

Electronic properties of Kagome metal YbV_3Sb_4 : A first-principles study

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We have investigated the vanadium-based Kagome metal YbV_3Sb_4 using density functional theory (DFT) combined with the Wannier function analysis. We explore the electronic properties, de Haas-van Alphen (dHvA) effect, and Fermi surface. Our calculations reveal the metallic characteristic in which the majority of the states around the Fermi energy E_F is contributed by the V-3d orbitals, while the localized Yb-4f states are positioned below it. The inclusion of spin-orbit coupling (SOC) induces the splitting of Yb-4f states, while its impact on the V-3d states is moderate. Furthermore, we have incorporated U + SOC, where the Hubbard parameter, which drastically changes the Yb-4f states, creates additional splitting, leading to three distinct peaks in the density of states (DOS). Meanwhile, the V-3d atoms with the Kagome lattice contribute the maximum to the transport properties, exhibit flat bands near the E_F , while being protected under SOC and U + SOC. Herein, we report the vulnerability of the Yb-4f states under SOC and U + SOC. Furthermore, the Fermi surface is found to comprise quasi-2D cylindrical sheets centered at the Γ point, along with smaller pockets near the Brillouin zone boundaries, which, under combined U + SOC, a small spherical pocket emerges, and the cylindrical sheet exhibits slight deformations. The dHvA frequencies reach as high as 70 kilotesla, which increases with tilt angle, exhibiting a nearly parabolic trend as expected for cylindrical orbits, while a low-frequency branch remains below 1 kilotesla. Only the U + SOC case shows noticeable modification in both the Fermi surface and the dHvA oscillation. Crucially, the Z_2 invariant calculation identifies YbV_3Sb_4 as a strong topological metal ($\nu_0 = 1$). These findings not only advance our understanding of the underlying quantum phenomena in rare-earth Kagome systems, but also establish YbV_3Sb_4 as a compelling and promising platform for exploring intertwined topology and electron correlations in Kagome lattices, thereby offering valuable insights for engineering quantum phases in layered materials.

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I. INTRODUCTION

Kagome materials have been of intensive research interest recently in solid-state physics due to their unique electronic properties, as they provide an opening into various quantum phenomena, including the formation of charge density waves [1], nontrivial topology [2], and superconductivity, among a few [3,4]. The lattice geometry of Kagome materials comprising the Japanese basket weave pattern of interlaced triangles and corner-sharing triangles with geometrically frustrated two-dimensional (2D) lattices plays a key role in the creation of the flat band in the electronic structure, van Hove

singularities, and Dirac cones naturally [5–9]. It also displays tunable Dirac band gaps [10,11], Chern numbers, and Chern gaps [12]. It was recently noted that acoustic Kagome lattices exhibit higher-order non-Hermitian skin effects (NHSE) [13], and in topological invariants, such as the Z_2 invariant [14–16], which further illustrate the interaction between geometry and topology in these systems. The Fermi surface reconstructions revealed by de Haas-van Alphen studies have been used to investigate electronic correlations of Kagome materials [17–21], while nematicity and symmetry-breaking phenomena [22,23] emphasize the role of electronic interactions.

Emergent quantum behaviors, such as the Nernst effect [24–26] and the anomalous Hall effect [27–31] are further revealed by transport measurements, signs of Berry curvature and chiral quasi-particles, and also unconventional superconductivity [32,33] that emerges under doping or pressure. These findings position Kagome materials at the forefront of research into quantum materials, bridging topology, frustration, and strong correlations.

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In addition to the research on the frustrated quantum magnetism of Kagome materials, the recent research interest has been directed towards their electronic, magnetic and topological quantum transport properties. Multiple materials have been found to support Kagome lattices and are seen to exhibit new Kagome-derived phenomena [34]. Some examples having Kagome-type lattices are Fe_3Sn_2 showing giant spin-orbit coupling [10,11], magnetic Weyl semimetals $\text{Co}_3\text{Sn}_2\text{S}_2$ [28,35,36], charge density wave (CDW) ordering compound ScV_6Sn_6 [37], nematicity and multigap superconductivity in titanium-based Kagome metal, CsTi_3Bi_5 [38], FeSn antiferromagnet [39], a skyrmionlike triple-Q state in breathing Kagome lattices [40], Chern-gapped, Dirac fermions in ferromagnetic TbMn_6Sn_6 [12], the noncollinear antiferromagnet in Mn_3Sn [41], and h-BN-induced Kagome ordering in transition metal monolayers on heavy metallic substrates [42]. Recently, a superconducting behavior in quasi two dimensional (2D) Kagome metals AV_3Sb_5 ($A = \text{K}, \text{Rb}, \text{and Cs}$) [43–48] and high-temperature superconductivity in hydrogen-based systems AH_3Li_5 ($A = \text{C}, \text{Si}, \text{P}$) has been reported up to 120 K in PH_3Li_5 under compression [49].

