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## ABSTRACT:

### Hierarchical Generation of Transferable Interatomic Interactions Coupling Chemical and Thermal Degrees of Freedom in Multicomponent Alloys

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Modeling high-temperature diffusion in multicomponent alloys—e.g., using the kinetic Monte Carlo (kMC) method—requires accurate descriptions of interatomic interactions that capture both chemical and thermal degrees of freedom. Conventional brute-force parameterization based on cluster expansion often suffers from rapidly increasing complexity with the number of elements and limited transferability across compositions and alloy subsystems.

In this work, we introduce a hierarchical framework for generating transferable interatomic interactions in multicomponent alloys. Inspired by the CALPHAD-type thermodynamic modeling, interactions in higher-order systems are systematically constructed from well-characterized lower-order subsystems. This enables reuse of optimized interactions while preserving consistent thermodynamic and kinetic information from low- to high-order systems required for modeling multicomponent diffusion. We demonstrate the approach for the ternary Mo–Ta–W refractory alloy system across the full composition space, where ternary interactions are derived from the Mo–Ta, Mo–W, and Ta–W binary subsystems. Thermal effects beyond configurational contributions are incorporated by including vibrational free energies obtained from machine-learning interatomic potentials trained on DFT data.

Using this coupled chemical–thermal framework, we investigate the influence of thermal vibrations—particularly anharmonic effects—on phase stability, order–disorder transitions, and short-range order across different alloy compositions. The results highlight the importance of temperature-dependent vibrational contributions and demonstrate the capability of the proposed hierarchical approach to bridge ab initio information with large-scale kinetic modeling.