How to tune the tilt of a Dirac cone by atomic manipulations?

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We decipher the microscopic mechanism of the formation of tilt in the two-dimensional Dirac cone of $8Pmmn$ borophene sheet. With the aid of ab initio calculations, we identify relevant low-energy degrees of freedom on the $8Pmmn$ lattice and find that these atomic orbitals reside on an effective honeycomb lattice (inner sites), while the high-energy degrees of freedom reside on the rest of the $8Pmmn$ lattice (ridge sites). Local chemical bonds formed between the low- and high-energy sublattices provide the required off-diagonal coupling between the two sectors. Elimination of high-energy ridge sites gives rise to a remarkably large effective further neighbor hoppings on the coarse grained (honeycomb) lattice of inner sites that determine the location and tilt of the Dirac cone. This insight based on real space renormalization of the $8Pmmn$ lattice enables us to design atomic scale substitutions that can lead to desired change in the tilt of the Dirac cone. We furthermore encode the process of renormalization into an effective tight-binding model on a parent honeycomb lattice that facilitates numerical modeling of various effects such as disorder/interactions/symmetry-breaking for tilted Dirac cone fermions of $8Pmmn$ structure. The tilt parameters determine a spacetime metric, and therefore the ability to vary the tilt over distances much larger than the atomic separations opens up a paradigm for fabricating arbitrary solid-state spacetimes.

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Introduction. Every periodic structure in quantum condensed matter is mounted on a mathematical object called lattice. Irrespective of which atoms one wishes to place on the sites of a given lattice, they come in 230 possible structures [1]. The presence of lattice breaks translation and rotation, and some times parity and time reversal invariance of the vacuum [2]. The lattice therefore breaks the Poincaré group [3] thereby the connection between spin and statistics of the particles is lost and therefore one may have fermions with integer spin that is enforced by the irreducible representations of its space group (SG) [4]. Is there any other interesting consequence that can be associated with the underlying SG? To set the stage for answering this question, let us start by a profound observation [2]: Consider a simple quantum mechanical hopping process on a lattice and think about the wave equation in the continuum limit. On the square lattice the Hamiltonian becomes $-\hbar^2 \nabla^2/(2m^*)$, while on the honeycomb lattice it becomes $i\hbar v_F \sigma \cdot \nabla$, namely the massless Dirac Hamiltonian [5]. Therefore despite that in the continuum limit the lattice spacing is immaterial, but still the microscopic symmetries of the pertinent SG are imprinted on the long-distance behavior and decide whether the structure of spacetime is Galilean or Minkowski. This can be regarded as an example of metamorphosis of atomic scale symmetry (SG) to a long-distance geometrical structure.

Then an interesting question would be, how does the duality between the microscopic structure and the long-distance (low-energy) characteristics manifest in more complicated lattice structures? The long-distance behavior of interest for us is the tilted Dirac cone band whose Hamiltonian is $\propto (\sigma \cdot \nabla) + \sigma_0 \zeta \cdot \nabla$ [6–11] where $\sigma_0$ is the $2 \times 2$ unit matrix. A vector-looking quantity $\zeta$ here determines the tilt of the Dirac cone. But at a much deeper level, it can be encoded into an emergent spacetime metric $ds^2 = -(v_F dt)^2 + (dx - \zeta v_F dt)^2$ [9, 10, 12–17], where $v_F$ is the Fermi velocity. In this work we decipher the microscopic mechanism that determines the tilt parameter $\zeta$. For this purpose we focus on the SG number 59 that describes the $8Pmmn$ structure 1 of borophene [9, 19]. We show that in this structure, the low-energy and high-energy degrees of freedom are nicely separated into two sublattices denoted by gray and teal circles in Fig. 1(a), respectively.

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1 The tilted Dirac cone has been experimentally observed in the so called [18]
Protection of the Dirac node. The relevant orbitals in the boron (as well as C) atom are 2p orbitals. The possibility of formation of $sp^2$ and $sp^3$ hybridization establishes the honeycomb lattice [20], and structures such as 8Pmmm that involve buckled honeycomb networks as natural lattices for these atoms. As can be seen in Fig. 1(a), there is a backbone (buckled) honeycomb sub-lattice denoted with gray circles that are called inner (I) sites. The rest of the lattice are called ridge (R) sites and are denoted by teal circles. First principle calculations indicate that the resulting Dirac cone is tilted [21, 22] which is shown as red (low-energy) band in Fig. 1(b) and the three dimensional reconstruction of the band structure is shown in panel (c). The first thing that the 8Pmmm SG implies about the tilted Dirac cone is that at X and Y points in the Brillouin zone (BZ) of Fig. 1(d), two bands ”stick together” (as Kittel puts it [23]) where the two-dimensional irreducible representations are protected by non-symmorphic elements [23]. Then the compatibility relations gives the qualitative band picture of cat’s cradle shape [24] shown in panel (d). For pedagogical details of the derivation of this figure with group theory methods see the supplementary material (SM).

Of course the protection of the tilted Dirac cone by the underlying SG is enough for many purposes. But it does not explain why and how the tilt parameter $\zeta$ is formed. In order to “manipulate” the tilt of the Dirac cone at will, one needs a microscopically detailed understanding of the root cause of formation of tilt in the Dirac cone. To achieve this, we need to identify the low-energy degrees of freedom that give rise to the tilted Dirac cone dispersion. For this purpose in Fig. 1(e) we have plotted an orbital projected representation of the band structure that resolve the contribution of atoms 2 (I) and 5 (R). As can be seen, the dominant contributions to the tilted Dirac dispersion comes from the $p_z$ orbitals of the I atoms (top left plot in panel (e)). The R atoms also contribute via their $p_z$ and $p_x$ orbitals (bottom left and center). The remaining two boxes on the top row indicate little contributions from the $p_x$ and $p_y$ orbitals of the I atoms that is due to buckling of the honeycomb sublattice.
FIG. 2: (a) The lattice structure, unit cell, and hopping processes in the 8Pmmn lattice and (b) its BZ with two tilted Dirac cones. (c) The "effective" honeycomb lattice of I atoms (low-energy degrees of freedom) obtained by elimination of R sites from the 8Pmmn lattice. (d) two representations (rhombus and hexagonal) of the BZ of the effective honeycomb lattice. The effective second/third neighbor hoppings (green/red) in (c) arise from the corresponding hopping path in (a) via the process of renormalization (see the text). As indicated in (d), the red (third neighbor) hopping shifts the Dirac cone, while the green (second neighbor) hoppings tilt the cone.

TABLE I: (top) ab initio hopping matrix elements (in eV) for borophene and C-doped borophene obtained from Wannier functions. Conventions for labeling of the hopping matrix elements are given in Fig. 2(a). (bottom) Renormalized parameters of Fig. 2(c). ζ is the tilt parameter and $k_D/k_Y$ quantifies the location of Dirac node.

|        | $t_{36}$ | $t_{65}$ | $t_{33}$ | $t_{81}$ | $t_{38}$ | $t_{72}$ | $t_{78}$ |
|--------|----------|----------|----------|----------|----------|----------|----------|
| B$_8$  | 2.09     | -2.66    | 2.09     | -1.87    | -1.87    | -1.87    | -2.54    |
| B$_6$C$_2$-I | 1.93     | -2.52    | 1.96     | -1.52    | -1.52    | -1.55    | -2.34    |
| B$_6$C$_2$-R | 2.14     | -2.33    | 2.12     | -2.23    | -2.21    | -2.20    | -2.43    |

|        | $t$      | $t^p$    | $t^z$    | $t$      | ζ        | $k_D/k_Y$ | ζ$^{DPT}$ |
|--------|----------|----------|----------|----------|----------|-----------|-----------|
| B$_8$  | -2.21    | -2.36    | -1.07    | -1.99    | -2.51    | 0.46      | 0.48      | 0.49      |
| B$_6$C$_2$-I | -2.37    | -1.75    | -0.95    | -1.62    | -2.05    | 0.36      | 0.66      | 0.47      |
| B$_6$C$_2$-R | -2.05    | -2.49    | -1.09    | -2.24    | -2.85    | 0.59      | 0.32      | 0.66      |

In panel (a) of Fig. 2 we have labeled atomic hopoings paths with green and red dashed lines that connect I sites by virtual hoppings through R sites. There is only first neighbor direct hopping between the I sites denoted by black arrows. The appropriate atomic orbitals involved in forming the above microscopic $t_{ij}$ hoppings can be extracted from the DFT calculation. Working in a gauge that all $t_{ij}$’s are real, the hermiticity implies $t_{ij} = t_{ji}$. Panel (b) depicts the BZ of original 8Pmmn lattice. The insight from the projected bands in the left and center columns in the second row of Fig. 1(e) is that both $p_x$ and $p_z$ orbitals of the R atoms are of comparable importance and must be incorporated into the atomic scale computation of the $t_{6,5}$ (dark green) and $t_{87}$ (light green). Similarly the first column of Fig. 1(e) suggests that the $p_z$ orbitals of R and I atoms dominate in $t_{3,6} = t_{35}$ hopping process. Tab. I shows the calculated values of these hopping parameters for pristine borophene (B$_8$) and C-doped borophene B$_6$C$_2$ using Wannier function [25, 26]. The purpose of substituting C for B is to study its effect in the tilt of the Dirac cone. The substituted carbon dimers are placed in R and I positions, respectively. Using these parameters one can re-construct the ab initio bands with four $p_z$ orbitals of four inner sites, and eight $p_x$ and $p_z$ orbitals of ridge sites. The nice coincidence of the original DFT bands with Wannier-interpolated bands in Fig. 8 of SM shows that the obtained $t_{ij}$ values are reliable and the used atomic orbitals are adequate. Although such a atomic picture might be satisfactory if one wishes to focus on the low-energy features of the tilted Dirac cone around the Fermi surface, but still working with a 12-band Hamiltonian is neither convenient, nor the essential long-range physics depends on so many short-distance details. To achieve an effective two-band model, we need to decimate the 8Pmmn lattice into an effective honeycomb lattice shown in Fig. 2(c) whose two possible BZ’s are depicted in panel (d). On such a coarse grained lattice, the virtual atomic hopping paths will be replaced by
effective hoppings of the same color in panel (c). The connection between these effective hoppings and atomic hoppings \( t_{ij} \) is a nice example of renormalization.

