

Weyl nodes in CeRu₄Sn₆ studied by dynamical mean field theory

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 (Received 27 August 2025; revised 16 January 2026; accepted 26 January 2026; published 23 February 2026)

The heavy fermion compound CeRu₄Sn₆ was recently shown to exhibit a spontaneous nonlinear Hall effect, indicating its topological nature. This is consistent with the lack of inversion symmetry that allows for the existence of Weyl nodes. Here, we employ density functional theory combined with dynamical mean field theory, which is state of the art for strongly correlated materials, and study the topology of CeRu₄Sn₆. We find five inequivalent Weyl nodes of either type I or II, each having either 8 or 16 symmetry-related replicas. These Weyl nodes bridge the Kondo insulating gap, which is a direct but not an indirect gap. The Weyl points closest to the Fermi level are situated only 0.5 meV below it and have a very flat dispersion. Our *ab initio* results establish CeRu₄Sn₆ as a model system for investigating the interplay between strong electronic correlations and nontrivial topology. These findings provide a theoretical foundation for future studies of quantum transport and interaction-driven topological phases in heavy fermion systems.

DOI: [10.1103/8wcd-blpn](https://doi.org/10.1103/8wcd-blpn)

I. INTRODUCTION

Quantum materials [1] with nontrivial electronic topology [2–5] are in high demand for next-generation electronic and quantum devices [6,7]. Strongly correlated electron systems represent fertile ground for emergent quantum phases, including heavy fermion metals, Kondo insulators, and unconventional superconductors [8]. When strong electronic interactions interplay with crystalline symmetries, correlation-driven topological phases may arise [9]. They can be gapped, like in topological Kondo insulators [10,11], or gapless, like in topological Kondo semimetals [8,12,13]. Intriguing properties have been put forward in several candidate materials, including bulklike excitations [14] and heavy surface states [15] in the mixed-valent insulator [16,17] SmB₆, a giant spontaneous Hall effect in the Kondo semimetal Ce₃Bi₄Pd₃ [18], and a colossal anomalous Nernst effect in the ferromagnet UC_{0.8}Ru_{0.2}Al [19]. The many-body physics thought to underlie these interesting quantum phenomena make a theoretical description challenging, in particular with *ab initio* methods.

Of direct pertinence to the present work is the Weyl-Kondo semimetal [18,20–22]. Theoretically, this new phase was introduced through a study of the periodic Anderson model on a noncentrosymmetric lattice. In this case, the space group symmetry constraints on the Kondo-driven low-energy

electronic states create Weyl nodes of heavy quasiparticles at the Fermi level and span the underlying Kondo insulator gap [21,22]. Experimentally, the linearly dispersing ultraflat electronic bands associated with this state were identified by specific heat measurements [20], and evidence for Weyl nodes—sources and sinks of Berry curvature—near the Fermi energy was provided by a giant spontaneous Hall signal [18]. Furthermore, magnetic field-tuning experiments revealed the annihilation of Weyl nodes at a topological quantum phase transition before the underlying narrow Kondo insulator gap closes at a larger field [23].

Here, we study the compound CeRu₄Sn₆, which crystallizes in a noncentrosymmetric tetragonal crystal structure of the space group $I\bar{4}2m$ (No. 121) [24]. Early electrical resistivity [25] and optical conductivity data [26] on single crystals and NMR data on powder [27] led to the interpretation of CeRu₄Sn₆ as a “failed” Kondo insulator. With decreasing temperature, a Kondo insulator gap starts to form but ultimately fails to develop fully, leading to a semimetallic ground state. Later, from a treatment using density functional theory (DFT) plus the Gutzwiller approximation, it was proposed that CeRu₄Sn₆ might be a correlated Weyl semimetal [28]. Most recently, the hallmark of a strongly correlated Weyl semimetal—a giant spontaneous nonlinear Hall effect [13,18] originating from the Berry curvature monopoles at Weyl nodes near the Fermi energy [20–22]—was indeed identified in low-temperature experiments on CeRu₄Sn₆ [29].

Furthermore, the low-temperature electronic specific heat of CeRu₄Sn₆ was understood as a convolution of quantum critical and T^3 contributions [29]. The latter is another key signature of the Weyl-Kondo semimetal [20–22]: It is direct evidence of the linear Weyl dispersion, with Weyl nodes pinned to the Fermi energy, and a prefactor that allows for the extraction of the Weyl velocity. Just as in Ce₃Bi₄Pd₃ [20], the Weyl velocity of CeRu₄Sn₆ is experimentally found to be less

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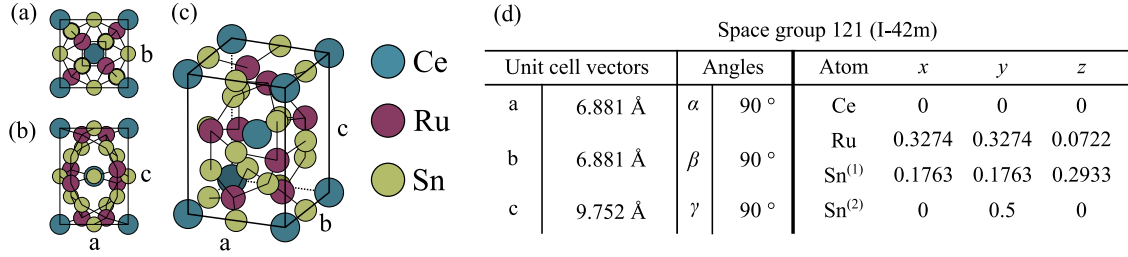


FIG. 1. Crystal structure of CeRu₄Sn₆. (a) and (b) show projections of the crystal structure along the (001) and (010) directions, respectively; (c) shows a three-dimensional view of the unit cell. In (d), the atomic coordinates are expressed in units of the lattice vectors. The crystallographic parameters are taken from [24].

than 1 km/s, orders of magnitude lower than in noninteracting systems [29].

Motivated by these findings, we investigate the situation employing state-of-the-art DFT plus dynamical mean field theory (DMFT) [30–35] and follow the Berry curvature to detect the Weyl nodes. We find that the hybridization between Ce 4*f* and conduction electrons leads to a direct (but not an indirect) gap throughout the Brillouin zone. However, this direct gap is bridged along some low-symmetry directions by 64 Weyl nodes.

