NEUP Nuclear Energy University Programs
U.S. Department of Energy

High Throughput Computational Platform for Predictive Modeling of Thermochemical and Thermophysical Properties of Fluoride Molten Salts

PI: Shun-Li Shang – Pennsylvania State University

Program: MS-FC-1: Understanding, Predicting, and Optimizing the Physical Properties, Structure, and Dynamics of Molten Salt

Collaborators:
Hojong Kim – Pennsylvania State University
Zi-Kui Liu – Pennsylvania State University
Shenyang Hu – Pacific Northwest National Lab
Tatiana G. Levitskaia – Pacific Northwest National Lab

ABSTRACT:

The proposed research aims to (i) understand critical salt characteristics of fluoride molten salts such as atomic structure, melting points, heat capacity, free energy of potential corrosion reactions, solubility of fission, and corrosion products in a model system of F-(K-Li-Na)-(Cr-Ni)-(Pu-U) by means of the density functional theory (DFT) based molecular dynamics (MD) simulations and advanced experiments; (ii) predict and optimize critical salt characteristics using thermodynamic database created by high throughput (H-T) thermodynamic modeling with validation and refinement by key experiments; (iii) develop an open-source H-T computational platform with an automated process from DFT-based first-principles calculations, DFT-based MD simulations, machine learning (ML) predictions, to CALPHAD (CALculations of PHAse Diagrams) modeling of thermodynamic properties; and (iv) provide a publicly accessible H-T computational platform with Python-based open-source codes and thermodynamic models that has a capability to integrate both experimental and computational data for continued advancement in understanding complex molten salt systems.

Considerable simulations are required to create a valid thermodynamic description for the present F-(K-Li-Na)-(Cr-Ni)-(Pu-U) system, calling for efficient CALPHAD modeling with extensive data as input. To address this issue, the proposed project will employ and develop an open-source high throughput computational platform with automated high throughput calculations from DFT and ML predictions to CALPHAD modeled database. The use of open source codes in the fast-growing Python programming language for high throughput approaches will enable efficient dissemination and transfer of the developed knowledge and computational tools for molten salt research community and beyond. The model predictions of molten salt properties will be validated through targeted electrochemical and thermal measurements.

The newly created high throughput approaches, open source codes, and public-accessible data will (i) support the goal of US industries to commercialize MSR technologies and (ii) educate and train the next generation workforces, which are critical to the future development and deployment of nuclear energy.