

Type-I and type-II saddle points and a quasiflat band in a Bi-pyrochlore superconductor CsBi₂

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The divergence of the electron density of states (DOS) plays an important role in enhancing many-body interactions and inducing various quantum phases in low-dimensional systems. However, such unique electronic structures remain experimentally elusive in three-dimensional (3D) systems, particularly those with strong spin-orbit coupling (SOC). Using angle-resolved photoemission spectroscopy and first-principles calculations for a Laves-phase superconductor CsBi₂, which features a Bi-pyrochlore 3D network with strong SOC, we identify two characteristic electronic structures with a large DOS. One is a quasiflat band within a topologically nontrivial band sector with *p*-orbital character, locally formed around the U-K line, which enhances DOS near the Fermi level. The other involves type-I and type-II saddle points connected by a quasiflat band, which cooperatively produce an enhancement in the DOS. Our findings lay a foundation for exploring exotic phenomena driven by the interplay of multiple singularities with a large DOS, nontrivial topology, and strong SOC in 3D pyrochlores.

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I. INTRODUCTION

Exploring materials and mechanisms that produce a divergent density of states (DOS) is a frontier in condensed-matter physics research. Achieving a divergent DOS becomes increasingly challenging as the dimensionality increases. For

instance, in one-dimensional (1D) systems like nanotubes, the energy extremum of a simple parabolic band can cause a divergent DOS [1,2], but this no longer occurs in two-dimensional (2D) systems. A promising source of a large DOS in 2D and quasi-2D materials is a saddle point (SP), characterized by concave and convex energy dispersions along different directions in momentum space. The SP generates a van Hove singularity (VHS) with a logarithmic divergence in the DOS [3], as in cuprates, pnictides, ruthenates, and kagome metals [4–9], potentially promoting various instabilities such as high-temperature superconductivity and unconventional density waves [10–19]. Another key source of high DOS is a flat band [20–24], which originates from interference of extended wave functions within special crystalline lattices, such as the kagome lattice and magic-angle twisted bilayer graphene [25–31]. Flat bands in these systems have been a focus of intensive research because of their presumed links to

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exotic correlated insulating, superconducting, magnetic, and strange-metal states [32–38].

In contrast to 1D and 2D cases, three-dimensional (3D) platforms with a divergent DOS are quite scarce. A possible material class is the pyrochlore lattice, a 3D extension of the kagome lattice. Similar to the kagome lattice, the pyrochlore lattice is predicted to host SPs and flat bands, but with 3D characteristics [39,40]. While 3D SPs typically do not cause a DOS divergence [3], 3D flat bands can, as recently reported in pyrochlores [41–43]. However, the ideal flat-band character is present only in systems with relatively weak spin-orbit coupling (SOC), as strong SOC is predicted to increase the flat-band width. Therefore, realizing a divergent DOS in pyrochlores with strong SOC, which could lead to intriguing correlated topological and fractionalized properties [44–47], remains an important challenge.

In this Article, we report a DOS enhancement in a 3D pyrochlore with strong SOC, CsBi₂, by conducting density functional theory (DFT) calculations and angle-resolved photoemission spectroscopy (ARPES) measurements. This enhancement originates from the coexistence of type-I and type-II SPs, defined as SPs at time-reversal-invariant momentum (TRIM) point and non-TRIM point, respectively [48,49], and a quasiflat band connecting these SPs. We also demonstrate an enhancement of the DOS near the Fermi energy (E_F) due to a quasiflat band formed in specific momentum space. Our findings pave the way for exploring a large DOS and associated unconventional properties in 3D pyrochlore systems with strong SOC.

II. METHODS

Density functional theory calculations were carried out by using the Vienna *ab initio* Simulation Package [50,51], within the projector augmented wave method [52]. The generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof functional was adopted as the exchange-correlation functional [53–55]. The plane wave truncation energy was selected as 500 eV and the Brillouin zone (BZ) was sampled with a $12 \times 12 \times 12$ and a $18 \times 18 \times 18$ k -mesh for structural relaxation and the density of states, respectively. The force convergence criterion was -0.01 eV/Å, and the convergence accuracy of the self-consistent iteration was set to be 1×10^{-6} eV/atom. The optimized lattice constants are $a = b = c = 6.9587$ Å, which agree well with the experimental data ($a = b = c = 6.901$ Å). The Green's function iterative method implemented in the wanniertools software package [56] was adopted to demonstrate the surface electronic properties.

High-quality single crystals of CsBi₂ were synthesized with high-purity Bi (Alfa Aesar, 99.9999%) and Cs (Alfa Aesar, 99.9%) as starting materials by a Bi self-flux technique. The starting materials were weighed and loaded into an Al₂O₃ crucible carefully, and then transferred into a fused silica tube. The tube was evacuated and sealed to prevent any exposure of the alkaline metals to air. After that, this assembly was subjected to a meticulous heating protocol, initially reaching 650 °C, where it was maintained for a period of 8 h to ensure thorough homogenization. Followed by cooling down to 300 °C at a rate of 5 °C/h, at which the excess Bi flux was removed through centrifugation. Finally, tetrahedrally shaped CsBi₂

crystals with a typical size approximately $2 \times 2 \times 2$ mm³ were obtained. To avoid chemical reactions of CsBi₂ in air, all sample preparations prior to ARPES measurements were carried out in an Ar-filled glove box. Photon-energy ($h\nu$) tunable vacuum ultraviolet ARPES measurements were performed with MBS-A1 spectrometers at BL5U and BL7U in UVSOR. Additional measurements were conducted at micro-ARPES beamline at BL-28A in Photon Factory, KEK [57]. The energy and angular resolutions were set to be 10–30 meV and 0.3°, respectively. Samples were cleaved *in situ* along the (111) plane in an ultrahigh vacuum better than 5×10^{-11} Torr, and all data were recorded within 6 h after the cleavage. During this period, no discernible surface degradation was observed. The samples were kept at $T = 30$ K during measurements.

III. RESULTS AND DISCUSSION

ABi₂ ($A = \text{K, Rb, and Cs}$) [58,59] is a C15-type Laves-phase material that crystallizes in a cubic structure ($Fd\bar{3}m$ space group; No. 227), with A and Bi atoms arranged in diamond and pyrochlore sublattices, respectively [Fig. 1(a); see Fig. 1(b) for the corresponding Brillouin zone]. ABi₂ exhibits intriguing properties, including strong SOC of the Bi-pyrochlore sublattice, superconductivity ($T_c \sim 4$ K), and nonsaturating large magnetoresistance [58–62]. We first built the electronic tight-binding (TB) Hamiltonian for the 16c Wyckoff positions of space group $Fd\bar{3}m$ (No. 227) of CsBi₂ by the MagneticTB package [63]. For the case of s orbitals without SOC, the TB band dispersion presented in Fig. 1(c) shows an ideal twofold degenerate flat band (labeled as bands 3 and 4) crossing the entire BZ, along with two dispersive bands (bands 1 and 2) that are symmetric around -2 eV. In addition to the SPs (black circles) located at the L point for the bands 1 and 2 (hereafter, each SP is labeled by the location of the high-symmetry point with band numbers, e.g., L1 and L2 for these SPs), further SPs are identified at K1, U1, K2, and U2 (see Appendix A for the 3D band structures of these SPs). When SOC is included for s orbitals, the corresponding TB band structure in Fig. 1(d) reveals that the originally flat band becomes dispersive; however, quasiflat segments locally emerge along the U-K high-symmetry line. Moreover, the SPs identified in the SOC-free case are preserved, and additional SPs appear, as marked by black dots. Importantly, although the flat-band width is globally broadened by SOC, DOS remains nearly divergent at energies near the locally formed flat bands and newly emerged SPs around 2 and 4 eV.

To verify such large DOS in a real material, we performed our band-structure calculations with SOC for CsBi₂ [Fig. 1(e)]. As confirmed by previous band-structure calculations for ABi₂ and ARPES results for RbBi₂, there are multiple symmetry-enforced Dirac points (DPs) at the X point (indicated by red points) [58,59,64] and two quadratic contact DPs at the Γ point (orange points; see Appendix B for details of the band topology). In addition, as expected from the presence of strong SOC, ideal flat bands are absent. However, calculated DOS in Fig. 1(f) shows notable enhancements characterized by a hump near E_F and multiple spikes at higher binding energies (E_B 's), similar to the high-DOS peaks in the TB model.

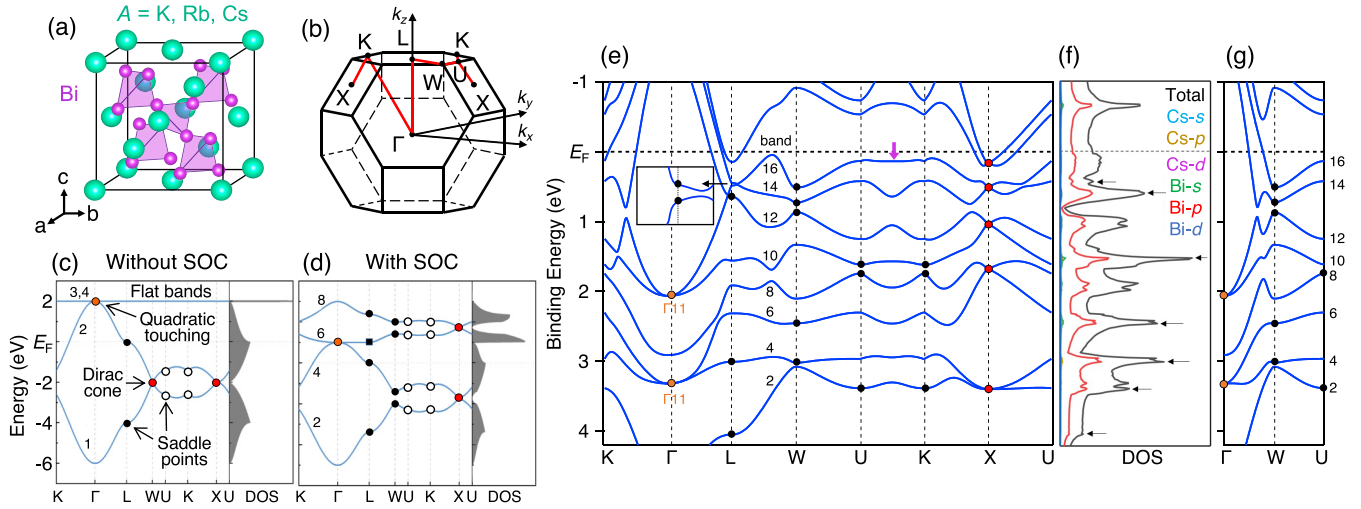


FIG. 1. (a) Crystal structure of cubic CsBi₂. Bi-pyrochlore network is highlighted by purple tetrahedrons. The graphic was drawn by vesta [71]. (b) BZ of CsBi₂. (c), (d) Band structures of pyrochlore lattice (left) obtained by the TB model without and with SOC, respectively, together with the corresponding DOS (right) [69]. The momentum paths are indicated by red lines in panel (b). (e) Calculated band structure with SOC for CsBi₂. Occupied bands are sequentially numbered. Red, orange, and black dots indicate the positions of DP, quadratic touching, and SP, respectively. Inset shows an enlarged view for the two SPs at L near E_F . (f) Calculated orbital-resolved DOS. Black arrows highlight spikes due to SPs. (g) Same as panel (e), but along different momentum paths for visualizing type-II SPs (black dots) at W.

