Transfer learning for predicting the dynamics of complex atomic ensembles

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Multiscale modeling based on machine learning (ML) enables the exploration of broad regions of thermodynamic parameters. For multicomponent systems, calculations of transport properties or phase diagrams remain challenging. Creating training datasets for ML interatomic potentials (MLIPs) requires thousands of configurations, making the process inefficient. A solution is multi-stage transfer learning. First, accurate but slow graph neural networks, pre-trained on large quantum-chemical databases, are used. They are then fine-tuned on a small number of *ab initio* DFT configurations. Then, fast fully connected networks are developed, enabling calculations with millions of atoms. This approach reduces the volume of training data by an order of magnitude and allows adapting MLIPs to non-standard DFT. The methodology was applied to predict a phase diagram for the Ca–Fe–Ni ternary system over a wide pressure range (0–500 GPa), which is of interest to materials science and geophysics. Fine-tuning of the MLIP potential required 10,000 DFT configurations. The results are consistent with known data. Stable CaFeNi phases were predicted. The study demonstrates the effectiveness of transfer learning for accurate and resource-efficient modeling of complex atomic systems under extreme conditions [1].

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