Topological Luttinger semimetallic phase accompanied with surface states realized in silicon

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By means of systematically first-principles calculations and model analysis, a complete phase diagram of the body-centered silicon (BC8-Si) via lattice constant \(a\) and internal atomic coordinate \(x\) is explored, which demonstrates that BC8-Si is a topological Luttinger semimetal (LSM) accompanied with topologically nontrivial surface states, and the electronic properties of BC8-Si can be further tuned to a normal insulator or topological Dirac semimetal by very tiny changing of \(a\) and \(x\). These results successfully explain the contradictory transport reports of BC8-Si. More importantly, the topological surface states in the LSM phase fill in the gap between the topological matters and silicon, which provide an opportunity to integrate the topological quantum devices and silicon chips together.

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Introduction—Silicon is the most important material for electronic and photovoltaic industry due to its excellent electronic properties and mature technology. Especially, almost 90% of electronic chips are equipped based on the diamond cubic silicon (DC-Si). Nonetheless, the miniaturization of Si-based chips is facing the end of Moore’s Law due to the limitation of quantum effects. Searching and devising the next-generation of electronic devices are the most urgent and challenging task.

In the past decades, topological matters with nontrivial boundary modes have attracted intensive attentions due to their novel properties such as backscattering suppression, spin-momentum locking and non-abelian braiding, which are expected to be a significant platform for the next-generation electronic and spintronic devices. In order to integrate the topological quantum devices and silicon chips together, it is highly desirable to realize the topological boundary modes in silicon. However, these two fields have no overlap until now, because DC-Si is well known as semiconductor without band inversion, which makes it impossible to hold the topological boundary modes.

Fortunately, silicon has more than 13 allotropes. Among them, a body-centered cubic structure, named as BC8-Si, was reported to be stabilized under ambient conditions, but its electronic properties are under debate. While previous experiments and calculations suggest that BC8-Si is a semimetal with band overlap, a contrary literature reports that it is a narrow band gap semiconductor recently. In particular, the topological properties of BC8-Si have never been studied yet. In this paper, by means of the first-principles calculations, we investigate the electronic and topological properties of BC8-Si systematically, and demonstrate that it is a topological Luttinger semimetal (LSM) with band inversion, on the surface of which, topological surface states can be stabilized. Moreover, our numerical results indicate that the electronic and topological properties of BC8-Si are sensitive to the lattice constant \(a\) and internal atomic coordinate \(x\). A complete phase diagram via \(a\) and \(x\) is explored, which demonstrates that the topological LSM phase of BC8-Si can be tuned to a normal insulator (NI) without band inversion or a topological Dirac semimetal (DSM) by very tiny changing of \(a\) and \(x\). Such changing can be achieved by varying the applied pressure during crystal synthesis. Our results successfully explain the controversial reports on electronic properties of BC8-Si. More importantly, the topological properties of BC8-Si fill in the gap between the topological matters and silicon, which provides an opportunity to integrate the next-generation electronic quantum devices and silicon chips together.

Crystal structure and methodology—As shown in Fig. 1(a), BC8-Si adopts the body-centered cubic lattice with space group \(Ia\overline{3}\) (No.206), where the lattice constant \(a\) equals 6.636 Å and Si atoms are located at 16c Wyckoff position with coordinate \(x = 0.1003\). These most reported experimental crystal parameters are used in our calculations, otherwise they will be explicitly pointed out. Compared with DC-Si, Si atoms form a slightly distorted tetrahedral structure with two types Si-Si distance \(A = 2.305\) Å and \(B = 2.391\) Å in BC8-Si. The first Brillouin zone (BZ) of the primitive cell and its projection on the (001) surface of the unit cell are displayed in Fig. 1(b). Our first-principles calculations are performed by the Vienna ab initio simulation package with the projected augmented wave method. The energy cutoff is set as 400 eV, and 7 × 7 × 7 k-meshes are adopted. Perdew-Burke-Ernzerhof type of the exchange-correlation potential, and Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional with Hartee-Fock exchange factor 0.35 are used in all calculations to obtain the accurate electronic structures. Spin-orbit coupling (SOC) interaction is considered consistently. Sym-
symmetry preserving Wannier functions are constructed by the Wannier90 package. The surface states are calculated by iterative Green’s function method as implemented in the WannierTools package.

*Luttinger semimetal* — The electronic configuration of Si atom is $3s^23p^2$. Because each Si atom is tetrahedrally connected with other four Si atoms, the main chemical bonding in BC8-Si is $sp^3$ hybridization, which is similar to the chemical bonding in DC-Si. As a result, the calculated band structures in Fig. 2(a) show that the $sp^3$ bonding states are almost fully occupied and contribute to the valence bands, while the $sp^3$ antibonding states are almost empty and form conduction bands. However, different from semiconductor DC-Si, one antibonding state in BC8-Si is lower than its bonding states at $H$ point as shown in the inset of Fig. 2(a) and Fig. 2(b), which leads to a band inversion in BC8-Si and makes it a semimetal. Due to the presence of inversion symmetry ($I$) and time reversal symmetry ($T$), each band in BC8-Si is doubly degenerate at every momentum $k$, which means that the band touching at Fermi level ($E_F$) is fourfold degeneracy.

