

# DOE-ID NEPA CX DETERMINATION

**SECTION A. Project Title: Learning-based Computational Study of the Thermodynamic, Structural, and Dynamic Properties of Molten Salts at the Atomic and Electronic Scale and Experimental Validations – University of Illinois at Urbana-Champaign and Argonne National Laboratory**

**SECTION B. Project Description**

The University of Illinois at Urbana-Champaign (UIUC), in collaboration with Argonne National Laboratory (ANL), proposes to obtain the thermophysical, thermochemical, and transport properties, construct the phase diagrams, and build empirical physical models of molten salts using simulations driven by machine-learned high-dimensional statistical learning modules combined with experimental validations. The tasks associated with this project are (1) Use machine learning (ML) to generate neural network potentials (NNPs) for molten salts from first-principles calculations; (2) Perform large-scale and longtime Molecular Dynamics (MD) simulations with the machine-learned NNPs, compute thermodynamic, structural, and dynamic properties and construct phase diagrams and empirical models of the thermophysical and thermochemical properties of the molten salts; and (3) Perform neutron/X-ray scattering and thermodynamic experiments to validate the empirical models. Existing laboratory facilities will be used.

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

Chemical Use/Storage, Chemical Waste Disposal, and Hazardous Waste Generation – About 100 g of FLiNaK salt will be studied in this project. Used chemical samples will be disposed of by the Division of Safety Research at UIUC as well as Oak Ridge National Laboratory (ORNL) and ANL.

Radioactive Material Use and Radioactive Waste Generation – Radioactive material will be used because natural or depleted uranium will be added to the salts in small quantities (<1000 g total). Any radioactive waste generated by this work will be LLW and can be disposed of through ANL’s waste disposal procedures.

Chemical Use/Storage and Chemical Waste Disposal – Chemical use is inherent to the synthesis of salts. Chemicals to be used include alkali halides such as LiF, LiCl, KF, KCl, and NaF. A total of 6 kg of fluoride salts and 6 kg of chloride salts will be synthesized and sent to UO+IUC. ANL has procedures in place for the acquisition, tracking, handling, and disposal of chemicals.

**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 university-scale research activities to determine the properties of molten salts that are relevant to Molten Salt Reactors.

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 08/14/2019