On-the-fly Machine Learning Potential Accelerates Accurate Lattice Thermal Conductivity Prediction of the Pentagonal Structured Monolayer Materials

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In this study, we propose an innovative approach that combines the phonon Boltzmann transport equation (PBTE) with on-the-fly machine learning potential (FMLP) to accelerate the accurate prediction of lattice thermal conductivity of pentagon structured monolayer materials with composite two types of atoms. We overcome the traditional trade-off between accuracy and speed by integrating the precision of density functional theory (DFT) with the computational efficiency of empirical potentials. This way to hugely speed up these calculations is by using force fields and parametrizations of the potential energy. Our method is applied to predict the thermal conductivity of various penta-structured monolayers, revealing insights into their thermal transport properties. These findings have implications for designing advanced materials for thermoelectric applications and thermal management.

Keywords: Lattice thermal conductivity, monolayer material, pentagonal structures, machine learning