Electric-field-induced lowest state in bilayer zigzag graphene nanoribbon

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Abstract. We investigated the lowest state in the bilayer zigzag graphene nanoribbon by taking the electric field into account. In this calculation, we considered five collinear configurations of magnetic moment of carbon atoms at the four edges. We found that the lowest state changes as the electric field is applied. We also showed that at the high electric field, those five configurations almost become degenerate. This suggests that the lowest state is not robust to the electric field so that the electric field can control the lowest state in the bilayer zigzag graphene nanoribbon.

1. Introduction

Zigzag graphene nanoribbon, a one-dimensional form of graphene, has many interesting electric and magnetic properties, such as half-metallic property [1,2] and spin stiffness [3-8]. Such properties are very benefit to develop spintronic devices with low cost. The model of zigzag graphene nanoribbon itself was initially introduced by Fujita et al. when they considered a theoretical model of one-dimensional version of graphene [9].

As reported in the previous works [10], the ground state of monolayer zigzag graphene nanoribbon is an antiferromagnetic state for the non-doped case, in which the magnetic moments of carbon atoms at two edges are aligned antiferromagnetically. When the hole-electron doping is introduced in the monolayer case, the ground state changes from antiferromagnetic stated → canted state → ferromagnetic state. This means that the appearing ground state depends on the doping [11].

We investigate the influence of electric field on the ground state in bilayer zigzag graphene nanoribbon. The electric field is important to generate half metallicity in the graphene nanoribbon when the hybrid exchange functional is used [1,2]. In this case, we do not use such functional because we focus on the change of ground state. All the collinear calculations only include a ferromagnetic state, three antiferromagnetic states, and a ferrimagnetic state, as provided in Sawada et al. [12]. We find the ground state depends on the electric field, which is similar to the hole-electron doping case.

We provide the structure model of bilayer zigzag graphene nanoribbon, in which the carbon atoms at the edges have different directions of magnetic moments, in section 2. In the next section, we classify the interval of electric field at which the ground state appears and show the degenerate condition at high electric field.
2. Methods
Our collinear structure model is based on the AB-stacking bilayer zigzag graphene nanoribbon, as shown in Figure 1.

![Figure 1](image)

**Figure 1.** Model of AB-stacking bilayer zigzag graphene nanoribbon from x-y plane (a) and y-z plane (b). The small and large circles are addressed to the hydrogen and carbon atoms, respectively.

In this model, the lattice constant in the x-direction is 0.246 nm while the interlayer distance is 0.335 nm. Those values were obtained from the experiment result of graphite. The electric field was then applied in the y-axis, as shown in Figure 1(a). Following Sawada et al. [12], we constructed five states, as shown in Figure (2). Here, the antiferromagnetic state has three types, i.e., A-antiferromagnetic, C-antiferromagnetic, and G-antiferromagnetic states. In this calculation, we only consider the ribbon width of 10, which involves 40 carbon atoms and 4 hydrogen atoms in the primitive unit cell.

Based on the density functional theory, we specified two s orbitals and two p orbitals as basis set for the carbon atoms with the cutoff radius of 6.0 Bohr. Meanwhile, an s orbital and a p orbital as basis set for the hydrogen atoms were specified in the cutoff radius of 6.0 Bohr. All the numerical calculations were carried out by using the OpenMX code [13], a free package using linear combination of localized orbitals as basis set. In addition, an exchange correlation potential in this magnetic system was also
numerically evaluated via generalized gradient approximation (GGA-PBE) [14] with the k-point sampling of $65 \times 1 \times 1$.

![Figure 2. Configuration of magnetic moments of carbon atoms for ferromagnetic state (a), A-antiferromagnetic state (b), C-antiferromagnetic state (c), G-antiferromagnetic state (d), ferrimagnetic state (e).](image)

3. Results and discussions

As shown in table 1, we see that the ground state of bilayer zigzag graphene nanoribbon is not robust on the electric field. For the low electric field, the insulating state (antiferromagnetic state) dominates the ground state while the C-antiferromagnetic has the large piece. When the electric field increases up to the sufficiently high electric field, the magnetic state (ferromagnetic or ferrimagnetic states) takes the role. This means that the role of electric field in the bilayer zigzag graphene nanoribbon is to generate the metallic property.

| States         | E (Volt/nm) |
|----------------|-------------|
| FM             | 0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 |
| A-AFM          | ●           |
| C-AFM          | ●, ●, ●, ●, ● |
| G-AFM          | ●, ●, ●, ●, ● |
| Ferrimagnetic  | ●, ●, ●     |

The interesting case can be seen when we observe the energy difference between the highest and lowest states when taking the electric field into account. As shown in Fig. 3, the highest energy difference is reached at the electric field of 0.4 V/nm where the A-antiferromagnetic state is the lowest state. When we compare table 1 with Fig. 3, we deduce that the energy difference tends to reduce at the same ground state when increasing the electric field. In addition, we immediately see that all the states are almost
degenerate starting from the electric field of 0.8 V/nm even though the precise calculation still achieves the ground state.

![Figure 3](image)

Figure 3. Trend of total energy difference between the highest and lowest states with respect to electric field.

Compared to Sawada et al. [12], who studied the ground state in the same structure by introducing the hole-electron doping, our results do not show specific intervals, at which the ground state emerges. The same trend is that their results show that the antiferromagnetic state (insulating properties) dominates the low concentration while the ferromagnetic state (magnetic properties) dominates the high concentration. In addition, the same model with the same configurations but in the noncollinear structure can also produce the different ground state when varying the interlayer distance [15]. Interestingly, this ground state will influence the spin stiffness that is useful for examining the carbon-based spintronics.

4. Conclusions
We found that the ground state can be tuned by increasing the electric field in the bilayer zigzag graphene nanoribbon for the five collinear magnetic configurations. We also showed that the insulating properties take part in the low electric field, otherwise, the magnetic properties take the role in the high electric field. This means that increasing electric field leads to the magnetic properties in the bilayer zigzag graphene nanoribbon.

Acknowledgements
Personal high computer was used to perform the calculations.

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