



Glenn T. Seaborg Center Seminar

Exploring Actinide Chemistry by Computation

Colin J. Marsden

*Université P. Sabatier
Toulouse, France*

Wednesday, June 2, 2010

4:00 - 5:00 pm

Building 70A, Room 3377

I shall start with a brief summary of what seem to me to be the most important notions in contemporary quantum chemistry, with particular reference to applications involving the actinides. I shall try to describe orbital polarization, correlation, density functional theory (DFT), multireference character, relativistic effects and pseudopotentials.

I shall then present some examples that show how computations can be helpful in actinide chemistry. Among the systems that I shall consider are:

- the uranyl ion, UO_2^{2+} , and several systems related to it
- UO_2^+ , UO_2 , UO_2^- , US_2 ;
- the reaction between Th atoms and NH_3 to give $\text{HN}=\text{ThH}_2$;
- the reaction between U atoms and NH_3 to give $\text{U}:\text{NH}_3$, $\text{H}_2\text{N}-\text{UH}_2$ and $\text{HN}=\text{UH}_2$;
- the reaction between U atoms and NF_3 to give $\text{N}\equiv\text{UF}_3$.

The ability of DFT to predict vibrational frequencies with high accuracy will be emphasized.

I shall then move to work in progress, involving various AnO and AnS species ($\text{An} = \text{Ac} - \text{Cm}$). The focus here will be on the ability (or otherwise) of standard DFT to provide reliable data for bond energies and ionization energies.