Dirac Fermions in Antiferromagnetic FeSn Kagome Lattices with Combined Space Inversion and Time Reversal Symmetry

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Symmetry principles play a critical role in formulating the fundamental laws of nature\textsuperscript{1}, with a large number of symmetry-protected topological states identified in recent studies of quantum materials\textsuperscript{2,3}. As compelling examples, massless Dirac fermions are jointly protected by the space inversion symmetry $P$ and time reversal symmetry $T$ supplemented by additional crystalline symmetry\textsuperscript{4-8}, while evolving into Weyl fermions when either $P$ or $T$ is broken\textsuperscript{4,9-11}. Strikingly, such massless Dirac fermions are expected to survive when each of the $P$ and $T$ symmetries is individually broken but the combined $PT$ symmetry is preserved\textsuperscript{12}. To date, this conceptually intriguing prediction remains to be experimentally validated. Here, based on angle-resolved photoemission spectroscopy (ARPES) aided by first-principles calculations, we present the first experimental observation of massless Dirac fermions in a layered FeSn crystal containing
antiferromagnetically coupled ferromagnetic Fe kagome layers. In this system, each of the $P$ and $T$ symmetries is individually broken, but the stable Dirac points are protected by the combined $PT$ symmetry with additional non-symmorphic $S_{2z}$ symmetry. We further demonstrate that by breaking the $PT$ or $S_{2z}$ symmetry, we can transform the massless Dirac fermions into massless Weyl or massive Dirac fermions. The present study substantially enriches our fundamental understanding of the intricate connections between symmetries and topologies of matter, especially with the spin degree of freedom playing a vital role.

Topological materials have been extended to include gapless systems that are characterized by the nontrivial topology of bulk bands and its associated robust surface states. Such topological semimetals host electronic structures with linear band-contact nodes or lines\textsuperscript{4-8,13,14}. Existing studies of three-dimensional (3D) Dirac semimetals have been primarily restricted to nonmagnetic materials\textsuperscript{4-8} with both $T$ and $P$ symmetries, where the electronic bands are doubly degenerate at each momentum and two of such doubly degenerate bands accidentally cross to form a Dirac point. This four-fold degenerate Dirac point can be stable against spin-orbit coupling (SOC) under additional crystalline symmetry such as glide mirror symmetry or screw rotation symmetry\textsuperscript{4,15,16}. Recently, Shou-Cheng Zhang and his colleagues presented the conceptually intriguing proposal that Dirac fermions can also be hosted even in antiferromagnetic (AFM) materials, where both $T$ and $P$ are broken but their combination $PT$ is respected\textsuperscript{12}. However, experimental realization of the Dirac fermions in realistic AFM systems remains to be accomplished.

The kagome lattices have attracted much attention for the emergence of both linearly dispersive bands and dispersionless flatbands\textsuperscript{17-22}. In Fe$_3$Sn$_2$ containing ferromagnetic (FM) kagome lattices, an ARPES experiment reported the existence of massive Weyl states\textsuperscript{20}. Meanwhile, in Mn$_3$Sn containing AFM kagome lattices\textsuperscript{19} and Co$_3$Sn$_2$S$_2$ containing FM kagome lattices\textsuperscript{22}, massless Weyl states were experimentally measured. Here, we demonstrate the first experimental realization of stable Dirac points in the AFM FeSn system with $PT$ symmetry.

Figure 1a shows the structure of FeSn consisting of stacked Fe$_3$Sn kagome and Sn honeycomb layers, where Fe atoms form a kagome lattice. The X-ray diffraction (XRD) pattern of FeSn single crystal validates its high crystalline quality (Fig. 1b). Specifically, the cross-sectional transmission electron microscopy (TEM) image of the (210) plane reveals the well-ordered layer-stacked atoms in Fe$_3$Sn
and Sn layers (Fig. 1c). The FeSn(001) surface is shown to be terminated by Sn layer, by means of combined scanning-tunneling-microscopy (STM) imaging and density-functional-theory (DFT) calculations (see Fig. 1d, Extended Data Fig. 1 and Supplementary Note 1).