The origins of the DOS enhancements are twofold. First, examining the band dispersions reveals that nearly flat bands can exist in specific momentum cuts (e.g., along U-K) like the TB model with SOC, and one of such local flat bands (purple arrow) produces the hump near E_F . Second, analysis of the 3D band structures around high-symmetry points clarifies multiple SPs [black points in Fig. 1(e)], whose energies match some spikes in Fig. 1(f) (black arrows). These SPs are present not only at the TRIM point L (0.5, 0.5, 0.5), but also at non-TRIM points, such as W (0.5, 0.25, 0.75), U (0.625, 0.25, 0.625), and K (0.375, 0.375, 0.75). For instance, SPs at the L point characterized by opposite band velocities along two orthogonal momentum cuts, i.e., Γ -L and L-W, are identified for bands numbered as 2, 4, 12, 14, and 16 in Fig. 1(e). Similar SP characteristics are found at the W point for bands 4 and 6 [Fig. 1(g); see Appendix C for more details]. This unveils the coexistence of type-I SPs at TRIM points and type-II SPs at non-TRIM points [48,49]. An important consequence of the multiple SP formation is that the SPs at the same energy (U2 and K2, L4 and W4) generate one single logarithmic spike in the DOS [Fig. 1(f)], which echoes the prediction that two SPs corresponding to the same value of $E(k)$ might produce one single VHS in the DOS [3]. It is also noteworthy that the energetically degenerate SPs at the same branch are connected by a nearly dispersionless local flat band (U2-K2 and L4-W4), which would further contribute to the DOS enhancement.

To characterize the global topology of the occupied bands, we computed the parity products at TRIM points for the globally gapped occupied manifolds 1- n with $n = 8, 12$, and 16 (Table I) [65–67]. The corresponding $\mathbb{Z}_2$ invariants are (0, 000), (1, 000), and (1, 000), respectively, indicating that the fully occupied bands 1–12 and 1–16 form topologically nontrivial sectors (see Appendix D). The quasiflat segment observed experimentally along the U-K path (band 16) and the saddle-point connectivity along the L-W path (band 4)

reside within these nontrivial sectors (bands 1–16 and bands 1–12, respectively). This distinguishes them from trivial flat atomic bands derived from localized orbitals. However, we emphasize that the $\mathbb{Z}_2$ invariants characterize the global topology of the occupied manifolds and do not establish that the local flatness of the quasiflat segments is topologically protected. The enhanced DOS arises from the coexistence of SPs and quasiflat dispersions within these nontrivial band sectors,

TABLE I. Parity eigenvalues at TRIM points and parity products for the occupied bands 1- n ($n = 2, 4, 6, 8, 10, 12, 14, 16$) of CsBi₂. The coordinates of eight TRIM points are Γ (0, 0, 0), X_1 (0.5, 0.5, 0), X_2 (0.5, 0, 0.5), X_3 (0, 0.5, 0.5), L (0.5, 0.5, 0.5), F_1 (0.5, 0, 0), F_2 (0, 0.5, 0), and F_3 (0, 0, 0.5). The + (−) denotes the positive (negative) parity eigenvalue. Rigorous $\mathbb{Z}_2$ topological invariants are defined only for $n = 8, 12$, and 16, where the occupied manifolds are separated from higher bands by global gaps. For $n = 2, 4, 6, 10$, and 14, the occupied manifolds are gapless due to Dirac crossings at X or Γ ; the listed values are algebraic parity products and are not rigorous $\mathbb{Z}_2$ invariants. The quasiflat segments observed experimentally along the U-K path (band 16) and the L-W path (band 4) reside within the topologically nontrivial sectors (bands 1–16 and bands 1–12, respectively).

Band index	Parity				Product of parity				$\mathbb{Z}_2(v_0, v_1 v_2 v_3)$
	Γ	3X	L	3F	Γ	3X	L	3F	
2	−	+	+	−	−	+	+	−	(0, 111)
4	−	−	+	−	+	−	+	+	(1, 000)
6	−	+	+	−	−	−	+	−	(1, 111)
8	−	−	−	+	+	+	−	−	(0, 000)
10	−	+	+	−	−	+	−	+	(0, 111)
12	−	−	+	−	+	−	−	−	(1, 000)
14	−	+	−	+	−	−	+	−	(1, 111)
16	+	−	+	−	−	+	+	+	(1, 000)

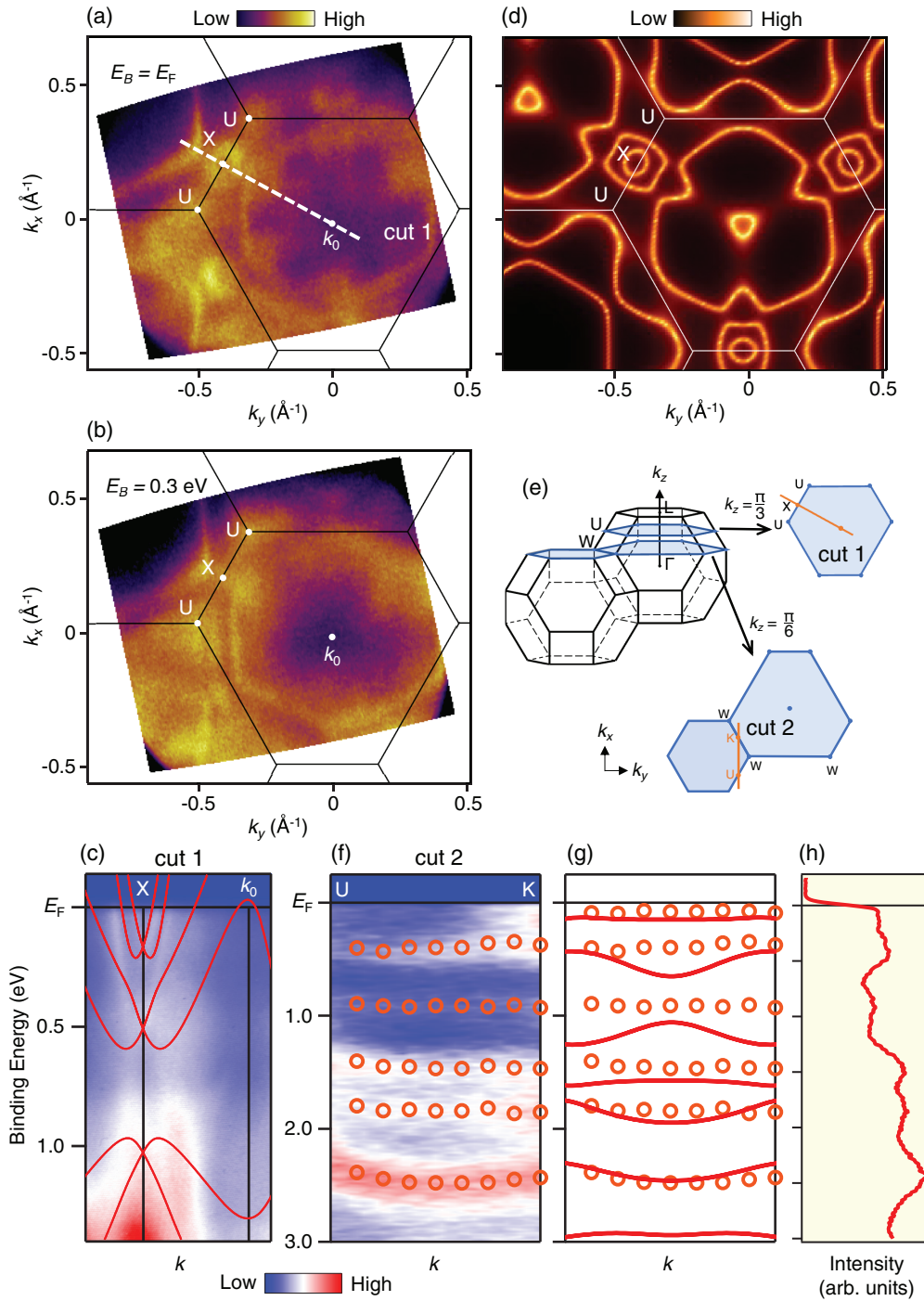


FIG. 2. (a) ARPES-intensity map at E_F as a function of k_x and k_y at $k_z \sim \pi/3$, measured with 21-eV photons. (b) Same as panel (a), but at $E_B = 0.3$ eV. (c) ARPES intensity and calculated band structure along cut 1 [white dashed line in panel (a)]. (d) Calculated Fermi surface at $k_z = \pi/3$. (e) Schematic of $k_z = \pi/3$ and $\pi/6$ planes in the bulk BZ, displayed with (left) 3D and (right) top views. (f) ARPES intensity along U-K [cut 2 in panel (e)], measured with 120-eV photons. (g) Calculated band structures along U-K. Orange circles in panels (f) and (g) show peak positions of energy distribution curves (EDCs). (h) Integrated EDC obtained with data in panel (f).

rather than from a topological protection mechanism of the flatness itself. Furthermore, while strong SOC is typically expected to broaden flat bands, our realistic band calculations with multiorbitals clarify its constructive role. Notably, SOC induces orbital hybridizations that effectively produce sharper DOS peaks compared to the SOC-free case (see Appendix E for a comparison of band dispersions).

To compare the calculated and experimental band structures in CsBi₂, we mapped out a 2D ARPES intensity. The map at E_F [Fig. 2(a)] reveals a large Fermi surface at the BZ center and a small circular pocket at the BZ boundary. When increasing E_B to 0.3 eV [Fig. 2(b)], the former expands into a large hexagonal shape, while the latter disappears. These features originate from a highly dispersive band and

