Investigation of electron-phonon interaction in hydrogenated graphene through ab-initio calculations

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The role of electron-phonon interaction is an important issue to be addressed, since it can provide information regarding the ultimate intrinsic mobility limit (μ) of a material. Such an issue is even more relevant, when investigating electrical properties of a new material like hydrogenated graphene. Graphene hydrogenation has been demonstrated [1] to be a viable solution in order to induce an energy gap in graphene, which could path the way to its exploitation in digital electronic applications. However, due to its novelty, many questions still remains unanswered. Simulations based on a multi-scale approach have been recently performed [2], showing that, within the ballistic assumption, 50% and 100% hydrogenated graphene can represent a potential candidate for next-generation nanoscale devices. Such calculations however provide an upper limit for device performance, so that, in order to get a clear understanding of the real potential of such new material, it is of primary importance to take into account source of non-idealities like electron-phonon coupling.

In this work, we address electron-phonon interaction by means of DFT simulations, focusing on 50% and 100% hydrogenated graphene. The electron mobility, which provide a figure of merit of the material under investigation, is computed within the Deformation Potential Approximation, considering longitudinal acoustic phonons, and following the approach described in [3] to compute the deformation potential and the one in [4] to calculate mobility. All the simulations have been performed by means of the Quantum Espresso code [5].

In Fig. 1, we show the atoms position for the 50% and 100% hydrogenated graphene. In the case of 50% hydrogenation, we consider H atoms lying on the top of the pristine graphene, while in the 100% case, H atoms are placed on both sides.

In Figs. 2 and 3, the Phonon Density of States as well the phonon spectra for the 50% and 100% hydrogenated graphene are shown. In both cases, acoustic and optical modes are well separated, especially for the top highest optical branches, and Kohn anomalies are observed in the 100% case, as also shown in [6]. The sound velocity v_s can be extracted from the acoustic branches. In particular, we obtain v_s=1.7x10^4 m/s and v_s=1.63x10^4 m/s for the 100% and 50% case, respectively.

In Table I, we show the computed relative effective masses m^* in the conduction and in the valence band, both in the x and y direction. In the case of 100% hydrogenated graphene, both heavy and ligth holes are reported. As can be seen, the top and the bottom of the conduction band are isotropic, i.e. they show almost the same m^* in both directions.

The deformation potentials for the longitudinal acoustic phonons are also shown, as well as carrier mobilities. As can be seen, mobility in hydrogenated graphene is comparable to mobility expected in graphene (of the order of 10^5 cm^2/Vs as in [7]). Heavy holes in 100% hydrogenated graphene show instead the smallest mobility.

In conclusion, we have investigated electron-phonon interaction through ab-initio simulations, evaluating, for the first time, carrier mobility in hydrogenated graphene. Hydrogenated graphene could represent a viable option for future nanoelectronic devices, since, despite graphene, it presents a large energy gap, while retaining almost the same carrier mobility.

References

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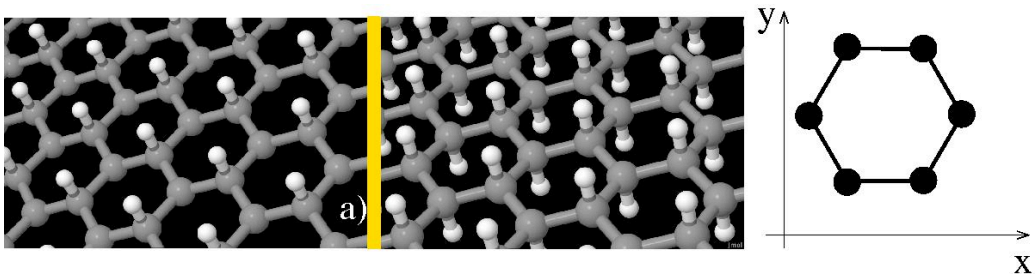

Fig.1: Atoms position in a) 50% and b) 100% hydrogenated graphene

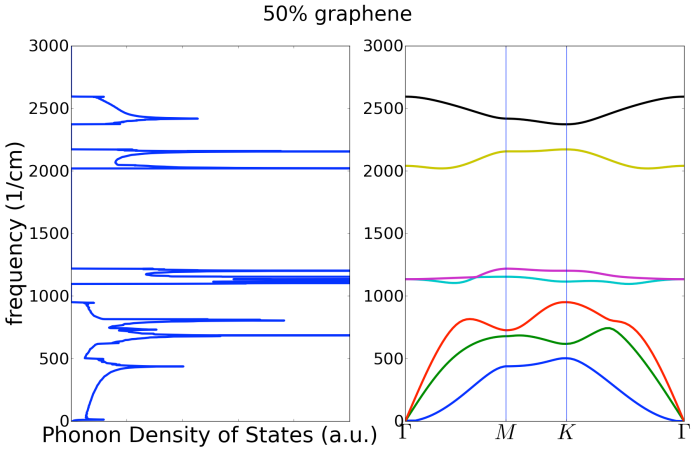

Fig.2: Phonon Density of States and phonon spectra for 50% hydrogenated graphene (spin up)

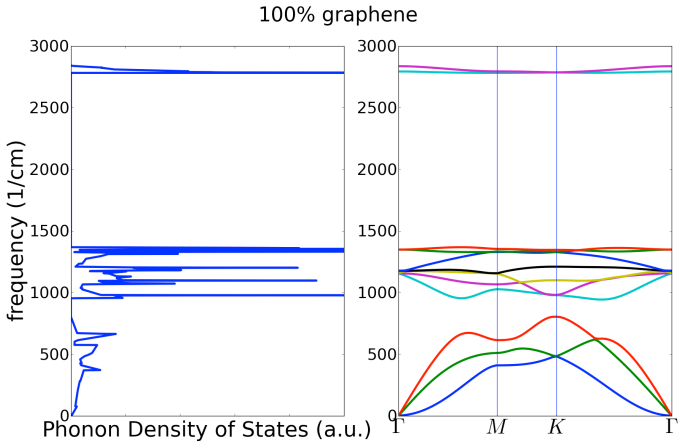

Fig.3: Phonon Density of States and phonon spectra for 100% hydrogenated graphene

Table I

%	m_{ex}^*	m_{ey}^*	m_{hhx}^*	m_{hhy}^*	m_{lhx}^*	m_{lhy}^*	D_{ace} (eV)	D_{achh} (eV)	D_{aclh} (eV)	μ_e (cm^2/Vs)	μ_{hh} (cm^2/Vs)	μ_{lh} (cm^2/Vs)
50	1.315	1.346	1.540	1.478	-	-	2	3.74	-	$1.62x10^5$	$1.189x10^5$	-
100	1.029	1.027	0.622	0.641	0.278	0.270	5.228	7.532	7.532	$1.09x10^5$	$5.18x10^4$	$2.833x10^5$

m_{ex}^* and m_{ey}^* are the relative effective masses of electrons along the *x* and *y* direction, respectively. m_{hhx}^*, m_{hhy}^*, m_{lhx}^* and m_{lhy}^*, are the heavy and light hole relative effective masses along the *x* and *y* direction. D_{ace}, D_{achh} and D_{aclh} are the deformation potential for the electrons and the heavy and light holes. μ_e, μ_{hh} and μ_{lh} are the mobility computed for electrons, and heavy and light holes.