Substrate dependence of the Raman 2D line of graphene

Alejandro Molina-Sanchez and Ludger Wirtz

Laboratory for the Physics of Advanced Materials, University of Luxembourg, Luxembourg
alejandro@molina.uv.es

We present ab-initio calculations of phonons of graphene on hexagonal boron-nitride which is an example for an ideal flat insulating substrate with a minor presence of charge traps or corrugation.

The measured double-resonant Raman spectra display shifts of the G and 2D lines comparing, e.g., the spectrum of graphene on silicon dioxide with the spectra of suspended graphene [1] and of graphene on hexagonal boron nitride [2]. In this work, we investigate the influence of the dielectric screening by the substrate on the electron-phonon coupling between the highest-optical phonon branch and the \((\pi,\pi^*)\)-bands of graphene [3]. The calculation of the electron-phonon coupling elements is performed with the GW method, that gives an accurate description of the electronic structure and corrects the underestimation of the band gap given by the local density approximation (LDA). Moreover, GW properly includes the effect of screening by the environment.

This enables us to give an explanation for the substrate dependence of the Raman 2D peak position in terms of dielectric screening of the Coulomb interaction. Thus, the frequency of the 2D band will increase due to the presence of the substrate with respect to suspended graphene, which is in agreement with the available Raman spectra.
References