Recently, a novel class of vanadium Kagome bilayer, viz AV_6Sb_6 , AV_3Sb_5 ($A = \text{K}, \text{Rb}, \text{Cs}$) has been reported [50]. Among these new compounds, AM_3X_4 —consisting of A : La, Ce, Sm, Ca, Yb, Eu, Gd; M : V, Ti; X : Sb, Bi—is particularly fascinating. It is distinguished by the presence of zigzag chains made of A -site ions that run parallel to their somewhat-distorted M -based Kagome sublattices [51–56]. Due to the wide variety of A cations available, members of this group include both magnetically ordered and non-magnetic materials. Its crystal structure is significantly more layered, exfoliable, and quasi-2D, making it an intriguing research subject.

In this work, we study the compound YbV_3Sb_4 , a recent addition to the larger AM_3X_4 family. Despite its intriguing structural motifs and the potential emergence of rare-earth physics, YbV_3Sb_4 remains mostly unexplored, with limited experimental reports and first-principles studies to-date. Its distinct structural motifs of vanadium-based Kagome lattices scattered with divalent Yb^{2+} ions arranged in zigzag chains make this compound containing rare-earth atoms an ideal candidate for a thorough investigation. Between 300 K and 60 mK, this compound is found to exhibit no discernible thermodynamic changes and is nonmagnetic [52]. Here, using *ab initio* methods, we examine the electronic characteristics of YbV_3Sb_4 . Utilizing density functional theory, we investigate the dHvA effect, examine the Fermi surface, and utilize Wannier centres to compute the topological invariant Z_2 .

II. COMPUTATIONAL DETAILS

Our *ab initio* calculations were carried out using the FPLO (full potential local orbital) package, version 22.00-62 [57,58]. We employed the Perdew-Burke-Ernzerhof form of generalized gradient approximation (GGA) for the exchange-correlation potential [59,60].

To accurately account for the strong electron interactions among the strongly correlated V $3d$ and Yb $4f$ valence electrons in our system, an effective Hubbard interaction (U_{eff})

TABLE I. Coordinates of the high-symmetry points in the Brillouin zone (BZ) employed for band-structure calculations, expressed in fractional coordinates relative to $2\pi/a$, $2\pi/b$, and $2\pi/c$.

Point	$k_x [2\pi/a]$	$k_y [2\pi/b]$	$k_z [2\pi/c]$
Γ	0	0	0
k1	0.69153348986391	0	0
A	0.3649862854056	0.57144308943088	0
Y	0	0.5714430894309	0
Γ	0	0	0

within the DFT + U approximation has been applied, with fully screened Coulomb and exchange interaction parameters (J). Based on previous studies on Yb-based intermetallics and vanadium compounds [61–66], the parameters were set to $U_{\text{Yb}} = 6.0$ eV, $J_{\text{Yb}} = 0.5$ eV, $U_{\text{V}} = 3.4$ eV, and $J_{\text{V}} = 1.0$ eV. To verify the robustness of this choice, we performed systematic sensitivity tests by varying the Hubbard parameters over a broad range. In particular, U_{Yb} was varied from 5.0–7.0 eV and U_{V} from 2.0–4.0 eV, while keeping the corresponding J values fixed. Additionally, we tested the sensitivity to Hund's exchange by varying J_{Yb} between 0.0–1.0 eV and J_{V} between 0.5–1.5 eV. We find that the low-energy electronic structure near E_F and the main conclusions of this work remain essentially unchanged within these ranges (see Figs. S1 and S2 of the Supplemental Material (SM) [67]). Furthermore, spin-polarized calculations were performed to examine the possible emergence of local magnetic moments. In all tested cases (GGA, GGA + SOC, GGA + U , and GGA + U + SOC), the total moment remains below $0.03 \mu_B/\text{f.u.}$, confirming the absence of a stable long-range magnetic solution within the explored U and J ranges (see Table I and Fig. S3 of the SM [67]).

We relaxed the atomic coordinates until the residual forces on each atom were less than 10^{-3} eV/Å. The convergence criterion was set to 10^{-8} for the charge density and 10^{-8} Hartree for the total computed energy in all calculations. The integration over the Brillouin zone was carried out using the Blöchl-corrected linear tetrahedron approach using a k -points grid of $12 \times 12 \times 12$ points. This k -points mesh was used consistently across both scalar and fully relativistic calculations and for analyzing both the band and densities of states (DOS). Full-relativistic effects, including spin-orbit coupling (SOC), were treated using the FPLO's implementation of the full four-component Dirac formalism [57,58]. The magnetization direction was fixed via the global spin quantization axis setting. Following the established methodology described in [52,68], we adopted the conventional high-symmetry k -path in the Brillouin zone, along which the band structures were computed, as shown in Fig. 1 and in Table I. The tight-binding Hamiltonian model was built using Wannier functions optimized through maximal projection, obtained through the PYFPLO module of the FPLO code [58] (see Fig. S4 of the SM [67]). The local Wannier basis set consisted of orbitals of Yb [$4f$, $5d$], V [$3d$, $4s$], and Sb [$5p$, $5s$]. To ensure consistency, the same $12 \times 12 \times 12$ k -points mesh was used in the self-consistent calculations. The Hamiltonian data were used in the Z_2 invariant calculations.

