



Glenn T. Seaborg Center Seminar

Integrating Modeling and Experiment to Understand Actinide Chemistry

Bert A DeJong
Pacific Northwest National Laboratory
Wednesday, December 9, 2009
4:00 - 5:00 pm
Building 70A, Room 3377

Computational chemistry has reached the point where it makes significant contributions to the fundamental understanding of actinide chemistry, and plays an important role in interpretation of experimental data and the prediction of chemical and physical properties of actinide complexes. This presentation will discuss results of: 1) Understanding chemical bonding by combining sensitive experimental gas-phase measurements on actinides with the interpretative power of ab initio computational chemistry, and 2) Modeling the dynamical behavior of actinides in solution and at interfaces using newly developed and highly scalable heavy-element chemistry software capability in NWChem.