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Possible polaron formation of zigzag graphene nano-ribbon in the presence of Rashba spin–orbit coupling

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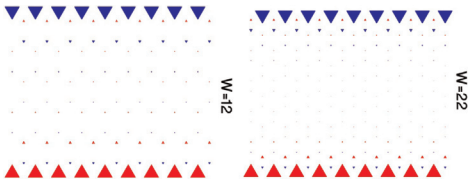
HIGHLIGHTS

- A tight binding study of Rashba spin–orbit coupling in a zigzag graphene nanoribbon is presented.
- We show that even for small values of Rashba spin–orbit coupling the anti-ferromagnetic phase on the zigzag edges is disappeared.
- Our results show the spin-dependent polaron formation energy in zigzag nanoribbon.

GRAPHICAL ABSTRACT

We study the effect of Rashba spin–orbit coupling and the electron–phonon interaction on the electronic structure of zigzag graphene nanoribbon.



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ABSTRACT

In this article we study the role of Rashba spin–orbit coupling and electron–phonon interaction on the electronic structure of zigzag graphene nanoribbon with different width. The total Hamiltonian of nanoribbon is written in the tight binding form and the electron–electron interaction is modeled in the Hubbard term. We used a unitary transformation to reach an effective Hamiltonian for nano ribbon in the presence of electron–phonon interaction. Our results show that small Rashba spin orbit coupling annihilates the anti-ferromagnetic phase in the zigzag edges of ribbon and the electron–phonon interaction yields small polaron formation in graphene nano ribbon. Furthermore, Rashba type spin–orbit coupling increases (decreases) the polaron formation energy for up (down) spin state.

1. Introduction

The recent theoretical and experimental works in the field of carbon nanostructure show the enormous potential of carbon for future technologies. The graphene nanoribbon is a 1D strip of graphene with armchair and zigzag edges. Theoretical works predicted the antiferromagnetism in the zigzag edge of graphene nano ribbon (ZGNR) [1–4]. It was shown that the Hubbard term is an effective Hamiltonian for description of magnetic properties in carbon nanostructures like graphene nanoribbon and graphene quantum dots [5–10]. Actually the presence of substrate and thermal vibrations change the electronic and other properties of nanomaterials. Kane and Mele introduced an effective tight-binding model to study the intrinsic and Rashba spin–orbit coupling in graphene [11,12]. The Rashba spin–orbit coupling (RSOC) is related to the presence of substrate or external electric field perpendicular to the graphene plane. Although the strength of intrinsic spin–orbit coupling of graphene was overestimated in the prior works [13,14]. But there are some experimental evidences for relatively large strength of RSOC in graphene that is related to the substrate [15,16]. Also considerable RSOC splitting for π bands is predicted for graphene with adsorbed Au atoms [17]. An experimental method was proposed to determine the strength of RSOC and Dresselhaus spin–orbit coupling by measuring the charge and spin currents [18–20]. There are many theoretical investigations of natural spin polarized transport through nanostructures in the presence of spin–orbit interaction [9,10,20–23].

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Phonon modes of graphene play an important role in charge carrier dynamics. In the ZGNR the interaction between electron and phonon can change different properties of ribbon. Polaron formation and the effect of electron–phonon coupling on energy spectrum of graphene were discussed in literature [24–26]. Combined effects of electron–phonon interaction and spin–orbit coupling on energy spectrum of low dimensional structures are another important issue that inspires the construction of spintronic devices [27–33]. Even some of the studies claim that the strength of electron–phonon interaction was enhanced with spin–orbit coupling mechanism [27–31], the others showed that the RSOC decreases this strength [32,34]. Moreover, the combination between these effects induces a unique character for each spin orientation.

Here, we study the role of RSOC and the electron–phonon interaction on the electronic properties and polaron formation energy of ZGNR. The tight binding is a simple and effective model to study different effects. We used a single orbital tight binding model to describe the non-interacting Hamiltonian and add the Hubbard term, SOC and electron–phonon interaction to study the role of environment effects on the nano structures. By using the unitary transformation method we obtained an effective tight binding Hamiltonian for zigzag and other periodic structures in the presence of electron–phonon interaction. By considering different interactions in the ribbon we reached to a relatively real physical system.

2. Model and method

The atomic structure and unit-cell of ZGNR for $W=12$ atoms is plotted in Fig. 1. In the first step we consider the electronic structure of ZGNR and add the electron–electron, RSOC and electron–phonon interaction terms one by one. The total Hamiltonian in the presence of different kind of the above mentioned interactions can be written as

$$H_{T-GQD} = \sum_{i,\sigma} \varepsilon_i C^{\dagger}_{i,\sigma} C_{i,\sigma} - \sum_{<i,j>,\sigma} t_{i,j}[C^{\dagger}_{i,\sigma} C_{j,\sigma} + C^{\dagger}_{j,\sigma} C_{i,\sigma}] + U \sum_{i,\sigma} C^{\dagger}_{i,\sigma} C_{i,\sigma} C^{\dagger}_{i,-\sigma} C_{i,-\sigma} + i\lambda_{RSO} \sum_{<i,j>,\sigma} C^{\dagger}_{i,\sigma} C_{j,-\sigma} (Sd_{ij})^{\sigma,-\sigma}_{z} + \hbar\omega_0 \sum_{\vec{q}} b^{\dagger}_{\vec{q}} b_{\vec{q}} + \frac{g}{\sqrt{N}} \sum_{\vec{i},q,\sigma} C^{\dagger}_{i,\sigma} C_{i,\sigma} (b_{\vec{q}} + b^{\dagger}_{-\vec{q}}), \quad (1)$$

