



Glenn T. Seaborg Center Seminar

First-principles calculations for lanthanides and actinides: applications to nuclear separations and new nuclear detection materials

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and
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Wednesday, September 23, 2009
4:00 - 5:00 pm
Building 70A, Room 3377

I will discuss the application of density functional based approaches to f state systems and in particular the use of the LDA+U extension to improve on the local density approximation for f state systems. I will then present some applications of this approach to Ce and Eu doped gamma ray detector materials and Pu, Ce and U ligand complexes related to nuclear separations.