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Supplemental Information

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Supplementary Materials

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Note S1. Dirac-like field with chirality – Flavor Weyl field

The Dirac fields obey the famous Dirac equation, $(-i\alpha^i\partial_i + m\beta)\psi(x) = i\partial_0\psi(x)$, where $\alpha^i = \tau_x \otimes \sigma_i$ and $\beta = \tau_z \otimes \sigma_0$. Its field operators furnish a 4D irreducible representation of the Lorentz group. Such a group can be written as a combination of two disconnected pieces—$O(3,1) = SO(3,1) + P\,SO(3,1)$, where $SO(3,1)^1$ is a connected subgroup of $O(3,1)$. The reducible representation of $SO(3,1)$, i.e., $(0,1/2)\oplus(1/2,0)$, in the presence of P, becomes irreducible for the Lorentz group $O(3,1)$, giving rise to the Dirac fields. However, seldom considered is the possibility of elementary spin-1/2 particles described by four-component fields having $(1/2,0)\oplus(1/2,0)$ (or equivalently, $(0,1/2)\oplus(0,1/2)$). To achieve such fields, P should be broken, reducing the corresponding

symmetry group to $SO(3,1)$. Therefore, $(1/2,0)\oplus(1/2,0)$ would become a reducible representation, corresponding to a field that naturally decomposes into two Weyl fields. Second, additional internal symmetries need to be assumed to elevate the symmetry hierarchy of the system, rendering $(1/2,0)\oplus(1/2,0)$ representation irreducible. Internal symmetry operations are required to decouple the space-time operations according to the Coleman–Mandula theorem[2]. Furthermore, we selected them to form an $SU(2)$ group connecting two Weyl fields with the same chirality, analogous to the $SU(2)$ flavor symmetry in high-energy physics. Specifically, it is analogous to the isospin symmetry proposed by Heisenberg, pairing a proton and a neutron forming an $SU(2)$ doublet.[3]

Such isospin symmetry can stabilize free and causal quantum fields that follow the representation $(1/2,0)\oplus(1/2,0)$ (and $(0,1/2)\oplus(0,1/2)$). The corresponding fields are called flavor Weyl fields, described by the following massless Dirac-like equation:

$$i\alpha^i\partial_i\psi(x) = \pm i\partial_0\psi(x), \tag{1}$$

where $\psi(x)$ denotes a four-component free field operator and $\alpha^i = \tau_i\otimes\sigma_0$. Furthermore, the energy spectrum of equation (1) is doubly degenerate owing to the protection of the additional $SU(2)$ group, resembling the role of P in the Dirac equation.

To construct such flavor Weyl field, we firstly assume that inversion symmetry is broken such that left-handed Weyl field and right-handed Weyl field could exist individually. Then, we further assume a four component Dirac field can be written as the form $\psi = \begin{pmatrix}\psi_L^1\\ \psi_L^2\end{pmatrix}$ where ψ_L^1 and ψ_L^2 are two left-handed and 2-component Weyl fields following the irreducible representation $(1/2,0)$ of the proper orthochronous Lorentz transformation. Then the representation matrices of the angular momentum operators and boost operators

of proper orthochronous Lorentz transformation are $\boldsymbol{\mathcal{J}} = \frac{1}{2}\tau_0 \otimes \boldsymbol{\sigma}$, $\boldsymbol{\mathcal{K}} = -\frac{i}{2}\tau_0 \otimes \boldsymbol{\sigma}$, where τ_i and σ_j (i = 0, x, y, z) are Pauli matrices.

Such field is reducible under proper orthochronous Lorentz transformation, to stabilize this field, we further assumes that there is an internal $SU(2)$ symmetry group with generators represented as $\boldsymbol{\mathcal{J}} = \frac{1}{2}\boldsymbol{\tau} \otimes \sigma_0$, which implies that the elements of $SU(2)$ group transform on $\psi = \begin{pmatrix} \psi_L^1 \\ \psi_L^2 \end{pmatrix}$ by $exp(-i\boldsymbol{\theta} \cdot \frac{1}{2}\boldsymbol{\tau}) \begin{pmatrix} \psi_L^1 \\ \psi_L^2 \end{pmatrix}$, identical to the transformation properties of $SU(2)$ isospin symmetry on two quantum fields in standard model. Then, it is obvious that such field describe one particle formed by two Weyl fields connected by the internal $SU(2)$ symmetry group.