Furthermore, the dispersions around the fourfold degenerate node are always parabolic as shown in Fig. 2(b) and Fig. 6. We further transform Eq. 7 to the SOC representation as shown in Fig. 2(b) and Fig. 6. We further transform Eq. 7 to the SOC representation $|J, J_z\rangle$ as described in appendix B, where $J = L + S$ is the total angular momentum, and $J_z$ is its projections on the $z$-axis. Under the basis of $|p_x\rangle^+, |p_y\rangle^+, |p_z\rangle^+$ and $|s\rangle^-$ with the superscript +/- denoting parity, the generators of $T_h$ can be expressed by the matrix form as shown in Eq. 2 and the Hamiltonian without SOC is constructed as Eq. 3 (see details in appendix A). In Table 1, the parameters of the effective model are obtained by fitting with first-principles calculations. The fitted band structures are plotted in Fig. 5 which give rise to a triply degenerate node formed by the bonding orbitals at $H$ point due to the protection of $C_{3v}$.

By considering SOC, the Hamiltonian under the spinful basis $\left(|p_{x\uparrow}\rangle^+, |p_{y\uparrow}\rangle^+, |p_{z\uparrow}\rangle^+, |s\rangle^+ \otimes (|\uparrow\rangle | \downarrow\rangle)\right)$ is given in Eq. 7 where the $H_{soc}$ is shown in Eq. 6 with atomic SOC strength parameter $\lambda$. With $\lambda = 0.0152$ eV, the energy eigenvalues of the eight-band model well reproduce the band structures from first-principles calculations as shown in Fig. 2(b) and Fig. 6. We further transform Eq. 7 to the SOC representation $|J, J_z\rangle$ as described in appendix B, where $J = L + S$ is the total angular momentum, and $J_z$ is its projections on the $z$-axis. Under the basis of $|\frac{3}{2}, \frac{1}{2}\rangle^+|\downarrow\rangle, |\frac{3}{2}, \frac{3}{2}\rangle^+|\uparrow\rangle, |\frac{3}{2}, -\frac{1}{2}\rangle^+|\downarrow\rangle, |\frac{1}{2}, \frac{3}{2}\rangle^+|\uparrow\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle^+|\downarrow\rangle, |\frac{1}{2}, \frac{1}{2}\rangle^+|\uparrow\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle^+|\downarrow\rangle$, the new Hamiltonian is written in Eq. 10 which explicitly shows that the $|J = \frac{3}{2}\rangle^+$ doublet is pushed down $2\lambda$ while $|J = \frac{3}{2}\rangle^+$ quartet is pushed up $\lambda$ at $H$ point by SOC interaction. As a result, the energy difference between $|J = \frac{3}{2}\rangle^-$ and $|J = \frac{3}{2}\rangle^+$ at $H$ point can be described as $\Delta = E_{ab} - E_{b} - \lambda$. According to the fitted parameters list in Table 1 we get $\Delta = -78$ meV $< 0$, which means that the band inversion is well reproduced by our model and parameters. One important consequence of the band inversion is that the fourfold degenerate node formed by the $|J = \frac{3}{2}\rangle^+$ states is leaved at the $E_F$ exactly. Since $k^2$ is the leading order in the $|J = \frac{3}{2}\rangle^+$ subspace, the band dispersions around the fourfold degenerate node are always parabolic. These results theoretically clarify...
that BC8-Si is a LSM with band inversion.

TABLE I. Fitted parameters of the eight-band $k \cdot p$ Hamiltonian. $E_0$ and $E_{ab}$ are the on-site energies of bonding and antibonding states at $H$ point. $t_1$, $t_2$, $t_3$ and $t_4$ are the mass terms in bonding and antibonding subspace, respectively. $t_5$ is the coupling between the bonding and antibonding subspace, while $t_6$ is the coupling within the bonding subspace.

$$H_{4 \times 4} = H_0 + H', \quad H_0 = \begin{bmatrix}
M_0(k) & -\frac{t_0 k_{x-kz}}{\sqrt{3}} & V_1(k) & 0 \\
-\frac{t_0 k_{x-kz}}{\sqrt{3}} & M_1(k) & 0 & V_1(k) \\
V_1^*(k) & 0 & M_1(k) & -\frac{t_0 k_{x-kz}}{\sqrt{3}} \\
0 & V_1^*(k) & -\frac{t_0 k_{x-kz}}{\sqrt{3}} & M_0(k)
\end{bmatrix}, \quad H' = \frac{t_0^2}{-\Delta} \begin{bmatrix}
\frac{1}{6} k_{k-kz} & \frac{2k^2}{3} & -\frac{k_z k_x}{\sqrt{3}} & \frac{k_z^2}{2\sqrt{3}} \\
-\frac{k_z k_x}{\sqrt{3}} & \frac{2k^2}{3} & 0 & -\frac{k^2}{2\sqrt{3}} \\
\frac{k_z k_x}{\sqrt{3}} & \frac{2k^2}{3} & 0 & \frac{k^2}{2\sqrt{3}} \\
0 & \frac{k_z k_x}{\sqrt{3}} & \frac{2k^2}{3} & \frac{1}{6} (k_{k-kz} + \frac{2k^2}{3})
\end{bmatrix}$$

