



Glenn T. Seaborg Center Seminar

EXPLORING SPECTROSCOPIC AND PHOTOCHEMICAL PROPERTIES OF ACTINIDE COMPOUNDS WITH QUANTUM CHEMICAL METHOD

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**Thursday, July 5, 2012
2:00 - 3:00 pm
Building 70A, Room 3377**

Quantum chemical methods are perfectly suited for the calculation of spectroscopic properties of heavy ions. In such ions, the manifold of electronic states is very dense and electron correlation and spin-orbit effects are intertwined. We will illustrate the potentialities and limitations of present quantum chemical methods for the calculation of the electronic spectra of bare and solvated uranyl(VI) and uranyl(V) complexes.

We will also discuss the mechanism for the photochemically induced isotope-exchange reaction $U^{17/18}O_2^{2+}(aq) + H_2^{16}O \rightarrow U^{16}O_2^{2+}(aq) + H_2^{17/18}O$. We were able to identify the nature of the excited states where the yl-exchange reaction takes place.