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Electronic properties of nanoribbon junctions

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Abstract

We investigate the effects of nitrogen impurities on the electronic properties of quantum dots realized in Z-shaped graphene nanoribbon junction. The system is studied using first principle calculations, based on the local spin density approximation (LSDA). Our results indicate that the presence of the impurities drastically changes the configuration of the localized states in the quantum dot.

Keywords: Quantum dots; Nanoribbon; Graphene

The electronic and optical properties of carbon-based nanoscaled materials such as carbon nanotubes, single or bi-layer graphene, and nanoribbons [1–3] are being intensively studied due to their fundamental and technological interest. Recent studies have shown that the electronic structure of graphene nanoribbons (GNRs) exhibits remarkable geometric-dependent properties: it can have metallic or semiconductor behavior depending on the ribbon width and on the arrangement of the atoms on its side edges. It has been demonstrated that the transport and optical properties of GNRs are strongly affected by the edge shape, in particular in the case of ribbons with zigzag edges due to the existence of localized edge states which gives a sharp peak in the density of states (DOS) at the Fermi level [4,5]. Different device junctions based on patterned GNRs have been proposed [6–8] and constructed which can confines electronic states realizing quantum-dot like structures. The electronic states of these confined GNRs structures can be manipulated by chemical edge modifications or impurities addition. In this work we use first principle calculations to perform a theoretical study on the effects of nitrogen impurities on the electronic properties of Z-shaped GNRs junctions.

The system investigated is composed by two $N = 4$ armchair GNRs joined by two Z-shaped GNR junctions where each junction contains a finite $N = 2$ zigzag GNRs (N denotes the number of lines of carbon atoms). The edges of the ribbon are terminated with hydrogen atoms. A schematic view of the structure unit cell is shown in Fig. 1.

In order to carry out first principle calculations we repeat periodically the structure in the space, separating in 20 Å the planes of the ribbon and separating each ribbon on the same plane by a distance of 20 Å. The proposed

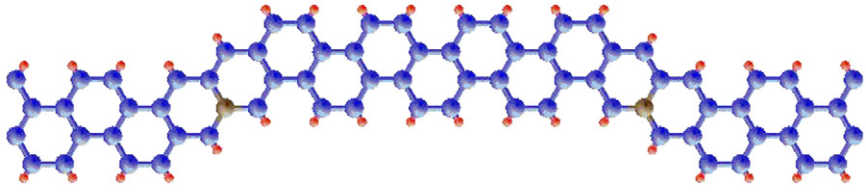

Fig. 1. Structure doubly doped.

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geometry is estimated using the method DIIS with a criteria for having less than 10^{-4} Hartree/bohr of residual force. Then, the band structure and the DOS are determined using first principle calculations; based on the pseudo-potentials method and using the LSDA approach. The convergence criterion for SCF calculation is 10^{-6} Hartree. We use a 150 Ry cutoff energy and the borders are passivated with hydrogen atoms. Calculations were made using the Openmx Code [9–12].

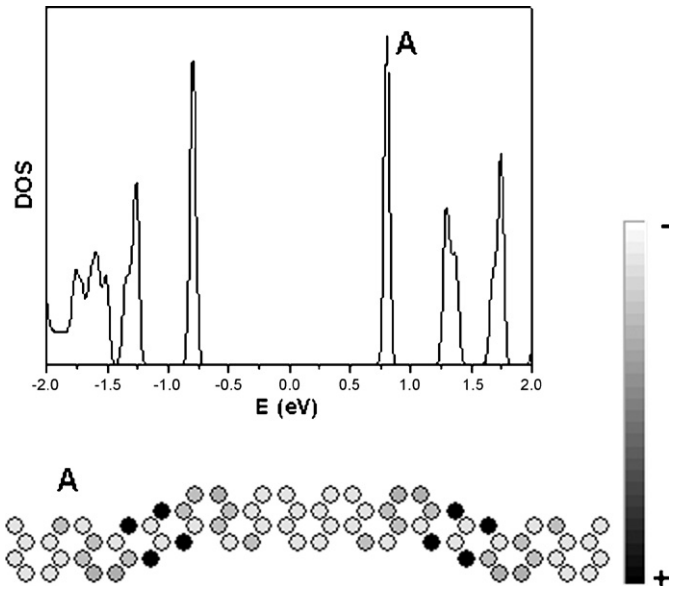

Fig. 2. Pristine structure.

