Understanding the Speciation and Molecular Structure of Molten Salts Using Laboratory and Synchrotron based In Situ Experimental Techniques and Predictive Modeling

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ABSTRACT:

Deployment of advanced nuclear energy technologies in the near future is essential to reduce greenhouse gas emissions and meet the projected worldwide energy demand. As part of the Generation IV reactor initiative, high temperature molten salt reactors (MSR) are expected to provide increased operating efficiency in addition to incorporating passive safety features and as a result industry is actively developing MSR designs. As such, it is of critical importance to understand the physical and chemical properties of molten salts, and how these properties vary as a function of composition, speciation and structure.

The objective of the proposed research is to develop a methodology to correlate speciation and structure of molten salts to their physical properties. The proposed research will use a combination of atomistic modeling and both laboratory and synchrotron-based in situ experimental techniques, to understand the speciation and atomistic structure of molten salts and their effect on properties such as density, thermal conductivity, and volatility.

The research objectives will be pursued via the following specific tasks:

- Design and develop an *in situ* system to simultaneously obtain Raman, UV-Visible absorption and near-Infrared (NIR) spectra from molten salts (currently UNR has an unique custom designed *in situ* Raman spectroscopy system for molten salts and INL has built an *in situ* UV-Vis system)
- Develop a methodology using above laboratory techniques and synchrotron-based scattering and diffraction techniques to determine the structure and speciation of molten salts
- Apply density functional theory (DFT) to predict the structure and chemical bonding of molten salts using the combination of quantum molecular dynamics (QMD), density-functional perturbation theory (DFPT), and natural bond orbital (NBO) analysis, and modify the method based on experimental data
- Study the effect of addition of various cations (Sm, Eu and Gd) on the structure of the other existing species in the molten salt and/or the properties such as redox potential
- Study the effect of addition of F^- (smaller than Cl^-) and I^- (larger than Cl^-) anions to a chloride based molten salt and study the changes in coordination number as a function of concentration.

The deliverable is an experimental methodology and predictive modeling for determining the speciation and structure of molten salts.