

Extremely large magnetoresistance in nodal-net semimetal $\text{Pd}_3\text{Ti}_2\text{S}_2$ with kagome lattice

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Materials with a kagome lattice naturally host topological electronic structures, giving rise to many intriguing quantum states within this family. In this study, we performed calculations of the electronic structure and Fermi surface, and measured the longitudinal resistivity $\rho_{xx}(T, B)$, Hall resistivity $\rho_{yx}(T, B)$, and quantum oscillations of the magnetization as a function of temperature and magnetic field for $\text{Pd}_3\text{Ti}_2\text{S}_2$, a kagome-lattice material. We observed an unsaturated extremely large magnetoresistance of 14 500% at 2 K and 9 T, the highest reported in kagome lattice materials, which was attributed to the carrier compensation supported by the Hall resistivity measurements. The band structure calculations, along with the observation of nontrivial Berry phases in the de Haas–van Alphen oscillations, demonstrate that $\text{Pd}_3\text{Ti}_2\text{S}_2$ is a topological nodal-net (Hopf link) semimetal.

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I. INTRODUCTION

Recently, materials with a kagome lattice have attracted much attention due to their naturally featuring Dirac fermions, flat bands, and van Hove singularities in the electronic structure, allowing for the realization and discovery of a series of topological kagome magnets and superconductors with exotic properties. Numerous emerging phenomena resulting from the quantum interactions between geometry, topology, spin, and correlation have been reported [1]. Many kagome lattice materials host one-dimensional band crossing in momentum space, protected by reflecting symmetry, forming a linear band degeneracy along closed loop, and exhibiting nodal line semimetal behaviors [2–9]. For example, an endless Dirac nodal line emerges in the nonmagnetic Shandite compounds $\text{Ni}_3\text{In}_2\text{S}_2$ and $\text{Ni}_3\text{In}_2\text{Se}_2$, as evidenced by angle-resolved photoemission spectroscopy (ARPES) experiments,

density functional theory (DFT) calculations, magnetoresistance, and Hall resistivity measurements [10–15]. For the ferromagnetic Shandite kagome lattice $\text{Co}_3\text{Sn}_2\text{S}_2$, the nodal ring transforms into Weyl nodes under strong spin-orbit coupling (SOC), resulting in a large anomalous Hall angle and giant anomalous Hall resistivity due to its intrinsic Berry curvature [16–20]. Since $\text{Ni}_3\text{In}_2\text{S}_2$, $\text{Ni}_3\text{In}_2\text{Se}_2$, and $\text{Co}_3\text{Sn}_2\text{S}_2$ belong to the $M_3X_2Z_2$ family (M = transition metals; X = In, Sn, Sb, Pb, Bi, Tl; Z = S, Se) [21], which hosts two-dimensional (2D) kagome lattice layers forming by M atoms, it is reasonable to expect exotic topological states and novel physical properties in other members, particularly homologous compounds such as $\text{Pd}_3\text{Ti}_2\text{S}_2$, which should exhibit similar electronic band structures. Although the structure of $\text{Pd}_3\text{Ti}_2\text{S}_2$ was reported years ago [22], its physical properties remain unexplored, prompting interest in investigating its intriguing properties.

In this article, we report that a complex nodal net structure (Hopf link), formed by multiple interconnected nodal lines protected by inversion symmetry $\mathcal{P}$ and time-reversal symmetry $\mathcal{T}$, emerges in $\text{Pd}_3\text{Ti}_2\text{S}_2$, which shares the same kagome structure as $\text{Co}_3\text{Sn}_2\text{S}_2$, as revealed by DFT calculations. We then successfully grew $\text{Pd}_3\text{Ti}_2\text{S}_2$ single crystals and systematically performed longitudinal resistivity, Hall resistivity, and magnetoresistance (MR) measurements. It was found that $\text{Pd}_3\text{Ti}_2\text{S}_2$ exhibits almost all the characteristics of extremely large magnetoresistance (XMR) semimetals [23]: the nearly quadratic field dependence of MR, a field-induced upturn in

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resistivity followed by a plateau at low temperatures, and high carrier mobilities. It should be noted that $\text{Pd}_3\text{Tl}_2\text{S}_2$ exhibits record-high MR ($\sim 14500\%$ at 2 K and 9 T) and mobility ($\sim 16700 \text{ cm}^2/\text{Vs}$) among materials with a kagome lattice structure. Furthermore, the nontrivial Berry phase, derived from de Haas–van Alphen (dHvA) oscillations, suggests that $\text{Pd}_3\text{Tl}_2\text{S}_2$ is a nontrivial topological nodal-net semimetal.

II. EXPERIMENTAL AND COMPUTATIONAL METHODS

$\text{Pd}_3\text{Tl}_2\text{S}_2$ single crystals were synthesized using a self-flux method. Stoichiometric amounts of Tl chunks, Pd, and S powders were placed in an alumina crucible, which was then sealed in an evacuated silica tube. The mixture was heated to 1050°C over three days and maintained at this temperature for 24 hours in an electronic furnace. Afterward, it was slowly cooled down to 600°C at a rate of $2^\circ\text{C}/\text{h}$. Finally, the mixture was rapidly cooled to room temperature by turning off the furnace power. Single crystals with typical dimensions of $1.5 \times 1 \times 0.4 \text{ mm}^3$ (as shown in the inset of Fig. S1 in the Supplemental Material [24]) were mechanically exfoliated from the flux.

