



## Glenn T. Seaborg Center Seminar

### *Coordination of Actinyl Ions to Nitrogenous Heterocyclic Ligands: A Joint Theoretical and Experimental Study*

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**Pacific Northwest National Laboratory, Richland, Washington, 99352**

**Thursday, October 9, 2014**

**4:00 - 5:00 pm**

**Building 70A, Room 3377**

Nuclear energy represents a critical tool available to meet the demand of increasing energy supply, at the same time reducing green house gas emission. To reduce the need for long-term nuclear waste storage, it is important to develop efficient strategies for selective separation. A better molecular-level understanding of the coordination modes and affinity of ligands with multiple binding sites to actinyl ions can pave the way to designing new ligand with improved extraction efficiency and selectivity. We will discuss the coordination chemistry to actinyl ions with ligands composed of multiple competitive binding sites including sulfur, nitrogen and oxygen chelating groups. We will present the interactions between actinide centers and the selected nitrogenous heterocyclic ligands using first-principle methods that include relativistic effects and electron correlation. The theoretical results will be further validated by gas phase collision-induced dissociation experiments and solution spectroscopic characterizations.