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Impact of the electron-electron correlation on phonon dispersion:Failure of LDA and GGA DFT functionals in graphene and graphite. MICHELE LAZZERI, IMPMC, Paris, France, CLAUDIO ATTACCALITE, ETSF, Universidad del Pais Vasco, Spain, LUDGER WIRTZ, IEMN, ISEN, Villeneuve d'Asq, France, ANGEL RUBIO, ETSF, Universidad del Pais Vasco, Spain, FRANCESCO MAURI, IMPMC, Paris, France — GW is nowadays the most accurate ab-initio method to determine electronic bands. So far GW has never been used to determine neither the electron-phonon coupling (EPC) nor phonon dispersions. We show that GW approach [1] can be used to compute the EPC and the phonon dispersion. In particular, in graphene and graphite, standard DFT (LDA and GGA) underestimates, by a factor of 2, the slope of the highest optical branch at the zone boundary (K) and the square of its EPC by almost 80%. On the contrary, GW reproduces the experimental phonon dispersion near K, the value of the EPC, and the electronic band dispersion, in agreement with phonon dispersions from inelastic x-ray scattering and Raman spectroscopy. Comparing these results with other computational methods, the B3LYP hybrid functional gives phonons close to GW but overestimates the EPC at K by about 30%. Within Hartree-Fock, the graphene structure displays an instability under a distortion following the A'1 phonon at K. [1] M. Lazzeri et al., Phys. Rev. B 78, 081406(R) (2008).

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