Dirac cone, flat band and saddle point in kagome magnet YMn₆Sn₆

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Kagome-lattices of 3d-transition metals hosting Weyl/Dirac fermions and topological flat bands exhibit non-trivial topological characters and novel quantum phases, such as the anomalous Hall effect and fractional quantum Hall effect. With consideration of spin-orbit coupling and electron correlation, several instabilities could be induced. The typical characters of the electronic structure of a kagome lattice, i.e., the saddle point, Dirac-cone, and flat band, around the Fermi energy (E_F) remain elusive in magnetic kagome materials. We present the experimental observation of the complete features in ferromagnetic kagome layers of YMn₆Sn₆ helically coupled along the c-axis, by using angle-resolved photoemission spectroscopy and band structure calculations. We demonstrate a Dirac dispersion near E_F, which is predicted by spin-polarized theoretical calculations, carries an intrinsic Berry curvature and contributes to the anomalous Hall effect in transport measurements. In addition, a flat band and a saddle point with a high density of states near E_F are observed. These multi-sets of kagome features are of orbital-selective origin and could cause multi-orbital magnetism. The Dirac fermion, flat band and saddle point in the vicinity of E_F open an opportunity in manipulating the topological properties in magnetic materials.

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he frustrated kagome lattice, made up of the geometry of corner-sharing triangles, has been studied intensively due to the magnetic frustration-induced quantum spin liquid state. Meanwhile, the construction of topological band theory in recent years has greatly enriched in the electronic band structure of kagome lattice. Theoretical studies show the kagome lattice systems as an ideal platform for understanding the topological states with novel topological excitations. For example, a flat band (FB) can be constructed by completely destructive interference of Bloch wave functions in two-dimensional (2D) kagome lattice with nearest-neighbor (NN) interaction. Such FBs, just like a counterpart of the Landau level, can be characterized by a Chern number. Representing a highly degenerate and quenched kinetic energy of electron state may give rise to the abundant exotic emergent effects, such as ferromagnetism, high-temperature superconductivity, Wigner crystal, and fractional quantum Hall effects. Besides, the kagome lattice system shares similar topological physics with honeycomb, Dirac cone-type dispersions in the momentum-space in the vicinity of $K$ point, a saddle point at BZ boundary, and a FB over the whole BZ. They show negligible $k_z$ dispersion, suggesting the major 2D characters of the kagome structure constituted of 3d-transition metallic element, i.e., large intrinsic anomalous Hall effect originating from the Berry curvature of Dirac cone-type dispersion of K point both in ferromagnetic (FM) and antiferromagnetic (AFM) materials. Another important feature is the dispersionless electronic structure in magnetic kagome materials and paramagnetic (PM) kagome materials. In PM kagome materials, extremely flat bands close to $E_F$ have been reported in CoSn$_2$, Co$_3$Sn$_2S$_2, and YCr$_6$Ge$_6$. However, in magnetic systems, the direct evidence of the FBs is either unobserved (Fe$_3$Sn$_2$, FeSn$_2$, CoSn$_2$, Co$_3$Sn$_2S$_2), or far away from $E_F$ (FeSn$_2$), due to the strong correlation of 3d electrons, the complexity with magnetic structure, and the interplay between electron correlation and topological properties. Thus, searching for the flat band, and saddle point, in addition to the Dirac fermion near $E_F$ in magnetic kagome systems serves as the main objective to manipulate the topological properties in magnetic materials.

In this paper, we study the electronic structure of kagome lattice YMn$_6$Sn$_6$ with in-plane ferromagnetism and helical antiferromagnetism along $c$-axis by combining angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT + DMFT) calculations. We report the first experimental observation of the complete characters of kagome electronic structure: Dirac cone, flat band, and saddle point, in such a magnetic system. One complete set of the characteristic of kagome lattice includes a Dirac point (DP1) above $E_F$, a saddle point (SP1) near $E_F$ and a flat band (FB1) located at ~0.4 eV below $E_F$ across the whole BZ. They show negligible $k_z$ dispersion, suggesting the major 2D characters of the kagome structure in YMn$_6$Sn$_6$. The DFT + DMFT calculations with orbital-resolved electronic structures further confirm the 2D features with the in-plane orbital composition of $d_{xy}/d_{x^2-y^2}$. Moreover, we detected the existence of extra kagome characters, including a Dirac point (DP2) and a flat band (FB2) in the vicinity of $E_F$. The DP2 has a $d_{xy}/d_{x^2-y^2}$ with mixture of $d_{z^2}$ orbital.