where $H_0$ comes from the upper left $4 \times 4$ block ($|J = \frac{1}{2} \rangle$ subspace) of the eight-band model in Eq. 10 with $M_0(k) = E_0 + \lambda + \frac{1}{2} \left[ (t_1 + 4t_2 + t_3) k_{x-kz}^2 + (4t_1 + t_2 + t_3) k_{k-z}^2 + (t_1 + t_2 + 4t_3) k_{k-z}^2 \right]$, $M_1(k) = E_0 + \lambda + \frac{1}{2} \left[ t_1 (k_{x-kz}^2 + k_{z-kx}^2) + t_2 (k_{y-kz}^2 + k_{z-y}^2) + t_3 (k_{x-z}^2 + k_{y-z}^2) \right]$, $V_1(k) = -\frac{1}{2\sqrt{3}} \left[ k^2 \right.$ ($t_1 + t_2 + t_3 + k_{k-kz}^2 (t_1 - t_3) + 2t_0 k_{x-kz} k_y$, $k^2 = k_{x-kz}^2 + k_{z-kx}^2$, $k_z = k_z \pm ik_y$, $H'$ is the influence part from $|J_e = \pm \frac{1}{2} \rangle$-

Topological characters — Maxim Kharitonov et al. have confirmed that the four-band 3-dimensional LSM is topological and can exhibit surface states, if its 2-dimensional (2D) reductions to some planes in momentum space passing the quadratic node are topologically non-trivial [22]. The topological properties of the reduced 2D nodal semimetal is determined by the phase diagram in $(|\beta_0_1|, |\beta_0_2|)$ parameter plane, as shown in Fig. 2. Here, $\beta_1$ is the coefficient of the pauli matrix $\sigma_y$ characterizing a chiral symmetric 2D LSM, and $\beta_0$, $\beta_2$ are the coefficients of $\sigma_0$ and $\sigma_z$ describing the breaking of the chiral symmetry. In Fig. 2, the gray region $|\beta_0| > \sqrt{|\beta_0|^2 + |\beta_2|^2}$ means that the system is no longer a semimetal, the pink region labeled by 0 is trivial semimetal, the blue and yellow region labeled by topological number 1 and 2 are the non-trivial LSM accompanied of one and two edge states, respectively.

To explore the topological properties of BC8-Si, the eight-band model in Eq. 10 is downfolded to four-band Hamiltonian by perturbation theory [23], the details of downfolding are shown in appendix C. Under the basis of $|\frac{3}{2}, \frac{1}{2} \rangle$, $|\frac{3}{2}, -\frac{1}{2} \rangle$, $|\frac{1}{2}, \frac{3}{2} \rangle$, $|\frac{1}{2}, -\frac{3}{2} \rangle$, a simple Hamiltonian describing the low energy physics of LSM in BC-8 Si is written as Eq. 1 up to its leading term of $k$:

$$H_4 \times 4 = H_0 + H', \quad H_0 = \begin{bmatrix}
M_0(k) & -\frac{t_0 k_{x-kz}}{\sqrt{3}} & V_1(k) & 0 \\
-\frac{t_0 k_{x-kz}}{\sqrt{3}} & M_1(k) & 0 & V_1(k) \\
V_1^*(k) & 0 & M_1(k) & -\frac{t_0 k_{x-kz}}{\sqrt{3}} \\
0 & V_1^*(k) & -\frac{t_0 k_{x-kz}}{\sqrt{3}} & M_0(k)
\end{bmatrix}, \quad H' = \frac{t_0^2}{-\Delta} \begin{bmatrix}
\frac{1}{6} k_{k-kz} & \frac{2k^2}{3} & -\frac{k_z k_x}{\sqrt{3}} & \frac{k_z^2}{2\sqrt{3}} \\
-\frac{k_z k_x}{\sqrt{3}} & \frac{2k^2}{3} & 0 & -\frac{k^2}{2\sqrt{3}} \\
\frac{k_z k_x}{\sqrt{3}} & \frac{2k^2}{3} & 0 & \frac{k^2}{2\sqrt{3}} \\
0 & \frac{k_z k_x}{\sqrt{3}} & \frac{2k^2}{3} & \frac{1}{6} (k_{k-kz} + \frac{2k^2}{3})
\end{bmatrix}$$