Then, following the process of constructing field operator provided in Ref. [4], we can see that ψ can be constructed for describing massless spin-1/2 particles. It could also be shown that this field obeys the following equation

$$\left(-\partial_0 + \alpha^i \partial_i\right)\psi(x) = 0, \tag{4}$$

where $\alpha^i = \sigma_0 \otimes \sigma_i$. This 4-component field have 4 independent variables, however, when we do not assume internal $SU(2)$ symmetry group, the field operator will reduce to operators with two independent variables.

Note S2. Spin space groups and description of magnetic materials without spin-orbit coupling

Because spin and orbit degrees of freedom are partially decoupled in magnetic systems when SOC effect is weak, we follow the notations by Litvin et al. that write spin and spatial

operations in separate slots and denote spin rotations and spatial rotations as $U_{\boldsymbol{n}}(\theta)$ and $C_{\boldsymbol{m}}(\varphi)$, respectively[5,6], where $\boldsymbol{n}$ and $\boldsymbol{m}$ denote are rotation axes and θ and φ the rotation angles. By considering time reversal T, spatial inversion symmetry P and translation symmetry $\boldsymbol{t}$, all elements of a spin space group can be written as the following form:

$$\{T^{n_1} U_{\boldsymbol{n}}(\theta)||P^{n_2} C_{\boldsymbol{m}}(\varphi)|\boldsymbol{t}\},$$

with $n_1 = 0,1$ and $n_2 = 0,1$. Although time-reversal T could reverse momentum in the reciprocal space, both T and $U_{\boldsymbol{n}}(\theta)$ can be seen as the symmetries of spin in real space when analyzing the symmetry. P, $C_{\boldsymbol{m}}(\varphi)$ and $\boldsymbol{t}$ are spatial symmetries. Thus, we separate the 5 types of symmetry into spin symmetries, T and $U_n(\theta)$, and spatial symmetries, P, $C_{\boldsymbol{m}}(\varphi)$ and $\boldsymbol{t}$, by a double vertical line.

When spin-orbit coupling is neglected in magnetic materials, spin and lattice DOF are decoupled, rendering three kinds of operation, i.e., pure spin operation, pure spatial operation and operation of combined spin and spatial operation. This allows the definition of two types of spin group, i.e., nontrivial and a trivial spin group, where the nontrivial spin group is composed of spatial operations or/and combined operations of spatial and spin operations, and the trivial spin group is formed by pure spin operations. It has been shown that every spin group can be written as the direct product of a nontrivial and a trivial spin group[5].

The recent discussions about spin group symmetry mainly focus on nontrivial spin groups, especially nontrivial spin point groups. In ref. [7], symmetry invariants of all nontrivial spin point groups, used for classifying projective representations based on the second group cohomology, are listed. In ref. [8], energy band degeneracy and topological

insulating phases protected by the combined operations of spin rotation and spatial rotation are discussed. Nevertheless, even if the complex spiral incommensurate magnetic structures are excluded from consideration, spin point groups with trivial part containing more than identity element cannot be neglected in general. This is because the collinear or coplanar magnetic structures, commonly existing in realistic materials, have trivial part containing symmetry elements that could usually contribute to spin degeneracy and quasiparticle excitations. Most importantly, the spin point groups of magnetic structures corresponding to type-IV magnetic groups have additional trivial part being significant which contribute to flavor Weyl points discussed in the main text.

