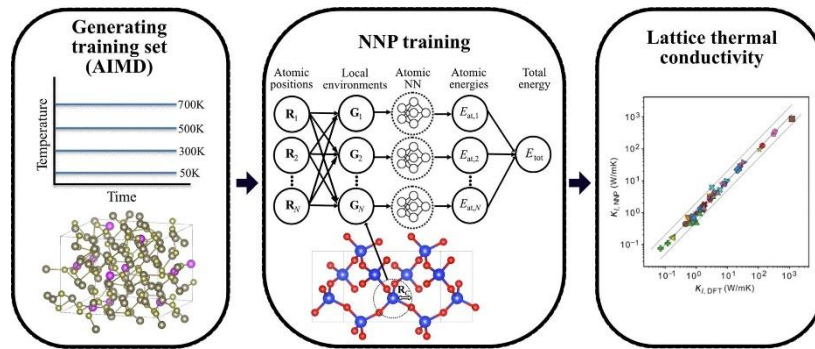# Accelerated computation of lattice thermal conductivity by NNP

With the development of the density functional theory (DFT) and ever-increasing computational capacity, an accurate prediction of lattice thermal conductivity (LTC) based on the Boltzmann transport theory becomes computationally feasible. However, steep computational costs in evaluating interatomic force constants limit the theoretical investigation of LTC to relatively simple crystals. Currently, machine learning potentials (MLPs) are garnering attention as an efficient surrogate model of DFT. However, the applicability of MLPs to a wide range of materials has yet to be demonstrated. Furthermore, establishing a standard training set that provides consistent accuracy and computational efficiencies across a variety of materials would be useful. Herein, we test a various methods of training set construction, and compute LTC of materials with diverse symmetries and a wide range of LTC using MLP. The current work will establish a robust framework for accurately computing LTC with MLPs. This work was published at Computational Materials Science 2022 **211**, 111472