

# DOE-ID NEPA CX DETERMINATION

## Idaho National Laboratory

### SECTION A. Project Title: Electronic and Thermodynamic Properties of Unconventional Superconductors

### SECTION B. Project Description and Purpose:

Unconventional superconductors, especially the ones on the verge of magnetism represent a fascinating topic in condensed matter physics. This class of materials covers a wide range of systems, of which heavy fermion superconductors (the ones containing 4f and 5f-electron elements) are a subset. These superconductors are characterized by a significant band renormalization that leads to the strong electron mass enhancement being orders of magnitude larger than bare electron mass. Such materials typically contain elements such as Ce (Cerium), U (Uranium), Np (Neptunium), or Pu (Plutonium), in which the effects of strong electronic correlations and f-sp-d-electron hybridization are the cause of the effective mass enhancement. Uranium superconductors, in particular, are being intensively investigated due to the possibility of exhibiting triplet superconductivity with p-type of the order parameter. However, despite intensive experimental and theoretical studies, the nature of superconductivity and its relationship to the electron hybridization process and Fermi surface topology is still unclear. We propose to study the electronic structure, by angle resolved photoemission spectroscopy (ARPES), and thermodynamic properties of U6X systems. The ARPES technique is one of the best methods to determine the electronic band structure of materials because the ARPES measurements are based on the photoemission process, where photon hits the surface of a sample with certain energy ejecting electrons out of the surface of the measured material. Then, the electrons' kinetic energy and momentum are determined by the hemispherical analyzer of ARPES.

The U6X system is unique because it shows superconductivity with a relatively high  $T_c$  as compared to other uranium-based superconductors,  $T_c \sim 1$  K. Superconductivity in U6X was first discovered in 1958 by Chandrasekhar and Hulm, where they found U6Mn [(Uranium)6 Manganese], U6Fe [(Uranium)6 Iron], and U6Co [(Uranium)6 Cobalt], to be superconducting with transition temperatures  $T_c$ , of 2.3, 3.9, and 2.3 K, respectively. Furthermore, the U6X system was suggested to be close to the boundary between superconducting and ferromagnetic ground states, which has been extensively studied for ferromagnetic superconductors in heavy fermion systems, UCoGe (Uranium Cobalt Germanium) and URhGe (Uranium Rhodium Germanium) in particular.

To date, no experimental work has been carried out to precisely determine the electronic properties of the U6X materials. Hence, here, we propose to perform detailed studies of U6Co, U6Mn, and U6Fe single crystals by the ARPES technique focusing on: (i) Fermi surface mapping in this family by changing photon energies, (ii) observation of dispersion maps along with various high symmetry directions at the preformed and above the superconducting transition temperature, (iii) detection of energy dispersions in U6X near the Fermi level and to compare them with the calculated energy band dispersions. If the energy dispersion is narrow/broad, then it will indicate the localized/itinerant character of the 5f electrons. The photoemission studies will be conducted at the Advanced Light Source (ALS), which is a user facility located at Lawrence Berkeley National Laboratory (LBNL). By using synchrotron radiation (produced by a linear accelerator), we will be able to obtain high-resolution dispersion maps using different photon energies and polarization-dependent measurements. All these studies will be complemented by thermodynamic measurements, specifically detailed, high-resolution thermal expansion, magnetostriction, and heat capacity measurements performed at low temperatures and high magnetic fields. All of these will allow us to unveil the electronic behaviors and their coupling to other degrees of freedom such as phonons, spins, and quantum topology. Special attention will be devoted to understanding the influence of the 5f-ligand hybridization on their unusual normal state and superconducting properties. It is worth noting that good-quality single crystals of U6X phases are already available at INL Research Center (IRC, Lab C6) for the proposed studies. Furthermore, the proposed research can be conducted, due to (i) possession of a specially designed vacuum suitcase that will be used to cleave and carry radioactive samples from IRC to ALS. The system has a battery support that can retain high vacuum ( $\sim 10^{-10}$  Torr) for more than 60 hours and has already been approved to be used at ALS for our uranium samples, (ii) Presence of a state-of-the-art system for precise dilatometry measurements of radioactive samples at low temperatures, high magnetic fields, strain, and rotation. Finally, the topological behaviors in quantum materials are currently the hottest research topic in the condensed matter and material science community. The realization of these properties in uranium-based materials is novel, and the proposed studies will strongly impact the condensed matter physics community. In addition, the knowledge of electronic properties of uranium intermetallics will not only help to understand the nature of 5f electrons in general but will also advance fuel research, since the electronic properties govern the electronic thermal transport, hence important in advanced nuclear fuel materials.

The samples will be shipped in accordance with Department of Transportation requirements. The samples will be returned to the INL Research Center at the conclusion of the project.

### SECTION C. Environmental Aspects or Potential Sources of Impact:

#### Air Emissions

N/A

#### Discharging to Surface-, Storm-, or Ground Water

N/A

#### Disturbing Cultural or Biological Resources

N/A

#### Generating and Managing Waste

Samples will be returned to the IRC upon conclusion of the project. Some industrial waste is anticipated to be generated at the ALS facility.

#### Releasing Contaminants

N/A

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**Using, Reusing, and Conserving Natural Resources**

N/A

**SECTION D. Determine Recommended Level of Environmental Review, Identify Reference(s), and State Justification:** Identify the applicable categorical exclusion from 10 Code of Federal Regulation (CFR) 1021, Appendix B, give the appropriate justification, and the approval date.

For Categorical Exclusions (CXs), the proposed action must not: (1) threaten a violation of applicable statutory, regulatory, or permit requirements for environmental, safety, and health, or similar requirements of Department of Energy (DOE) or Executive Orders; (2) require siting and construction or major expansion of waste storage, disposal, recovery, or treatment or facilities; (3) disturb hazardous substances, pollutants, contaminants, or Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)-excluded petroleum and natural gas products that pre-exist in the environment such that there would be uncontrolled or unpermitted releases; (4) have the potential to cause significant impacts on environmentally sensitive resources (see 10 CFR 1021). In addition, no extraordinary circumstances related to the proposal exist that would affect the significance of the action. In addition, the action is not "connected" to other action actions (40 CFR 1508.25(a)(1) and is not related to other actions with individually insignificant but cumulatively significant impacts (40 CFR 1608.27(b)(7)).

**References:**

10 CFR 1021 Appendix B to subpart D, Item B3.6, "Small-scale research and development, laboratory operations, and pilot projects."

**Justification:**

The proposed R&D activities are consistent with CX B3.6 "Siting, construction, modification, operation, and decommissioning of facilities for small-scale research and development projects; conventional laboratory operations (such as preparation of chemical standards and sample analysis); small-scale pilot projects (generally less than 2 years) frequently conducted to verify a concept before demonstration actions, provided that construction or modification would be within or contiguous to a previously disturbed area (where active utilities and currently used roads are readily accessible). Not included in this category are demonstration actions, meaning actions that are undertaken at a scale to show whether a technology would be viable on a larger scale and suitable for commercial deployment."

Is the project funded by the American Recovery and Reinvestment Act of 2009 (Recovery Act)       Yes     No

Approved by Jason L. Anderson, DOE-ID NEPA Compliance Officer on: 04/18/2022