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"Fast and Accurate Interatomic Potentials by Genetic Programming."

Abstract: In recent years there has been great progress in the use of machine learning algorithms to develop interatomic potential models. Machine-learned potential models are typically orders of magnitude faster than density functional theory but also orders of magnitude slower than physics-derived models such as the embedded atom method. We demonstrate that machine learning, in the form of genetic programming, can be used to develop accurate and transferable many-body potential models that are as fast as the embedded atom method, making them suitable to model materials on extreme time and length scales. The key to our approach is to explore a hypothesis space of models based on fundamental physical principles and to select models from this hypothesis space based on their accuracy, speed, and simplicity. We demonstrate our approach by developing fast and accurate interatomic potential models for copper that generalize well to properties they were not trained on. Our approach requires relatively small sets of training data, making it possible to generate training data using highly accurate methods at a reasonable computational cost.