This paper is organized as follows: In Sec. II we briefly recapitulate the computational methods used, discussing the DFT + DMFT approach in Sec. II A and the Weyl node search algorithm in Sec. II B. In Sec. III we present the results obtained, starting with the DFT + DMFT spectra and self-energies in Sec. III A before turning to the topological properties in Sec. III B. Section IV summarizes our results, and the Appendix lists the symmetry operations for obtaining all 64 Weyl nodes from the five inequivalent ones.

II. COMPUTATIONAL DETAILS

A. DFT + DMFT

As the first step of our DFT + DMFT study, the electronic band structure of CeRu₄Sn₆ is calculated using the FPLO code [36] and, for comparison, the WIEN2K [37] full potential linearized augmented plane wave package. The details of the crystal structure of CeRu₄Sn₆ [24] are summarized in Fig. 1. Following previous studies [28,38], we calculate the electronic band structure using the local density approximation with the Perdew-Wang exchange-correlation potential [39] and a dense ($6 \times 6 \times 6$) *k* mesh to determine the electronic band structure. After the calculation converges, we take the resulting ground state density as the starting point for another self-consistent computation, where we increase the *k* mesh to ($12 \times 12 \times 12$). This computation converges immediately, which confirms that the initial *k* mesh is sufficient. All calculations were performed in a fully relativistic framework, with spin-orbit coupling explicitly included.

To simplify our DMFT calculations and to improve numerical accuracy, we employ a tight-binding Hamiltonian based on the FPLO calculation. The tight-binding parametrization is motivated by the fact that subsequent calculations involve extensive sampling at different *k* points, where the reduced basis significantly improves computational efficiency. The new basis consists of 90 orbitals, giving a 90×90 Hamiltonian

matrix. These orbitals are Ce 4*f* orbitals (total of 14: 6 $f_{5/2}$ and 8 $f_{7/2}$ orbitals), Ru 4*d* orbitals (total of $4 \times 10 = 40$: 4×6 $d_{5/2}$ and 4×4 $d_{3/2}$ orbitals), and Sn 5*p* orbitals (total of $6 \times 6 = 36$ orbitals: 6×4 $p_{3/2}$ and 6×2 $p_{1/2}$ orbitals).

The energy range spanned by all orbitals extends from -5 to 5 eV, which is sufficient to capture the relevant electronic behavior near the Fermi level. Since the six Ce $4f_{5/2}$ orbitals and the Sn and Ru orbitals that hybridize with them near the Fermi level are essential for accurately describing the low-energy Weyl points, a reduction to a model containing only a few orbitals is, unfortunately, not feasible. The full Hamiltonian is available in the dataset accompanying this paper.

This tight-binding Hamiltonian is supplemented by a Coulomb interaction *U* for the Ce $4f_{5/2}$ manifold. Since the Ce $4f_{7/2}$ bands are above the Fermi energy, we treat their interaction in a static way as a Hartree-like shift and treat only that of the Ce $4f_{5/2}$ manifold dynamically. The intraorbital (*U*) and interorbital (*V*) Coulomb interaction potentials are set to the same value of 5.5 eV for the Ce $4f_{5/2}$ bands, consistent with values used in the literature [38]. Consequently, the Hund’s coupling is set to zero [$J = (U - V)/2 = 0$], which is justified to some extent by the fact that Ce is in a $4f^1$ configuration. Hence, the Hund’s exchange is relevant for only excited states and multiplet admixing. To avoid double counting correlation effects that are partially included in the DFT functional, they are subtracted using the Anisimov formula $V_{DC} = U(\langle n \rangle - \frac{1}{2})$ [40]. For CeRu₄Sn₆, with a Ce 4*f* shell filling of $\langle n \rangle \approx 0.73$ from DFT calculations, this correction is $V_{DC} = 1.27$ eV.

Subsequently, the previously defined Hamiltonian is solved by DMFT using the open-source code W2DYNAMICS [41], with continuous-time quantum Monte Carlo (QMC) in the hybridization expansion [42] as a DMFT impurity solver. In DMFT, the complex many-body problem is mapped onto an effective Anderson impurity model that is solved self-consistently [31,32] (see the schematics in Fig. 2). Here, the Anderson impurity model consists of the six interacting Ce $4f_{5/2}$ orbitals coupled to the same number of auxiliary bath sites, which are together described by $\mathcal{G}_0$ in Fig. 2. This noninteracting $\mathcal{G}_0$ is supplemented by the local Coulomb interaction *U*, and the thus defined impurity model is solved (here by QMC). In this way DMFT captures the local electronic correlations of the Ce $4f_{5/2}$ orbitals, and from the solution of the impurity, one obtains dynamical, i.e., frequency-dependent, Ce $4f_{5/2}$ self-energies (as mentioned above, for Ce $4f_{7/2}$ a static Hartree shift is sufficient).

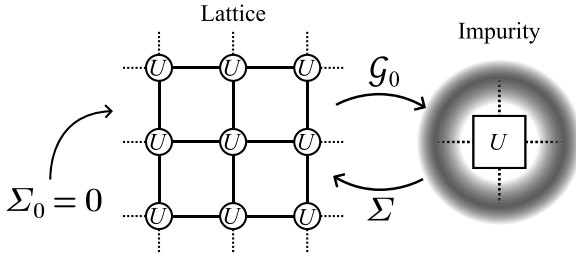


FIG. 2. Self-consistency cycle of dynamical mean field theory. The Dyson equation for the lattice model (left) is solved using the initial self-energy $\Sigma_0 = 0$. The dynamic Weiss field G_0 (i.e., the noninteracting impurity Green's function) is then extracted (see text) and supplemented by the same on-site Coulomb potential U as in the lattice model. The thus defined Anderson impurity model (right) is solved and a local (impurity = lattice) self-energy Σ is obtained. This self-energy is then used in turn as input in the lattice model to update G_0 . The cycle is repeated until the convergence of the self-energy is achieved.

