Mobility gap and quantum transport in a functionalized graphene bilayer

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Abstract
In a Bernal graphene bilayer, carbon atoms belong to two inequivalent sublattices A and B, with atoms that are coupled to the other layer by $p_\sigma$ bonds belonging to sublattice A and the other atoms belonging to sublattice B. We analyze the density of states and the conductivity of Bernal graphene bilayers when atoms of sublattice A or B only are randomly functionalized. We find that for a selective functionalization on sublattice B only, a mobility gap of the order of 0.5 eV is formed close to the Dirac energy at concentration of adatoms $c \geq 10^{-2}$. In addition, at some other energies conductivity presents anomalous behaviors. We show that these properties are related to the bipartite structure of the graphene layer.

Keywords: graphene bilayer, quantum transport, electronic structure, functionalization

(Some figures may appear in colour only in the online journal)

1. Introduction

Electronic properties at nanoscale are the key to the novel applications of low-dimensional and nanomaterials in electronic and energy technologies. In particular, a lot of research has been devoted to understanding the remarkable electronic structure and transport properties of bilayer (or multilayers) of graphene [1–14]. Depending on the stacking, the charge carriers were shown, both theoretically [15–21] and experimentally [22–27], to behave like massless Dirac particles or massive particles with chirality. Electronic properties can be tuned by various means and in particular by electrostatic gate or by adding of static defects and functionalization by adatoms or admolecules of monolayer (MLG) [7, 13, 14, 28–42] and bilayer (BLG) [20, 21, 24, 26]. For example, one can open a band gap in this system by electrostatic gating [22, 23]. Recently such locally coupled structures have been also observed in chemical vapor deposition (CVD) graphene samples [26, 41] where, due to rippling, the layers were decoupled in some regions, while being connected in others. It has also been shown that UV irradiation, which results in water dissociative adsorption on graphene of few % of adsorbates, can induce a tunable reversible gap [42].

In this work, we investigate the density of states and the conductivity of a Bernal bilayer graphene (BLG) when the upper layer is functionalized by adatoms. There are two types of site on the upper layer, as shown in figure 1. Sites of sublattice A are above a carbon atom of the lower layer whereas sites of sublattice B are not. Therefore it is possible in principle to functionalize selectively atoms which belong to sublattice A or to sublattice B only. We consider here, that, within the functionalized sublattice, the repartition of the functionalized atoms is random. As a main result we find that, when only sublattice B is functionalized a mobility...
gap of the order of 0.5 eV is formed close to the Dirac energy at concentration of adatoms $c \geq 10^{-2}$. Furthermore for both sublattice functionalization the conductivity increases in some Fermi energy window, when the concentration of functionalized sites increases. This is because the functionalization is not just introducing scattering centers but deeply changes the electronic structure. As we show, the creation of the gap and the abnormal behavior of the conductivity are related to the bipartite nature of the monolayer and bilayer graphene.

2. Method

The BLG studied here consists of the bottom layer 1 and of the top layer 2 as shown in figure 1. The top layer 2 is functionalized whereas the bottom layer 1 keeps its perfect structure. There are four carbon atoms in the unit cell, two carbons $A_1, B_1$ in layer 1 and $A_2, B_2$ in layer 2 where $A_2$ lies on the top of $A_1$. We use an electronic model where only $p_z$ orbitals are taken into account, since we are interested in the low energy physics i.e. electronic states close to the Dirac energy. The adsorbates which create a covalent bond with a carbon atom of the graphene upper layer is represented by removing the $p_z$ orbitals of the functionalized carbon atoms [7, 31, 43–46]. The missing $p_z$ orbitals are distributed randomly only on sites of the top layer 2 in the sublattice A or B. The tight-binding (TB) Hamiltonian for $p_z$ orbitals has the form:

$$\hat{H} = \sum_{\langle i,j \rangle} t_{ij} \left( c_i^\dagger c_j + c_i^\dagger c_j^\dagger \right)$$

where $c_i^\dagger$ and $c_i$ create and annihilate respectively an electron on site $i$, $\langle i,j \rangle$ is the sum on index $i$ and $j$ with $i \neq j$, and $t_{ij}$ is the hopping matrix element between two $p_z$ orbitals $i$ and $j$. We analyze the average local density of states (LDOS) on the sublattices A or B of each plane, and the conductivity as a function of the position of the Fermi energy. Densities of states are computed by recursion (Lanczos algorithm) [47] in real-space on sample containing a few $10^7$ carbon atoms with periodic boundary conditions. Within the Kubo-Greenwood formalism we compute the microscopic conductivity $\sigma_m(E)$ [37] using the real-space method developed by Mayou, Khanna, Roche and Triozon [48–52] (see supplementary material section 4 (stacks.iop.org/JPhysCM/30/195701/mmedia)). $\sigma_m$ is the semi-classical conductivity that does not take into account the quantum corrections due to multiple scattering effects. Typically this quantity represents a room temperature conductivity when multiple scattering effects are destroyed by dephasing due to the electron–phonon scattering.

