

Conductance of Armchair GNRs with side-attached organic molecules

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Abstract

In this work we show a theoretical study of the transport properties of armchair graphene nanoribbon at which linear poly-aromatic hydrocarbon molecules (LPHC) are side-attached on the ribbon edge. We describe the system by a tight-binding model and calculate the local density of states and the conductance within the Green's function formalism. We found that the conductance curves reflect the energy spectra of the attached molecules, suggesting that AGNRs could be used as a spectrograph device.

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The fabrication under controlled experimental conditions of graphene nanoribbons (GNRs) has attracted a lot of scientific interest in the last years. Recently, experimental works have been reported, all related with possible applications of GNRs as a gas sensors and nanoelectronic devices [1,2]. From the theoretical point of view, distinct designs of GNRs are proposed to highlights their peculiar transport properties [3].

In this work we present a study on transport properties of armchair nanoribbons (AGNRs) at which linear chains of hexagons are pinned at the ribbon edge. These structures could describe the presence of benzene-based molecules attached on the ribbon edge, Fig. 1. We considered a semi-metallic $N = 5$ AGNR and two configurations of attached molecules: (i) a finite number of linear poly-aromatic hydrocarbon molecule (LPHC) of the same length L equally spaced into the ribbon edge and (ii) two LPHC of different length L , separated by a distance d (in units of the AGNR primitive-cell length). The LDOS of the systems reflects the attached-molecules energy spectra, whereas the conductance presents a series of dips at defined energy levels. These evolve as a function of the molecule lengths L and also with the number M of attached molecules. These dips emerge in a system where discrete states coexist

with the energy continuum, and they are known as Fano antiresonances (FARs) [4].

We adopt a single π -band nearest-neighbor tight-binding Hamiltonian (with $\gamma = 2.75$ eV). The LDOS and the conductance of the systems are obtained within the Green's function formalism based on real-space renormalization techniques. The system is partitioned into three parts: the central conductor (the AGNR and attached molecules) and two leads (two semi-infinite pristine AGNRs). The conductance is calculated using the Landauer formula (for more details see Ref. [3]). The energies are written in terms of γ and the Fermi level is taken as the zero of the energies.

Results of the conductance (upper panel) and the LDOS (down panel) for a $N = 5$ AGNR with a finite number of octacene ($L = 8$ LPHC) are shown in Fig. 2. The number

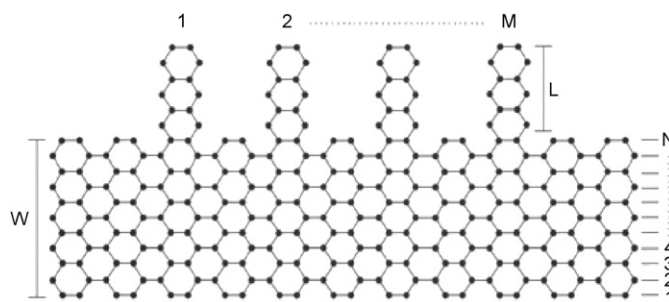


Fig. 1. Schematic view of the considered system.

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of attached molecules is taken from $M = 1$ to 5. For comparison we include the LDOS of a pristine $N = 5$ AGNR (black dash online). The LDOS curves show the

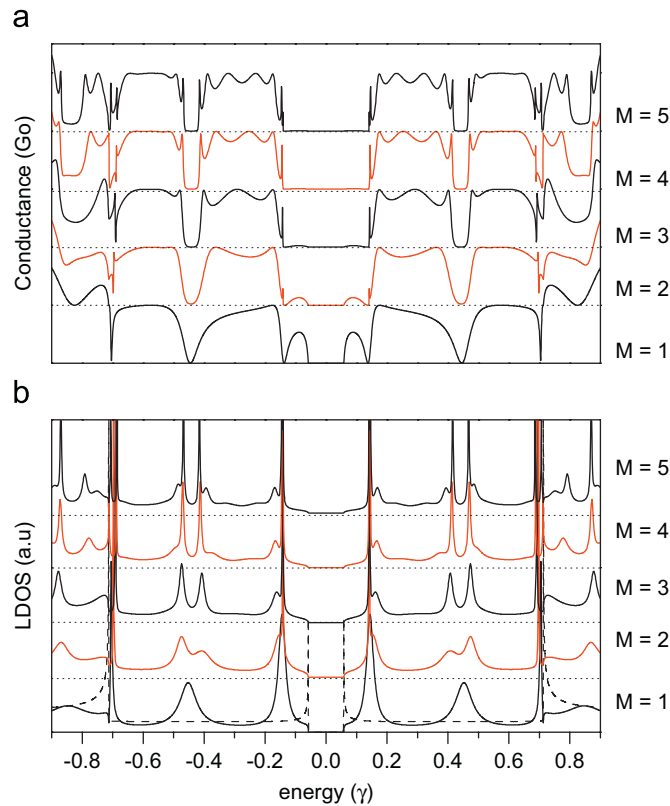


Fig. 2. (a) Conductance and (b) LDOS for a $N = 5$ AGNR with M octacene molecules.

