Chiral Dirac-like fermion in spin-orbit-free antiferromagnetic semimetals

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PUBLIC SUMMARY

- A counterpart of isospin SU(2) symmetry is predicted to exist in crystalline solids
- Such symmetry is realized in some collinear antiferromagnets in nonrelativistic limit
- CoNb₃S₆ is a representative material manifesting Dirac-like fermions with chirality
Chiral Dirac-like fermion in spin-orbit-free antiferromagnetic semimetals

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INTRODUCTION

Dirac semimetal is a phase of matter whose elementary excitation is described by the relativistic Dirac equation. In the limit of zero mass, its parity-time symmetry enforces the Dirac fermion in the momentum space, which is composed of two Weyl fermions with opposite chirality, to be non-chiral. Inspired by the flavor symmetry in particle physics, we theoretically propose a massless Dirac-like equation yet linking two Weyl fields with the identical chirality by assuming SU(2) isospin symmetry, independent of the space-time rotation exchanging the two fields. Dramatically, such symmetry is hidden in certain solid-state spin-1/2 systems with negligible spin-orbit coupling, where the spin degree of freedom is decoupled with the lattice. Therefore, the existence of the corresponding quasiparticle, dubbed as flavor Weyl fermion, cannot be explained by the conventional (magnetic) space group framework. The 4-fold degenerate flavor Weyl fermion manifests linear dispersion and a Chern number of ±2, leading to a robust network of topologically protected Fermi arcs throughout the Brillouin zone. For material realization, we show that the transition-metal chalcogenide CoNb3S6 with experimentally confirmed collinear antiferromagnetic order is ideal for flavor Weyl semimetal under the approximation of vanishing spin-orbit coupling. Our work reveals a counterpart of the flavor symmetry in magnetic electronic systems, leading to further possibilities of emergent phenomena in quantum materials.

RESULTS

Theory of Dirac-like fermion with chirality

In high-energy physics, a Dirac field is a four-component field with field operators furnishing a 4D irreducible representation of Lorentz group. Such a field is non-chiral because P connects two 2D representations of proper orthochronous Lorentz group supporting two Weyl fields with opposite chirality. To construct a chiral Dirac-like four-component field, one requires additional internal symmetries (i.e., commute with space-time operations) connecting two Weyl fields with identical chirality. A famous type of internal symmetry in particle physics is the isospin symmetry relating a proton and a neutron forming an SU(2) doublet. In analogy, we can choose a condensed-matter counterpart of such SU(2) flavor symmetry to construct a massless four-component field with chirality, named flavor Weyl field (see Note S1).

In condensed matter solids with elementary excitations (quasiparticles), although spin is an internal degree of freedom of an electron, its rotational operations are completely locked to the rotations of the lattice owing to the relativistic SO(3) effect. However, the symmetry description of compounds composed of light elements with negligible SOC requires decoupled spin and lattice operations, forming symmetry groups called spin groups. We next show that the combination of translation and spin rotation in certain magnetic compounds with long-range magnetic order leads to a hidden SU(2) symmetry group, supporting the emergence of flavor Weyl fermions.

We considered a collinear AFM system belonging to the type-IV Shubnikov space group, as schematically shown in Figure 2A. We used a four-band model with two orbitals separately located at sublattices $A$ and $B$ and the Neel vector along the $z$ axis to describe such a system. Three elements in the spin space group were considered, including a 2-fold spin rotation perpendicular to the magnetic moment followed by a fractional translation symmetry, $U_1^{12} = \{U_{\alpha}(\pi)\}E_{\tau_1/2}$, and a spin rotation operation along magnetic moments with an infinitesimal rotation angle, $U_2(\theta) = E_{\sigma_0}$, where $U_{\alpha}(\theta)$, represents pure spin rotation $\alpha$ along $n$ axis and $E_{\tau_1/2}$ denotes the half translation along the $z$ axis (see Note S2). We can write the general form of the single-electron Hamiltonian as $H(k) = \sum_{j=1}^{4} t_{j} f_{j}(k) \tau \otimes \sigma$, where $\tau$ and $\sigma$ operate on spin and site degrees of freedom, respectively, and $f_{j}(k)$ represents real functions of $k$. After that,
symmetry connecting two Weyl fermions, rendering the role of the two Weyl fermions with distinct spatial wave functions.

