I. INTRODUCTION

Monolayer material science is one of the most active fields of condensed matter physics in this decade. It has begun with graphene and been extended to the group IV monolayer materials including silicene, germanene, stanene, and antimonene. Furthermore, experimental success of phosphorene has opened a field of the group V monolayer materials including arsenene and antimonene. A search for new monolayer materials is extended to the group III monolayer materials including borophene and aluminene. Especially, several types of borophene are proposed by first-principles calculation. Recently, several types of borophene is synthesized on Ag(111) and have been extended to the group IV monolayer material.

In particular, borophene experimentally manufactured on the silver surface is quite interesting. Dirac fermions are clearly observed by the ARPES experiments as well as by first-principles calculation. The band structure is well reproduced by a tight-binding model, where it is enough to take into account only the $p_z$ orbitals of its perfect planar structure. The unit cell contains five atoms as in Fig. 1(a). The lattice has a perfectly flat structure as in Fig. 1(b). It can be constructed by adding atoms indicated in yellow into the honeycomb lattice.

In this paper we study the band structure of borophene based on the tight-binding model. In particular we explore the band touching problem at high symmetry points. We then confirm the above results. In Sec.VI, we study edge states of borophene nanoribbons, where five different types of edges are introduced corresponding to the unit cell number.

II. $\beta_{12}$ LATTICE

The lattice structure of borophene is illustrated in Fig. 1(b). The unit cell contains five atoms as in Fig. 1(a). The "a" and "e" atoms have four bonds, the "b" and "d" atoms have five bonds, and the "c" atoms have six bonds, leading to the basic properties of the lattice structure, the Brillouin zone and the symmetry for $\beta_{12}$ borophene. In Sec. III, we start with a five-band model comprised of the $p_z$ orbitals of Boron. We compare three types of models. One is a homogeneous model, where we take an identical transfer energy and an identical on-site energy. The second is the inversion symmetric model, where the transfer and on-site energies are chosen so as to respect the inversion symmetry. The third is the inversion non-symmetric model, where on-site energies breaks the inversion symmetry. We show that Dirac fermions are gapless (gapped) when the inversion symmetry is present (absent). In Sec.IV, we derive an effective Dirac theory for general parameters and confirm the above results. In Sec.V, we derive effective theories of fermions at three-band touching points. It is shown that the set of fermions at the $X$ or $M$ point is unitary equivalent to the triplet of the pseudospin ($J = \pm 1, 0$). In Sec.VI, we study edge states of borophene nanoribbons, where five different types of edges are introduced corresponding to the unit cell number.

III. Band Structure

Borophene is a monolayer materials made of boron. A perfect planar borophene called $\beta_{12}$ borophene has Dirac cones and they are well reproduced by a tight-binding model according to recent experimental and first-principles calculation results. We explicitly derive a Dirac theory for them. Dirac cones are gapless when the inversion symmetry exists, while they are gapped when it is broken. In addition, three-band touching points emerge together with pseudospin triplet fermions when all transfer energy is equal and all on-site energy is equal. The three-band touching is slightly resolved otherwise. We construct effective three-band theories for triplet fermions. We also study the edge states of borophene nanoribbons, which show various behaviors depending on the way of edge terminations.
ficient on-site potentials.

The Brillouin zone is a rectangular given by \(-\pi/a \leq k_x \leq \pi/a\) and \(-\pi/(\sqrt{3}a) \leq k_y \leq \pi/(\sqrt{3}a)\), as shown in Fig. 2(a). However, it is convenient to use a shifted Brillouin zone \(0 \leq k_x \leq 2\pi/a\) and \(-\pi/(\sqrt{3}a) \leq k_y \leq \pi/(\sqrt{3}a)\). The area of the Brillouin zone of \(\beta_{12}\) borophene is one half of that of the honeycomb lattice. This is understood as follows. The \(\beta_{12}\) lattice without the "c" atoms is identical to the honeycomb lattice, where the unit cell contains four atoms. On the other hand, the honeycomb lattice has only two atoms in the unit cell. Namely, the Brillouin zone of the \(\beta_{12}\) borophene must be one half of that of the honeycomb lattice.