**Fig. 1** Crystal and electronic structures of YMn$_6$Sn$_6$. a Confinement of electron eigenstate induced by destructive interference in kagome lattice with NN hopping. b Tight-binding calculation of band structure of kagome lattice with NN in-plane hopping without SOC, featuring the Dirac cone at the BZ corner $K$ point, a saddle point at BZ boundary $M$ point, and a FB over the whole BZ. c Crystal structure of YMn$_6$Sn$_6$ with space group $P6/mmm$ (No. 191). d 3D and projected BZs of YMn$_6$Sn$_6$ with marked high-symmetry points. e Photoemission intensity plot measured with 138-eV photons at $E_F\pm 10$ meV in the $k_z$ = 0 plane. Hexagonal BZs are marked with red lines. f Magnetization as a function of temperature with zero field-cooling and field-cooling at $B = 0.5$ T along the [100] direction. Temperature dependence of longitudinal resistivity $\rho_{xx}$ and $\rho_{zz}$ with zero-field.
character, and presents a weak dispersion along \( k_z \), while the FB2 becomes more clearly seen in second derivative plots (Fig. 2b). This \( \beta \) band shows a little variation, further confirming the speculation of the orbital characters in the \( \alpha \) band. Moreover, the temperature dependence of longitudinal resistivity \( \rho_{xx} \) and \( \rho_{zz} \) with zero-field shows a metallic behavior with weak anisotropy, similar to GdMn\(_6\)Sn\(_6\) [40].

**The complete characteristics of kagome structure.** In order to investigate the kagome lattice related topological electronic structure, we measured the band structures in the 1st BZ at \( E_F \sim 0 \) plane along with the high-symmetry lines. The intensity plots along the \( \Gamma–K–\Gamma \) line and the corresponding second derivative plots are shown in Fig. 2a, b, respectively. Along \( \Gamma–M \), one can clearly see a quadratic band (QB) with its bottom at about 0.4 eV below \( E_F \) at \( \Gamma \) dispersing upward towards \( M \), and gradually becoming flat at the \( M \) point. Along \( M–K \), an electron-like band disperses linearly upward towards \( E_F \) and across \( E_F \) about one third between \( M \) and \( K \), forming the \( \beta \) FS in Fig. 1c. At \( M \) point, it conforms to the dispersion of SP1 at \( E_F \sim 40 \) meV, as marked in Fig. 2b. From intensity plot along \( \Gamma–K–\Gamma \), the \( \beta \) band passes through the \( E_F \), forming a large holelike FS around \( K \) point, which can be more clearly seen in second derivative plots (Fig. 2b). This \( \beta \) band forms a Dirac point (DP1) at about 0.3 eV above \( E_F \) by linear extrapolation, as indicated by the blue circle in Fig. 2c. Another feature is a flat band at about 0.4 eV below \( E_F \), FB1, which exists through the whole BZ. It can be regarded as a direct consequence of quantum phase interference effects in the kagome lattice, as shown in Fig. 1a. This flat band feature has a narrow bandwidth and the intensity is more visualized along \( \Gamma–K \) due to the matrix element effect. The band dispersion closely follows the DFT + DMFT calculations shown in Fig. 2c. In particular, it exhibits the complete characteristics of kagome electronic structure, a flat band (FB1) over the whole BZ touching a quadratic band at \( \Gamma \) point that emerges from the Dirac band (DP1) at \( K \) point and forms a saddle point (SP1) at \( M \).

At the \( K \) point, a linearly dispersing Dirac point (DP2) is found at around 45 meV below \( E_F \), which is also characteristic of the band structure as a result of kagome lattice similar as previously observed in FeSn and CoSn [25,29,29]. According to our DFT + DMFT calculated orbital-resolved electronic structures in FM configuration, the DP2 belongs to the spin-polarized band with minority-spin state, as shown in the Supplementary Fig. 5. The DP2 can also be clearly seen from the momentum distribution curves (MDCs) and energy distribution curves (EDCs) in Fig. 2f, g, respectively. With consideration of SOC, a small bandgap <10 meV will open at DP2, adding a mass term to the linearly dispersive band, and a massive Dirac fermion thus can be formed. In consideration of in-plane FM configuration, it could realize a spin-polarized Dirac fermion with a non-trivial Chern gap in YMn\(_6\)Sn\(_6\) as previously observed in TbMn\(_6\)Sn\(_6\) by scanning tunneling microscopy/spectroscopy (STM/S) measurement [18]. In our result, this non-trivial Dirac fermion is in the occupied state and closer to \( E_F \) than in TbMn\(_6\)Sn\(_6\), and contributes to the intrinsic anomalous Hall effect at high magnetic field in transport measurement [34].