Earlier neutron diffraction and Mössbauer experiments\textsuperscript{23,24} reported that FeSn has an AFM coupling of adjacent Fe\textsubscript{3}Sn layers with a Néel temperature $T_N \approx 367$ K. The magnetization in each Fe\textsubscript{3}Sn kagome lattice was measured to point along the [3.732,1,0] direction\textsuperscript{24}, as shown in Extended Data Fig. 3. Our measured magnetization as a function of temperature shows a peak at $T_N \approx 366$ K (Fig. 1e), consistent with previous results\textsuperscript{23,24}. This observed AFM order is supported by our DFT calculations (see Extended Data Fig. 4 and Supplementary Note 2).

The low-energy electronic structure of the FeSn(001) surface was measured by ARPES. We employed large photon energies ranging from 90 to 160 eV to acquire the ARPES data between the K-$\Gamma$-K’ and H-A-H’ lines, which enable us to examine the bulk states. Figure 2a shows the ARPES data of photon energies between 105 eV and 130 eV, representing the energy bands from $k_z = 0$ (Fig. 2b) to $k_z = \pi/c$ (Fig. 2c) (see Extended Data Fig. 5 and Supplementary Note 3). There exist two linearly dispersive band crossings at the K and K’ points around 0.4 eV below $E_F$. Remarkably, the positions of these Dirac points are nearly identical with increasing photon energy, implying nodal lines along the K-H and K’-H’ lines. Due to the limited energy resolution of ARPES, at this stage we cannot resolve whether the observed Dirac points and nodal lines are gapped or gapless.

To provide an interpretation of the ARPES data, we performed DFT calculations for the band structure of bulk FeSn. The calculated band structure in the absence of SOC shows that all the spin-up and spin-down bands are degenerate with each other because of $PT$ symmetry. As shown in Fig. 2d, there are two Dirac nodal lines (DNLs) DNL\textsubscript{1} and DNL\textsubscript{2} along the K-H line around -0.4 eV. Since the crystalline symmetry of FeSn belongs to the space group P6/mmm (No. 191) with the point group $D_{6h}$, two additional DNLs also exist along the K’-H’ line. It is noted that along the K-H and K’-H’ lines, the system has the three-fold rotational symmetry $C_{3z}$ around the $z$ axis, and $PT$ symmetry, thereby preserving the four-fold degeneracy of the DNLs in the absence of SOC\textsuperscript{12,25}. As shown in Fig. 2g and 2h, the band-touching point H along DNL\textsubscript{1} exhibits a singularity of the Berry curvature. Further, the topological $Z_2$ index, defined as $\zeta_i = \frac{1}{\pi} \oint dk \cdot A(k)$ where $A(k) = -i <u_k|\partial_k|u_k>$ is the Berry connection.
of Bloch bands, along a closed loop encircling each DNL is calculated to be $\pm 1$, indicating that the DNLs are stable against perturbations without breaking the $C_{3z}$ and $PT$ symmetries.

Meanwhile, the bulk band structure with including SOC reveals that the four-fold degeneracy at the band-crossing points along the K-H (K’-H’) line is lifted, but is still preserved at the H (H’) point (see Fig. 2e and 2i). Consequently, the SOC gaps of less than $\sim$30 meV appear along the DNLs, and the massless Dirac points exist at the H and H’ points. Since magnetization is parallel to the [3.732,1,0] direction as observed by experiment\textsuperscript{24}, the system has the magnetic point group of $D_{2h}$, which contains a two-fold screw rotation along the $z$ axis ($S_{2z}$) and $PT$ symmetries. Such a non-symmorphic symmetry $S_{2z}$ (equivalent to the combination of $C_{2z}$ and a half translation along the $z$ direction) protects the Dirac points at the Brillouin zone boundary points H and H’\textsuperscript{4,12,15}. Thus, the AFM FeSn hosts the massless Dirac states even in the presence of SOC.