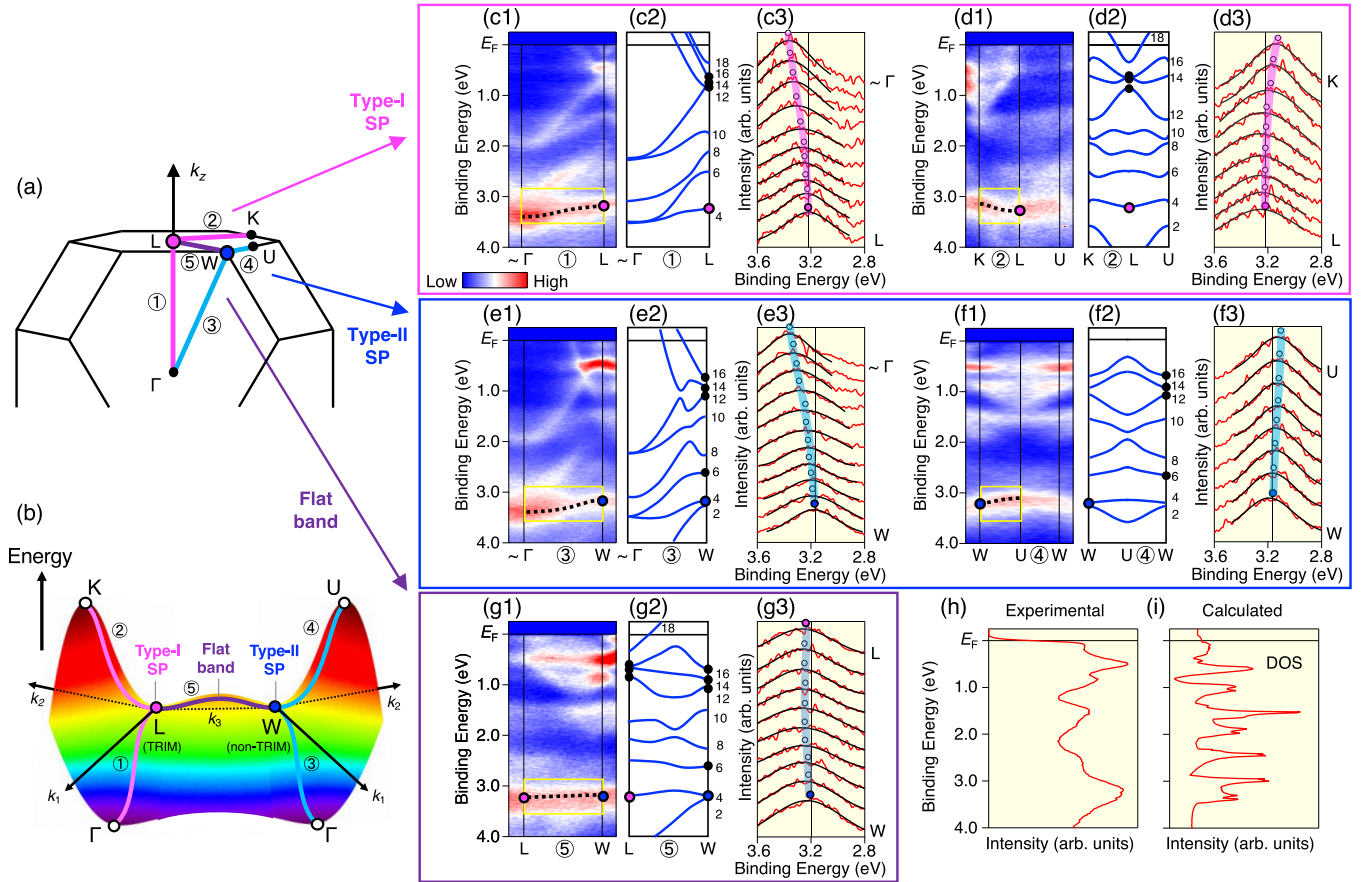


FIG. 3. (a) BZ of CsBi₂. (b) Schematic of type-I and type-II SPs at the L and W points, respectively, connected by a flat dispersion for band 4. (c) Plots of (c1) ARPES intensity along $\sim\Gamma$ -L, (c2) corresponding calculated band structure, and (c3) EDCs in the yellow rectangle region in panel (c1). Black dashed line in panel (c1) is a guide for the eyes to trace band 4. Circles in panel (c3) represent peak positions of EDCs. (d)–(g) Same as panel (c), but along L-K/U, $\sim\Gamma$ -W, W-U, and L-W, respectively. (h) Integrated EDC of panel (g1). (i) Calculated total DOS of CsBi₂ [same as the black curve in Fig. 1(f)].

a shallow electron band, both of which cross E_F , as seen in Fig. 2(c) [cut along white dashed line in Fig. 2(a)]. We also conducted normal-emission measurements to clarify the three dimensionality of the band structure (see Appendix F), and found that the data in Figs. 2(a)–2(c) reflect the electronic states near the $k_z = \pi/3$ plane. As shown by the red curves in Fig. 2(c) and the calculated Fermi surface in Fig. 2(d), the highly dispersive band and the shallow pocket are qualitatively reproduced by the DFT calculations for $k_z = \pi/3$ (see also Appendix G for additional data suggesting the DP formation at the X point).

Next, to experimentally identify the near- E_F quasiflat band, one of the key predictions from the DFT calculations, we measured the band dispersion along the U-K cut at $k_z = \pi/6$ [cut 2 in Fig. 2(e)]. Figure 2(f) shows several less-dispersive bands in this momentum region, which reasonably agree with the DFT calculations [compare orange circles and red curves in Fig. 2(g); see Appendix H for the numerical fitting to extract the peak position]. We note some quantitative differences such as a flattening of the band at $E_B \sim 1.0$ eV, which is an extrinsic effect arising from angle-integrated signals generated by high DOS (see Appendix I). Importantly, the band near E_F corresponds to the predicted quasiflat band along

U16-K16 and produces a near- E_F peak in the local DOS obtained by integrating energy distribution curves (EDCs) between U and K [Fig. 2(h)], consistent with the predicted DOS enhancement. A recent STM/STS study discussed a possible relationship between this DOS enhancement and the strong-coupling superconductivity [68] (see also Appendix J), although its microscopic role remains to be clarified.

We next focus on another key prediction, the presence of type-I and type-II SPs at nearly the same E_B and their connection by a flat band, whose characteristics would be most clearly seen along L4-W4 [see schematics in Figs. 3(a) and 3(b)]. Figures 3(c1)–3(c3) and 3(d1)–3(d3) show a comparison of experimental and calculated band dispersions along $\sim\Gamma$ -L and L-K/U (Appendix K). Along $\sim\Gamma$ -L, the experiment reveals relatively shallow electron pockets within 0.5 eV of E_F and deeper holelike dispersions centered at the L point [Fig. 3(c1)], which overall agree with the calculations [Fig. 3(c2)]. Notably, band 4, located at $E_B = 3.2$ – 3.4 eV, exhibits a holelike dispersion topped at the L point [black dashed line in Fig. 3(c1)], as confirmed by tracing the peak position in the magnified view of EDCs at $E_B = 3.0$ – 3.5 eV [Fig. 3(c3); see also Appendix L]. In contrast, along the L-K/U cut, this band has the bottom of an electronlike dispersion

at the L point [Figs. 3(d1) and 3(d3); see Appendix M for a magnified view near E_F]. The observed opposite band curvature with respect to the L point confirms the formation of a type-I SP at the TRIM point, in agreement with the calculations [Figs. 3(c2) and 3(d2)]. Furthermore, the existence of a type-II SP at the W point (non-TRIM) is supported by a comparison of Figs. 3(e1)–3(e3) and 3(f1)–3(f3), where band 4 shows the holelike and electronlike dispersions centered at W along $\sim\Gamma$ -W and W-U, respectively. Remarkably, these two SPs are located at approximately the same E_B of ~ 3.25 eV [see black circles in Figs. 3(c3)–3(e3)] and connected by a quasiflat band along the L-W path [Figs. 3(g1)–3(g3)], resulting in a clear peak in the momentum-integrated EDC in Fig. 3(h), consistent with the enhancement in the calculated DOS [Fig. 3(i)]. Intriguingly, our analysis also identifies another SP at the U point (Appendix N). According to the recent theoretical classification of singularities in 3D materials [69], the SP at the U point in pyrochlores is a noncritical SP, which represents a distinct class of electronic singularities.

We now discuss the implications of the present results. First, our observation expands the scope of flat-band materials. Unlike the d -orbital flat bands reported in 3D systems such as CaNi_2 and CeRu_2 [41,43], the flat bands in CsBi_2 exhibit dominant p -orbital character [Fig. 1(f)]. This finding is particularly timely, as p -orbital flat bands have been recently predicted theoretically to host unique correlated phases [70] but have remained experimentally elusive in 3D kagome/pyrochlore networks until now. Second, the identification of type-II SP is noteworthy because it has been theoretically linked to unconventional superconductivity, especially topological odd-parity superconductivity [48,49]. Therefore, it is an intriguing future work to explore pyrochlores hosting type-II SPs near E_F . Finally, the coexistence of type-I and type-II SPs connected by a quasiflat band provides a pathway to DOS enhancement in 3D pyrochlores with strong SOC. These bands are at nearly the same energy and collectively lead to an enhanced DOS. This finding is unexpected from general hypotheses that (1) 3D SP-band systems do not exhibit such an enhanced DOS and (2) strong SOC diminishes the ideal flat-band character to broaden the singularity of the DOS in pyrochlores. Since the essential features are well reproduced in the TB model [Fig. 1(d)], multiple singularities and resonant DOS enhancement can be found in other pyrochlores.

IV. CONCLUSION

In conclusion, we presented DFT and ARPES investigations of a Laves-phase superconductor CsBi_2 . The results demonstrated several unique band structures: (1) an incipient quasiflat band close to E_F , (2) multiple SPs with both type-I and type-II characteristics, and (3) a quasiflat dispersion bridging two SPs in the same branch within a topologically nontrivial band sector. Multiple SPs connected by a flat band lead to a DOS enhancement. These findings contribute to our deeper understanding of unique physical properties of CsBi_2 and suggest a pathway to realize a DOS enhancement and associated instabilities in 3D pyrochlores with strong SOC.

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DATA AVAILABILITY

The data that support the findings of this study are available within the main text and Appendixes. Any other relevant data are available from the corresponding authors upon reasonable request.

APPENDIX A: SADDLE-POINT BAND DISPERSIONS IN TIGHT-BINDING CALCULATIONS

Figure 4(a) shows the tight-binding band dispersion for the case of s orbitals without spin-orbit coupling. The 3D band dispersions of saddle points (SPs) located at L2, K2, U2, L4, K4, and U4 (filled and hollow circles) are displayed in Fig. 4(c). The TB band structure with SOC for s orbitals is shown in Fig. 4(b). In addition to the SPs identified in the SOC-free case, additional SPs appear, as illustrated in Fig. 4(d).

APPENDIX B: THEORETICAL ANALYSIS OF BAND TOPOLOGY

To illustrate the band topology, the irreducible representations (irreps) of the little group at distinct $\mathbf{k}$ points in BZ are obtained [72]. Regarding the high-symmetry Γ point (0,0,0), the little group has five generating elements, i.e., C_{4x}^+ , $\bar{C}_{31}^-$, C_{2b} , I , and T . Here, C_{4x}^+ denotes $\{C_{4x}^+ | \frac{1}{4} \frac{1}{4} \frac{1}{4}\}$, $\bar{C}_{31}^-$ indicates $\{\bar{C}_{31}^- | 000\}$, C_{2b} stands for $\{C_{2b} | \frac{1}{4} \frac{1}{4} \frac{1}{4}\}$, I represents $\{I | \frac{1}{4} \frac{1}{4} \frac{1}{4}\}$, and T is the time-reversal symmetry. Then, the obtained irreps, written in the Bilbao Crystallographic Server convention [73,75], of Γ would be Γ_{11} , and the effective Hamiltonian model $\mathcal{H}(\mathbf{k})$ for the emergent particle at the Γ

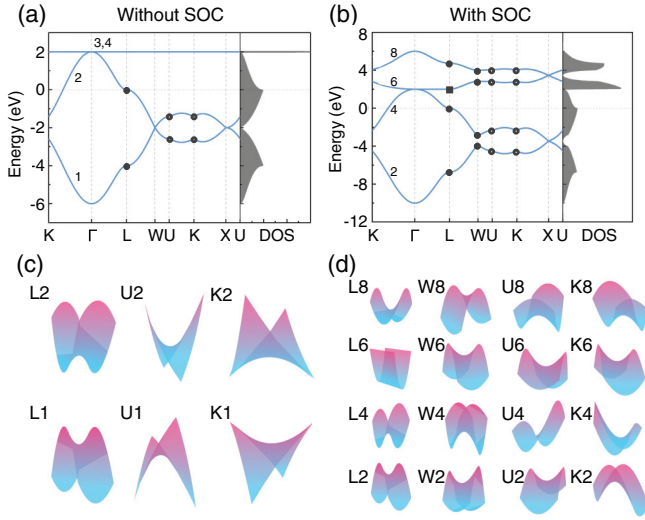


FIG. 4. (a) Electronic structures of the pyrochlore lattice without SOC based on the TB Hamiltonian [69]. (b) Same as panel (a), but calculated with SOC [69]. The TB models were built on s orbitals with nearest-neighbor hopping. For panel (a), the hopping parameter is $t_1 = -1$, and for panel (b), the hopping parameters are $t_1 = -1$ and $t_2 = 1$. In the band dispersions, the ordinary van Hove singularities are highlighted by black solid circles, while the noncritical VHSs are marked by black hollow circles. The black solid square in panel (b) denotes a higher-order VHS. Panels (c) and (d) display the corresponding 3D band structures for the singularities plotted in panels (a) and (b), respectively.

point is constrained by $\Delta(\mathcal{O})\mathcal{H}(\mathbf{k})\Delta^{-1}(\mathcal{O}) = \mathcal{H}(\hat{\mathcal{O}}\mathbf{k})$ [74]. Here, $\mathcal{O} \in \{C_{4x}^+, \bar{C}_{31}^-, C_{2b}, I, T\}$ is one of the five operators and $\Delta(\mathcal{O})$ denotes the corresponding matrix representation at the Γ point [74]. The obtained model given in Ref. [74] reveals that the set of bands whose irreps is $\Gamma 11$ forms a quadratic nodal point, namely, a quadratic contact Dirac point.

