



Glenn T. Seaborg Center Seminar

Probing the Electronic Structures of Actinide Complexes by Anion Photoelectron Spectroscopy

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4:00 - 5:00 pm

Bldg 54 Room 130 (Perseverance Hall)

Electrospray ionization coupled with a magnetic-bottle time-of-flight photoelectron analyzer has been used to probe the intrinsic electronic properties of singly and multiply charged anions from solution samples in the gas phase. This presentation discusses our recent investigations of actinide complexes. Being the heaviest naturally occurring element, uranium occupies a unique position in the periodic table and in society at large. Combining photoelectron spectroscopy (PES) and *ab initio* calculations allows us to probe the electronic structure of uranium compounds, revealing new insight into the chemical bonding of f-orbitals and help the elucidation of the actinide-ligand binding. The uranyl ion (UO_2^{2+}) is known to be the most stable form of uranium in solution and readily forms complexes with anionic ligands or solvent molecules. Various equatorial ligands can have weak interactions with U through the d- and f-type orbitals. A discussion of how this interaction can influence the electronic structure and bonding properties of UO_2^{2+} , will be presented through a series study of dianions $\text{UO}_2\text{X}_4^{2-}$ (X = F and Cl) and monoanions UO_2X_3^- (X = F, Cl, Br, and I). In addition, new experimental results for lower oxidation state uranium complexes (UF_5^- , UF_6^- , UCl_5^- , UCl_6^- , UCl_6^{2-} , and $\text{U}(\text{SCN})_5^-$) can help to explore the f-orbital participation in chemical bonding. I will also discuss our second generation cryogenic ion trap technique, which creates vibrationally and rotationally cold anions and significantly improve our spectral resolution.