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Ab initio description of electron-phonon and phonon-phonon scattering processes in density functional theory for the calculation of charge and heat transports

The future sparsity of carbon-based fuels, the increasing energy cost, together with the growing concern of society over environmental problems, make the performance improvement of energy conversion devices –thermoelectricity, photovoltaics –a topic of high importance. Such devices are mainly designed by using macroscopic models -the drift-diffusion for electronic transport, or the Fourier formalism for heat/energy transport- which assume local equilibrium and simplified (averaged) material properties for the carrier relaxation times. Huge progress has however been achieved in the description of scattering processes with methods based on the density functional perturbation theory (DFPT). We will show that electron transport characteristics of bulk semiconductors are well described within the approach that couples DFPT electron-phonon scattering rates with the semi-classical Boltzmann transport equation (BTE), and the same is true for DFPT phonon-phonon scattering rates and BTE for phonon that yield the thermal conductivity, with bismuth as an example. We will also discuss the electron and phonon coupled equations for thermoelectricity –the so-called phonon-drag effect -as well as the effect of nano-structuring on the Seebeck coefficient.

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[1] P. Giannozzi et al., *Advanced capabilities for materials modelling with QUANTUM ESPRESSO.* J. Phys.: Condens. Matter, 29:465901, 2017.

[2] S. Ponce, E. R. Margine, C. Verdi, and F. Giustino. *EPW: Electron-phonon coupling, transport and superconducting properties using maximally localized Wannier functions.* Comp. Phys. Comm., 209:116, 2016.

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