Figures 2b and 2c show that the ARPES spectra with 105- and 130-eV photon energies are well reproduced by the DFT bulk bands at $k_z = 0$ and $\pi/c$, respectively. We note that there are some extra electronic states near $E_F$ (see Fig. 2a-c), which mainly arise from the topmost Fe$_3$Sn layer, as discussed below. In particular, the bulk Fermi surface measured with a 130-eV photon energy (Fig. 2k) is in excellent agreement with that obtained from the SOC-included DFT calculation (Fig. 2l). Compared to the ARPES spectra with a 105-eV photon energy (Fig. 2b), that with a 130-eV photon energy exhibits more Dirac-like bands below -0.4 eV as well as some fuzzy features around the A point (Fig. 2c). This difference between the two ARPES spectra can be explained by the DFT results: i.e., (i) DNL$_1$ and DNL$_2$ in Fig. 2d are close to each other at the K (K’) point but separated by $\sim$0.2 eV at the H (H’) point, and (ii) multiple bands with the concave-upward and concave-downward dispersions appear around the A point (see the orange lines in Fig. 2c).

It is noteworthy that the symmetry protection of Dirac points in FeSn can be manipulated via spin reorientation. Our SOC-included DFT calculations show that, when the spin orientations are still in the (001) plane, i.e., along the [210], [110] directions, the gapless Dirac points at the H and H’ points are preserved (see Extended Data Fig. 6). However, as shown in Fig. 2f and 2j, the calculated band structure with the [001] spin orientation perpendicular to the (001) plane opens a gap of $\sim$70 meV at the H and H’ points, due to breaking of the non-symmorphic symmetry $S_{2z}$. Because of a tiny magnetic anisotropy energy of $\sim$0.03 meV/unit-cell in FeSn, we anticipate that external perturbations, e.g., spin-
orbit torque, can readily manipulate the spin orientations to control the mass of Dirac fermions$^{26,27}$.

By applying external electric field, the $PT$ symmetry can also be broken to split the Dirac point into two Weyl points, which can be realized near the surface by the naturally developed surface electric potential. To verify this point, we acquired the ARPES data with a low photon energy of 35 eV. Strikingly, as shown in Fig. 3a-b, the ARPES data along the $\overline{K}-\Gamma-\overline{K}'$ line reveal the crossings of two linearly dispersive bands at the $\overline{K}$ and $\overline{K}'$ points only around -0.2 eV, differing from the bulk Dirac points around -0.4 eV (Fig. 2a). Furthermore, the observed Fermi surface shows that the circular patterns around the $\overline{K}$ and $\overline{K}'$ points develop typical Weyl cones with varying chemical potential (Fig. 3e).

Our calculated band structures of FeSn(001) show that the surface-induced Stark effect splits each Dirac band into two spin-polarized nondegenerate Weyl bands, which reside in neighboring Fe$_3$Sn subsurface layers with interlayer AFM coupling: i.e., one species located at the lower Fe$_3$Sn layer still remains around -0.4 eV (Extended Data Fig. 7), while the other species located at the upper Fe$_3$Sn layer shifts toward a higher energy up to $\sim$-0.2 eV at the $\overline{K}$ and $\overline{K}'$ points (Fig. 3c-d), consistent with the ARPES results.

We have demonstrated that the versatile topological properties can be entangled with the spin configurations and magnetic symmetries in the AFM FeSn kagome lattices. Besides the spin reorientation effect as discussed earlier, turning the interlayer coupling from AFM to FM can also induce the splitting of the Dirac point into two two-fold degenerate Weyl points (see Extended Data Fig. 8). As summarized in Fig. 4, symmetry control can effectively tune the topological quantum states. Thus, the spin degree of freedom in this AFM kagome system serves as a new knob to effectively tune the topological behaviors. The present findings therefore not only enrich the already fascinating kagome physics$^{17-22}$, but also pave a way for designing the topological AFM devices that can be utilized for future spintronics applications.

Methods

**Growth of FeSn single crystal.** FeSn single crystals were grown by Sn-flux method with Fe:Sn = 1:19 molar ratio. Fe and Sn powders were mixed together to put into an alumina crucible and were
then sealed in a quartz ampoule under vacuum. The sealed quartz ampoule was heated to keep at 1323 K for 4 hours, and then cooled down to 1183 K with 30 K/h. Subsequently it was cooled down to 853 K with a rate of 6 K/h, at which the ampoule was taken out from the furnace and was decanted with a centrifuge to separate FeSn crystals from Sn flux. After the centrifugation process, most of the flux contamination was removed from the surfaces of crystals. The grown crystals are shaped as hexagons, as shown in the inset of Extended Data Fig. 9.

