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Coupling of first-principles calculation and Boltzmann transport for accurate and computationally effective thermoelectric transport

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Abstract

Thermoelectricity is a promising approach to the reversible energy conversion, such as power generation and refrigeration. The thermoelectric (TE) efficiency is quantified by the dimensionless temperature-dependent figure of merit *ZT*. *ZT* values of TE materials are determined by the Seebeck coefficient, electrical conductivity, and thermal conductivity, which are correlated through band structure and carrier concentration. Here we present a method to compute the transport coefficients by coupling first-principles density-functional theory (DFT) band structure calculations with the Boltzmann transport equation (BTE) with energy/momentum/band dependent scattering rates. Based on DFT and density-functional perturbation theory (DFPT), we compute the electronic band structures, phonon dispersion relations, and electron-phonon matrix elements, which we use to extract deformation potentials. Then we use an advanced home-developed numerical simulator to which can consider the full energy and momentum dependencies of electron-phonon, ionized impurity, and alloy scattering to compute the electronic transport properties. This approach enables the full integration of DFT, DFPT, and BTE for the accurate and computationally effective first principles modelling of advanced thermoelectric materials. We demonstrate this method for simple Si and GaAs semiconductors, but also promising TE materials such as Mg_3Sb_2.