With this DMFT Ce $4f_{5/2}$ self-energy, the Hartree Ce $4f_{7/2}$ self-energy, and zero self-energy for the Ru and Sn orbitals, we then solve the lattice Dyson equation with the DFT-derived 90×90 Hamiltonian to get a 90×90 Green's function. Summing over momenta and projecting onto the Ce $4f_{5/2}$ orbitals yield a local Ce $4f_{5/2}$ Green's function. Through the impurity Dyson equation we obtain a new noninteracting impurity model given by $G_0 = [G^{-1} + \Sigma]^{-1}$ for the six Ce $4f_{5/2}$ orbitals. This impurity model is solved again and again until convergence. For further details on DFT + DMFT, see, e.g., [35].

The combined DFT + DMFT [35,43,44] approach enables the extraction of momentum-resolved spectral functions, self-energies, and renormalized bands for real materials [34,35]. Furthermore, it is possible to extract topological features from the renormalized band structures, such as Weyl points and surface states for finite-volume systems.

The DMFT loop is iterated for 10 self-consistency steps. In each step, 2×10^8 QMC warm-up and 10^7 measurement sweeps are performed. This procedure is independently repeated at multiple temperatures T to capture the thermal evolution of the correlated electronic structure. The calculations are in the paramagnetic phase, which correctly captures the experimental situation [29]. After completion of the DMFT iterations, we obtain Green's functions $G(i\omega_n)$ and self-energies $\Sigma(i\omega_n)$ at Matsubara frequencies $i\omega_n = (2n + 1)\pi/\beta$ for the correlated Ce $4f_{5/2}$ orbitals. These $G(\text{in})$ and (in) are then analytically continued to real frequencies ω using the open-source maximum entropy analytical continuation package ANA_CONT [45]. The spectral function $A(\omega)$ is connected to $G(\omega)$ through the relation $A(\omega) = -\frac{1}{\pi} \text{Im}G(\omega)$.

To represent the many-body effects of DMFT, we further employ a quasiparticle renormalization of the DFT bands by expanding Green's functions around the Fermi level. The quasiparticle weight Z for the different Ce $4f_{5/2}$ states is calculated from the real part of the self-energy:

$$Z = \left(1 - \frac{\partial \text{Re}\Sigma(\omega)}{\partial \omega} \bigg|_{\omega=0} \right)^{-1}. \quad (1)$$

The quasiparticle representation then yields the renormalized Hamiltonian matrix

$$H_{\text{qp}}(\mathbf{k}) = \sqrt{Z}[H(\mathbf{k}) + \text{Re}\Sigma(0) - \mu\mathbb{I} - V_{\text{DC}}]\sqrt{Z}. \quad (2)$$

Here, $H(\mathbf{k})$ is the original tight-binding Hamiltonian matrix, and $\mathbb{I}$ is the identity matrix; Z , $\text{Re}\Sigma(0)$, and V_{DC} are in (diagonal) matrix form and have only nonzero elements for the Ce $4f_{5/2}$ manifold. With $H_{\text{qp}}(\mathbf{k})$, the quasiparticle Green's function

$$G_{\text{qp}}(\omega, \mathbf{k}) = Z \cdot [\omega - H_{\text{qp}}(\mathbf{k})]^{-1} \quad (3)$$

is then used to compute $\mathbf{k}$ -resolved quasiparticle spectral functions and to determine the topology of the DFT + DMFT electronic structure.

B. Weyl node search algorithm

An important quantity defining the Weyl nodes is the Berry curvature $\Omega_n(\mathbf{k})$, which characterizes the geometrical structure of Bloch bands. For a given band n , the Berry curvature is defined as a curl of the Berry connection $A_n(\mathbf{k})$ [46]:

$$\Omega_n(\mathbf{k}) = \nabla \times A_n(\mathbf{k}), \quad (4)$$

with

$$A_n(\mathbf{k}) = i \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n\mathbf{k}} \rangle. \quad (5)$$

Here, $u_{n\mathbf{k}}$ is the periodic part of the Bloch function for the n th band. The topological “charge” of the Weyl nodes is defined by the Chern number, which is computed by integrating $\Omega_n(\mathbf{k})$ over a closed surface S :

$$C_n = \frac{1}{2\pi} \oint_S \Omega_n(\mathbf{k}) dS. \quad (6)$$

Weyl nodes come in pairs, characterized by their Chern numbers C_n : +1 for a source and −1 for a sink of the Berry curvature $\Omega_n(\mathbf{k})$ in $\mathbf{k}$ space. This behavior is analogous to magnetic monopoles and electric charges in real space.

There are various methods to find Weyl nodes. The brute-force approach is to take the full lattice cell, subdivide it into smaller pieces, and compute the Berry flux in each cell. If they are small enough to have only one Weyl node per cell, it is possible to pinpoint the location of these nodes by continuously making the cells smaller. However, this method is numerically demanding, especially if the nodes are relatively close to each other, and very small cells can be prone to numerical inaccuracies when the Berry flux is calculated.

We use a more efficient method that is visualized in Fig. 3 and is available as part of the TIGHTBINDINGTOOLBOX [47]. It has been employed successfully to identify Weyl points in the heavy fermion compound Ce₃Bi₄Pd₃ [48]. The locations of the Weyl nodes are obtained by introducing particles with Chern “charge” at random starting points in the Brillouin zone, which then follow the Berry curvature. Depending on this charge, the particles will approach the nodes with either $C_n = +1$ or $C_n = -1$. This resembles the motion of charged test particles toward an opposite charge at a fixed position. In this way, it is possible to obtain accurate locations of the Weyl nodes at much lower computational costs.

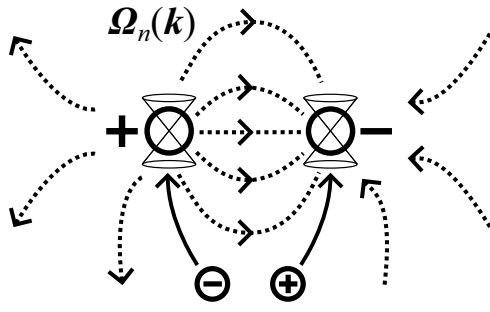


FIG. 3. Schematic representation of the Weyl node search algorithm [47]. Randomly placed “particles” with Chern positive or negative “charges” ($\oplus$, $\ominus$) are created and follow the Berry curvature “field lines” $\Omega_n(\mathbf{k})$ (dotted lines) toward the Weyl points (symbolized by a circle with a cone dispersion). Depending on the charge of the particles, they will move toward Weyl nodes with Chern numbers of $+1$ or -1 .

