Topological Edge States Induced by Zak’s Phase in A₃B Monolayers

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In crystalline systems, charge polarization is related to Zak’s phase determined by bulk band topology. Nontrivial charge polarization induces robust edge states accompanied with fractional charge. In Su-Schrieffer-Heeger (SSH) model, it is known that the strong modulation of electron hopping causes nontrivial charge polarization even in the presence of inversion symmetry. Here, we consider a bi-atomic honeycomb lattice to introduce such strong modulation, i.e., A₃B sheet. By tuning hopping ratio and onsite potential difference between A and B atoms, we show that topological phase transition characterized by Zak’s phase occurs. Furthermore, we propose that C₃N and BC₃ are the possible realistic materials on the basis of first-principles calculations. Both of them display topological edge states induced by Zak’s phase without spin-orbital couplings and external fields unlike conventional topological insulators.

I. INTRODUCTION

Concept of topology leads to a new class of electronic materials, such as topological insulators topological crystalline insulators and Weyl semimetals. In topological materials, topologically protected edge states (TES) emerge owing to nontrivial bulk band topology. These TES are robust to defects and edge roughness, and can be exploited for applications to low-power-consumption electronic and spintronic devices. One origin of TES is nonzero Berry curvature introduced by spin-orbit couplings. Berry curvature is a geometric field strength in momentum space. Its integration over momentum space yields magnetic monopole that is characterized by Chern number.

Recently two of us have found that, even under zero Berry curvature, Berry connection – a geometric vector potential whose curl yields Berry curvature – can also lead to TES. Integration of Berry connection over momentum space (also called as Zak’s phase) results in an electric dipole moment that generates robust fractional surface charges. Such dipole field related to Zak’s phase brings a new type of topological materials, i.e., topological electrides.

To obtain nonzero Zak’s phase even in the presence of inversion symmetry, modulation of electron hopping is necessary. Employing Su-Schrieffer-Heeger (SSH) model on two-dimensional (2D) square lattice, nontrivial Zak’s phase emerges when the inter-cellular hopping is larger than the intra-cellular hopping. This can be successfully demonstrated in the photonic system by mimicking the electronic tight-binding model. In addition, this idea can also be extended to honeycomb lattice systems with Kekulé pattern. However, no realistic materials of nonzero Zak’s phase have been proposed in this framework yet. Also, the model proposed in Ref. 19 is hard to apply for designing atomistic model, since it demands strong hopping modulation in monatomic sheets.

To overcome this difficulty, we consider biatomic system of honeycomb lattice, i.e., A₃B atomic sheet. We show that TES emerge owing to different electron hopping and onsite potentials between A and B atoms. Furthermore, we propose two possible realistic materials, i.e., C₃N and BC₃ based on first-principles calculations. Both C₃N and BC₃ display TES induced by Zak’s phase. Remarkably, both BC₃ and C₃N have already been successfully synthesized by several experiments.

The paper is organized as follows. In Sec. II, we relate charge polarization to Zak’s phase in terms of Berry connection in 2D crystalline systems. We especially discuss the cases where energy bands are degenerate. In Sec. III, we investigate electronic states of A₃B monolayer and their zigzag nanoribbon (NR) on the basis of tight-binding model. We show the bulk-boundary correspondence, i.e., emergence of TES and nonzero Zak’s phases. In Sec. IV, we analyze the electronic structures of C₃N and BC₃ sheets and their nanoribbons on the basis of first-principles calculations. We verify the existence of TES in energy bands for π electrons in these materials. We summarize our results in Sec.V.

II. CHARGE POLARIZATION AND ZAK’S PHASE

Charge polarization can be regarded as geometric center of electronic wavefunctions. For 1D crystalline system, the charge polarization of n-th energy band is given as a Wannier center, i.e., $P^n = \langle w_n(x) | x | w_n(x) \rangle$, where $w_n(x)$ is a Wannier function of n-th energy band. Owing to gauge freedom of Wannier functions, $P^n$ is well-defined up to a lattice constant.

