Ab-initio study of the electric field effects produced by nitrogen and boron dopants on the transport and electronic properties of the bilayer graphene

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Abstract
Graphene, with its extraordinary electronic properties, has all the features to be a potential candidate for the future nanotechnology. Thanks to its peculiar band structure with linear dispersion near the Fermi level, graphene charge carriers behave like massless Dirac particles allowing ballistic transport properties [1]. However the absence of an energy gap restricts its application in nanoelectronics. Also bilayer graphene has no band gap between its conduction and valence bands, but in this case the gap opening can be externally tuned through an electric field effect [2]. A similar or even enhanced result can be obtained by properly doping the two graphene sheets.
In this context, our work focuses on the theoretical study of a bilayer graphene in which one layer is doped with nitrogen (N) atoms, while the other is doped with boron (B) atoms. Our approach relies on the density functional theory (Kohn-Sham equations on localized basis set of atomic orbitals) coupled with the non-equilibrium Green's function technique and the Büttiker-Landauer transport formalism [3]. The structural, electronic, and transport properties have been worked out for different densities of dopants and various geometries. First of all, we verified an energy gap opening for almost all the structures considered, comparable to that generally obtainable in the pristine bilayer graphene. Moreover, the band structure of each layer undergoes an energy shift: because of the required alignment of Fermi levels, the N-doped layer electronic states shift down, while the B-doped ones shift in the opposite direction. Such an effect, also present in the electric field biased bilayer but with a minor extent, should give rise to a very different conducting behaviour of the two layers. A further contribution to this global effect comes from the strong internal electric field due to the charge transfer from N to B dopants, being B less electronegative. This asymmetry between the two layers produces some energy intervals in which the states are localized on one sheet only.
To study the electronic transport, the doped bilayer has been contacted with graphene electrodes (see Fig. 1). One effect is a small reduction of the transmission probability due to the presence of scattering centers, i.e. the dopant atoms. More in detail, each N-B pair creates local electronic states which produce a double effect: while on one side such states do not contribute significantly to the transport and also perturb the near carbon states reducing their propagation, on the other side the N-B interaction allows the electrons to transfer themselves between the two layers, opening a new channel for the intra-layer electron transport. This transfer takes place through a N-B molecular orbital or thanks to an easier tunneling due to a reduction of the potential barrier between the layers. The electronic current, which can be directly compared with experimental measurements, has been obtained via energy integration of the transmission probability in the presence of an applied bias. In the ballistic regime, typical of these graphene-based nanosystems, the voltage-current characteristic, reported in Fig. 2, shows a weak increasing for low voltages and tends to a linear quasi-ohmic behavior for higher voltages. All the above mentioned aspects concur to the peculiar features of a particular junction constituted by two graphene electrodes, one contacted to the B-doped layer and the other to the N-doped one (see Fig. 3). This nanojunction breaks the symmetry between the two leads, setting a preferential direction to the current. Consequently, the electric current takes up a diode-like dependence on the applied voltage. Indeed, the internal electric field facilitates the transport from N-doped layer to the B-doped one, while it hampers it in the opposite direction (see Fig. 4).
These results are very promising in order to use such systems as constituents for electronic devices. The demonstrated possibility of engineering the doped graphene-based systems [4] allows us to nourish hopes for their future applications in nanoelectronics and optoelectronics fields.

References
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Figures

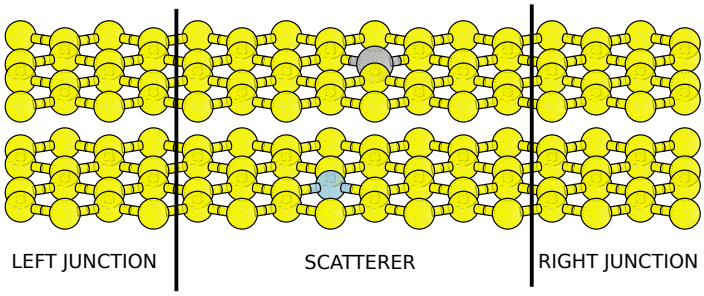

Figure 1 Geometry of the BN doped junction. The upper layer contains the nitrogen atom while the lower layer contains the boron one.

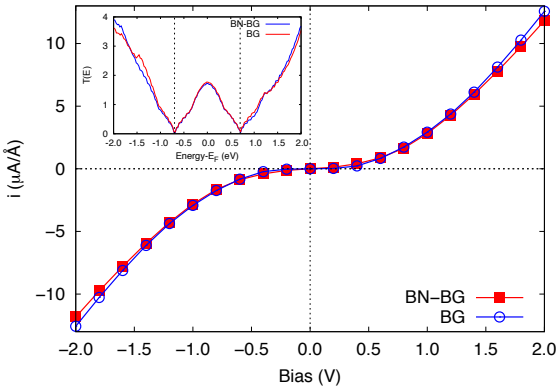

Figura 2 I-V characteristic of the system reported in Fig. 1. The inset reports the transmission probability at ΔV=-1.4 V.

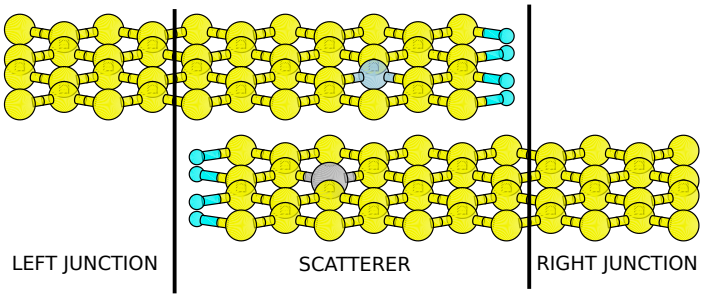

Figure 3 Geometry of the n-p BN doped nanojunction. The upper layer contains the nitrogen atom while the lower layer contains the boron one.

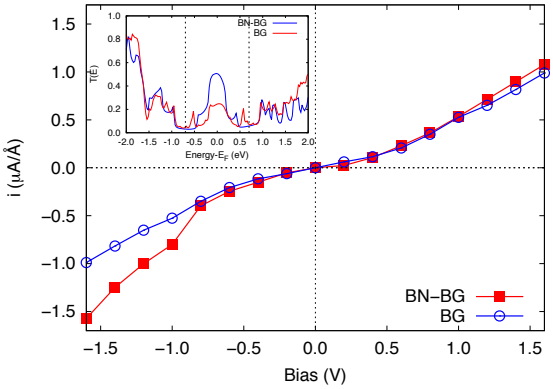

Figura 4 I-V characteristic of the system reported in Fig. 3. The inset reports the transmission probability at ΔV=-1.4 V.