III. RESULTS

A. DFT + DMFT calculations

Figure 4 shows the DMFT-computed spectral functions for the Ce $4f_{5/2}$ orbitals at three different temperatures: 290, 97, and 23 K. As the temperature decreases, a spectral peak develops at the Fermi energy and strongly increases in height for the $m_j = \pm 3/2, \pm 1/2$ components [see Figs. 4(e) and 4(f)]. This behavior is characteristic of the gradual formation of the Kondo resonance at low temperatures, which in our case is saturated at 23 K [the spectral function at 50 K (not shown) is essentially the same as that for 23 K]. In contrast, the $m_j = \pm 5/2$ components exhibit a significantly weaker temperature dependence, showing only minor changes in the studied energy range [Figs. 4(a) and 4(d)].

Figure 5 presents the real and imaginary parts of the self-energy for different m_j projections of the Ce $j = 5/2$ manifold. At room temperature, each m_j component shows

different intensities and pole positions. The latter correspond to a (damped) $1/\omega$ behavior of the real part of the self-energy in Fig. 5(a) and a maximum in the imaginary part in Fig. 5(c). These poles lead to a correlation-induced splitting of the DFT bands. Here, two poles split off the Hubbard bands from the quasiparticle band, and the one for $\omega > 0$ is more pronounced since the splitting between the quasiparticle band and the upper Hubbard band is larger (which requires a larger prefactor of the $1/\omega$ pole). The $m_j = \pm 1/2$ component exhibits minor glitches near $\omega = 0$, which likely arise from numerical artifacts in the analytic continuation.

At lower temperatures (23 K), the pole of $\Sigma(\omega)$ for $m_j = \pm 1/2$ is shifted to higher energies [Fig. 5(b)], and the region where $\text{Im}\Sigma(\omega)$ is small at the Fermi energy becomes broader [Fig. 5(d)]. This indicates enhanced quasiparticle lifetimes, concomitant with the development of a sharp Kondo resonance. The self-energy of the other orbitals ($m_j = \pm 5/2, \pm 3/2$) becomes nearly degenerate at lower temperatures.

From the DMFT self-energy, we computed Z and $\text{Re}\Sigma(0)$ for each m_j projection of the Ce $4f_{5/2}$ manifold at two temperatures: 290 and 23 K. For the results, see Table I. In all cases Z remains similar and approximately 0.1. On the other hand, $\text{Re}\Sigma(0)$ is nearly temperature independent for the $m_j = \pm 1/2$ bands, while it is largest for the $m_j = \pm 5/2$ manifold. For $m_j = \pm 3/2, \pm 5/2$, $\text{Re}\Sigma(0)$ becomes smaller as the temperature is reduced. Also shown in Table I is the occupation of these different $4f$ orbitals. With decreasing temperature, we see that the $m_j = \pm 1/2$ occupation increases toward half filling, whereas the other orbitals depopulate. This agrees with previous DFT + DMFT calculations at higher temperatures [38] and x-ray spectroscopy [49].

Figure 6 shows the $\mathbf{k}$ -resolved spectral function at 290 and 23 K. The original DFT bands are overlaid; they are gapped, representing an insulator. Importantly, they fail to describe the correlated spectral function $A(\omega, \mathbf{k})$ around the Fermi energy. The reason is that they lack the Kondo resonance

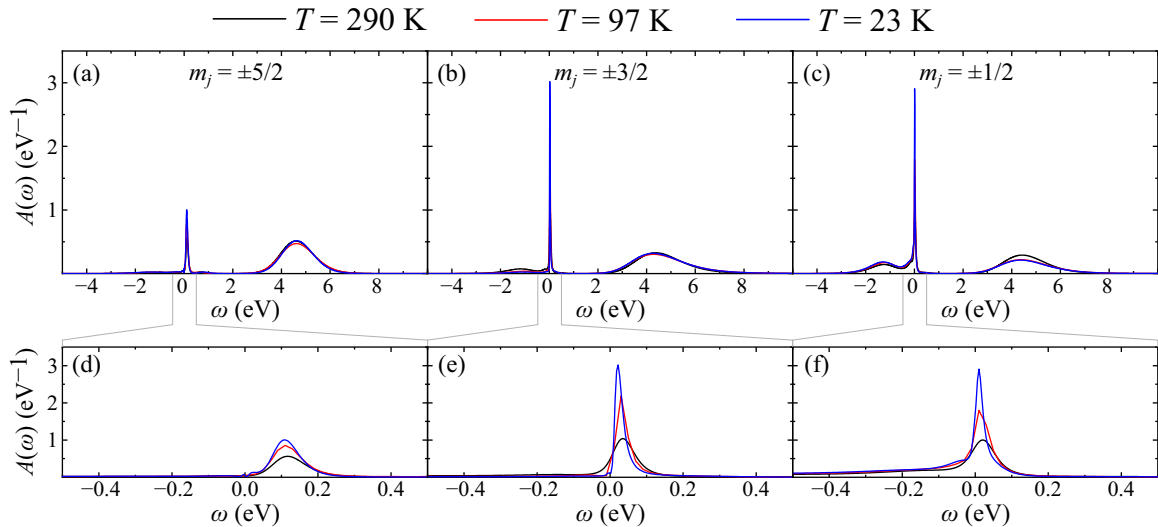


FIG. 4. DMFT spectral functions $A(\omega)$ for the 3×2 Ce $4f_{5/2}$ states at three different temperatures: $T = 290$ K (black), $T = 97$ K (red), and $T = 23$ K (blue). Results are resolved by total angular momentum projections: (a) and (d) $m_j = \pm 5/2$, (b) and (e) $m_j = \pm 3/2$, and (c) and (f) $m_j = \pm 1/2$. The graphs in (a)–(c) show the full energy range, while (d)–(f) are zoomed-in views near the Fermi energy.