Renormalization via molecular orbitals: Anderson in his book maintains that renormalization is one of the pillars of condensed matter physics [27]. In this section we will show that the same concept is in a remarkable way encoded into a local quantum chemistry of the \( 8\text{Pmmn} \) borophene. Since we are not interested in higher energy features that take place away from the tilted Dirac node, we build an effective picture based on Fig. 2(c) where the "effective" hoppings must be evaluated from the atomic scale data in the upper part of Tab. I. The low-energy degrees of freedom are dominated by the \( p_z \) orbitals of the I sites. So we decimate the \( 8\text{Pmmn} \) lattice by elimination of the R sites. In doing so, the effective coarse-grained lattice becomes the honeycomb lattice in Fig. 2(c). The nearest neighbor hoppings denoted by black arrows take place within the low-energy subspace and are responsible for the formation of a parent Dirac cone from the \( p_z \) orbitals of the I sites. Slight anisotropy in the black arrows is known to shift the location of the Dirac cone [28] within the rhombus BZ of panel (d) that we ignore here. Green/red hopping processes are associated with the second/third neighbors of the honeycomb backbone that arise via the renormalization from the corresponding atomic process \( t_{ij} \) of panel (a).

|2⟩ |3⟩ |7⟩

\( t_{27} = \Delta \)

\( t_{37} = \Delta \)

\( E = 0 \)

\( E = 0 \)

\( E = 2\Delta \)

\( E_1 = \Delta - \sqrt{2t_{27}^2 + \Delta^2} \)

\( E_2 = \Delta + \sqrt{2t_{27}^2 + \Delta^2} \)

FIG. 3: (a) Virtual hopping via the ridge site 7 generates an effective hopping \( t^p \) between 2 and its third neighbor site 3 – i.e. site 3 in the neighboring unit cell in Fig. 2 – (b) The odd parity combination of 2 and 3 remains decoupled, but the even parity combination hybridizes with ridge site and lowers its energy.

Let us see how the atomic processes \( t_{ij} \) in Fig. 2(a) are related to the effective hopping processes in Fig. 2(c). For example consider the simplest third neighbor R sites 2 and 3 in Fig. 1(a) that becomes possible via atomic hoppings \( t_{27} \) and \( t_{37} \) of Fig. 2(a). The hopping process via the R site 7 is depicted in Fig. 3(a). Assuming an on-site energy offset \( 2\Delta \) for the R sites with respect to I site, an electron starting at the site 2 virtually hops to R site 7 and then returns to low-energy sector at site 3. In this process it gains the following energy

\[ t^p = \Delta - \sqrt{2t_{27}^2 + \Delta^2} < 0, \]

Even in the limit of \( \Delta \to 0 \) this gives an energy lowering \(-2|t_{27}|\) that can be regarded as effective hopping between the third neighbor sites 2 and 3 of the I sublattice. To intuitively understand this formula, note that in the absence of the I site, \( t_{27} = t_{37} = 0 \), and hence both even and odd combinations of third neighbor atomic orbitals \(|2⟩\) ± \(|3⟩\) remain inert. But once the inner site is present, the atomic hopping \( t_{27} \) causes a coupling of \(|7⟩\) with the even-parity state \(|2⟩ + |3⟩\), leaving the odd parity state \(|2⟩ - |3⟩\) decoupled at zero energy. The coupling with the even parity combination provides a channel to lower the energy given by the effective hopping in Eq. (1). Furthermore, in the limit of \( \Delta \gg |t_{27}| \) the above formula reduces to the perturbatively appealing form \(-2t_{27}^2/\Delta \). For pedagogical details of the above computation, please refer to section II of SM.
As a second example, consider the I site 3 and the same site in the unit cell above it (that we denote by 3’ in Fig. 1(a). These sites will be second neighbor on the coarse grained lattice and there are two hopping pathways 3 → 6 → 5 → 3’ and 3 → 8 → 7 → 3’ connecting them that are denoted by light and dark green dashed lines in Fig. 2(a). The process of the calculation of the effective hopping amplitude 3 → 3’ is similar for the above two paths. So we focus on the first one. In principle one must consider the energy gained by the lowest molecular orbitals formed by the above chain of sites. This has been done in section III of SM. But the end result allows for a nice interpretation as depicted in Fig. 4. First, due to hopping $t_{65}$, the R sites 5 and 6 form bonding and anti-bonding molecular orbitals denoted by $|\phi_1\rangle$ and $|\phi_3\rangle$ in Fig. 4(a). Then as depicted in panel (b), an electron gains by virtually hopping via the anti-bonding orbital $|\phi_3\rangle$ whose energy is now offset by $t_{65} + 2\Delta$. The hoppings connecting 3 to $|\phi_3\rangle$ are $t_{65}/\sqrt{2}$ because the normalized $|\phi_3\rangle = (|\phi_5\rangle - |\phi_6\rangle)/\sqrt{2}$. In the final step as shown in Fig. 4(c), the even-parity combination of $|3\rangle$ and $|3'\rangle$ is mixed with $|\phi_3\rangle$ to give an energy gain $E_{\text{even}} = (t_{56}/2 + \Delta) - \sqrt{(t_{56}/2 + \Delta)^2 + t_{65}^2}$. A similar contribution arises from the second path. Adding the two contributions we obtain the total renormalized hopping $\tilde{t}$ of Fig. 2(c) as

$$\tilde{t} = \frac{t_{56} + t_{87} + 4\Delta}{2} - \sqrt{\left(\frac{t_{56}}{2} + \Delta\right)^2 + t_{63}^2} - \sqrt{\left(\frac{t_{87}}{2} + \Delta\right)^2 + t_{73}^2}$$

In the above formula, the hopping parameters $t_{65}$ and $t_{87}$ are dominantly contributed by the $p_x$ and $p_z$ orbitals as the intensity of the $p_x$, $p_z$ orbitals in the second row of Fig. 1(e) is dominant, while $p_y$ is faint. Similarly the two other renormalized hopping parameters $t^p$ and $t^z$ can be computed. For details please refer to SM where we have shown that the elimination of higher energy states actually corresponds to the above simple molecular orbital analysis.

This is how the renormalized parameters of the coarse grained honeycomb lattice model in the bottom part of Tab. I are computed from the ab initio data of the top part of the table. Note that if instead of $8Pmnmn$ structure, we had a simple honeycomb lattice (such as in graphene), such a large values of second or third neighbor hopping given in Tab I would be unthinkable as hopping between the atomic orbitals exponentially decays with distance. Therefore the virtual hopping via the ridge sites attaches a great importance to them as providers of channels for energy gain and ultimate formation of renormalized hoppings on a coarse grained lattice of inner sites. Furthermore, this is an example of how the molecular orbital play a significant role in the formation of longer range hoppings on the decimated $8Pmnmn$ lattice.

**Effective coarse-grained model:** Now that we have identified the $p_z$ orbitals residing at the inner sites as the low-energy degrees of freedom, and have computed various renormalized hoppings between second and third neighbors, we are ready to write down a physically clear low-energy effective model that will straightforwardly demonstrate how the renormalized parameters $t^p$, $t^z$, $t$ and $\tilde{t}$ can provide information about the position and the amount of the tilt.

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**FIG. 4:** (a) Formation of bonding and anti-bonding orbitals between the ridge atoms 5 and 6. (b) Effective hopping $\tilde{t}$ between second neighbor inner sites 3 and 3 can be formed by virtual hopping via the anti-bonding orbital $|\phi_3\rangle$ of two ridge atoms.
The first neighbor hoppings denoted by black arrows in Fig. 2(c) and are present even when there are no R sites. In the two-dimensional Hilbert space of A and B sublattice of such a honeycomb lattice, these hoppings contribute the usual off-diagonal term $F_0(k) = -\sum_{\alpha=1,2,3} e^{i k \cdot \delta_{\alpha}}$, where sum over $\alpha$ runs over three first neighbors in Fig. 2(c). This is responsible for the formation of a pair of upright Dirac cones. Slight anisotropy of the honeycomb lattice of R sites will amount to a shift in the location of the Dirac node [28] which is irrelevant for our purposes. For concrete calculations, we assume a regular effective honeycomb lattice of bond length $a$ for which the Dirac nodes in the rhombus BZ are at $K^\pm = \frac{\pi}{3a}(i \pm \frac{1}{\sqrt{3}}j)$ [20].

Next let us consider the third neighbor hoppings denoted by red arrows in Fig. 2(c) labeled by $t^p$ ($p$ for pseudo, as they give rise to pseudogauge fields that shift the location of the Dirac node) and $t^z$ ($z$ to emphasize the role of $p_z$ orbitals of R sites). They contribute another off-diagonal term denoted by $F_{3p}(k) = t^p e^{2iak_x} + 2t^z e^{-iak_z} \cos(\sqrt{3}ak_y)$. Expanding this form factor around the Dirac nodes $K^\pm$ above, gives rise to (i) a shift $\Delta k_D = 2(t^p - t^z)/(\mp 3at \pm at^z)$, where $t$ is the nearest neighbor hopping (assumed to be 1) and (ii) anisotropy in the Fermi velocity given by $v_{Fp} \rightarrow v_{Fp} \left(1 + \frac{2t^z + 2t^p}{3t} \right)$ and $v_{Fy} \rightarrow v_{Fy} \left(1 - \frac{2t^z}{3t} \right)$. Therefore the first and third neighbor hoppings establish the location of the (still upright) Dirac node and determine its Fermi velocities.

Now let us focus on the second neighbors (green arrows) in Fig. 2(c) that are the root cause of tilt formation [7]. Since these hoppings are driven via virtual hopping through different arrangements of molecular orbitals, there are two types of them denoted by solid (f) and dashed (f). These hoppings being second neighbor, connect two atoms on the same sublattice, and therefore contribute to the diagonal terms, namely $AA$ and $BB$ components of the effective $2 \times 2$ Hamiltonian matrix. Among the matrices $\sigma_\mu$ with $\mu = 0 \ldots 3$, only $\sigma_0$ and $\sigma_z$ can contribute diagonal terms. So now one has to decide whether these diagonal terms come with the same sign ($\sigma_0$ term $\rightarrow$ tilt) or opposite signs ($\sigma_z$ term $\rightarrow$ gap). There are two ways to see that the term must be proportional to the $\sigma_0$: (i) Analysis of the irreducible representations and compatibility relations of the original $8Pmnn$ structure in Fig. 1(d) shows that the crossing of the red bands is protected by the glide elements of the $8Pmnn$ lattice (see SM for details). Since the effective theory has to obey this protection against gap opening, the $\sigma_z$ term is ruled out. (ii) Consider the renormalized lattice itself and focus on the solid green line in Fig. 2(c). If the hopping between 1 and 3 in Fig. 1(a) contributes to AA term, the hopping between 2 and 4 contribute to BB term. Both these contributions arise from the $p_z$ orbitals of these atoms via intermediate hopping through $p_x$ orbital of atom 5. Apparently for $p_z$ orbitals the "northwest" (1 $\rightarrow$ 5 $\rightarrow$ 3) and "northeast" (4 $\rightarrow$ 5 $\rightarrow$ 2) hoppings are identical. Similar arguments holds for the dashed green line in Fig. 2(c). In this case AA (BB) term is generated by 3 $\rightarrow$ 6 $\rightarrow$ 5 $\rightarrow$ 3 (2 $\rightarrow$ 6 $\rightarrow$ 5 $\rightarrow$ 2) path. Again the $p_z$ orbitals of the 5, 6 atoms symmetrically connects 3 $\rightarrow$ 3 and 2 $\rightarrow$ 2, thereby giving identical AA and BB terms in the effective Hamiltonian.