APPENDIX C: SADDLE-POINT BAND DISPERSIONS IN DENSITY FUNCTIONAL THEORY CALCULATIONS

To see SPs at the time-reversal invariant momentum point L, calculated band dispersions between the L and various high-symmetry points are plotted in Fig. 5. As marked by black circles in Fig. 5, there are SPs (type-I SPs) at L2, L4, L12, L14, and L16. Three-dimensional $E(\mathbf{k})$ relationships of these SPs are shown in Fig. 6. Type-II SPs at non-TRIM points K, U, and W are found in Figs. 7, 8, 9, 10, 11, and 12.

APPENDIX D: TOPOLOGICAL CLASSIFICATION

Flat bands can be briefly divided into three categories [23], i.e., the flat atomic bands (FABs), the flat topological bands (FTBs), and the flat obstructed atomic band (FOAB). Specifically, a set of bands that are flat in all/some particular directions should be FABs and they form a band representation (BR) that can be derived from local orbitals. However, when a set of flat bands do not form any BR, i.e., cannot be induced from local orbitals, the set of bands forms a set of FTBs. The FOAB would lie at the interface between the polar opposites FAB and FTB. In addition, according to the theory of topological quantum chemistry [75–79], the band topology of a nonmagnetic system can be described by three effective schemes: $\mathbb{Z}_2$ index, the Wilson loop, and the symmetry-data vector [80]. In this work, the $\mathbb{Z}_2$ index was calculated. According to the definition of $\mathbb{Z}_2$, for a 2D system, a single $\mathbb{Z}_2$ invariant is expressed as

$$(-1)^v = \prod_{i=1}^4 \delta_i,$$

where δ denotes the parity eigenvalue at the i th TRIM point. In 3D, there exist eight TRIM points, leading to four independent $\mathbb{Z}_2$ invariants. The first invariant ν_0 is defined as the product

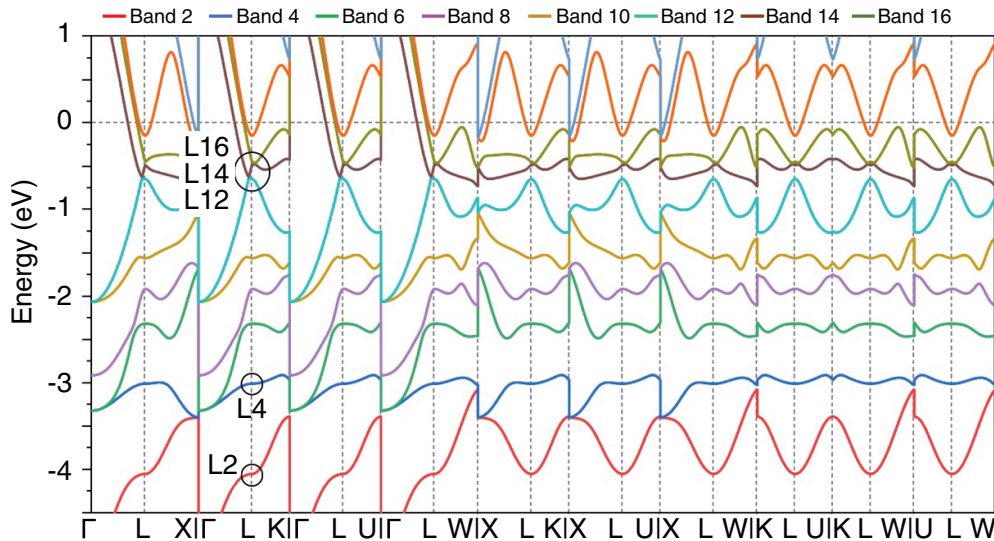


FIG. 5. Calculated band structures of the Γ -L-X| Γ -L-K| Γ -L-U| Γ -L-W|X-L-K|X-L-U|X-L-W|K-L-U|K-L-W|U-L-W paths. Circles represent the SPs L2, L4, L12, L14, and L16.

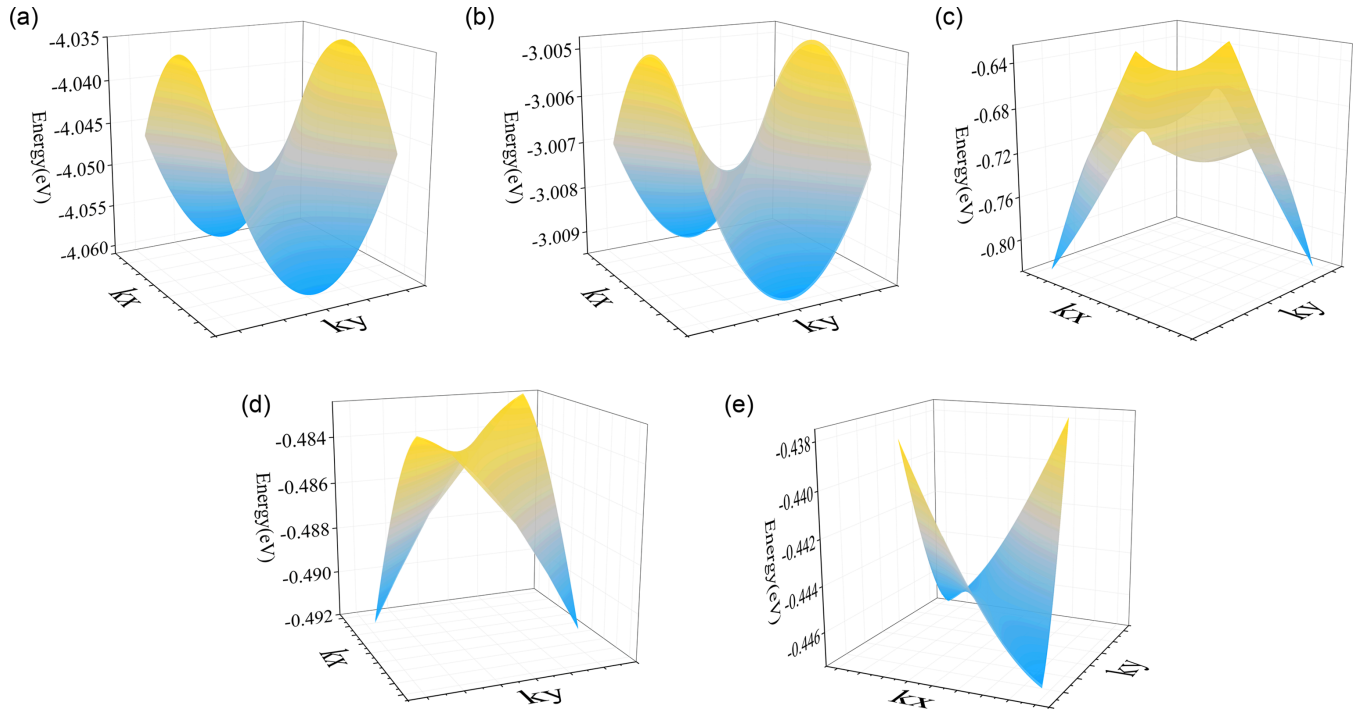


FIG. 6. The 3D band dispersion of the SPs (a) L2, (b) L4, (c) L12, (d) L14, and (e) L16.

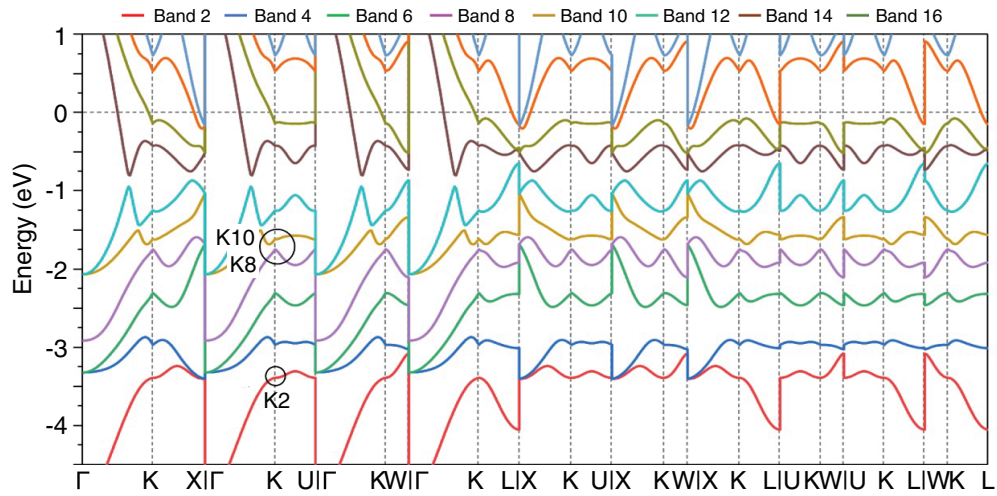
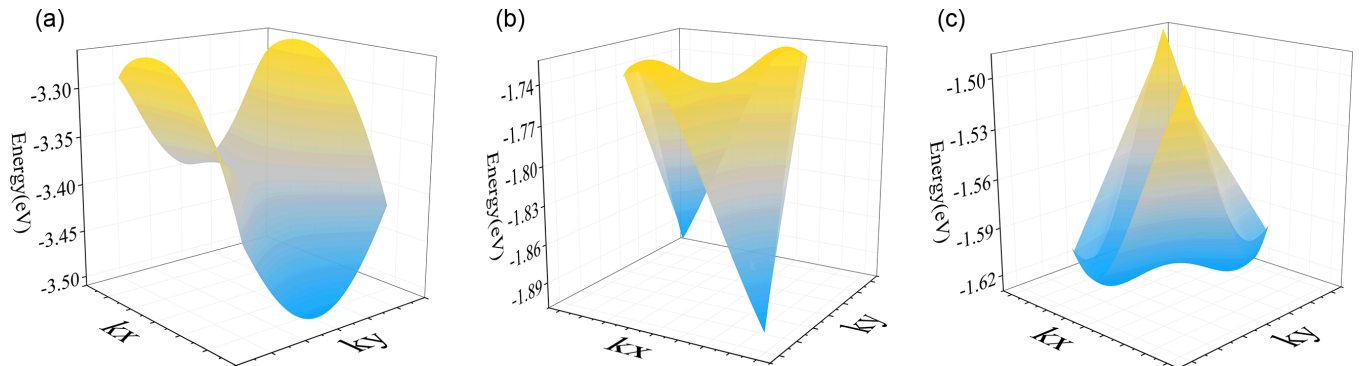
FIG. 7. Calculated band structures of the Γ -K-X| Γ -K-U| Γ -K-W| Γ -K-L|X-K-U|X-K-W|X-K-L|U-K-W|U-K-L|W-K-L paths. Circles represent the SPs K2, K8, and K10.

FIG. 8. The 3D band dispersion of the SPs (a) K2, (b) K8, and (c) K10.