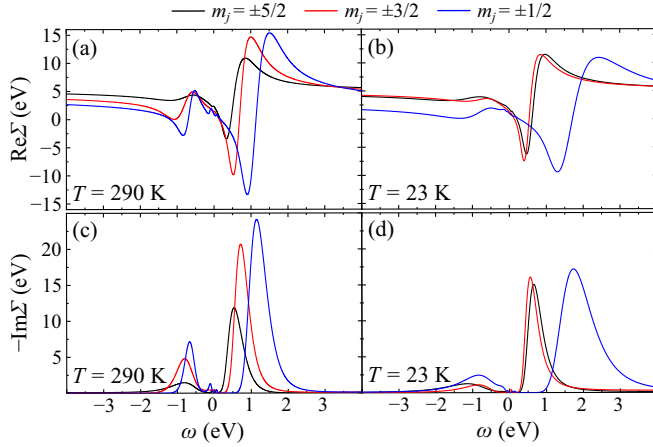


FIG. 5. (a) and (b) Real and (c) and (d) imaginary parts of the DMFT self-energy $\Sigma(\omega)$ at two different temperatures: (a) and (c) 290 K and (b) and (d) 23 K. Results are resolved for different m_j of the Ce $4f_{5/2}$ manifold.

(or quasiparticle peak). In contrast, the overlaid renormalized quasiparticle bands provide a reliable representation of the many-body spectral function at low energies.

At $T = 23$ K [Fig. 6(b)], within the low-energy quasiparticle band, a direct gap of ~ 5 meV appears at most wave vectors across the Brillouin zone, in excellent agreement with experiments [27]. This gap becomes visible only at low temperatures, where lifetimes are long enough that the resolution of the bands improves. The reason for the gap opening is the hybridization of the Ce $4f$ states with the conduction bands—the hallmark of a Kondo insulator. However, because the gap is very small and the bands disperse, there is no indirect band gap across the entire Brillouin zone: From Fig. 6, as well as the m_j -resolved spectrum in Fig. 7, it can be seen that there are bands that cross the Fermi level.

As we will show in Fig. 9 below, electronic correlations also lead to *topological* band crossings of the Kondo insulator gap, with a linear dispersion around the Weyl points. These Weyl points do not, however, lie on the high-symmetry lines displayed in Fig. 6. Note that in Ref. [38], which used Hirsch-Fye QMC as the DMFT impurity solver, such low temperatures could not be reached. The use of continuous-time QMC and the improved Weyl node search algorithm are essential for the advance presented here.

TABLE I. Calculated quasiparticle parameters and electron filling for the full Ce $4f_{5/2}$ manifold from DMFT calculations at two different temperatures: 290 and 23 K. The chemical potential μ is for the 90-orbital basis set.

T (K)	m_j	μ (eV)	Z	$\text{Re}\Sigma(0)$ (eV)	$\langle n \rangle$
290	$\pm 1/2$	-0.080	0.132	0.951	0.569
	$\pm 3/2$		0.107	1.336	0.293
	$\pm 5/2$		0.126	2.217	0.096
	$\pm 1/2$		0.112	1.013	0.734
23	$\pm 3/2$	-0.059	0.104	1.257	0.095
	$\pm 5/2$		0.123	1.754	0.107
	$\pm 1/2$				

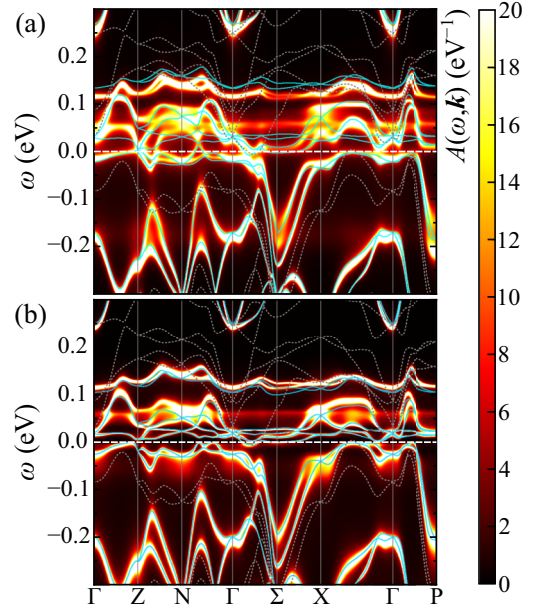


FIG. 6. Total DMFT spectral function $A(\omega, \mathbf{k})$ of all bands at (a) 290 K and (b) 23 K. Overlaid white dashed lines are the initial DFT bands; blue solid lines are the renormalized quasiparticle bands. The latter are in good agreement with the DMFT $A(\omega, \mathbf{k})$ around the Fermi energy.

B. Topological analysis

The search for Weyl nodes in CeRu₄Sn₆ at the Fermi level is carried out using the Weyl node search algorithm from [47]. We focus on the physically most relevant Ce $4f_{5/2}$ orbital with $m_j = (-)1/2$ and use the renormalized quasiparticle Hamiltonian (2) with DMFT self-energy at $T = 23$ K as the input. Additionally, an FPLO-generated primitive unit cell is used, with all $\mathbf{k}$ points expressed in fractional units of the primitive reciprocal lattice vectors. In total, we identify five inequivalent low-energy Weyl points, which are presented in Table II. Some of them are located above the Fermi level, and others are located below it, with the closest node only 0.5 meV (6 K) below the Fermi level.

With the eight symmetry operations of the D_{2d} point group in real space and pure time reversal in momentum space, the symmetry transformations generate 16 Weyl nodes for every inequivalent Weyl point. However, Weyl points I and IV in Table II are high-symmetry points and thus generate only 8 symmetry-related nodes. All transformation operations are discussed in the Appendix. Some symmetry-related nodes at the same energy and opposite Chern number are relatively close to each other; see $|\Delta \mathbf{k}_{\min}|$ in Table II.