Single-crystal x-ray diffraction was performed at room temperature using a Rigaku diffractometer with $\text{Cu } K_{\alpha 1}$ radiation [see Fig. S1 of the Supplemental Material]. Only $(0\ 0\ l)$ ($l = 3, 6, 9, \dots$) peaks were observed, with an estimated $c = 14.05 \text{ \AA}$, consistent with previous reports [22]. The chemical composition of the crystal was analyzed via energy-dispersive x-ray spectroscopy (EDXS) using a Zeiss Supra 55 scanning electron microscope, with a representative EDX spectrum provided in Fig. S2 of the Supplemental Material. The longitudinal resistivity and Hall resistivity were measured using a Quantum Design physical property measurement system (PPMS-9T), while magnetization measurements were performed with a Quantum Design magnetic property measurement system (SQUID-VSM-7T).

The DFT calculations were performed using the Vienna *ab initio* simulation package (VASP) [25,26]. A plane-wave basis up to a 400 eV energy cutoff and a $12 \times 12 \times 12$ Γ -centered k -point mesh sampling the Brillouin zone were chosen for both the spin-orbit coupling (SOC) and non-SOC calculations. Throughout the calculations, the PBEsol approximation [27] was employed in the lattice relaxation and self-consistent calculations. The lattice parameters were fully optimized until the force on each atom was less than $1 \text{ meV/\AA}$ and the internal stress was less than 0.1 kbar. The calculated lattice constants, $a = 5.726 \text{ \AA}$ and $c = 13.946 \text{ \AA}$, are consistent with experimental results [22]. Based on the optimized lattice parameters, self-consistent calculations, band structure, and density of states (DOS) were performed. After the DFT calculations, the obtained band structure was fitted to a tight-binding (TB) Hamiltonian with 27 atomic orbitals, including Pd-4*d*, S-3*p*, and Tl-6*p*, using the Wannier function method [28]. The resulting Hamiltonian was symmetrized using the WannSymm code [29]. Using the symmetrized TB Hamiltonian, we calculated the Berry phase around each nodal line and the surface state with WannierTools [30].

III. RESULTS AND DISCUSSION

$\text{Pd}_3\text{Tl}_2\text{S}_2$ crystallizes in a hexagonal lattice (space group $R\bar{3}m$, No. 166) with a quasi-2D Pd-Tl layer where Pd atoms

form a perfect kagome lattice [see Figs. 1(a) and 1(b)], similar to $\text{Co}_3\text{Sn}_2\text{S}_2$. Based on this structure, we calculated the electronic band structure and Fermi surface (FS) of $\text{Pd}_3\text{Tl}_2\text{S}_2$. As shown in Fig. 1(c), five bands cross the Fermi energy (E_F), forming three hole pockets [Figs. 1(d)–1(f)] and four electron pockets [Figs. 1(g)–1(j)]. The states near E_F are primarily composed of the *d* orbitals of Pd atoms in the kagome lattice. To match the experimentally measured dHvA frequencies (discussed below), the Fermi level E_F in the DFT calculations was shifted upward by 20 meV. The band structure around the E_F hosts several Dirac nodal lines between the highest valence bands and the lowest conduction bands when SOC is neglected [Figs. 1(l) and 1(m)]. Unlike the endless nodal lines observed in $\text{Ni}_3\text{In}_2\text{S}_2$ [10], the nodal lines in $\text{Pd}_3\text{Tl}_2\text{S}_2$ interweave and form complicated nodal net structures (Hopf link) [31–38], consisting of multiple interconnected nodal lines protected by $\mathcal{PT}$ symmetry. Notably, the bands cross along the P-L and P_1 - L_1 [Fig. 1(c)], very close to the Fermi level E_F , giving rise to the nodal lines NL_1 and NL_4 [Figs. 1(m)], marked with cyan lines, which are related by inversion symmetry. The NL_1 , NL_2 , and NL_3 (NL_4 , NL_5 , and NL_6) lie on the $k_x = k_y$ ($k_y = k_z$, $k_x = k_z$) mirror plane, mutually related by C_3 rotation symmetry. The other nodal lines are away from the mirror plane. By integrating the Berry connection along a circle enclosing the nodal line, we obtain a Berry phase of π , as shown in Fig. 1(m). Therefore, in the presence of $\mathcal{PT}$ symmetry, the stability of the Hopf link nodal structures is guaranteed, as the band crossings are robust against symmetric perturbations due to the π Berry phase associated with any loop linking a nodal line [39–41].

We show the $[1\bar{1}0]$ surface state in the absence of SOC in Fig. 1(l). The drumhead surface states, marked as Ss_1 , Ss_2 , and Ss_3 , emerge around the E_F , connecting two bulk nodal points. The surface state Ss_4 connects the valence band and the conduction band, also exhibiting nontrivial topological properties. When SOC is included, small gaps open at the gapless points [Fig. 1(c)], leaving the hole and electron bands around the E_F fully gapped. By examining the parities of the occupied bands at the time-reversal invariant momenta (TRIM) [42], the $\mathbb{Z}_2$ classification of $\text{Pd}_3\text{Tl}_2\text{S}_2$ is $(0; 111)$. In the $[1\bar{1}0]$ surface [Fig. 1(m)], the SOC induces the Rashba spin splitting for all surface states due to the lack of inversion symmetry at the surface. The nodal lines near the E_F are expected to give rise to a polarized surface charge, which significantly enhances the Rashba spin splitting at the surface [43]. As a result, large Rashba spin splittings are observed in the current Hopf link nodal semimetal $\text{Pd}_3\text{Tl}_2\text{S}_2$, as illustrated in Fig. 1(m). Although all the nodal points are gapped by SOC, the massive Dirac nodal lines may still lead to unconventional transport and optical phenomena [43,44].

