Determination of Molecular Structure and Dynamics of Molten Salts by Advanced Neutron and X-ray Scattering Measurements and Computer Modeling

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Program: RC-2.3: Understanding the Structure and Speciation of Molten Salt at the Atomic and Molecular Scale

ABSTRACT:

The design and development of fully functional Molten-Salt Reactors (MSR) require detailed knowledge of the molten salt properties in order to understand and predict the salt's behavior. Fundamental properties of interest include molecular structure and speciation, as well as dynamic properties such as diffusion coefficients for the salt and corrosion and fission products dissolved in it. Computer modeling is necessary to predict changes in physical and chemical properties due to irradiation and burning of dissolved fuel. The modeling requires measurement data, and advanced neutron and x-ray scattering and spectroscopy provide the most reliable and direct determination of the structure (Pair-Distribution Functions, PDF), and dynamics (diffusion coefficients).

This proposal deals with both fluoride and chloride salts. The PDF's will be measured 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. We will utilize 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. Although some similar measurements have been done before, modern advanced neutron and x-ray-scattering techniques will allow collecting the data at much higher resolution and in wider range of temperatures. Importantly, fluoride salts were not studies by neutron scattering. The importance of impurities and their effects on salt properties have become apparent recently and so new methods of salt purification were developed. We will take advantage of these developments to produce reliable data, which will be used for computer simulations of both clean salts and those with added fission and corrosion products most relevant for MSR's.

Ab initio molecular dynamics simulations will be performed to understand the multi-component liquid solution, in particular solubility of impurities and thermodynamic interactions in relation to the ionic-cluster structure of the fluid. We will then apply machine learning 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.

The liquid state is a very difficult state of matter to understand and describe. However, detailed understanding is necessary for the development of novel molten-salt reactors. Thus, the objective of this project is to gain crucial new knowledge about molecular structure and dynamics of molten salts, to inform the design of new MSR's.