



## Glenn T. Seaborg Center Seminar

# Exploring actinide chemistry with multiconfigurational quantum chemical methods

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**Wednesday, February 11, 2009**  
**4:00 - 5:00 pm**  
**Building 70A, Room 3377**

Quantum chemistry is a mature science that can be applied to the study of systems containing any atom in the periodic table. In this lecture I will discuss our latest results in actinide chemistry. I will present the study on Pu-oxides [1] that has allowed us to resolve the controversy between different experiments concerning the value of the ionization potential of  $\text{PuO}_2$ . A similar study on Np-oxides is in progress.

I will then describe our ongoing study on actinide-actinide multiply bonded compounds [2] and uranium-poly-nitrogen species that may represent a way to stabilize all-nitrogen molecules and may open new routes to the formation of high energy density materials.

[1] G. La Macchia, I. Infante, J. Raab, J. K. Gibson, L. Gagliardi *A theoretical study of the ground state and lowest excited states of  $\text{PuOO}^{0/+/+2}$  and  $\text{PuO}_2^{0/+/+2}$*  Phys. Chem. Chem. Phys., 2008, 10, 7278–7283

[2] B.O. Roos, A. Borin and L. Gagliardi *The maximum multiplicity of the covalent chemical bond* Angew. Chem. Int. Ed., 2007, 46, 1469 -1472