The symmetry properties guarantee the following topological features that are permitted without SOC, forming the spin space group $\text{SU}(2)$ and methods for details about density functional theory (DFT) calculation). We adopt the experimental magnetic configuration and (3) presence of spin-group symmetry $\text{SU}(2)$, and (3) nondegeneracy of spin-group symmetry $\text{SU}(2)$.

**Material realization: CoNb$_3$S$_6$**

To realize flavor WSM in realistic materials, we first summarize the required conditions as following design principles: (1) collinear AFM order, (2) broken $P$ and $PT$ symmetry, and (3) presence of $\text{SU}(2)$ symmetry. We note that (1) and (3) ensure the presence of spin-group symmetry $\text{SU}(2)$ and $\text{SU}(4)$ without SOC. Based on these principles, we propose that the chiral transition-metal chalcogenide CoNb$_3$S$_6$ is a representative flavor WSM that hosts flavor Weyl points around the Fermi level. Among them, transition-metal chalcogenide CoNb$_3$S$_6$ is a representative flavor WSM that hosts flavor Weyl points around the Fermi level. Figure 3A shows that CoNb$_3$S$_6$ crystallizes in the chiral space group $\text{P6}_322$. It has an AFM order with magnetic moments directed along a crystal axis within the $a$-$b$ plane below the Neel temperature, $T_{\text{N}}$, of $26$ K.\(^{32}\) This structure corresponds to the type-II magnetic space group $P6_322$ (No. 182). It has one 2-fold rotation along the $z$ axis ($\langle 0, 0, 1 \rangle$) and two screw rotations {$(\langle 0, 1, 0 \rangle) \parallel C2, z = 0$, $\langle 0, 1, 0 \rangle \parallel C2, z = 0$}, and non-symmetric time-reversal $(\langle 0, 1, 0 \rangle \parallel C2, z = 0)$. We achieve this pattern of spin space groups by the role of spin space groups. Some symmetry operations beyond the conventional magnetic space group, including $\{E\} | \langle 0, 1 \rangle \rangle | \langle 0, 1 \rangle \rangle$ and $\{T_{\text{N}}\} | \langle 0, 1 \rangle \rangle | \langle 0, 1 \rangle \rangle$, are permitted without SOC, forming the spin space group $P6_322$ (see Note S3).

In contrast to the previous calculations using nonmagnetic or alternative AFM configurations,\(^{34}\) we adopt the experimental magnetic configuration observed by neutron scattering.\(^{33}\) The band structure calculation (Figure 3C) shows that CoNb$_3$S$_6$ is a metal with multiple hole pockets near the $\Gamma$ point, consistent with the experiments showing holes as major system carriers (see materials and methods for details about density functional theory [DFT] calculation).\(^{34}\) The symmetry properties guarantee the following topological features that appear in the band structure. First, the spin space group does not have $P$.
the two degenerate energy bands have identical rotation eigenvalues on the high-symmetry lines. Therefore, the three 2-fold rotation operations can provide additional protection for flavor Weyl points. We note that although CoNb$_3$S$_6$ belongs to chiral space group, implying that all point-like degeneracies are chiral fermions, the occurrence of flavor Weyl nodes does not require a chiral space group in general.\(^\text{36}\)

Remarkably, there are multiple flavor Weyl points located around the Fermi level and four flavor Weyl points at \(-0.7\) eV above the Fermi level. The latter points are located along \(\Gamma - X\) and \(\Gamma - Y\) lines. We found that the crossing bands along these high-symmetry lines have opposite eigenvalues of \(\{E|\hat{C}_x(\pi)|0\}\) and \(\{E|\hat{C}_y(\pi)|\gamma_{x=0}\}\), indicating that the flavor Weyl points are protected by \(C_2\) rotation. The Berry curvature calculation (see Figure 3D) shows that the two Weyl points along \((-X) - \Gamma - X\) act as the source of Berry curvature, and the other two act as the drain, manifesting their chiral nature. Further calculation of the Wilson loop showed that the Chern number over a spherical surface around a Weyl point along \(\Gamma - X - \gamma\) was \(-2\) (see Figure S1). Therefore, we name the flavor Weyl points along \(\Gamma - X - \gamma\) as \(N_1, N_2, P_1, P_2\). We obtained the Dirac-like \(k \cdot \hat{p}\) Hamiltonian in the following by applying the symmetry operations, \(U_{2\zeta}^2, U_{k\cdot\hat{p}}\) and \(\{T|\hat{C}_z(\pi)|\gamma_{x=0}\}\), to the low-energy Hamiltonian near \(N_1\):