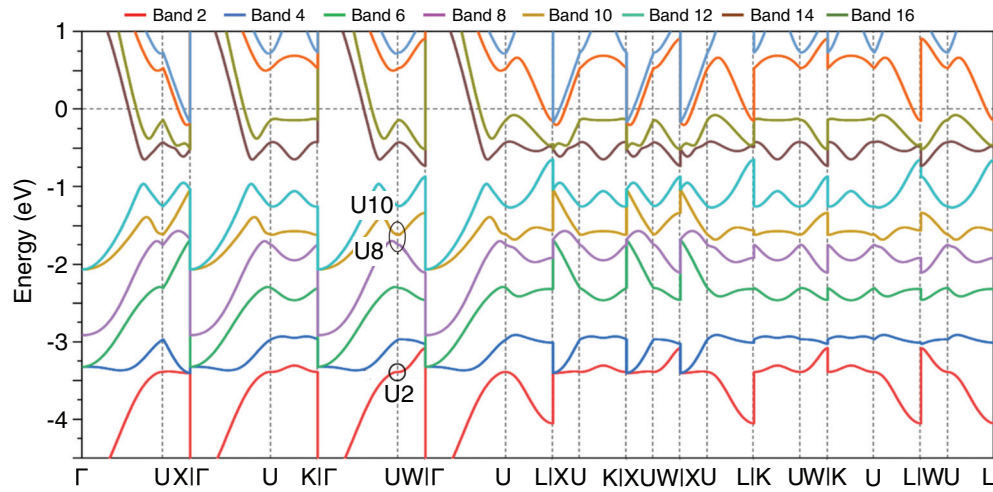


FIG. 9. Calculated band structures of the Γ -U-X| Γ -U-K| Γ -U-W| Γ -U-L|X-U-K|X-U-W|X-U-L|K-U-W|K-U-L|W-U-L paths. Circles represent the SPs U2, U8, and U10.

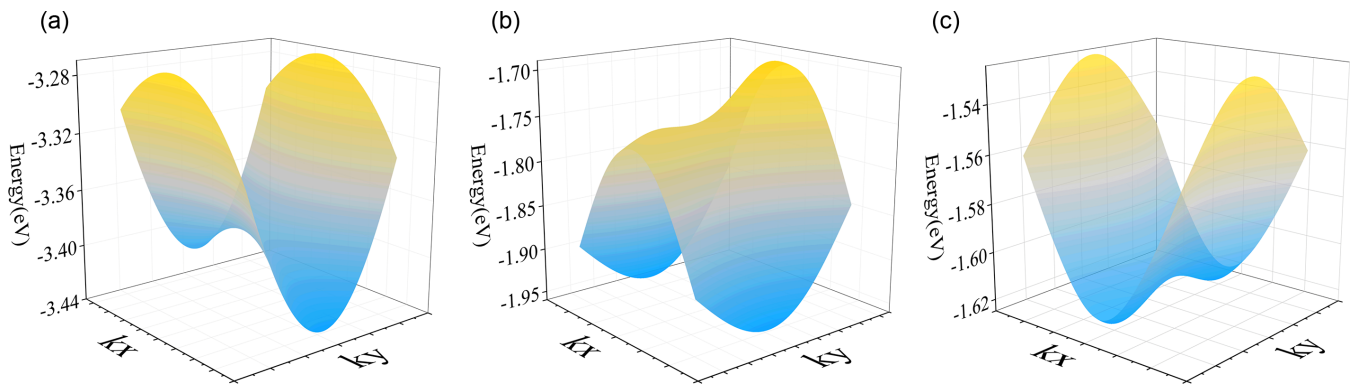


FIG. 10. The 3D band dispersion of the SPs (a) U2, (b) U8, and (c) U10.

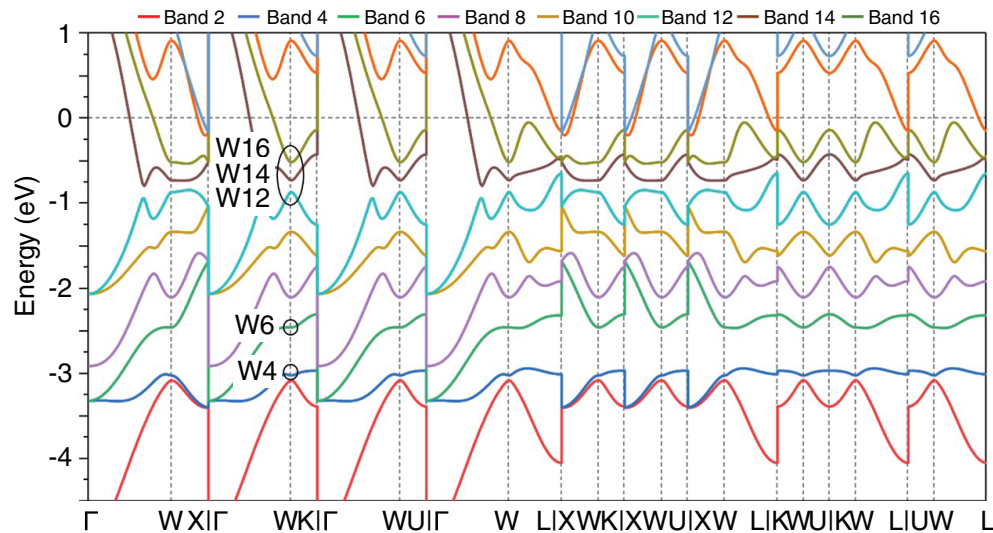


FIG. 11. Calculated band structures of the Γ -W-X| Γ -W-K| Γ -W-U| Γ -W-L|X-W-K|X-W-U|X-W-L|K-W-U|K-W-L|U-W-L paths. Circles represent the SPs W4, W6, W12, W14, and W16.

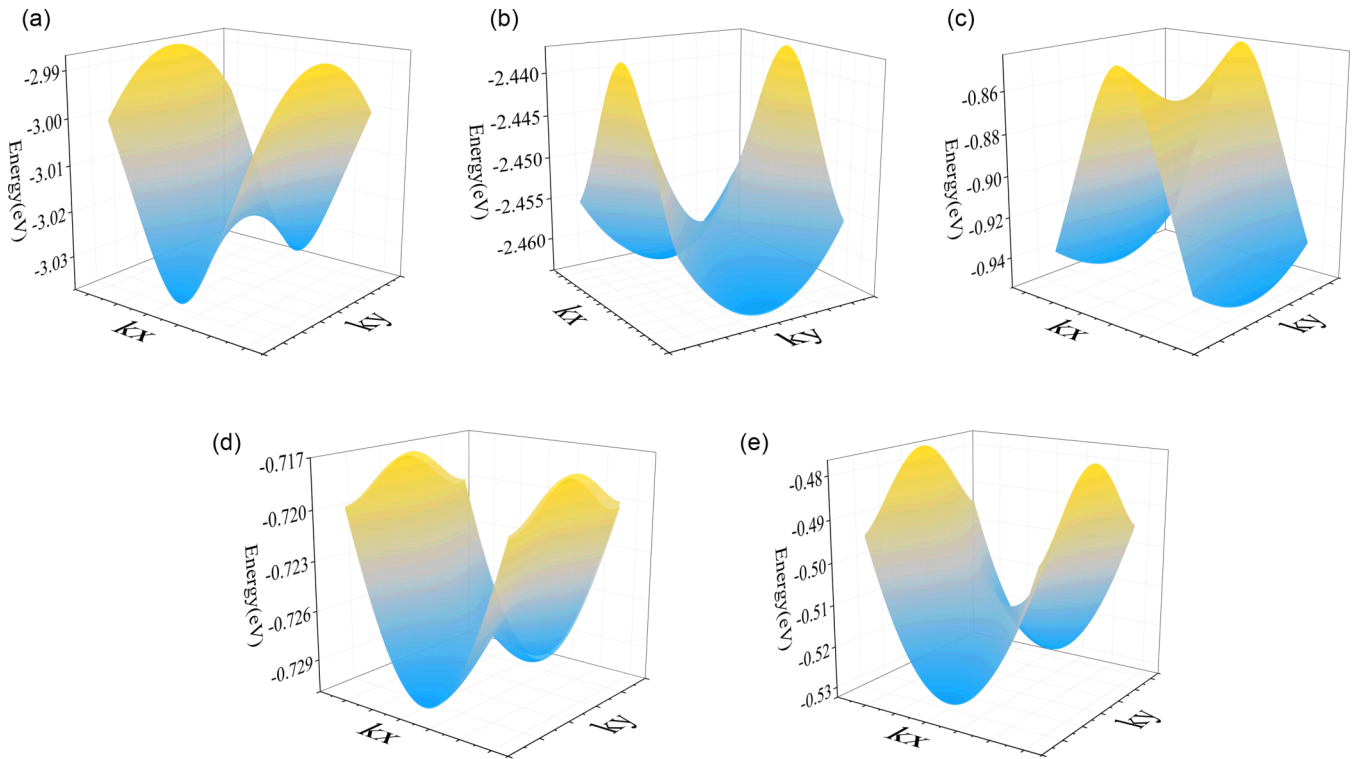


FIG. 12. The 3D band dispersion of the SPs (a) W4, (b) W6, (c) W12, (d) W14, and (e) W16.

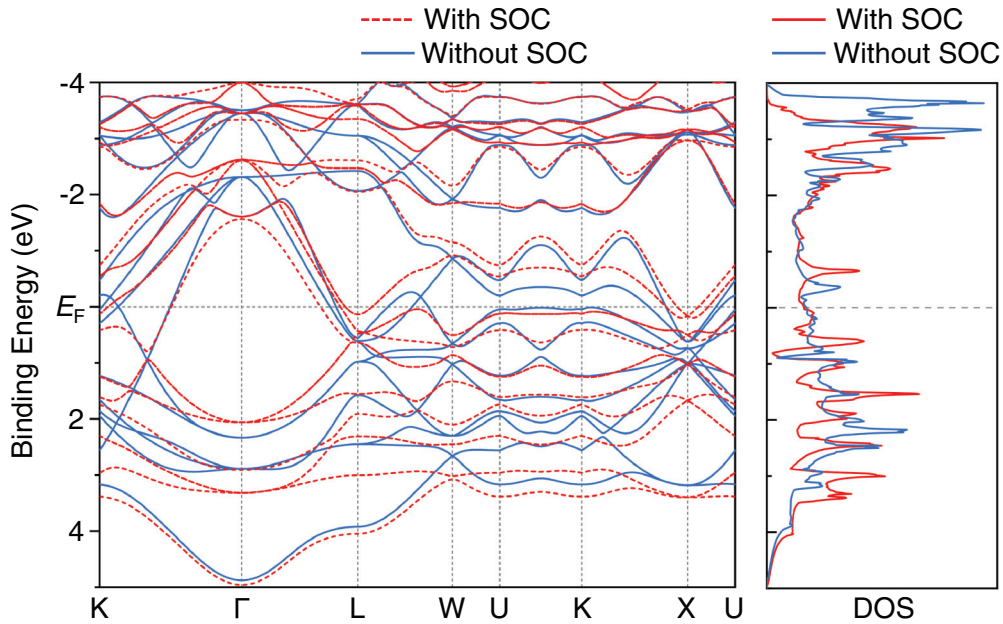


FIG. 13. Calculated band structures and DOS with and without SOC.

TABLE II. Calculated bandwidths ΔE for different $Un-Kn$ and $L4-W4$ routes without SOC (w/o SOC) and with SOC, respectively.