The symmetries of the lattice are the inversion symmetry \(I\), the two mirror symmetries with respect to the \(x\) and \(y\) axes, \(M_x\) and \(M_y\). There is a relation \(I = M_x M_y\). On the other hand, the \(C_3\) rotation symmetry is absent in the \(\beta_{12}\) lattice, which exists in the honeycomb lattice.

III. FIVE-BAND MODEL

A recent first-principles calculation demonstrates that the system is well described only in terms of the \(p_z\) orbitals of the boron atoms\(^{19}\) implying that the tight-binding model is five dimensional,

\[
H_5 = \begin{pmatrix}
\varepsilon_a & t_{ab}g^* & t_{ac}f^* & 0 & t_{af}c \\
-t_{ab}g & \varepsilon_b & t_{bc}f^* & 0 & 0 \\
t_{ac}f & t_{bc}g & \varepsilon_c & t_{cd}f & t_{ce}g \\
0 & -t_{bc}f & \varepsilon_d & t_{de}f & t_{de}g \\
t_{af}c & 0 & t_{cd}g & -t_{de}f & \varepsilon_e
\end{pmatrix} \quad (1)
\]

with

\[
f = e^{iak_x/\sqrt{3}}, \quad g = 2e^{-iak_y/2\sqrt{3}} \cos ak_x/2. \quad (2)
\]

The parameters obtained by fitting first-principles calculation results are summarized as\(^{20}\),

\[
t_{ab} = t_{de} = -2.04, \quad t_{ac} = t_{ce} = -1.79, \quad t_{ae} = -2.12, \\
t_{be} = t_{cd} = -1.84, \quad t_{bd} = -1.91. \quad (3)
\]

The parameters obtained by fitting first-principles calculation results are summarized as\(^{20}\),

\[
U_1^{-1}H_5(K_{\pm}) U_1 = t \text{ diag.} \left(0, 0, 1 \pm \sqrt{5}, -2\right) \quad (6)
\]

with the use of a unitary transformation \(U_1\). (These two points are customarily called the \(K\) and \(K'\) points.) It is interesting
that there are different types of three-band touching points. Their positions in the Brillouin zone are shown in Fig.2(b). One is at the point $X = (\pi/a, 0)$, where the energy is given by

$$U_3^{-1} H_5 (X) U_2 = t \text{ diag.} (1, 1, 1, -1, -2).$$

(7)

The second one is at the point $M = (\pi/a, \pi/\sqrt{3}a)$, where the energy is given by

$$U_3^{-1} H_5 (M) U_3 = t \text{ diag.} (-1, -1, -1, 1, 2).$$

(8)

The third one is at the points $\Lambda_{x} = (\pm \pi/(3a), \pi/(\sqrt{3}a))$, where the energy is given by

$$U_4^{-1} H_5 (\Lambda_{x}) U_4 = t \text{ diag.} (-2, -2, -2, 2, 4).$$

(9)

We show the detailed band structures of Dirac fermions and triple-point fermions in Fig.4(a1), (b1), (c1) and (d1).

We may investigate both the inversion symmetric and nonsymmetric models in a similar way. Their overall band structures are very similar to that of the homogeneous model, as shown in Fig.3(b1) for the inversion nonsymmetric model. However, there arise differences with respect to the degeneracy at the band touching points. First, the Dirac fermions remain gapless in the inversion symmetric model but get gapped in the inversion nonsymmetric model. On the other hand, three-band touching points are slightly resolved both in the inversion symmetric and nonsymmetric models. We show the detailed band structure at these points in Fig.4.

