Orbital-Selective Dirac Fermions and Extremely Flat Bands in the Nonmagnetic Kagome Metal CoSn

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Two-dimensional layered Kagome-lattice 3d transition metals are emerging as an exciting platform to explore the frustrated lattice geometry, electronic correlation and quantum topology. However, the typical Kagome electronic bands, characterized by sets of the Dirac-like bands capped by a phase-destructive flat band, have not been clearly observed in these materials, mainly due to the complicated electronic structures induced by magnetism, their orbital physics are even less well investigated. Here, we present the orbital-selective Dirac fermions and extremely flat bands in the nonmagnetic Kagome metal CoSn, which contains Co Kagome lattice in single CoSn layers. Without complications from the magnetism and with a perfect in-plane Kagome lattice, the Kagome bands of CoSn are clearly determined both experimentally and computationally. We directly visualize that the extremely flat band with out-of-plane $d_{x^2-y^2}$ orbital characters runs through the whole Brillouin zone (BZ) and features in touch with a quadratic band at the BZ center, which is a key feature to distinguish from the flat band in heavy fermions and Morii lattice. This key evidence of Kagome flat band is critically missing in previous experiments. The flat band top with in-plane $d_{x^2}/d_{y^2}$ orbital characters is just at about -0.07 eV below the Fermi level. If the chemical potential were tuned properly, superconductivity at even higher temperature could be realized. The energy gap induced by spin-orbit interaction at the Dirac cone with out-of-plane orbital characters is much smaller than that with in-plane orbital characters, suggesting orbital-selective character of the Dirac fermions. Our findings explicitly unveil orbital-selective topological electronic states, and provide insight into the recent discoveries of multiple types of topological electronic excitations in 3d transition Kagome metals.

Because of geometry frustration and competing magnetic interactions, materials with Kagome lattices exhibit abundant magnetic behaviors, which have been intensively investigated in condensed-matter physics [1][2]. Recently, the investigations of topological theories discover that symmetry-protected topological excitations could cause novel transport properties in two-dimensional (2D) 3d transition Kagome metals. For instance, large intrinsic anomalous Hall effects associated with Dirac/Weyl nodes near the Fermi energy ($E_F$) in antiferromagnetic (AFM) [3] and ferromagnetic (FM) [4][7] Kagome metals have been reported. A typical band structure of Kagome material is characterized by a Dirac-like band capped by a flat band, which can be produced by using the tight-binding method with single-orbital nearest-neighbor hopping. However, the materials with clearly typical Kagome bands near $E_F$ still remain elusive. Recently, the linearly dispersive energy bands and dispersionless flat bands have been observed in magnetic metals Fe$_3$Sn$_2$ [8][10], Fe$_7$GeTe$_5$ [11][12], Co$_3$Sn$_2$S$_2$ [5][7][13] and FeSn [14][15]. Topologically protected linearly dispersive bands show distinctly different behaviors from the traditional parabolic bands. When such bands are tuned to $E_F$, the low-energy quasiparticle excitations would be drastically different from that of the conventional parabolic-band fermions and thus lead to novel transport properties [16][18]. Further, with consideration of spin-orbit coupling (SOC), a small band gap can open, adding a mass term to the linearly dispersive band, and a massive Dirac fermion thus can be formed [9]. Contrasting with the linear band hosting massless or lightweight quasiparticles, flat band is dispersionless over a finite range of momentum, usually with super-heavy localized electrons, extremely singular density of states, and correlated states with broken symmetries. Because of the similarity with 2D continuum Landau levels, flat bands can induce novel quantum behaviors, like Mott insulators, FM or AFM magnetism, fractional quantum Hall states at even high temperature and superconductivity [19][21], as predicted in twisted bilayer graphene [22][23]. In Kagome metals, the extremely light band (Dirac fermions) and extremely heavy band (flat bands) coexist. Unconventional phenomena would happen if either of the two bands is tuned close to $E_F$.