Next, we discuss the longitudinal and Hall resistivity measured for $\text{Pd}_3\text{Tl}_2\text{S}_2$ at different magnetic fields. Figure 2(a) illustrates the temperature dependence of the in-plane (ρ_{xx}) and out-of-plane resistivity (ρ_{zz}) for a $\text{Pd}_3\text{Tl}_2\text{S}_2$ crystal. At $T = 300 \text{ K}$, $\rho_{xx} = 50.79 \mu\Omega \text{ cm}$, and $\rho_{zz} = 208.65 \mu\Omega \text{ cm}$, yielding an anisotropy ratio of $\rho_{zz}/\rho_{xx} = 4.1$. This indicates that the electronic properties are more three-dimensional (3D) than 2D. With decreasing temperature, both $\rho_{xx}(T)$ and $\rho_{zz}(T)$ decrease monotonically to $\rho_{xx}(2\text{K}) = 0.16 \mu\Omega \text{ cm}$ and

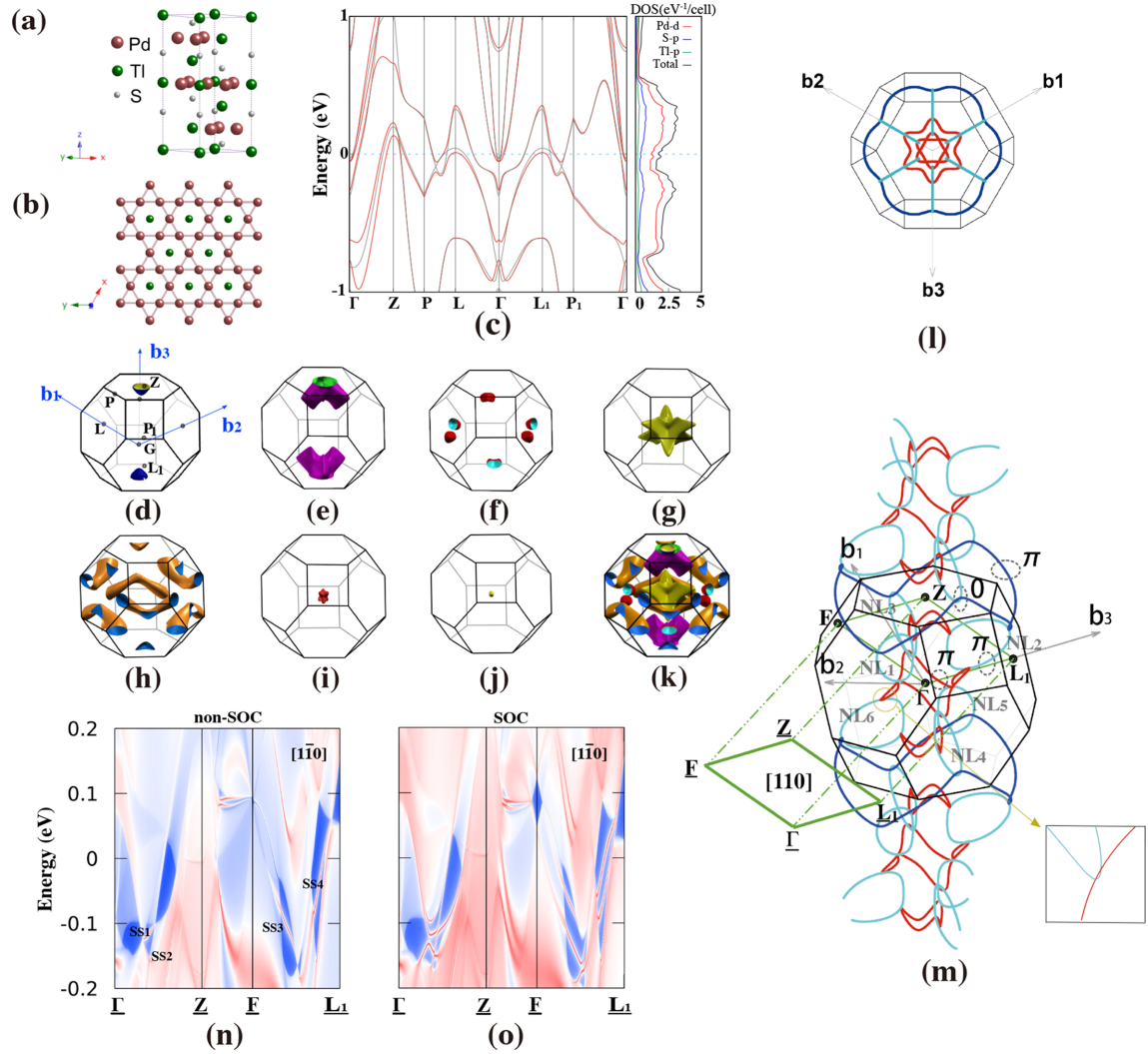


FIG. 1. (a) Crystal structure of $\text{Pd}_3\text{Tl}_2\text{S}_2$ with a Shandite $\text{Ni}_3\text{Pb}_2\text{S}_2$ -type structure. Pd, Tl, and S atoms are represented by violet, green, and gray spheres, respectively. (b) Kagome lattice observed within the Pd-Tl plane. (c) Band structure and DOS of $\text{Pd}_3\text{Tl}_2\text{S}_2$. The black/red lines are corresponding to the band structure without/with SOC. (d)–(k) The Fermi surfaces of $\text{Pd}_3\text{Tl}_2\text{S}_2$ in the presence of SOC. (d)–(f) Three hole pockets; (g)–(j) four electron pockets; (k) all pockets combined together. (l), (m) The top view and side view of Hopf link nodal structures of $\text{Pd}_3\text{Tl}_2\text{S}_2$ in the absence of SOC. Three types of nodal line interweave to form a complicated nodal net. The equivalent nodal lines are shown in the same color. In the inset, Hopf link nodal structure is demonstrated. Such nodal structure exists between all the interweaved nodal lines. (n), (o) $[1\bar{1}0]$ surface state of $\text{Pd}_3\text{Tl}_2\text{S}_2$ in the absence and presence of SOC. The surface Brillouin zone is illustrated in (m) with green solid line.