FIG. 4: Band structures in the vicinity of the Dirac point ($K$) indicated by a magenta circle and the three-band touching points ($X$, $M$, $\Lambda$) indicated by cyan circles: (a1) for the homogeneous model; (a2) for the inversion symmetric model; (a3) for the inversion nonsymmetric model. Dirac fermions become gapped in the inversion symmetric model and nonsymmetric models. We show the detailed band structures of Dirac fermions and triple-point fermions in Fig.4(a1), (b1), (c1) and (d1).
it is constructed solely for the homogeneous model. The dispersion is isotropic only when \( \epsilon = 0 \). The fact that the Brillouin zone is enlarged twice since the unit cell Expanded in the vicinity of the \( \Gamma \) point, the two-band Hamiltonian is

\[
H_2 = \begin{pmatrix}
(\epsilon_b + \epsilon_e)/2 & F \\ F^* & (\epsilon_a + \epsilon_d)/2
\end{pmatrix},
\]

with

\[
F = \frac{t_{ae} + t_{bd}}{2} e^{-iak_y/\sqrt{3}} + (t_{ab} + t_{de}) e^{iak_y/\sqrt{3}} \cos \frac{ak_x}{2}.
\]

It is identical to the Hamiltonian of the anisotropic honeycomb lattice with on-site potentials which corresponds to the lattice without the "c" atoms. This correspondence is due to the fact that the amplitude of the wave function at the "c" sites is zero at the zero energy.

The gap closes at

\[
\tilde{K} = \left( \frac{2}{\alpha} \arccos - \frac{(t_{ae} + t_{bd})}{2(t_{ab} + t_{de})}, 0 \right),
\]

when \( \epsilon_a - \epsilon_b + \epsilon_d - \epsilon_e = 0 \). Especially, the gap closes in the presence of the inversion symmetry since \( \epsilon_a = \epsilon_e \) and \( \epsilon_b = \epsilon_d \). The gap closing point shifts from the original \( K \) point when \( t_{ae} + t_{bd} \neq t_{ab} + t_{de} \). The gap opens when \( \epsilon_a - \epsilon_b + \epsilon_d - \epsilon_e \neq 0 \) with the gap \( |\epsilon_a - \epsilon_b + \epsilon_d - \epsilon_e|/2 \). We estimate the gap is 0.254 eV by using the parameters in the inversion nonsymmetric model.

We show the band structure along the \( k_y \) axis of the two-band model as well as the five-band model in Fig. 5b. The Dirac fermions at the \( K \) point is well reproduced, while the Dirac fermions at the \( \Gamma' \) point disappear. This is due to the fact that the Brillouin zone is enlarged twice since the unit cell becomes half compared with that of the four-band model, as shown in Fig. 2. It is necessary to construct another two-band model by expanding at the \( K' \) point, which is done precisely in the similar way.

In the vicinity of the \( K' \) point, the two-band Hamiltonian is expanded as

\[
H^K_2 = \frac{\epsilon_a - \epsilon_b + \epsilon_d - \epsilon_e}{4} \tau_z - \frac{\epsilon_a - \epsilon_b + \epsilon_d - \epsilon_e}{4} \tau_0
\]

\[
- \sqrt{4(t_{ab} + t_{de})^2 - (t_{ae} + t_{bd})^2} \frac{4}{4} \alpha(k_x - \tilde{K}) \tau_x
\]

\[
+ \sqrt{3} \frac{4}{4} (t_{ae} + t_{bd}) ak_y \tau_y,
\]

which describe a Dirac cone. The dispersion is isotropic only for the homogeneous model.

In passing, it is intriguing to see that the four-band theory describes precisely two bands of the \( X \) and \( M \) points though it is constructed solely for the \( K \) and \( K' \) points in Fig. 5.
with \( k_x' = k_x \mp \frac{\pi}{3} \). The corresponding wave functions are
\[
\psi_0 = \{0, i \sin \theta, \cos \theta\}^t, \quad (19)
\[
\psi_{\pm} = \frac{1}{\sqrt{2}} \{\pm i, -i \cos \theta, \sin \theta\}^t. \quad (20)
\]
The Berry phase is zero for each band,
\[
\Gamma_B = -i \int d\theta \langle \psi_0 | \frac{\partial}{\partial \theta} | \psi_0 \rangle = -i \int d\theta \langle \psi_{\pm} | \frac{\partial}{\partial \theta} | \psi_{\pm} \rangle = 0. \quad (21)
\]
Since the band carries no topological charge, the \( X \) point can exist by itself. Furthermore, it indicates that the three-band touching point is not topologically protected.