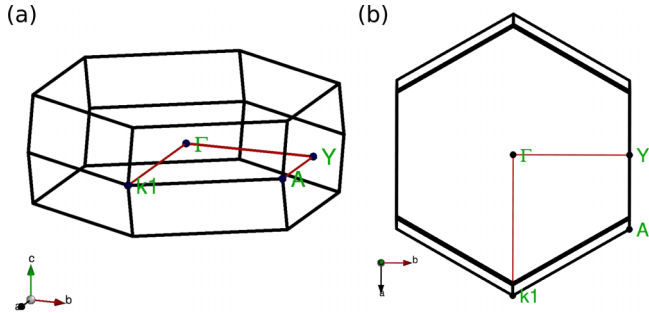


FIG. 1. (a) The path connecting the high-symmetry points of the first Brillouin zone. (b) Top-down view of the Brillouin zone.

III. RESULTS AND DISCUSSION

A. Structural properties

YbV_3Sb_4 crystallizes in a face-centered orthorhombic system and is assigned to space group $Fmmm$ (No. 69, Hall symbol: $-F 22$); see Fig. 2. The experimentally obtained [52] lattice parameters chosen for the computations are $a = 5.623 \text{ \AA}$, $b = 9.840 \text{ \AA}$, $c = 23.652 \text{ \AA}$. The corresponding point group is D_{2h} , indicating the presence of an inversion symmetry. The structure is symmorphic. The atomic positions are detailed in Table II, following the corresponding Wyckoff positions. The unit cell of YbV_3Sb_4 features zigzag layers of Yb atoms (depicted in gold), interleaved with V (blue spheres), and Sb (red spheres) atoms, arranged in a pattern combining hexagonal motifs and layered structures [see Fig. 2(a)]. The Kagome structure is slightly distorted, as is shown in Fig. 2(b). A Kagome network is formed by the V atoms, with $2.81 \text{ \AA}$ and $2.83 \text{ \AA}$ V-V bond lengths, indicating that every bond deviates by at most $0.02 \text{ \AA}$ from the ideal Kagome lattice. The zigzag chain running along the a axis forms an angle of 93.90° , with intrachain atomic separations of approximately $3.9 \text{ \AA}$, as illustrated in Fig. 2(c), whereas the closest atomic neighbor inter-chain spacing is $\sim 5.7 \text{ \AA}$.

TABLE II. Atomic positions and symmetry labels for YbV_3Sb_4 .

Element	Type	X	Y	Z	Wyckoff position	Symmetry
Yb	70	0.00000	-0.50000	0.30552	8i	mm2
Sb	51	0.00000	-0.50000	0.43536	8i	mm2
Sb	51	-0.50000	-0.32904	-0.50000	8h	m2m
Sb	51	-0.50000	0.34123	0.31426	16m	m..
V	23	-0.50000	-0.50000	0.40981	8i	mm2
V	23	-0.25000	0.25000	0.40577	16j	..2

B. Electronic properties

To perform the comprehensive study, we have computed the electronic properties of YbV_3Sb_4 , which includes the orbital resolved band structure and the corresponding DOS assuming different approximations GGA, GGA + U, GGA + SOC, and GGA + U + SOC within the DFT formalism. We also verified that the ground state is nonmagnetic, regardless of the methodology used to incorporate electronic correlations and spin-orbit coupling, in accordance with the experimental report [52].

In a first step, we performed the comparative study of electronic properties by calculating the density of states and band structure from GGA and GGA + U. In both cases, YbV_3Sb_4 is found to be metallic [Figs. 3(a), 3(b) and Figs. 4(a), 4(b)]. The DOS and orbital-resolved band structure reveal that V-3d states, especially d_{xz} , d_{yz} , d_{xy} , and $d_{x^2-y^2}$ orbitals, are predominant at the Fermi energy E_F . Flat-bandlike (denoted by FB) features are observed near E_F , mainly contributed by the d_{xz} , d_{yz} (green line), and states below Fermi level at -1.5 eV is contributed by d_{xy} and $d_{x^2-y^2}$ (red line) [Figs. 3(a) and 4(a)]. While the d_{z^2} states are mostly seen in intermediate energies, the Yb-4f orbitals are absent at the Fermi level, indicating that the 4f manifold remains largely localized and only weakly hybridized with the itinerant V-3d Kagome-derived conduction bands. This behavior is consistent with a predominantly localized Yb-4f manifold in Yb-based intermetallics, where the 4f states lie slightly below E_F and do not contribute strongly to the low-energy transport [69,70]. Importantly, our