where $H_0$ comes from the upper left $4 \times 4$ block ($|J = \frac{1}{2} \rangle$ subspace) of the eight-band model in Eq. 10 with $M_0(k) = E_0 + \lambda + \frac{1}{2} \left[ (t_1 + 4t_2 + t_3) k_{x-kz}^2 + (4t_1 + t_2 + t_3) k_{k-z}^2 + (t_1 + t_2 + 4t_3) k_{k-z}^2 \right]$, $M_1(k) = E_0 + \lambda + \frac{1}{2} \left[ t_1 (k_{x-kz}^2 + k_{z-kx}^2) + t_2 (k_{y-kz}^2 + k_{z-y}^2) + t_3 (k_{x-z}^2 + k_{y-z}^2) \right]$, $V_1(k) = -\frac{1}{2\sqrt{3}} \left[ k^2 \right.$ ($t_1 + t_2 + t_3 + k_{k-kz}^2 (t_1 - t_3) + 2t_0 k_{x-kz} k_y$, $k^2 = k_{x-kz}^2 + k_{z-kx}^2$, $k_z = k_z \pm ik_y$, $H'$ is the influence part from $|J_e = \pm \frac{1}{2} \rangle$-

Phase diagram — Since it has been reported that the electronic property of BC8-Si is sensitive to lattice constant $a$ and internal atomic coordinate $x$ [34, 35], we further investigate their impacts on the band structures and topological properties by first principles calculations. The calculated phase diagram with various $a$ and $x$ consists of three subregions, NI, topological LSM and DMS, labeled by different colors in Fig. 3(a). Our results demonstrate that the electronic properties of BC8-Si are more sensitive to the atomic coordinate $x$. Keeping $a = 6.636 \text{ Å}$ as a constant ($a\% = 0.0$ in Fig. 3(a)), it shows that: (1) BC8-Si is a NI without band inversion when $x$ is less than 0.0998; (2) it falls into the topological LSM phase for the medium value of the reported results 0.1008 $> x > 0.0998$ [30, 41], where the parameters used in Fig. 2 are marked by a red star; (3) BC8-Si becomes topological DSM consisting both the Dirac point and the quadratic node, when $x$ exceeds 0.1008. In general, pressure (strain) will shorten (enlarge) the distance between the SI atoms by increasing (decreasing) $x$ and compressing (elongating) $a$ [54], which indicates the various electronic states of BC8-Si illustrated in Fig. 3(a), as discussed in $\alpha$-Sn [37] and Cu$_2$Se [58].

Normal insulator — Actually, different structural pa-
we would like to emphasize that the coordinate $x$ bital projections shown in the inset of Fig. 3(b). Finally, in the NI phase, which is clearly illustrated by the or- 

logical LSM phase, the energy difference $\Delta$ is positive gap of 5 meV of the NI state, which gives rise to a direct band 

we plot the calculated band structures as a representa- 

is determined by the crossing between $|E_x\rangle$ and $|E_p\rangle$, which makes the fourfold degenerate node 

increasing, which makes the fourfold degenerate node 

between antibonding and bonding states is enhanced as 

and model analysis. It demonstrates that BC8-Si is a 

topological DSM on its (001) surface of the unit cell, where black point represents location of projected Dirac point.

**Conclusion**—The electronic and topological properties of BC8-Si are explored by the first-principles calculations and model analysis. It demonstrates that BC8-Si is a topological LSM characterized by the band inversion at $H$ point and three quadratic nodes are located at $E_F$ exactly, which can hold the stabilized topological surface state on its (001) surface of the unit cell. Our calculations further suggest that LSM can be tuned to a NI or topological DSM by tiny changing of the crystal parameters, which can be achieved by the variation of the applied pressure during crystal synthesis. These results can well explain the previous contrary reports on the electronic properties of BC8-Si. More importantly, the topological surface states in BC8-Si could be a good connection between the topological quantum devices and silicon chips, which will stimulate more efforts on the promising elec- 

cia a topological DSM with $x$ exceeding 0.1008, and Fermi 

arcs formed by the topological surface states would be 

expected on its surface. By constructed the maximally 

localized Wannier functions, we carry out the Green’s 

function calculations on the semi-infinite (001) surface 

of the unit cell, and plot the corresponding LDOS in 

Fig. 4(d), which evidently shows two Fermi arcs origin- 

ated from the projected Dirac point and buried into the 

bulk states. We note that the presence of two Fermi arcs in 

Fig. 4(d) is because two bulk Dirac points are pro- 

jected to the same point on (001) surface as marked in 

Fig. 4(d).

