

Abstract Submitted
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Phonon-defect scattering and thermal transport in semiconductors: developing guiding principles¹ CARLOS POLANCO, LUCAS LINDSAY, Materials Theory Group, Oak Ridge National Laboratory — First principles calculations of thermal conductivity have shown remarkable agreement with measurements for high-quality crystals. Nevertheless, most materials contain defects that provide significant extrinsic resistance and lower the conductivity from that of a perfect sample. This effect is usually accounted for with simplified analytical models that neglect the atomistic details of the defect and the exact dynamical properties of the system, which limits prediction capabilities. Recently, a method based on Greens functions was developed to calculate the phonon-defect scattering rates from first principles. This method has shown the important role of point defects in determining thermal transport in diamond and boron arsenide, two competitors for the highest bulk thermal conductivity. Here, we study the role of point defects on other relatively high thermal conductivity semiconductors, e.g., BN, BeSe, SiC, GaN and Si. We compare their first principles defect-phonon scattering rates and effects on transport properties with those from simplified models and explore common principles that determine these. Efforts will focus on basic vibrational properties that vary from system to system, such as density of states, interatomic force constants and defect deformation.

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