For non-spiral magnetic structures classified into conventional type-I and type-III magnetic space group, the spin point group part of spin space group has trivial part being $\{E\}$ for noncoplanar magnetic structures, Z_2^K for coplanar but not collinear magnetic structures , and $Z_2^K \times SO(2)$ for collinear magnetic structures, where $SO(2)$ is the spin rotation group with rotation operations along the axis of magnetic order x, and $Z_2^K = \{\{E||E|0\}, \{U_{\boldsymbol{n}}(\pi)T||E|0\}\}$ is the group generated by the combined operation of a spin rotation operation perpendicular to the magnetic moments and a time reversal operation. All of the 597 nontrivial spin point groups, which directly applies to noncoplanar spin arrangements, are listed in ref. [6]. For spin arrangements being coplanar and collinear, there are 252 and 90 possible spin point groups, derived in ref. [8]. However, for spiral magnetic structures described by any type of magnetic space group or non-spiral magnetic structures described by type-IV magnetic space group, the spin point group part of spin space group could go beyond $\{E\}$, Z_2^K and $Z_2^K \times SO(2)$ because of the existence of operations of the form $\{R||E|\boldsymbol{\tau}\}$ where $\boldsymbol{\tau}$ is a lattice translation with $\{E||E|\boldsymbol{\tau}\}$ is not contained in the spin

space group. Specifically, if a nonchiral magnetic structure belongs to type-IV magnetic space group, the existence of time reversal symmetry combined with translation symmetry $\{T||E|\boldsymbol{\tau}\}$ would add a group $Z_2^T = \{\{E||E\}, \{T||E\}\}$ to the trivial spin point group and the spin group would be $Z_2^T \times Z_2^K \times SO(2)$ or $Z_2^T \times Z_2^K$. Most importantly, the combination of Z_2^T and Z_2^K will lead to spin flip symmetry $\{U_{\boldsymbol{n}}(\pi)||E\}$ which corresponds to the combined symmetry of 180 degree of spin rotation and half translation in spin space group, $\{U_{\boldsymbol{n}}(\pi)||E|\boldsymbol{\tau}_{1/2}\}$. This symmetry $\{U_{\boldsymbol{n}}(\pi)||E|\boldsymbol{\tau}_{1/2}\}$ is contained in the little group of every momentum in the Brillouin zone, which could lead to effective $SU(2)$ isospin symmetry if there is additionally a SO(2) group, as is shown in the main text.

Note S3. Symmetry properties of $CoNb_3S_6$ when neglecting spin-orbit coupling

We know that without consideration of magnetic order in $CoNb_3S_6$, the crystal structure belongs to the space group $P6_322$, following Hermann–Mauguin notation, while, with magnetic order, the structure corresponds to type-IV magnetic space group $P_B2_12_12$. If using notations of spin group (Ref. [6]), the magnetic space group is ${P_B}^{2_x}{2_1}^{2_y}{2_1}^{2_z}2$, with all spatial rotation combined with a spin rotation of the same angle around the same axis. This group commute with the single electron Hamiltonian of this system with spin orbit coupling (SOC), and there cannot be more symmetry operations beyond this group (Ref. [5,8,9]).

If we neglect SOC now, the spin rotations and spatial rotations are not forced to be operated simultaneously, i.e., be operated at the same time with the same angle and the same rotation axis. Thus, in addition to the magnetic group ${P_B}^{2_x}{2_1}^{2_y}{2_1}^{2_z}2$, decoupled spin and orbit rotation operations appear to commute with the Hamiltonian of our system[8].