Altogether, this results in a total of $3 \times 16 + 2 \times 8 = 64$ Weyl points, with half carrying a Chern number of +1 and the other half having a Chern number of -1. Not all of them were detected in the DFT+Gutzwiller band structure [28], which could be due to the more advanced DMFT treatment. Note that the Gutzwiller approximation corresponds to a DMFT approximation for the Gutzwiller wave function [50]. Given that Xu *et al.* [28] found Weyl nodes close to high-symmetry lines with, e.g., $k_y \approx 0$ it is also possible that the improved

TABLE II. Fractional coordinates of the inequivalent Weyl nodes in momentum space of a primitive unit cell. Also shown are the total number of symmetry-related nodes N , their type (I or II), the minimal distance $|\Delta\mathbf{k}_{\min}|$ between symmetry-related opposite Chern charge nodes, energy relative to the Fermi level, the geometric mean of the Weyl velocities $(v_x v_y v_z)^{1/3}$, and the Ce $4f_{5/2}$ spectral weight $w_{4f_{5/2}}$. Only one set of nodes with a Chern number of +1 are listed; others can be obtained by symmetry transformations (see the Appendix). Chern numbers are computed by integrating the Berry curvature over a sphere with a radius of 0.01, centered at each node. Node types, node energies, and Weyl velocities are obtained from the band structure in the vicinity of the nodes, with the velocities computed from the linear slope of the bands along Cartesian directions. The spectral weight of Ce $4f_{5/2}$ is extracted from $A(\omega, \mathbf{k})$ at the corresponding node coordinates.

Node	Coordinates	N	Type	$ \Delta\mathbf{k}_{\min} $ ($\text{\AA}^{-1}$)	Energy (meV)	$(v_x v_y v_z)^{1/3}$ (km/s)	$w_{4f_{5/2}}$ (%)
I	[+0.032, -0.179, -0.032]	8	I	0.1442	-1.5	51	67
II	[+0.043, -0.432, +0.448]	16	I	0.3245	22.1	10	81
III	[+0.244, -0.127, +0.060]	16	I	0.0021	-0.5	7	77
IV	[-0.127, +0.127, -0.038]	8	I	0.0519	-3.8	17	81
V	[+0.125, +0.001, -0.003]	16	II	0.0861	12.2	26	67

search algorithm used in the present work helped us identify more Weyl points.

Figures 8(a) and 8(b) display the Weyl points in a projection onto $k_z = 0$ and $k_y = 0$, respectively. Blue and green circles indicate Chern numbers of +1 and -1; overlaid are the projected DMFT spectral functions computed at the Fermi energy. For both the Weyl points and the spectrum, the projections respect the D_{2d} symmetries around the $k_x = k_y$ and

$k_x = -k_y$ planes. The density of the Weyl nodes is larger in the vicinity of the Γ point.

In Fig. 9, the dispersion around two exemplary Weyl points of types I and II along the k_y direction is shown at 23 K. For both nodes, the band structure exhibits linearly dispersing crossings close to the Fermi energy, forming Dirac conelike structures. The type II Weyl node shown in Fig. 9(b) is tilted

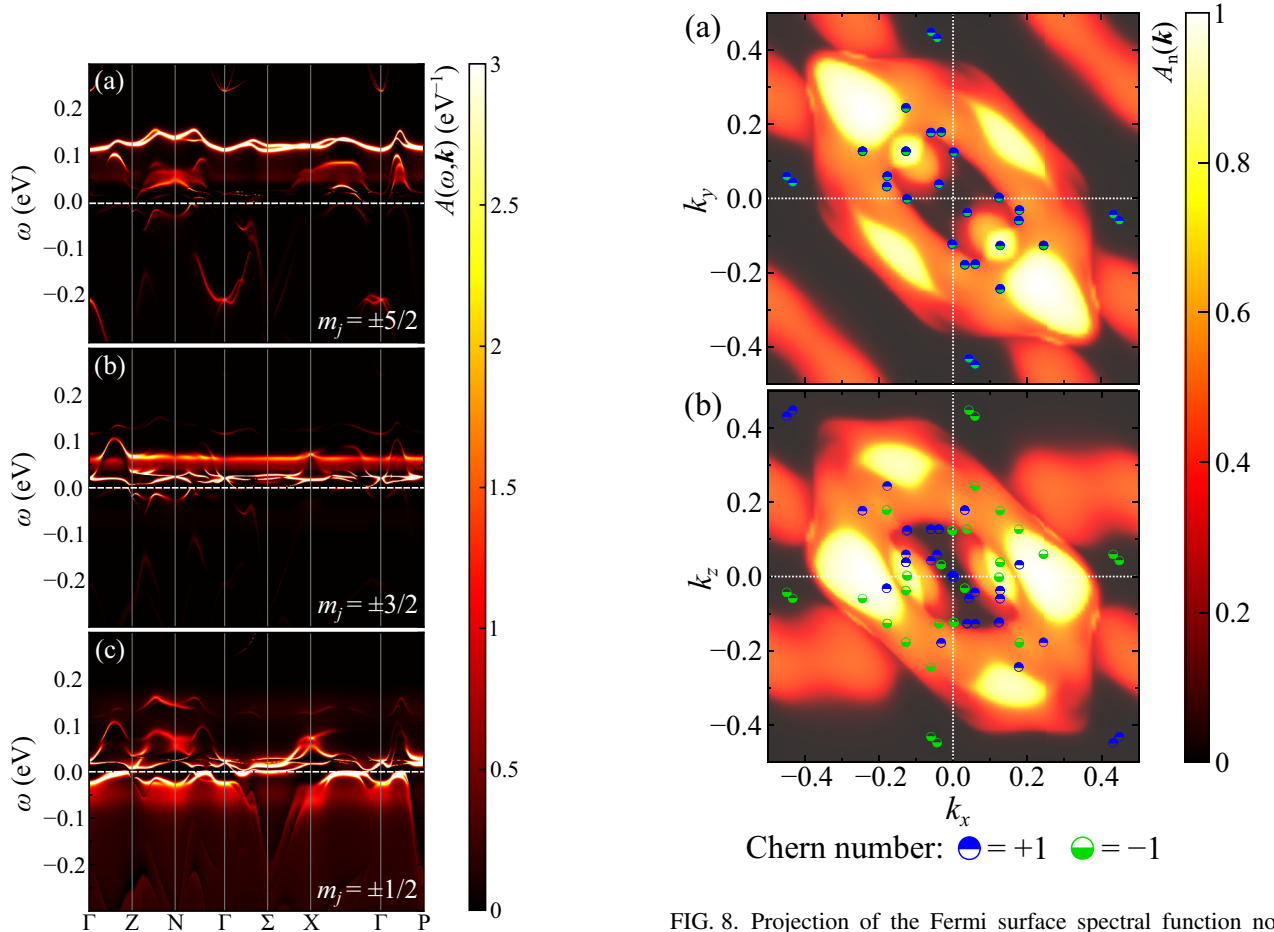


FIG. 7. Contribution of the different Ce $4f_{5/2}$ orbitals to the spectral functions at 23 K: (a) $m_j = \pm 5/2$, (b) $m_j = \pm 3/2$, and (c) $m_j = \pm 1/2$.