Figure 2b shows a series of constant energy evolution maps in the \( k_z \sim 0 \). We notice that the \( \beta \) band constitutes a hole pocket and the \( \alpha \) band holds an electron pocket around \( K \) point. Along with the energy going from \( E_F \) to higher binding energy, the hole pockets gradually expand and the branches of \( \beta \) band get closer to each other along \( K–M–K \), finally touching at SP1 with the binding energy \( \sim 40 \) meV. Further away from the energy, the band forms a hole band along \( \Gamma–M \). At \( M \) point, the band dispersion conforms a saddle point at \( \sim 40 \) meV below \( E_F \). The \( \alpha \) pocket firstly shrinks into a single point at \( K \) and then expands forming a Dirac point at about \( E_F \sim 45 \pm 10 \) meV.

In Fig. 3a, b, we show the ARPES data along \( \Gamma–K–M–K \) with photon energies from 70 to 180 eV, which covers near four BZs along \( k_z \). In Fig. 3a, one can see that the band dispersions show no qualitative change at various photon energies. Especially, the \( \beta \) band shows no noticeable \( k_z \) dependence, which is also identified by the constant crossing point of \( k_{F\beta} \) in Fig. 3b. The FB1 at about 0.4 eV below \( E_F \) is also presented in every photon energy, with a limited bandwidth (does not exceed 150 meV) along \( \Gamma–A \) as shown in Fig. 3d, indicating a near 2D character of the band. Figure 3b shows the integrated intensity at \( E_F \pm 10 \) meV in TK–AH plane which covers part of \( K–M–K \) at extended in-plane BZs. The \( \beta \) band shows a little variation, further confirms the 2D-like character and ensures the 2D Dirac cone of DP1. The Dirac-related \( \alpha \) band around \( K \) also displays a negligible dispersion along \( k_z \), which has intensity modulation associated with matrix element effect, similar to FeSn and CoSn [25,29]. The \( k_z \) dependence supports the quasi-2D characters of the DP1, DP2, and FB1 bands. An explanation to the 2D-like band structure is that the bands mainly originate from the orbitals confined by the kagome lattice.

To confirm the speculation of the orbital characters in the helical magnetic state along \( c \)-axis, we carry out the DFT + DMFT calculations in FM configuration with SOC and show the results in Fig. 3e and (in Supplementary Fig. 4). In the DFT + DMFT calculated spectra, we downshift the chemical potential of 76 meV to match the experiment value \( E_{\text{exp}} \) mostly caused by a chemical doping of the sample. The calculations in the FM
configurations agreed well with the observation, the orbital-resolved ARPES without SOC shows that the $\beta$ band mainly originates from the minority-spin branch of $d_{x^2-y^2}$ orbitals (Supplementary Fig. 5). The DP1 locates at $-0.3$ eV above $E_F$ and shows negligible dispersion along $K-M$ as shown in Fig. 3e. The FB1 passing through the whole in-plane BZ originates from the minority-spin branch of the in-plane $d_{x^2-y^2}$ orbitals, and has a limited bandwidth at the entire BZ district.

