



THE GLENN T. SEABORG CENTER  
SCIENCE AND EDUCATION FOR HEAVY ELEMENTS AND THE ENVIRONMENT



**Dr. Zhiyong Zhang**  
Computing Sciences  
Lawrence Berkeley National Laboratory

## **Relativistic Chemistry And Its Applications to Actinides**

Thursday, April 25, 2002  
5PM-6PM  
Bldg. 70A- Room 3377

---

**Host: Dr. Linfeng Rao**

### **ABSTRACT**

We have developed spin-orbit configuration interaction and spin-orbit DFT programs for the calculation of systems with heavy elements. For systems with open shell electrons and strong spin-orbit effects, it is necessary to use multi-reference methods with spin-orbit interaction capabilities. We have applied the spin-orbit interaction method to the calculation of the electronic states of uranyl and UO and the results agree very well with experiments. The second part of the talk will focus on the application of DFT methods to actinide systems. We will discuss the calculated trends of structure and spectra of some uranyl-anion systems. We will also discuss the results on uranyl fluoride hydrolysis reactions.

For more information please contact the Center at 486-7535