Therefore the effective Hamiltonian becomes
\[ H_{\text{eff}}(k) = \begin{pmatrix} f_{\text{tilt}}(k) & f(k) \\ f^*(k) & f_{\text{tilt}}(k) \end{pmatrix}, \quad f(k) = F_{xy}(k) + F_0(k), \]
\[ f_{\text{tilt}}(k) = 2i \cos \left( \sqrt{3}ak_y \right) + 4i \cos(3ak_x/2) \cos \left( \sqrt{3}ak_y/2 \right). \]

Taylor expanding the diagonal \( f_{\text{tilt}} \) term around the Dirac node obtained from the rest of the terms gives,

\[ \zeta_x = 0, \quad \zeta_y = \pm 2 \frac{\tilde{t} - \bar{t}}{\tilde{t}}. \]  

The above equation indicates that the tilt arises from the second neighbor hoppings \( \tilde{t} \) and \( \bar{t} \) that in turn are generated via the \( p_x \) and \( p_z \) orbitals of the R atoms. An immediate suggestion of the above model is to (partially) replace the R sites boron atoms by carbon atoms to see whether the tilt is changed or not. In Fig. 5 we have replaced two of the boron atoms with C atoms. For this purpose there are two choices: (i) To place a carbon dimer on the R sites as in the panel (a) or (ii) to place the carbon atoms in the I sites as in panel (f). The results are summarized in Tab. I. For case (i), the location of the Dirac node is shifted towards the \( \Gamma \) pint and its tilt increases. Placing carbon atoms in the R sites shifts the 5 and 6 sites to higher energies, thereby generating larger \( \tilde{t} \) and \( \bar{t} \) (see Tab. I) that ultimately increases the tilt from the \( \zeta_y = 0.46 \) of the pristine borophene to \( \zeta_y = 0.59 \) in \( \text{B}_6\text{C}_2\text{-R} \). Our picture provides also a way to decrease the tilt parameter. In this case, the hybridization of the \( p_z \) orbitals of sites 2, 3 with the R sites (5, 6) reduces as in Tab. I and hence the resulting \( \tilde{t} \) and likewise \( \bar{t} \) are scaled down, thereby reducing the tilt to 0.36 in \( \text{B}_6\text{C}_2\text{-I} \). The above values of the tilt \( \zeta_y \) are calculated based on Eq. (2) and as detailed in SM are in good agreement with the corresponding values directly extracted from DFT bands.

**Summary and outlook.** Based on our ab initio calculations, we have identified the \( p_z \) orbitals of the I sites as real space sublattice on which the low-energy degrees of freedom in \( 8\text{Pmmn} \) lattice reside. The effective hoppings between these sites are obtained via renormalization that encodes the virtual hopping to R sites. These gives a physically clear picture of the formation of the tilt in two-dimensional Dirac cone of \( 8\text{Pmmn} \) borophene. In our picture, tilt arises from a competition between two renormalized hoppings \( \tilde{t} \) and \( \bar{t} \) between the second neighbor I sites. The former involves virtual hopping via two R sites, while the latter involves one R site. Therefore, replacing the ridge (inner) atoms by C increase (decreases) the tilt. The rest of the effective hoppings determine the location of the (protected) Dirac node and the anisotropy in the Fermi velocity. Our picture clearly shows how do certain atomic scale manipulations control the tilt of the tilted Dirac cone materials. Since the tilt of the Dirac cone can be attributed to an underlying spacetime metric, the ability to tune the tilt parameter is tantamount to controllability of the ensuing solid-state spacetime structure by electric forces. Dirac materials subject to gravitational disorder [29, 30] find their materialization in the present context when the carbon is randomly for boron.

On the technical side, our current work presents a concrete example of decimation and renormalization on a lattice that belongs to a non-trivial SG and shows how can an non-trivial geometry emerge at long wave lengths. This logic can be used to discover more materials in other SGs [31]. On the fundamental physics side, our proposal opens up a practical paradigm for designing interesting spacetime geometries that might have no analogs in the cosmos. The effects of spacetime curvature [32, 33] are expected to be much stronger in such solid-state spacetimes.

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Supplemental materials to the manuscript: How to tune the tilt of a Dirac cone by atomic manipulations?

In this supplementary material, we provide pedagogical derivations of all the relations and figures referred in the text.

I. SYMMETRY ANALYSIS

In this section, we illustrate the application of group theory methods in classification and labeling of the band structures by way of example of $8Pmmn$ borophene. This section is based on chapter 10 of C. Kittel’s Quantum Theory of Solids [1]. For a quick and concise introduction to the theory of groups and their representations, we recommend chapter 3 of G. Mahan’s Applied Mathematics [2].

Here, the two-dimensional rectangular lattice of pristine borophene $B_8$ has symmetry group of $Pmmn$. The crystal structure of the pure $8Pmmn$ borophene and the character table for the double group of $D_{2h}$($Pmmn$) are presented in Fig. 6(a) and Table. II respectively [3, 4]. The generators of $Pmmn$ space-group are given by two screw operations $C_{2x} = \{C_{2x}\mid \frac{1}{2}00\}$ and $C_{2y} = \{C_{2y}\mid 0\frac{1}{2}0\}$ together with an inversion operation $P = \{P\mid000\}$, where $\tilde{C}_{2x}$ ($\tilde{C}_{2y}$) is a nonsymmorphic operator meaning the twofold rotation $C_{2x}$ ($C_{2y}$) around the $x$($y$) axis is followed by a translation $\frac{1}{2}$($\frac{1}{2}$) as indicated in Fig. 6. These three independent operations can produce all other symmetry operations of the $Pmmn$ space group as follow:

$\tilde{M}_x = P\tilde{C}_{2x}, \tilde{M}_y = P\tilde{C}_{2y}$
$\tilde{C}_{2x} = \tilde{C}_{2x}\tilde{C}_{2y}, \tilde{M}_z = P\tilde{C}_{2z}$

FIG. 6: (a) The crystal structure of the pure $8Pmmn$ borophene $B_8$. Dark and light blue circles exhibit inner boron atoms $B_I$ and ridge boron atoms $B_R$ respectively. $\tilde{C}_{2x} = \{C_{2x}\mid \frac{1}{2}00\}$ and $\tilde{C}_{2y} = \{C_{2y}\mid 0\frac{1}{2}0\}$ shown above, are two generators of $Pmmn$ space-group. (b) Rectangular first Brillouin zone of $8Pmmn$ borophene. (c) decomposition of elementary band representation of the $8Pmmn$ space group with time-reversal symmetry labeled according to notations of Bilbao crystallography server.

$D_{2h}(8Pmmn)$ group has eight 1D irreducible representations given in character Table. II. The two other 2D representations belong to the double group which is obtained by taking the spin of the electrons into account and is indicated with a bar over the representation label. We are interested in the little group representations at each high symmetry points in the BZ [1]. The little group of $\Gamma$ point (top panel of Fig. 6(b)) is always the entire point group of lattice, in this case $D_{2h}$. The other important high symmetry $X$ and $Y$ points have little double group $C_{2h}$ and generated by operators $(\tilde{C}_{2x}, \tilde{M}_x, P)$ and $(\tilde{C}_{2y}, \tilde{M}_y, P)$ respectively. We apply the action of the point group elements on the spin and molecular orbitals to construct the elementary band representation matrices $\rho^i$[5, 6].
matrix), the matrices related to the action of \( \{ \pi \} \) rotation by \( \pi \) acts as a rotation by \( \pi \), and therefore one finds,

\[
\sigma_z \otimes i s_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \otimes i \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}.
\]

Similarly, \( \{ C_{2x} | 0 \frac{b}{2} \} \) acts as a rotation by \( \pi \) but it does not interchange the sublattices. Hence

\[
\rho^\Gamma(\{ C_{2x} | 0 \frac{b}{2} \}) = \sigma_0 \otimes e^{i \frac{\pi}{2} s_1} = \sigma_0 \otimes i s_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes i \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \end{bmatrix}.
\]

Lastly, we need to examine inversion \( \tilde{P} \) and time-reversal \( \tilde{T} \) representations. Since \( \tilde{P} \) interchanges the two sublattices, the band representations are given by

\[
\rho^\Gamma(\{ \tilde{P} | 000 \}) = \sigma_z \otimes e^{i \tilde{z} s_0} = \sigma_z \otimes i s_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \otimes i \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \end{bmatrix},
\]

while the time-reversal becomes,

\[
\rho^\Gamma(\{ T \}) = i s_2 \otimes \sigma_0.
\]

Having constructed the above matrix representations, comparing the trace of each of these matrices to the characters in Table. II, we see that little group representations for the energy bands in borophene at \( \Gamma \) is decomposed into two irreducible representations of the little group of \( \Gamma \) point in Table. II as follows:

\[
\rho^\Gamma \sim \Gamma_5 + \Gamma_6.
\]

Now we need to repeat the same procedure for \( X \) and \( Y \) points. The little group of \( X \) and \( Y \) points are isomorphic to \( C_{2h} \) and generated by \( (C_{2x}, \tilde{P}) \) and \( (C_{2y}, \tilde{P}) \) respectively. Character tables for the little co-group \( C_{2h} \) of \( X \) and \( Y \) for both single and double-valued representations are given in Table. III. We deduce by similar argument that little group representations at \( X \) and \( Y \) points decompose as

\[
\rho^X \sim \tilde{X}_3 + \tilde{X}_4, \rho^Y \sim \tilde{Y}_3 + \tilde{Y}_4
\]
TABLE III: The character table for the double little group of \( C_{2h} \) related to \( X \) and \( Y \) points.

| Rep | \( E \) | \( C_{2v} \) | \( \bar{I} \) | \( M_{x} \) | \( CE \) | \( C\bar{I} \) |
|-----|-----|-----|-----|-----|-----|-----|
| \( X_{1}^{-} \) | 1 | 1 | 1 | 1 | 1 | 1 |
| \( X_{1}^{+} \) | 1 | 1 | -1 | -1 | 1 | -1 |
| \( X_{2}^{-} \) | 1 | -1 | 1 | -1 | 1 | -1 |
| \( X_{3} \) | 2 | 0 | 2 | 0 | -2 | 2 |
| \( X_{4} \) | 2 | 0 | -2 | 0 | -2 | 2 |

