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Influence of Local Electric Field on Electronic States of Graphene Nanoribbons

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Abstract

Using density functional theory with the effective screening medium method, we studied the electronic properties of graphene nanoribbons with zigzag and armchair edges under an external electric field. Our calculations showed that a nearly free electron (NFE) state emerges in the vacuum region outside edge atomic sites of the ribbons and shifts downward with increasing the electric field. We also found that the mutual arrangement and shapes of graphene nanoribbons with respect to the electric field is important to control the energy of NFE states.

1. Introduction

Following the synthesis of garaphene, graphene and its derivatives are now attracting much attention as the emerging materials for electronic, spintronic, sensing, and photovoltaic devices due to its peculiar electronic structure arising from their dimensionality and hexagonal covalent network. As for the graphene application for the above devices, graphene inherently forms hybrid structures with foreign materials and external environments. Under these hybrid structures, electronic structure of graphene is sensitively modulated from that of the isolated one. Among these foreign materials and environmental condition, an external electronic field plays an important role for the application of graphene to various devices. An electric field occasionally affects the electronic structure of graphene and graphite. In the case of bilayer graphene the metal-semiconductor-metal transition occurs by applying the electric field normal to graphene layers [1]. Similar electronic structure modulations are also found in the graphene nanoribbon under the lateral electric field. In the case, we found that the lateral electric field basically opens or increases the energy gap of the ribbons [2]. However, it is still unclear how the electronic structure of the ribbons is further modulated by the strong lateral electric field. Thus, in this work, we study the electronic structure of graphene nanoribbons under the lateral electric field to investigate the possibility for injection of free carriers outside the ribbons.

2. Methods and Models

All calculations are performed in the framework of density functional theory [3, 4] using the Simulation Tool for Atom Technology (STATE) [5]. For the exchange correlation energy among electrons, we use the local density approximation (LDA) with the functional form Perdew-Zunger [6, 7]. An ultrasoft pseudopotential generated using the Vanderbilt scheme is adopted to describe the electron-ion interaction.[8] The valence wave functions and charge density are expanded in terms of the plane waves of which cutoff energy is 25 Ry and 225 Ry, respectively. Here, we consider the graphene nanoribbons with zigzag and armchair edges under parallel (θ=0 degree) to perpendicular (θ=90 degree) electric field (Fig. 1). To investigate the graphene nanoribbons under the parallel electric field, we sandwich the graphene nanoribbons between two planar electrodes simulated by an effective screening medium with infinite permittivity. Under the model, we adopt the effective screening medium method to solve the Poisson equation including the external electric field [9]. Atomic structures are fully optimized under zero electric fields. For the calculations under the condition of a finite electric field up to 5 V/nm, the geometries are fixed to those under the condition of a zero electric field.

3. Results

Figure 2 shows the electronic energy band of graphene nanoribbons with zigzag edges under the electric field. We found that the quadric dispersion band at the Γ point in the bottom of conduction bands. The state possesses unusual feature: The wave function of this state is distributed in the vacuum region outside the graphene ribbon and extended along the edge with the free electron nature (Fig. 3). Thus, this state possesses similar feature to the nearly free electron (NFE) state of graphene which is distributed above the graphene layer [10]. Figure 4 shows the eigen value of NFE states of graphene nanoribbons as a function of the external electric field. In the parallel electric field, NFE state distributed at the ribbon side rapidly shifts downward with increasing the electric field, while the NFE state distributed above and below the ribbon is insensitive to the field. In the normal electric field, both NFE states are insensitive to the electric field. These results imply that the direction of electric field with respect to the ribbon is important to control electronic structure of graphene nanoribbons. Furthermore, filed concentration around the ribbon edges enhances the decrease the electrostatic potential around the edge atomic site leading to the carrier injection outside the graphene nanoribbons that decreases the barrier for carrier injection into graphene nanoribbons via electrodes [11].

4. Conclusions

We studied the electronic structures of hydrogenated graphene nanoribbons under a lateral electric field using density functional theory with the effective screening medium method. We found that the NFE state appears not only in the vacuum region above/below the graphene atomic layer, but also in the vacuum region alongside the edge atomic sites.

