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ABSTRACT:

Accelerating First-Principles Predictions of Thermodynamics and Diffusion in Complex Concentrated Alloys

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Finite-temperature, non-dilute diffusion coefficients of multicomponent alloys are important inputs for predicting kinetic properties and microstructure evolution. Computing vacancy-mediated diffusion coefficients from first principles requires estimating thermodynamic parameters, equilibrium vacancy concentrations, and Onsager transport coefficients of concentrated alloys at elevated temperatures. Obtaining these quantities from electronic structure calculations remains a significant challenge, particularly in alloys containing three or more elements, where the large number of local chemical environments makes accurate energy predictions difficult. This talk will outline how on-lattice cluster expansions, chemical embedding schemes, machine-learning techniques, and rigorous statistical mechanics can be combined to compute the parameters needed to estimate diffusion coefficients in complex concentrated alloys. The methodology will be applied to elucidate vacancy-mediated diffusion mechanisms on the BCC crystal structure in a prototypical multicomponent refractory alloy. These calculations will shed light on the roles of alloying chemistry, short-range order, and temperature in controlling diffusion in multicomponent alloys.