**Signature of phase-destructive flat band near $E_F$.** A feature that is faint in the 1st BZ but more clearly visible in the 2nd BZ is the existence of another flat band near $E_F$ at the BZ center, labeled as FB2 in Fig. 4. In Fig. 4a, the ARPES intensity plots and the corresponding second derivative plots along the $\Gamma-M-K-\Gamma$ lines of the 2nd BZ at $k_z \approx 0$ plane are shown. In the 2nd BZ, a spectral weight close to $E_F$ with binding energy $-60 \pm 20$ meV is clearly seen and extends over a large part of the BZ except around the $K$ points due to the intensity leakage from the Dirac bands. In comparison, the intensity of the $\beta$ and FB1 bands are stronger in the 1st BZ but become feeble in the extended BZ. We assign the contrasting behaviors between FB2 and $\beta$ bands to the Brillouin-Zone-selection effects that show the different signal intensity in the first BZ and extended BZ$^{16,37}$ due to the different parity, symmetries or spin-polarization of the bands. In Fig. 4b, we present the DFT + DMFT calculations of the band structure in the FM state with SOC, with a downshift adjustment of the chemical potential of 76 meV as in Fig. 3e. Figure 4c, d show EDC plots over more than one BZ along the high-symmetry line as marked in the insets. The contrast of the intensity among different BZs is shown, and the flat bands (FB1 and FB2) and the Dirac point (DP2) can be confirmed unambiguously. For the FB1, it is predicted to degenerate with the QB at the center of the BZ ($\Gamma$) without SOC. With the consideration of SOC, the two bands further hybridize and open a gap $\sim 40 \pm 10$ meV, which is similar to the results in PM CoSn$_2$. The FB2 declines weakly close to $M$ and $K$ points. It is noticed that the peak width becomes broader and the intensity becomes weaker near $M$ and $K$ points, which cause the expected Dirac points feature blurry and nearly indistinguishable, in agreement with the DFT + DMFT calculations in Fig. 4b. In conventional DFT calculations, there should be more band features in magnetic state, and several kagome-related structures are expected. However, in the DFT + DMFT calculations with consideration of the correlation effect which is normally present in the magnetic system, the broadness and the weaker intensity cause the smearing out of the band, the ARPES measurements normally observe fewer bands than DFT predictions, i.e., some band features around $M$, $K$, and along $M-K$.

We also present the evolution of the FB2 as a function of out-of-plane momentum $k_z$ measured in the in-plane-2nd-BZ along $\Gamma-A'$ as shown in Supplementary Fig. 3. The FB2 displays a weak dispersion over more than one BZ along $k_z$. Combining its in-plane flat dispersion in the $k_z \approx 0$ plane, weak dispersion along $k_z$, and the DFT + DMFT calculated orbital-resolved ARPES as shown in Supplementary Fig. 5, we assign the orbital character of FB2 to $d_{x^2-y^2}$ orbitals. It is worth notice that there exists an
out-of-plane $d_{z^2}$ orbital with a steep $k_z$ dispersion and crossing $E_F$ at certain $k_z$, it thus might contribute to the $c$-axis conductivity in our transport measurements. Further, the FB1 displays a limited bandwidth (<150 meV) along $k_z$ in the 2nd BZ as shown in Supplementary Fig. 3. It is consistent with results in the 1st BZ with the in-plane $d_{xy}/d_{x^2-y^2}$ orbital composition, as discussed earlier. According to the spin-polarized DFT + DMFT calculations, FB2 with a high density of states (DOS) around the $E_F$ is from the majority-spin state, indicating its singly spin degenerate origin. FB2 is the first momentum-space evidence of the flat band really close to $E_F$ in the magnetic kagome system, which could give interesting phenomena such as orbital magnetism.

The band calculations. To take into account the strong electronic correlation effect of the Mn 3$d$ electrons, in the DFT + DMFT calculations, we include an onsite Coulomb interaction parametrized with a Hubbard $U = 4.0$ eV and a Hund’s coupling $J = 0.7$ eV among the Mn 3$d$ electrons in both the PM and FM states. In the PM state, the mass enhancements of the Mn 3$d$ electrons near the $E_F$ are about 5–7, which are similar to the values in some iron chalcogenide superconductors. The fluctuating local moment of Mn 3$d$ electrons, namely, the average value of $g[S(S+1)]^{1/2}$, is about 3.9 $\mu_B$ with an effective spin $S = 1.5$, indicating YMn$_6$Sn$_6$ has a large fluctuating local moment due to the Hund’s rule coupling. Combining with its metallic behavior, we conclude that YMn$_6$Sn$_6$ is a strongly correlated Hund’s metal.

When the Mn 3$d$ local moments are partially frozen and form long-range static FM order in the hexagonal $ab$ plane, the mass enhancements of the Mn 3$d$ electrons near the $E_F$ are substantially reduced to about 2–3. The fluctuating local moment of Mn 3$d$ electrons remains the same value as in the PM state whereas the statically ordered moment is 2.1 $\mu_B$, which is in excellent agreement with experimental measurement.

Discussion
In the PM state, the YMn$_6$Sn$_6$ has two major characters, including the strong electronic correlation and the kagome related features. The kagome structure has a flat band, while the strong correlation gives extra mass enhancement. These combinations will contribute large DOS around $E_F$ and could cause several instabilities, such as charge density waves, superconductivity, or magnetic instability. In the magnetic state, the spin degeneracies are lifted, and a few spin-polarized branches shift below $E_F$.