Besides, five 3d orbitals dominate the low-lying electronic states in the 3d Kagome materials, resulting in the presence of multiple orbital physics. Along with the increased filling of the electronic 3d shell, the orbital characters of the low-energy
bands near $E_F$ can be tuned. The crystal field can also affect the orbital energy-levels in Kagome lattice. The Dirac-like bands and the flat bands with specified orbital characters have been reported in Kagome paramagnetic YCr$_6$Ge$_6$ ($d^8$)\cite{24}, as well as in helically coupled FM Kagome layers of YMn$_6$Sn$_6$ ($d^9$)\cite{25} and antiferromagnetically coupled FM Kagome layers of FeSn ($d^6$)\cite{14}. Furthermore, when SOC opens band gaps at the Dirac points, orbitals with different SOC strengths will cause various sizes of the band gaps. If the sizes of the band gaps have obvious distinctions among the orbitals, the Dirac cones with small gaps would be largely responsible for the novel topological excitations, leading to orbital-selective Dirac fermions.

In this work, we demonstrate the orbital-dependent Dirac fermions and extremely flat bands in the nonmagnetic Kagome CoSn by means of angle-resolved photoemission spectroscopy (ARPES), scanning tunneling microscopy/spectroscopy (STM/S), and in combination with theoretical calculations. Because of representation of the group $D_{6h}$, five 3$d$ orbitals are divided into three groups: in-plane $d_{xy}/d_{xz},$ out-of-plane $d_{yz}/d_{z^2},$ and $d_{2z}$ orbitals, with individual sets of feature for each group. We find that the SOC induced energy gap at the Dirac cone with $d_{xy}/d_{xz}$ orbital characters is much larger than that with $d_{yz}/d_{z^2}$ orbital characters, suggesting that the latter can be predominant in the Dirac-like fermionic excitations. While, the extremely flat bands near $E_F$ are mainly dominated by $d_{xy}/d_{xz}$ and $d_{yz}/d_{z^2}$ orbitals, respectively. The $d_{2z}$ orbital sinks downward to higher binding energy and mainly contributes dispersions in a narrow range of momentum space around $k_z \sim \pi$ plane, indicating 2D character of the flat bands of CoSn.

CoSn is isostructural to FeSn, crystallizing in a hexagonal structure with $P6/mmm$ (No. 191) space group, in which Co Kagome lattice in single Co$_3$Sn$_2$ layer is the one closest to the 2D limit, as shown in Fig. 1(a). The corresponding Brillouin zone (BZ) with high-symmetry points and two mirror planes ($\sigma_h$ and $\sigma_v$) are shown in Fig. 1(b). High-quality single crystals were synthesized by the Sn flux method [see more details in Supplemental Material (SM)\cite{26}]. The samples used for the experimental studies were characterized by X-ray diffraction [Fig. S1\cite{24}] and transport measurements [Figs. S2 and S3\cite{26}]. The electrical resistance of CoSn as a function of temperature is shown in Fig. S2, from which a clear metallic behavior is observed as the resistance decreases rapidly upon cooling the sample. Further, Fig. S3 demonstrates a nonmagnetic metal as the electrical resistance shows no variation between zero field cooling and field cooling. Without complicated magnetism, the electronic bands of CoSn would be advantageous for clearly addressing the fundamental questions of Kagome physics both theoretically and experimentally.

![Image of CoSn crystal structure with high-symmetry directions and Dirac cones](imageurl)

