Thermal and electronic properties of twisted bilayer ZnO

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Abstract

ZINC oxide (ZnO) based materials are the foremost metal oxides in technological utilization, with both monolayer and bilayer configurations experimentally verified. In this work, we developed interatomic potentials for studying the lattice thermal conductivity of monolayer and bilayer ZnO. We show that the structural parameters of the monolayer and bulk wurtzite can accurately be described by Stilinger-Weber (SW potential). Kolomogrov-Crespi potential is optimized for capturing the interlayer interaction of the bilayer system. We also show that the resulting potentials can be used to investigate structural relaxation in twisted bilayer ZnO. We studied the effect of twist angle on the thermal conductivity of the bilayer ZnO.

Figures

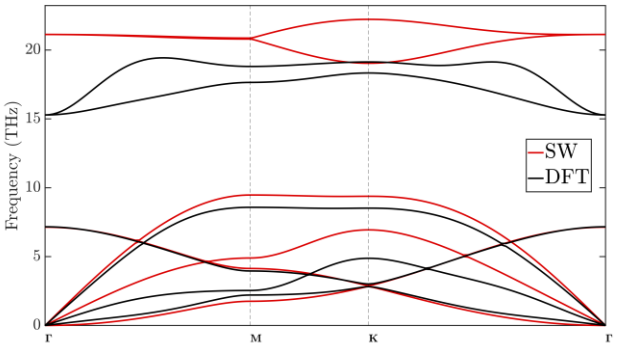

Figure 1: Phonon dispersion curves obtained using the DFT (black lines) and SW potential (red lines).