

SECTION A. First-principles free energies by hybrid thermodynamic integration for phase equilibria and fission product solubility in molten salts – Rensselaer Polytechnic institute**SECTION B. Project Description**

Rensselaer Polytechnic Institute (RPI) proposes to model phase diagrams and solubility of actinides and lanthanide-fission products in molten salts for molten salt reactors (MSRs). The project aims to improve understanding of phase diagrams, equations of state and transport properties of binary and ternary molten salt mixtures as well as solubility of fuel, fission products and reactor-wall corrosion products. *Ab initio* computational prediction of these properties will help design future materials and supplement measurements involving short-lived radioactive species. After modeling, a series of experiments will be performed to experimentally validate the models using *in-situ* x-ray diffraction (XRD) and spectroscopic measurements of the compositions under the conditions modelled.

SECTION C. Environmental Aspects / Potential Sources of Impact

Radioactive Material Use / Radioactive Waste Generation / Chemical Use/Storage – RPI's Radiation Safety Office (RSO) has approved the PI's laboratory for storage and use of depleted uranium under RPI's license issued by the New York State Department of Health and is monitored on a regular basis by RPI's Radiation Safety Officer. Experiments to be conducted will involve handling depleted uranium-containing samples for characterization and testing. Samples will be stored in the environmental-controlled glovebox and waste will be disposed of following the guidance of RPI RSO. The procedures in handling, processing and sintering uranium-containing samples have been established and approved by RPI RSO.

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 7/20/2020