\[
H(K) = \begin{pmatrix}
\mathbf{a}_0 + \mathbf{a}_1 K_x \tau_x \otimes \sigma_0 + (\mathbf{a}_2 K_z + \mathbf{a}_3 K_y) \tau_y \otimes \sigma_x + (\mathbf{a}_4 K_x + \mathbf{a}_5 K_y) \tau_z \otimes \sigma_y
\end{pmatrix} \tag{Equation 2}
\]

The results of our DFT calculation can be used to obtain the parameters of Equation 2, giving rise to an anisotropic Dirac cone. By implementing the spin rotation \(e^{-i\mathbf{k}\cdot\mathbf{p}/2}\) to Equation 2 (transforming \(\sigma_1\) terms into \(\sigma_2\) terms), the Hamiltonian is block-diagonalized into two Weyl Hamiltonians of the same chirality.

The topological charges of the flavor WSM imply the existence of Fermi arc surface states connecting two flavor Weyl points with opposite chirality. However, flavor Weyl points with opposite chirality are not connected by any symmetry owing to the lack of inversion, roto-inversion and their combinations with \(T\). Therefore, we found an energy difference of \(0.7\) meV between \(P_1\) and \(N_1\). Moreover, flavor Weyl points, \(P_1\) and \(P_2\) \((N_1, N_2)\), are connected by a 2-fold spatial rotation. Hence, they are located at the same energy. There are two disconnected electron Fermi pockets, separately enclosing \(P_1\) and \(P_2\), and two disconnected hole pockets, separately enclosing \(N_1\) and \(N_2\), for the (001) surface when Fermi energy exists between the two. Every electron pocket is connected to a hole pocket by a branch of Fermi arc surface states due to the enclosure of the different topological charges in electron and hole pockets, forming a network across the Brillouin zone (see Figure 4A). Interestingly, the surface states are also doubly degenerate because \(\{U_{2\zeta}(\pi)|E|\gamma_{x=0}\}\) is preserved on this surface (and so as the hidden SU(2) symmetry), in sharp contrast to the conventional topological insulators or DMSs where the surface bands are spin-polarized and nondegenerate. The degenerate Fermi arc surface states are split into two branches for the (100) surface with broken symmetry of \(\{U_{2\zeta}(\pi)|E|\gamma_{x=0}\}\), as shown in Figure 4B. The various Fermi arc surface states are robust against perturbations, maintaining the collinear A-type AFM order in the absence of SOC. On the contrary, topological protection for the surface states on the conventional DSM does not exist.\(^\text{37}\)

The Chern number of a 2D slice in the Brillouin zone changed in the multiples of 2 because the flavor Weyl points have chiralities of \(\pm 2\). Figure 4C shows that the Chern number of the slice perpendicular to the \(z\) axis changes as a function of \(k_y\). The Chern number calculated on slice near \(\Gamma\) between flavor Weyl points with opposite chirality is \(\pm 2\). The result is consistent with the Berry curvature calculation (Figure 3D), where Berry curvature flows from \(N_1\) to \(N_2\) and \(P_1\) to \(P_2\). Figure 4D shows the corresponding edge states with two branches of chiral surface states connecting the conduction and valence bands that are doubly degenerate at SU(2)-preserved edge and nondegenerate at SU(2)-broken edge, further validating the interplay between the Weyl points and the hidden SU(2) symmetry. We note that the energies of the flavor Weyl points \(P_{1,2}\) and \(N_{1,2}\) \((-0.7\) eV) depend on the \(U\) value (3 eV) of Co-3d electrons we adopt for correlation effects. When \(U\) is set to 1 eV, the energies of these points shift to \(-0.5\) eV, whose Fermi arc states might be observed by angle-resolved photoemission spectroscopy.

