Glenn T. Seaborg Center Seminar

Charge Transfer and Vibronic Interaction in Actinide Compounds

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4:00 pm – 5:00 pm
Bldg. 70A, Room 3377

The competition of ionic and covalent metal-ligand interactions in actinide compounds creates a rich spectrum of electronic and structural dynamics accessible to optical spectroscopy. Except the intra-configuration $5f^n$ and inter-configuration $5f^n$-$5f^{n-1}6d$ electronic transitions, charge transfer transitions probed by using optical spectroscopic methods provide fundamental information on electronic structures and bonding properties. We will discuss recent experimental and theoretical results from actinyl compounds and havey-5f elements including Cf(III) that exhibits anomalous electronic properties. Beyond the well-understood characteristics in the spectra of uranyl charge transfer vibronic transitions, our interest is in understanding the spectroscopic complication induced by bending the linear structure of O=U=O. Based on the Franck-Condon theory for vibronic transitions, excitation and emission spectra of non-linear uranyl species in the complex of UO_2Cl_2-$(phen)_2$ will be discussed in comparison with linear uranyl in tetrachloride crystals. In the second part of the seminar, we will focus our attention on the spectroscopic properties of Cf(III) compounds recently reported by Albrecht-Schmitt and co-workers.[Nature-Chemistry, DOI: 10.1038/NCHEM.1896] Our analysis suggests that the anomalous broadband emission is originated from a ligand-to-metal charge transfer that converts Cf(III) into Cf(II) in borate compounds. To be further discussed, this assignment brings out several important issues as regarding to the electronic energy levels and stabilities of Cf in the 3+ and 2+ oxidation states.

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