Routes		U2-K2	U4-K4	U6-K6	U8-K8	U10-K10	U12-K12	U14-K14
ΔE (eV)	w/o SOC	0.1129	0.1351	0.3315	0.2055	0.0842	0.3271	0.4684
	with SOC	0.0871	0.0398	0.1696	0.2118	0.0615	0.1983	0.2263
Routes		U16-K16	U18-K18	U20-K20	U22-K22	U24-K24	L4-W4	
ΔE (eV)	w/o SOC	0.0310	0.1435	0.6553	0.2168	0.5157	0.2079	
	with SOC	0.0185	0.1508	0.5354	0.1187	0.3448	0.0858	

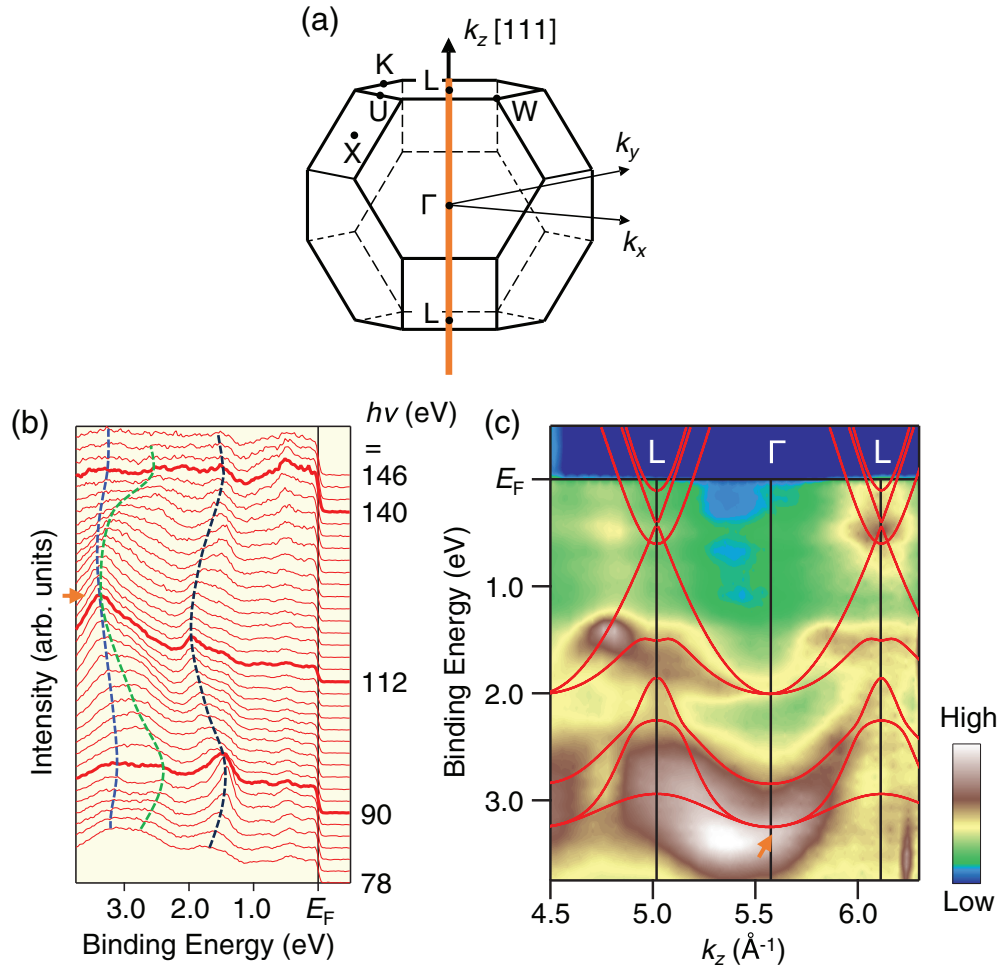


FIG. 14. (a) Bulk BZ of CsBi₂. (b) $h\nu$ dependence of the normal-emission EDCs measured with $h\nu = 78\text{--}146$ eV with a 2 eV interval, which traces the band dispersion along the orange line in panel (a). Dashed lines are a guide for the eyes to trace the band dispersions. (c) Intensity plot of panel (b) as a function of binding energy and k_z . The inner potential V_0 of 4.5 eV was used to calculate k_z values. Red curves are the calculated band dispersions.

over all eight TRIM points:

$$(-1)^{v_0} = \prod_{i=1}^8 \delta_i.$$

The remaining three invariants v_k ($k = x, y, z$) are determined by the product of four TRIM points lying on planes orthogonal to the k th axis:

$$(-1)^{v_k} = \prod_{n_j=0,1, n_i=0,1} \delta_{(n_1, n_2, n_3)}, \quad k = x, y, z,$$

where n_1 , n_2 , and n_3 index the TRIM points in the Brillouin zone. The obtained $\mathbb{Z}_2$ indices are tabulated in Table I. It is important to note that the $\mathbb{Z}_2$ invariants characterize the global topology of the occupied manifolds and do not by themselves imply that the local flatness of the quasiflat segments is topologically protected. As an obvious consequence, the electronic DOS would become localized around the flat band, which can be found in the DOS of Fig. 2.

APPENDIX E: INFLUENCE OF SPIN-ORBIT COUPLING ON THE BAND STRUCTURE

Here, we discuss the influence of SOC on the flat band, SP, and DOS by DFT calculations. The band structures and DOS without considering SOC are displayed in Fig. 13 (light blue curves), which differ from those results with SOC (red curves). To describe the flatness, the bandwidth ΔE , i.e., the difference between the highest energy and the lowest energy of the quasiflat segments [23] along set routes (U-K and L4-W4), is introduced. As shown in Fig. 13 and Table II, one can find that SOC makes most of the band structures along U-K more dense (except U8-K8 and U18-K18), i.e., with a smaller ΔE when SOC is considered. As a result, the DOS becomes more localized and gives rise to a larger peak value at specific E_B 's (Fig. 13). These results indicate that SOC plays a constructive role in generating the unique electronic singularities of this system. Since the primary DOS enhancement resides away from E_F , the present results hint at a pathway where the DOS contributing to the superconducting and other properties of CsBi₂ might be enhanced by SOC if the chemical potential is tuned, e.g., via carrier doping.

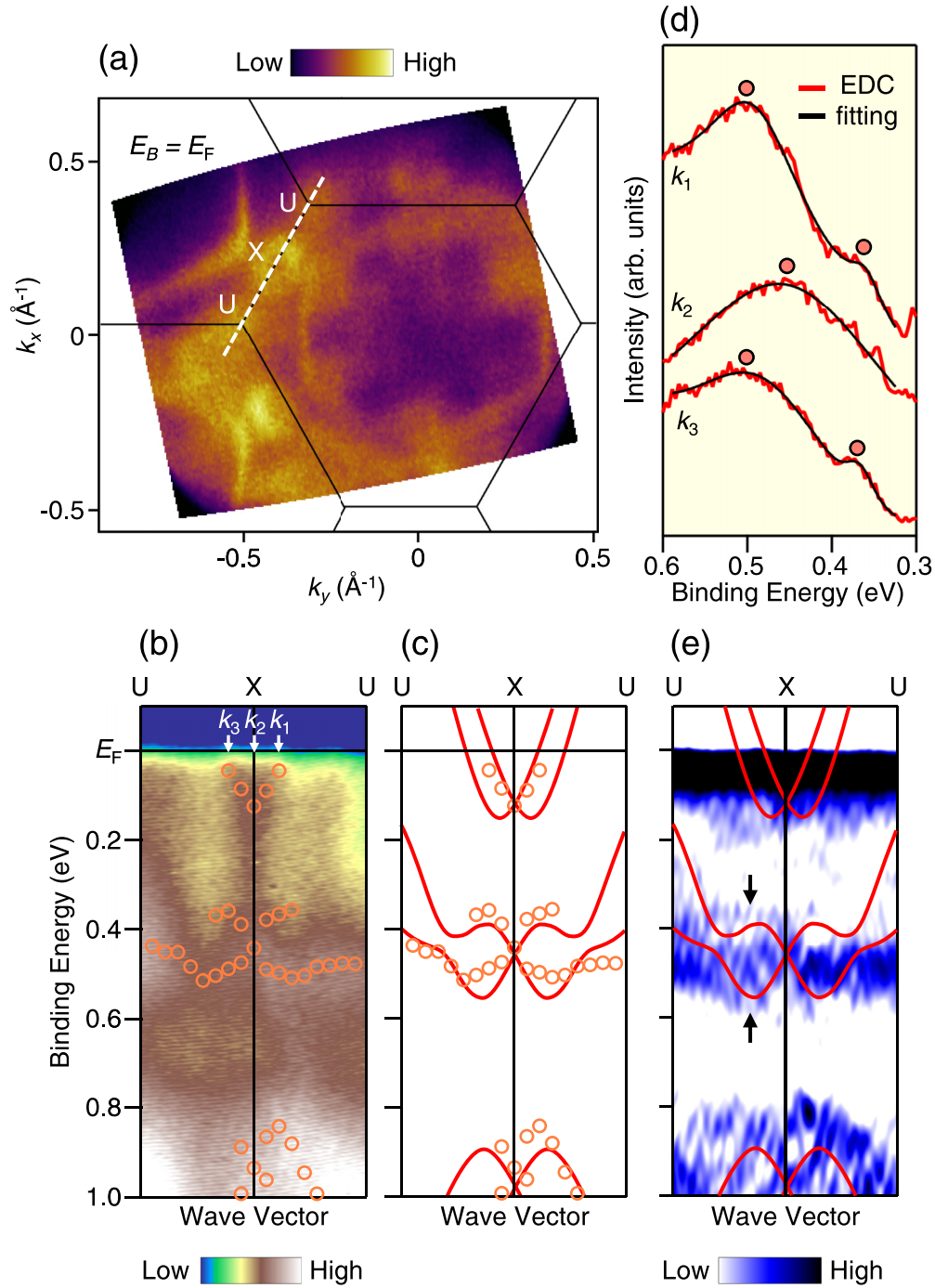


FIG. 15. (a) Fermi-surface mapping at $k_z \sim \pi/3$, probed by 21-eV photons [same as Fig. 2(a)]. (b), (c) ARPES intensity plot and calculated band structure along the U-X-U cut [white dashed line in panel (a)], respectively. Orange circles show the peak positions of EDCs. (d) EDCs (red curves) obtained at momenta k_1 – k_3 indicated by white arrows in panel (b). Fitting results (black curves) are overlaid. (e) Plots of second-derivative intensity of panel (b), compared with the calculated band dispersion (red curves).

