Center for Actinide Science & Technology (CAST)
EFRC Director: Thomas Albrecht-Schmitt
Lead Institution: Florida State University
Start Date: August 2016

Mission Statement*: To unite materials chemists, separations scientists, condensed-matter physicists, and theoreticians into a cohesive research unit with the common goal of solving long-standing problems associated with the nuclear legacy of the Cold War.*

Cultivating new technologies that solve the vast challenges associated with nuclear waste from the Cold War will require an advanced science-based understanding and predictive capabilities for controlling *f*-element (actinide and lanthanide) molecules and materials in solution and solid state that utilizes the most advanced spectroscopic tools available. The Center for Actinide Science & Technology (CAST) brings together groups of scientists with *f*-element expertise from Florida State University, the National High Magnetic Field Laboratory, Florida International University, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Purdue University, and the University of Pennsylvania to facilitate synergistic cross-fertilization between chemists, physicists, materials scientists, and theoreticians. Our focus is on developing our unique expertise in synthesis, spectroscopy, and theory to develop first-principals, predictive electronic structure approaches to achieve the design, synthesis, and characterization of both low-temperature and high-temperature waste forms as well as new molecular systems that gain unprecedented control of chemical selectivity during processing. We will develop new synthetic methodologies, providing a detailed understanding of electronic structure from both experimental and computational perspectives, and addressing new separations schemes treating tank waste. A key impact of this research will be to develop practical, resilient, and experimentally-verified computational tools for describing complex chemistry, physics, and materials science both in the solid state and in solution. These advancements in experiment and theory will provide a revolutionary understanding of actinide materials under normal and extreme conditions, and in turn lead to wide-ranging applications in the nuclear sciences. This will advance our predictive capabilities in *f*-element science with implications across the periodic table.

Synthesis of Solid State, Complexes, and Molecular Materials. The actinide extended structure and molecular materials systems that are the focus of CAST will utilize the unique synthetic capabilities at FSU, LANL, and LBNL. A host of critical physical property measurements on these materials will take place at the NHMFL making use of both the unique facilities that will allow us to probe properties under a variety of extreme magnetic field, temperature, pressure, etc. conditions. Similarly, the synthesis of specialized actinide complexes and molecular materials will take place at FSU, LANL, LBNL/UC-Berkeley, and partner laboratories. The preparative efforts will include the design, synthesis, and optimization of new and existing ligands containing light atoms (B, C, N, O containing conjugated ligands) for the development and evaluation of transuranic separations. The ligand design and complexation studies with lanthanide, thorium, and uranium will take place at the University of Pennsylvania and Purdue University.

Electronic Structure. There are no broadly available, reliable predictive electronic structure approaches for the strongly correlated materials, both solid and molecular, that are the focus of CAST. We are expanding our approaches to employ high-accuracy electronic structure methods for the reliable predictions of the properties of actinide compounds. Results from the calculations will be validated through synergistic collaborations with experiment. Hard X-ray XES and RXES also will be used to determine precise *f*-occupancies. Complementary to the aforementioned occupied state probe will be unoccupied state measurements conducted using ligand K-edge XAS and non-resonant inelastic X-ray scattering, for which LANL has unique expertise.

Solution Chemistry. The solution chemistry effort will focus on revolutionizing the predictive capability for actinide complexation/exchange reactions with specific focus on developing new actinide separation strategies. Interplay between the theoretical and experimental efforts will center on quantifying *f*-element-ligand interactions and fine-tuning these interactions to maximize selectivity. The combined CAST X-ray spectroscopic expertise (XAFS, XES, RIXS, ligand K-edge XAS) will be utilized to probe the electronic structure and speciation of *f*-element species dynamics relevant to separations processes in solution with actinide-light atom bonds, and used to benchmark the theoretical and simulation efforts. Adding to the X-ray approaches, will be the unique capabilities of the CAST team in solution thermodynamics (including calorimetry), kinetics, and advanced optical spectroscopies will be focused onto the same systems.

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