Now, we need all the possible paths where crystal symmetries force bands to be joined to find appropriate band structure. Compatibility relations [1] express that the irrepresentation along the high-symmetry lines are completely determined by the irrepresentation that appear at high-symmetry points. We apply it to connection line \( \Delta (\Sigma) \) between pair of \( k \)-points \( \Gamma \) and \( X (Y) \) according to notations of Bilbao crystallography server [7]. Since that there is only a single 2D representation \( \bar{\Delta}_{5}(2) (\bar{\Sigma}_{5}(2)) \) allowed at the \( \Gamma \rightarrow X \) (\( \Gamma \rightarrow Y \)) line, we have

\[
\rho_{\Delta} \sim \bar{\Delta}_{5}(2) + \bar{\Delta}_{5}(2), \quad \rho_{\Sigma} \sim \bar{\Sigma}_{5}(2) + \bar{\Sigma}_{5}(2)
\]

Using Compatibility relation (see Table. IV), we find one possibility is to have a (tilted) cone crossing along the \( Y \) path. For this purpose a "sticking together" (as Kittel puts it) of \( \bar{X}_{3}, \bar{X}_{4} \) and also \( \bar{Y}_{3}, \bar{Y}_{4} \) is necessary. Such sticking together is protected by glid/screw elements [1]. In our case it is the screw-symmetry \( \bar{C}_{2h}y \). Other possibilities are to have the crossing along the \( \Gamma X \) path, or to have a crossing between the blue and red bands of Fig. 6(b). The later possibilities are ruled out by the \( ab \) initio data presented in Fig. 1(b) of the main text.

TABLE IV: Compatibility relation of space group \( P_{mmn} \)

| \( C_{2v} \) | \( C_{2h} \) | \( D_{2h} \) |
|-----|-----|-----|
| \( \bar{\Sigma}_{5}(2) (\bar{\Delta}_{5}(2) \bar{X}_{3}(2), \bar{X}_{4}(2) \bar{Y}_{3}(2), \bar{Y}_{4}(2) \bar{\Gamma}_{5}(2), \bar{\Gamma}_{6}(2) \) |

II. 8PMMN MOTIVATED TIGHT-BINDING MODEL FOR TILTED DIRAC FERMIONS

As pointed out in the main text, effective degrees of freedom are \( p_{z} \) orbitals of inner sites the projection of which on the \( xy \) plane will be a honeycomb lattice. In this effective model, the buckling of honeycomb lattice sites are ignored. This can be absorbed into effective hybridization with \( p_{x} \) orbitals of the ridge sites. Furthermore, the projection of the inner sites of \( 8P_{mmn} \) lattice into \( xy \) plane will not be a regular honeycomb lattice. Ignoring this will amount to a shift in the location of the Dirac node. This shift can also be absorbed into various effective hoppings. Therefore for modeling purposes, it is enough to start with an "effective regular honeycomb lattice” on which the relevant degrees of freedom (the \( p_{z} \) orbitals of the inner sites) reside. In this section we pedagogically derive all the details related to the formation, movement and titling of the Dirac cone based on the effective honeycomb lattice. As is shown in the main text, the picture arising from an effective model can accurately reproduce the DFT tilt parameters. Furthermore, having a tight binding two-band model allows to study various effects such as disorder/interactions/symmetry breaking.

A. Theory without ridge atoms

Without ridge atoms (faint teal sites in Fig. 1(a) and Fig. 2(a) of the main text), life is simple and one basically needs a theory of graphene which will be pedagogically and quickly reviewed below to build upon. We therefore start with Fig. 7 that depicts a regular honeycomb lattice and its associated first Brillouin zone.
FIG. 7: (a) The honeycomb lattice with two electrons per unit cell. The lattice constant is $a$ and three vectors connecting to nearest neighbors are denoted by $\delta_i$, $i = 1, 2, 3$ (b) Two representations of the first Brillouin zone. The hexagonal Brillouin zone is the Wigner-Seitz cell in the reciprocal lattice and manifests the symmetries better. The rhombic Brillouin zone better indicates two independent Dirac cones at wave vectors at $K_{\pm b}$.

The three vectors connecting every site from a given sublattice to three nearest neighbors from the opposite sublattice in Fig. 7(a) are

\[
\begin{align*}
\delta_1 &= \frac{a}{2}(1, \sqrt{3}), \\
\delta_2 &= \frac{a}{2}(1, -\sqrt{3}), \\
\delta_3 &= -a(1, 0).
\end{align*}
\]

The primitive lattice basis vectors are

\[
\begin{align*}
\vec{a}_1 &= \frac{3}{2}a\hat{i} + \frac{\sqrt{3}}{2}a\hat{j}, \\
\vec{a}_2 &= \frac{3}{2}a\hat{i} - \frac{\sqrt{3}}{2}a\hat{j}.
\end{align*}
\]

Using $\vec{a}_i, \vec{b}_j = 2\pi\delta_{ij}$ gives the following basis for the reciprocal space,

\[
\begin{align*}
\vec{b}_1 &= 2\pi\left(\frac{1}{3a}\hat{i} + \frac{1}{\sqrt{3}a}\hat{j}\right), \\
\vec{b}_2 &= 2\pi\left(\frac{1}{3a}\hat{i} - \frac{1}{\sqrt{3}a}\hat{j}\right),
\end{align*}
\]

where $a$ is the distance between two neighbouring atoms. In the hexagonal Brillouin zone it appears the there are six corners $K$. But in fact two of them are independent and fall into two categories related to each other by a reciprocal lattice vector constructed from the above vectors. For example the corners of Brillouin zone shown in Fig. 6(b) labeled by $K_{\pm a}$ and $K_{\pm b}$ are given by,

\[
\begin{align*}
K_{a}^+ &= \frac{4\pi}{3\sqrt{3}a}\hat{j}, & K_{a}^- &= -\frac{4\pi}{3\sqrt{3}a}\hat{j} \\
K_{b}^+ &= \frac{2\pi}{3a}(\hat{i} + \frac{1}{\sqrt{3}}\hat{j}), & K_{b}^- &= \frac{2\pi}{3a}(\hat{i} - \frac{1}{\sqrt{3}}\hat{j})
\end{align*}
\]

As can be seen adding $\vec{b}_2$ to $K_{a}^+$ gives $K_{b}^-$ and hence they are equivalent. Similarly $K_{a}^-$ and $K_{b}^+$ are equivalent. So in the calculations, one can pick a convenient one. The effective theories around equivalent $K$ points are the same within a gauge transformation that will be discussed below. The $K_{b}^\pm$ points indicated in the rhombic Brillouin zone of Fig. 7(b) manifestly emphasizes that there are two independent corners that can not be connected to each other by a reciprocal lattice vectors.
Denoting by $a, b$ the field operators for the annihilation of electrons in $p_z$ orbitals of the $A$ and $B$ sublattices of the honeycomb lattice, the parent Hamiltonian is basically the theory of graphene and is given by,

$$H_0 = -t \sum_{i,j} a_i^\dagger b_j + \text{h.c.}$$

Fourier transformation of the above Hamiltonian becomes,

$$H = -t \sum_{k,\alpha=1,2,3} a_k^\dagger b_k e^{ik\cdot\delta_\alpha} + \text{h.c.}$$

that begs for a matrix representation as

$$H = \sum_k (a_k^\dagger b_k^\dagger) \left( \begin{array}{cc} 0 & F_0(k) \\ F_0^*(k) & 0 \end{array} \right) \left( \begin{array}{c} a_k \\ b_k \end{array} \right).$$

This is how the spinor structure emerges. The form factor connects the opposite sublattices, and hence is off-diagonal in the above sublattice space and is given by,

$$F_0(k) = \sum_\delta t e^{i k \cdot \delta}$$

Plugging in the Cartesian representations of $\delta_1, \delta_2, \text{and} \delta_3$ given above and carrying out the summation over the three neighbors, the famous formula of graphene literature can be obtained,

$$F_0(k) = t e^{-i k_x a} + 2t e^{i k_x a} \cos \left( \frac{\sqrt{3}}{2} k_y a \right)$$

The above form factor vanishes at the corners of the hexagonal Brillouin zone. Expanding it around two independent corners, e.g. $K_a^\pm$ gives,

$$F(K_a^\pm + k) = F(K_a^+) + \frac{\partial F}{\partial k_x}|_{k=K_a^\pm} k_x + \frac{\partial F}{\partial k_y}|_{k=K_a^\pm} k_y,$$

$$= -\frac{3}{2} a t i (k_x \mp i k_y).$$

The overall factor of $-i = e^{-i\pi/2}$ can be gauge transformed by rotating the overall phase of the wave function in one sublattice. For example gauge transforming the amplitude of wave function on sublattice $B$ as $\phi_B \rightarrow i \phi_B$, eliminates the $-i$ factor above and we have

$$F_0(k) \rightarrow \frac{3a t}{2} (k_x \mp i k_y)$$

Upon the above gauge transformation the behavior of the Hamiltonian around the crossing points is given by,

$$H_0(k) = \frac{3at}{2} \left( \begin{array}{cc} 0 & k_x \mp i k_y \\ k_x \pm i k_y & 0 \end{array} \right) = \frac{3at}{2} (k_x \sigma_x \pm k_y \sigma_y)$$

Defining $3at/2 = \hbar v_F$, this formula gives two representations of the Dirac theory $H_{\text{Dirac}}(k) = \alpha_x k_x + \alpha_y k_y + \beta m$ with $\alpha_x = \sigma_x, \alpha_y = \pm \sigma_y$ and $m = 0, \beta = \sigma_z$, hence massless Dirac electrons. These two representations are connected to each other by time-reversal operator $\vec{k} \rightarrow -\vec{k}$ followed by $T = i \sigma_y K$ where $K$ is complex conjugation.
FIG. 8: (a) The crystal structure of $8Pmnn$ borophene which consists of two different types of B atoms ($B_R$ and $B_I$). The coarse grained lattice of inner sites form a honeycomb structure. Black arrows indicate direct hopping between the atomic $p_z$ orbitals. There are additionally green path (second neighbor) and red path (third neighbor) hopping on the effective honeycomb lattice that becomes possible via the molecular orbitals involving $p_x$ and $p_z$ orbitals of ridge site atoms. (b) The first Brillouin zone of original borophene ($B_8$) lattice. (c) The effective honeycomb-like crystal structure of $8Pmnn$ borophene after decimation. The role of higher energy ridge site atoms is replaced by effective hoppings denoted by a single path of corresponding color, namely green for second neighbors and red for the same neighbors. The dashed and solid lines correspond to two different types of virtual processes. (d) The first Brillouin zone of effective hexagonal system. The two Dirac cones in (d) are born from two Dirac cones at (b), albeit shifted and tilted by effective green and red path hoppings of (c).