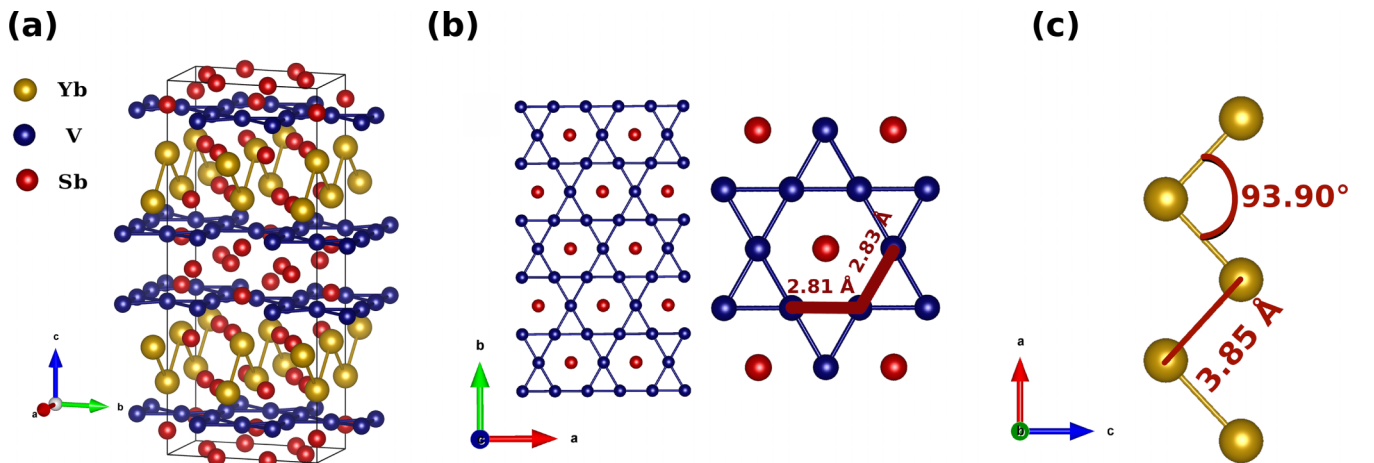


FIG. 2. Crystal Structure of YbV_3Sb_4 : (a) The unit cell of YbV_3Sb_4 includes Yb atoms (shown in gold) with V atoms represented as blue spheres and Sb atoms as red spheres. (b) Crystal Structure of YbV_3Sb_4 , highlighting the V-based Kagome Network. (c) Structure of the Yb ions' zigzag sublattices.

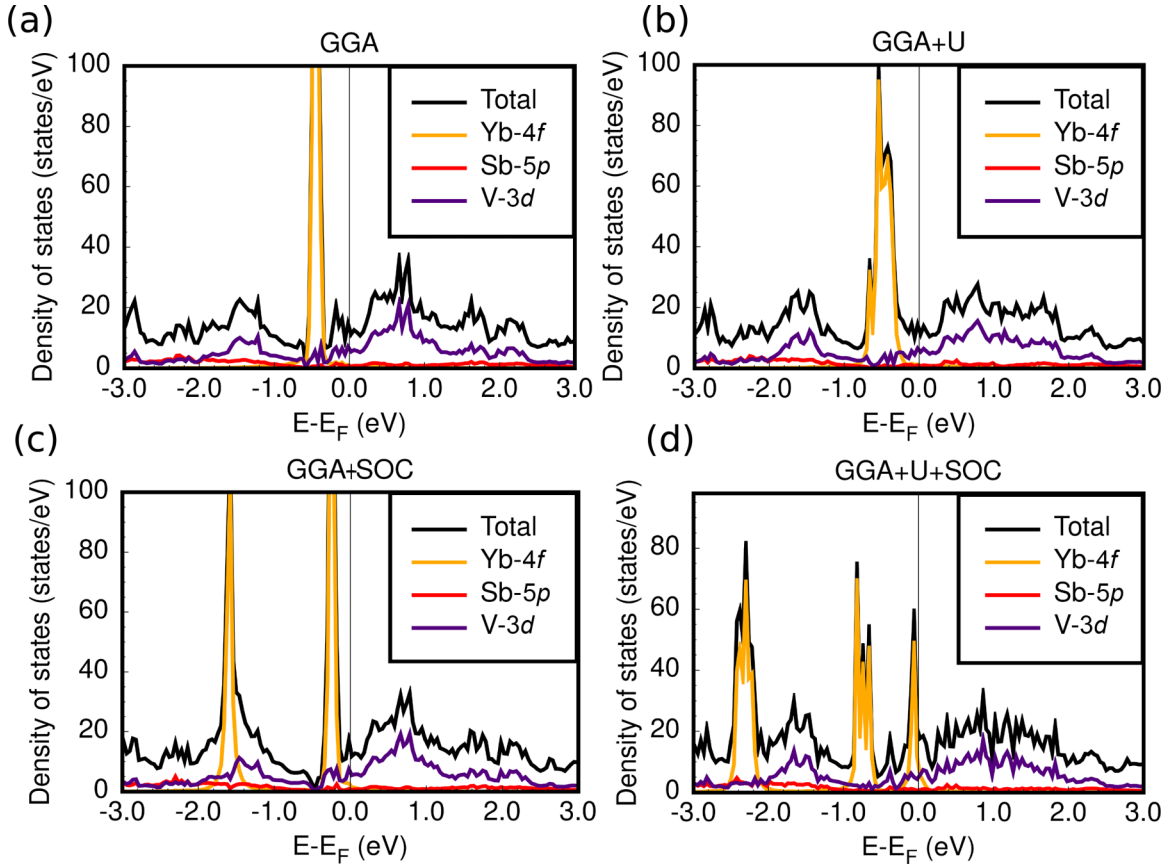


FIG. 3. Comparison of the total and partial density of states (DOS and PDOS) as a function of energy (eV) for: (a) GGA, (b) GGA + U, (c) GGA + SOC, and (d) GGA + U + SOC. The total DOS is shown in black, while the PDOS from Yb-4*f*, Sb-5*p*, and V-3*d* orbitals are shown in yellow, red, and blue, respectively. The Fermi level is set as a reference energy, indicated with solid lines.