To relate $P^n$ to Berry connection, one can apply Fourier transformation to $w_n$ and $x$, which result in

$$P^n = \frac{1}{2\pi} \int_0^{2\pi} \langle \psi_n | i \partial_k | \psi_n \rangle dk,$$

where $\psi_n$ is the periodic part of Bloch function of n-
th energy band, and $A^n = \langle \psi_n | i \partial k | \psi_n \rangle$ is Berry connection. We refer to the integration part of Eq. (1) as Zak’s phase. In a finite chain, fractional charge $P = \pm \sum_{n=0}^{n_{\text{occ}}} P^n$ accumulate at the ends of the chain, where the summation is taken over all the occupied energy bands. When inversion symmetry is present, $P^n$ is quantized to 0 or 1, and is determined by the winding number of associated sewing matrix of wavefunctions. In following discussions, we interchangeably use Zak’s phase and “charge polarization” to mean same quantity.

Now we extend Eq. (1) to 2D crystalline systems. Suppose that there are two independent directions denoted as $i$ and $j$. In 2D systems, charge polarization becomes a vector such as $\mathbf{P}^n = (P^n_i, P^n_j)$, and $P^n_i, P^n_j$ depend on the wavevectors $k_i(=k)$, $k_j$ along directions $j, i$, respectively. Charge polarization along $i$-direction is given as

$$ P^n_i(k) = \frac{1}{|P|} \int_A A^n(k_i, k_j) \cdot \mathbf{n}_i dk_i, \tag{2} $$

where $P$ is a straight path connecting two equivalent $k$ points in momentum space, $\mathbf{n}_i$ is a unit vector for $i$-direction and $A^n = \langle \psi_n | i \partial k | \psi_n \rangle$ is Berry connection of $n$-th energy band in 2D momentum space. Similar to 1D systems, fractional charge $\sum_{n=0}^{n_{\text{occ}}} \mathbf{P}^n \cdot \mathbf{n}$ accumulates on the edge if a material possesses finite charge polarization. The derivation of Eq. (2) is given in supplement of Ref. [33].

When inversion symmetry is present, $P^n_i(k = 0)$ is simply determined by the parities at inversion-invariant points in BZ. In hexagonal lattice, polarization along $i$-direction at $k = 0$ is given as

$$ P^n_i(k = 0) = \frac{1}{2}(q^n_i \text{ modulo } 2), \quad (-1)^n_i = \frac{\eta^n(M_i)}{\eta^n(\Gamma)}, \tag{3} $$

where $i = 1, 2$, and $\eta^n(k)$ is the eigenvalue of $\pi$ rotation along the out-of-plane direction for $n$-th energy band.

According to Stoke’s theorem, the relation of $P^n_i(k_a)$ and $P^n_i(k_b)$ is given by

$$ \Delta P^n_{k_a, k_b} = P^n_i(k_a) - P^n_i(k_b) = \frac{1}{2\pi i} \int_{\mathcal{F}} F^n(k, k') dk dk', \tag{4} $$

where $F^n = \partial_i A_j - \partial_j A_i$ is Berry curvature of $n$-th energy band, and the integration is taken over the area $|\{k_a - k_b \times \mathcal{P}\}|$. Combining Eqs. (3) and (4), one can obtain $P^n_i(k)$ at arbitrary $k$ from the parities and Berry curvature of wavefunction of $n$-th energy band.

In degenerate systems, both Berry connection and Berry curvature are written in the non-abelian forms. In this situation, we need to use more generic gap-opening condition: $E_n(k) \neq E_n(k)$ for all $k$, where $n \in I$ and $n' \notin I$ for $I = \{n_1, n_2, \ldots, n_{\text{occ}}\}$. However, when we consider Zak’s phase exactly at degenerate $k$ point, even the generic gap-opening condition cannot be satisfied. In such the cases, we apply an inversion-symmetry-preserving perturbation to lift those degeneracies, as far as the perturbation does not alter the order of parities of energy bands at inversion-invariant $k$ point. If such the generic gap-opening condition cannot be satisfied by imposing the perturbation, Eqs. (3) and (4) can be applied only for the region without degeneracies.