B. Role of ridge atoms

The $8Pmnn$ borophene’s lattice consists of two different types of B atoms, which we will call inner B ($B_I$) and ridge B ($B_R$) atoms in Fig. 8(a). The $B_I$ atoms form a hexagonal graphene-like lattice and $B_R$ atoms look like one-dimensional chains passing through the effective honeycomb lattice as in Fig. 8(c). As pointed out, in absence of $B_R$ atoms, the structure looks like a distorted graphene lattice. This lattice naturally includes the nearest neighbor (black path hoppings in panel (c)) that gives rise to two Dirac cones described above. Deviations of the honeycomb lattice from planar structure allows for mixing with $p_z$ orbitals of the ridge sites, while the deviations of the projected honeycomb lattice from perfect $C_6$ symmetry of graphene accounts for shift in the location of the Dirac cones. Therefore the schematically depicted Dirac cones in panel (d) above are shifted and tilted as described below to form the two Dirac cones in panel (b) of the original $8Pmnn$ lattice.

If there were not ridge sites, in a pure honeycomb lattice, hoppings between 2nd and 3rd neighbors via atomic orbitals would be negligibly small. Therefore there would be no green and red hoppings as in panel (c). However, ridge atoms provide dotted hopping paths of panel (a) that facilitate a hopping between 2nd and 3rd neighbors of the parent honeycomb-like lattice via virtual hopping through the ridge atoms. The connection between the microscopic paths in (a) and effective hoppings in (c) will be discussed in next section. For the purpose of present sub-section, we only need to focus on the effective green and red hoppings in panel (c) above. The corresponding hoppings as depicted in Fig. 2(c) of the main text are $t$ and $t'$ for the green path (2nd neighbor). Two different symbols correspond to two different virtual processes depicted in panel (a) above. Similarly for the red paths there are two hoppings $t''$ and $t'''$ as depicted in Fig. 2(c) of the main text. As we will see shortly, $t''$ (and $t'''$) acts like a pseudo-gauge field that shifts the location of the Dirac cone. The superscript $x$ in $t''$ is meant to emphasize a special role played by the $p_z$ orbitals of the ridge atoms that will be discussed in the next section. The $t''$ and $t'''$ being 3rd neighbor hoppings connect a site from A sublattice to one in the B sublattice. Therefore the corresponding form factor $F_{xp}(\vec{k})$ will contribute off-diagonally to the effective Hamiltonian. Furthermore, the hoppings $t$ and $t'$ being 2nd neighbor hoppings connect atoms on the same site, and therefore the corresponding form factors $\tilde{F}(\vec{k})$ and $\bar{F}(\vec{k})$ contribute diagonally to the effective Hamiltonian in the sublattice space. So we end up with

$$H = \sum_k (\bar{a}_k^\dagger b_k^\dagger) \begin{pmatrix} \bar{F}(\vec{k}) + \bar{F}(\vec{k}) & F_0(\vec{k}) + F_{xp}(\vec{k}) \\ F_0^*(\vec{k}) + F_{xp}^*(\vec{k}) & \bar{F}(\vec{k}) + \bar{F}(\vec{k}) \end{pmatrix} (a_k \ b_k)$$

where $F_0(\vec{k})$ provides a upright Dirac cone to begin with (as discussed in the previous sub-section).

$$F_0(K^\pm_x + k) = -\frac{3\alpha i}{2} (k_x + ik_y)$$

Using the third nearest-neighbor vectors $\delta_p = -\frac{2}{3}(\alpha_1 + \alpha_2) = -2\alpha \hat{i}$, $\delta_1 = \alpha \hat{i} + \sqrt{3} \alpha \hat{j}$, $\delta_2 = \alpha \hat{i} - \sqrt{3} \alpha \hat{j}$ where “$\alpha$” is an “effective” lattice constant for the parent honeycomb lattice, the $F_{xp}(\vec{k})$ form factor and its Taylor expansion near the Dirac
crossing become,
\[
F_{xp}(k) = t^p e^{2iak_x} + 2t^x e^{-iak_x} \cos(\sqrt{3}ak_y)
\]
\[
F_{xp}(K_a^\pm + k) = t^p - t^x \pm 3at^x k_y + i\alpha(2t^p + t^x)k_x
\]
As can be seen the difference \(t^p - t^x\) between the 3rd neighbor hoppings generated via two different microscopic paths effectively shifts the \(k_y\) of the opposite valleys by opposite values. Furthermore, the coefficients of the \(k_x\) and \(k_y\) above that arise from \(t^x\) and \(t^p\) contribute to the re-definition and anisotropy of the Fermi velocity. Remembering to affect the gauge transformation \(\phi_B \rightarrow -i\phi_B\) of the previous sub-section, the off-diagonal form factor giving still an upright (but shifted) Dirac cone becomes,
\[
f_{\text{Dirac}}(K_a^\pm + k) \rightarrow a(\frac{3t^p}{2} + 2t^p + t^x)k_x - i(\frac{3at}{2} \pm 3at^x)(k_y + \frac{t^p - t^x}{\pm \frac{3at}{2} \pm 3at^x})
\]
(3)
This form makes it manifest how the third neighbor hoppings shift the Dirac cones and make their velocities anisotropic. The difference \(t^p - t^x\) is responsible for the mutual movement of the Dirac cones along the \(k_y\) direction. The Dirac point at \(K^+_a\) move downward by \((t^p - t^x)/(3at^x - \frac{3at}{2})\) and Dirac point at \(K^-_a\) move upward by the same value. An illustration of this shift is indicated in Fig. 8(d) by red arrows. So, by increasing difference \((t^p - t^x)/(3at^x - \frac{3at}{2})\), the Dirac-nodes at \(K^+_a\) move toward \(\Gamma\). Equivalently, this means that the Dirac-nodes at \(K^+_a\) move away from \(\Gamma\) as indicated by red arrows.

**Formation of the tilt:** We are now ready to discuss the green path hoppings in Fig. 8(c) that are second neighbor hoppings on the effective honeycomb structure. The form factors \(\tilde{F}(k)\) and \(\bar{F}(k)\) correspond to the real-space displacements
\[
\tilde{\delta}_1 = \tilde{a}_1 - \tilde{a}_2 = \sqrt{3}a\hat{j}, \quad \tilde{\delta}_1 = (0, \sqrt{3}a)
\]
\[
\tilde{\delta}_2 = \tilde{a}_2 - \tilde{a}_1 = -\sqrt{3}a\hat{j}, \quad \tilde{\delta}_2 = (0, -\sqrt{3}a)
\]
and,
\[
\bar{\delta}_1 = \bar{a}_1 = \frac{3}{2}a\hat{i} + \frac{\sqrt{3}}{2}a\hat{j}
\]
\[
\bar{\delta}_2 = -\bar{a}_1
\]
\[
\bar{\delta}_3 = \bar{a}_2 = \frac{3}{2}a\hat{i} - \frac{\sqrt{3}}{2}a\hat{j}
\]
\[
\bar{\delta}_4 = -\bar{a}_2,
\]
respectively. The \(\tilde{F}(k)\), \(\bar{F}(k)\), in the diagonal part of Hamiltonian are thus
\[
\tilde{F}(k) = \tilde{t}(e^{i\sqrt{3}ak_y} + e^{-i\sqrt{3}ak_y}) = 2\tilde{t} \cos(\sqrt{3}ak_y)
\]
\[
\bar{F}(k) = 2\bar{t}(\cos(k.\tilde{a}_1) + \cos(k.\bar{a}_2)) = 4\bar{t} \cos(\frac{3}{2}ak_x) \cos(\frac{\sqrt{3}}{2}ak_y)
\]
that add up to give a tilt form factor, \(f_{\text{tilt}}\)
\[
f_{\text{tilt}}(k) = \tilde{F}(k) + \bar{F}(k) = 2\tilde{t} \cos(\sqrt{3}ak_y) + 4\bar{t} \cos(\frac{3}{2}ak_x) \cos(\frac{\sqrt{3}}{2}ak_y)
\]
Expanding around the Dirac point \(K_a^\pm\), the total AA matrix element becomes,
\[
f_{\text{tilt}}(K_a^\pm + k) = -(\tilde{t} + 2\bar{t}) \pm 3a(\tilde{t} - \bar{t})k_y
\]
(4)
Note that the BB matrix element is the same as above. Remember that the gauge transformation \(\phi_B \rightarrow -i\phi_B\) does not change the BB matrix element as a factor \((-i)^+(-i)\) gives 1. From the above formula we read:
\[
\zeta_x = 0, \quad \zeta_y = \pm \frac{\tilde{t} - \bar{t}}{\tilde{t}}
\]
(5)
Eqs. (3) and (5) derived for our model system are great guiding principles. Eq. (3) shows that the 3rd neighbor (red) hoppings are responsible for the location and anisotropy of the upright Dirac cone. Eq. (5) simply means that the tilt (a long distance property) depends on the difference between the microscopic parameters \(\tilde{t} - \bar{t}\), namely the difference in the hopping via two different green paths in Fig. 8(e). This model shows how the presence of ridge atoms move and tilt the Dirac cone. In the following section we are going to show how the effective hoppings in panel (c) of Fig. 8(c) arise from microscopic hoppings in panel (a).
III. EFFECTIVE HOPPING TERMS: RENORMALIZATION VIA MOLECULAR ORBITALS

If one considers the honeycomb-like structure formed by inner sites only, the hopping between 2nd and 3rd neighbors are quite negligible. This is because in a tight-binding approach, the overlap between the atomic orbitals exponentially decays with the distance. But when the ridge sites (denoted by teal color in Fig. 8(a)) are added, they act as virtual sites thorough which a renormalized hopping between the ($p_z$) atomic orbitals of the inner sites is formed. In this section we provide a simple picture of renormalization based on the molecular orbitals theory that explains why relatively large hoppings between 2nd and 3rd neighbors are obtained. The remarkable agreement of the tilt parameters extracted within such a local quantum chemistry picture indicates its validity. So in this section using molecular orbital theory, we first analytically derive these renormalized hopping parameters of new effective honeycomb lattice in term of hopping parameters of original $8Pmmn$ lattice. This will show that the ridge atoms ($B_R$) play a crucial role in mediating strong hoppings between the 2nd and 3rd inner sites atoms. Then we discuss the connection between the present molecular orbital treatment with a picture of renormalization procedure by considering Dyson equation for the local quantum clusters of the $8Pmmn$ lattice.