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ence Foundation of China (11874022).
APPENDIX A: \( k \cdot p \) MODEL

The matrix form of the generators under the basis of \( |p_x^+\), \( |p_y^+\), \( |p_z^+\) and \( |s^−\) are given:

\[
C_{3}^{111} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, C_{2y} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, K, \tag{2}
\]

where \( K \) represents the complex conjugate operation. Hamiltonian at \( H \) point without spin-orbit coupling(SOC) is constructed with the generators and method of invariants as follows((up to quadratic order in \( k \)):

\[
H_{\text{non-SOC}}(k) = \begin{bmatrix} E_b + t_3k_x^2 + t_2k_y^2 + t_1k_z^2 & t_6k_zy & t_6k_zk_y & it_5k_x \\ t_6k_zy & E_b + t_1k_x^2 + t_3k_y^2 + t_2k_z^2 & t_6k_zk_y & it_5k_y \\ t_6k_zk_y & t_6k_zk_y & E_b + t_2k_x^2 + t_1k_y^2 + t_3k_x^2 & it_5k_z \\ -it_5k_x & -it_5k_y & -it_5k_z & E_{ab} + t_4(k_x^2 + k_y^2 + k_z^2) \end{bmatrix}. \tag{3}
\]

The parameters of model in Eq. (3) can be obtained by fitting band structures from first-principles calculations. First of all, we will consider the band structures along \( k_x \) direction. The non-SOC model along \( k_x \) direction, i.e. \( k_y = k_z = 0 \):

\[
H_{\text{non-SOC}}(k_x) = \begin{bmatrix} E_b + t_3k_x^2 & 0 & 0 & it_5k_x \\ 0 & E_b + t_1k_x^2 & 0 & 0 \\ 0 & 0 & E_b + t_2k_x^2 & 0 \\ -it_5k_x & 0 & 0 & E_{ab} + t_4k_x^2 \end{bmatrix}. \tag{4}
\]

with the value of \( t_1, t_2, t_3, t_4 \) and \( t_5 \) given in Table.I, the energy eigenvalues of four-band model are well fitted to the band structures from first-principles calculations as shown in Fig. 5(a).

To obtained the value of \( t_6 \), the band structures along \( k_x = k_y , k_z = 0 \) directions are considered. The corresponding model reads:

\[
H_{\text{non-SOC}}(k_xk_y) = \begin{bmatrix} E_b + t_3k_x^2 + t_2k_y^2 & t_6k_zy & t_6k_zk_y & 0 \\ t_6k_zy & E_b + t_1k_x^2 + t_3k_y^2 & 0 & 0 \\ t_6k_zk_y & 0 & E_b + t_2k_x^2 + t_1k_y^2 & 0 \\ 0 & -it_5k_x & -it_5k_y & E_{ab} + t_4(k_x^2 + k_y^2) \end{bmatrix}. \tag{5}
\]

With the values of \( t_6 \) given in Table.I, the energy eigenvalues of four-band model are well fitted to the band structures from first-principles calculations as shown in Fig. 5(b).

Finally, band structures along \( k_x = k_y = k_z \) and high symmetry lines are considered to check the model parameters that derived from \( k_x \) and \( k_y = k_z \) lines as shown in Fig. 5(c) and (d).

Considering SOC, only the atomic SOC strength parameter \( \lambda \) is counted in Eq. 5. The SOC effect under the basis of \( \phi |p_x^+, |p_y^+, |p_z^+, |s^−\) \( \otimes (|\uparrow \rangle |\downarrow \rangle) \) is written:

\[
H_{\text{soc}} = \lambda \begin{bmatrix} 0 & -i & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ i & 0 & 0 & 0 & 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{6}
\]

The eight-band Hamiltonian with SOC is obtained in Eq. 7

\[
H = \sigma_0 \otimes H_{\text{non-SOC}} + H_{\text{soc}}. \tag{7}
\]

With \( \lambda = 0.0152 \text{ eV} \), the energy eigenvalues of eight-band model are well fitted to the band structures from first-principles calculations as shown in Fig. 6 which means the low energy physics around \( H \) point can be described well by our model and parameters in Table.I.
APPENDIX B: BASIS TRANSFORMATION

Considering SOC, the eigenstates can be written as $|J, J_z\rangle$ representation, where $J$, $J_z$ indicate total angular momentum and its z-direction component. In order to transform the basis $\phi$ to $\psi \left[ |\frac{3}{2}, \frac{1}{2}\rangle^+, |\frac{3}{2}, \frac{3}{2}\rangle^+, |\frac{3}{2}, -\frac{3}{2}\rangle^+, |\frac{3}{2}, -\frac{1}{2}\rangle^+, |\frac{3}{2}, \frac{1}{2}\rangle^+, |\frac{1}{2}, -\frac{1}{2}\rangle^+, |\frac{1}{2}, -\frac{3}{2}\rangle^+, |\frac{1}{2}, \frac{3}{2}\rangle^-, |\frac{1}{2}, -\frac{1}{2}\rangle^-\right]$, the specific combination form between two bases are as follows:
The trace of Hamiltonian is same, \( uH u^{-1} = H' \), we get:

