

Anisotropic Phonon Transport and Thermal Conductivity in Black Phosphorus

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Black phosphorus is a layered van der Waals material, which could have potential applications in electronics and optoelectronics due to its intriguing properties. In this work, we study the phonon transport and thermal conductivity in bulk black phosphorus using the state-of-art first-principles-based Boltzmann transport equation method. Large degree of anisotropy of its thermal conductivity is observed along three crystal axes. In contrary to the conventional wisdom that the anisotropy of the thermal conduction of an anisotropic material comes from the group velocity of phonons, we identify the important roles of direction-dependent phonon relaxation times. The anisotropy of phonon relaxation times comes from the different response of phonon population under the heat flux along different directions.