evolution of the molecular states as a function of M . For instance, for $M = 1$ the smooth and wide states around $\pm 0.47\gamma$, become two sharp states for $M = 5$, emerging a forbidden mini-band centered at the levels of the isolated molecule. The same behavior is obtained for higher and lower energies, Fig. 2b. These mini-bands are clearly reflected in the conductance of the system. A series of well defined energy regions in which the conductance is completely suppressed, is shown in Fig. 2a. This effect arises from the quasi-periodic structure formed by the attached molecules at the ribbon. A similar effect was found before in quantum wires with a finite number of side-attached nanowires [5].

In what follow, we consider the $N = 5$ AGNR at which two molecules of different length L (a tetracene and an octacene) are pinned at the ribbon. We consider molecules separated by a distance: (a) $d = 1$, and (b) $d = 10$. The conductance of this system is shown in Fig. 3a and b (black solid online). The conductance for a system of two tetracenes (blue dot online) and one of two octacenes (dash red online) is included for comparison. In both cases, the conductance shows FARs at the same defined energies, independent of the relative distance of the attached molecules. Furthermore, the energy position of the FARs match perfectly with those corresponding to each individual molecule. This result suggests that AGNRs could detect different molecules simultaneously.

In summary, we have described the transport properties of AGNR with benzene-based molecules attached on the ribbon. The AGNRs conductance reflects the molecule energy spectra. Based on these results, it could be proposed a detailed study of systems considering a large number of

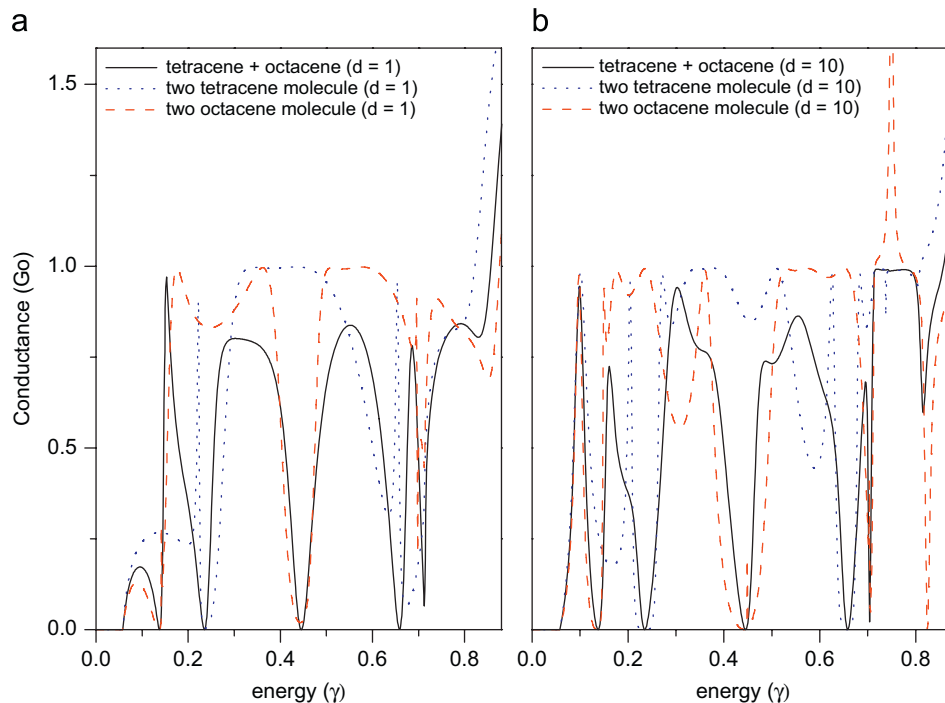


Fig. 3. Conductance of a $N = 5$ AGNR with a tetracene and an octacene attached on the ribbon.

molecules, randomly distributed along the ribbon. The charge distribution effects also could be included.

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