**Formation of effective third neighbor hopping:** Let us illustrate the basic principle by considering inner sites $B_2$ and $B_3$ in Fig. 8(a) and see how the ridge site $B_7$ facilitates a hopping between them. In Fig. 9(a) we have depicted an energy diagram where sites $B_2$ and $B_3$ (by symmetry) are at the same atomic energy levels $|2\rangle$ and $|3\rangle$, respectively. The site $B_7$ is assumed at state $|7\rangle$ energetically lying $2\Delta$ above the inner sites. The atomic hopping $t_{27}$ and $t_{37}$ connecting sites $B_2$ and $B_3$ to site $B_7$ that can be derived from Wannier states are indicated. These two (real) hoppings are the same by symmetry. The basic principle can be seen in the limit where $t_{27} = t_{37} \ll 2\Delta$. In this limit a virtual second order in $\Delta$ hopping via higher energy atomic orbital $|7\rangle$ stabilizes the energy of the states $|2\rangle$ and $|3\rangle$ by $-2t_{27}^2/\Delta$. The factor 2 comes from two different ways of performing such a virtual process: $|2\rangle \rightarrow |7\rangle \rightarrow |3\rangle$ and $|3\rangle \rightarrow |7\rangle \rightarrow |2\rangle$. The analytical extension of this result to arbitrary $2\Delta$ is straightforward.

In Fig. 9(b) we have denoted the energy level $E = 0$ and $E = 2\Delta$ of the inner and atomic sites before the hybridization $t_{27}$ by red and teal colors. The sites $B_2$ and $B_3$ are equivalent and hence symmetry adopted basis based on the even and odd representation of a two-element group including identity operation and operator that exchanges $B_2$ and $B_3$ is given by,

$$|\Phi_1\rangle = \frac{|2\rangle + |3\rangle}{\sqrt{2}}$$

$$|\Phi_2\rangle = |7\rangle$$

$$|\Phi_3\rangle = \frac{|2\rangle - |3\rangle}{\sqrt{2}}$$

The states $|\Phi_1\rangle$ and $|\Phi_2\rangle$ are even parity and mix with each other by atomic hopping $t_{27} = t_{37}$, while the state $|\Phi_3\rangle$ being odd parity decouples from the others. In fact state $|\Phi_{1(3)}\rangle$ is a bonding (anti-bonding) molecular orbital and is composed of atomic
orbitals of inner sites $B_2$ and $B_3$. The matrix elements and Hamiltonian in this basis are

$$\langle \Phi_2 | H | \Phi_3 \rangle = \langle 7 | H | \frac{\langle 2 \rangle - \langle 3 \rangle}{\sqrt{2}} \rangle = 0, \quad \langle \Phi_1 | H | \Phi_3 \rangle = 0,$$

$$\langle \Phi_2 | H | \Phi_1 \rangle = \langle 7 | H | \frac{\langle 2 \rangle + \langle 3 \rangle}{\sqrt{2}} \rangle = \sqrt{2} t_{27},$$

that give,

$$\begin{bmatrix}
0 & \sqrt{2} t_{27} & 0 \\
\sqrt{2} t_{27} & 2 \Delta & 0 \\
0 & 0 & 0
\end{bmatrix}$$

As can be seen when $t_{27} = 0$, the bonding/anti-bonding states have zero energy (equal to the energy of atomic orbitals $\langle 2 \rangle$ and $\langle 3 \rangle$) and hence bonding/anti-bonding degrees of freedom are inert in this limit. Upon turning on the atomic hopping to ridge site $B_7$, the above structure of the Hamiltonian, still leaves the anti-bonding orbital $\langle \Phi_3 \rangle$ decoupled and hence it remains at zero energy, while the bonding (even parity) combination $\langle \Phi_1 \rangle$ is mixed with $\langle \Phi_2 \rangle = \langle 7 \rangle$ giving rise to two split-off states at energies $\Delta \pm \sqrt{2 t_{27}^2 + \Delta^2}$. The energy of the $E_1 = \Delta - \sqrt{2 t_{27}^2 + \Delta^2}$ state is always less than energy $E = 0$ of the original $B_2$ and $B_3$ sites. The low-energy sub-space that – involving only the inner sites $B_2$ and $B_3$ – the high-energy site $B_7$ is eliminated (or integrated out in the renormalization group terminology), this lowering of energy can be interpreted as an effective hopping between $B_2$ and $B_3$,

$$t_{23}^{\text{eff}} = \Delta - \sqrt{2 t_{27}^2 + \Delta^2}.$$  \hfill (6)

This is so, because in a sub-space composed of only inner orbitals $\langle 2 \rangle$ and $\langle 3 \rangle$, placing such a off-diagonal hopping between the two states at energy zero, correctly reproduces the energy lowering of $E_1$ with respect to $E = 0$. This effective hopping in the main text has been denoted by $t_p$ and is responsible for a pseudo-gauge field that shifts the location of the Dirac node. Note that the in the $\Delta \gg t_{27}$ limit, the above expression reduces to the perturbative result $-2 t_{27}^2/\Delta$ cited above, while in the opposite limit $\Delta \ll t_{27}$ it becomes $-\sqrt{2 |t_{27}|}$.

**Formation of effective second neighbor hopping:** As a second example of how longer range hoppings on the parent honeycomb-like lattice of inner atoms are formed, let us consider in Fig. 6(a) the effective hopping between site $B_3$ in one unit cell and the same $B_3$ in the lower unit cell (let’s call it $B_3'$). This process will be achieved by two virtual paths: $3' \rightarrow 5 \rightarrow 6 \rightarrow 3$ and $3' \rightarrow 8 \rightarrow 7 \rightarrow 3$. Let us consider the first virtual path indicated by dotted green path in Fig. 8(a). Denoting by $\langle 3 \rangle$ and $\langle 3' \rangle$ the atomic orbitals on the two $B_3$ sites, and by $\langle 5 \rangle$ and $\langle 6 \rangle$ the atomic orbitals on the intermediate $B_5$ and $B_6$ sites, respectively, the four dimensional Hilbert space is broken into even sector

$$\langle \phi_1 \rangle = \frac{\langle 5 \rangle + \langle 6 \rangle}{\sqrt{2}}, \quad \langle \phi_2 \rangle = \frac{\langle 3 \rangle + \langle 3' \rangle}{\sqrt{2}},$$

and odd sector

$$\langle \phi_3 \rangle = \frac{\langle 5 \rangle - \langle 6 \rangle}{\sqrt{2}}, \quad \langle \phi_4 \rangle = \frac{\langle 3 \rangle - \langle 3' \rangle}{\sqrt{2}}.$$

The hopping matrix elements between the atomic orbitals are shown in Fig. 10 and by symmetry $t_{53} = t_{63}$. The hopping between $B_5$ and $B_6$ is associated with a $\pi$-bonding between the $p_x$ orbitals of these two sites. Taking the energy offset $2\Delta$ for the ridge sites with respect to the inner sites into account, the even block of the Hamiltonian and its eigenvalues become,

$$\begin{bmatrix}
t_{56} + 2 \Delta & t_{63} \\
t_{63} & 0
\end{bmatrix}, \quad E_{\text{even}}^{\pm} = \frac{t_{56}}{2} + \Delta \pm \sqrt{\left(\frac{t_{56}}{2} + \Delta\right)^2 + t_{63}^2}$$

while for the odd sector we have

$$\begin{bmatrix}
2 \Delta & t_{63} \\
t_{63} & 0
\end{bmatrix}, \quad E_{\text{odd}}^{\pm} = \Delta \pm \sqrt{\Delta^2 + t_{63}^2}$$

In fact replacement $\Delta \rightarrow \Delta + t_{56}/2$ maps the odd sector to even sector. This can be interpreted as the fact that the even sector take advantage of the $t_{56}$ hopping term between the $p_x$ atomic orbitals of the ridge atoms and generate larger stabilization.
Therefore for the $3' \rightarrow 5 \rightarrow 6 \rightarrow 3$ path, a contribution to the effective second neighbor hopping between the two $B_3$ inner sites will become,

$$t_{33}^{\text{eff}}(3' \rightarrow 5 \rightarrow 6 \rightarrow 3) = \left(\frac{t_{56}}{2} + \Delta\right) - \sqrt{\left(\frac{t_{56}}{2} + \Delta\right)^2 + t_{63}^2}$$  \hspace{1cm} (7)

A similar contribution arises from the path $3' \rightarrow 8 \rightarrow 7 \rightarrow 3$ by simply replacing $(5, 6) \rightarrow (8, 7)$ that gives

$$t_{33}^{\text{eff}}(3' \rightarrow 8 \rightarrow 7 \rightarrow 3) = \left(\frac{t_{87}}{2} + \Delta\right) - \sqrt{\left(\frac{t_{87}}{2} + \Delta\right)^2 + t_{73}^2}$$  \hspace{1cm} (8)

Adding these two terms gives the green $\tilde{t}$ in Fig. 2(c) of the main text,

$$\tilde{t} = \left(\frac{t_{56}}{2} + \Delta\right) - \sqrt{\left(\frac{t_{56}}{2} + \Delta\right)^2 + t_{63}^2} + \left(\frac{t_{87}}{2} + \Delta\right) - \sqrt{\left(\frac{t_{87}}{2} + \Delta\right)^2 + t_{73}^2}$$  \hspace{1cm} (9)

It is rather surprising to note that the Eq. (7) for the virtual hopping path $3' \rightarrow 5 \rightarrow 6 \rightarrow 3$ can be obtained by a simple intuitive picture as follows: As shown in Fig. 10(a), first an anti-bonding orbital from the ridge sites $B_5$ and $B_6$ is formed that has been denoted by $|\phi_3\rangle$. The upward shift of the anti-bonding orbital with respect to the initial level $2\Delta$ of the ridge atoms is given by the off-diagonal element $t_{53}$ in the space of $|5\rangle$ and $|6\rangle$. Then $|\phi_3\rangle = (|5\rangle - |6\rangle)/\sqrt{2}$ will have hopping matrix elements $t_{53}/\sqrt{2}$ and $t_{36}/\sqrt{2}$ to sites $3'$ and 3, respectively. Then a virtual hopping with these amplitudes via the intermediate state $|\phi_3\rangle$ at energy $t_{53} + 2\Delta$, precisely gives Eq. (7).