The energy eigenstate of the Hamiltonian \((18)\) is given by \( E = -t, -t \pm \sqrt{k_x'^2 + k_y^2} \). Hence it is unitary equivalent to the following Hamiltonian,
\[
H = -t + ta(k_x'J_x + k_yJ_y), \quad (22)
\]
where \( J = (J_x, J_y, J_z) \) is the pseudospin operator obeying \( [J_x, J_y] = J_z \), etc., whose magnitude is \( J = 1 \). Namely, the three bands are members of a pseudospin triplet with \( J \). On the other hand, the middle band becomes a perfect flat band in the three-band model \((3)\) as Fig.3(a2).

\( M \) point: In the vicinity of the \( M \) point, we obtain the following effective three-band model,
\[
H^M_3 = t \begin{pmatrix}
F_{aa}^M & F_{ab}^M & F_{ac}^M \\
F_{ba}^M & F_{bb}^M & F_{bc}^M \\
F_{ca}^M & F_{cb}^M & F_{cc}^M
\end{pmatrix}, \quad (23)
\]
where
\[
F_{aa}^M = F_{bb}^M = F_{cc}^M = \frac{1}{2} \left( \cos \frac{ak_x'}{\sqrt{3}} + \sqrt{3} \sin \frac{ak_y}{\sqrt{3}} \right),
\]
\[
F_{ab}^M = (-1)^{2/3} \cos \frac{ak_x}{2} \left( \sqrt{3} \sin \frac{ak_y}{2\sqrt{3}} - \cos \frac{ak_y}{2\sqrt{3}} \right),
\]
\[
F_{ac}^M = \frac{\sqrt{3}}{2} \left( -1 \right)^{5/6} \left( \sin \frac{ak_y}{2\sqrt{3}} - \sqrt{3} \cos \frac{ak_x}{\sqrt{3}} \right),
\]
\[
F_{bc}^M = (-1)^{1/6} \sqrt{3} \cos \frac{ak_x}{2\sqrt{3}} \left( \sin \frac{ak_y}{2\sqrt{3}} + \sqrt{3} \cos \frac{ak_y}{2\sqrt{3}} \right). \quad (24)
\]
in the case of the homogeneous model. See Appendix for general parameters.

We show the band structure in Fig.6(b1). In Fig.6(b2), comparing the band structure of the three-band model \( H^M_3 \) along the \( k_y = \pi / \sqrt{3} a \) line with that of the five-band model \( H_5 \), we find that the three-band model \( H^M_3 \) perfectly reproduces the two-bands given by \( E = t \pm 2 \cos \frac{ak_x'}{2} \) all over the region. On the other hand, the middle band becomes a perfect flat band in the three-band model \( H^M_3 \), while it is dispersive in the five-band model \( H_5 \).

We expand the three-band Hamiltonian in the vicinity of the \( M \) point as
\[
H^M_3 = t + ta \begin{pmatrix}
0 & 0 & e^{5i\pi/6}k_y' \\
0 & 0 & -\sqrt{3}e^{-i\pi/6}k_x' \\
e^{-5i\pi/6}k_y' & -\sqrt{3}e^{i\pi/6}k_x' & 0
\end{pmatrix} \quad (25)
\]
with \( k_x' = k_x - \pi/a \), \( k_y' = k_y - \pi/(\sqrt{3}a) \). The energy is obtained as \( E = t, t \pm \sqrt{3}k_x'^2 + k_y'^2 \). Hence it is unitary equivalent to the following Hamiltonian,
\[
H = t + ta(\sqrt{3}k_x'J_x + k_yJ_y). \quad (26)
\]
The three bands are members of a pseudospin triplet with \( J = \pm 1, 0 \). The Berry phase is zero for each band. Consequently, the \( M \) point is not accompanied by a partner. These properties are quite similar to those of the \( X \) point.