Let us take graphene as an example of degenerate systems. Figure 1(a) displays graphene lattice structure and its bulk energy bands, and Fig. 1(b) displays its corresponding BZ where yellow and blue areas indicate valid and invalid ranges of applying Eqs. (3) and (4), respectively. In graphene, energy bands are degenerate at $K$ and $K'$ points guaranteed by inversion symmetry, and Eqs. (3) and (4) can only be applied in the range $-\pi/3 < k < \pi/3$, if $\mathbf{b}_1$ is chosen in the direction of
charge polarization, \( i.e. P_1(k) \). Outside this range, only Eq. (2) is applicable.\(^{22}\)

III. TIGHT-BINDING MODEL

Let us introduce a tight-binding model for \( \pi \) electrons up to nearest-neighbor hopping on a biatomic honeycomb lattice \( A_3B \). We show that TES appear due to nonzero Zak’s phase in \( A_3B \) atomic sheet. The lattice structure of \( A_3B \) is displayed in Fig. 2(a), whose unit cell is a rhombus made up by six \( A \)-atoms (black circles indexed from 1 to 6) and two \( B \)-atoms (white circles indexed as 1 and 2). We denote hopping between \( A \)-\( A \) (\( A \)-\( B \)) atoms as \(-\gamma \) (\(-\gamma' \)), and onsite potential of \( A \) (\( B \)) atoms as \( V_A \) (\( V_B \)). Figure 2(b) shows the corresponding first Brillouin zone (BZ), where the reciprocal lattice vectors are \( b_1 = \frac{2\pi}{\sqrt{3}}(0, 2) \) and \( b_2 = \frac{2\pi}{\sqrt{3}}(\sqrt{3}, 1) \).

The tight-binding Hamiltonian of \( A_3B \) can be written as

\[
\hat{H} = \sum_{m,n} \sum_{j,j'} \sum_{\alpha} f^\alpha(j, j') a_{m,j}^\dagger \alpha_{m,j} \gamma\alpha \sum_{m',m''} a_{m',m''}^\dagger b_{m''} + \text{H.c.},
\]

where \( m, n \) are unit cell indices, \( j, j' \) (\( j, j' = 1, 2 \cdots 6 \) for \( A \) atoms and \( j, j' = 1, 2 \) for \( B \) atoms) are indices of atomic orbitals in each unit cell, and \( \alpha = a, b, a^\dagger, b^\dagger \) and \( a(b) \) mean creation and annihilation operators of \( p_e \) electronic orbital on atom \( A \) (\( B \)), respectively. \( \cdot \cdot \cdot \cdot \) indicates the summation between the nearest-neighbor sites. Here

\[
f^\alpha(j, j') = \begin{cases} 
-\gamma & \text{if } j \neq j' \text{ and } \alpha = a, \\
V_A & \text{if } j = j' \text{ and } \alpha = a, \\
V_B & \text{if } j = j' \text{ and } \alpha = b.
\end{cases}
\]

Note that, the electronic states of graphene recover when \( \gamma = \gamma' \approx 3 \text{eV} \) and \( V_A = V_B = 0 \).

A. Symmetry analysis

Before showing the detailed results, we briefly look at the symmetries of \( A_3B \) structure. This structure has time-reversal and \( C_{6v} \) point group symmetries. The two \( B \) atoms in unit cell play similar role of two nonequivalent sublattices in graphene, since both of them are mutually transformed under \( C_6 \) rotation. On the other hand, the six \( A \) atoms in unit cell play similar role of benzene rings in hexagonal 2D SSH model.\(^{22}\) Thus, two of energy bands of \( A_3B \) resemble energy bands of graphene, and the other six energy bands resemble energy bands of hexagonal 2D SSH model discussed in Ref. \(^{13}\).