\[
H' = 
\begin{bmatrix}
M_0(k) & -\frac{t_{zk}}{\sqrt{3}} & V_1(k) & 0 & -\frac{t_{zk}}{\sqrt{3}} & V_2(k) & -\frac{\sqrt{3/5}t_{zk}}{\sqrt{3}} & 0 \\
-\frac{t_{zk}}{\sqrt{3}} & M_1(k) & 0 & V_1(k) & V_3(k) & -\frac{t_{zk}}{\sqrt{3}} & \frac{\sqrt{3/5}t_{zk}}{\sqrt{3}} & 0 \\
V_1^*(k) & 0 & M_1(k) & 0 & 0 & 0 & 0 & 0 \\
-\frac{t_{zk}}{\sqrt{3}} & -\frac{t_{zk}}{\sqrt{3}} & M_0(k) & -V_2(k) & 0 & 0 & 0 & 0 \\
-\frac{t_{zk}}{\sqrt{3}} & V_2^*(k) & \frac{t_{zk}}{\sqrt{3}} & -\frac{t_{zk}}{\sqrt{3}} & M_2(k) & 0 & 0 & 0 \\
\sqrt{\frac{2}{3}t_{5}k_{z}} & V_3(k) & \frac{t_{zk}}{\sqrt{3}} & \frac{t_{zk}}{\sqrt{3}} & -\frac{t_{zk}}{\sqrt{3}} & -\frac{\sqrt{3/5}t_{zk}}{\sqrt{3}} & 0 & 0 \\
\sqrt{\frac{2}{3}t_{5}k_{z}} & -V_3^*(k) & \frac{t_{zk}}{\sqrt{3}} & \frac{t_{zk}}{\sqrt{3}} & 0 & \frac{\sqrt{3/5}t_{zk}}{\sqrt{3}} & 0 & 0 \\
\frac{t_{zk}}{\sqrt{6}} & 0 & -\frac{t_{zk}}{\sqrt{6}} & -\frac{\sqrt{2/3}t_{5}k_{z}}{\sqrt{6}} & \frac{t_{zk}}{\sqrt{6}} & \frac{t_{zk}}{\sqrt{6}} & 0 & 0 \\
\frac{t_{zk}}{\sqrt{6}} & \frac{t_{zk}}{\sqrt{6}} & 0 & -\frac{\sqrt{2/3}t_{5}k_{z}}{\sqrt{6}} & \frac{t_{zk}}{\sqrt{6}} & \frac{t_{zk}}{\sqrt{6}} & 0 & 0 \\
\end{bmatrix}
\]
where \( k_+ = k_x + ik_y \), \( k_- = k_x - ik_y \) and

\[
M_0(k) = \frac{6E_0 + 6\lambda + (t_1 + 4t_2 + t_3)k_x^2 + (4t_1 + t_2 + t_3)k_y^2 + (t_1 + 2 + 4t_3)k_z^2}{6}
\]

\[
M_1(k) = \frac{2E_0 + 2\lambda + t_1(k_x^2 + k_y^2) + t_2(k_x^2 + k_z^2) + t_3(k_x^2 + k_y^2)}{2}
\]

\[
M_2(k) = \frac{3E_0 - 6\lambda + (t_1 + t_2 + t_3)(k_x^2 + k_y^2 + k_z^2)}{3}
\]

\[
M_3(k) = E_{ab} + t_4(k_x^2 + k_y^2 + k_z^2)
\]

\[
V_1(k) = \frac{k_x^2(-t_1 + t_2) + k_y^2(-t_2 + t_3) + k_z^2(t_1 - t_3) + 2it_6k_xk_y}{2\sqrt{3}}
\]

\[
V_2(k) = \frac{k_x^2(t_1 - t_2 + 2t_3) + k_y^2(t_1 - 2t_2 + t_3) + k_z^2(-2t_1 + t_2 + t_3)}{3\sqrt{2}}
\]

\[
V_3(k) = \frac{k_x^2(t_1 - t_2) + k_y^2(t_2 - t_3) + k_z^2(-t_1 + t_3) - 2it_6k_xk_y}{\sqrt{6}}.
\]

From Eq. 10 and 11, the onset energy difference between \( |J = \frac{3}{2}\rangle^\dagger \) and \( |J = \frac{1}{2}\rangle^\dagger \) is \( 3\lambda \). Therefore, the value of \( \lambda \) is determined by the onsite energy of the band structures from first-principles calculations, i.e. \( \lambda = 0.0152 \text{ eV} \) which is consistent with the values in Table I.

**APPENDIX C: DOWNFOLDING**

In order to explore the topological properties, the eight-band model in Eq. 10 is downfolded to four-band Hamiltonian under the basis of \( |\frac{1}{2}, \frac{1}{2}\rangle^\dagger, |\frac{1}{2}, \frac{3}{2}\rangle^\dagger, |\frac{3}{2}, -\frac{1}{2}\rangle^\dagger \) and \( |\frac{3}{2}, -\frac{1}{2}\rangle^\dagger \) up to the leading term of \( k \). The influences from \( |J = \frac{1}{2}\rangle^\dagger \) orbitals to \( |J = \frac{3}{2}\rangle^\dagger \) subspace are second-order of \( k \) terms while the influences from \( |J = \frac{1}{2}\rangle^\dagger \) orbitals are fourth-order of \( k \) terms. Therefore, the influences from \( |J = \frac{1}{2}\rangle^\dagger \) orbitals are ignored while only the influences from \( |J = \frac{3}{2}\rangle^\dagger \) orbitals are considered. By perturbation theory,

\[
H_{4 \times 4} = H_{ul}(k) + H_{\frac{3}{2} \frac{1}{2}}^{\dagger} (p) \frac{1}{H_{\frac{3}{2} \frac{3}{2}}^{\dagger} (0) - H_{\frac{1}{2} \frac{3}{2}}^{\dagger} (0) } H_{\frac{3}{2} \frac{3}{2}} (p)
\]

