Theoretical Study of Edge States in BC_2N Nanoribbons with Zigzag Edges

Kikuo Harigaya[1], Tomoaki Kaneko[2]

[1]Nano-scale Theory Group, NRI, AIST, Higashi 1-1-1, Tsukuba, Ibaraki 305-8565, Japan
[2]First-Principles Simulation Group, CMSU, NIMS, Sengen 1-2-1, Tsukuba, Ibaraki 305-0047, Japan
k.harigaya@aist.go.jp

Abstract

Graphene is an atomically thin carbon sheet in which carbon atoms are arranged in a honeycomb lattice. Due to their outstanding electronic structure and electron transport properties, graphene attracts much interest for future electronic devices. Graphene nanoribbons are finite width graphene sheets. The electronic properties of graphene nanoribbons strongly depend on the edge structures [1]. Graphene nanoribbons with zigzag edges have the so-called flat bands at the Fermi level [1]. The states corresponding to the flat bands are localized at the zigzag edges [1]. For the so-called edge states, the A- (B-) sublattice structure plays decisive role, i.e., the distribution of electronic charge of the edge states becomes finite only one sublattice sites including the outermost sublattice. Recently, graphene nanoribbons were fabricated by e-beam lithography [2] and unzipping of carbon nanotubes [3], and were synthesized using bottom-up processes [4]. Furthermore, quite recently, the edge states in graphene nanoribbons were confirmed by STM/STS measurement [5].

On the other hand, boron and nitrogen atoms behave as acceptors and donors, respectively. Therefore, boron-carbon-nitride, i.e., graphene sheet doped with B and N, should show interesting electronic properties with controllability by doping. BC_2N sheet is organic analogous of graphene, which can be regarded as one of example of boron-carbon-nitride. Graphite-like BC_2N was synthesized using chemical vapor depositions of boron trichloride, BCl_3, and acetronitrile, CH_3CN [6]. The electronic properties of BC_2N sheets depend on the atomic arrangement [7]. The electronic properties of nanoribbons made with BC_2N were investigated by several authors [8]. However, there are no reports on the presence of the flat bands and edge states in BC_2N nanoribbons.

In this paper, we investigate the electronic properties of BC_2N nanoribbons with zigzag edges using a tight binding model. In the tight-binding model, B and N atoms are described by higher and lower site energy, E_B and E_N, compared with that of C atom, E_C, respectively [9]. Let N be a number of the zigzag lines. We shall consider three different structures of BC_2N nanoribbons with zigzag edges as shown in the left part of Fig. 1 (a). In this figure, B and N atoms are indicated by the black and white circles, and C atoms are located the empty vertices. It should be noted that atoms are arranged as B-C-N-C along the zigzag line in these BC_2N nanoribbons.

Figure 1 (b) shows calculated results of the band structures of BC_2N nanoribbons for N = 10. We observed the flat bands at E = 0. However, we confirm that the flat bands are absent if atoms are not arranged as B-C-N-C along the zigzag lines. Therefore, we can conclude that B-C-N-C arrangement along the zigzag line is necessary to obtain the flat bands. In the right part of Fig. 1 (a), the local density of states (LDOS) at E = 0 for several structures are shown by the circles. In this figure, the radii of the circles are proportional to the magnitude of the LDOS at each site. The electronic charge is localized at the BC_2N nanoribbons edges, showing the presence of the edge states. As discussed below, the edge states in BC_2N nanoribbons is different from those in conventional graphene nanoribbons.

In the model-1, the charge distributions at the both edges are different each other, i.e., the charge distribution at the edge, where the outermost sites are occupied with C atoms, is similar to that at the conventional zigzag edge, while the charge of the edge states at the edge, where the outermost sites are occupied with B and N atoms, distributes the both sublattice sites. Recently, Kaneko et al. showed that the edge states in zigzag graphene nanoribbons are robust on the substitution of outermost C atoms with B and N atoms alternately [10]. However, such substitution causes change in charge distribution, i.e., the sublattice structure is broken [10]. The edge states at the edge, where the outermost sites are occupied with B and N atoms alternately, are similar to those discovered by Kaneko et al. [10]. In the model-2 nanoribbon, the charge distribution of the edge states is similar to that of graphene nanoribbons, but the sublattice structure is broken inside the nanoribbons. In the model-3 nanoribbon, the charge distributes over both sublattice sites, showing the similarity of those discovered by Kaneko et al. [10].

