Electron-phonon interactions in graphene: going beyond the limitations of plane-wave density-functional theory for 2D materials

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Abstract: With The coupling of electrons to acoustic phonons in graphene includes the unscreened gauge field, screened deformation potential [1,2], and the coupling to out-of-plane phonons in certain cases. In the process of simulating those, we are faced with key limitations of plane-wave density-functional perturbation theory (DFPT) with local functionals in 2D materials. The first limitation is the treatment of electron correlations in the calculation of the zero-momentum limit of the gauge field, relevant for transport. The second one is the use of periodic boundary conditions, implying the presence of periodic images of the 2D system in the out-of-plane direction. The periodic images lead to anomalous screening of the deformation potential at small momentum. It also implies that the coupling to out-of-plane phonons is zero due to the reflection symmetry with respect to the graphene plane. This is not the case in most experimental setups where this symmetry is broken by the use of an external electric field to dope graphene. We develop novel approaches to surpass those limitations. To surpass the first limitation, we propose a method [2] to calculate the coupling to acoustic phonons within the GW approximation. We interpret the zero-momentum limit of in-plane acoustic phonons as a strain of the crystal unit cell and link electron-phonon coupling parameters to the strain-induced fields. This allows the extraction of the gauge field parameter from band structure calculations in strained graphene, which can be carried out within the GW approximation. This “static strain” method also gives access to the bare deformation potential. To surpass the second limitation, we eliminate the interactions between periodic images by truncating the long-range Coulomb interactions in the out-of-plane direction. This is first implemented for the linear response of the electronic density to an external potential [3]. This allows us to calculate the static dielectric function of graphene and deduce the screened deformation potential. The truncation is then implemented for the calculation of total energy, forces, phonons and electron-phonon interactions. This allows us to simulate 2D materials doped in a field-effect setup and explore the possibility of coupling to out-of-plane phonons. We expect those new methods to be useful for numerous applications of 2D materials beyond the case of graphene presented here.

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[2] T. Sohier, M. Calandra, C.-H. Park, N. Bonini, N. Marzari, and F. Mauri, Phys. Rev. B **90**, 125414 (2014).
[3] T. Sohier, M. Calandra, and F. Mauri, Phys. Rev. B **91**, 165428 (2015).