RC-2: Salt Behavior in Molten Salt Reactors

RC-2.1: UNDERSTANDING, PREDICTING, AND OPTIMIZING THE PHYSICAL PROPERTIES, STRUCTURE, AND DYNAMICS OF MOLTEN SALT

RC-2.2: UNDERSTANDING THE STRUCTURE AND SPECIATION OF MOLTEN SALT AT THE ATOMIC AND MOLECULAR SCALE

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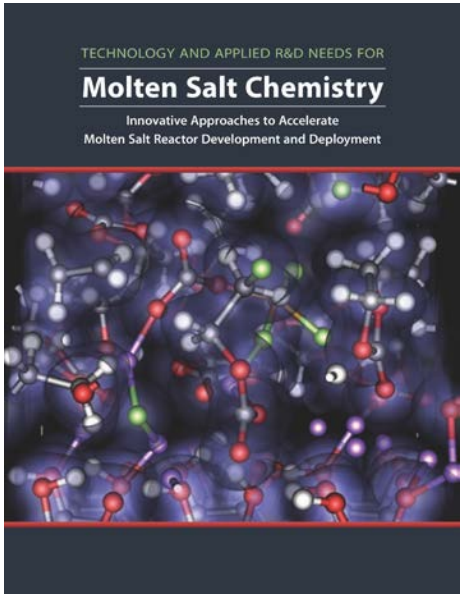
ELIGIBLE TO LEAD: UNIVERSITIES ONLY
Up to 3 years; $800K

In April 2017, the Office of Nuclear Technology Research and Development sponsored a Molten Salt Chemistry Workshop at Oak Ridge National Laboratory. A report entitled "*Technology and Applied R&D Needs for Molten Salt Chemistry*" is available at: https://www.ornl.gov/content/molten-salt-chemistry-workshop



The report identified six priority research directions:

- ✓ Understanding, Predicting and Optimizing the Physical Properties of Molten Salts
- ✓ Understanding the Structure, Dynamics, and Chemical Properties of Molten Salts
- ✓ Understanding Fission and Activation Product Chemistry and Radiation Chemistry
- ✓ Understanding Materials Compatibility and Interfacial Phenomena
- ✓ Guiding Next Generation Materials for Molten Salt Reactors
- ✓ Creating a Virtual Reactor Simulation

RC-2.1: UNDERSTANDING, PREDICTING, AND OPTIMIZING THE PHYSICAL PROPERTIES, STRUCTURE, AND DYNAMICS OF MOLTEN SALT

Thermodynamic models are needed to predict critical salt characteristics such as melting points, heat capacity, free energies for potential corrosion reactions, and solubilities for fission and corrosion products as function of temperature and composition.

Proposals are requested to better understand, predict, and optimize the physical properties and thermochemical behavior of molten salts. Our goal is to develop and use first-principles molecular dynamics simulations and computational electronic structure method to extend the limited experimental data sets in covering a broader range of chemical evolution and environments.

- Apply molecular dynamics simulations to predict thermophysical and transport properties;
- Build multi-component models for prediction of phase diagrams; and
- Develop advanced models to guide the experimental efforts to manipulate the molten salt thermophysical properties are especially encouraged

RC-2.2: UNDERSTANDING THE STRUCTURE AND SPECIATION OF MOLTEN SALT AT THE ATOMIC AND MOLECULAR SCALE

To understand how the structure and dynamics of molten salts impact their physical and chemical properties—such as viscosity, solubility, volatility, and thermal conductivity—it is necessary to determine the speciation of salt components as well as the local and intermediate structure at operationally relevant temperatures.

Proposals are requested to take advantage of recent breakthroughs in advanced characterization tools and instrumentation methods to provide information at the atomic and molecular scale. The goals are to determine the local structure and bonding of chemical species in salt solution and to develop innovative real-time analytical methods for microscopic and macroscopic property measurements to underpin and support molten salt reactor design and development.

- ❑ Determine salt molecular structure using scattering and spectroscopic methods;
- ❑ Develop novel electrochemistry and spectroscopy methods for in-situ monitoring and predictive modeling; and
- ❑ Develop molten salts optical basicity scale to determine corrosivity and solubility of actinides