**Fig. 1.** (Color online) (a) Crystal structure of CoSn with space group $P6/mmm$ (No. 191). (b) 3D bulk BZ with marked high-symmetry points and two mirror planes: $\sigma_h$ ($\Gamma-K-M$) and $\sigma_v$ ($\Gamma-A-H-K$). $\Gamma-K-M$ plane is a projected 2D BZ. (c) Intensity plots at $E_F \pm 10$ meV in 2D BZ. The red lines indicate high-symmetry directions and the first BZ projected on the (001) surface. (d) Intensity plots at $K$ and $H$ points along cut 1 as indicated in (c) in $\sigma$ and $\pi$ geometries, respectively. Dirac cones (DP) and flat bands (FB) are indicated by the white and red arrows, respectively. (d$_1$)-(g$_1$) Corresponding second derivative plots of (d$_1$)-(g$_1$). (h) MDCs around the Dirac cones at $K$ point in $\sigma$ geometry show two close Dirac cones at about $-0.6$ eV below $E_F$, as indicated by the dashed square in (d). The Dirac-like bands are indicated by the black dashed lines. (i) MDCs around the Dirac cones at $H$ point in $\sigma$ geometry show two Dirac cones at about $-0.42$ eV and $-0.68$ eV below $E_F$, respectively, as indicated by the dashed square in (f$_1$). Two close Dirac cones (DP 1, 2) at about $-0.6$ eV and a flat top of the hole-like band (FB 1) at about $-0.07$ eV below $E_F$ are indicated in (d$_1$) and (d$_2$) under $\sigma$ geometry. The two Dirac cones (DP 1, 2) at about $-0.6$ eV and a flat band (FB 2) at about $-0.3$ eV below $E_F$ are indicated in (e$_1$) and (e$_2$) under $\pi$ geometry. (f$_1$) and (f$_2$) show a flat band (FB 1) and two Dirac cones (DP 2, DP 3) in $\sigma$ geometry. (g$_1$) and (g$_2$) show a flat band (FB 2) and the Dirac cone (DP 3) in $\pi$ geometry.
We performed polarization- and photon-energy-dependent ARPES measurements on (001) surfaces of CoSn. The experimental setup shows the high-symmetry directions and the normal of the sample surface defined a mirror plane [Fig. S4](26). The $\pi$ ($\sigma$) geometry refers to the electric fields of the incident photons within (normal to) the mirror plane. The even (odd) orbitals with respect to the mirror plane are detected in $\pi$ ($\sigma$) geometry. With selected experimental symmetries, certain orbitals combinations, e.g. $d_{xz}$ (odd) and $d_{x^2-y^2}$ (even) [d$_{yz}$ (even) and d$_{z^2}$ (odd)], could be enhanced or suppressed individually, thus the Dirac cones and the flat bands features could be more prominent under certain conditions.

Figs. 1(a)–1(d) show ARPES intensity plots along cut1, which is perpendicular to $\Gamma-K$ line, as marked on the Fermi surface (FS) plot [Fig. 1(c)]. One can clearly see the feature of typical Kagome bands characterized by the Dirac-like dispersion capped by a phase-destructive flat band, in spite of the weak electron correlation effect in CoSn. At $K$ point, the two close Dirac cones at around -0.6 eV below $E_F$ are shown in both geometries, as shown in Figs. 1(a), 1(b), 1(e), and 1(f). The two close cones can be more clearly seen from the momentum distribution curves (MDCs) in Fig. 1(h). The two flat bands at about -0.07 and -0.3 eV below $E_F$ are revealed in $\sigma$ [Figs. 1(d1) and 1(d2)] and $\pi$ geometries [Figs. 1(e1) and 1(e2)], respectively. The former is an extremely flat top of a hole-like band, which contributes a hotspot around $K$ point at $E_F$, as shown in Fig. 1(c). The latter entangles with the Dirac-like bands and looks like a break at the center of the $K$ point. At $H$ point, two Dirac cones locate at about -0.42 eV and -0.68 eV below $E_F$, respectively, as shown in Figs. 1(f1) and 1(f2). The two cones can also be determined from the MDCs in Fig. 1(i). With the same binding energies as at the $K$ point, the two flat bands at $H$ point are also revealed in $\sigma$ [Figs. 1(f1) and 1(f2)] and $\pi$ geometries [Figs. 1(g1) and 1(g2)], respectively, indicating that the flat bands have negligible $k_z$ dispersions. We applied the projected 2D BZ ($\Gamma-K-M$) in our studies of the flat bands unless further stated, due to the weak $k_z$ dispersions and the limitation of $k_z$ resolution in ARPES experiments.