As there are both time-reversal and inversion symmetries, Berry curvature in \( A_3B \) is guaranteed to vanish everywhere except energy-degenerate \( K \) and \( K' \) points in momentum space. To apply Eqs. (3) and (4), we lift these degeneracies by adding onsite potentials \( \delta_m \approx m\gamma/100 \) (\( m = 1, 2, 3 \)) on \( A \) atoms to break \( C_6 \) point group symmetry as shown in the inset of Fig. 2(a). After imposing such the perturbation, degeneracies are lifted except for the central two energy bands around \( E = 0 \) at \( K \) and \( K' \) points. Thus, when one of the central two energy bands is occupied, Eqs. (3) and (4) can be applied only for \(-2\pi/3 < k < 2\pi/3 \).

B. Effect of variable hopping

Figures 3(a)-(c) show energy band structures of \( A_3B \) sheet for different ratios of \( \gamma' / \gamma \) with \( V_A = V_B = 0 \). The red and blue circles at \( \Gamma \) and \( M_1 \) points indicate even and odd parities of wavefunctions. Yellow regions indicate that Zak’s phase along \( b_1 \) is \( \pi \), resulting in charge polarization of 1/2.

In Figs. 3(a)-(c), \( P_{\gamma}^n(k = 0) \) is calculated from the parities of wavefunction for \( n \)-th energy band at \( \Gamma \) and \( M_1 \) points by applying Eq. (3). Note that all three nonequivalent \( M \) points have same parity. Then we obtain Zak’s phase at other \( k \) points by applying Eq. (4) except for the central two energy bands which have similar nature of graphene.

For the central two bands, they have degenerate points \( K \) and \( K' \) guaranteed by inversion symmetry. Thus, Equation (4) is applied for a limited range \(-2\pi/3 < k < 2\pi/3 \) where gap-opening conditions are satisfied. However, we cannot apply Eq. (4) for the path which go beyond the region \(-2\pi/3 < k < 2\pi/3 \) to relate with the region \( k < -2\pi/3 \) or \( k > 2\pi/3 \), because \( F^n \) is not well defined at the degenerate points. In this situation, only Eq. (2) is applicable for central two bands.\(^{22}\) Thus, if one of these two central energy bands is occupied, the value distribution of Zak’s phase is dissociated into two distinct regions as displayed by Fig. 1(b). Otherwise, Zak’s phase is uniform over whole BZ.

Same procedure can be applied for \( b_2 \) direction, and \( b_1 \) and \( b_2 \) directions are equivalent owing to \( C_{6v} \) point group symmetry.

As we see from Fig. 3, \( A_3B \) atomic layer always possesses finite Zak’s phase irrespective of the ratio between \( \gamma' \) and \( \gamma \). In case of \( \gamma' = \gamma \), Figure 3(b) reproduces the energy band structure of graphene, which possesses finite Zak’s phase around zero energy.\(^{22}\) In the case of \( \gamma' < \gamma \) [Fig. 3(a)], it is similar to the case of \( \gamma = \gamma' \). In the case of \( \gamma < \gamma' \) [Fig. 3(c)], besides graphene-like energy bands, upper and lower bands possess finite Zak’s phase due to band inversions. Thus, emergence of TES is expected in \( A_3B \) system for any ratio between \( \gamma' \) and \( \gamma \).

To show TES induced by Zak’s phase, we study the energy band structures of \( A_3B \) NRs. Figure 4(a) displays lattice structure of \( A_3B \) NR with zigzag edges. For zigzag NR the corresponding Zak’s phase is along \( b_1 \) or \( b_2 \) direction. We assume that all the edge atoms are terminated by hydrogen atoms and no dangling bond exists. The width of NR is given by number of zigzag chains \( N_z \).

