Materials Science of Actinides (MSA)
EFRC Director: Peter C. Burns
Lead Institution: University of Notre Dame
Start Date: August 2009

Mission Statement*: To conduct collaborative, multidisciplinary, novel and transformative research on actinide materials emphasizing actinide ceramic, metallic, hybrid, and nanoscale materials; effectively integrate experimental and computational approaches; and solve research questions that are critical to the energy future of the nation.*

The Materials Science of Actinides Center unites researchers to conduct research in actinide materials science, with an emphasis on control at the nanoscale. Actinides are, in many ways, at the frontier of exploration of the periodic table, as their chemistry is complicated by the importance of the 5*f* electrons, relativistic effects of the electrons, their complex redox chemistry, and their radioactivity. Owing to this complexity and the relative difficulty of working with actinides, research in actinide chemistry and actinide-based materials has lagged far behind that of most other elements in the periodic table, both in theory and synthesis and design for special properties, such as radiation resistance of actinide-bearing materials.

In actinides, the delocalization/localization of 5*f* electrons presents the possibility of control of materials processes at the level of electrons. These properties emerge from the complex correlations of atomic (composition and short and long-range order) and electronic (f-electron) constituents. In this center, we heavily emphasize new synthesis approaches for actinide materials that are likely to lead to revolutionary new forms of matter with tailored properties. New materials that we emphasize are based upon the self-assembly of actinides into nanoscale materials with the potential to create new technologies. Radiation in actinide materials creates a system that is very far away from equilibrium, and a core focus of this center is to examine the behavior of actinide-based materials under extreme conditions of radiation, pressure and temperature.

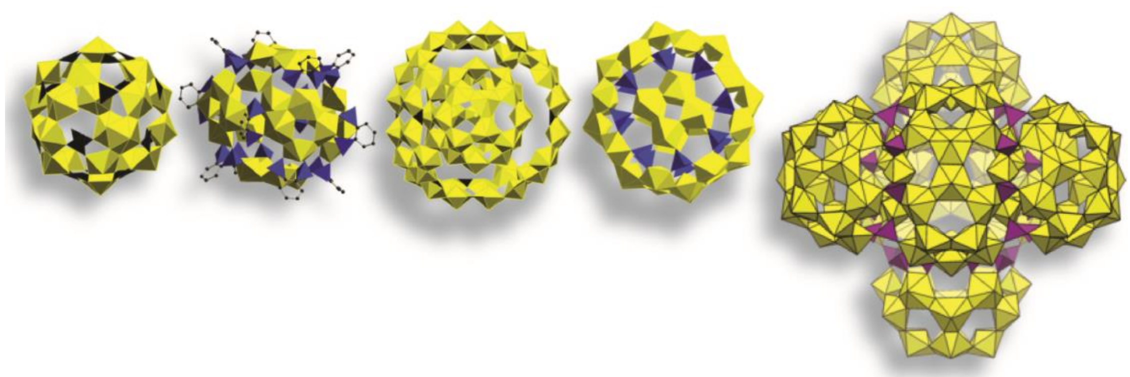

Figure 1. Examples of uranyl peroxide cage clusters containing uranyl polyhedra and, from left to right: phosphite, carboxyphosphonate, nitrate, molybdate, and phosphate (Qiu et al. *Chemical Reviews* **113**, 1097-1120 (2013)).

Three major Research Themes in actinide materials science are central to MSA's efforts. These themes are: (i) Nanoscale cage clusters, (ii) complex ceramic and metallic materials, and (iii) materials under extreme environments. Four cross-cutting themes are: (i) Novel synthesis methods for actinide materials across length scales, (ii) thermodynamics of actinide materials across length scales, (iii) integration of computational analysis and experimental results for actinide materials, and (iv) relevance of research to the nuclear fuel cycle.

The **nanoscale cage clusters theme** focuses on the self-assembly and properties of a large family of nanoscale actinyl-based cage clusters discovered by this group (Fig. 1). We seek to develop a fundamental understanding of the science of nanoscale actinide materials. Emphasis is on the assembly mechanisms, solution behavior, aggregation, stability, bonding, and ion pairing of these clusters.

The **complex ceramic and metallic materials theme** extends rigorous experimental determination and computational simulation of thermodynamic parameters of important actinide materials including oxides, selected metals, intermetallics, nitrides, and carbides containing plutonium, neptunium, or uranium. Work includes measurement of heat capacity, thermal expansion, and elasticity of a variety of actinide materials to guide theory and to provide critical data for next-generation nuclear reactors.

The **materials under extreme environments theme** addresses the many phenomena in actinide solids that are radiation dose, temperature, and/or pressure dependent – such as, order-disorder transformations, other phase transitions, and chemical decomposition. The coupling effects of extreme temperature and pressure environments with strong radiation fields are emphasized.

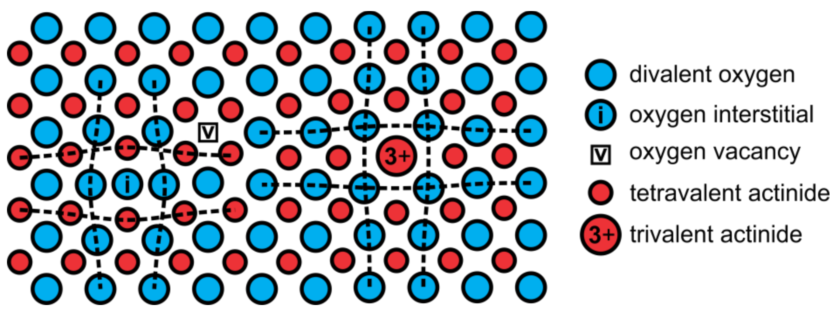

Figure 2. Cation reduction causes structural distortions in the actinide oxide lattice that are identical to that caused by Frenkel defects (Tracy et al. Nature Communications **15**, 507-512 (2016)).

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