f-Block Chemistry at the Frontier: How *f*-Orbitals Shape Bonding and Electronic Structure

Seminar

Friday,
March 14, 2025

12:15 – 1:15 p.m.

Beaupre Center,
Room 105

Understanding the principles that govern actinide-ligand (An–L) bonding and electronic structure is crucial for advancing nuclear industry applications, environmental remediation strategies, and our fundamental knowledge of actinide chemistry. Strategies such as modifying ligand symmetry, electronic softness, or metal oxidation states offer powerful tools to tune covalency and electronic properties in An–L interactions, driving both experimental and computational efforts. On the metal side, reducing the oxidation state leads to more diffuse and destabilized *f*- and *d*-orbitals, enhancing covalency with suitable ligands and enabling novel bonding modes. Despite their potential in areas like separation chemistry, these bonding modes remain largely unexplored.

In this presentation, I will share my recent investigations into the chemical bonding and electronic structure of heavy elements across the lanthanide and actinide series, focusing on the effects of oxidation state and ligand design. Through close collaboration with experimental teams, this work demonstrates the powerful synergy between theory and experiment in uncovering new actinide bonding paradigms. These findings not only deepen our understanding of *f*-element chemistry but also open new pathways for innovative applications driven by *f*-electron interactions.

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Spring 2025 Seminar Series

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