Because the distribution of magnetic moments does not guarantee 6-fold rotations or 3-fold rotations of the form $\{U_{\boldsymbol{n}}(\pi)||C_z(\pi/3)|\boldsymbol{\tau}\}$ or $\{U_{\boldsymbol{n}}(\pi)||C_z(2\pi/3)|\boldsymbol{\tau}\}$, the rotations of the highest order of the system are still two fold rotations. Thus, the nontrivial spin space group of this system can be written as the magnetic space group, ${P_B}^2{2_1}^2{2_1}^22$. From Ref. [8], the trivial spin space group of this collinear magnetic system is unique to be $SO(2) \times Z_2^K$. Then, the full spin space group of this system can be written as product of these two groups $({P_B}^2{2_1}^2{2_1}^22)(SO(2) \times Z_2^K)$. By selecting the proper nontrivial part of this group, we can write the group as direct product of a trivial group and a nontrivial group, $({P_B}^1{2_1}^1{2_1}^12) \times (SO(2) \times Z_2^K) = {P_B}^1{2_1}^1{2_1}^12^{\infty m}1$, where ${}^{\infty m}1$ represents the trivial part of spin space group $SO(2) \times Z_2^K$. The elements of this full spin group are shown in Table S1.

Note that there could be more than one choice of the nontrivial part of a spin space group, such that the full spin space group can be written as the direct product of the nontrivial one with a trivial group. In the case of spin space group ${P_B}^1{2_1}^1{2_1}^12^{\infty m}1$, by replacing every time reversal operation contained in the elements of the group ${P_B}^1{2_1}^1{2_1}^12$ to a spin rotation $U_{\boldsymbol{y}}(\pi)$ (or any other spin rotations $U_{\boldsymbol{n}}(\pi)$, with $\boldsymbol{n} \parallel cos\varphi\hat{y} + sin\varphi\hat{z}, \varphi \in (0, \pi]$), the resulting group still commutes with ${}^{\infty m}1$, thus we can write the full spin space group as the direct product of this group with ${}^{\infty m}1$.

Table S1. Group elements of the magnetic space group and spin group describing $CoNb_3S_6$.

	Spin space group	Group elements
w/ SOC	${P_B}^2{2_1}^2{2_1}^22$	H: $\{E\|\|E\|0\}, \{U_x(\pi)\|\|\mathrm{C}_x(\pi)\|0\}, \{U_y(\pi)\|\|\mathrm{C}_y(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{b}+\boldsymbol{c})/2}\}, \{U_z(\pi)\|\|\mathrm{C}_z(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{b}+\boldsymbol{c})/2}\}$

		M: $\{T\|\|E\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{b})/2}\},\{TU_x(\pi)\|\|\mathrm{C}_x(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{b})/2}\},$ $\{TU_y(\pi)\|\|\mathrm{C}_y(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{c})/2}\},\{TU_z(\pi)\|\|\mathrm{C}_z(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{c})/2}\}$
w/o SOC	Nontrivial: $P_B{}^1 2_1{}^1 2_1{}^1 2$	H: $\{E\|\|E\|0\},\{\mathrm{E}\|\|\mathrm{C}_x(\pi)\|0\},$ $\{E\|\|\mathrm{C}_y(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{c})/2}\},\{E\|\|\mathrm{C}_z(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{c})/2}\}$ M: $\{T\|\|E\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{b})/2}\},\{T\|\|\mathrm{C}_x(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{b})/2}\},$ $\{\mathrm{T}\|\|\mathrm{C}_y(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{b}+\boldsymbol{c})/2}\},\{\mathrm{T}\|\|\mathrm{C}_z(\pi)\|\boldsymbol{\tau}_{(\boldsymbol{b}+\boldsymbol{c})/2}\}$
	Trivial: ${}^{\infty m}1$	$\{TU_n(\pi)\|\|E\|\|0\}\ (n \parallel cos\varphi\hat{y} + sin\varphi\hat{z}, \varphi \in (0,\pi])$ $\{U_x(\theta)\|\|E\|\|0\}\ (\theta \in (0,2\pi])$

$\boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{b})/2} = (1/2,1/2,0), \boldsymbol{\tau}_{(\boldsymbol{b}+\boldsymbol{c})/2} = (0,1/2,1/2), \boldsymbol{\tau}_{(\boldsymbol{a}+\boldsymbol{c})/2} = (1/2,0,1/2)$;

H/M: elements with/without time-reversal symmetry.

