Deformation potentials and simulations of thermoelectric properties using first principles: The case of Mg_3Sb_2

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We present a first-principles framework to derive the deformation potential from the electron-phonon coupling matrix elements, which can be further used to investigate the scattering and transport properties of thermoelectric materials within the Boltzmann transport equation. We have chosen the well-studied Si and GaAs as examples of non-polar and polar materials to benchmark our method. We compare the Wannier interpolated electron-phonon matrix elements with that obtained by direct calculation within density functional perturbation theory (DFPT). For the non-polar material, we consider the acoustic deformation potential (ADP) and optical deformation potential (ODP) for intravalley and intervalley transitions. For the polar material, we consider in addition the piezoelectric scattering and polar optical phonon scattering due to the long-range contributions. Then we applied this method to Mg_3Sb_2 to understand the ADP and ODP for holes and electrons, especially for the intervalley transitions in the conduction band. The presented framework can be readily applied to other non-polar and polar materials.