

NUCLEAR ENERGY UNIVERSITY PROGRAMS

Computational Design of Advanced Nuclear Fuels

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Abstract

The main objective of this project is to develop a novel computational method capable of fully treating the complex character of f electrons and to apply this method to study the electronic, magnetic, and lattice properties of the actinide elements. This project will concentrate on a class of systems relevant for the design of nuclear fuels—uranium and plutonium oxides, nitrides, and carbides, as well as their mixtures with fission product elements such as Np, Cm, and Am. The team will also study the properties of metallic binary alloys U–Zr, Pu–Al, U–Mo, and U–Cr. The project will address the issues connected to their lattice instabilities and phonon and magnon dynamics, as well as thermal conductivity. Building a robust theory to predict these materials' complex behavior has great potential for future computational design of advanced nuclear energy systems via computer simulations of phase diagrams, structural stability, lattice dynamics, and magnetic, transport and spectroscopic properties of many promising actinide compounds.