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# Learning-based Computational Study of the Thermodynamic, Structural, and Dynamic Properties of Molten Salts at the Atomic and Electronic Scale and Experimental Validations

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**ABSTRACT:**

Despite increasing excitement of Molten Salt Reactors (MSRs), the fundamental thermophysical and thermochemical behaviors and the transport properties of molten salts identified for MSR applications are still not well understood. Large variations are evident across existing data sets for many of these properties. For instance, the variation of the melting point, the heat capacity, the free energy for potential corrosion reactions, the solubility of fission and corrosion products, and the effect of tritium cannot be accurately predicted as a function of temperature and composition with current data sets. This knowledge gap of molten salt behavior poses a major roadblock in the development and commercialization of MSR technology. The objective of this proposal is to obtain the thermophysical, thermochemical, and transport properties, construct the phase diagrams, and build empirical physical models of molten salts that are relevant to Molten Salt Reactors (MSRs) with first-principles accuracy using Molecular Dynamics (MD) simulations driven by Machine-Learned (ML) high-dimensional Neural Network Potentials (NNPs) combined with neutron/X-ray scattering and thermodynamic experimental validations. The achievement of this proposed project can help eliminate some of the basic obstacles towards the design and construction of MSRs.