# Edge States and Stacking Effects in Nanographene Systems

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Bilayer graphene nanoribbon with zigzag edge is investigated with the tight binding model. Two stacking structures,  $\alpha$  and  $\beta$ , are considered. The band splitting is seen in the  $\alpha$  structure, while the splitting in the wave number direction is found in the  $\beta$  structure. The local density of states in the  $\beta$  structure tend to avoid sites where inter-layer hopping interactions are present.

### I. INTRODUCTION

The graphite, multi-layer, and single-layer graphene materials have been studied intensively, since the electric field effect has been found in atomically thin graphene films.<sup>1</sup> These materials can be regarded as bulk systems. On the other hand, nanographenes with controlled edge structures have been predicted to have localized states along the zigzag edges.<sup>2</sup> The presence of the edge states has been observed by experiments of scanning tunneling spectroscopy.<sup>3,4</sup> Thus, the studies of the edge states are one of the interesting topic of the field. The recent atomic bottom-up fabrication of nanoribbons really promotes experimental and theoretical investigations.<sup>5</sup>

Previously, one of the present authors has studied the stacking effects of the nanographene by considering weak inter-layer hopping interactions in the tight binding model.<sup>6,7</sup> The cluster calculations have been performed, and compared with experiments of the magnetic properties. It has been found that open shell nature of the electronic orbital of the each layer is important. The existence of the spin in the each layer gives rise to the magnetism of the stacked nanographene. Therefore, the simple tight binding model is effective.

In this paper, bilayer graphene nanoribbon with zigzag edge is investigated with the tight binding model. Two stacking structures,  $\alpha$  and  $\beta$ , are considered. The band splitting is seen in the  $\alpha$  structure, while the splitting in the wave number direction is found in the  $\beta$  structure. The local density of states in the  $\beta$  structure tend to avoid sites where inter-layer hopping interactions are present.

This paper is organized as follows. In the next section, the model is explained. The results are shown in Section 3. The paper is closed with summary in Section 4.

## II. MODEL

We consider the following tight binding model

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{H.c.})$$



FIG. 1. A-B stacked bilayer graphene nanoribbon with zigzag edges. The upper layer is shown by the solid lines, and the lower layer by dotted lines. In the  $\alpha$  structure (a), the upper layer is shift by the bond length downward to the position of the lower layer. The region surrounded by the dashed line is the unit cell in the direction of the one dimensional direction. At the circles, two carbon atoms of the upper and lower layers overlap completely, and there is the weak hopping interaction  $t_1$  here. In (b), the  $\beta$  structure is shown, where the lower layer is shift right-down direction so the stacking pattern is different from that of the  $\alpha$  structure. The convention of the  $\alpha$  and  $\beta$  structures are the same used in the paper.<sup>8</sup> (c) The detailed view around the edge atom in the  $\beta$  structure is displayed.

$$-t \sum_{\langle i,j\rangle,\sigma} (d^{\dagger}_{i,\sigma}d_{j,\sigma} + \text{H.c.}) -t_1 \sum_{\langle i,j\rangle,\sigma} (c^{\dagger}_{i,\sigma}d_{j,\sigma} + \text{H.c.}),$$
(1)

where  $c_{i,\sigma}$  and  $d_{i,\sigma}$  are the annihilation operators of electrons at the lattice site *i* of the spin  $\sigma$  on the upper



FIG. 2. Energy band structures for the single layer (a),  $\alpha$  structure (b), and  $\beta$  structure (c). Details near the Brillouin zone edge are magnified for the single layer (d),  $\alpha$  structure (e), and  $\beta$  structure (f). In (e) and (f), the energy bands of the single layer are shown by the red lines for comparison.



FIG. 3. Number of states against the energy for the single layer (a),  $\alpha$  structure (b), and  $\beta$  structure (c).

and lower layers, respectively. The quantity t is the hopping integral of  $\pi$  electrons between neighboring lattice sites. Two stacking patterns, shown in Figs. 1 (a) and (b), are considered. They are named as  $\alpha$  and  $\beta$  structures, respectively. This convention has been used in the literature.<sup>8</sup> There are  $N_z = 6$  zigzag lines in upper and lower layers. The detailed view near the edge atom in the  $\beta$  structure is displayed in Fig. 1 (c). There is a weak hopping integral  $t_1$  along the dashed line.

### III. RESULTS

In order to see effects of inter-layer interactions, the tight binding model is solved numerically. The model is solved using the Bloch theory of the band calculation. Energy band structures of the  $N_z = 20$  systems are displayed in Fig. 2, for the single layer (a),  $\alpha$  structure (b), and  $\beta$  structure (c). The interlayer interaction strength

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is  $t_1 = 0.1t$ . In (b), the split of the energy bands is seen compared with Fig. (a). In contrast, split in the perpendicular direction is small in Fig. (c). In order to see split structures clearly, details near the Brillouin zone edge are magnified for the single layer (d),  $\alpha$  structure (e), and  $\beta$  structure (f). In (e) and (f), the energy bands of the single layer are shown by the red lines for comparison. The nearly flat band due to the edge state in  $-\pi < kd < -2\pi/3$  is present at the energy  $E \sim 0$  in (d). where d is the unit cell length of the one dimensional direction of Figs. 1 (a) and (b). The energy bands starts at E = 1.0t at  $kd = \pi$ , typical to the graphene structure. In (e), the energy split is magnified again. However, in (f), the energy split is not seen, and split in the wave number direction is found. This property is confirmed by looking at the numerical data, also.

It is interesting to look at how such the difference of the band split in the  $\alpha$  and  $\beta$  structures appear, in the quantization of conductance. Number of states in the energy window for the positive wave number is calculated for the single layer,  $\alpha$ , and  $\beta$  structures. Fig. 3 displays the calculated results for the parameters  $N_z = 20$  and  $t_1 = 0.1t$  again. Around the energy E = 0 of the single layer (a), the energy band is singly degenerate, as shown in Fig. 2 (d). At the energy E = 0.4t, the energy window reaches the first parabolic band, and the number of states jumps by two. The energy window reaches the second parabolic band at the energy E = 0.65t. In this way, a series of jumps by two is realized in (a). For the  $\alpha$  structure (b), number of states near the energy E = 0is two due to the bilayer property. There are two steps of the jump of two around the energy E = 0.4t, owing to the energy split of the first parabola. Also, two steps are present closely around the energy E = 0.7t due to the second parabolic band. On the other hand, each jump of the number of states becomes four for the  $\beta$  structure (c) due to the split in the wave number direction. The dependence of the energy reflects the band structures, and this will appear quantization of conductance experimentally.

### IV. SUMMARY

In summary, weak inter-layer interactions have been considered for the bilayer graphene nanoribbon with zigzag edge. The  $\alpha$  and  $\beta$  stacking structures have been considered. The band splitting is seen in the  $\alpha$  structure, while the splitting in the wave number direction is found in the  $\beta$  structure. The local density of states in the  $\beta$  structure tend to avoid sites where inter-layer hopping interactions exist.

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