![Fig. 10: (a) Energy diagram for bonding and anti-bonding orbitals arise from the linear combination of atomic orbitals |5⟩ and |6⟩. (b) Energy levels of two successive inner ($B_3$) and anti-bonding orbitals (|$\Phi_3$⟩) stem from ridge $B_5$ and $B_6$ atoms (c) Energy diagram after the formation of molecular states which connect $B_3$ to one of its successive third nearest neighbors through anti-bonding orbitals (|$\Phi_3$⟩).](image)

**Relation with renormalization:** Now we are ready to show that the effective hoppings obtained in this way, admit a nice interpretation in terms of renormalization. As an example, let us elaborate on Eq. (6) and show that it can be alternatively obtained from a renormalization picture. This will establish that the molecular orbital theory that was explained in the previous part is indeed equivalent to a renormalization procedure.

Imagine the situation we discussed for effective third neighbor hopping energy between $B_2$ and $B_3$. Denoting as before the atomic basis $|2\rangle$, $|3\rangle$, and $|7\rangle$, and breaking the three dimensional Hilbert space into a two dimensional subspace composed of low-energy states $|2\rangle$, $|3\rangle$ and a one-dimensional high energy subspace described by $|7\rangle$, the Hamiltonian $H$ can be split as, where the subscripts L (H) stand for low-energy (high-energy) sectors. As described in the textbook of Grosso and Pastori

$$H = \begin{pmatrix} 0 & 0 & t_{27} \\ 0 & 0 & t_{27} \\ t_{27} & t_{27} & 2\Delta \end{pmatrix} = \begin{pmatrix} H_{LL} & H_{LH} \\ H_{HL} & H_{HH} \end{pmatrix} = \begin{pmatrix} H_{LL} & 0 \\ 0 & H_{HH} \end{pmatrix} + \begin{pmatrix} 0 \\ H_{HL} \end{pmatrix}$$

Paravicini, the application of Dyson’s equation leads to a renormalized (effective) Hamiltonian in the low-energy subspace of the following form,

$$H_{LL}^{\text{eff}}(E) = H_{LL} + H_{LH} \frac{1}{E - H_{HH}} H_{HL}$$

...
that depends on energy. Plugging the various sub-matrices in the above equation gives,

\[ H_{\text{eff}}^{LL}(E) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{E - 2\Delta} \begin{bmatrix} t_{27}^2 \\ t_{27} \end{bmatrix} = \frac{1}{E - 2\Delta} \begin{bmatrix} t_{27}^2 \\ t_{27} \end{bmatrix} \]

Now we have to evaluate the operator, whose matrix elements are energy-dependent as,

\[ \frac{1}{E - 2\Delta} \begin{bmatrix} t_{27}^2 \\ t_{27} \end{bmatrix} \Psi = E\Psi. \]

The eigenvalues are given by,

\[ \det \begin{bmatrix} -E & t_{27}^2 \\ -E & -2\Delta \end{bmatrix} = 0, \]

that immediately becomes,

\[ E = \Delta \pm \sqrt{2t_{27}^2 + \Delta^2}. \]

This is exactly the result (6) of our simple molecular orbital theory. The same logic applies to all other effective hoppings. Therefore the process of virtual hopping via the inner sites that involves molecular orbitals is actually equivalent to formation of renormalized hoppings in the low-energy sector of the theory (residing on the inner sites) as a result of elimination of higher-energy degrees of freedom that reside on ridge sites.

IV. AB INITIO CALCULATION: RELAXATION, ELECTRONIC STRUCTURE, AND STABILITY

The crystal structure of pure 8Pmnn borophene is presented in Fig. 6(a). The basic unit cell is rectangular and contains eight B atoms. For DFT calculation we use pseudopotential Quantum Espresso code [8] based on plane wave basis set within the GGA in the Perdew-Burke-Ernzerhof (PBE) parameterization [9]. Simulation of borophene rectangular unit cells is based on the slab model having a 25 Å vacuum separating slabs. We also consider monolayer of 8Pmnn structure, where some of the B atoms are substituted by C atoms in the form of B_{8-x}C_x (x=0, 1, 2). We have depicted the crystal structure for situation where a single B atom in the ridge (inner) sites is replaced by C atom, denoted by B_{7}C_1-R (B_{7}C_1-I) in Fig. 11(a) (Fig. 11(b)). An interesting situation where a dimer of B atoms in ridge (inner) sites is replaced by a dimer of C atoms is denoted by B_{6}C_2-R (B_{6}C_2-I) and is shown in Fig. 11(c) (Fig. 11(d)). The uniform k-point grids of 24×24×1 are used for the self-consistent field calculations of all systems. The Kinetic energy cut-offs for the wavefunctions and the charge density are 850 and 8500 eV, respectively. For each systems, the Broyden-Fletcher-Goldfarb-Shanno quasi-Newton algorithm is used to relax the internal coordinates of the B and C atoms and possible distortions with convergence threshold on forces for ionic minimization as small as 10^{-4} eV/Å. The obtained structural properties after the ionic relaxations such as lattice parameters, \(a\), \(b\), and \(c\) component of the B and C atoms in crystal coordinates are shown in Table V for pure borophene and in Table VI for C doped systems B_{8-x}C_x.

| TABLE V: Optimized lattice parameters (in Å) and atomic position of two-dimensional pure borophene. |
|--------------------------------------------------|
| \(a=4.5200\) \(b=3.2600\) \(c=26.0\)         |
| atom \(x\) \(y\) \(z\)                          |
| B_1  0.3333  0.0000  0.4840                      |
| B_2  0.1850  0.5000  -0.4840                      |
| B_3  -0.1850  0.5000  -0.4840                     |
| B_4  -0.3333  0.0000  0.4840                      |
| B_5  0.0000  0.2470  0.4570                       |
| B_6  0.0000  -0.2470  0.4570                      |
| B_7  0.5000  0.2470  -0.4570                      |
| B_8  0.5000  -0.2470  -0.4570                     |
TABLE VI: Optimized lattice parameters (in \(\text{\AA}\)) and atomic position for a system in which: (1) a single B atom in ridge sites is replaced by C atom, B\(_7\)C\(_1\)-R, (2) a single B atoms in inner sites is replaced by C atom, B\(_7\)C\(_1\)-I, (3) a dimer of B atoms in ridge sites is replaced by C atoms B\(_6\)C\(_2\)-R, and (4) a dimer of B atoms in inner sites is replaced by C atoms B\(_6\)C\(_2\)-I.

| B\(_7\)C\(_1\)-R | B\(_7\)C\(_1\)-I |
|-----------------|-----------------|
| \(a=4.5686\)   | \(a=4.5191\)   |
| \(b=3.2297\)   | \(b=3.2700\)   |
| \(c=26.0\)     | \(c=26.0\)     |
| atom            | atom            |
| \(x\) | \(y\) | \(z\) | \(x\) | \(y\) | \(z\) |
| B\(_1\) | 0.3169 | 0.0333 | 0.4880 | B\(_1\) | 0.2991 | 0.0000 | 0.4832 |
| B\(_2\) | 0.1864 | 0.5120 | -0.4831 | C\(_2\) | 0.1757 | 0.5000 | -0.4872 |
| B\(_3\) | -0.1864 | 0.5120 | -0.4841 | B\(_3\) | -0.1982 | 0.5000 | -0.4852 |
| B\(_4\) | -0.3169 | 0.0333 | 0.4810 | B\(_4\) | -0.3385 | 0.0000 | 0.4854 |
| B\(_5\) | 0.0000 | 0.2451 | 0.4574 | B\(_5\) | 0.0000 | 0.2470 | 0.4460 |
| C\(_6\) | 0.0000 | -0.2459 | 0.4594 | B\(_6\) | 0.0000 | -0.2470 | 0.4440 |
| B\(_7\) | 0.5000 | 0.2091 | -0.4527 | B\(_7\) | 0.5000 | 0.2470 | -0.4420 |
| B\(_8\) | 0.5000 | -0.2922 | -0.4537 | B\(_8\) | 0.5000 | -0.2470 | -0.4450 |

| B\(_6\)C\(_2\)-R | B\(_6\)C\(_2\)-I |
|-----------------|-----------------|
| \(a=4.3721\)   | \(a=4.4132\)   |
| \(b=3.5053\)   | \(b=3.1501\)   |
| \(c=26.0\)     | \(c=27.0\)     |
| atom            | atom            |
| \(x\) | \(y\) | \(z\) | \(x\) | \(y\) | \(z\) |
| B\(_1\) | 0.3218 | 0.0000 | 0.4743 | B\(_1\) | 0.3133 | 0.0000 | 0.4866 |
| B\(_2\) | 0.2095 | 0.5000 | -0.4713 | C\(_2\) | 0.1924 | 0.5000 | -0.4863 |
| B\(_3\) | -0.2095 | 0.5000 | -0.4703 | C\(_3\) | -0.1924 | 0.5000 | -0.4863 |
| B\(_4\) | -0.3218 | 0.0000 | 0.4723 | B\(_4\) | -0.3133 | 0.0000 | 0.4866 |
| C\(_5\) | 0.0000 | 0.2721 | 0.4619 | B\(_5\) | 0.0000 | 0.2457 | 0.4452 |
| C\(_6\) | 0.0000 | -0.2721 | 0.4619 | B\(_6\) | 0.0000 | -0.2457 | 0.4482 |
| B\(_7\) | 0.5000 | 0.1970 | -0.4613 | B\(_7\) | 0.5000 | 0.2528 | -0.4475 |
| B\(_8\) | 0.5000 | -0.1970 | -0.4611 | B\(_8\) | 0.5000 | -0.2528 | -0.4485 |

As we have shown in the main text and the previous sections of SM, the formation of the Dirac nodes is controlled by those atoms residing at the inner sites, while the location and tilting properties are controlled by the atoms residing at the ridge sites. With the aim of finding new materials with tilted Dirac cone, as well as, in order to confirm our analytical model, in this section we investigate whether and to what degree the location and tilt of Dirac-cone would change if boron atoms replaced by another atoms like carbon. We establish that the coarse grained honeycomb lattice of tilted Dirac fermions presented in the main text, is fully supported by ab initio calculations.

For instance, for the case of substitution of single C atom in ridge sites B\(_7\)C\(_1\)-R, we obtain that lattice parameters and position of atoms are not too different from the pure B\(_8\) (borophene) and, as a consequence, the shape of band structure including location and tilt of Dirac-cone does not change much (see first part of Table VI and Fig. 11(e)). On the other hand, the situation is different in the case of substitution of single C atom in inner sites, B\(_7\)C\(_1\)-I due to the breaking of C\(_x\)y and C\(_y\) symmetry (it breaks C\(_x\)z and inversion symmetries when we consider effective hexagonal lattice). So, single C atoms in hexagonal lattice gap out the tilted Dirac cone bands, as presented in Fig. 11(f). This observation confirms that the atoms at the inner (honeycomb-like) sites are responsible for the formation of the parent Dirac-cone.

