

SECTION A. Project Title: Determination of Molecular Structure and Dynamics of Molten Salts by Advanced Neutron and X-Ray Scattering Measurements and Computer Modeling – Massachusetts Institute of Technology**SECTION B. Project Description**

The Massachusetts Institute of Technology (MIT), in collaboration with Oak Ridge National Laboratory, proposes to measure pair-distribution functions (PDFs) by a combination of neutron and x-ray diffraction. The diffusion coefficients for salt and impurity ions will be extracted from neutron inelastic scattering measurements. The techniques of isotope substitutions, a very powerful tool available for neutron-scattering, as well as anomalous x-ray diffraction, a relatively new tool available at synchrotrons, will be utilized. *Ab initio* molecular dynamics simulations will be performed to understand the multicomponent liquid solution, in particular solubility of impurities and thermodynamic interactions in relation to the ionic-cluster structure of the fluid. Machine learning will be applied to regress from the simulation and experimental data in order to develop a fast-acting model that can handle molten salt with arbitrary (>10) number of chemical elements and be able to predict chemical potential as a function of composition and temperature.

SECTION C. Environmental Aspects / Potential Sources of Impact

Radioactive Waste Generation – A few grams of low-level activated fluoride and chloride salts will be generated, as well as a few small crucibles (a few cm³ in volume) from neutron diffraction measurements at Oak Ridge National Laboratory (ORNL) neutron user facilities. The total activation level is expected to be less than μ Ci levels due to very small sample sizes and small total neutron flux. Standard procedures exist at ORNL to dispose of user samples generated during user experiments. Alternatively, MIT could receive and dispose of these samples, which will be well within MIT license limits for receiving, handling, and disposing of such material.

Chemical Use/Storage – Various fluoride and chloride salts (a few grams in total) will be stored and used. Small amounts (~ 1 L) of standard organic solvents (i.e., isopropanol) to clean lab-ware will also be stored and used.

Chemical Waste Disposal – Small amounts of chemical waste might be generated due to the use of organic solvents. Standard procedures exist at MIT to dispose of this waste through the MIT Environmental Safety and Health (ESH) office. Very small amounts of chloride and fluoride salts (a few grams) might be disposed.

Hazardous Waste Generation – A few milliliters of generated chemical waste might contain trace amounts of Berillium. MIT EHS has standard procedures for disposal of such waste.

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 used to produce reliable data for computer simulations of both clean salts and those with added fission and corrosion products most relevant for 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 08/03/2018