MACHINE LEARNING INTERATOMIC POTENTIALS FOR ATOMISTIC SIMULATION OF THERMODYNAMIC PROPERTIES AND PROCESSES IN COMPLEX MATERIALS

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Atomistic simulations play an important role in understanding thermodynamic properties and phase transformations in materials. Molecular dynamics simulations provide detailed insight into microscopic mechanisms of processes such as melting, crystallization, and nucleation. However, traditional atomistic modeling methods are limited by the trade-off between accuracy and computational cost. First-principles calculations based on density functional theory (DFT) provide high accuracy but are restricted to relatively small systems and short timescales. In recent years, machine learning interatomic potentials (MLIPs) have emerged as a powerful approach that bridges this gap [1,2]. In this framework, the potential energy surface of a system is approximated using flexible many-body functions, typically based on neural networks trained on datasets obtained from ab initio calculations. As a result, MLIP-based molecular dynamics simulations can achieve near-DFT accuracy while being orders of magnitude faster, enabling large-scale simulations of complex materials and thermodynamic processes. In this work we present recent results obtained using MLIP-based simulations for compositionally complex materials, including multicomponent metallic melts, high-entropy alloys, and refractory carbides. Particular attention is paid to atomistic modeling of thermodynamic processes such as crystallization and melting, as well as to the calculation of structural and transport properties of liquids. Finally, we discuss an emerging paradigm in the development of MLIPs based on foundation models [3]. These large universal potentials are pre-trained on extensive databases of first-principles calculations and demonstrate improved transferability across different compositions and thermodynamic conditions. Such models open new opportunities for predictive atomistic simulations of complex materials and their thermodynamic behavior.

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