U/J sensitivity tests confirm that this feature is robust and does not originate from a fine-tuned choice of Hubbard parameters (see Figs. S1, S2 of the SM [67]).

Moreover, characteristic Dirac-like crossings, coherent with the vanadium Kagome network, appear in the vicinity of the high-symmetry points k_1 and A , while the Yb-4*f* states are localized below -0.3 eV, indicating limited hybridization with the conduction bands. The orbital-resolved band weights further confirm that these Dirac-like crossings originate predominantly from V-3*d* states, whereas the Yb-4*f* bands remain nearly dispersionless and localized below E_F , supporting weak $4f - 3d$ hybridization near the Fermi level.

On incorporation of the Hubbard U parameter to treat strong electron-electron correlation effect, we have noticed no significant changes, rather than the slight shift of the V-3*d* bands towards the lower energy below E_F [see Figs. 3(b) and 4(b)]. Moreover, the Yb-4*f* bands show noticeable broadening in which the DOS peak spans roughly from -0.2 eV to -0.8 eV [Fig. 3(b)]. This broadening reflects enhanced correlation-driven redistribution of the Yb-4*f* spectral weight, while the V-3*d* bands remain dispersive near E_F , indicating that the low-energy states retain predominantly V-3*d* character.

In contrast, the GGA + SOC brought major changes in the band profile by splitting the Yb-4*f* states into two distinct peaks at approximately -0.2 eV and -1.6 eV, attributed to $F_{7/2}$ and $F_{5/2}$, respectively, in accordance to Hund's rule [see

Figs. 3(c), 4(c) shown in yellow]. This splitting is primarily driven by the atomic spin-orbit interaction of the Yb-4*f* shell, which lifts the degeneracy of the $J = 7/2$ and $J = 5/2$ states. Such a two-peak multiplet structure is a characteristic fingerprint of the atomlike SOC-split Yb-4*f* manifold in Yb-based intermetallic systems [71–73]. These bands are seen to remain extremely flat. We have also observed the shift of $F_{7/2}$ states closer to the Fermi level. The splitting factor ($\Delta \sim F_{5/2} \rightarrow F_{7/2}$) is found to be ~ 1.4 eV, reflecting the strong atomic spin orbit interaction in Yb *f*-orbitals [71–73], whereas the V-3*d* contribution at E_F remains essentially unchanged. The V-3*d* bands continue to dominate at E_F , exhibiting the band crossings which may be indicative of SOC-induced band inversions and emergent topological behavior; see Fig. 4(c). The flat-bandlike characteristics drawn by V-3*d* orbital remain protected under SOC. It seems that the V-3*d* orbitals are more immune to relativistic effects and drive metallic transport channels.

The comparison between the DOS and band structures from GGA + SOC and GGA + U + SOC is shown in Figs. 3(c), 3(d) and Figs. 4(c), 4(d). The introduction of Hubbard U to GGA + SOC has split the $F_{7/2}$ multiplet into two sub peaks by $\Delta \approx 0.7$ eV, one shifts downwards to ~ -0.8 eV and another shifts upwards at the proximity of the E_F . The $F_{5/2}$ shift further downwards at ~ -2.2 eV, creating 3 distinct energy states. The additional splitting compared to the SOC-only case likely originates from the combined effect of on-site