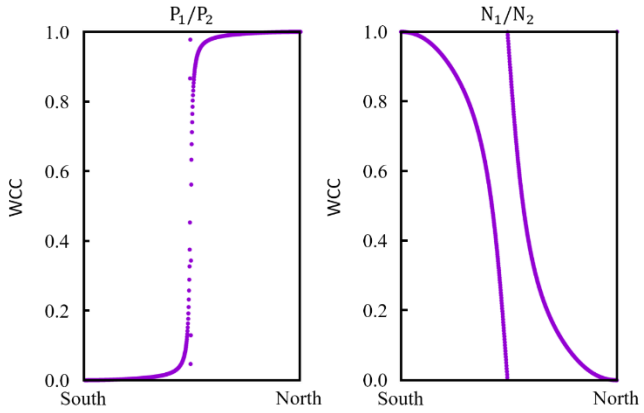

Fig. S1. Evolution of Wannier charge centers (WCCs) calculated on a spherical surface enclosing $\mathrm{P}_1/\mathrm{P}_2$ and $\mathrm{N}_1/\mathrm{N}_2$. The calculation results show that the Dirac points P_1 and P_2 have chirality $+2$ and the Dirac points N_1 and N_2 have chirality -2.

Note S4. The other material candidates

In Table S2 we provide the list of flavor Weyl materials according to the symmetry filters. Such procedure has screened out 62 material candidates. Then, we further carry out DFT calculations on these candidates without considering spin-orbit coupling. In this step,

we rule out the materials that are insulating, and focus on the flavor Weyl point near the Fermi level (within ~1 eV around the Fermi level).

Table S2. Collinear antiferromagnetic materials realizing flavor Weyl semimetal. The label and chemical formula in the table are from the Bilbao MAGNDATA database.

1.32:Lu_2MnCoO_6	1.565:Pb_2CoOsO_6	1.429:$BaFe_2Se_3$	1.184:$Na_2Co_2TeO_6$
1.330:Lu_2CoMnO_6	1.592:Pb_2NiOsO_6	1.111:GdBiPt	1.192:$SmMn_2O_5$
1.438:$BaCoF_4$	1.325:$PrMn_2O_5$	1.232:CuMnSb	1.335:Nd_2Pd_2In
1.64:$BaNiF_4$	1.374:HoNiGe	1.58:$La_2O_2Fe_2OSe_2$	1.586:PrFeAsO
1.100:Cu_2MnSnS_4	1.583:$La_{1.5}Ca_{0.5}CoO_4$	1.120:$BaFe_2Se_3$	1.18:MnS_2
1.440:$CrPS_4$	1.55:Na_2MnF_5	1.79:Li_2CoSiO_4	1.439:$BaCoF_4$
1.459:$CeFe_3(BO_3)_4$	1.136:$AgCrS_2$	1.589:$Fe_{0.967}Nb_3S_6$	1.472:CaOFeS
1.7:$NdFe_3B_4O_{12}$	1.561:$GeNi_2O_4$	1.349:$CoNb_3S_6$	1.71:$SrCo_2V_2O_8$
1.90:$YFe_3(BO_3)_4$	1.563:$GeNi_2O_4$	1.50:$AgNiO_2$	1.101:LuMnO3
1.20:$HoMnO_3$	1.341:$TmMnO_3$	1.86:GeV_4S_8	1.298:$BaCdVO(PO_4)_2$
1.263:$Ca_3Ru_2O_7$	1.33:ErAuGe	1.504:GdCuSn	1.505:GdAgSn
1.506:GdAuSn	1.353:$SmNiO_3$	1.354:$EuNiO_3$	1.43:$PrNiO_3$
1.45:$NdNiO_3$	1.463:$Sr_2Fe_3Se_2O_3$	1.172:$NiTa_2O_6$	1.281:$YBaCuFeO_5$
1.24:ZnV_2O_4	1.574:NdBiPt	1.156:$LaMn_3Cr_4O_{12}$	1.165:Ni_3TeO_6
1.581:$FeTiO_3$	1.91:$TbFe_3(BO_3)_4$	1.233:CuMnSb	1.265:CuMnSb
1.424:UCu_5	1.275:$Ba_6Co_6ClO_{15.5}$		