ARPES data reveal the existence of flat band with large DOS and Dirac point near $E_F$ in YMn$_6$Sn$_6$, these bands are thus of singly...
spin degenerate branches. With consideration of SOC, Chern gaps are opened and Chern numbers are assigned to each band correspondingly.

YMn$_6$Sn$_6$ possesses a ferromagnetic bilayers which anti-ferromagnetically couple with neighboring bilayers. At low temperature, it exhibits an incommensurate magnetic phase along $c$-axis. With the breaking of the combined symmetry of inversion and time-reversal symmetry $PT$, the electron bands become spin-polarized. In order to confirm the spin configuration of individual bands and the corresponding flat band and Dirac point (Weyl point), further spin-polarized ARPES measurements are needed.

These spin-polarized bands carry Berry curvatures and also cause the orbital magnetism. The existence of an orbital magnetic moment has been reported in Co$_2$Sn$_2$S$_2$, and was attributed to the kagome flat band. However, the ARPES observation of flat band near $E_F$ has not been reported in Co$_2$Sn$_2$S$_2$ yet. The orbital magnetism of the flat band of tight-binding model in kagome lattice with Kane–Mele SOC was calculated in Supplementary Fig. 7, which is closely related to the Berry curvature. Both the flat band with non-zero group velocity part and the massive Dirac fermion will contribute to the orbital magnetism. Our ARPES results first reveal FB and Dirac fermion near $E_F$ with orbital-selective characters, so multiorbital-magnetisms are expected.

In summary, based on ARPES measurement and in combination with theoretical calculations, we have fully revealed the band structure of magnetic kagome YMn$_6$Sn$_6$, and presented the first experimental observation of the complete characteristics of kagome lattice near $E_F$ with spin polarization and non-trivial topological properties. The Dirac point and flat band near $E_F$ arise from the spin-polarized band with intrinsic Berry curvature may explain the anomalous Hall effect observed in transport measurements, and the orbital magnetic moment observed in STM/S measurement. As an ideal candidate for magnetic kagome lattice material with the electronic structure near $E_F$, it opens up a new avenue to comprehend the intrinsic properties of magnetic topological electronic material. Furthermore, if the non-trivial band structures–Dirac points, flat band and/or saddle point are further tuned properly, it would possibly realize more versatile quantum phenomena in such material.

Methods
Sample growth and characterizations. Single crystals of YMn$_6$Sn$_6$ were grown by using Sn flux. Y lumps (purity 99.99%), Mn granules (purity 99.9%), and Sn grains (purity 99.9%) with a molar ratio of Y: Mn:Sn = 1:6:30 were put into an alumina crucible and sealed in a quartz ampoule under partial argon atmosphere. The sealed quartz ampoule was heated up to 1273 K and held for 24 h. Then it was cooled down slowly to 873 K at a rate of 5 K/h. Finally, the ampoule was taken out from the furnace and decanted with a centrifuge to separate YMn$_6$Sn$_6$ crystals from excess Sn flux. Magnetization and electrical transport measurements were carried out by using Quantum Design PPMS-14 T.

ARPES measurements. ARPES measurement were performed at the Dreamline and 63U beamline of the Shanghai Synchrotron Radiation Facility (SSRF), and 1-squared ARPES end-station of BESSY. The optimal energy and angular resolutions were set to 20 meV and 0.2°, respectively. Samples were cleaved in situ along (001) surface. During the measurements, the temperature was kept at 25 K and the pressure was maintained less than 5 x 10$^{-11}$ Torr.

DFT + DMFT calculations. The electronic structures of YMn$_6$Sn$_6$ were computed by using DFT + DMFT. The DFT part is based on the full-potential linear augmented plane wave method implemented in WIEN2k. The Perdew–Burke–Ernzerhof generalized gradient approximation is used for the exchange correlation functional. DFT + DMFT was implemented on top of WIEN2k and was described in detail. 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 method with Hubbard $U = 4.0$ eV and Hund’s rule coupling $J = 0.7$ eV. The experimental crystal structure (space group P6/mmm, No. 191) of YMn$_6$Sn$_6$ with lattice constants $a = b = 5.512$ Å and $c = 8.984$ Å was used in the calculations.

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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**Author contributions**

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**Competing interests**

The authors declare no competing interests.