**Effects of SOC**

While SOC is a universal relativistic property existing in all materials, for most materials, even with strong SOC, e.g., 10 to 100 meV, its influence on the electronic structure is still limited compared with those caused by exchange splitting and crystal field, etc. Therefore, we can take the SOC-free Hamiltonian, which is described by spin-group symmetry, as a good starting point to understand magnetic materials with SOC by treating SOC as a

Figure 2. Hidden SU(2) symmetry in antiferromagnetic materials (A) The magnetic lattice with collinear antiferromagnetic order allows spin-group symmetry operations, \(U_{k\cdot\hat{p}}\) with \(k\) and \(\hat{p}\) (see the main text). (B) Bloch sphere of the SU(2) symmetry group, transforming the basis of a Weyl cone \(|\mathbf{A}, \uparrow\rangle, |\mathbf{B}, \uparrow\rangle\rangle\) (blue arrow) to any linear combinations (up to a phase factor) \((\alpha|\mathbf{A}, \uparrow\rangle + \beta|\mathbf{B}, \uparrow\rangle\), \(\alpha|\mathbf{A}, \uparrow\rangle + \beta|\mathbf{A}, \downarrow\rangle\)), and transforming \(|\mathbf{B}, \downarrow\rangle, |\mathbf{A}, \downarrow\rangle\rangle\) (red arrow) to an orthogonal one \(-|\mathbf{A}, \uparrow\rangle + |\mathbf{B}, \downarrow\rangle\rangle\). The basis transformation under the rotation axis (gray line) \(n = \cos(\omega_n)\sin(\omega_n)\) and rotation angle \(\theta\) are also shown. The mixing coefficients are \(\alpha = \cos(\theta/2)\) and \(\beta = -i\sin(\theta/2)e^{i\phi}\).

Figure 3. Crystal and bulk electronic properties of CoNb$_3$S$_6$ (A) The crystal structure of CoNb$_3$S$_6$. (B) Bulk and surface Brillouin zones of CoNb$_3$S$_6$. (C) The band structure of CoNb$_3$S$_6$ without spin-orbit coupling. There are two flavor Weyl points at \(-0.7\) eV above the Fermi level, \(N_1\) and \(P_1\), and another two flavor Weyl points, \(N_2\) and \(P_2\) (not shown), that are connected to \(N_1\) and \(P_1\) through 2-fold rotation. (D) Distribution of in-plane components of the surface states with Fermi arc on the planes, where \(N_1\) and \(P_1\) denote the source and sink, respectively.
perturbation that breaks certain spin-group symmetries. Specifically, since the flavor Weyl points are charge-2 monopoles of Berry curvature, the sub-Hilbert space on a spherical surface encircling a flavor Weyl point of opposite chirality in CoNb$_3$S$_6$ does not lie at the same energy, and there is a small spin splitting at the Weyl points. However, despite the gapped phase and spin-split surface states, the features of Fermi arc still resemble those without SOC, as shown in Figures 5B and 5C. The difference is that the Fermi arc surface states are now trivial rather than nontrivial, connecting an electron (hole) pocket with an electron (hole) pocket. Recall the successful measurement of the Fermi arc states in DSMs, such spin-group-induced feature could also be visible for experiments. For flavor Weyl points near the Fermi level (Figure 5D), small spin splitting causes some flavor Weyl points to split into twin-pair Weyl points rather than being gapped, as shown in Figures 5E and 5F. The spin splitting at the Fermi points is only $\sim$0.3 meV, which is a small perturbation to the flavor Weyl points protected by spin group.38–41

Overall, even if SOC effect is generally not negligible in CoNb$_3$S$_6$, the flavor WSM phases can still be considered as a starting point to understand its topological nature that cannot be fully described by magnetic space group. Interestingly, the SOC-free approximation of the flavor symmetry studied here also makes a nice analogy to the flavor symmetry in particle physics, which is also an approximate symmetry. Recall that isospin symmetry is good enough in prediction of the possibility and rates of nuclear reaction when the masses of the two particles, for example, proton (938.27 MeV) and neutron (939.57 MeV), are similar, spin-group symmetry protects degeneracies, topological charges, and surface states of certain topological materials when SOC is weak.42