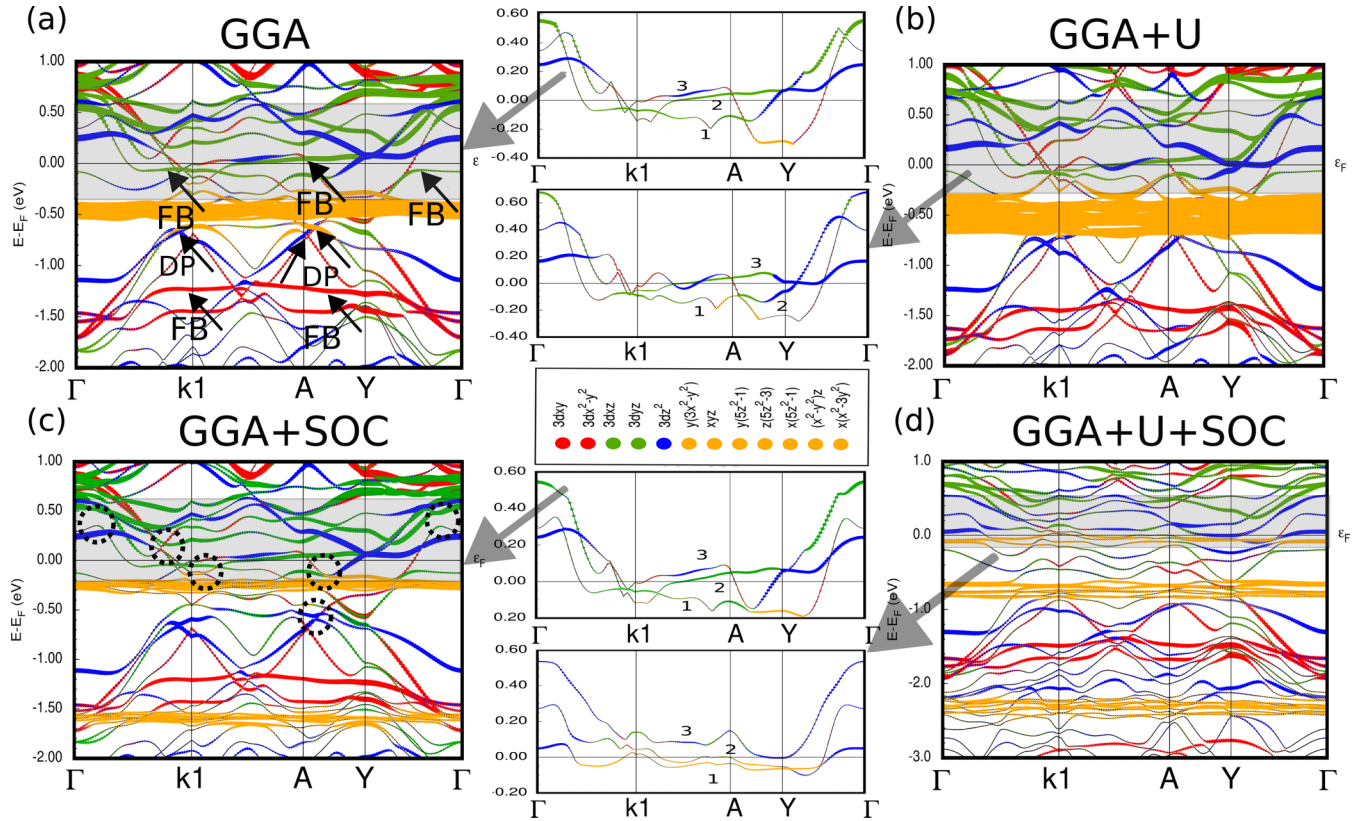


FIG. 4. DFT calculated electronic properties of YbV_3Sb_4 , showing orbital-resolved band structures obtained by: (a) GGA, (b) GGA + U, (c) GGA + SOC, and (d) GGA + U + SOC. Flat bands (FB) and Dirac points (DP) are indicated in the GGA panel (a), and the visible gaps induced by SOC are circled in panel (c). Orbital characters are displayed in different colors. A zoomed-in view of the three orbital resolved bands, which are crossing the Fermi level under different approximations, is consistently labeled as 1, 2, and 3 across all panels; band 2 (the highest occupied band) is used for the Z_2 invariant calculation. The Fermi level is set to zero energy (solid horizontal line).

correlations and SOC, which further separates the correlated $4f$ levels and can enhance the lifting of degeneracies within the SOC-split multiplets. As a result, the combined effect of SOC and on-site correlations produces a three-peak structure in the $\text{Yb-}4f$ spectral weight.

The splitting of f -orbitals into three spectral states reflects the interplay of SOC and Hubbard potential (U) under the influence of crystal field splitting [69,74,75]. The $\text{Yb-}4f$ states are found to be dominated almost entirely by the $y(5z^2 - 1)$ orbital character at the Fermi level. In contrast, we have not observed major changes in V-3d PDOS in both cases while assessing the sensitivity of the $\text{Yb-}4f$ orbitals to SOC and U when considered simultaneously. As usual, the out-of-plane d_{z^2} orbital becomes strongly dominant near the Fermi energy, whereas the in-plane d_{xy} and $d_{x^2-y^2}$ orbitals have less contribution. The out-of-plane d_{xz}/d_{yz} (green) bands remain dispersive but with noticeably lower weight and narrowed bandwidth around the Fermi level, driving the out-of-plane d_{z^2} orbital and $\text{Yb-}4f$ $y(5z^2 - 1)$ orbital to dominate the low-energy states. Furthermore, we observe band flattening and also gap formations, especially around k_1 and A, which may indicate correlation-assisted band inversions in the presence of SOC.

These observations motivate the analysis of the Fermi surface topology employing de Haas-van Alphen oscillations and a direct calculation of the Z_2 invariant to demonstrate the existence of nontrivial topological phases.