APPENDIX F: NORMAL-EMISSION MEASUREMENTS

To determine the band dispersion along the wave vector perpendicular to the sample surface, i.e., k_z [orange line in Fig. 14(a)], we measured energy distribution curves with various $h\nu$'s in the normal-emission setup [Fig. 14(b)]. These EDCs show that a peak at a binding energy (E_B) = 1.5 eV at $h\nu = 90$ eV moves to higher E_B with increas-

ing $h\nu$, reaches a local minimum at $E_B \sim 2.0$ eV around $h\nu = 112$ eV, and then returns to lower E_B , as traced by a black dashed curve. In addition, a shoulder structure at $E_B \sim 2.5$ eV at $h\nu = 90$ eV (green dashed curve) disperses toward higher E_B as $h\nu$ approaches 112 eV and seems to merge into another band at $E_B \sim 3.2$ eV (blue dashed curve). Based on the observed periodic dispersions that qualitatively

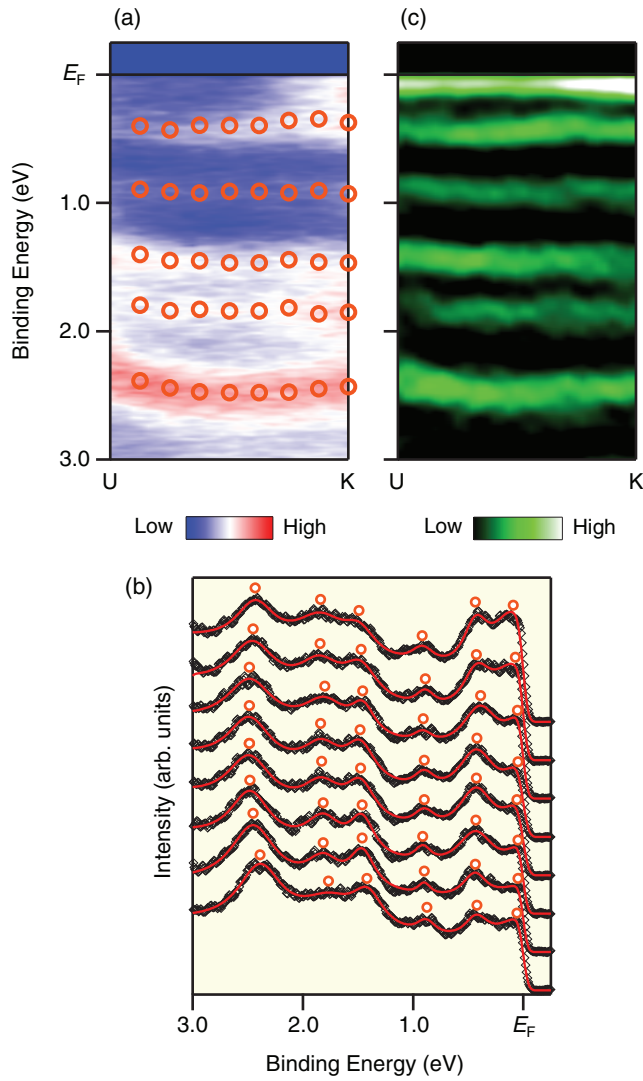


FIG. 16. (a) ARPES intensity plot along the U-K cut measured with 120-eV photons. (b) Series of EDCs along the U-K cut (black circles) together with numerical fits (red curves) using six Lorentzian peaks and a moderate background, multiplied by the Fermi-Dirac distribution function at $T = 30$ K. The peak positions obtained from the fits are indicated by orange open circles, and are also reproduced in panel (a). (c) Second-derivative ARPES intensity plot along the U-K cut, confirming the existence of a quasiflat band near E_F .

agree with the calculation along the Γ L axis, we estimated the inner potential to be 4.5 eV and plotted the ARPES intensity as a function of E_B and k_z in Fig. 14(c). The result shows an overall agreement with the band calculations for the bands at high E_B 's. It is noted that, although the near- E_F band dispersions around the L point are not clearly determined due to their weak spectral intensities in Figs. 14(b) and 14(c), measurements in a different momentum cut [Fig. 3(c1)] reveal electronlike and holelike dispersions that seem to cross with each other at $E_B \sim 0.5$ eV at the L point, in agreement with the calculations. One important implication here is that the band degeneracy at the Γ point is consistent with the predicted quadratic touching DP (orange arrow).

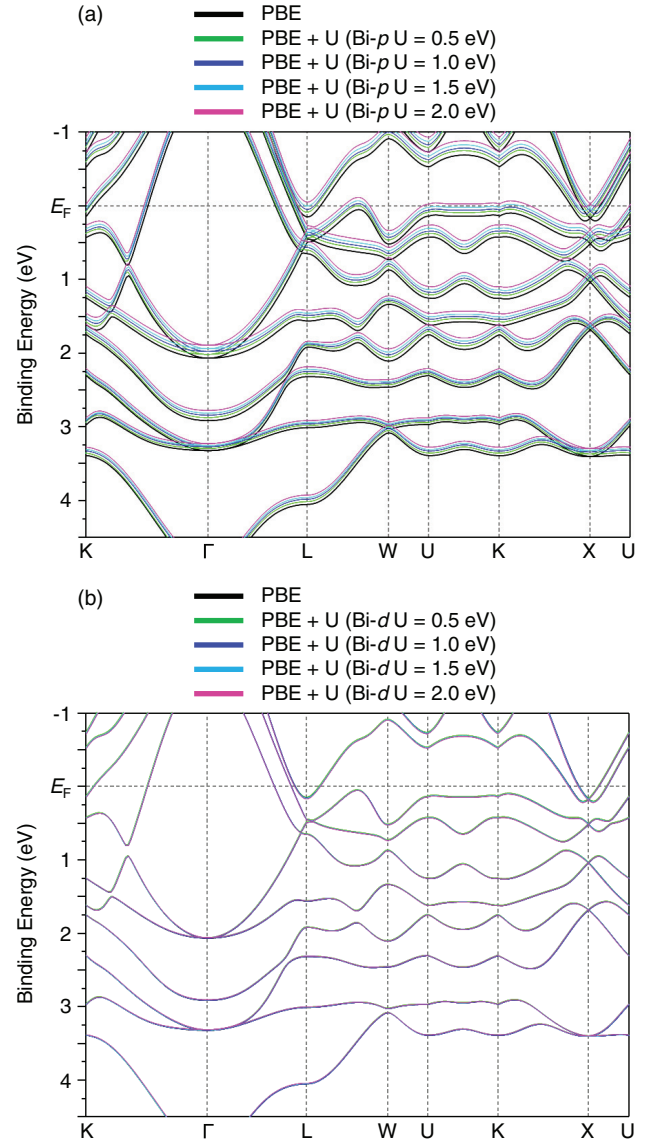


FIG. 17. Electronic structures of CsBi_2 using GGA + U method. The Coulomb repulsion parameter U on the (a) p and (b) d orbitals of Bi is set to be 0.0 (black), 0.5 (green), 1.0 (blue), 1.5 (light blue), and 2.0 (red) eV, respectively. The SOC is included in all the computations.

APPENDIX G: SIGNATURE OF DIRAC-CONE DISPERSION

To find an experimental signature of the Dirac-cone formation, we measured the band dispersion along the U-X-U cut [white dashed line in Fig. 15(a)] as shown in Fig. 15(b). According to the calculations [Fig. 15(c)], the shallow electron pocket may be composed of a pair of electronlike bands forming a DP at $E_B \sim 0.1$ eV. The calculations also suggest that another DP could be formed at $E_B \sim 0.45$ eV. To clarify this point, we extracted EDCs at three-momentum positions k_1 – k_3 indicated by white arrows in Fig. 15(b). The result plotted in Fig. 15(d) suggests that a single peak at k_2 (the X point) splits into two peaks at k_1 and k_3 (slightly off the X point), consistent with the DP formation at the X point. This is also

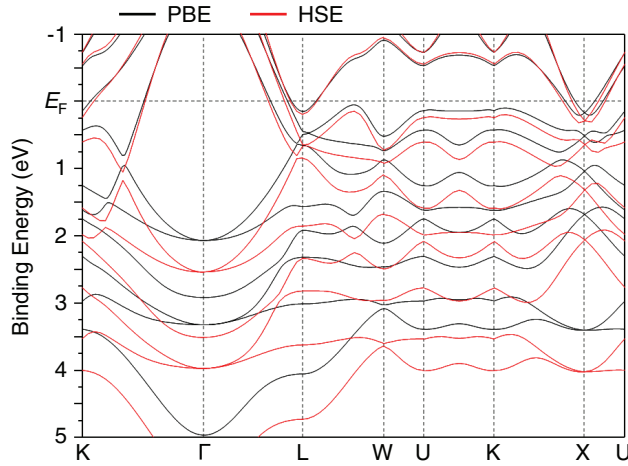


FIG. 18. The electronic structures of CsBi₂ investigated using both the PBE (black) and HSE06 (red) methods, with contributions from spin-orbit coupling.

supported by a reasonable agreement between experimental peak positions and calculated band energies [orange circles and red curves, respectively, in Fig. 15(c); the existence of the upper and lower branches of the Dirac cone is also seen in the second-derivative intensity plot in Fig. 15(e), as indicated by black arrows]. It is noted that, while the two branches producing the Dirac cone near E_F are not clearly resolved likely due to their proximity to each other, their DP crossing may be protected similarly to the Dirac-cone band at $E_B = 0.4\text{--}0.6$ eV because the protection mechanism (namely, the screw symmetry of the pyrochlore lattice) is the same.

APPENDIX H: NUMERICAL FITTING TO THE QUASIFLAT BANDS

Figures 16(a) and 16(b) show the ARPES intensity along the U-K path and the corresponding energy distribution

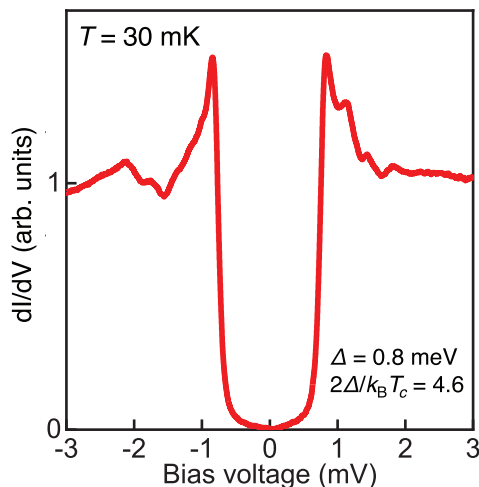


FIG. 19. dI/dV spectrum as a function of bias voltage measured at $T = 30$ mK. Coherence peaks and the superconducting gap are clearly resolved.

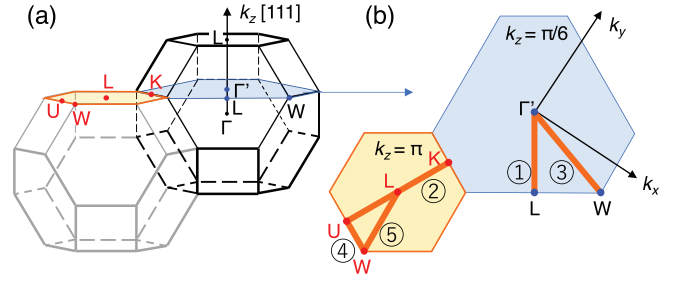


FIG. 20. Schematics of the k_z planes (light blue and orange planes) probed by $h\nu = 120$ eV: (a) a 3D view of the bulk BZ and (b) a top view. Orange lines indicate the measured momentum cuts k_1 ①–⑤, defined in Fig. 3.

curves, respectively. The EDCs exhibit multiple peaks that are well reproduced by assuming six bands within 3 eV from E_F , consistent with the DFT calculations. In particular, one can clearly find peaks near E_F , which supports the formation of a quasiflat band near E_F (note that the peak position of this band is not displayed in the intensity plot for its better visual confirmation). The existence of the near- E_F quasiflat band is further corroborated by the second-derivative plot in Fig. 16(c).

APPENDIX I: INFLUENCE OF ELECTRONIC CORRELATIONS

GGA method is generally not accurate enough to describe the electronic structures of strongly correlated systems. It is well known that strong on-site Coulomb repulsive effects are commonly observed in the d (f) orbitals of transition metal elements and the p orbitals of nonmagnetic elements in magnetic compounds such as superoxides AO_2 ($A = K, Rb, Cs$). To verify possible Coulomb repulsive interactions of CsBi₂, we performed the GGA + U and hybrid functional (HSE06) calculations and then compared their electronic structures. Specifically, for the GGA + U scenario, the band structures of CsBi₂ are obtained with the Coulomb repulsion on the p (d) orbitals of Bi element, using U values of 0.5, 1.0, 1.5, and 2.0 eV, respectively (Fig. 17). As shown in Fig. 17(a), when the Coulomb repulsion is applied to the p orbitals, the band structures retain their shape but shift uniformly up or down relative to E_F . This indicates that the flat band along U-K path might be tuned closer to E_F with a stronger Coulomb repulsion interaction. Moreover, when Coulomb repulsion is applied to the d orbitals, the overall band structures maintain their pristine energy positions [Fig. 17(b)], indicating that the Coulomb repulsive effect is negligible for the inner d orbitals of Bi atoms. Additionally, as shown in Fig. 18, although the HSE06 band structures are more dispersive than those obtained within the GGA scheme (Fig. 17), key features such as Dirac points and flat bands are preserved. These results strongly suggest that electronic correlations of CsBi₂ are weak and hence our DFT calculations are reliable. Therefore, the band flattening at ~ 1 eV is not caused by electron correlations but is most likely an extrinsic effect, possibly related to the aforementioned high-DOS background at $E_B \sim 1.0$ eV, and it does not affect our main conclusions regarding the SPs and the flat topological band at higher E_B 's.