**DISCUSSION**

We discuss the possible experimental phenomena associated with flavor Weyl fermions. First, flavor WSM manifests unique and robust surface states enforced by topological charges. On SU(2) preserved surfaces, the surface states would be Weyl-like; while on SU(2) breaking surfaces, the surface states would be Dirac-like. In contrast, robust surface states of DSMs are rare except for specific nonsymmorphic symmetries to protect the surface states.43–45 Owing to the protection of topological charge, even if sizable SOC exists, flavor Weyl points could split into a twin-pair of conventional Weyl points with the same chirality rather than being gapped immediately. These characteristics are potentially observable by angle-resolved photoemission spectroscopy. More importantly, the robust Fermi arc surface states of flavor WSM potentially lead to unexplored emergent transport and optical properties. For example, the flavor Weyl points of opposite chirality in CoNb$_3$S$_6$ do not lie at the same energy, possibly leading to a large and quantized response to circularly polarized light.46

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**Figure 5. Effects of spin-orbit coupling on energy bands** (A) Band structure around the Fermi level. (B) Iso-energy topological surface states without SOC (B) and with SOC (C). The energy is set between those of $N_1$ and $P_3$. (B) Band structure around the Fermi level. (E and F) Zoom-in bands of a flavor Weyl point without SOC (E) and with SOC (F). The coordinate of points labeled are $A = (0.5, 0.2572, 0); A' = (0.5, 0.2575, 0); \Delta = (0.05, 0, 0).$
Furthermore, the net anomalous Hall conductivity and spin Hall conductivity in CoNb3S6 should be zero owing to the presence of $\{ T \} | E | r_{az} $ symmetry and $\{ T \} | u | (e | r_{az} ) $ symmetry. However, breaking $\{ T \} | E | r_{az} $ symmetry and $\{ T \} | u | (e | r_{az} ) $ symmetry through the small SO effect and small tilting of magnetic moments may lead to a large anomalous Hall conductance because of the uncompensated Berry curvature and multiple Fermi arcs emerging from the charge-2 flavor Weyl points. It has been observed in CoNb3S6, accompanied by small out-of-plane components of the magnetic moments.34

Poincare symmetry is generally broken in solid-state lattices, while certain crystalline symmetries such as nonsymmetric symmetry are absent in high-energy physics. Because of these differences, there are various types of quasiparticle excitation in condensed matter physics that do not have counterparts in high-energy physics, including 3-, 6- or 8-fold degenerate points,45–46 line-like,47–49 chain-like,50,51 and plane-like band crossings,52 et cetera. Besides, there are also emergent quasiparticles composed of two Weyl points of opposite chirality, like Dirac fermions, but with different velocities, indicating that energy bands around the 4-fold degenerate points are generally nondegenerate.52,53 We note that such quasiparticles sometimes are also attributed to a type of DSM with a looser definition, which allows band splitting around Dirac points.5 In addition, previous literature also reported four-component Weyl fermions with nonzero Chern number ± 2 or ± 4 in both electrons,52,23,25–27 and phonons systems.58,59 We note that the main difference between these quasiparticles and the flavor Weyl fermions in the presented work is 2-fold. First, these quasiparticles are stabilized by the little groups with high-order rotation operations or the little groups without nonsymmorphic symmetry operations. Therefore, these elementary excitations can only appear at specific high-symmetry moments of the Brillouin zone. However, the flavor Weyl points can appear at generic momenta. This property implies the emergence of dense flavor Weyl points within a small energy range, possibly leading to stronger topological effects. Second, the previously studied 4-fold degenerate points with nonzero Chern number inevitably have nondegenerate energy bands away from the high-symmetry points. Therefore, they do not strictly fulfill the massless four-component equation in quantum field theory. However, our flavor WSM model was derived from the quantum field theory perspective with doubly degenerate dispersions around the Dirac-like points, stabilized by the hidden SU(2) isospin symmetry.