In Figs. 4(b)-(d), we show the energy band structures
FIG. 2. (a) Lattice structure of $A_3B$ biatomic sheet. Shaded yellow rhombus indicates unit cell, which contains six A-atoms (black circles indexed as $1, \ldots, 6$) and two B-atoms (white circles indexed as 1 and 2). $a_1 = (a, 0)$ and $a_2 = (-a, \sqrt{3}a)$ are primitive lattice vectors. Inset displays non-uniform onsite potentials $\sigma_m \sim m\gamma/100$ ($m = 1, 2, 3$) on A atoms, which breaks $C_6$ point group symmetry and preserves inversion symmetry. (b) Corresponding first BZ of $A_3B$ atomic sheet.

$\mathbf{b}_1 = \frac{2\pi}{\sqrt{3}a}(0, 2)$ and $\mathbf{b}_2 = \frac{2\pi}{\sqrt{3}a}(\sqrt{3}, 1)$ are primitive reciprocal vectors.

FIG. 3. Energy band structures of 2D $A_3B$ sheet with (a) $\gamma' = \frac{1}{12}$, (b) $\gamma' = \gamma$, and (c) $\gamma' = 1.5\gamma$. Onsite potentials are considered to be zero, i.e. $V_A = V_B = 0$. Red (blue) circles at $\Gamma$ and $M_1$ points indicate the positive (negative) parity of wavefunction. Note that all three nonequivalent $M$ points have the same parity. The yellow regions indicate the range where Zak’s phase are nonzero.

of NR for different hopping ratios $\gamma'/\gamma$. It can be clearly observed that TES appear in the subband gap regions (indicated by yellow) where Zak’s phases are $\pi$. In case of $\gamma'/\gamma \leq 1$, TES appear within the central subband gap for zigzag NR. For $\gamma'/\gamma > 1$, band inversions occur in upper and lower energy regions away from $E = 0$, resulting in nonzero Zak’s phases and consequent emergence of TES. It is noted that the TES at $E=0$ only appear within the region $-2\pi/3 < k < 2\pi/3$ that is same as graphene zigzag NR. These zero energy edge states are nonbonding molecular orbitals, whose analytic form can be derived in similar manners of Refs. 37 and 38 as detailed in Appendix A. Outside this range, Zak’s phase cannot be calculated by Eqs. (3) and (4), which is shaded as blue.

C. Effect of onsite potential

In $A_3B$ sheet, onsite potentials of A and B atoms are different due to their distinct chemical elements. Here, we study effect of different onsite potentials on A and B atoms. The corresponding energy band structures are displayed in Figs. 5(a) and (b), where the yellow regions indicate nonzero Zak’s phase.

According to Fig. 5, $A_3B$ systems always possess non-trivial energy bands in either the upper or lower energy region depending on the values of $V_A$ and $V_B$. When $V_A < V_B$, the central and upper subband gaps have nonzero Zak’s phase as shown in Fig. 5(a). For $V_A > V_B$, the central and lower subband gaps have nonzero Zak’s phase as shown in Fig. 5(b). Thus, TES emerge in either upper or lower subband gaps when onsite potentials between A and B atoms are different.

Figures 5(a)-(c) show the energy band structures of
FIG. 4. (a) Lattice structure of A<sub>3</sub>B zigzag NR. Thick and thin bonds represent the intra-cell ($\gamma$) and inter-cellular ($\gamma'$) hopping, respectively. The yellow rectangle indicates unit cell. Energy band structures of A<sub>3</sub>B zigzag NRs for the hopping ratios $\gamma'/\gamma$ with (b) 1.0/1.5, (c) 1.0 and (d) 1.5. TES (red curves) appear in non-zero Zak’s phase (yellow shaded region). Blue shaded region indicates the ranges that Eqs. (3) and (4) cannot be applied.