In this paper, we also performed the first-principles calculations based on the density functional theories within projector-augmented wave method and the local density approximation implemented in VASP code. We shall discuss the comparison of the results within the tight-binding model with those within the density functional theories.

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Figure

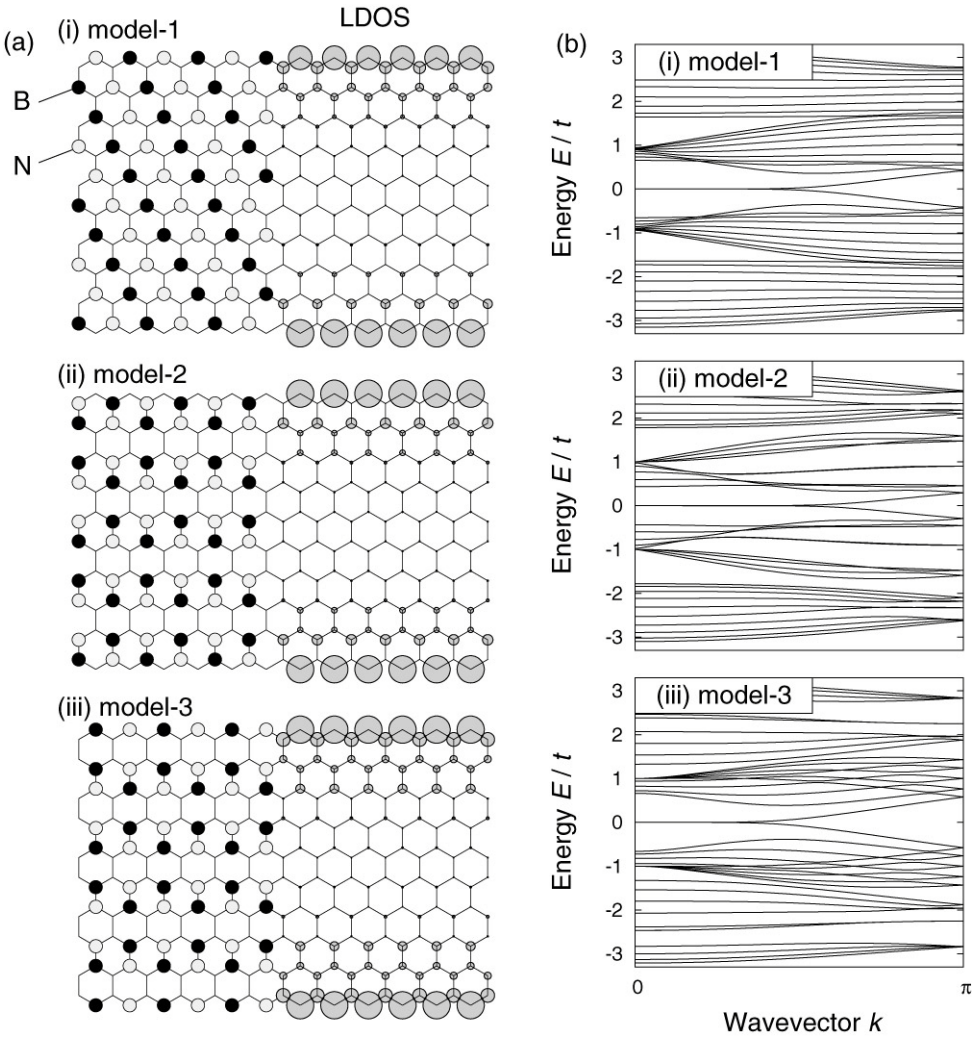

Fig. 1: (a) Schematic illustration of BC_2N nanoribbons (left side) and corresponding LDOS at E=0 for N=10 (right side). In this schematic illustration, the black and white circles represent B and N atoms, respectively. (b) The band structures of BC_2N nanoribbons with N=10.