Fig. 2 shows the DOS for the pristine structure. There are two sharp peaks around the Fermi energy which correspond to edge states localized mainly in both Z-shaped junctions. This can be confirmed by the local DOS (LDOS) across the structure which we have displayed, for the peak labeled A, in the isosurface plot within the same figure. To study the effects, on the confined states, due to the presence of impurities in the quantum dot regions, we analyze two kind of doping profiles. In both cases we have plotted the DOS and the corresponding spatial distribution of the LDOS for different peaks of the DOS corresponding to energies near the Fermi energy. The asymmetrical profile (ADP) contains one nitrogen atom placed just in one of the Z-junctions (Fig. 3), and the symmetrical (SDP) has one nitrogen atom in both Z-junctions (Fig. 4). The comparison between the results obtained for the two doping configurations help us to understand the modifications induced by the impurity on the confined states in the graphene quantum dot. We should note that the DOS peaks labeled B, C, E, F of the ADP structure coincide very well with those labeled I, J, K, L of the SDP structure. The contribution to the DOS at these energies comes mainly from atoms belonging to the junction where the impurity is located. Otherwise, the peaks D and G are present only in the ADP structure and the contribution to the DOS at these energies comes mainly from states localized in the quantum dot free of impurities.

We have confirmed the existence of confined states in quantum dots formed in Z-shaped graphene junctions. We have also shown that the electronic spectrum of localized states is strongly modified by the presence of nitrogen impurities in these graphene quantum dots.

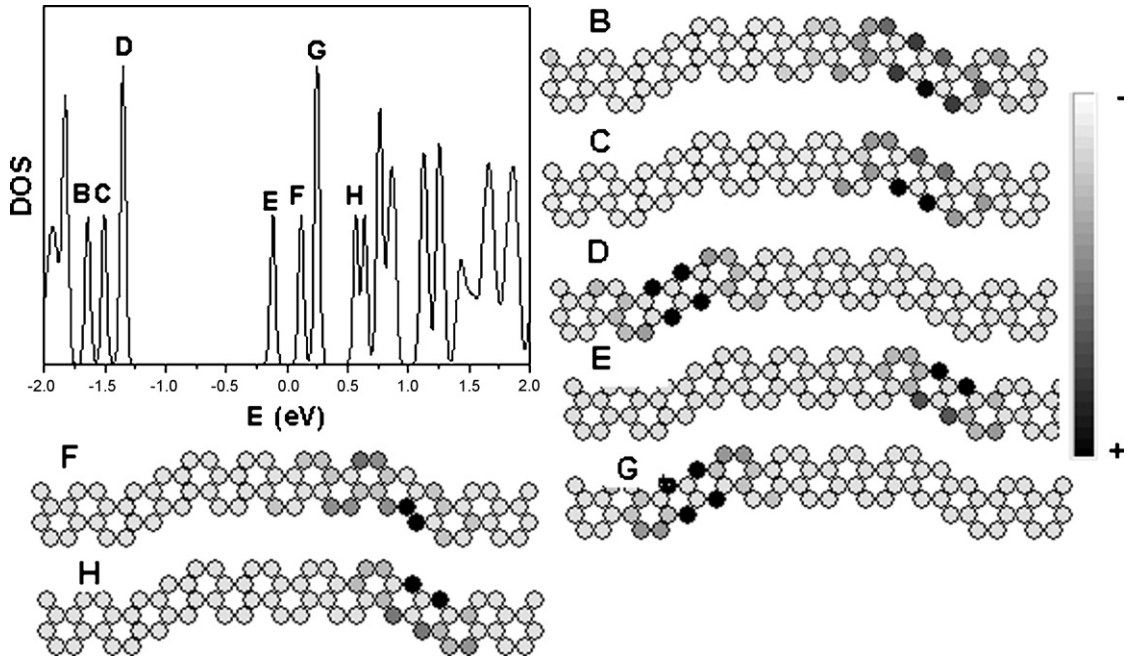

Fig. 3. Structure asymmetrically doped, a nitrogen atom substitutes one carbon atom only at the right Z-shaped junction.

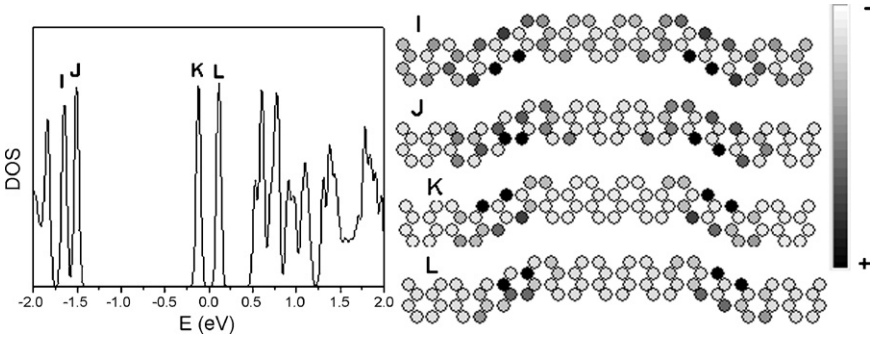

Fig. 4. Structure symmetrically doped, there is one nitrogen atom in each Z-shaped junction of the structure.

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