3. Results

We present first calculations performed with the standard nearest neighbor hopping Hamiltonian (TB1): $t_0 = 2.7$ eV for intra-layer hopping between A and B atoms, and $t_1 = 0.34$ eV for nearest neighbor inter-layer hopping between $A_1$ and $A_2$ atoms. The advantage of this simple Hamiltonian TB1 is to allow a detailed physical discussion of the physical mechanism involved. These results are confirmed by analyzing a more realistic Hamiltonian description that takes into account hopping beyond the nearest neighbor hopping model (TB2) (supplementary material, section 1). TB2 has been used successfully to study the electronic structure in rotated bilayer of graphene [17–19] in good agreement with STM density of states measurements [53, 54] and for transport calculations [21, 35, 37, 38].

3.1. Results with nearest-neighbor hopping Hamiltonian (TB1)

The total density of states for both layers (TDOS), $n(E)$, are shown figures 2(a.1) and (b.1) respectively for A and B vacant atoms in layer 2. As explained in the following and in supplementary material (section 2), each missing orbital in the A2 sublattice (resp. B2 sublattice) of the top layer 2 produces one midgap states at Dirac energy $E_D = 0$ that spreads on $\{A_1, B_2\}$ sublattices (resp. $\{A_2, B_1\}$). This is similar to the case of a monolayer of graphene where vacancies in sublattice A (resp. B) produce midgap states at Dirac energies $E_D = 0$ that are located in sublattice B (resp. A) [44, 55]. In figures 2(a.1), (b.1) and (c) the midgap states at $E_D = 0$ are not included in plotted DOSs and in the calculation of the conductivity (supplementary material sections 2 and 4). Vacancies on the A2 sublattice do not produce a gap in the TDOS, whereas B2 vacancies induce a quasi-gap clearly seen around $E_D = 0$. Its width, $\Delta E_g = 2E_0$, increases when $c$ increases and saturates at a value $2t_0$. In B2 vacancies case, unphysical small oscillations appeared in the total DOS and local DOSs. Those oscillations are numerical artifacts related to the termination of the continuous fraction expansion of the Green function used in the recursion method (see supplementary material sections 2 and 3, and [47]). The presence of these unphysical oscillations in the case of B2 vacancies whereas there is no oscillations in the cases of A1 vacancies, confirms the emergence of a gap by B2 vacancies.

The conductivity $\sigma_m(E)$, is shown figures 2(a.2) and (b.2) for $A_2$ vacant atoms and $B_2$ vacant atoms, respectively. In both cases, the conductivity at large energies $|E| \gg 1$ eV is inversely proportional to the concentration $c$ of vacancies. This is expected from the Boltzmann theory if the vacancies are seen only as scattering centers which give a finite lifetime to the eigenstates of the perfect Bernal bilayer. For smaller energies, corresponding to usual $E_F$ values, the variation of the conductivity with the concentration $c$ of vacancies is not

![Figure 1. Bilayer structure with sublattice $\alpha = \{A_1, B_2\}$ (square), and sublattice $\beta = \{A_2, B_1\}$ (circle).](image-url)
consistent with Boltzmann theory. Indeed, with vacancies on A2 sublattice, for small $E$ values, $\sigma(E)$ increases strongly when $c$ increases. With vacancies on B2 sublattice, for energies above the quasi-gap, i.e. $E > E_b$, if $c < c_l \simeq 1.5\%$, $\sigma(E)$ decreases when $c$ increases (as expected in Boltzmann theory); whereas for $c > c_l$, $\sigma(E)$ increases when $c$ increases.

All these spectacular results show that the effect of selective functionalization is not just to induce scattering for the states of the perfect bilayer. This is also confirmed by analyzing the selective functionalization of a sublattice of the MLG. As shown in figure 2(c), it leads to the creation of a quasi-gap which width increases with concentration of adatoms. Let us recall that for a monolayer and bilayer with vacancies that are randomly distributed on the two sublattices A and B ([21, 37, 46, 56] and Refs. there in) the low energy DOS presents a peak which is reminiscent of the midgap states but has a finite width.