FIG. 5. Energy band structures of 2D A<sub>3</sub>B biatomic sheet in presence of onsite potentials, $V_A$ and $V_B$. The parameter values are chosen as follows: (a) $V_A = -0.5\gamma$, $V_B = 0.5\gamma$, (b) $V_A = 0.5\gamma$, $V_B = -0.5\gamma$. Here red (blue) circles at $\Gamma$ and $M_1$ points indicate the positive (negative) parity of wavefunction. Yellow regions depict nonzero Zak’s phase. Note that, the hopping ratio $\gamma'/\gamma$ is 1 for all plots.

A<sub>3</sub>B zigzag NRs in presence of different onsite potentials between A and B atoms. TES appear in yellow shaded region where the Zak’s phase is nonzero. In case of $V_A < V_B$, TES appear in the central and upper energy regions. When $V_A > V_B$, TES appear in the central and lower energy regions. In presence of different onsite potentials, note that TES emerge in the energy regions away from $E = 0$ even when $\gamma' = \gamma$.

FIG. 6. Energy band structures of A<sub>3</sub>B zigzag NR for the following onsite potential values: (a) $V_A = -0.5\gamma$ and $V_B = 0.5\gamma$, (b) $V_A = 0$ and $V_B = 0$ and (c) $V_A = 0.5\gamma$ and $V_B = -0.5\gamma$. The yellow shaded region has nonzero Zak’s phase, where the TES (red curves) appear. Blue shaded region indicates that Eqs. (3) and (4) cannot be applied. Note that, the hopping ratio $\gamma'/\gamma$ is 1 for all plots.

IV. DENSITY FUNCTIONAL THEORY

So far, on tight-binding calculations, we have demonstrated that A<sub>3</sub>B sheet possesses nonzero Zak’s phase, which consequently induces TES. Here we investigate the electronic structure of C<sub>3</sub>N biatomic sheet as a realistic candidate with nonzero Zak’s phase on the basis of first-principles calculations using SIESTA.\textsuperscript{22}

The conditions of first-principles calculations are summarized as follows. Perdew-Burke-Ernzerhof (PBE) exchange and correlation functional have been considered within generalized gradient approximations with double zeta polarized (DZP) basis set. To avoid any interactions within adjacent unit cells, we have created sufficiently large vacuum regions in the non-periodic directions. The energy cut-off for real space mesh size is 400 Ry energy. The $k$-point sampling in BZ is taken over $30 \times 30 \times 1$ of Monkhorst-Pack grid for the relaxation of 2D C<sub>3</sub>N sheet, and $70 \times 1 \times 1$ for that of C<sub>3</sub>N zigzag NRs. The atomic positions are relaxed until the force on each atom reaches 0.04 eV/Å. For calculations of electronic states for optimized NRs, we take the $k$-points sampling in BZ as $300 \times 1 \times 1$ of Monkhorst-Pack grid.

Figure 7(a) shows energy band structure of C<sub>3</sub>N sheet, where Fermi energy is zero. Blue curves indicate the energy bands that originate from $\pi$ electrons, which nicely match with the energy band structures obtained by using tight-binding model shown in Fig. 4(b). Since nitrogen
has one excess electron than carbon, it should be noted that the Fermi energy is upward shifted owing to the electron doping by nitrogen substitution. From Fig. 5(b), the middle and low subband gaps possess finite Zak’s phases. Thus, TES induced by Zak’s phase are expected to appear in C$_3$N.

Figure 7(b) shows energy band structure of C$_3$N zigzag NR with $N_z = 20$. Red and blue curves indicate the energy bands arising from $\pi$ electrons. Especially, red curves indicate TES. Edge states of partial flat bands appear near $-2.5$eV, $-7.0$eV and $-8.0$eV, consistent with the tight-binding calculations [see Fig. 6(c)]. Wavefunction of the flat band near $-2.5$eV at $\Gamma$ point is shown in Fig. 7(c), which suggests strong localization of electrons near edges. In addition, we also show wavefunction of the flat band near $-7.0$eV at BZ boundary ($k = \pi/a$) in Fig. 7(d), which displays localized wavefunction at ribbon edges.