$\rho_{zz}(2\text{K}) = 1.60 \mu\Omega \text{ cm}$, a typical metallic behavior. The corresponding residual resistivity ratio, $\text{RRR} = \frac{\rho_{xx}(300\text{K})}{\rho_{xx}(2\text{K})} = 317$, indicative of the high quality of our sample. The $\rho_{xx}(T)$ curves measured at various fields ($B = 0\text{--}9\text{ T}$) applied along the c axis are shown in Fig. 2(b). Similar to many other non-trivial and trivial topological semimetals [45–54], $\text{Pd}_3\text{Tl}_2\text{S}_2$ exhibits an XMR behavior. Besides, an up turn in $\rho_{xx}(T)$ curves under applied magnetic field occurs at low temperatures, i.e., ρ_{xx} increases with decreasing temperature then saturates.

Figure 2(c) shows the MR as a function of magnetic field at various temperatures with the conventional definition $\text{MR} = \left[\frac{\rho_{xx}(B) - \rho_{xx}(0)}{\rho_{xx}(0)} \right] \times 100\%$, where $\rho_{xx}(B)$ and $\rho_{xx}(0)$ are the resistivity at field B and zero field, respectively. The measured MR is extremely large at low temperatures, reaching $1.45 \times 10^4\%$ at 2 K and 9 T, and shows no sign of saturation

up to the highest field (9 T) applied in our measurements. With increasing temperature, the MR decreases rapidly; however, it still reaches 10.8% at 100 K and 9 T. As we know, the MR in our $\text{Pd}_3\text{Tl}_2\text{S}_2$ crystal is the largest observed among materials with a kagome lattice. For comparison, in $\text{Ni}_3\text{In}_2\text{S}_2$, which exhibits one of the largest recorded MR values, it reaches about 8000% at 2 K and 9 T [11]. Moreover, it is found that MR can be described by the Kohler scaling law: $\text{MR} = f\left(\frac{B}{\rho(0)}\right)$ [55]. As shown in Fig. 2(d), all MR data from $T = 2\text{ K}$ to 100 K collapse onto a single line when plotted on a logarithmic scale as $\text{MR} \sim \frac{B}{\rho(0)}$. However, the collapsed curve exhibits a sigmoidal shape, rather than the linear behavior expected from a simple power law. This phenomena has also been observed in that of PdSn_4 and PtSn_4 [56]. Jo *et al.* suggested that this may indicate a crossover from the low-temperature limit to high-temperature limit in terms of the dimensionless

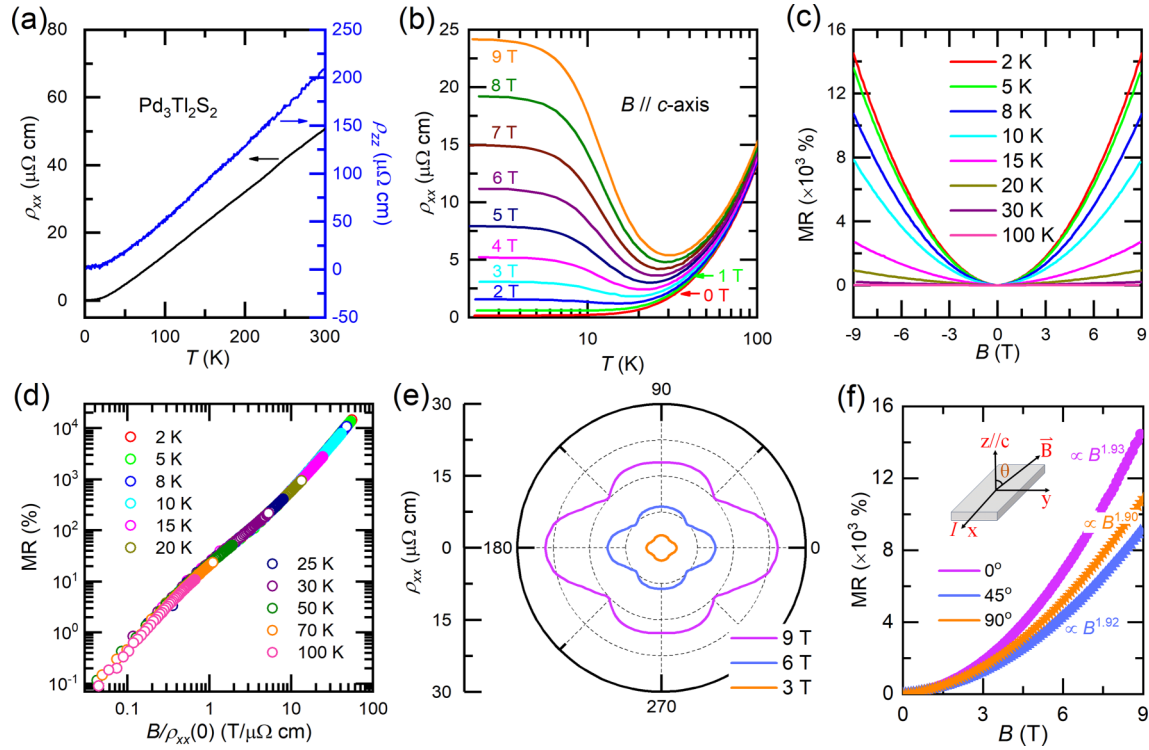


FIG. 2. (a) Temperature dependence of the in-plane resistivity ρ_{xx} and the out-of-plane resistivity ρ_{zz} ; (b) Temperature dependence of the in-plane resistivity $\rho_{xx}(T)$ under various magnetic fields with $B \parallel c$ axis, measured below 100 K. (c) Field dependence of MR of $\text{Pd}_3\text{Tl}_2\text{S}_2$ at various temperatures. (d) MR plotted against $B/\rho_{xx}(0)$ on a logarithmic scale to highlight scaling behavior. (e) In-plane resistivity ρ_{xx} versus magnetic field B for various tilt angles θ at 2 K. (f) Angular dependence of resistivity at 2 K under different magnetic fields, illustrating the anisotropic response.

