An Automated Workflow for Thermodynamic Properties Prediction via Bayesian Free-Energy Reconstruction

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In this work, an automated tool for predicting thermodynamic properties of materials is developed. The framework reconstructs Helmholtz free-energy surfaces [1] from molecular dynamics simulations using Gaussian Process Regression [2] with zero-point energy corrections [3]. It accounts for statistical uncertainties, mitigates finite-size effects, and provides uncertainty-aware estimates of thermodynamic quantities. The framework is applicable to both solid and liquid phases within NVT and NPT ensembles. An active learning strategy is employed to adaptively select simulation points, reducing computational cost while preserving accuracy [4]. This enables systematic analysis of thermodynamic and mechanical properties, as well as melting behavior. The approach is tested on cubic structures using classical and machine-learned interatomic potentials [5].

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