Coupling the CALPHAD Method and First Principles Simulations for the Prediction and Modelling of the Thermal Transport Properties in Complex Solid Salt Systems

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The design of materials for nuclear molten salts reactors (NMSR) or concentrated solar power (CSP) require an accurate knowledge of thermodynamic and thermal transport properties for solid phase. For several systems of interest, a severe lack of experimental data is observed for both thermodynamic and thermal transport properties. Very few data on thermal conductivity and thermal diffusivity are reported for binary and higher order salts compounds, especially for those of CSP and NMSR interest. To a lesser extent, a similar lack of data may be observed on thermal expansion and heat for many compounds. To alleviate this severe lack of data, we report here a CALPHAD based method to build reliable models describing the thermophysical properties as a function of temperature by explicitly considering the phonon and the electrons density of state. Note that the developed models describing molten salts properties are derived from physical principles. For example, the thermal conductivity model is derived from Boltzmann kinetic theory. The model parameters are determined via Density Functional Theory (DFT) simulations. The methodology has shown a good predictive capability for simple as well as complex systems. Several examples on materials related to CSP and MNS illustrating the methodology are presented. The predicted thermal conductivity, thermal expansion and heat capacity is compared with experimental data when available and to simulated properties via classical (Newtonian) Equilibrium Molecular Dynamics (EMD) where the force field describing the interaction between ions is determined via DFT. The tensorial aspect of the thermal properties will be discussed.