**MATERIALS AND METHODS**

The first-principles calculations were carried out using projector-augmented-wave (PAW) method62, implemented in Vienna ab initio simulation package (VASP)63 within the framework of density-functional theory.62,63 Contributions of exchange and correlation effects were accounted by the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) formalism.64 An energy cut off of 520 eV is used in our calculations. The whole Brillouin-zone was sampled by $5 \times 8 \times 4$ Monkhorst-Pack grids for all cells. Due to the local magnetic moments contributed from 3d electrons in Co atoms, GGA+U approach within the Dudarev scheme65 is applied and we set the U on Co to be 3 eV, which produces local magnetic moments of 2.2 $\mu_B$ consistent with the experiments.44 A tight-binding Hamiltonian is obtained based on locally maximized Wannier functions13,17 of Co-3d, Nb-4d, S-3p orbitals, from which the topological surface states, Berry curvature and Chern number are calculated. The iterative Green’s function implemented in WannierTools package is used for surface states calculations.66

**REFERENCES**

1. Novoselov, K.S., Geim, A.K., Morozov, S.V., et al. (2005). Two-dimensional gas of massless Dirac fermions in graphene. Nature 438, 197–200.

2. Fu, L., Kane, C.L., and Mele, E.J. (2007). Topological insulators in three dimensions. Phys. Rev. Lett. 98, 106803.

3. Moore, J.E., and Balents, L. (2007). Topological invariants of time-reversal-invariant band structures. Phys. Rev. B 75, 121306.

4. Wang, P., Ge, J., Li, J., et al. (2021). Intrinsic magnetic topological insulators. Innovation 2, 100098.

5. Song, S., Zuo, X., and Chen, Q.-X. (2012). Dirac semimetal in three dimensions. Phys. Rev. Lett. 108, 140405.

6. Yang, B.-J., and Nagaosa, N. (2014). Classification of stable three-dimensional Dirac semimetals with nontrivial topology. Nat. Commun. 5, 4898.

7. Young, S.M., and Kane, C.L. (2015). Dirac semimetals in two dimensions. Phys. Rev. Lett. 115, 126803.

8. Watanabe, H., Po, H.C., and Vishwanath, A. (2018). Structure and topology of band structures in the 1651 magnetic space groups. Sci. Adv. 4, eaat8685.

9. Yu, X., Elcoro, L., Song, Z.-D., et al. (2020). High-throughput calculations of magnetic topological materials. Nature 586, 702–707.

10. Elcoro, L., Wieder, B.J., Song, Z., et al. (2021). Magnetic topological quantum chemistry. Nat. Commun. 12, 5965.

11. Peng, B., Jiang, Y., Fang, Z., et al. (2022). Topological classification and diagnosis in magnetic materials. Nature 598, 231358.

12. Yu, Z.-M., Zhang, Z., Liu, G.-B., et al. (2022). Encyclopaedia of emergent particles in three-dimensional crystals. Sci. Bull. 67, 375–380.

13. Tang, F., and Wang, X. (2021). Exhaustive construction of effective models in 1651 magnetic space groups. Phys. Rev. B 104, 085137.

14. Brinkman, W.F., and Elliott, R.J. (1966). Theory of spin-space groups. Proc. R. Soc. A 294, 343–358.

15. Litvin, D.B., and Okechowski, W. (1974). Spin groups. Physica 76, 538–554.

16. Liu, P., Li, J., Han, J., et al. (2022). Spin-group symmetry in magnetic materials with negligible spin-orbit coupling. Phys. Rev. X 12, 021016.

17. Yang, J., Liu, Z.-X., and Fang, C. (2021). Symmetry invariants of spin space groups in magnetic materials. Preprint at arXiv. https://arxiv.org/abs/2105.12738.

18. Cortijo, A., Moessner, R., and McClarty, P.A. (2022). Spin-space groups and magnon band topology. Phys. Rev. B 105, 064430.

19. Coleman, S., and Mandula, J. (1967). All possible symmetries of the s matrix. Phys. Rev. 159, 1251–1256.

20. Heisenberg, W. (1932). Uber den bau der atomkerne. I. Z. Physik 77, 1–11.

21. Chang, G., Xu, S.-Y., Sanchez, D.S., et al. (2016). A strongly robust type II Weyl fermion semimetal state in TaS2. Sci. Adv. 2, e1600295.

22. Anzenhofer, K., Van Den Berg, J.M., Cossee, P., and Helle, J.N. (2017). The crystal structure and magnetic susceptibilities of MnNb3S6, FeNb3S6, CoNb3S6 and NiNb3S6. J. Phys. Chem. Solids 31, 1057–1067.