C. Fermi surface and de Haas-van Alphen (dHvA) oscillation

To further understand the low-energy electronic structure, we computed the Fermi surface of YbV_3Sb_4 . To ensure maximum accuracy, the Fermi surface was computed using a self-adaptive k-point mesh. The Fermi surface was constructed through iterative mesh refinement using an isosurface method. We used a mesh of k-points set on a grid of $(48 \times 48 \times 48)$, achieved through three bisections of an initial grid of $(6 \times 6 \times 6)$. Figures 5(a)–5(d) present the Fermi surface of YbV_3Sb_4 , calculated using the GGA, GGA + U, GGA + SOC, and GGA + U + SOC approaches. The Fermi surface arises from the contributions of three bands: Band 1, Band 2, and Band 3. The detailed band-resolved Fermi surfaces are provided in the Supplemental Material (see Fig. S5 [67]). Here, the labels Band 1, Band 2, and Band 3 correspond to the three dispersive bands crossing the Fermi level in the orbital-resolved band structure shown in Fig. 4. These three bands are the only contributors to the Fermi surface topology and are therefore used for the band-resolved dHvA frequency analysis presented below. Among them, Band 2 corresponds to the highest occupied band and is also used to evaluate the Z_2 invariant. Notably, the Fermi surface consists of multiple cylindrical-like sheets positioned around the Γ -point, along with small sheetlike features near the boundaries of the BZ. The overall topology remains largely unchanged with the

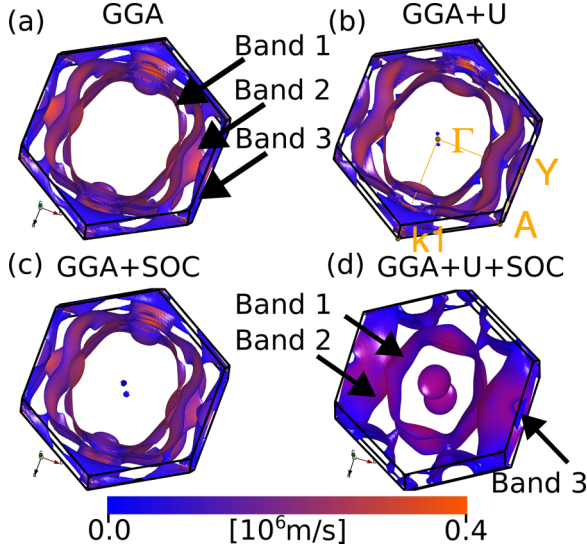


FIG. 5. The calculated Fermi surface of YbV_3Sb_4 , computed under four approaches: (a) GGA, (b) GGA + U, (c) GGA + SOC, and (d) GGA + U + SOC. Three bands—Band 1, Band 2, and Band 3—contribute to the Fermi surface by crossing the Fermi level. The scale at the bottom is for the Fermi velocity.

inclusion of both U and SOC. However, a small spherical feature at the center becomes more pronounced, and the cylindrical sheets exhibit slight deformation under their combined effect. From the orbital-resolved band weights, this spherical pocket originates mainly from Band 1 and is dominated by the $V-3d_{z^2}$ orbital character. Similar cylindrical Fermi surfaces have been reported in various titanium- and vanadium-based Kagome materials [16,76–81].

Based on Onsager's relation Eq. (1), the dHvA oscillation frequency F is directly proportional to the cross-sectional area A of the Fermi surface [76,82,83]:

$$F = \frac{\hbar}{2\pi e} A. \quad (1)$$

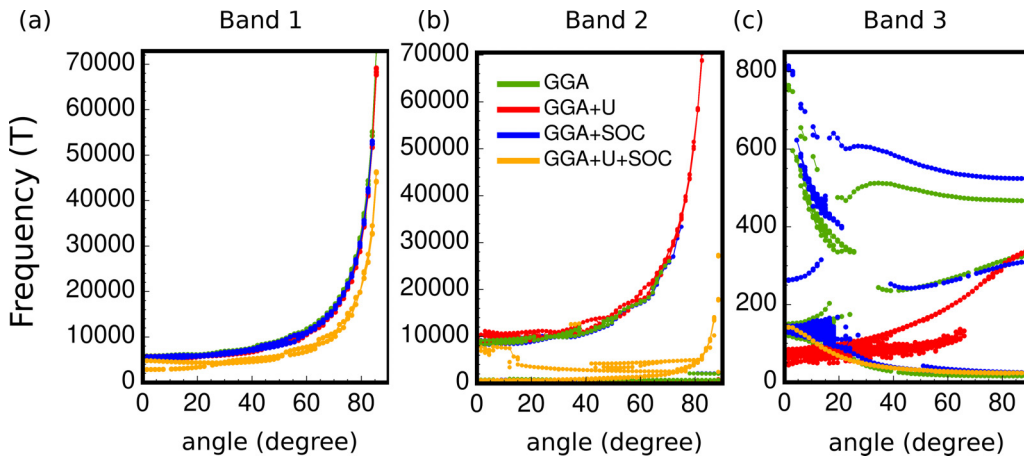


FIG. 6. Theoretical dHvA frequencies of YbV_3Sb_4 computed using Onsager's relation at various tilt angles of the magnetic field. Frequencies derived from (a) Band 1, (b) Band 2, and (c) Band 3, incorporating the effects of GGA (green), GGA + U (red), GGA + SOC (blue), and GGA + U + SOC (yellow) in all three panels. The frequencies from Band 1 and Band 2 exhibit nearly parabolic angular dependence, whereas those from Band 3 show a decreasing trend with increasing tilt angle.

