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Electronic states of zigzag graphene nanoribbons with edges reconstructed with topological defects

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ABSTRACT

The energy spectrum and electronic density of states (DOS) of zigzag graphene nanoribbons with edges reconstructed with topological defects are investigated within the tight-binding method. In case of the Stone–Wales *zz*(57) edge the low-energy spectrum is markedly changed in comparison to the pristine *zz* edge. We found that the electronic DOS at the Fermi level is different from zero at any width of graphene nanoribbons. In contrast, for ribbons with heptagons only at one side and pentagons at another one the energy gap at the Fermi level is open and the DOS is equal to zero. The reason is the influence of uncompensated topological charges on the localized edge states, which are topological in nature. This behavior is similar to that found for the structured external electric potentials along the edges.

1. Introduction

Currently, there is a growing interest in studies of edge states in graphene structures. It has been found that zigzag graphene nanoribbons (ZGNRs) possess a localized edge state at the Fermi energy which has a crucial influence on their electronic properties. In particular, the energy band gap of the ZGNRs is zero due to the existence of edge states and, consequently, these nanoribbons are always metallic. The presence of energy gap is necessary for various applications in nanoelectronics and, therefore, an important problem is to control and manipulate the edge states in ZGNRs.

Recently, the influence of external electric potentials applied along the edges of ZGNRs has been investigated. It was found that such potential can induce a spectral gap thus converting the metallic behavior of the ZGNR into a semiconducting one. As was mentioned in [1] this effect originates from the sensitivity of the spinorial edge states to electric potentials. What is interesting, the edge states are topological in nature [2,3]. Therefore one could expect a similar influence in case of topological charges situated along the edges. In order to check it we consider an artificial ZGNR with edges reconstructed with pentagons at one side and heptagons at the opposite side. For our motivation, it was shown in works [4,5] that heptagonal defects influence the electronic structure of the graphene nanostructure significantly.

Our task is to study the electronic band structure of ZGNRs with reconstructed edges and to calculate the density of states (DOS). For this purpose, we employ the well approved tight-binding method [6] which has been successfully used in studies of edge states in pristine ZGNRs [7]. The paper is organized as follows. In the next section, we give a brief description of the tight-binding method. Then, we study the energy band structure and the electronic DOS of endless ZGNRs containing periodically repeating structures with edges reconstructed with two different kinds of topological defects. A separate section is devoted to an analysis of the stability of the investigated structure by using the programs Avogadro [8] and GAMESS [9]. Finally, we present a brief conclusion.

2. Tight-binding method

The tight-binding method assumes the numerical solution of the stationary Schrödinger equation

$$H\psi = E\psi, \tag{1}$$

where the Hamiltonian is written for π electrons in graphene lattice with nearest-neighbors taken into account, ψ is the linear

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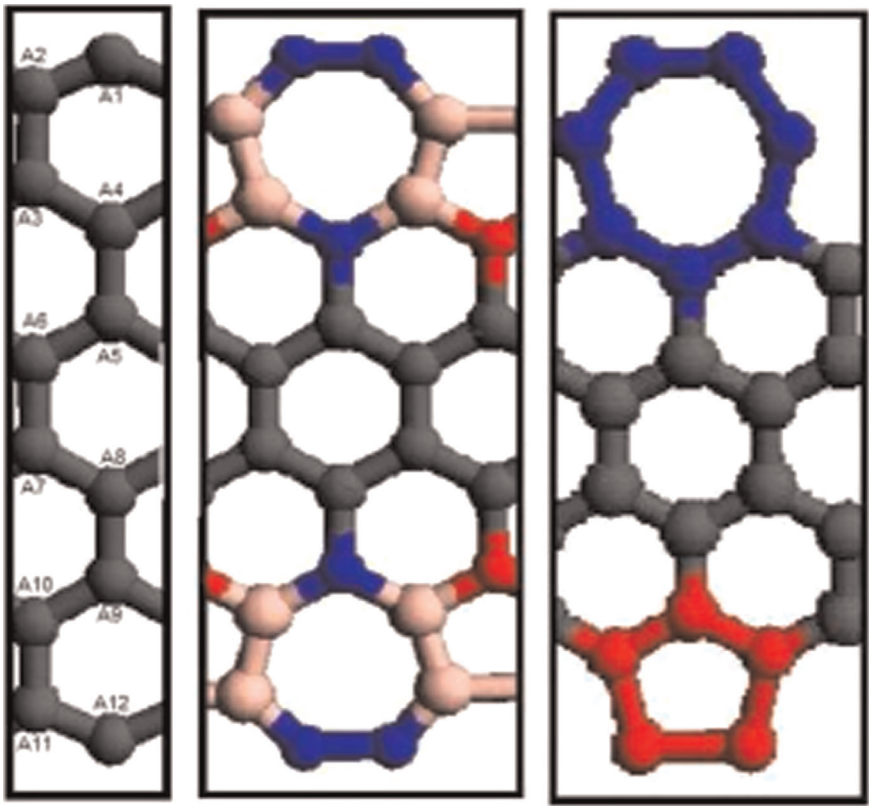