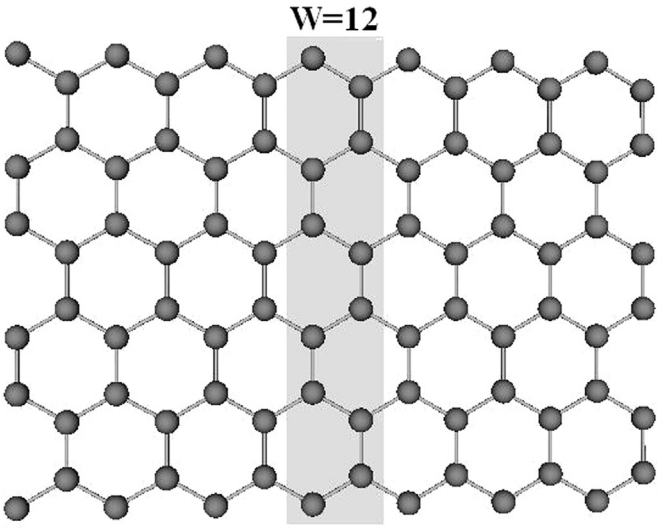

Fig. 1. Top view of ZGNR with 12 atoms width.

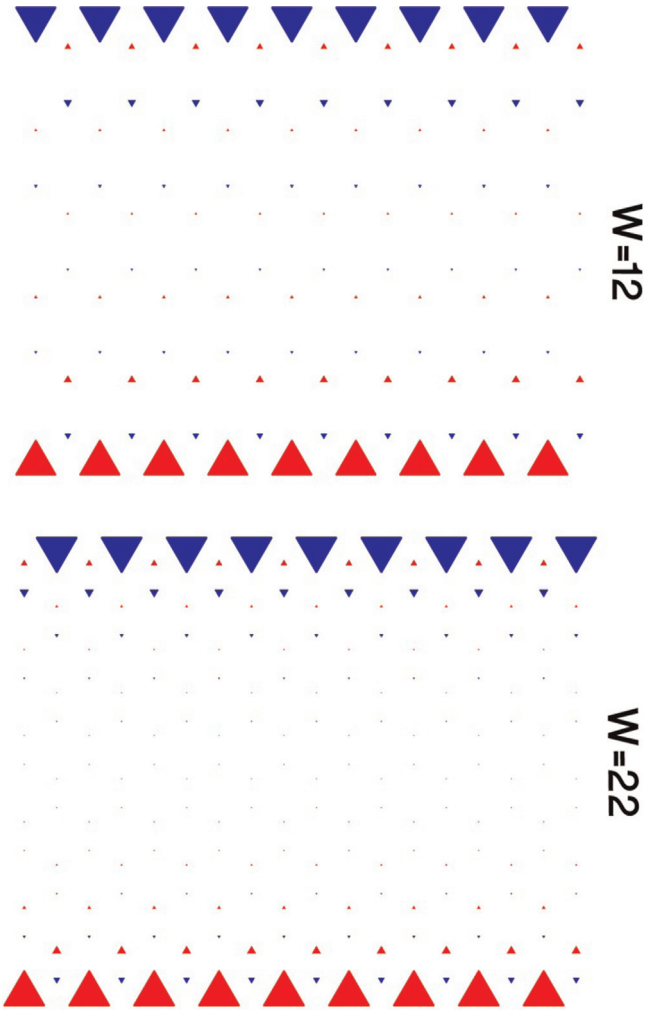

Fig. 2. The atomic magnetization in the unit of Bohr magnetron for two zigzag nanoribbon with $W=12$ and $W=22$ in the absence of Rashba spin–orbit interaction.

where the $C^{\dagger}_{i,\sigma}(C_{i,\sigma})$ is the electron creation (annihilation) operator for π electron states with spin σ at ith site of ZGNR. The first two terms are the non-interacting Hamiltonian for the on-site energy and hopping between ZGNR atomic sites. The third part is the well-known Hubbard term that explains the electron–electron interaction between two electrons in a same site with different spin orientations. We used the mean-field approximation to solve the Hubbard Hamiltonian. The electron–electron interaction is decoupled into two parts for spin up and down states $H_{Mean\ field} = U\sum_{i,\sigma}\langle n_{i,\sigma}\rangle C^{\dagger}_{i,-\sigma} C_{i,-\sigma}$. Accordingly the on-site energy is spin-dependent and corresponds to the density of opposite spin [5–10,35–37]. The decoupled Hamiltonian of spin up and down states should be solved in a self-consistent manner for a starting point. The fourth term in Eq. (1) that was proposed by Kane and Mele is an effective Hamiltonian for the Rashba spin–orbit coupling. The d_{ij} is a unit vector for ith and jth nearest neighbor atoms, S is the Pauli matrix and λ_{RSO} shows the strength of RSOC [10–12]. The last two terms in Eq. (1) represent the bare phonon and Hubbard–Holstein Hamiltonians, respectively [24]. Here, the $b^{\dagger}_{\vec{q}}(b_{\vec{q}})$ is the creation (annihilation) operator for phonon with wave vector q and $\hbar\omega_0 \simeq 0.15$ eV is the frequency of out-of plane phonon mode [24,38], N is the number of atoms in the unit cell of nanoribbon and g is the coupling parameter of the electron–phonon interaction. Actually Eq. (1) is the Kane–Mele–Hubbard