm
Building 70A, Room 3377

The complicated electronic structure of actinide complexes leads to their versatility of chemical reactivity, spectral and magnetic properties, and dynamical behaviors. We will show that computational chemistry modeling can be used as an effective tool to provide a first-principle description yielding insight into these spectroscopic and dynamical properties of actinide complexes. Two areas will be presented in this talk. We start by discussing metal-ligand bonding and the excitation of ligand based core electrons using time-dependent density functional theory. The simulated spectra are found in good agreement with the high-quality direct experimental probing of the bonding using K-edge X-ray Absorption Spectroscopy, lending support to the computational description of chemical bonding. We will also present simulation results of the dynamical behavior of actinide species interacting with minerals and water with a focus on the adsorption and complexation of uranyl at the water-mineral interface. These fundamental findings provide a solid foundation towards a more complete and accurate understanding of the physico-chemical properties of actinide complexes in the natural environment.

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