FIG. 8. Projection of the Fermi surface spectral function normalized as $A_n(\mathbf{k}) = A(\mathbf{k})/\max[A(\mathbf{k})]$ (a) in the $[k_x, k_y, 0]$ plane and (b) in the $[k_x, 0, k_z]$ plane. Projected Weyl nodes are marked by blue and green circles, corresponding to Chern numbers of +1 and -1, respectively.

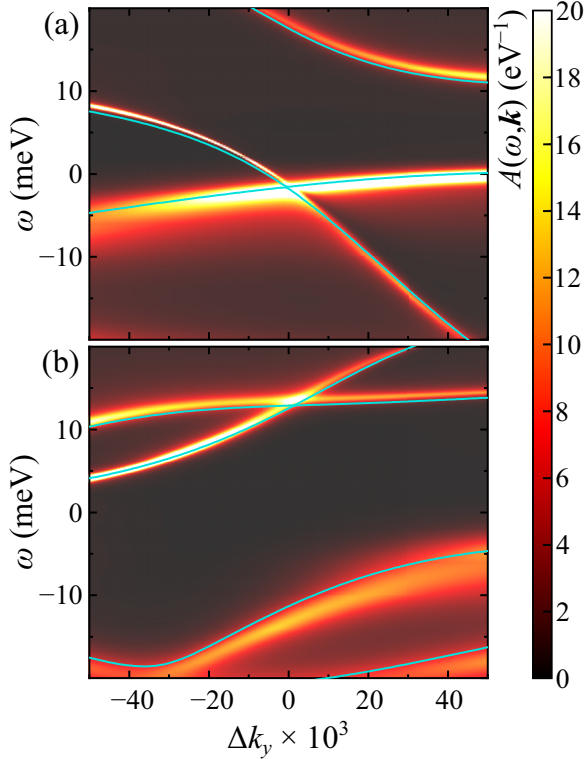


FIG. 9. Quasiparticle bands (lines) and DMFT k -resolved spectral functions (color overlay) in the vicinity of two selected Weyl nodes: (a) type I node at $[0.032; -0.179; -0.032]$ and (b) type II node at $[0.125; 0.001; -0.003]$. Δk_y is the momentum deviation from the nodes along the k_y direction, while other components are held fixed.

along the (shown) k_y direction. Band crossings in Fig. 9 confirm the presence and topological nature of the identified Weyl points.

From the linear dispersion relations near each Weyl point, we computed the geometric mean of the velocities $(v_x v_y v_z)^{1/3}$ (Table II). These values, in some cases below 10 km/s, are orders of magnitude smaller than those in weakly correlated Weyl semimetals. Such reduced velocities enhance the low-temperature density of states and specific heat and can significantly amplify nonlinear transport responses.

Let us also note that the low-energy Weyl points that we identified are within the Kondo resonance. This Kondo resonance—and hence the low-energy Weyl points—emerge due to electronic correlations when the temperature is lowered to the order of the Kondo temperature. Due to the poles of the DMFT self-energy, there are three copies of the DFT Ce $4f_{5/2}$ orbitals in the form of the lower and upper Hubbard bands and the quasiparticle band. These three hybridize with other noninteracting (conduction electron) bands at other k points. As a consequence, the Kondo effect leads to additional and qualitatively different Weyl points compared to the original DFT band structure.

IV. CONCLUSION AND DISCUSSION

We studied the topology of the low-energy quasiparticle bands of CeRu₄Sn₆ using DFT + DMFT. We found five

inequivalent Weyl points, or 64 in total close to the Fermi level, bridging the Kondo insulator gap induced by the hybridization between $4f$ and conduction electrons. Besides the Kondo temperature, which is of the order of 100 K in DMFT, additional energy scales are set by (1) the size of the direct Kondo gap, which is about 5 meV (60 K), (2) the energy range by which the bands above and below this direct Kondo gap cross the Fermi energy, which is up to about 1 meV (12 K), and (3) the distance of the various Weyl points from the Fermi energy, the smallest being 0.5 meV (6 K). This will lead to a complex temperature dependence, as different phenomena become apparent when crossing the various temperature scales.

Experimentally, CeRu₄Sn₆ was evidenced to be an emergent Weyl-Kondo semimetal, exhibiting a spontaneous nonlinear Hall effect below 1 K [29]. It is of the same order of magnitude as the smallest separation of a DMFT Weyl node from the Fermi energy (6 K). There is also overall agreement in terms of the Weyl velocities, which in both experiment and DMFT are reduced by orders of magnitude compared to those of noninteracting Weyl semimetals.

Inelastic neutron scattering experiments [51] further found an ω/T scaling, which motivated an extended DMFT study of a quantum critical Weyl-Kondo semimetal state [29] and indicates Kondo destruction quantum criticality in CeRu₄Sn₆ below a scale of 10 K. While quantum criticality and Kondo destruction can, in principle, be described by DMFT, we have no indications of such physics in our calculations, which describe a Fermi liquid. However, nonlocal correlations that are not included in DMFT can compete with the Kondo effect captured in DMFT. This competition can alter the physics if, with decreasing temperature, nonlocal correlations become strong.