Thus, C$_3$N can be considered as one possible realistic material that possess TES protected by nonzero Zak’s phase. Especially the TES near $-2.5$eV have similar electronic properties of edge states in zigzag graphene edges, they provide a perfectly electronic transport channel which is robust to edge roughness and impurities as long as the intervalley scattering are suppressed. Besides C$_3$N, we also investigate the electronic structure of honeycomb BC$_3$ sheet on the basis of first-principles calculations. The details are presented in Appendix B.

V. SUMMARY

In summary, we have studied the electronic structures of A$_3$B biatomic sheet on the basis of tight-binding model. This system shows topological phase transition by tuning the electron hopping and onsite potentials. Instead of Berry curvature, this topological phase transition is characterized by non-zero Zak’s phase, which induces TES. Based on our tight-binding analysis, we further propose realistic material candidates, e.g., C$_3$N and BC$_3$. Within first-principles calculations we successfully demonstrate the emergence of TES in such materials.

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FIG. 7. (a) Energy band structure of C$_3$N sheet. Blue curves indicate $\pi$-electronic bands. (b) Energy band structure of C$_3$N zigzag NR. Blue and red curves indicate $\pi$-electronic bands. Especially, red curves indicate TES. Wavefunction of TES near the edge at energies of (c) $-2.5$eV and (d) $-7.0$eV.

FIG. 8. Lattice structure of A$_3$B biatomic sheet. Each unit cell contains eight sublattices denoted by $P,Q,R,S,T,U,V,W$. 
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Appendix A: Edge states

As we have shown in Figs. 4(b)-(d), zigzag A3B NRs have the partial flat bands at $E = 0$ for $|k| \leq 2\pi/3$, where electrons are localized near the edges, i.e. edge states. In this section, we derive the condition of $k$-region for which edge states can exist in zigzag A3B NRs by constructing an analytic solution of edge state for semi-infinite A3B sheet with a zigzag edge, according to the manner presented in Refs. 37 and 38.

In order to derive the wavefunctions of the edge states, we divide the graphene lattice into eight sublattices, namely, $P, Q, R, T, U, V$ and $W$ as shown in Fig. 8. We define the wavefunction at $m$-th row as

$$
\Psi_m = (\psi_{m,P}, \psi_{m,Q}, \ldots, \psi_{m,V}, \psi_{m,W}).
$$

(A1)

Here we have assumed the translational invariance along the ribbon direction.

Thus, the set of equation of motions for nearest-neighbor tight-binding model can be written as

$$
\begin{align*}
\psi_{m,P} &= -\gamma^* \eta \psi_{m,S} - \gamma \eta^* \psi_{m,Q} - \gamma \eta \psi_{m,U}, \\
\psi_{m,Q} &= -\gamma^* \eta \psi_{m,R} - \gamma \eta^* \psi_{m,P} - \gamma \eta \psi_{m,R}, \\
\psi_{m,R} &= -\gamma \eta \psi_{m,Q} - \gamma^* \eta^* \psi_{m,W} - \gamma^* \eta \psi_{m,S}, \\
\psi_{m,S} &= -\gamma \eta \psi_{m,R} - \gamma \eta^* \psi_{m,R} - \gamma^* \psi_{m,R}, \\
\psi_{m,T} &= -\gamma \eta \psi_{m,W} - \gamma \eta^* \psi_{m,S} - \gamma \eta \psi_{m,Q}, \\
\psi_{m,W} &= -\gamma \eta \psi_{m,P} - \gamma^* \eta \psi_{m,T} - \gamma \eta \psi_{m,U}, \\
\psi_{m,U} &= -\gamma \eta \psi_{m,Q} - \gamma \eta^* \psi_{m,L} - \gamma \eta \psi_{m,V}, \\
\psi_{m,V} &= -\gamma \eta \psi_{m,R} - \gamma \eta^* \psi_{m,W} - \gamma \eta \psi_{m,U}, \\
\psi_{m,U} &= -\gamma \eta \psi_{m,W} - \gamma \eta^* \psi_{m,S} - \gamma \eta \psi_{m,Q}.
\end{align*}
$$

