

SECTION A. Project Title: Probing Speciation of Light Elements in Molten Salts by Electrochemistry, High Temperature Liquid NMR, and Neutron Diffraction – University of California, Berkeley**SECTION B. Project Description**

The University of California, Berkeley (UCB) proposes to investigate the speciation of solutes and the impact of light-element solutes on solvent structure for the following elements: hydrogen (tritium is an activation product in coolants containing Be or Li), beryllium metal (used for redox control), and carbon (present in abundance for graphite-moderated reactors and of importance to corrosion of metal alloys). The relationship between solvent structure and solvation of light elements will be probed; the solvent structure of 2LiF-BeF₂ (FLiBe) will be investigated over a range of BeF₂ compositions, representative of a range of fluorobasicity and of oligomer network structures. The molecular structure of melts and solutes will be predicted by Ab-Initio Molecular Dynamics (AIMD). Experimentally determined pair-distribution functions (from X-ray and neutron scattering) will then be used for validating the AIMD predictions. Liquid NMR will provide indication of distributions of elements among the different possible chemical environments such as content of bridging fluoride ions in oligomeric structures. NMR in conjunction with results from AIMD models will be used to identify the molecular structure of the solvent and of the species solvated in the solvent. Fluorobasicity will be measured by electrochemical measurements, employing fluoride ion-selective thermodynamic reference electrodes. Electrochemical measurements will also be employed to measure solubility, activity coefficient, activation energy of diffusivity and reactivity of hydrogen, carbon, and beryllium metal solutes in FLiBe. The following tasks are proposed: 1) Electrochemical Studies – chemical activity, apparent solubility, and reactivity of solutes; 2) AIMD – prediction of solvent structure, solute speciation, and the impact of solutes on solvent structure; 3) Scattering Methods - validation of solvent structure; and 4) High temperature liquid NMR - validation of solute speciation.

SECTION C. Environmental Aspects / Potential Sources of Impact

Work will be done with FLiBe and other chemicals. Beryllium-contaminated waste will be generated and disposed of through UC Berkeley EH&S.

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). For purposes of this category, “demonstration actions” means actions that are undertaken at a scale to show whether a technology would be viable on a larger scale and suitable for commercial deployment. Demonstration actions frequently follow research and development and pilot projects that are directed at establishing proof of concept.

Justification: The activity consists of the first demonstration of neutron diffraction and synchrotron studies on FLiBe or any other molten salts containing BeF₂.

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

Approved by Jason Anderson, DOE-ID NEPA Compliance Officer, on 09/17/2021.