In any case, our theoretical calculations form an *ab initio* basis for understanding the Weyl semimetal nature of CeRu₄Sn₆. It is a strongly correlated “failed” Kondo insulator, with (1) some of the topologically trivial bands crossing the Fermi level and (2) Weyl nodes bridging the Kondo insulator gap. Our work highlights the importance of many-body correlations in CeRu₄Sn₆ and heavy fermion systems in general and offers a framework for investigating interaction-driven topology, nonlinear transport, and quantum criticality across a wider range of materials.

ACKNOWLEDGMENTS

We thank M. Wallerberger, A. Smolyanyuk, D. Kirschbaum, and Q. Si for very helpful discussions. The support of the Research Unit FOR5249 “QUAST” of the Deutsche Forschungsgemeinschaft [Austrian Science Funds (FWF) Grant DOI: 10.55776/15868] and Spezialforschungsbereich (SFB) Q-M and S FWF Grant DOI: 10.55776/F86 is gratefully acknowledged. The computational results were achieved in part using the Austrian Scientific Computing (ASC) infrastructure.

DATA AVAILABILITY

The data that support the findings of this article are openly available [52].

TABLE III. D_{2d} symmetry matrices that transform $\mathbf{k} = (k_x, k_y, k_z)^T$ on its eight symmetrically related replicas, represented in conventional and primitive reciprocal lattice bases, and the transformation effect on the Chern charge.

Symmetry operation	Conventional matrix α	Primitive matrix $B^{-1}\alpha B$	Chern charge
Identity E	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	Unchanged
Twofold rotation around x , C_{2x}	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} -1 & -1 & -1 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	Unchanged
Twofold rotation around y , C_{2y}	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 1 \\ -1 & -1 & -1 \\ 1 & 0 & 0 \end{bmatrix}$	Unchanged
Twofold rotation around z , C_{2z}	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ -1 & -1 & -1 \end{bmatrix}$	Unchanged
Mirror in $x = y$ plane $\sigma_{x=y}$	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\mathcal{C} \rightarrow -\mathcal{C}$
Mirror in $x = -y$ plane $\sigma_{x=-y}$	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & -1 & -1 \end{bmatrix}$	$\mathcal{C} \rightarrow -\mathcal{C}$
Fourfold rotoinversion around z , S_{4z}^+	$\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} -1 & -1 & -1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$	$\mathcal{C} \rightarrow -\mathcal{C}$
Fourfold rotoinversion around z , S_{4z}^-	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 1 \\ -1 & -1 & -1 \\ 0 & 1 & 0 \end{bmatrix}$	$\mathcal{C} \rightarrow -\mathcal{C}$

APPENDIX: D_{2d} SYMMETRY OPERATIONS IN A PRIMITIVE UNIT CELL

To represent the found Weyl nodes, we have chosen a primitive lattice, and we express all momentum coordinates in fractional units of the corresponding reciprocal lattice vectors. In order to convert from this lattice to a conventional lattice, one can change the coordinate system by applying a transformation matrix.

The unit vectors for a primitive cell of CeRu_4Sn_6 are (in Å)

$$\begin{aligned} \mathbf{a}_1 &= (-6.502, +6.502, +6.502), \\ \mathbf{a}_2 &= (+6.502, -6.502, +6.502), \\ \mathbf{a}_3 &= (+9.214, +9.214, -9.214). \end{aligned}$$

The corresponding reciprocal lattice vectors are (in Å⁻¹)

$$\begin{aligned} \mathbf{b}_1 &= (0.000, 0.483, 0.341), \\ \mathbf{b}_2 &= (0.483, 0.000, 0.341), \\ \mathbf{b}_3 &= (0.483, 0.483, 0.000). \end{aligned}$$

The transformation matrix B is constructed by placing the reciprocal vectors as columns:

$$B = \begin{bmatrix} b_{1x} & b_{2x} & b_{3x} \\ b_{1y} & b_{2y} & b_{3y} \\ b_{1z} & b_{2z} & b_{3z} \end{bmatrix} = \begin{bmatrix} 0.000 & 0.483 & 0.483 \\ 0.483 & 0.000 & 0.483 \\ 0.341 & 0.341 & 0.000 \end{bmatrix}.$$

To map a node from primitive cell coordinates to conventional cell coordinates, the node's coordinate vector must be

multiplied by B . This transformation yields the coordinates of the Weyl node expressed in the basis of the conventional reciprocal lattice vectors. It is also possible to go from the conventional lattice basis to a primitive one by inverting B .

D_{2d} symmetry operations also take a different form in the primitive cell. To obtain their representation in reciprocal coordinates consistent with the primitive cell, the conventional symmetry matrices α_C can be transformed as follows:

$$\alpha_P = B^{-1}\alpha_C B. \quad (\text{A1})$$

This procedure ensures that the symmetry operations act correctly on the reduced $\mathbf{k}$ -space coordinates defined in the primitive basis. Additionally, these transformations are consistent with the changes in the Chern charge associated with the Weyl nodes, ensuring that the symmetry operations correctly map not only the node locations but also their corresponding topological characteristics. All eight D_{2d} symmetry operations in both conventional and primitive cells are summarized in Table III, together with the effects on the Chern charge of the Weyl nodes. Furthermore, the time-reversal symmetry relates each Weyl node to a partner with the same Chern charge; its momentum can be obtained by changing the sign of all the momentum components. This operation can be combined with the D_{2d} symmetry transformations discussed above, yielding 16 symmetrically related

Weyl points in total. However, there is a possibility that Weyl nodes are at high-symmetry points. In this case, only some of the 16 points generated by the symmetry operations are equivalent. This occurs for Weyl points I and IV in Table II.

For example, Weyl node I with $\mathbf{k} = [+0.032, -0.179, -0.032]$ and a Chern number of +1 (see Table II) has eight symmetry-related replicas. Applying, for instance, C_{2x} yields

another Weyl node at $\mathbf{k} = [+0.179, -0.032, -0.179]$ (see Table III for a primitive cell) with the same Chern number of +1. Applying other transformations such as mirror symmetry ($\sigma_{x=y}$) also yields symmetry-related Weyl nodes with opposite Chern numbers. Additionally, the combined application of the time reversal and C_{2y} rotation maps the Weyl node onto itself, $\mathbf{k} = [+0.032, -0.179, -0.032]$, due to its high-symmetry position.

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