Except for $CoNb_3S_6$, we show another representative candidate, i.e., GdCuSn, for ideal flavor Weyl points near the Fermi level. GdCuSn adopts an orthorhombic crystal structure and a collinear AFM order with the magnetic moments originated from Gd 4f electrons (Supplementary Fig. S2a). Different from $CoNb_3S_6$, GdCuSn is nonchiral, yet supporting flavor Weyl points. We thus plot its band structure in the AFM phase (Fig. S2b) and identify two inequivalent flavor Weyl points occurring at the generic momenta, as shown in Figs. S2c-S2f. Each of the two Weyl points represents four equivalent flavor Weyl points connected by nonsymmorphic glide reflection symmetries with the glide mirrors perpendicular to the x and y axis.

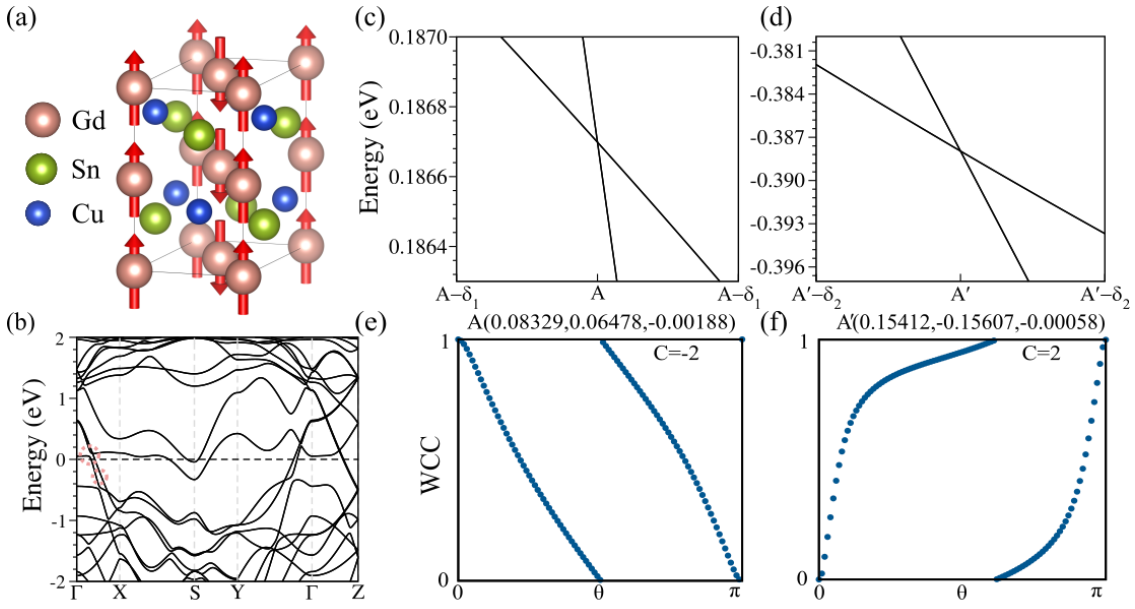

Figure S2: (a) The crystal and collinear AFM magnetic structure of GdCuSn. The red arrow denotes the direction of the magnetic moment. (b) The band structure of GdCuSn without spin-orbit coupling. The black dashed line and pink dashed circles denote the Fermi level and the rough positions of the flavor Weyl points, respectively. (c,e) the electronic structure near the flavor Weyl point. There are four flavor Weyl points at ~ 0.19 eV above the Fermi level which are labeled by A, and another four flavor Weyl points at ~ 0.39 eV below the Fermi level A'. Note that . (e,f) The Wannier charge centers (WCCs) of the flavor Weyl points and their Chern numbers.

Supplementary References

1. For simplicity, we only consider the orthochronous part of the Lorentz group because time-reversal symmetry is not relevant for the discussion of the conventional and chiral Dirac fields.
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