First-principles method for electron-phonon coupling and electron mobility - DTU Orbit (11/08/2019)

First-principles method for electron-phonon coupling and electron mobility: Applications to two-dimensional materials

We present density functional theory calculations of the phonon-limited mobility in n-type monolayer graphene, silicene, and MoS2. The material properties, including the electron-phonon interaction, are calculated from first principles. We provide a detailed description of the normalized full-band relaxation time approximation for the linearized Boltzmann transport equation (BTE) that includes inelastic scattering processes. The bulk electron-phonon coupling is evaluated by a supercell method. The method employed is fully numerical and does therefore not require a semianalytic treatment of part of the problem and, importantly, it keeps the anisotropy information stored in the coupling as well as the band structure. In addition, we perform calculations of the low-field mobility and its dependence on carrier density and temperature to obtain a better understanding of transport in graphene, silicene, and monolayer MoS2. Unlike graphene, the carriers in silicene show strong interaction with the out-of-plane modes. We find that graphene has more than an order of magnitude higher mobility compared to silicene in the limit where the silicene out-of-plane interaction is reduced to zero (by substrate interaction, clamping, or similar). If the out-of-plane interaction is not actively reduced, the mobility of silicene will essentially be zero. For MoS2, we obtain several orders of magnitude lower mobilities compared to graphene in agreement with other recent theoretical results. The simulations illustrate the predictive capabilities of the newly implemented BTE solver applied in simulation tools based on first-principles and localized basis sets.

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