Molten Salts in Extreme Environments (MSEE)
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Lead Institution: Brookhaven National Laboratory
Class: 2022 – 2026

Mission Statement: *To provide fundamental and predictive understanding of molten salt bulk and interfacial chemistry that will establish robust principles to guide the technologies needed to deploy molten salt nuclear reactors.*

Molten salt reactors (MSRs) are a potentially game-changing nuclear reactor technology that is likely to shape the future of nuclear power generation. MSRs could provide a cost-competitive, safe, and more sustainable commercial nuclear power option. MSRs are designed to operate above 500 °C and include molten salts as coolants for solid-fueled reactors, and liquid-salt-fueled reactors containing the nuclear fuel constituents 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.

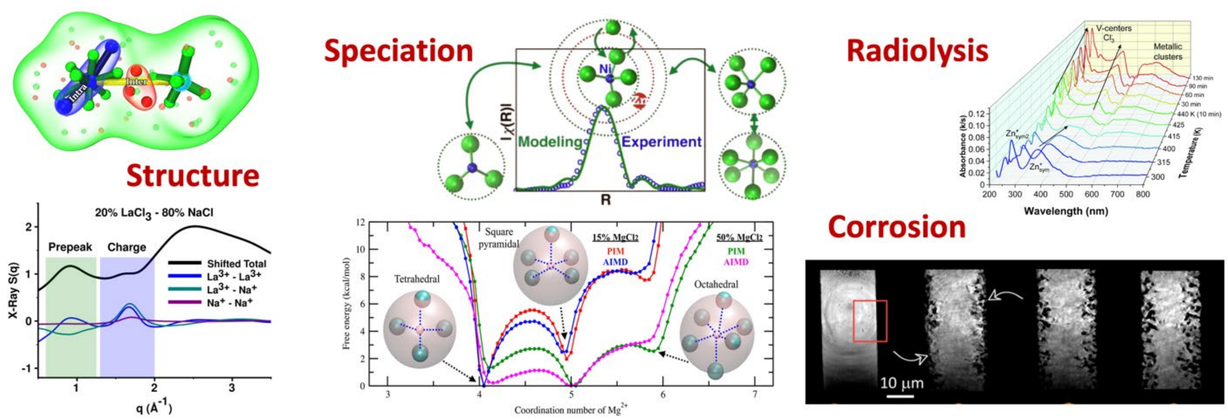
Though made from simple ionic components, molten salts are complex, structured liquids that are subject to intricate physical and chemical processes, particularly in the extreme environments encountered in reactors. Their behavior with solutes, including fuel actinides, and in contact with reactor materials, introduces complex interactions for which fundamental understanding is needed across the range of conditions relevant to reactor operation.

To address this challenge, the integrated, high-level science goals of MSEE over the next four years are:

i. to understand how molten salt atomic-scale structures and interactions control salt dynamical properties and chemical speciation and reactivity, in the bulk and at interfaces, by advancing the state-of-art in experimental and computational methods;
ii. to develop a mechanistic understanding of metal corrosion processes in molten salt systems, ranging from atomistic chemical processes to mesoscale structure and transport; and
iii. to build a comprehensive description of radiation-driven chemical reactivity in bulk fuel salt and at interfaces, to anticipate and mitigate undesirable product formation and material degradation in MSR systems.

MSEE pursues these goals through three synergistic thrusts and one crosscutting theme. The purpose of Thrust 1 (*Molten Salt Structure, Dynamics and Properties*) is to understand the structure and dynamics of neat salts and salt mixtures in the bulk phase across a range of concentrations and temperatures. The purpose of Thrust 2 (*Speciation and Redox Processes*) is to identify and predict the multi-faceted behaviors of the accumulating fission and corrosion products in the salt. The purpose of Thrust 3 (*Interfacial Phenomena*) is to investigate the structure and reactivity of molten salt interfaces with metals and model materials. The purpose of the crosscutting theme of *Radiation-Driven Processes* is to obtain mechanistic understanding of how ionizing radiation changes the speciation of molten salt constituents through redox reactions, leading to new products that alter the properties of the salt system, and driving chemical reactivity at interfaces. These objectives can only be accomplished by closely-coordinated efforts among researchers from multiple disciplines working as a team. Our experience has shown that theoretical insight is essential to properly interpret complex experimental results, for example the coordination environments of technologically important metal ions such as U^{3+} and Ni^{2+}, and counterintuitive changes in the nanoscale ordering of monovalent-divalent salt mixtures with increasing temperature.

A deeper knowledge of 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 greater understanding of the speciation, solubilities and chemical reactivities of dissolved species such as actinides and fission and corrosion products will contribute to better predictions of precipitation and particle formation, participation in corrosion reactions, and ultimately enable stable reactor operation over a wide range of composition, temperature and radiation flux. Improved molecular knowledge of the interfacial processes that drive corrosion, including mass and charge transfer, chemical reactions, and microstructural evolution will suggest ways to mitigate challenges to the endurance of nuclear reactor materials. MSEE will focus on filling these 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.



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