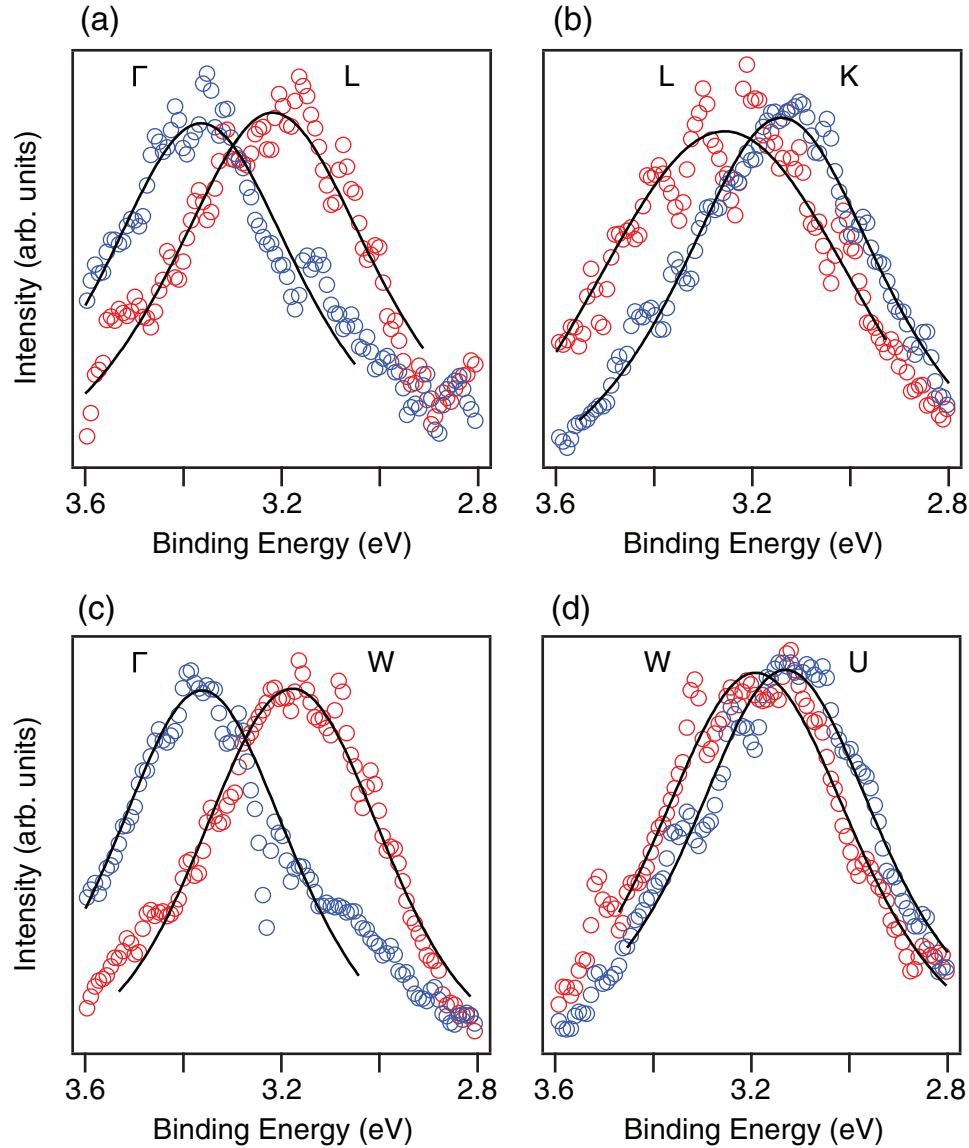


FIG. 21. Direct comparison of EDCs at high-symmetry points, reproduced from Fig. 3: (a) L and Γ points from Fig. 3(c3), (b) L and K points from Fig. 3(d3), (c) W and Γ points from Fig. 3(e3), and (d) W and U points from Fig. 3(f3).

APPENDIX J: STRONG-COUPLING SUPERCONDUCTIVITY

We observed a quasiflat band slightly below E_F , called an incipient flat band, coexisting with a highly dispersive band crossing E_F . This observation is intriguing because theory predicts that the large DOS from the flat band, combined with pair scattering between the flat and dispersive bands, could trigger unconventional superconductivity [81–83]. Although the importance of this mechanism in CsBi₂ needs further clarification, our scanning tunneling spectroscopy/microscopy measurements (Fig. 19) reveal a large superconducting gap ($\Delta = 0.8$ meV; $2\Delta/k_B T_c = 4.6$). This observation is consistent with a strong-coupling scenario [68] and may warrant further investigation of a possible connection to the near- E_F quasiflat band.

APPENDIX K: DETAILS OF MEASUREMENT PATHS

ARPES data presented in Fig. 3 were measured at $h\nu = 120$ eV, which probes $k_z \sim \pi/6$ at $k_x = k_y = 0$ (light blue plane in Fig. 20) and $k_z \sim \pi$ in the neighboring Brillouin zone (see light orange hexagon). The orange lines in Fig. 20(b) indicate the measured momentum paths ①–⑤ ($\sim\Gamma$ -L, L-K/U, $\sim\Gamma$ -W, W-U, and L-W lines, respectively). It is noted that $\sim\Gamma$ of the paths ① and ③ corresponds to the $(0, 0, \pi/6)$ point defined as Γ' .

APPENDIX L: TYPE-I AND TYPE-II SADDLE POINTS AT L AND W POINTS

Figures 21(a) and 21(b) directly compare the EDCs at two high-symmetry points: L (red) and Γ (blue) in Fig. 21(a),

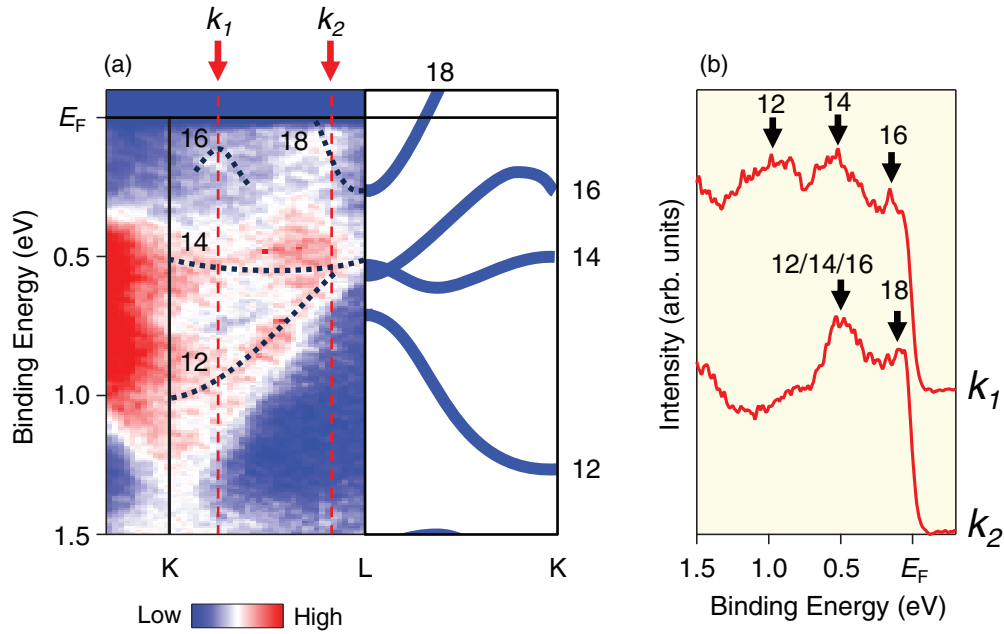


FIG. 22. (a) Left: ARPES intensity plot along the K-L cut with the experimental band dispersions (black dotted curves). Right: corresponding calculated band dispersion. (b) EDCs at two representative k points, k_1 and k_2 [red arrows in panel (a)]. Black arrows indicate the peak positions.

and L (red) and K (blue) in Fig. 21(b). Independent of the details of the fitting procedure, the raw EDCs show opposite energy shifts with respect to the L point along the Γ -L and L-K/U cuts, supporting the formation of a saddle point around L. Similarly, the direct comparison of EDCs in Figs. 21(c) and 21(d) supports the saddle-point character around W.

APPENDIX M: MAGNIFIED VIEW OF THE NEAR- E_F BAND DISPERSION

Figure 22 displays a magnified view near E_F and corresponding EDCs shown along the K-L cut. The results resolve

four bands, i.e., 12, 14, 16, and 18, within ~ 1 eV of E_F , in reasonable agreement with the DFT calculations [right panel in Fig. 22(a)].

APPENDIX N: OBSERVATION OF A NONCRITICAL SADDLE POINT

Along the Γ -U-W path, two bands are observed below $E_B = 3$ eV [Fig. 23(a); labeled as bands 2 and 4 in Fig. 23(b)], as evidenced by two peaks in the EDC at the U point in Fig. 23(c). Band 2 exhibits the characteristic dispersion of an SP: it disperses toward higher E_B 's from the U to Γ points

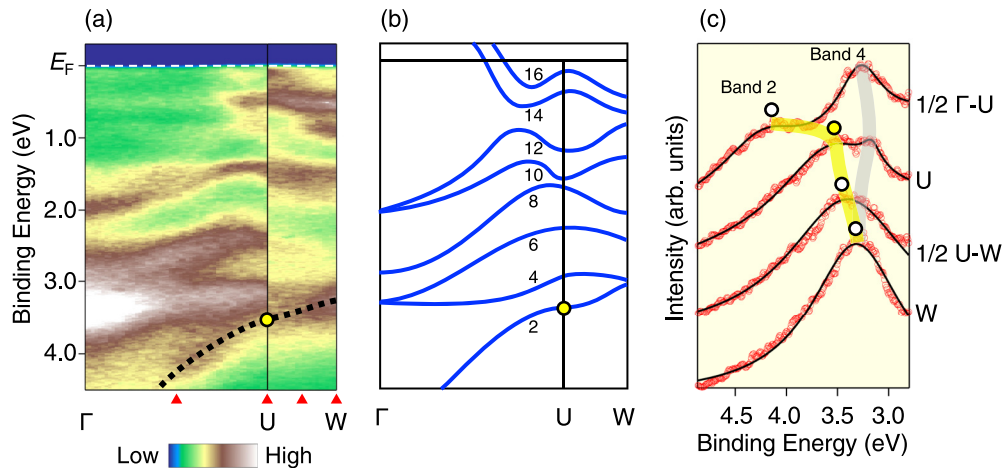


FIG. 23. (a) The ARPES-intensity plot along the Γ -U-W path and (b) corresponding calculated band structures. The dotted black line in panel (a) represents a guide for the eyes to trace band 2, which forms the SP at the U point. (c) ARPES spectra at four characteristic momentum points [indicated by red triangles in panel (a)], where circles indicate the energy positions of band 2 determined by numerical fittings, supporting the SP nature of the dispersion.

(convex shape with respect to the U point), while it shifts toward lower E_B 's upon approaching the W point (concave shape). According to recent theoretical classification of singu-

larities in 3D materials, the SP at the U point in pyrochlores is identified as a distinct class dubbed noncritical SP [69] (see also Fig. 4 and its caption).

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