Fine-tuning universal force fields for rapid and accurate lattice thermal conductivity

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Lattice thermal conductivity (κ_l) is a fundamental materials property that is vital for applications such thermoelectrics and power electronics. Over recent decades, predicting lattice thermal conductivity has primarily relied on classical molecular dynamics or first-principles calculations. However, these methods often suffer from insufficient accuracy or high computational costs. Recent advancements in universal machine learning models for materials offer a promising solution to these limitations. In this study, we conducted extensive calculations of κ_l using three universal models and compared their performance against ab initio calculations for 25 zincblende and wurtzite compounds. Our findings indicate that all off-the-shelf models consistently underpredict phonon frequencies and thermal conductivity. However, we demonstrate that this phonon softening can be effectively addressed by fine-tuning with small amounts of additional data. In particular, the fine-tuned MACE-MP-0 model displays remarkable accuracy while requiring several orders of magnitude less computational cost than first-principles calculations. Our approach has the potential to significantly accelerate the materials discovery process