parameter $\omega_c\tau$, where ω_c is the cyclotron frequency and τ is the relaxation time. In the high magnetic field (or low-temperature) regime, $\omega_c\tau > 1$, meaning that electrons can complete multiple rotational orbits before being scattered. In this case, the motion of electrons is primarily constrained by the magnetic field rather than by scattering events, inducing a large MR. Conversely, in the high-temperature (or low-magnetic-field) regime, $\omega_c\tau < 1$. Here, the motion of electrons in the magnetic field is strongly disturbed by scattering, leading to a weakened MR effect.

To investigate the anisotropy of the FS, we also measured the resistivity anisotropy at 2 K in $B = 3, 6, 9$ T, with the current I applied along the x axis and by rotating the magnetic field in the yz plane (the z axis corresponds to the c axis of crystal), as shown in the inset of Fig. 2(f). Figure 2(e) shows the angular resistivity polar plot, which exhibits twofold symmetry, i.e., $\rho(\theta) = \rho(\theta + \pi)$. The resistivity decreases quickly from a maximum at $\theta = 0^\circ$ (where $B \parallel c$ axis) to a minimum at $\theta = 45^\circ$, then increases again to another relatively wide maximum at $\theta = 90^\circ$ (where $B \parallel ab$ plane). This behavior is consistent with the layered structure of $\text{Pd}_3\text{Tl}_2\text{S}_2$ [22]. We then measured the field dependence of MR for the magnetic field orientation corresponding to the extrema, i.e., $\theta = 0^\circ, 45^\circ$, and 90° . As shown in Fig. 2(f), the MR curves for the three field orientations exhibit similar, nearly parabolic behavior, indicating that the anisotropy of electronic structure in $\text{Pd}_3\text{Tl}_2\text{S}_2$ is not as large as that in $\text{Ni}_3\text{In}_2\text{S}_2$ and $\text{Ni}_3\text{In}_2\text{Se}_2$ [10,13].

To reveal the origin of the XMR in $\text{Pd}_3\text{Tl}_2\text{S}_2$, we measured the Hall resistivity at different temperatures. Figure 3(a) displays the field dependence of the Hall resistivity, $\rho_{yx}(B)$, measured at $T = 2, 10, 50, 100$, and 300 K. The nonlinear behavior of $\rho_{yx}(B)$ at lower temperatures implies the presence of multiple bands, i.e., both electron and hole bands, similar to those observed in many topological trivial/nontrivial semimetals [45–54]. Then, we employed the two-band model to analyze the longitudinal and Hall resistivity data, i.e., the Hall conductivity $\sigma_{xy} = \frac{\rho_{yx}}{\rho_{yx}^2 + \rho_{xx}^2}$ and the longitudinal conductivity $\sigma_{xx} = \frac{\rho_{xx}}{\rho_{yx}^2 + \rho_{xx}^2}$ were calculated using the experimentally measured $\rho_{yx}(B)$ and $\rho_{xx}(B)$ data. In this model, the conductivity tensor is given by [57]

$$\sigma = \frac{en_e\mu_e}{1 + i\mu_e B} + \frac{en_h\mu_h}{1 - i\mu_h B}, \quad (1)$$

where n_e (n_h) and μ_e (μ_h) are the carrier concentrations and mobilities of electrons (holes), respectively. The Hall conductivity σ_{xy} and the longitudinal conductivity σ_{xx} are then given by

$$\sigma_{xy} = \frac{eBn_h\mu_h^2}{1 + \mu_h^2 B^2} - \frac{eBn_e\mu_e^2}{1 + \mu_e^2 B^2} \quad (2)$$

and

$$\sigma_{xx} = \frac{en_h\mu_h}{1 + \mu_h^2 B^2} + \frac{en_e\mu_e}{1 + \mu_e^2 B^2}. \quad (3)$$