Fig. 1. The unit cells for pristine (left), *zz*(57) (middle) and *zz*(5/7) (right) zigzag graphene nanoribbons.

combination of the wave functions which correspond to the particular atoms in the unit cell. In graphene lattice, the unit cell contains exactly two atoms while in graphene nanoribbons this number is much larger (see Fig. 1). Let us enumerate them as $A_1, A_2, \ldots, A_N$, where N is the total number of atoms in the unit cell. Then

$$\psi = C_1\psi_{A_1} + \cdots + C_N\psi_{A_N}, \tag{2}$$

and one can define the matrix coefficients

$$H_{ij} = \int \psi_i^* H \psi_j \, \mathrm{d}\vec{r}, \tag{3}$$

where $i, j \in \{A_1, \ldots, A_N\}$. Owing to orthogonality of ψ_i one gets

$$\sum_{j=1}^{N} C_j H_{ij} = C_i E S, \tag{4}$$

where the normalization condition is chosen to be $S = \int \psi_i^* \psi_i \, \mathrm{d}\vec{r}$ with S being the number of unit cells in the nanostructure. Finally, solving the matrix equation (4) we obtain the energy eigenvalues and thereby the electronic spectrum of the given nanostructure. The electronic DOS is written as

$$DOS(E) = \int_0^{2\pi} \delta(E - E(\vec{k})) \, \mathrm{d}\vec{k}. \tag{5}$$

In order to verify this consideration we have performed the numerical calculations of the electronic spectrum and the DOS for the ZGNR of given width. The results are shown in Fig. 2 and they are in perfect agreement with [7].

3. Zigzag graphene nanoribbons with reconstructed edges

Let us first consider ZGNRs with edges totally reconstructed

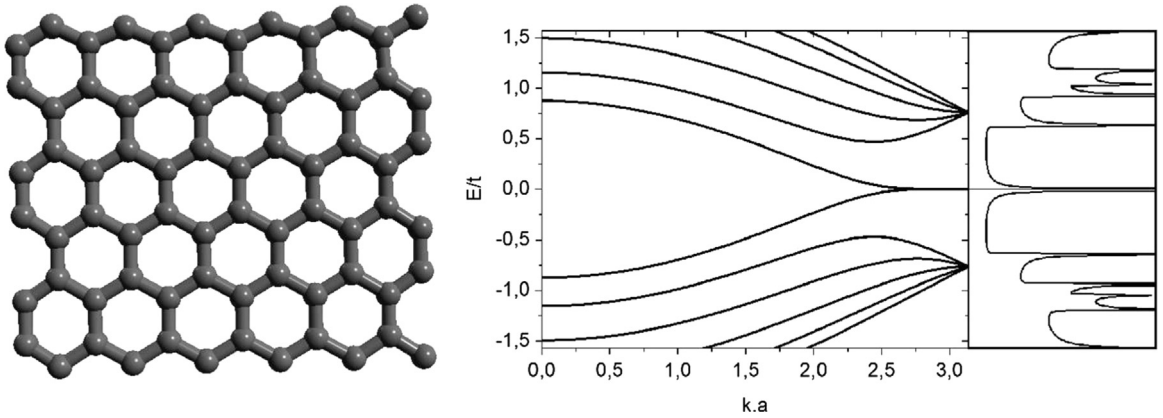

Fig. 2. Lattice structure, electronic spectrum and density of states of endless zigzag graphene nanoribbon. The results are in perfect agreement with [7].