The band structure along $\Gamma-K$ direction is shown in Fig. 2(a). The flat bands are indicated by the red dashed lines in Figs. 2a and 2b. The red solid lines appended on second derivative plots [Figs. 2c and 2d] are the density functional theory (DFT) calculated bands, renormalized by a factor of $\sim$1.4 to match the mainly ARPES dispersive features, indicating weak electron correlation effect in CoSn. At $K$ point, the extremely flat band top with the binding energy of ~0.07 eV can still be observed in both geometries, which is consistent with the observation along cut1 in Fig. 1. At $\Gamma$ point, the electron-like bands contribute the FSs around BZ center [Fig. 1(c)], and nearly flat band lays at about -0.3 eV below $E_F$. Figs. 2c and 2f show the energy distribution curves (EDCs) corresponding to Figs. 2a and 2b, respectively. The EDCs clearly exhibit the flat band (FB 3), the electron-like parabolic band (QB), and the flat band top (FB 1). As predicted by fundamental Kagome lattice model [10, 13], the nearly flat band (FB 3) degenerates with the quadratic band bottom at $\Gamma$ with the exclusion of SOC. The electron-like band extends

![FIG. 2](Color online) (a)-(d) Intensity plots and corresponding second derivative plots along the $\Gamma-K$ direction in $\sigma$ and $\pi$ geometries, respectively. Flat bands are indicated by the red dashed lines in (a) and (b). The red lines in (c) and (d) are DFT calculated bands renormalized by a factor of 1.4. (e) EDCs of (a). (f) EDCs of (b). The flat bands (FB 1, and FB 3) and the parabolic band (QB) are indicated by the black dashed lines and open circles, respectively.
to \( K \) point and forms Dirac cone above \( E_F \). In consideration of SOC, the two bands further hybridize and open an energy gap of \(-40\) meV, which can be estimated from the EDCs in our experimental data. We note that the flat band in touch with the quadratic band at BZ center is a key feature to distinguish from the flat band in heavy fermions and Morié lattice. This key evidence for Kagome flat band is critically missing in previous experiments. Besides, comparing intensity plots in two geometries, one can see that the electron-like band in \( \pi \) geometry is more enhanced than that in \( \sigma \) geometry, which may suggest the electron-like band along \( \bar{\Gamma} - \bar{K} \) direction with mostly even orbital character.

Analogously, the ARPES intensity plots and corresponding second derivative plots along \( \bar{\Gamma} - \bar{M} \) in two geometries are shown in Figs. 3(a)-3(d), respectively. The flat bands are indicated by the red dashed lines in Figs. 3(a) and 3(b), and the DFT calculated bands renormalized by a factor of \(-1.4\) in Figs. 3(c) and 3(d). Intensity contrast between two geometries along \( \bar{\Gamma} - \bar{M} \) line is similar to that along \( \bar{\Gamma} - \bar{K} \) line in Fig. 2. These plots, especially Fig. 3(c), show an extremely flat band at the binding energy of \(-0.27\) eV. Fig. 3(e) show EDCs of Fig. 3(a), also clearly exhibiting this extremely flat band through the \( \bar{\Gamma} - \bar{M} \) line. Complementary to ARPES measurements on the flat band of CoSn, we performed STM and STS experiments. Fig. 3(f) is a constant current STM topograph in which the atomic steps can be seen clearly. The atomic step height of 0.4 nm is consistent with the lattice constant of 0.42 nm along the \( c \) direction. Fig. 3(g) is the high-resolution STM topograph taken on the flat Co\(_3\)Sn terrace, and Fig. 3(h) shows the atomic-resolved STM topograph taken on Co\(_3\)Sn surface. In the scanning tunneling spectra (\( dI/dV \)), two peaks were observed at about -0.07 eV and -0.3 eV on both Co\(_3\)Sn plane and Sn plane. The peak at -0.07 eV corresponds well to the other peak reflects the flat band at about -0.3 eV below \( E_F \).

In order to study the orbital characters of the Dirac-like bands and the flat bands, we performed orbital-resolved DFT and dynamical mean-field theory (DMFT) calculations. Results of DFT calculation with SOC and DFT+DMFT calculation without SOC along high-symmetry directions are shown in Figs. 4(a) and 4(b), respectively. The SOC induced band gaps and \( 3d \) orbital projections are shown in the plots of DFT.
calculation results. Compared with calculated and observed low-energy band structures in other 3d transition AFM or FM Kagome metals \[5,6,9,11,12,14,15\], the calculated bands of CoSn are simpler and more accurate due to nonmagnetism and weak electron correlation, ideal for studying the intrinsic behavior of the Kagome metals. These calculations indicate a metallic CoSn with an electron-like FS at BZ center, and a nearly flat top of the hole-like band below \(E_F\) at BZ corner. Comparing to calculated bands, an extra electron-like band at \(\Gamma\) point in ARPES data [the \(\delta\) band in Figs. 3(e) and 4(e)] should be a shadow of the band above \(E_F\), as the calculated band at \(A\) and \(\Gamma\) point just above \(E_F\) in Fig. 4(b).