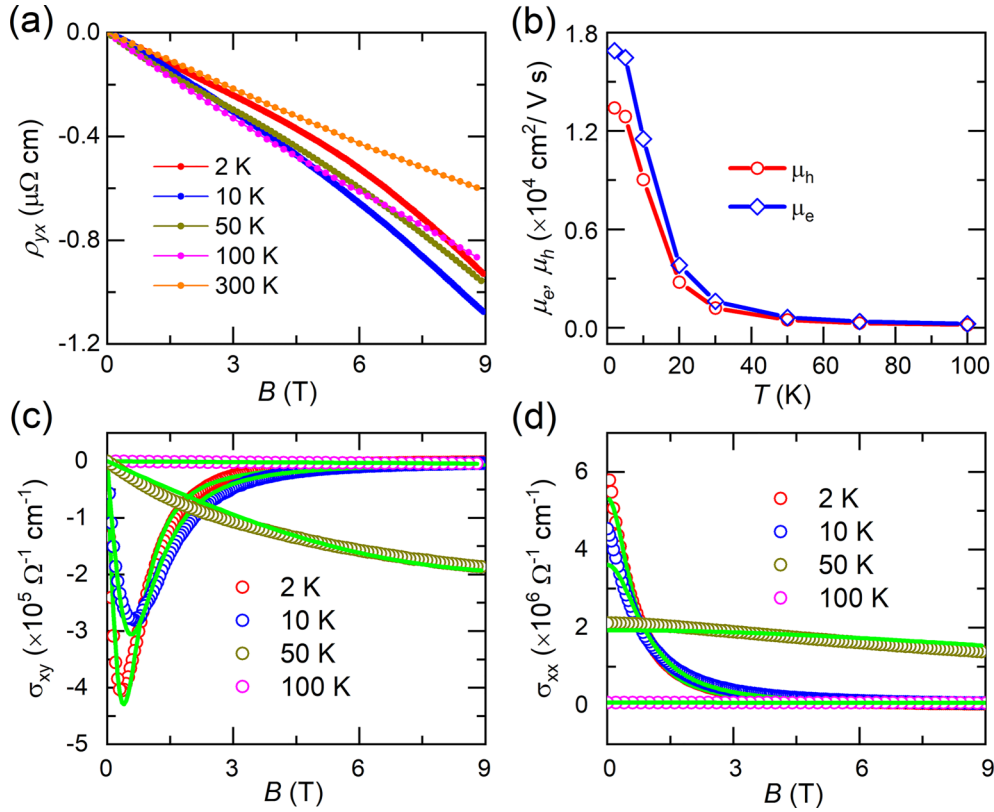


FIG. 3. (a) Field dependence of the Hall resistivity ρ_{xy} measured at several selected temperatures. (b) Temperature dependence of charge-carrier mobilities, μ_h and μ_e , extracted from the two-band model analysis. The components of the conductivity tensor, σ_{xy} and σ_{xx} , shown in panels (c) and (d), respectively, as functions of magnetic field at several selected temperatures ($T = 2, 10, 50$, and 100 K). Open circles indicate experimental data points, while the green solid lines represent the fitting curves derived from the two-band model. To enhance the clarity of the graph, we scaled the data for 50 K by a factor of ten.

Initially, we simultaneously fitted the σ_{xy} and σ_{xx} data to obtain reliable values for n_e (n_h) and μ_e (μ_h) at $T = 2$ K. Subsequently, we performed similar fits at other temperatures while fixing the values of n_e and n_h derived from the 2 K data. This approach was motivated by the observation that the MR in our $\text{Pd}_3\text{Ti}_2\text{S}_2$ crystals follows Kohler's rule well, implying that the carrier concentration likely remains constant below 100 K [58]. Figures 3(c) and 3(d) present the fitting results at $T = 2, 10, 50$, and 100 K. The close match between our experimental data and the two-band model confirms the coexistence of electrons and holes in $\text{Pd}_3\text{Ti}_2\text{S}_2$. Figure 3(b) depicts the temperature dependence of μ_e and μ_h across the range of 2 – 100 K. It should be noted that n_h and n_e are nearly identical, as exemplified at $T = 2$ K with $n_h = 1.08 \times 10^{21} \text{ cm}^{-3}$ and $n_e = 1.11 \times 10^{21} \text{ cm}^{-3}$. This suggests electron-hole compensation at low temperatures in $\text{Pd}_3\text{Ti}_2\text{S}_2$. In addition, the mobility μ_h and μ_e reach very large values of $13\,410 \text{ cm}^2/\text{V} \cdot \text{s}$ and $16\,700 \text{ cm}^2/\text{V} \cdot \text{s}$ at 2 K, respectively, significantly larger than those of other kagome-lattice materials. For comparison, RbV_3Sb_5 has a mobility of $450 \text{ cm}^2/\text{V} \cdot \text{s}$ at 2 K [59], $\text{Co}_3\text{Sn}_2\text{S}_2$ $2600 \text{ cm}^2/\text{V} \cdot \text{s}$ [60], YV_6Sn_6 about $7000 \text{ cm}^2/\text{V} \cdot \text{s}$ [61], and $\text{Ni}_3\text{In}_2\text{S}_2$, which previously had the highest mobility among kagome-lattice materials, ranging from 8600 to $14000 \text{ cm}^2/\text{V} \cdot \text{s}$ [11,12]. These results demonstrated that the emergence of XMR in $\text{Pd}_3\text{Ti}_2\text{S}_2$ is due to both the compensation and high mobilities of the carriers.

Finally, the evidence of topological nodal-net semimetal of $\text{Pd}_3\text{Ti}_2\text{S}_2$ can be provided from our experimental observation of quantum oscillations. Figure 4(a) shows the isothermal magnetization, $M(B)$, measured at various temperatures (2 – 10 K) up to 7 T ($B \parallel c$ axis) exhibiting pronounced dHvA oscillations. A subtle ferromagnetic response emerges in the $M(B)$ measurements at lower magnetic fields (<1 T), thus we measured the temperature dependence of susceptibility as shown in Fig. S3, $\chi(T)$, at $B = 1$ T, exhibiting a paramagnetic behavior except for an upturn below 30 K, which may be attributed to the presence of Pd magnetic impurities [$<1\%$, obtained from the fitting of $\chi(T)$ data below 30 K] [62]. For the dHvA oscillations observed in $M(B)$ curves at high fields, after subtracting a smooth background, periodic oscillations of ΔM with $1/B$ are clearly visible, as shown in Fig. 4(b). From the fast Fourier transform (FFT) analysis, we identified at least four major low frequencies [49 T (F_1), 140 T (F_2), 156 T (F_3), and 370 T (F_4)] and four major high frequencies [968 T (F_5), 1112 T (F_6), 1513 T (F_7), and 1666 T (F_8)] for $B \parallel c$ axis [Fig. 5(c)]. These oscillation frequencies are close to those observed in $\text{Ni}_3\text{In}_2\text{S}_2$, ranging from 11 to 1315 T [12]. Using the Onsager relation, $F = (\frac{\Phi_0}{2\pi^2})A_F$, where $\Phi_0 = 2.068 \times 10^{-15} \text{ Wb}$ is the magnetic flux quantum, and A_F represents the corresponding extremal areas of the FS pockets, the values of A_F were determined to be $0.47, 1.34, 1.49, 3.53, 9.24, 10.61, 14.44$, and 15.90 nm^{-2} for the above