(A2)-(A9)

Here $\eta = e^{ik/4}$ is the Bloch phase, and $\eta^*$ is its complex conjugate. Here we have defined the lattice constant as unit of length. Since we are interested in the wavefunctions of zero-mode ($\epsilon = 0$), we introduce the conditions:

$$
\begin{align*}
\psi_{m,P} &= 0, \psi_{m,R} = 0, \psi_{m,T} = 0, \psi_{m,V} = 0.
\end{align*}
$$

(A10)

We have numerically confirmed that the wavefunction at $(m, P), (m, R), (m, T)$ and $(m, V)$ sites for arbitrary $m$ is identically zero. Therefore, we can simplify the set of equation of motions:

$$
\begin{align*}
0 &= -\gamma \eta \psi_{m,S} - \gamma^* \eta^* \psi_{m,Q} - \gamma \eta^* \psi_{m,U}, \\
0 &= -\gamma \eta \psi_{m,Q} - \gamma \eta^* \psi_{m,W} - \gamma^* \psi_{m,S}, \\
0 &= -\gamma \eta \psi_{m,R} - \gamma \eta^* \psi_{m,U} - \gamma^* \psi_{m,T}, \\
0 &= -\gamma \eta \psi_{m,R} - \gamma \eta^* \psi_{m,W} - \gamma^* \psi_{m,V}.
\end{align*}
$$

(A11)-(A14)

From these equations, the wavefunction at $(m, U)$ and $(m, W)$ sites can be related to those at $(m, Q)$ and $(m, S)$ sites as following,

$$
\begin{align*}
\psi_{m,U} &= \eta \psi_{m,Q} + \frac{\eta'}{\gamma^*} \psi_{m,S} \\
\psi_{m,W} &= \eta^* \psi_{m,Q} + \frac{\eta'}{\gamma} \psi_{m,S}.
\end{align*}
$$

(A15)-(A16)

Therefore we obtain the following recurrence equations for charge densities between adjacent cells,

$$
\begin{align*}
|\psi_{m+1Q}|^2 &= 4|\psi_m Q|^2 (1 + \cos k)^2, \\
|\psi_{m+1S}|^2 &= 4|\psi_m S|^2 (1 + \cos k)^2.
\end{align*}
$$

(A17)-(A18)

Since the wavefunctions have to converge in the bulk region, the prefactors of above equations have to satisfy the following condition,

$$
4(1 + \cos k)^2 \leq 1.
$$

(A19)

Immediately, we obtain the condition for wavenumber to satisfy $\epsilon = 0$,

$$
-\frac{2\pi}{3} \leq k \leq \frac{2\pi}{3}.
$$

(A20)

This is nothing more than the region of flat bands as shown in Fig. 8.
Appendix B: Mixture of hopping energy and onsite potential

In Sec. [III] we discussed the effect of hopping energy and onsite potential separately. Here, we take into account both hopping energy and onsite potential simultaneously. The results well reproduce the energy band structures of BC$_3$ sheet.

Figure [3] (a) and (b) show the energy band structures of BC$_3$ sheet and zigzag BC$_3$ NR ($N_z = 8$), respectively, as obtained within first-principles calculations. Here, red curves indicate electron bands. TES appear near $E = 2.5$eV. If we choose the parameters $\gamma' = \gamma/1.3$, $V_A = -0.5V$, $V_B = 0.5V$ for tight binding model, the energy band structure of BC$_3$ NR is well reproduced as shown in Fig. [2] (c). Figures [2] (d) and (e) are the energy band structures of A$_3$B zigzag NRs obtained by tight-binding model, where TES clearly appear.