3.2. Results with Hamiltonian including hopping beyond nearest neighbor (TB2)

Now we present results calculated using TB2 model, including hopping beyond nearest neighbors, in place of TB1 model (supplementary material (section 1)). The TDOS, $n(E)$, the average LDOS, $n_i(E)$ with $i = A_1, A_2, B_1, B_2$, and the conductivity, $\sigma_m(E)$, are shown in figure 3 for A2 vacant atoms and B2 vacant atoms. In both cases the midgap states, produced by missing orbitals are displaced to negative energy by the effect of the hopping beyond nearest neighbors (TB2) as in MLG [35, 38, 44] and BLG with vacancies randomly distributed [21]. In addition these states appear in an energy window of a fraction of an eV that depends on the concentration of functionalized sites. It is interesting to note that the peak of vacancy states is split into a double peak when we increase the

![Figure 2. Electronic density of states and conductivity computed from TB1 in BLG: with (a.1) and (a.2) A2 vacant atoms, and with (b.1) and (b.2) B2 vacant atoms: (a.1) and (b.1) total DOS $n(E)$ (dashed lines TDOS without vacancy); (a.2) and (b.2) microscopic conductivity $\sigma_m(E)$. $c$ is the concentration of vacancies with respect to the total number of atom in BLG. (c) TDOS of MLG with A vacant atoms and (d) the corresponding $E_m^{\sigma}$ value versus the concentration $c_m$ of vacancies with respect to the total number of atom in MLG. As explained in the supplementary material (sections 2 and 4), theses plots do not include the midgap states at $E_D = 0$. Spectrum is symmetric with respect to Dirac energy $E_D = 0$.](image-url)
concentration of vacancies. That splitting indicates a coupling between vacancy states that are all located on the same sublattice. The symmetry of the electronic properties with respect to $E_B = 0$ of TB1 model is broken; but, qualitatively, the anomalous conductivity found in the case of TB1 model is still found with TB2 model. The main difference between TB1 and TB2 is in the energy window where the midgap states appear.

With $A_2$ vacant atoms, the average LDOS (figure 3(a.2)) shows that midgap states is located on $B_2$ orbitals of the same layer, as expected from the uncompensated theorem with TB1. For $c \geq c_1 \simeq 1\%$, $\sigma_M(E)$ increases strongly when $c$ increases (figure 3(a.3)). This increase is maximum (several order of magnitude) for energies close to $-0.6$ and $0.3$ eV, and it is smaller for energies corresponding to the midgap peak.

With $B_2$ vacant atoms, the average LDOS (figure 3(b.2)) shows that midgap states is located on $A_2$ orbitals (layer 2) and on $B_1$ orbitals (layer 1), as expected from a bipartite Hamiltonian analysis with TB1 [57]. The quasi-gap is found for $0 < E \leq E_m$, instead of $-E_b < E \leq E_b$ with TB1, since for negative energies midgap states are present in the case of TB2. $\sigma_M$ is very small for $E$ corresponding to midgap states, and these energys correspond at a mobility quasi-gap (figure 3(b.3)). As a result, similarly to TB1 model, a mobility quasi-gap is found for $-E_b < E \leq E_b$ with TB2 too. Moreover for $c \leq c_1 \simeq 1-1.5\%$ and for $E > E_m$, $\sigma(E)$ increases strongly when $c$ increases (as with TB1).

4. Discussion: interpretation of the results by bipartite lattice

We analyze now the origin for the formation of the gap in the MLG with selective functionalization on sublattices A (or B) and then show how it leads to the properties of the BLG. Quite generally an eigenstate with energy $E$ of the MLG with or without vacancies, can be written as $|\varphi\rangle = |\varphi_A\rangle + |\varphi_B\rangle$, with states $|\varphi_A\rangle$ ($|\varphi_B\rangle$) belonging to the sublattice $A$ ($B$). It is easy to show that $|\varphi_A\rangle$ and $|\varphi_B\rangle$ are eigenstates of the effective Hamiltonian $\hat{H} = \hat{H}_0^2$ with eigenvalue $E = \varepsilon_m$. $\hat{H}$ acts only within the sublattices $A$ and $B$ and does not couple them.

For example for the perfect MLG, $\hat{H}$ is the Hamiltonian of a triangular lattice of A atoms (B atoms),

$$\hat{H}_A = \sum_i \tilde{\varepsilon}_A c^\dagger_A c_A + \sum_{(i,j)} \tilde{\varepsilon}_0 c^\dagger_A c_B + \text{h.c.},$$

(2)

where $c^\dagger_A$ and $c_A$ creates and annihilates respectively a state of an electron $A$, and with $\tilde{\varepsilon}_A = 3\tilde{\varepsilon}_0$ and $\tilde{\varepsilon}_0 = \tilde{\varepsilon}_A$. The middle of $\hat{H}$ band ($E = 0$) corresponds to the lowest energy of $\hat{H}$ band ($E = \varepsilon_m^2 = 0$).