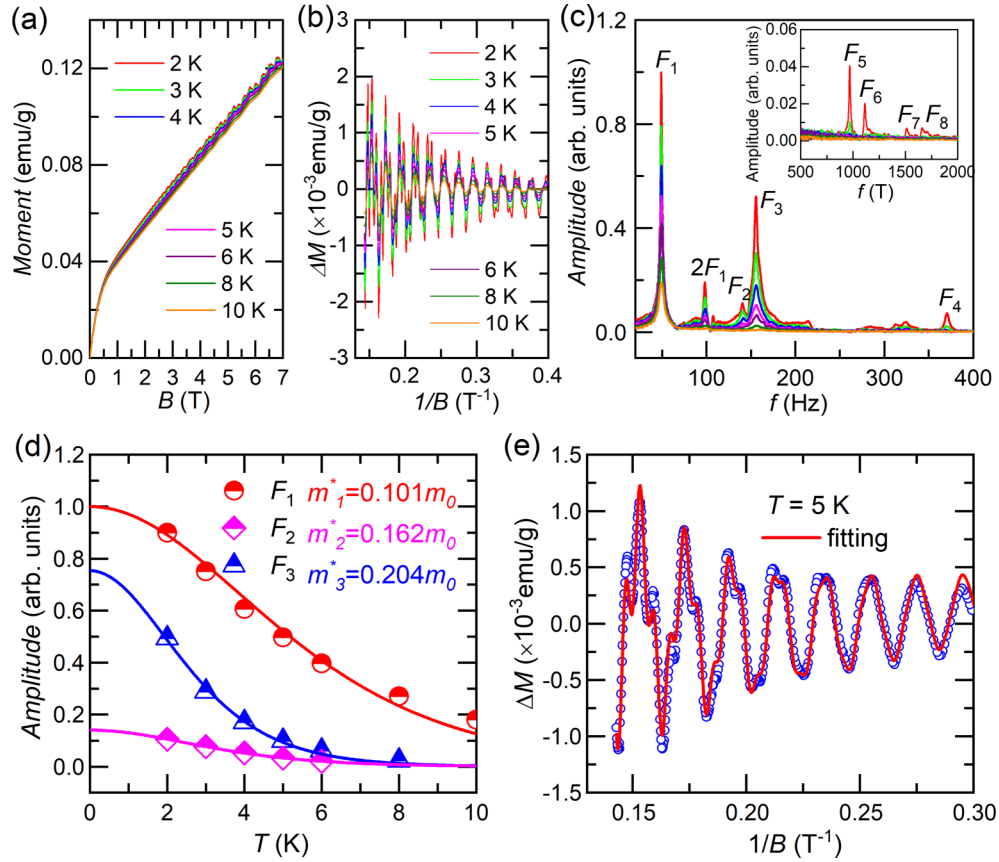


FIG. 4. (a) Magnetization as a function of field measured at various temperatures (2, 3, 4, 5, 6, 8, and 10 K) with $H \parallel c$ axis. Oscillatory component (b) and the FFT spectra (c) of ΔM . (d) Temperature dependence of relative amplitude in FFT spectra. Solid lines represent the corresponding fits to R_T . (e) The dHvA oscillation measured at 5 K and its fitting by the multiband LK formula.

eight frequencies. This indicates the presence of several pockets on the FS, consistent with the calculated results discussed above. Additionally, all the experimentally measured dHvA oscillation frequencies can match well with those obtained from DFT calculations (see Table I).

In general, the oscillatory magnetization of a 3D system can be described by the Lifshitz-Kosevich (LK) formula with the Berry phase (since the electron/hole pockets associated with frequencies F_1 and F_3 exhibit a more pronounced 3D nature rather than a 2D one, as elucidated in the subsequent analysis, the 3D LK formula has been employed in the main

text) [63]:

$$\Delta M \propto -B^{0.5} R_T R_D R_S \sin \left[2\pi \left(\frac{F}{B} - \gamma + \delta \right) \right], \quad (4)$$

$$R_T = \frac{\alpha T \mu}{B \sinh \left(\frac{\alpha T \mu}{B} \right)}, \quad (5)$$

$$R_D = \exp \left(-\frac{\alpha T_D \mu}{B} \right), \quad (6)$$

$$R_S = \cos \left(\frac{\pi g \mu}{2} \right), \quad (7)$$

TABLE I. Comparison of experimental and DFT-calculated frequencies, and parameters derived from dHvA oscillation fitting in $\text{Pd}_3\text{Ti}_2\text{S}_2$. For dHvA oscillation frequency F_3 , we find two DFT-calculated frequencies close to the experimental observation.