In the following, we will consider the situation in which a dimer of B atoms in the ridge (inner) sites is replaced by C atoms B\(_6\)C\(_2\)-R (B\(_6\)C\(_2\)-I). In the case of B\(_6\)C\(_2\)-R, Table VI indicates that atoms in ridge sites get closer to the inner atoms in hexagonal lattice. As a result, the ratio between the effective hopping energy differences and the first neighbor hopping \(t\), namely \((t^p - t^x)/(t - 2t^x)\) and \((t - \bar{t})/t\) (that according to our model in section II of SM, control location and tilting of the Dirac cone, respectively) are expected to be larger than pure borophene. The movement of Dirac cones can be qualitatively seen in panel (d) of Fig. 11 where a dimer of C atoms are replacing the corresponding B atoms on the ridge sites. A weaker movement can be seen in panel (a) as only one C has been replaced in the ridge site, and hence a weaker shift in the ratio \((t^p - t^x)/(t - 2t^x)\).

Now let us consider the opposite case, displayed in panel (c) of Fig. 11 where the C dimers replace B dimers on the inner sites, namely B\(_6\)C\(_2\)-I. In this case the ridge atoms move away from the \(xy\) plane (see Table VI), thereby giving rise to opposite effect of panel (d). Therefore in panel (c) the Dirac nodes move away from each other.
Due to high flexibility [15], the range of strain at which $8P_{mmn}$ borophene remains stable is very much higher than that of other 2D materials such as silicene [13], MoS$_2$ [14] and black phosphorene [12], and yet, slightly larger than graphene [10] and h-BN [11]. We expect it can also be able to withstand strong strain generated by carbon substitutions. Nevertheless, we need to confirm whether the $8P_{mmn}$ borophene remains stable by the chemical substitutions with C atoms. Study of phonon dispersion provides a way to investigate the dynamical stability of crystal structures. The calculated phonon dispersion of pure $8P_{mmn}$ borophene and two systems in which a dimer of C atoms is substituted into borophene are shown in Fig. 12. In this method, the negative value of imaginary phonon frequencies is an indication of dynamical instability. As can be seen in Fig. 12, there are no negative imaginary frequencies, and therefore all three systems studies here are stable with respect to substitution of C atoms for B atoms.

FIG. 11: Crystal structure and DFT-PBE band structure for system in which (a,e) a single B atom in ridge site is replaced by C atom, B$_7$C$_1$-R, (b,f) a single B atom in inner site is replaced by C atom, B$_7$C$_1$-I, (c,g) a dimer of B atoms in ridge sites is replaced by a C dimer, B$_6$C$_2$-R, and (d,h) a dimer of B atoms in hexagonal is replaced by C dimer, B$_6$C$_2$-I.

FIG. 12: The phonon dispersion of (a) pure $8P_{mmn}$ borophene B$_8$, and a system in which a dimer of B atoms residing in (b) ridge sites and (c) inner sites, is replaced by a dimer of C atoms.
V. AB INITIO HOPPING MATRICES ELEMENTS

The parameters of our coarse-grained 8_Pmmn structure are obtained from atomic scale hopping parameters \( t_{ij} \) depicted in panel (a) of Fig. 8. Based on these \( t_{ij} \) parameters, as explained in section III, the effective hopping parameters of our effective model defined on the parent honeycomb structure are calculated. The accurate determination of the effective parameters therefore depends on accurate ab initio calculation of atomic hopping amplitudes \( t_{ij} \) that can be extracted from the corresponding Wannier functions [16–18].

The honeycomb lattice tight-binding model presented in our paper to describe the formation of tilt in 8_Pmmn structure is rather generic, and the hopping parameters can span a wide range of values. Nevertheless for a specific material they are fixed numbers. In contrast to graphene where hopping energy to sites further away than nearest neighbours are much smaller than the first neighbor hopping, our renormalized hopping scenario predict large effective hopping mediated by B_R atoms in borophene. Even the graphene fits within our renormalized hopping picture, as in the case of pure graphene, there are no ridge sites, and hence all \( t_{ij} \) parameters other than the nearest neighbor hoppings are nearly zero. In contrast, in the 8_Pmmn structure, they are numerically on the scale of electron volts, giving rise to effective hopping parameters of the same order. So it is sufficient to calculate the atomic \( t_{ij} \) parameters.

We calculate the hopping energies for all considered systems using Wannier functions. The maximally localized Wannier functions (MLWFs) are constructed with the WANNIER90 library [25, 26]. It is worth noting that graphene show well-isolated \( \pi \) bands at the Fermi energy, which induces a simple single band model with \( p_z \) states. In borophene, our projected band-structure indicate that the \( p_x \) states of B_R atoms are not isolated from the \( p_z \) states. To verify the adequacy of the above orbitals and hence the validity of calculated Wannier functions, in Fig. 13 for three B_8, B_6C_2-R, and B_6C_2-I systems, we compare the DFT-PBE band structure (solid red) with the corresponding Wannier-interpolated bands (blue) obtained with \( p_z \) Wannier orbitals on the B_I site and the \( p_x \) and \( p_z \) Wannier orbitals on the B_R site. As seen from the band structures, the overall agreement between original and Wannier-interpolated bands is remarkably good. Small deviations appear for states far from the Fermi energy, which given our picture based on the renormalization, are irrelevant for the low-energy physics.

Now that we have established in Fig. 13 that the \( p_z \) orbitals of inner sites and \( p_x \) and \( p_z \) orbitals of ridge sites are relevant degrees of freedom, we are ready to calculate the \( t_{ij} \) parameters by inclusion of these orbitals. The results of ab initio hopping matrix elements for pure borophene, B_7C_1-I, B_7C_1-R, B_6C_2-I, and B_6C_2-R are presented in the left partition of Table VII. These values are then used to derive the parameters of the effective model in the right partition of the same table. When a dimer of B_R atoms occupying the ridge sites is replaced by a C dimer, B_6C_2-R, we obtain comparatively large matrix elements (except \( t_{6,5} \)). This is due to the fact that the ridge atoms come closer to the \( xy \) plane upon replacement by C atoms as depicted in Fig. 5(a) of main text. So, the ridge atoms mediate stronger hoppings in B_6C_2-R system, meaning that they can better connect further away inner sites on the effective honeycomb model. As a consequence, the tilt of Dirac-cone is considerably larger than the corresponding values in pristine borophene. The situation is reversed when B_I atoms of the inner sites are replaced by a dimer of C atoms B_6C_2-I. In this case, the ridge atoms move away from the plane of inner atoms, as a results, the hopping parameters are smaller than corresponding ones in pristine borophene. In this situation, the system tends to reduce the tilt of Dirac cone.

![FIG. 13: Comparison of the DFT-PBE band structures with the corresponding Wannier-interpolated band structures obtained with \( p_z \) Wannier orbitals of B_I atoms together with \( p_x \) and \( p_z \) Wannier orbitals of B_R atoms for (a) pure 8_Pmmn borophene B_8 (b) B_6C_2-R and (c) B_6C_2-I.](image-url)
Now that we have a picture of the formation of the Dirac cone, and an analytical model to produce it, we use the model parameters obtained in Table VII to construct a picture of tilted Dirac cone as a function of ($k_x$, $k_y$) in pure and C-doped borophene. The solution of the tight-binding model leads to the $\zeta_x = 0$, $\zeta_y = \pm 2(\bar{t} - \bar{t})/t$, where the further neighbor effective hoppings $\bar{t}$ and $\bar{t}$ of the model are calculate in the right partition of Tab. VII. As shown in Table VII, placing C atoms in the ridge sites generates larger $(\bar{t} - \bar{t})/t$ that ultimately increases the tilt from the $\zeta_y = 0.46$ of the pristine borophene to $\zeta_y = 0.59$ in $B_6C_2R$. Employing Eqs. (3) and (4) the energy dispersion for pristine borophene, $B_6C_2I$, and $B_6C_2R$ are reconstructed in Fig. 14 using the ab initio effective hopping amplitude reported in Tab. VII.

![3D plot band structures obtained based on our effective tight-binding model using ab initio hopping matrix elements for (a) pure $B_6$ (b) $B_6C_2I$, and (c) $B_6C_2R$.](image-url)

**FIG. 14:** 3D plot band structures obtained based on our effective tight-binding model using ab initio hopping matrix elements for (a) pure $B_6$ (b) $B_6C_2I$, and (c) $B_6C_2R$.

**Accuracy of tilt parameters:** The ultimate outcome of our model is to understand the mechanism of the formation of the tilt. Hence the value of tilt parameters are important. Let us close this supplementary material by a comparison between the values of the tilt parameter directly extracted from the DFT data, and the tilt parameter predicted by Eq. (5) of our model.

We extract the tilt directly from the DFT data by fitting the slopes $m_R$ and $m_L$ of the ab initio dispersion relations along the $\Gamma\bar{Y}$ direction as,

$$\zeta_y^{\text{DFT}} = \frac{m_R - m_L}{m_R + m_L}.$$

Using the direct DFT data, we find that the tilting parameter value $\zeta_y^{\text{DFT}}$ are 0.49, 0.47, and 0.66 in pristine borophene, $B_6C_2I$, and $B_6C_2R$ respectively. This is in qualitative agreement with the values obtained from our model, Eq. (5) and the trend in tilt values upon placing the carbon atoms in ridge/inner sites are correctly reproduced in our model (see Tab. VII). The physical picture emerging from both DFT data and our model is that the substitutions of $B_R$ atoms by C dimers where the two C atoms belong to the ridge sites can increase the tilt of Dirac cone. Moreover, the location of tilted Dirac-cone is very sensitive to the position of C atoms on the $8Pmnm$ lattice. This location has been quantified by the parameter $k_D/k_y$ to measure the distance from Dirac point to $\Gamma$ and the results are reported in Tab. VII. If C atoms are replaced in the ridge sites, Dirac-node moves closer to $\Gamma$ point.

To conclude, the tilted Dirac cone dispersion in $8Pmnm$ borophene can be well described by our effective tight-binding model. This effective model is not only important for understanding the origin of formation of the tilt in the Dirac cone in borophene, but it also increases considerably the predictive power to find new compounds possessing tilted Dirac cone. Furthermore, our concrete model paves the path for many other studies including the effects of interactions/disorder/symmetry breaking.
etc in a physically motivated model of tilted Dirac cone in $8Pmn$ space group.

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