NUCLEAR ENERGY UNIVERSITY PROGRAMS

Ab Initio Enhanced Calphad Modeling of Actinide-Rich Nuclear Fuels

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Abstract

The process of fuel recycling is central to the Advanced Fuel Cycle Initiative (AFCI), where plutonium and the minor actinides (MA) Am, Np, and Cm are extracted from spent fuel and fabricated into new fuel for a fast reactor. Metallic alloys of U-Pu-Zr-MA are leading candidates for fast reactor fuels and are the current basis for fast spectrum metal fuels in a fully recycled closed fuel cycle. Safe and optimal use of these fuels will require knowledge of their multicomponent phase stability and thermodynamics (Gibbs free energies). In additional to their use as nuclear fuels, U-Pu-Zr-MA contain elements and alloy phases that pose fundamental questions about electronic structure and energetics at the forefront of modern many-body electron theory. This project will validate state-of-the-art electronic structure approaches for these alloys and use the resulting energetics to model U-Pu-Zr-MA phase stability. In order to keep the work scope practical, researchers will focus on only U-Pu-Zr-{Np,Am}, leaving Cm for later study.

The overall objectives of this project are to:

- Provide a thermodynamic model for U-Pu-Zr-MA for improving and controlling reactor fuels.
- Develop and validate an *ab initio* approach for predicting actinide alloy energetics for thermodynamic modeling.