	dHvA(T)	DFT(T)	carrier type	m^*/m_0	T_D (K)	τ_q (ps)	μ_q (cm ² /Vs)	$\phi_B(\pi)$
F_1	49	55.9	electron	0.101	1.73	0.703	12240	1.69
F_2	140	103.2	electron	0.162				
F_3	156	148.1	electron	0.204	16.49	0.074	640	1.05
		227.0	hole					
F_4	370	368.3	hole					
F_5	968	892.1	hole					
F_6	1112	1116.6	electron					
F_7	1513	1269.7	electron					
F_8	1666	1622.5	hole					

where μ is the ratio of the effective cyclotron mass m^* to the free electron mass m_0 , T_D is the Dingle temperature, $\alpha = \frac{2\pi^2 k_B m_0}{\hbar e} = 14.7 \text{ T/K}$, and g is the effective Land factor. The phase factor $\gamma = \frac{1}{2} - \frac{\phi_B}{2\pi}$, where ϕ_B is the Berry phase, and $\delta = 1/8$ or $-1/8$ for a 3D system [the sign of δ ($\pm$) corresponds to the minima ($+$)/maxima ($-$) of the cross-sectional area on the FS for the case of an electron band; for a 3D hole band, the sign of δ is opposite] [64,65]. The effective mass m^* can be determined by fitting the temperature dependence of the oscillation amplitude $R_T(T)$. As shown in Fig. 4(d), the resulting m^* values are $0.101 m_0$, $0.162 m_0$, and $0.204 m_0$ for F_1 , F_2 , and F_3 , respectively. The effective masses are smaller than those of $\text{Co}_3\text{Sn}_2\text{S}_2$ [66], and comparable to those of $\text{Ni}_3\text{In}_2\text{S}_2$ and CsV_3Sb_5 [12,67], implying high mobilities in $\text{Pd}_3\text{Ti}_2\text{S}_2$. To simplify the fitting equation and derive the quantum mobility and Berry phase for the primary two oscillation frequencies (F_1 and F_3), we refitted the experimental data at $T = 5 \text{ K}$ using a two-frequency LK formula, as the oscillations of other frequencies can be negligible. The resulting Dingle temperatures T_D are 1.73 K and 16.49 K for F_1 and F_3 , corresponding to quantum relaxation times $\tau_q = \frac{\hbar}{2\pi k_B T_D}$ of 0.703 ps and 0.074 ps ; quantum mobilities $\mu_q = \frac{e\tau}{m^*}$ of $12\,240 \text{ cm}^2/\text{Vs}$ and $640 \text{ cm}^2/\text{Vs}$, respectively. It is reasonable that the mobilities obtained from the dHvA oscillations are smaller than those acquired from the two-band model fitting, because the mobility in the free electron model is not influenced by small-angle scattering, while μ_q is susceptible to momentum scattering in all directions [68]. The LK fit also yields a phase shift $\phi = -\gamma + \delta$ of 0.22 for F_1 and 0.9 for F_3 . Considering F_1 is related to the maximum cross section (Fig. S4 in the Supplemental Material) on the corresponding electron pockets around Γ [Fig. 1(j)] obtained from DFT calculation [69], $\delta = -1/8$ and $\phi_B = 1.69\pi$ are assigned to F_1 . The Berry phase ϕ_B of this electron pocket thus tends to indicate a topologically trivial property. For F_3 , however, we find two close oscillation frequencies (148.1 T and 227.0 T) from DFT calculations (Table I). The former frequency (148.1 T) is associated to the maximum cross section of electron pocket around Γ [Fig. 1(i)], when the magnetic field is along the c axis. The corresponding electronic band with a parabolic dispersion, however, is unlikely to relate to the π Berry phase, despite the calculated frequency being closer to the experimental dHvA oscillations. The latter frequency (227.0 T) is associated to the minimum cross section of the hole pocket around L [Fig. 1(f)], when magnetic field is parallel to the nodal line plane (e.g., the $k_x = k_y$ plane) [65]. Interestingly, the nodal ring (e.g., NL_1) is partially enclosed by this extremal cross section (see Fig. S5 in the Supplemental Material). Therefore, when electron travels along toroidal orbit on this hole pocket (the green circle in Fig. S5) with magnetic field along the c axis, the π Berry phase is expected to be observed from dHvA oscillations. In

3D LK fitting, δ is $-1/8$ for the minimum cross section of a hole pocket, yielding $\phi_B = 1.05\pi$, which indicates a topologically nontrivial property, consistent with our DFT results. A summary of the results is provided in Table I. Certainly, we also examined the case of a 2D FS. In this scenario, $\delta = 0$. The Berry phases corresponding to F_1 and F_3 have changed to 1.44π and 0.8π , respectively (see the Supplemental Material for the fitting results using the 2D-LK formula). We also try to obtain oscillation information for other frequencies. However, their amplitudes are very small, and rapidly diminish with increasing temperature, becoming nearly invisible. The nontrivial Berry phase for the pocket with oscillation frequency F_3 suggests the presence of topological nodal line in $\text{Pd}_3\text{Ti}_2\text{S}_2$. The complex nodal net structures (Hopf link) can be further verified through ARPES or angle dependence of the dHvA measurements.

IV. CONCLUSIONS

In summary, we report that the Shandite kagome lattice $\text{Pd}_3\text{Ti}_2\text{S}_2$ hosts a complex nodal net structure (Hopf link), formed by multiple interconnected nodal lines protected by $\mathcal{PT}$ symmetry, as revealed by DFT calculations. We then successfully grew $\text{Pd}_3\text{Ti}_2\text{S}_2$ single crystals and conducted a systematic study on its physical properties. It was found that $\text{Pd}_3\text{Ti}_2\text{S}_2$ exhibits an XMR of $14\,500\%$ at 2 K and 9 T , along with an impressive mobility of $16\,700 \text{ cm}^2/\text{V} \cdot \text{s}$, which are the highest reported to date among materials featuring a kagome lattice structure. In particular, the nontrivial Berry phase, derived from dHvA oscillations, suggests that $\text{Pd}_3\text{Ti}_2\text{S}_2$ is a promising candidate of topological nodal-net semimetal.

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DATA AVAILABILITY

The data supporting this study's findings are available within the article.

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