23. Parkin, S.S.P., Marseglia, E.A., and Brown, P.J. (1983). Magnetic structure of Co3TaS3 and Co3TaS2. J. Phys. C Solid State Phys. 16, 2755–2778.

24. Ghimire, N.J., Botana, A.S., Jiang, J.S., et al. (2018). Large anomalous hall effect in the chiral-antiferromagnet CoNb3S6. Nat. Commun. 9, 3280.

25. Smejkal, L., Gonzalez-Hernandez, R., Jungwirth, T., and Sinova, J. (2020). Crystal time-reversal symmetry breaking and spontaneous hall effect in collinear antiferromagnets. Sci. Adv. 6, eaaz8809.

26. Chang, G., Wieder, B.J., Schindler, F., et al. (2018). Topological quantum properties of chiral crystals. Nat. Mater. 17, 978–985.

27. Kargarian, M., Randeria, M., and Lu, Y.-M. (2016). Are the surface fermi arcs in Dirac semimetals topologically protected? Proc. Natl. Acad. Sci. USA 113, 8648–8652.

28. Yu, H., Wang, Z., Chen, C., et al. (2014). Evidence of topological surface state in three-dimen- sional Dirac semimetal Cd3As2. Sci. Rep. 4, 6106.

29. Xu, S.-Y., Liu, C., Kuswaha, S.K., et al. (2015). Observation of fermi arc surface states in a topological metal. Science 347, 294–298.

30. Moll, P.J.W., Nair, N.L., Helm, T., et al. (2016). Transport evidence for fermi-arc-mediated chirality transfer in the Dirac semimetal Cd3As2. Nature 535, 266–270.

31. Wu, Y., Jo, N.H., Wang, L.-L., et al. (2019). Fragility of fermi arcs in Dirac semimetals. Phys. Rev. B 99, 161113.

32. Zee, A. (2016). Group Theory in a Nutshell for Physicists (Princeton University Press).
54. Wieder, B.J., Wang, Z., Cano, J., et al. (2020). Strong and fragile topological Dirac semimetals. Phys. Rev. B 102, 115125.

55. Xu, Y., and Duan, L.M. (2016). Type-II Weyl points in three-dimensional cold-atom optical lattices. Phys. Rev. A 94, 053619.

56. Chang, G., Xu, S.-Y., Wieder, B.J., et al. (2017). Unconventional chiral fermions and large topological fermi arcs in RPh. Phys. Rev. Lett. 119, 206401.

57. Tang, P., Zhou, Q., and Zhang, S.-C. (2017). Multiple types of topological fermions in transition metal silicides. Phys. Rev. Lett. 119, 206402.

58. Zhang, T., Song, Z., Alexandradinata, A., et al. (2018). Double-Weyl phonons in transition-metal monosilicides. Phys. Rev. Lett. 120, 016401.

59. Miao, H., Zhang, T.T., Wang, L., et al. (2018). Observation of double Weyl phonons in parity-breaking FeSi. Phys. Rev. B 97, 134103.

60. Kresse, G., and Furthmüller, J. (1996). Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Phys. Rev. B 54, 11169.

61. Hohenberg, P., and Kohn, W. (1964). Inhomogeneous electron gas. Phys. Rev. 136, B864.

62. Kohn, W., and Sham, L.J. (1965). Self-consistent equations including exchange and correlation effects. Phys. Rev. 140, A1133.

63. Perdew, J.P., Burke, K., and Ernzerhof, M. (1996). Generalized gradient approximation made simple. Phys. Rev. Lett. 77, 3865 (1996). Phys. Rev. Lett. 78, 1396-1399.

64. Perdew, J.P., Burke, K., and Ernzerhof, M. (1996). Generalized gradient approximation made simple. Phys. Rev. Lett. 77, 3865.

65. Monkhorst, H.J., and Pack, J.D. (1976). Special points for brillouin-zone integrations. Phys. Rev. B 13, 5188.

66. Liechtenstein, A.I., Anisimov, V.I., and Zaanen, J. (1995). Density-functional theory and strong interactions: Orbital ordering in mott-hubbard insulators. Phys. Rev. B 52, R5467.