

**SECTION A. High Throughput Computational Platform for Predictive Modeling of Thermochemical and Thermophysical Properties of Fluoride Molten Salts – Pennsylvania State University****SECTION B. Project Description**

Pennsylvania State University proposes to study fundamental characteristics of molten fluoride salts in order to develop a thermodynamic model of this system. The project will study the atomic structure, melting point, heat capacity, free energy of potential corrosion reactions, solubility of fission and corrosion products in the F-(K-Li-Na)-(Cr-Ni)-(Pu-U) system using both density functional theory (DFT)-based molecular dynamics (MD) simulations and advanced experiments. Experimental measurements will be captured by x-ray diffraction (XRD), electromotive force (EMF), and differential scanning calorimetry (DSC).

**SECTION C. Environmental Aspects / Potential Sources of Impact**

Chemical Use/Storage / Chemical Waste Disposal – The experimental activities in this project will investigate physical properties of molten salts comprised of halide salts such as LiF, KF, and NaF.

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

Note: 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, including requirements of DOE orders; 2) require siting and construction or major expansion of waste storage, disposal, recovery, or treatment facilities; 3) disturb hazardous substances, pollutants, contaminants, or CERCLA-excluded petroleum and natural gas products that pre-exist in the environment such that there would be uncontrolled or unpermitted releases; 4) adversely affect environmentally sensitive resources. In addition, no extraordinary circumstances related to the proposal exist which would affect the significance of the action, and the action is not “connected” nor “related” (40 CFR 1508.25(a)(1) and (2), respectively) to other actions with potentially or cumulatively significant impacts.

References: 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); and 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 or developed 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 development.

Justification: The activity consists of an investigation into properties of molten salt systems.

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

Approved by Jason Sturm, DOE-ID NEPA Compliance Officer on 8/5/2020