\( \Lambda \) point: In the vicinity of the \( \Lambda \) point, we obtain the following effective three-band model,
\[
H^\Lambda_3 = t \begin{pmatrix}
F_{aa}^\Lambda & F_{ab}^\Lambda & F_{ac}^\Lambda \\
F_{ba}^\Lambda & F_{bb}^\Lambda & F_{bc}^\Lambda \\
F_{ca}^\Lambda & F_{cb}^\Lambda & F_{cc}^\Lambda
\end{pmatrix} \quad (27)
\]
with

\[ F_{\alpha\alpha}^{\Lambda} = F_{bb}^{\Lambda} = F_{cc}^{\Lambda} = -\frac{1}{4} \cos \frac{ak_y}{\sqrt{3}} + \sqrt{3} \sin \frac{ak_y}{\sqrt{3}} \]
\[ + 2\sqrt{3} \cos \frac{ak_x}{2} \left( \sqrt{3} \cos \frac{ak_y}{2\sqrt{3}} + \sin \frac{ak_y}{2\sqrt{3}} \right), \]
\[ F_{ab}^{\Lambda} = \frac{1}{4} (-1)^{2/3} \left[ -3 \cos \frac{ak_y}{\sqrt{3}} + \sqrt{3} \sin \frac{ak_y}{\sqrt{3}} \right. \]
\[ + 2 \cos \frac{ak_x}{2} \left( \sqrt{3} \sin \frac{ak_y}{2\sqrt{3}} - \cos \frac{ak_y}{2\sqrt{3}} \right), \]
\[ F_{ac}^{\Lambda} = \frac{\sqrt{3}}{2} e^{-ia k_y/\sqrt{3}} (-1)^{2/3} \left. + \frac{\sqrt{3}}{4} e^{ia k_y/\sqrt{3}} \right| \cos \frac{ak_x}{2} \]
\[ - \frac{3i}{2} e^{-ia k_y/2\sqrt{3}} \cos \frac{ak_x}{2}, \]
\[ F_{bc}^{\Lambda} = \left[ \frac{\sqrt{3}}{2} (-1)^{1/6} e^{-ia k_y/2\sqrt{3}} + \sqrt{3} e^{ia k_y/2\sqrt{3}} \right] \cos \frac{ak_x}{2} \]
\[ + \frac{3}{4} (-1)^{1/6} e^{ia k_y/\sqrt{3}}. \]  

(28)

We show the band structure in Fig.6(c1). In Fig.6(c2), we compare the band structure of the three-band model \( H_3^{\Lambda} \) along the \( k_y = \pi / \sqrt{3}a \) line with that of the original five-band model \( H_5 \), and find that the three-band model \( H_3^{\Lambda} \) perfectly reproduces the two bands given by \( E = -2t, t - 2 \cos \frac{ak_x}{2\sqrt{3}} \) all over the region.

In the vicinity of the \( \Lambda \) point, the Hamiltonian is expanded as

\[ H_3^{\Lambda} = -2t + \frac{\sqrt{3}}{2} ak_x + t a \left( \begin{array}{ccc} 0 & F_{ab}^{C'} & F_{ac}^{C'} \\ F_{ab}^{C' *} & 0 & F_{bc}^{C'} \\ F_{ac}^{C' *} & F_{bc}^{C' *} & 0 \end{array} \right). \]  

(29)

VI. BOROPHENE NANORIBBONS

When a nanoribbons is along the zigzag direction there are zigzag and beard edges in the case of the honeycomb system. This is because there are two atoms in the unit cell. There are five types of borophene nanoribbons with zigzag edges corresponding to the fact that the unit cell contains five atoms. For example, the edge terminated by "a", "b", "c" and "d" atoms forms a zigzag edge, while that terminated by "e" atoms forms a beard edge. Thus there are \( 5 \times 5 = 25 \) different nanoribbons.

