

SECTION A. Project Title: Electronic and transport properties of single-crystalline neptunium telluride

SECTION B. Project Description and Purpose:

Electronic and Transport Properties of Single-Crystalline Neptunium Telluride focuses on a fundamental understanding of the electronic and transport properties in neptunium telluride, NpTe_{1.75} crystals at the microscale, with special attention to potential topological phenomena governed by strong spin-orbit interactions. A similar compound, uranium ditelluride (UTe₂) is currently one of the most studied actinide materials, due to the unconventional superconductivity and topological ground state. To better understand the interplay of many-body physics and other degrees of freedom, such as topology and strong electronic correlations in similar NpTe_{1.75} crystals, the project will perform detailed electrical resistivity, magneto-resistivity, current-voltage (I-V) characteristics, thermal conductivity, and Hall effect studies that will be performed on micro-samples prepared by the plasma Focus Ion Beam (pFIB) method at low temperatures and high magnetic fields. The proposed project will lead to the understanding of the ground-state properties of this material that can be extended to other correlated actinide topological systems, transuranics in particular. This project will also help in establishing condensed matter physics and materials science as a lab core capability and enable a new research program related to actinide quantum materials.

The quantum effects associated with the spin-orbit interactions are directly related to atomic number and are strongest in heavy elements, such as actinides, where the relativistic shifting of the electron energy levels accentuates the spin-orbit coupling effect. In general, while the effect of electronic correlations is relatively well studied in cerium, ytterbium, and uranium (U)-based materials, there is still a lack of knowledge on how these collective phenomena impact magnetic, transport, and thermodynamic properties in transuranium intermetallics, neptunium (Np) in particular. The proposed research will make advances in the fundamental understanding of the electronic structure of NpTe_{1.75}, in particular and 5f-electron systems in general. This knowledge will be important for understanding the nature of 5f-states, especially in the context of quantum topological behaviors. In addition, the basic knowledge of the electronic structure of actinides will be also useful for understanding the electronic heat transfer in advanced nuclear materials.

Idaho National Laboratory (INL) has unique capabilities related to actinide materials that can be exploited to understand and harness emergent phenomena driven by strong electronic correlations and, especially, non-trivial electronic structure and topology. Examples include capabilities to study the magnetic, electronic, and spectroscopic properties of actinides under extreme conditions (low temperature, high magnetic fields, and pressure) and access to new state-of-the-art pFIB microscopes designed to work with nuclear materials. The new investigations of electronic and transport properties of NpTe_{1.75} have the potential to establish this material as a second known Np-based superconductor (after neptunium(1)palladium(5)aluminum(2), NpPd₅Al₂ and first Np-based topological material (low-risk, high-reward proposal). The proposed project will expand existing research activities and will be important in establishing a core Department of Energy (DOE), Basic Energy Science program at INL related to fundamental research of 5f-electron quantum materials and supports INL's Centre for Quantum Actinide Science and Technology. The advances in the understanding of the electronic structure of actinides would also benefit DOE Office of Nuclear Energy since the electronic properties govern the electronic heat transport in advanced fuels.

Data analysis for the project will be INL Research Center (IRC/IF-603/D11).

The transport properties will be measured using the Physical Property Measurement System (PPMS DynaCool-9) that allows measurements of the transport properties of radioactive samples in wide temperature (2–400 K) and magnetic field (0–9 T) ranges. All the measurements will be performed on micro-machined samples prepared by a pFIB technique. The usage of micro samples will unveil the electronic and transport behaviors of NpTe_{1.75} on a micro-scale, where quantum effects give rise to unusual electronic properties, with a particular focus on the effect of strong electronic correlations in 5f-electron systems. In addition, by using the micro-sized pFIB samples, we are also able to investigate how the electronic system changes as its physical dimension shrink below that length scale.

Therefore, to unveil the electronic and magnetotransport behaviors in the new NpTe_{1.75} system:

- (i) Prepare several NpTe_{1.75} lamellas by pFIB method having different contact configurations (“electrical resistivity” and “Hall effect”) and crystallographic orientations,
- (ii) Perform detailed transport studies with a focus on electrical resistivity, magnetoresistivity, I-V curve, thermal conductivity, and Hall effect. Measurements will be performed at low temperatures (down to 0.2 K), magnetic fields, and rotation (0-360 deg), and
- (iii) Special attention will be devoted to high magnetic field measurements, where quantum oscillations will be analyzed, the SdH effect in particular. All of the studies will enable full characterization of the electronic and transport behaviors in NpTe_{1.75}. The low-temperature measurements will fully characterize the ground state of this material (magnetic, superconducting, metallic, etc.) while the measurements in the magnetic field will enable detection of potential electronic and topological characteristics such as the presence of a Kondo hybridization gap, surface states, Berry curvature, or/and type and number of the electrical carrier, which can be probed by detailed transverse and longitudinal magnetoresistance and anomalous Hall effect studies.

The experimental work (FIBing and magnetotransport measurements) will be conducted at Materials and Fuels Complex (MFC) Irradiated Materials Characterization Laboratory (IMCL). The waste will include approximately 0.0005g of Np (~2 x10⁻⁷ Ci), which will result in low-level waste after final waste packaging in accordance with DOE O 435.1. Other low-level waste will be generated in the form of PPE, wipes, etc. and will amount to 0.1 ft³.

All of the studies will enable us to fully characterize the electronic and transport behaviors in NpTe_{1.75}. The low-temperature measurements will fully characterize the ground state of this material (magnetic, superconducting, metallic, etc.) while the measurements in the magnetic field will enable detection of potential electronic and topological characteristics such as the presence of

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a Kondo hybridization gap, surface states, Berry curvature, or/and type and number of the electrical carrier, which can be probed by detailed transverse and longitudinal magnetoresistance and anomalous Hall effect studies.

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

Final packaging of the Np contaminated waste will result in low-level waste and not TRU waste. Other low-level waste will be generated in the form of PPE, wipes, etc.

Releasing Contaminants

When chemicals are used during the project there is the potential for spills that could impact the environment (air, water, soil).

Using, Reusing, and Conserving Natural Resources

All materials will be reused and recycled where economically practicable. All applicable waste will be diverted from disposal in the landfill where conditions allow.

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, items 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: 05/17/2022