Nonadiabatic effects in graphene-based materials

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Abstract

Some of the most prominent features of quasi two dimensional (Q2D) materials issue from the electron-phonon coupling (EPC) and are easily tailored by strain and doping. Phonon mediated superconductivity is expected in a variety of Q2D materials, and because the superconducting transition temperature increases with increasing EPC, tailoring EPC provides a recipe for a more feasible realization of superconductors.
First-principles density functional theory (DFT) calculations of EPC properties of doped 2D systems, specifically graphene, graphane (hydrogenated graphene), molybdenum disulfide and arsenen will hereby be presented.
Doping equalizes energy scales of electron transitions and phonon frequencies, but using the adiabatic Born-Oppenheimer approximation, DFT assumes nuclear and electronic motion can be separated.
It will be shown that the mentioned approximation is not applicable on studied systems, since the adiabatically obtained phonon spectrum is at significant variance with the one containing nonadiabatic corrections. Nonadiabatic renormalization greatly modifies the EPC coupling strength.
The importance of including dynamical corrections is undisputable and care should be taken when neglecting nonadiabatic effects as they have a huge impact not only on the magnitude of EPC strength and the transition temperature, but also on the qualitative understanding of the system in question.