Computational Method for Bulk ZnO Thermal Conductivity

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It is generally shown that thermal conductivity of a ZnO bulk system is an important property of thermoelectric materials in transferring waste heat to electricity. In this work, we will study the computational method of calculating ZnO bulk system thermal conductivity using the Equilibrium Molecular Dynamics (or Green Kubo) simulation on MedeA and LAMMPS. The Green Kubo method and Non-equilibrium Molecular Dynamics (NEMD) method will be compared. The Green Kubo method with periodic systems is doing a better job with the zinc oxide system. We will also analyze the different factors affecting the accuracy of the thermal conductivity calculation. We have a result of ZnO bulk system at 300K that has a thermal conductivity of 123W/mK, which has proven to be reasonably close to the experimental data. With this method and code, we are able to do more calculations on the thermal conductivity of nanowire ZnO and doped ZnO bulk systems.