A Molten Salt Community Framework for Predictive Modeling of Critical Characteristics

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Program: FC-1.2 Understanding, Predicting, and Optimizing the Physical Properties, Structure, and Dynamics of Molten Salts

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ABSTRACT:

The proposed US-UK collaborative research aims to develop a molten salt community framework (**MOSAF**) to directly address the needs in advanced fuel cycles described in Workscope FC-1.2. This framework, when completed successfully, will provide the global molten salt community with high throughput computational approaches and tools, with underpinning databases, to understand, predict, and inversely design advanced molten salts that will offer a significant advancement to what is currently available.

Our unique efforts and the specific objectives include: **(1)** Understanding of molten salts through phonon collective excitations and supercritical state of matter to unveil underlaying physics based on molecular dynamics (MD) with an emphasis on machine learning (ML) accelerated ab initio MD (MLMD) simulations. **(2)** Predicting critical salt characteristics with uncertainty quantification (UQ) through CALPHAD-based computational thermodynamics and the implementation of advanced models such as the modified quasichemical model with quadruplet approximation (MQMQA) and the universal quasichemical (UNIQUC) model. **(3)** Optimizing inversely the selection of fit-for-purpose salt systems using ML-based conditional generative adversarial networks (cGAN) with input from simulations; and **(4)** iteratively verify and improve fundamental understanding, CALPHAD modeling, MD/MLMD simulations, and inverse design using key chloride salts. The present framework is achievable based on the PIs' previous successes in developing theories, software tools, and advanced experiments related to molten salts, including new theory of liquid, the world-leading flagship MD code, high throughput density functional theory calculations, high throughput CALPHAD modeling, and measurements by such as high-temperature rheometry and X-ray absorption fine structure (XAFS).

This US-UK collaborative research also has outstanding value for US taxpayers by leveraging $3 in UK funding for every $1 in US funding. This will enable the depth and breadth of our research to far exceed what could normally be achieved, to the mutual benefit of both US and UK nuclear research. The team consists of senior, middle career, and junior scientist along with postdoc fellows and graduate students, cultivating the workforce development of future subject matter experts for the molten salts and nuclear industry and delivery of outreach short courses and workshops for engagement across academia, industry, and the public.