Resonances Induced by Hydrogen-like Ad-atoms in Graphene Ribbons

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Abstract

The studied device consists of graphene nanoribbons patterned with two separated regions where hydrogen can be adsorbed as shown in Fig 1. Substrates can interact and open a gap in graphene (gapless itself), opening that can also be found when deposited on two-dimensional materials with hexagonal symmetry, such as hBN, germanene, silicine,… and group-VI dichalcogenides. We herein focus on the doped-nanoribbons and perform the calculations within a π-band approximation with a nearest-neighbor tight-binding Hamiltonian, well adapted for the low-energy properties of graphene. The C-H bonds are included with a one-parameter scheme [1], and the gap is introduced by a constant staggered potential, namely a local potential that acts with opposite signs in the two sublattices of graphene. The objective of this work is to study the electronic properties of the device presented above, concerning resonances and conductance.

Firstly, we report how resonances emerge in stripes made of two-dimensional materials due to the presence of hydrogen-like ad-atoms and their role on the electronic properties. By depositing hydrogens on the top of some carbons, we found that nanoribbons have states localized not only at neighbor atoms, the so-called defect induced states [2, 3], but along the nanostructure as resonances [4]. Secondly, we are able to establish the energies and spatial distributions of these localized states in ribbons from the rules obtained after folding the bands of certain simpler models [3], as shown in Figures 2 and 3. The ribbon width and the average distance between the hydrogenated regions define the foldings projected perpendicular or along the ribbon, respectively. In both directions, we obtain a set of discrete k-points that in the crossings with the envelop and defect bands determine in the density-of-states not only the energy but the width of the peaks, spread spatially in both graphene sublattices [5]. It is noteworthy that the same rules are applicable to metallic-gapless or semiconductor-gapped graphene ribbons. Finally, we have found that these peaks are crucial for the conductance, where resonances are seen at low concentrations independently of the random distribution of hydrogen atoms. These findings could be of relevance for STS and conductance measurements in graphene-like nanoribbons when doped with covalent bonds on top of carbon atoms.

References

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Figures

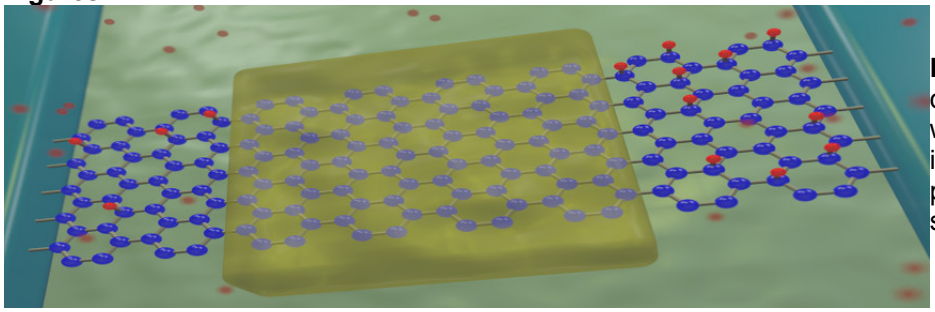

Fig. 1 Scheme of a device with two barriers where the hydrogenation is allowed and a protected separation structure.

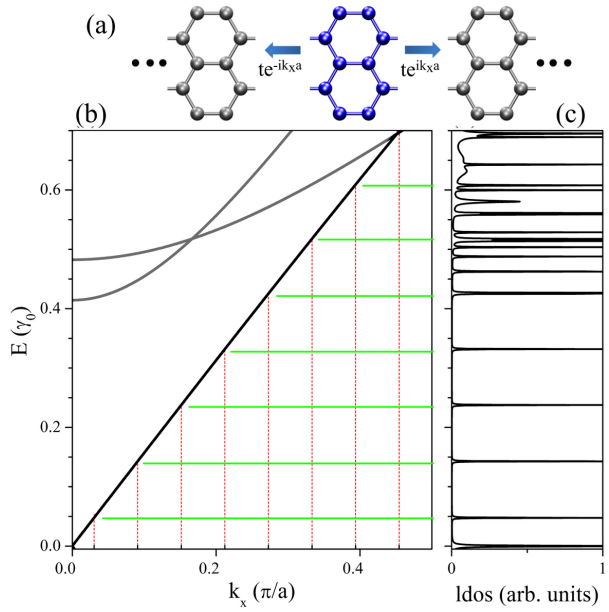

Fig. 2 (a) Model used for folding the electronic structure in the x-direction. (b) Band structure of the pristine metallic ribbon N = 11 with the quantizated k_X as vertical lines. The horizontal lines correspond to the energies where the first band and the quantization lines intersect, and they gives the equidistant resonances in (c) the density-of-states.

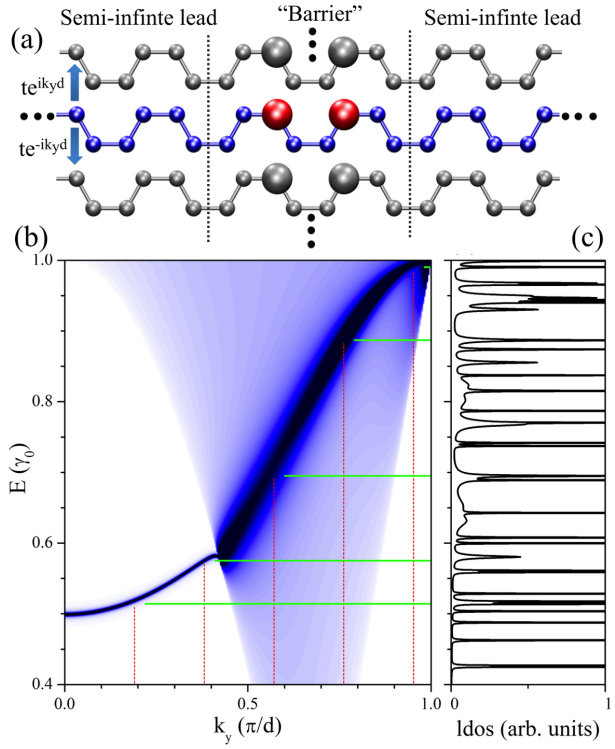

Fig. 3 (a) Model used for folding the electronic structure in the y-direction. (b) Projected density of states in the perpendicular k_Y-direction with the quantization lines for the ribbon L = 15 -presented as vertical lines-. The horizontal lines correspond to the energies where the projected density-of-states and the quantization lines intersect, these lines determine the interface states in (c) the density-of-states.