The effect of vacancies on the DOS away from zero energy can be understood by considering the effective Hamiltonian of the sublattice $A$ that contains the vacancies. This Hamiltonian has the form given in equation (2) but with functionalized sites that are simply deleted. Without vacancies the coordination $\eta$ of each atom of A sublattice is 6 (average number of A–A nearest neighbors of A sublattice). With a small concentration $c_m$ of vacancies in A sublattice, the average coordination is $\eta \equiv 6(1 - c_m[\%]/100)$. The center of the A band is fixed by on-site energies, $\tilde{\varepsilon}_A$, and it is not affected by vacancies; but the width of the band will decrease when $\eta$ decreases (i.e. when $c_m$ increases). As expected from this simple tight-binding argument, the minimum values, $E_m = E_m^0$, of the spectrum of $\hat{H}$, found numerically (figure 2(d)), is almost proportional to the concentration $c_m$ of vacancies. Consequently the average A DOS, $\tilde{\sigma}_A$, has a gap induced by vacancies for $0 \leq E \leq E_m^0$. This means that DOS in the A and B sublattices of MLG also presents a gap for $-E_m \leq E \leq E_m$ (figure 2(c)). Moreover, each vacancy in sublattice A also induces a zero energy midgap states in sublattice B. Note that similar results are obtained on a square lattice which is also a bipartite lattice (supplementary material, section 3).

Let us consider now the case of the bilayer with vacancies on the $A_2$ sublattice. In this case the midgap states of the top layer 2 are located only on sublattice $B_2$ and are not coupled to the lower layer 1. Therefore layer 1 is just coupled to a semi-conductor (top layer 2) with a gap in the energy range $-E_m \leq E \leq E_m$. The results shown above mean that $t_1$ is sufficiently small that the mixing between states of layer 1 and 2 is small. Therefore layer 1 has essentially the electronic structure of an isolated MLG without defects. This explains why the TDOS is similar to that of a graphene layer. In addition when the vacancies concentration increases, $E_m$ increases and the decoupling between the two layers is more efficient. Therefore at a given energy the lifetime of states in the lower layer 1 increases and the conductivity increases when concentration increases. Transport in the bilayer at these energies $-E_m \leq E \leq E_m$ is mainly through the lower layer 1.

The case of vacancies on the $B_2$ sublattice is slightly more complex. Again at energies $E$ such that $-E_m \leq E \leq E_m$ the mixing between states of layer 1 and states in the continuum of layer 2 is small. However in that case the midgap states of layer 2 are located on sublattice $A_2$ and are coupled to the sublattice $A_1$ of the lower layer 1. The effect of the interlayer coupling alone is to couple midgap states of $A_2$ with specific linear combinations of states of $A_1$ and to produce bonding and anti-bonding states at energies $t_1$ and $-t_1$. We consider now the case where the concentration of adatoms is sufficient to have $E_m \geq t_1$. Therefore at energies $E$ such that $-t_1 \leq E \leq t_1$ these specific states in sublattice $A_1$ appear as decoupled from the other states of layer 1. They act thus as vacancies in the MLG (layer 1) and this produces a quasi-gap with midgap states in sublattice $B$ of layer 1. For that reason, a quasi-gap exists in both layers in the energy range $-t_1 \leq E \leq t_1$ and it is seen in the TDOS. Similarly to the previous case, increasing the concentration can also increase the conductivity for energies $E$ such that $t_1 \leq |E| \leq E_m$.

These analyses of the effect of selective functionalization are confirmed by detailed studies of the bipartite Hamiltonian of BLG [57].
5. Conclusion

We have analyzed the density of states and the conductivity of graphene Bernal bilayer (BLG) when the upper layer is functionalized by adatoms. Since there are two inequivalent sublattices A and B, that correspond to carbon atoms that are more or less coupled to the lower layer, we study the effect of a selective functionalization of sublattices A or B. As we show...
this selective functionalization leads to the creation of a gap when sublattice B of the upper layer is randomly functionalized with a concentration of adatoms $c \gg 10^{-2}$. This gap is a fraction of one eV for the DOS and of at least 0.5 eV for the mobility. This phenomenon is intimately related to the bipartite structure of the graphene lattice and the maximum width of the gap is of the order of the interlayer coupling energy. Other functionalizations of sites are possible if both layers can be functionalized. In this case also we find that electronic structure and transport properties can be deeply modified by a selective functionalization [57]. We believe that the phenomenon due to selective functionalization could be observed in carefully prepared graphene bilayers or even in other 2D materials.

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