We show the band structure of typical nanoribbons in Fig.7(a)~(e). In Fig.7(f), we show the bulk band structure projected to the \( k_x \) axes for the sake of comparison. The band structure of nanoribbons are almost identical to those of the projected bulk band structure except for the edge states, which are marked by magenta curves. The edge states emerge in the region connecting between the Dirac point and the triple point. Among them, there emerge almost flat bands at the zero energy in Fig.7(e), which corresponds to the beard edge states. If the two terminations are different, the edge states are the sum of the two terminations.

VII. DISCUSSION

It is interesting that Dirac fermions or triplet fermions emerge in the \( \beta_{12} \) structure of borophene at the high symmetry points. There is a distinctive difference between them. On one hand, Dirac fermions emerge always in a pair: They emerge at the \( K \) and \( K' \) points just as in graphene. The reason is the Nielsen-Ninomiya theorem. Namely, the gapless Dirac fermions has \( \pm \pi \) Berry phase while the gapped Dirac fermion has \( \pm 1/2 \) Chern number. They appear in a pair so that the total topological number must be zero.

One the other hand, this is not the case for triplet fermions. There are no partners for the \( X \) and \( M \) points. Indeed, calculating the Berry phases of the bands at \( X \) and \( M \), we find them to be zero.

The lattice structure of \( \beta_{12} \) borophene has the inversion symmetry, where massless Dirac fermions are expected. However, the inversion symmetry is broken in the Hamiltonian together with the parameters presented in Ref.29 where Dirac fermions are gapped. The ARPES experiment shows that the gap is absent within the experimental resolution.

We note that there is a metallic band at the zero-energy in the five-band model, while it is absent in the effective lower-band theories. It is because that they are valid in the vicinity of the high symmetry points. We should use the five-band model when we calculate the conductivity and others.

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Appendix: Three-band theories with general parameters

In this appendix we present the matrix elements of the effective three-band theories \( 16 \) and \( 5 \) with general parameters \( \varepsilon_1 \) and \( \varepsilon_2 \).
X point:

\[ F_{aa}^X = \frac{\varepsilon_a + \varepsilon_e}{2} - t_{ac} \cos \frac{ak_y}{\sqrt{3}}, \]
\[ F_{bb}^X = \frac{\varepsilon_b + \varepsilon_d}{2} - t_{bd} \cos \frac{ak_y}{\sqrt{3}}, \]
\[ F_{cc}^X = \frac{\varepsilon_a + 4\varepsilon_c + \varepsilon_e}{6} - \frac{2t_{ac} - t_{ac} + 2t_{ee}}{3} \cos \frac{ak_y}{\sqrt{3}}, \]
\[ F_{ab}^X = \left( t_{ab} e^{i \frac{ak_y}{\sqrt{3}}} + t_{cd} e^{i \frac{ak_y}{\sqrt{3}}} \right) \cos \frac{ak_y}{2}, \]
\[ F_{ac}^X = \frac{\varepsilon_a - \varepsilon_e}{2 \sqrt{3}} + \frac{-t_{ac} + t_{cc}}{\sqrt{3}} \cos \frac{ak_y}{\sqrt{3}} + \frac{t_{ac} + t_{ce} + t_{ee}}{\sqrt{3}} \sin \frac{ak_y}{\sqrt{3}}, \]
\[ F_{bc}^X = -\left( t_{de} + 2t_{bc} \right) e^{-i \frac{ak_y}{\sqrt{3}}} \cos \frac{ak_y}{2}. \]  

(31)

