Transport properties of armchair graphene nanoribbon junctions between graphene electrode

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Abstract

In this paper [1], we present a first-principles study, by means of the non-equilibrium Green's functions (NEGF) technique, of the electronic properties of systems consisting of two semi-infinite graphene layers interconnected by a hydrogen-passivated armchair graphene nanoribbon (aGNR), see Fig. 1.

Very simple prototypes of these carbon-based molecular junctions have been investigated in order to characterize their transport properties. These systems present typical metal–semiconductor–metal behavior due to the electronic gap of the ribbons which depends on the their width. The electronic properties of the isolated subsystems, i.e. graphene electrodes and the nanoribbon, together with their interaction in contact regions determine the transport properties of the junction. For what concerns the coupling between the subsystems, this is very efficient and the contacts do not create an appreciable barrier for transport due to the same chemical species constituting the subsystems. Hence the transport properties are mainly determined by the shape (width and length) of the finite ribbon included in between the graphene leads. Larger molecules furnish more channels for convoying the electrons then the smaller ones and consequently the conductance is generally higher. In the energy gap region the transport occurs via electron tunneling between the electrodes and the efficiency decays simply with the linker length.

As an example, in Fig. 2 it is reported the density of states (DOS) in the EM region and the projected density of states (PDOS) on the ribbon region for the “4 lines-long/3 lines-large” aGNR (4L 3-aGNR), in comparison with the transmission function. The signature of the molecular energy levels is clear both in the DOS and PDOS, and the transmission function has higher intensity in correspondence to those peaks.

The effect of the applied bias on a longer ribbon, i.e. 8L 3-aGNR, is shown in Fig. 3 for different voltages up to 1.0 V. For any given bias voltage, the chemical potentials of the two leads are well recognizable, as they correspond to the left and right Dirac points where the DOS tends to zero. Within the bias window, the intensity of the transmission function increases with the bias. The two small peaks near the Dirac points of the two electrodes are assigned to the edge states appearing at the two zigzag electrodes [2]. At a small applied bias, the probability for an electron lying in an edge state to be transferred to the opposite lead is very small since the DOS at that energy is negligible. However, at finite bias, we can find distinct features in the transmission curves related to the presence of edge states.

Some additional representative configurations has been considered explicitly: for the thinnest ribbon, a torqued geometry has been studied to evaluate the effects of the misalignment of the π orbitals on different phenyl rings. The changes in transmission through HOMO and LUMO orbitals are noteworthy, while for energy levels farther from E_F they are negligible. Finally, graphene edges with different passivations and reconstructions have been considered and they do not significantly influence the calculated transport properties. In spite of the simple model adopted, the results on the electronic transport provide some parameters to control and engineer future carbon-based electronic devices [3].

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References

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Figures

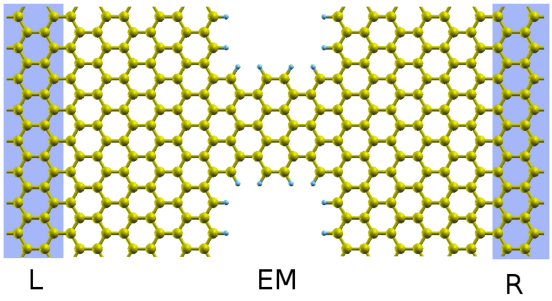

Fig. 1: System setup for a graphene nanoribbon junction (4L 7-aGNR). The left and right electrodes and the extended-molecule region are highlighted.

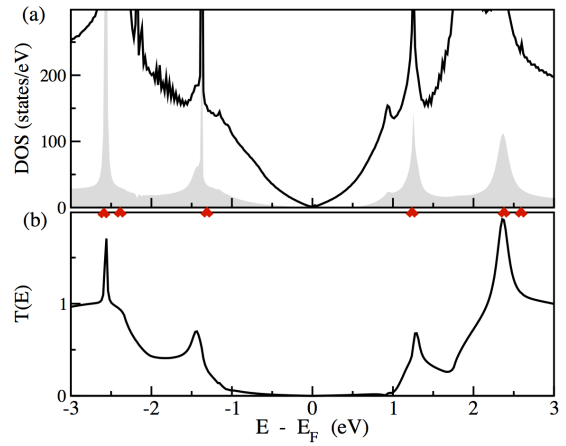

Fig. 2: Electronic and transport properties of 4L 3-aGNR. Upper panel (a): DOS (solid line) of the junction and PDOS (shaded grey area) on the ribbon region. Triangles represent the eigenstates of the isolated (unconnected and hydrogenated) 4L 3-aGNR linker. Lower panel (b): transmission function.

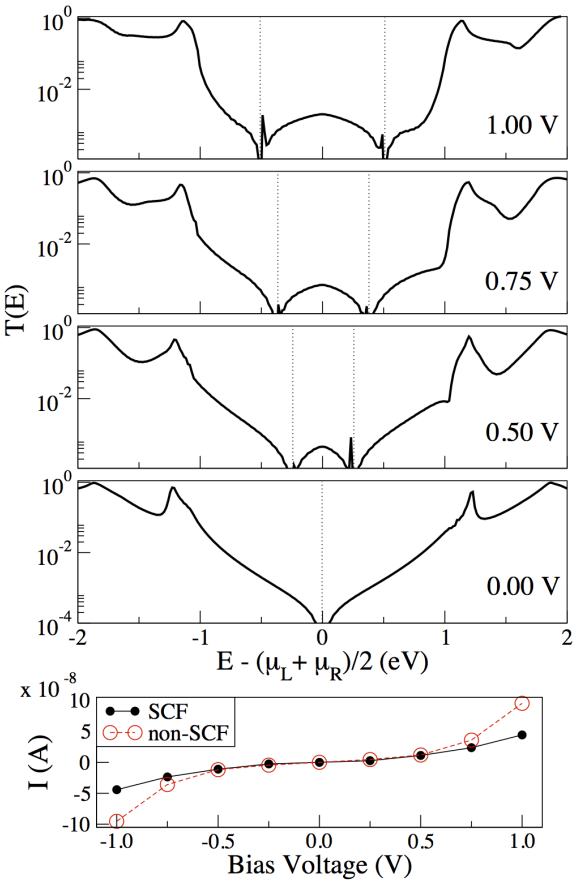

Fig. 3: Upper panels: transmission function of 8L 3-aGNR junction for four selected values of the bias voltage, as indicated in labels. The bias window is delimited by two vertical lines. Lower panel: current-voltage characteristics of 8L 3-aGNR junction.