Among them, \( H_{ul}(k) \) comes from the upper left \( 4 \times 4 \) block of the eight-band model in Eq. 10 and \( H_{\frac{3}{2} \frac{1}{2}}^{\dagger} (p), H_{\frac{3}{2} \frac{3}{2}} (p) \) and \( H_{\frac{1}{2} \frac{3}{2}}^{\dagger} (0) - H_{\frac{1}{2} \frac{1}{2}}^{\dagger} (0) \) are written

\[
H_{\frac{3}{2} \frac{1}{2}}^{\dagger} (p) = \begin{bmatrix}
\sqrt{\frac{2}{3}}t_5k_z & t_{sk_+} & 0 & -t_{sk_-} \\
t_{sk_+} & \sqrt{\frac{2}{3}}t_6k_z & -t_{sk_-} & 0 \\
0 & -t_{sk_-} & \sqrt{\frac{2}{3}}t_6k_z & t_{sk_+} \\
-t_{sk_-} & 0 & t_{sk_+} & \sqrt{\frac{2}{3}}t_5k_z
\end{bmatrix}
\]

\[
H_{\frac{3}{2} \frac{3}{2}}^{\dagger} (p) = \begin{bmatrix}
\sqrt{\frac{2}{3}}t_5k_z & -t_{sk_-} & 0 & t_{sk_+} \\
t_{sk_-} & \sqrt{\frac{2}{3}}t_6k_z & 0 & -t_{sk_+} \\
0 & t_{sk_+} & \sqrt{\frac{2}{3}}t_6k_z & -t_{sk_-} \\
-t_{sk_+} & 0 & t_{sk_-} & \sqrt{\frac{2}{3}}t_5k_z
\end{bmatrix}
\]

\[
H_{\frac{1}{2} \frac{3}{2}}^{\dagger} (0) - H_{\frac{1}{2} \frac{1}{2}}^{\dagger} (0) = \begin{bmatrix}
\frac{-\Delta}{2} & 0 & 0 \\
0 & 0 & \frac{-\Delta}{2}
\end{bmatrix}
\]

where \( \Delta = E_{ab} - E_b - \lambda \) is the energy difference between \( |J = \frac{1}{2}\rangle^\dagger \) and \( |J = \frac{3}{2}\rangle^\dagger \) states.

The second term in Eq. 12, i.e. the perturbation term from \( |J = \frac{1}{2}\rangle^\dagger \) orbitals is

\[
H_c(p) = \frac{t_6^2}{-\Delta} \begin{bmatrix}
\frac{1}{6}k_+k_- + \frac{2k^2}{3} & -\frac{k_xk_y}{6} & \frac{k^2}{2\sqrt{3}} & 0 \\
-\frac{k_xk_y}{6} & \frac{k_xk_y}{6} & 0 & \frac{k^2}{2\sqrt{3}} \\
-\frac{k_xk_y}{6} & \frac{k_xk_y}{6} & 0 & \frac{k^2}{2\sqrt{3}} \\
0 & \frac{k_xk_y}{6} & \frac{k_xk_y}{6} & \frac{1}{6}(k_-k_+) + \frac{2k^2}{3}
\end{bmatrix}
\]
Finally, the four-band Hamiltonian of BC8-Si under the basis of \(|\frac{3}{2}, \frac{1}{2}\rangle^+, |\frac{3}{2}, \frac{3}{2}\rangle^+, |\frac{3}{2}, -\frac{3}{2}\rangle^+\) and \(|\frac{3}{2}, -\frac{3}{2}\rangle^+\) is written as

\[
H_{4\times4} = \begin{bmatrix}
M_0(k) - \frac{t_0 k_z k_x}{\sqrt{3}} & V_1(k) & 0 & 0 \\
-\frac{t_0 k_z k_y}{\sqrt{3}} & M_1(k) & 0 & V_1(k) \\
0 & \frac{t_0 k_z k_y}{\sqrt{3}} & M_2(k) & 0 \\
0 & \frac{t_0 k_z k_x}{\sqrt{3}} & 0 & M_0(k)
\end{bmatrix} + \frac{t_2}{\Delta} \begin{bmatrix}
\frac{k_+ k_- + 2k^2}{3} & -\frac{k_+ k_y}{\sqrt{3}} & -\frac{k_+ k_z}{\sqrt{3}} & -\frac{k_+ k_y}{\sqrt{3}} \\
-\frac{k_+ k_y}{\sqrt{3}} & \frac{k_- k_y}{\sqrt{3}} & \frac{k_- k_z}{\sqrt{3}} & 0 \\
-\frac{k_+ k_z}{\sqrt{3}} & \frac{k_- k_z}{\sqrt{3}} & \frac{k_- k_y}{\sqrt{3}} & \frac{k_- k_y}{\sqrt{3}} \\
0 & \frac{k_- k_y}{\sqrt{3}} & \frac{k_- k_z}{\sqrt{3}} & 0
\end{bmatrix}
\]  \hspace{1cm} (17)