M point:

\[ F_{aa}^M = \frac{\varepsilon_a + \varepsilon_e}{2} + \frac{t_{ac}}{2} \cos \frac{ak_y}{\sqrt{3}} + \sqrt{3} t_{ae} \sin \frac{ak_y}{\sqrt{3}}, \]
\[ F_{bb}^M = \frac{\varepsilon_b + \varepsilon_d}{2} + \frac{t_{bd}}{2} \cos \frac{ak_y}{\sqrt{3}} + \sqrt{3} t_{bd} \sin \frac{ak_y}{\sqrt{3}}, \]
\[ F_{cc}^M = \frac{\varepsilon_a + 4\varepsilon_c + \varepsilon_e}{6} + \frac{2t_{ac} - t_{ac} + 2t_{ce}}{6} \left( \cos \frac{ak_y}{\sqrt{3}} + \sqrt{3} \sin \frac{ak_y}{\sqrt{3}} \right), \]
\[ F_{ab}^M = \left( \frac{e^{-2i \pi/3}}{4} t_{ab} e^{i \frac{ak_y}{\sqrt{3}}} + t_{de} e^{-i \frac{ak_y}{\sqrt{3}}} \right) \cos \frac{k_y}{2}, \]
\[ F_{ac}^M = \frac{e^{-i \pi/3} \left( 2t_{ac} - t_{ac} \right) e^{-i \frac{ak_y}{\sqrt{3}}} + (t_{ac} + t_{ce}) e^{-i \frac{ak_y}{\sqrt{3}}} + t_{ce} e^{-i \frac{ak_y}{\sqrt{3}}} + \frac{2t_{ee} + (-1)^{1/3} \left( t_{bc} + 2t_{cd} \right) e^{i \frac{ak_y}{\sqrt{3}}} \cos \frac{ak_y}{2}. \]  

(32)

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1. H. Tang and S. Ismail-Beigi, Phys. Rev. Lett. 99, 115501 (2007).
2. X. Wu, J. Dai, Y. Zhao, Z. Zhuo, J. Yang, and X. C. Zeng, ACS Nano 6, 7443 (2012).
3. E.S. Penev, S. Bhowmick, A. Sadrazadeh, and B. I. Yakobson, Nano Lett. 12, 2441 (2012).
4. A.J. Mannix, X.-F. Zhou, B. Kiraly, J. D. Wood, D. Alducin, B. D. Myers, X. Liu, B. L. Fisher, U. Santiago, J.R. Guest, M. J. Yacaman, A. Ponce, A.R. Oganov, M.C. Hersam, and N. P. Guisinger, Science 350, 1513 (2015).
5. Z. Zhang, Y. Yang, G. Guo, and B.I. Yakobson, Angew. Chem., Int. Ed. 52, 3156 (2013).
6. Y. Liu, J. Gao, and J. Zhao, Sci. Rep. 3, 3238 (2013).
7. T. Iimori, C. Lian, H. Li, L. Chen, B. Feng, J. Zhang, R.-Y. Liu, T. Iimori, C. Lian, H. Li, P. Cheng, S. Meng, L. Chen, and K. Wu, Nat. Chem. 8, 563 (2016).
8. B. Feng, J. Zhang, R.-Y. Liu, T. Iimori, C. Lian, H. Li, L. Chen, K. Wu, S. Meng, F. Komori, and I. Matsuda, Phys. Rev. B 94,
26 B. Feng, et.al., Phys. Rev. Lett. 118, 096401 (2017)
27 M. Ezawa, New J. Phys. 16 115004 (2014)
28 B. Bradlyn, et al, Science.aaf5037 (2016).
29 G. Chang, et.al., cond-mat/arXiv:1605.06831
30 H. Weng, C. Fang, Z. Fang, and X. Dai, Phys. Rev. B 93, 241202 (2016).
31 H. Weng, C. Fang, Z. Fang, and X. Dai, Phys. Rev. B 94, 165201 (2016).
32 Z. Zhu, G. W. Winkler, Q. S. Wu, J. Li, and A. A. Soluyanov, Phys. Rev. X 6, 031003 (2016).
33 M. Ezawa, Phys. Rev. B 94, 195205 (2016)
34 M. Ezawa, cond-mat/arXiv:1612.05857