Several sets of typical Kagome bands with their orbital characters are illustrated in Fig. 4(b). On \(\Gamma-K-M\) plane, the calculated bands is consistent well with the ARPES measurements. Two close Dirac cones at binding energy of \(-0.6\) eV at \(K\) point originate mainly from in-plane \(d_\sigma/d_{2\gamma-2}\) (red) and out-of-plane \(d_{\sigma z}/d_{\sigma z}\) (green) orbitals, respectively, corresponding to ARPES data in Figs. 3(d) and 4(e). The flat band at binding energy of \(-0.27\) eV with \(d_{\sigma z}/d_{\sigma z}\) orbital character is more prominent along \(\Gamma-M\) and \(\Gamma-A\) (\(k_z\) lines), corresponding to ARPES data in Fig. 3. Moreover, the electron-like band at \(\Gamma\) point extends to \(K\) point and forms Dirac cone above \(E_F\), as mentioned in Fig. 2. On \(A-H-L\) plane, the cone with \(d_{\sigma z}/d_{2\gamma-2}\) orbital characters ascends, the cone with \(d_{\sigma z}/d_{\sigma z}\) orbital characters descends to higher binding energy. The former caps a hole-like band with an utmost flat top, which locates around \(H(\bar{K})\) point at binding energy of \(-0.07\) eV, corresponding to ARPES data in Figs. 3(f) and 2. While, the \(d_{\gamma 2}\) (blue) orbital mainly contributes a typical Kagome band around \(k_z \sim \pi\) plane, showing a strong three-dimensional character. Comparing to calculated bands on the \(A-H-L\) plane, the measured cones at the \(H\) point [Fig. 1(f)] shift up about 0.1 eV possibly due to stronger electronic correlation induced by the extra band of \(d_{\gamma 2}\) than on the \(\Gamma-K-M\) plane.

Under the protection of time-reversal and spatial-inversion symmetry (\(T\cdot P\) symmetry), and a certain mirror symmetry \([\sigma_y\text{ in Fig. 1(b)}\)], the two cones at the \(K\) point form two nodal lines along the \(k_z\) direction when the SOC is neglected [Figs. S5-26]. With the inclusion of SOC, the two cones opening the energy gaps of \(-96.5\) meV \((d_{\gamma 2}/d_{2\gamma-2})\) and \(-8\) meV \((d_{\gamma z}/d_{\gamma z})\) in the DFT calculations [Fig. 4(a)], respectively, show that the strengths of SOC of in-plane orbitals are much stronger than that of out-of-plane orbitals, indicating an orbital-selective character of the SOC strength.

Based on the above experimental and calculational findings, we propose that a two-orbital model \[26\] can be used to describe the extremely flat band of \(d_{\gamma z}/d_{\gamma z}\) orbital. From DFT and DFT+DMFT calculations along \(k_z\) (\(\Gamma-A\) direction), we know that \(d_{\gamma z}/d_{\gamma z}\) bands are quite two-dimensional in the vicinity of \(E_F\). Hence, we can safely write down an effective model inside the Kagome plane. Based on \(D_{hh}\) point group and by including hopping integrals into second nearest neighbors, the two orbital model with \(d_{\gamma z}/d_{\gamma z}\) orbital can be constructed as \(H = H_{1N} + H_{2N} + H_{soc}\), where the \(H_{1N}\) and \(H_{2N}\) describe the nearest-neighbor and second nearest-neighbor hopping respectively. \(H_{soc}\) is the atomic SOC. We obtained that a nearly flat band passes through the whole BZ and features in touch with a quadratic band at BZ center [Fig. S7(b) \[26\]]. The degeneracy at \(\Gamma\) can further be lifted by introducing SOC [Fig. S7(c) \[26\]].