**XRD and TEM characterizations.** The micro-diffraction XRD was measured by Rigaku D/MAX-RAPID II with Mo Kα radiation (λ = 0.071 nm) at room temperature in State Key Laboratory for Mineral Deposits Research, Nanjing University. The large curved imaging plate detector with 210° aperture allows a two-dimensional diffraction image over a broad 2θ range in a single crystal, which can detect many other lattice planes without breaking the single crystal. The single-crystal XRD was measured by XRD (Panalytical X’pert PRO MPD) with Cu Kα radiation (λ = 0.154 nm) at room temperature. Cross-sectional TEM (FEI F20) measurement was performed to characterize the layered structure of FeSn crystal. The sample was prepared by cutting the side face of a single crystal with mechanical polishing, and argon-ion milling. The lattice parameters were determined to be a = b = 5.3 Å and c = 4.4 Å.

**STM measurement.** In order to characterize the surface structure, FeSn crystals were cleaved at about 80 K in an ultra-high vacuum chamber with a base pressure of 1×10⁻¹⁰ mbar and were then probed *in situ* at 80 K by a Createc low temperature STM.

**Magnetic measurements.** The bulk magnetic measurements were performed in a Quantum Design SQUID VSM magnetometer with the magnetic field of 500 Oe and the temperature-scan ranges between 2 and 400 K.

**ARPES measurements.** The ARPES experiments with a low photon energy of 35 eV were performed at beam line 13U of the National Synchrotron Radiation Laboratory in Hefei, China, using a Scienta Omicron DA30L analyzer. The angle resolution was 0.2°, and the combined instrumental energy resolution was better than 20 meV. The high photon energy (90-160 eV) ARPES measurements with higher photon energies between 90 and 160 eV were performed at the beam line 9U (Dream-line) of the Shanghai Synchrotron Radiation Facility (SSRF) using a Scienta Omicron DA30L analyzer. The energy resolution was better than 25 meV and the angular resolution was 0.2°. All the samples were
cleaved to measure at 10-20 K under a vacuum better than $5 \times 10^{-11}$ mbar.

**First-principles calculations.** Our DFT calculations were performed using the Vienna ab initio simulation package with the projector augmented-wave method\textsuperscript{29}. For the exchange-correlation energy, we employed the generalized-gradient approximation functional of Perdew-Burke-Ernzerhof (PBE)\textsuperscript{30}. A plane-wave basis was taken with a kinetic energy cutoff of 500 eV. All atoms were allowed to relax along the calculated forces until all the residual force components were less than 0.001 eV/Å. The optimized lattice parameters of the FM (AFM) phase are $a = b = 5.28$ Å and $c = 4.46$ (8.92) Å. The Fe$_3$Sn-terminated (Sn-terminated) surface was modeled by a periodic slab geometry consisting of the fifteen (seventeen) atomic layers with ~18 Å of vacuum in between the slabs. The $\mathbf{k}$-space integration was done with the $15 \times 15 \times 10$ and $15 \times 15 \times 1$ meshes in the bulk and surface Brillouin zones, respectively. The theoretical STM images were simulated using the Tersoff-Hamann approximation\textsuperscript{31}. We construct Wannier representations by projecting the Bloch wave functions (obtained using the first-principles calculations of bulk FeSn) onto Fe $d$, and Sn $s$, $p$ atomic orbitals, and generate a tight-binding Hamiltonian with a basis of maximally localized Wannier functions\textsuperscript{32}. Using the Wannier representations, we calculated the Berry curvature and Berry phase\textsuperscript{33}.  

**Data availability.** The datasets generated and analyzed during the current study are available from the corresponding author on reasonable request.

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Author contributions

C.Z. and J.H.C. designed and supervised the work. Z.L. and L.L. grew the FeSn single crystals and performed the XRD, TEM and magnetic measurements. P.W., Z.L., and Z.S. performed the ARPES measurements. Q.Z., Y.W., and Z.W. performed the STM measurements. C.W. and S.Y. performed the theoretical calculations. J.H.C., Z.L., C.W., and C.Z. analyzed the data and wrote the manuscript. All authors contributed to the scientific discussion and manuscript revisions.