Acknowledgements

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References

[1] M. Otani and S. Okada, J. Phys. Soc. Jpn. **79** (2010) 073701.
[2] A. Yamanaka and S. Okada, Jpn. J. Appl. Phys. **53** (2014) 06JD05.
[3] P. Hohenberg and W. Kohn: Phys. Rev. **136** (1964) B864.
[4] W. Kohn and L.J. Sham: Phys. Rev. **140** (1965) A1133.
[5] Y. Morikawa, K. Iwata, and K. Terakura: Appl. Surf. Sci. **169-170** (2000) 11.
[6] J.P. Perdew and A. Zunger: Phys. Rev. B **23** (1981) 5048.
[7] D.M. Ceperley and B.J. Alder: Phys. Rev. Lett. **45** (1980) 566.
[8] D. Vanderbilt, Phys. Rev. B **41** (1990) 7892.
[9] M. Otani and O. Sugino: Phys. Rev. B **73** (2006) 115407.
[10] A. Yamanaka and S. Okada, Appl. Phys. Express **7** (2014) 125103.
[11] A. Yamanaka and S. Okada, in preparation.

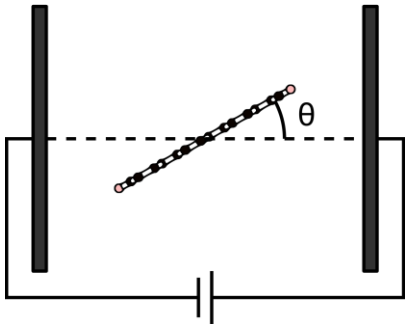


Fig. 1 Structural model of graphene nanoribbons under an electric field. Dark-shaded rectangles represent metal electrodes simulated by an effective screening medium.

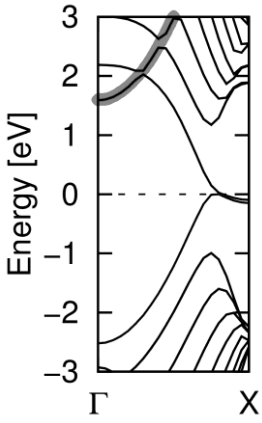


Fig. 2 Electronic structure of graphene nanoribbon with zigzag edges under the electric field of 2.5 V/nm. A gray thick line indicates the NFE state.

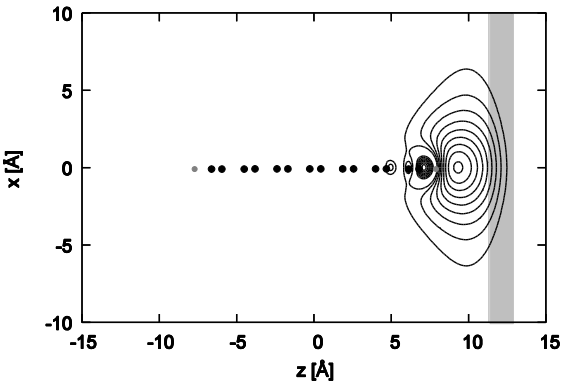
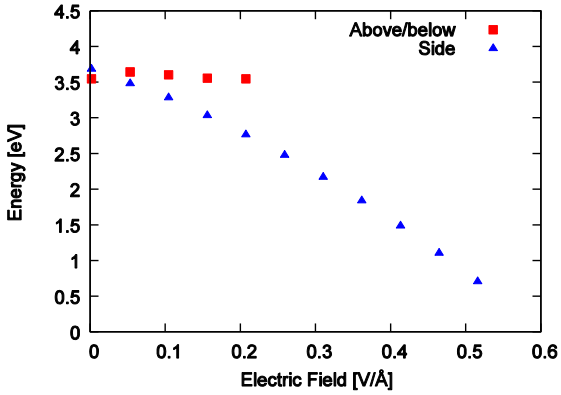


Fig. 3 Contour plot of NFE state of zigzag ribbon under 2.5 V/nm parallel electric field (θ=0). Black and gray circles denote carbon and hydrogen atomic position, respectively.

(a) Parallel electric field (θ=0)



(b) Normal electric field (θ=90)

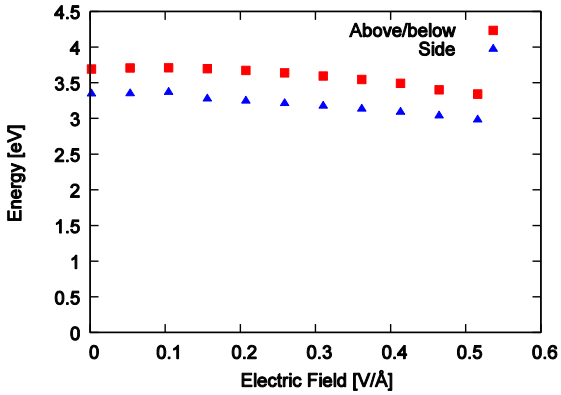


Fig. 4 Eigen values of NFE states of zigzag nanoribbons as a function of electric field. Squares and triangles denote the eigen values of NFE states appearing above/below and alongside of graphene nanoribbons, respectively.