Molten Salts in Extreme Environments (MSEE)
EFRC Director: James Wishart
Lead Institution: Brookhaven National Laboratory
Class: 2018 – 2022

***Mission Statement**: To provide a fundamental understanding of molten salt bulk and interfacial chemistry that will underpin molten salt reactor technology.*

Molten Salt Reactors (MSRs) are a potentially game-changing technology that could enable cost-competitive, safe, and more sustainable commercial nuclear power generation. Proposed designs employ molten salts in the temperature range of 500 – 900 ˚C acting as coolants for solid-fueled reactors or in other cases where the nuclear fuel dissolved in the molten salt as combined coolant and fuel. Consequently, the development of reliable MSRs requires a comprehensive understanding of the physical properties and chemistry of molten salts and of their interfacial interactions with reactor materials.

The Energy Frontier Research Center for Molten Salts in Extreme Environments (MSEE) will provide fundamental and predictive understanding of the bulk and interfacial chemistry of molten salts in the operating environments expected for MSRs. MSEE addresses this challenge through a coordinated experimental and theoretical effort to elucidate the atomic and molecular basis of molten salt behavior, including interactions with solutes (dissolved materials such as nuclear fuel and fission products) and interfaces, under the coupled extremes of temperature and radiation.

The research of MSEE is organized into two interrelated thrusts. The first is *Molten Salt Properties and Reactivity*, which aims to understand how molecular-scale interactions, structure and dynamics lead to macroscale properties. A key focus is to learn how the interactions between molten salts and solutes affect physical properties and control solubility and reactivity. The second thrust, *Interfacial and Corrosion Processes in Molten Salt Environments*, aims to understand the atomic-scale structure and dynamics at interfaces and related mechanisms of interfacial and corrosion processes between molten salts and materials, including the effects of extreme environments such as radiation and high temperature.

Thrust 1: Molten Salt Properties and Reactivity

Aim 1: Determine the structure and dynamics of molten salt solutions across scales of length and temperature. Powerful X-ray, neutron-scattering and optical spectroscopy techniques are employed and coupled with computational approaches to interpret observations and validate predictions in order to assemble a dynamic model of molten salt structure.

Aim 2: Elucidate the principles that control metal ion solvation, speciation and solubility in molten salts. The same methods are used to understand changes in solution structure, dynamics and thermal properties when solutes, including actinides and fission products, are dissolved in molten salts.

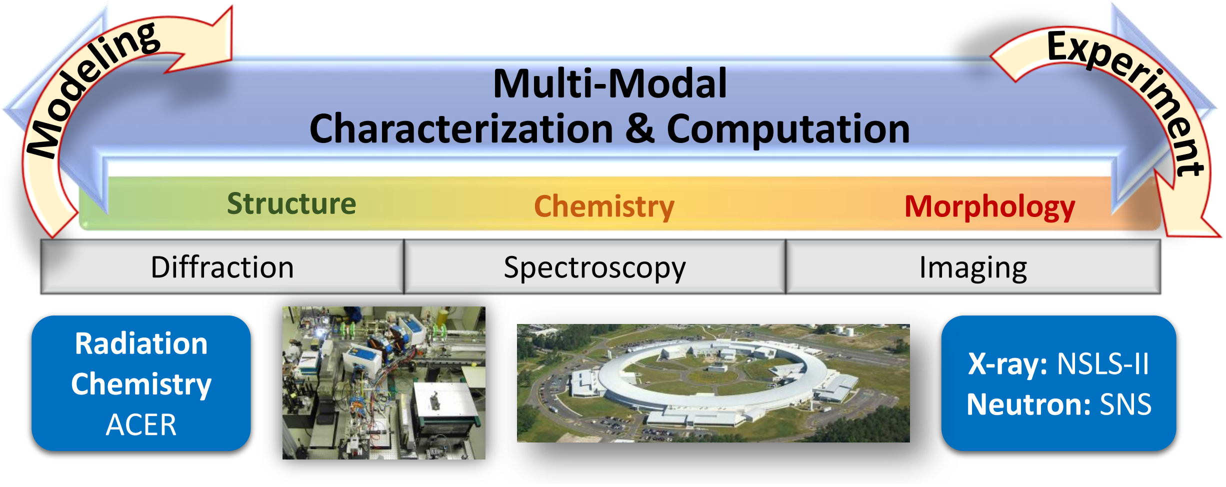
Aim 3: Understand how radiation affects salt solution chemistry and solute speciation. Radiation chemistry techniques are used to examine the radiation-driven reactions of molten salts and materials dissolved in them.

Thrust 2: Interfacial and Corrosion Processes in Molten Salt Environments

Aim 1: Measure and predict the structures and dynamics of molten salts at interfaces. X-ray and neutron reflectivity measurements are integrated with new modeling approaches to provide fundamental new information on surface ordering and dynamics of molten salts and to elucidate how these structures determine energy and charge transfer across the interface.

> *<u>Aim 2: Kinetics of interfacial reactions leading to corrosion.</u>* *In-situ* experimental techniques, enabled by advances in characterization capabilities, will provide unprecedented temporal and spatial resolution for quantifying interfacial reactions and help us understand and predict non-equilibrium, metastable states formed during the reactions at interfaces.

A deeper knowledge on molten salt structure and properties, and the behavior of the actinides, fission products and corrosion products in molten salt solution under radiolytic conditions, will strengthen the scientific foundation for the practical implementation of MSRs. A stronger understanding of redox chemistry and solvation of solutes such as fuel metal ions and fission products will contribute to better predictions of precipitation, participation in corrosion reactions, gas generation and failure to behave as desired in fission product separations. Improved molecular knowledge of the corrosive interactions of molten salts will suggest ways to mitigate challenges to the performance of nuclear reactor materials, and also in solar thermal collectors. MSEE will focus on filling those knowledge gaps to enable safer, higher performing and more reliable MSR systems, as well as to extend our scientific understanding of the general fundamental chemical processes in molten salts.



Molten Salts in Extreme Environments (MSEE)	
Brookhaven National Laboratory	James Wishart (Director), Eric Dooryhee, Simerjeet Gill, Anatoly Frenkel, Benjamin Ocko, Kotaro Sasaki
Idaho National Laboratory	Simon Pimblott (Deputy Director and Interim Thrust 2 Leader), Ruchi Gakhar, Gregory Horne, Lingfeng He
Oak Ridge National Laboratory	Shannon Mahurin (Thrust 1 Leader), Vyacheslav Bryantsev, Sheng Dai, Xiao-Guang Sun
University of Iowa	Claudio Margulis
University of Notre Dame	Jay LaVerne, Edward Maginn
Stony Brook University	Yu-Chen Karen Chen-Wiegart

Contact: James Wishart, Director, wishart@bnl.gov
631-344-4327, https://www.bnl.gov/moltensalts/