Additional information

Supplementary information is available in the online version of the paper. Reprints and permissions information is available online at www.nature.com/reprints. Correspondence and requests for materials should be addressed to C.Z., J.H.C., and Z.S.

Competing financial interests

The authors declare no competing financial interests.
Figure 1 | Structure and magnetism of FeSn single crystals. a, Crystal structure of an AFM FeSn system composed of alternating Fe$_3$Sn kagome and Sn honeycomb layers. Fe atoms with up and down spins are distinguished with red and blue circles, respectively. The three-dimensional Brillouin zone (BZ) and its projected surface BZ are given at the bottom. b, XRD data of the FeSn(001) crystal. c, Cross-sectional TEM image of the (210) plane with the atomic resolution of two different Fe$_3$Sn and Sn layers. d, Atomic resolution STM image of the Sn-terminated (001) surface, taken at $V_s = 0.1$ V. The corresponding simulated STM image is also given in the inset. e, Magnetization as a function of temperature under field-cooling with an applied magnetic field of 500 Oe along the [001] direction.
Figure 2 | ARPES spectra and electronic band structure of bulk FeSn. a, ARPES results between the K-Γ-K’ and H-A-H’ lines with changing photon energy from 105 eV to 130 eV. b,c, ARPES data (top) and their second derivatives (bottom) along the K-Γ-K’ ($k_z = 0$) and H-A-H’ ($k_z = \pi/c$) lines, respectively. Calculated band structure with SOC is superimposed by the orange lines at the bottom. d, Calculated band structure without SOC. e,f, Calculated band structures with SOC, where the spin orientations are along the [3.732, 1, 0] and [001] directions, respectively. g,h, Two crossing bands of DNL$_1$ and the Berry curvature component $\Omega_z$ around the H point in d. i, Two crossing bands around the Dirac point (DP) in e. j, Two bands around the H point in f. The Fermi energy $E_F$ is set at zero energy. k,l, Bulk Fermi surface obtained from ARPES measurement and DFT bands in e. The ARPES data are symmetrized with respect to $k_z=0$. 
Figure 3 | Electronic band structure of the FeSn (001) surface. a,b, ARPES data (a) with 35 eV-photon energy and their second derivatives (b) along the $\bar{K}$-$\bar{\Gamma}$-$\bar{K}'$ line. c,d, Projected band structures on the topmost Sn and Fe$_3$Sn surface layers without (c) and with SOC (d), where the radii of solid circles are proportional to the weights of the corresponding local density of states. Different colors of the circles with red and blue in c represent up and down spins, respectively. Two linearly dispersive bands at the $\bar{K}$ and $\bar{K}'$ points are highlighted with green color in d. e, Constant energy surface with respect to chemical potential, obtained by ARPES with 35 eV-photon energy. The ARPES data are symmetrized with respect to $k_x=0$. The regions surrounded by ellipses in b and d represent strong intensities along the $\bar{K}$-$\bar{M}$ and $\bar{K}'$-$\bar{M}'$ lines around -0.3 eV and around the $\bar{\Gamma}$ point at $\sim$-0.2 eV within a finite region of the Brillouin zone, showing a reasonably good agreement between ARPES and DFT results. The arrows in b and d indicate that the observed parabolic band around the $\bar{\Gamma}$ point is located at higher binding energy compared to the DFT result, which may be caused by an imperfect Sn-terminated surface in real samples. It is noted that the DFT bands without SOC in c show several spin-polarized surface states connecting the crossing points of two linearly bands located at $\sim$-0.2 eV, which is similar to the topologically nontrivial spin-polarized surface states observed at the surface of other Dirac semimetals$^{28}$. 
Figure 4 | Diagram of the topological phase transitions in bulk FeSn. 

**a,b.** Transition from massless Dirac to massless Weyl fermions via breaking $PT$ symmetry, such as surface stark effect or ferromagnetization. The calculated band structure of the FM phase of bulk FeSn shows the existence of massless Weyl points (see Extended Data Fig. 8).

**c.** Transition from massless Dirac to massive Dirac fermions via breaking $S_{2z}$ symmetry. Note that the manipulation of the Néel spin orientation can tune the magnetic symmetry to break $S_{2z}$ symmetry and generate non-zero mass in the originally massless Dirac bands.