The downfolding model in Eq. [17] can be written as \(\Gamma\) matrix.

\[
H_{4\times4} = H_{4l}(k) + \frac{t_2}{\Delta} \begin{bmatrix}
-\frac{k_- k_+}{3} & G_0 + (-\frac{k_- k_+}{6})G_1 & -\frac{k_- k_+}{3} & G_2 + \frac{k_- k_+}{6}G_3 - \frac{k_- k_+}{2\sqrt{3}}G_4 - \frac{2k_- k_+}{2\sqrt{3}}G_5
\end{bmatrix}
\]  \hspace{1cm} (18)

The \(\Gamma\) matrices are defined as \(\Gamma_0 = \tau_0 \otimes \sigma_0, \Gamma_1 = \tau_2 \otimes \sigma_z, \Gamma_2 = \tau_2 \otimes \sigma_x, \Gamma_3 = \tau_2 \otimes \sigma_y, \Gamma_4 = \tau_x \otimes \sigma_0, \Gamma_5 = \tau_0 \otimes \sigma_0\). \(\tau_0\) and \(\sigma_0\) are the 2 \(\times\) 2 identity matrices, \(\tau_x,\tau_y,\tau_z\) and \(\sigma_x,\sigma_y,\sigma_z\) represent the orbital and spin space, respectively.

**APPENDIX D: TOPOLOGICAL CHARACTERS**

Maxim Kharitonov et al. have confirmed that the four-band 3D LSM are topological, if its 2D reductions to some planes in momentum space passing the quadratic node are topologically nontrivial [52]. The topological property of the reduced 2D nodal semimetal is determined by the phase diagram in the \((|\beta_0|/\beta_1, |\beta_1|/\beta_1)) parameter plane, the 2D model in ref [52] is

\[
H^0_{2d}(p_x, p_y) = \begin{bmatrix}
\beta_0 + \beta_1 & p_x + p_y & \beta_1 p_x^2 & (\beta_0 - \beta_1) p_x + p_y
\end{bmatrix}
\]  \hspace{1cm} (19)

Next, we show the estimation of \(\beta_0, \beta_1\) and \(\beta_\perp\) in BC8-Si. In \(k_x, k_y\) plane, the 4 \(\times\) 4 Hamiltonian is decoupled into two pairs due to the \(T\) symmetry. The parameters \(\beta_0, \beta_1\) and \(\beta_\perp\) calculated from any one of the two \(2 \times 2\) Hamiltonians are same as the parameters calculated from the other one. For example, \(2 \times 2\) Hamiltonian under the basis of \(|\frac{3}{2}, \frac{3}{2}\rangle^+, |\frac{3}{2}, -\frac{1}{2}\rangle^+\) is considered

\[
H_{2\times2} = \begin{bmatrix}
\frac{t_0}{2}\left(\frac{k_-^2}{2}+k_x^2\right) & \frac{t_0}{2}\left(2t_0k_yk_z\right) & \frac{t_0}{2}\left(2t_0k_yk_z\right) & \frac{t_0}{2}\left(2t_0k_yk_z\right)
\end{bmatrix}
\]  \hspace{1cm} (20)

Here, the first term describes the electronic anisotropy of the crystal. However, the second term takes the leading role because of the small \(\Delta\). Moreover, one can further rewrite Eq. [20] as the following form

\[
H_{2\times2} = \begin{bmatrix}
\frac{1}{2}\left(\frac{t_0(t_0+2t_3)}{4t_0^2}\right) & \frac{t_0}{2}\left(2t_0k_yk_z\right) & \frac{t_0}{2}\left(2t_0k_yk_z\right) & \frac{t_0}{2}\left(2t_0k_yk_z\right)
\end{bmatrix} + \frac{t_2}{\Delta} \begin{bmatrix}
\frac{k_-k_+}{2} & -\frac{k_-k_+}{2\sqrt{3}} & -\frac{k_-k_+}{2\sqrt{3}} & \frac{k_-k_+}{6}
\end{bmatrix} + H_{anis}
\]  \hspace{1cm} (21)

where the first two terms are both isotropic as Eq. [19] and the anisotropic effect is attributed to \(H_{anis}\). Using the isotropic coefficients in Eq. [21] and the parameters in Table 1 of the main text, one can estimate \(\beta_0 = 13.7854, \beta_\perp = 10.1978, \beta_1 = -17.6633\), and \(\beta_0/\beta_1 = 0.7804, \beta_\perp/\beta_1 = 0.5733\), which strongly imply that BC8-Si is a topological LSM, similar to HgTe and \(\alpha\)-Sn.

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