Therefore, we computed all possible theoretical frequencies by evaluating the cross-sectional areas of the Fermi surface, as shown in Figs. 6(a)–6(c). As evident in the plot, the frequency increases with increasing tilt angle. Here, the tilt angle is defined as the angle between the c axis and the direction of the applied magnetic field— 0° corresponds to the field aligned along the c axis, while 90° indicates the field lies within the ab plane. The frequencies associated with Band 1 and Band 2 increase with tilt angle, reaching values as high as 70 kilotesla. Notably, the angular dependence exhibits a nearly parabolic trend, in agreement with expectations for a cylindrical Fermi surface. In contrast, the frequencies derived from Band 3 remain low (below 1000 T) and generally decrease with increasing tilt angle. This behavior can be understood from the geometry of the Band 3 Fermi surface. Unlike the quasi-cylindrical sheets associated with Bands 1 and 2, the Band 3 pocket exhibits a strongly three-dimensional character with pronounced curvature. As a result, the extremal cross-sectional area changes more weakly with tilt angle and can even decrease, leading to comparatively small dHvA frequencies. This supports the assignment of the low-frequency branch to Band 3, as shown in Fig. 6(c). As expected, except for the GGA + U + SOC case, the frequency curves from different methods largely overlap [see Figs. 6(a), 6(b)], indicating that the Fermi surface remains largely unaffected by the inclusion of U or SOC individually, but is noticeably modified when both effects are included simultaneously.

The angular dependence of Band 3 does not follow the $1/\cos\theta$ scaling characteristic of a quasi-two-dimensional cylindrical Fermi surface. Instead, it displays a weaker and nonmonotonic variation with tilt angle, suggesting that the corresponding Fermi surface sheet forms a closed pocket with appreciable three-dimensional character.

D. Z_2 invariant

To investigate the topological nature of YbV_3Sb_4 , four Z_2 topological invariants ($\nu_0; \nu_1\nu_2\nu_3$) were calculated following the method proposed by Fu and Kane [84,85]. The Z_2

invariants were evaluated using the Wannier charge center (WCC) approach within the PYFPL0 code [58]. Importantly, we calculated the Z_2 topological invariants for Band 2 (Fig. 4 under both GGA + SOC and GGA + U + SOC approximations), and in each case found that Band 2—which we identify as the highest occupied band—exhibits a strong topological index of $(\nu_0; \nu_1\nu_2\nu_3) = (1; 000)$. Hence, this result firmly establishes YbV_3Sb_4 as a material with robust topological character which hosts a nontrivial topological band structure. We further validated the topological invariants by examining the Wannier centers flow (see Fig. S6 of the SM [67]).

These Wannier centers on YbV_3Sb_4 show the evolution of Wannier charge centers as a function of k_y in four time reversal invariant planes ($k_z = 0$, $k_z = \pi$, $k_x = \pi$, and $k_y = \pi$). A well-defined linear reference line can be placed at a fixed value of θ . The crossing points of the Wannier center lines through this reference line are highlighted in red. We observe exactly one crossing on the $k_z = 0$ plane, and an even number of crossings (including zero) in the remaining planes, which results in $Z_2 = 1$, together with the observation that the Wannier center curves form continuous and smoothly connected patterns, provides strong evidence that the topological invariants are $(\nu_0; \nu_1\nu_2\nu_3) = (1; 000)$. In trivial cases, a region around θ can be found where the reference line either avoids intersecting any Wannier center trajectories or intersects them an even number of times. This yields a topological invariant of $(0; 000)$. Based on these results, YbV_3Sb_4 shows a non-trivial invariant Z_2 ($\nu_0 = 1$) for the plane $k_z = 0$ and trivial invariants for the remaining planes ($\nu_1, \nu_2, \nu_3 = 0$), confirming that YbV_3Sb_4 is a strong topological metal.

IV. CONCLUSION

We present the first ab initio DFT + Wannier investigation of the vanadium-based Kagome metal YbV_3Sb_4 , which reveals a nonmagnetic metallic ground state with V-3d derived

flat bands and Dirac-like crossings near E_F and localized Yb-4f states below it. The inclusion of Hubbard U + SOC splits the Yb-4f multiplets into three distinct peaks without opening a gap, while the V-3d-derived band topology remains preserved. The Fermi surface consists of quasi-2D cylindrical sheets, which show slight deformations under U + SOC, along with the emergence of a small pocket. The de Haas-van Alphen frequencies computed from these Fermi pockets reach up to ~ 70 kilotesla. Importantly, the Wannier-centre analysis reveals a strong Z_2 invariant ($\nu_0 = 1$), establishing YbV_3Sb_4 as a topological metal. Altogether, this rare-earth Kagome compound offers a unique and promising platform for exploring correlated and topological quantum phases.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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