We have unambiguously demonstrated the existence of sets of typical Kagome bands with their orbital characters in the nonmagnetic Kagome CoSn. Without complication from magnetism and strong electronic correlation effect, the electronic bands of CoSn are much simpler than in other Kagome metals, and exhibit more intrinsic band structures of Kagome metals both experimentally and theoretically. Experimental observation of the extremely flat band over the whole BZ and in touch with the quadratic band at the BZ center in CoSn is crucial. This key feature of the Kagome flat band in the fundamental Kagome model has been long sought by experiments. Additionally, the flat band top near \(E_F\) could induce
instabilities such as superconductivity or ferromagnetism at even high temperature, if the chemical potential were tuned properly. On the other hand, the band gap induced by SOC at the Dirac cone with \( d_{xy}/d_{xz}\) orbital characters is much smaller than that with \( d_{xy}/d_{x^2−y^2}\) orbital characters, and induces an orbital-selective Dirac fermions in topological low-energy excitations. With explicitly typical Kagome bands, CoSn not only plays a significant role in solving fundamental puzzles of Kagome physics, but also provides an ideal platform for further investigation and potential application on Kagome metals.

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Methods

Sample growth and characterization. High quality single crystals of CoSn were synthesized by the Sn flux method. The starting elements of Co (99.99%), Sn (99.99%) were put into an alumina crucible, with a molar ratio of Co : Sn = 3 : 20. The mixture was sealed in a quartz ampoule under partial argon atmosphere and heated up to 1173 K, then cooled down to 873 K with 2 K/h. The CoSn single crystals were separated from the Sn flux by using centrifuge. The samples were characterized by powder X-ray diffraction (XRD) and transport measurements, including temperature dependence of resistivity and magnetic susceptibility, and field dependence of magnetization, as shown in Figs. S1–S3.

ARPES experiments. ARPES measurements were performed at Dreamline and 03U beamlines of Shanghai Synchrotron Radiation Facility (SSRF). Experimental setup is shown in Fig. S4. Samples were cleaved in situ, yielding a flat mirror-like (001) surface. During measurements, the temperature was kept at \( T = 20 \) K. The pressure was maintained greater than \( 5 \times 10^{-11} \) Torr.

STM/S experiments. STM experiments were carried out with a Unisoku low-temperature STM at the base temperature of 4.3 K. CoSn single crystal samples were cleaved in situ under ultra-high vacuum and transferred immediately into STM head under the vacuum of \( 2 \times 10^{-10} \) Torr. STS measurements were done by using standard lock-in technique with 5 mV modulation at the frequency of 914 Hz.

Band calculations. The electronic structures of CoSn in the nonmagnetic and paramagnetic states are calculated with density functional theory (DFT) and in combination with dynamical mean field theory (DFT+DMFT). For the density functional theory calculations, we used the full-potential linear augmented plane wave method implemented in Wien2K\cite{27} in conjunction with Perdew-Burke-Ernzerhof generalized gradient approximation\cite{28} of the exchange correlation functional. DFT+DMFT is implemented on top of Wien2K and documented in Ref. \cite{29}. In the DFT+DMFT calculations, the electronic charge was computed self-consistently on DFT+DMFT density matrix. The quantum impurity problem was solved by the continuous time quantum Monte Carlo (CTQMC) method\cite{30,31}, at a temperature of 116 K and with a Hubbard \( U=5.0 \) eV and Hund’s rule coupling \( J=0.8 \) eV in the paramagnetic state. The same values as we used for many iron-based compounds\cite{32–34}. The experimental crystal structure (space group P6/mmm, No. 191) of CoSn with lattice constants \( a=b=5.275 \) Å and \( c=4.263 \) Å was used in the calculations.

Author contributions

Z.L., Z.Y., H.L., and S.W. provided strategy and advice for the research. Z.L., M.L., X.L., Y.H., D.S., and S.W. performed ARPES measurements; C.W., and S.Y. performed STM measurements; G.W., and Z.Y. carried out DFT and DFT+DMFT calculations; K.J., J.Y., and Z.W. proposed theoretical model; Q.W., and H.L. synthesized the single crystals. All authors contributed to writing the manuscript.

Competing interests

The authors declare that they have no competing financial interests.

Data availability

The authors declare that the main data supporting the findings of this study are available within the paper and its Supplementary Information files. Extra data are available from the corresponding authors upon request.

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