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GW Many-Body Perturbation Theory for Electron-Phonon Coupling Calculations[1]

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Within many-body perturbation theory (MBPT) and the GW approximation, we study the electron-phonon coupling (EPC) in carbon-based systems, taking as paradigmatic examples the fullerene molecule, graphene and diamond. It has been demonstrated by several groups that the strength of the electron-phonon coupling potential is in these cases significantly underestimated at the DFT-LDA level, while GW calculations offer an excellent agreement with experiments.[2] [3] [4] Similar results have been obtained for superconducting bismuthates and transition-metal chloronitrides.[5] However, the related computational costs of evaluating the EPC strength at the GW level are high and thus represent strong limitations to a widespread application. We therefore discuss the accuracy of two less demanding alternatives on the MBPT level, namely the static Coulomb-hole plus screened-exchange (COHSEX) approximation and further the constant screening approach. In the latter, variations of the screened Coulomb potential W upon small changes of the atomic positions along the vibrational eigenmodes are neglected. We show that this latter approximation is most reliable, whereas the static COHSEX ansatz leads to substantial errors.[6] These findings open the way for combining the present MBPT approach with efficient linear-response theories.

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