

Superconductivity in the nodal-line compound $\text{La}_3\text{Pt}_3\text{Bi}_4$

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Owing to the specific topological states in nodal-line semimetals, novel topological superconductivity is expected to emerge in these systems. In this Letter, we demonstrate that $\text{La}_3\text{Pt}_3\text{Bi}_4$ is a topologically nontrivial nodal-ring semimetal protected by the gliding-mirror symmetry using first-principles calculations. Meanwhile, we discover bulk superconductivity with a transition temperature of ~ 1.1 K and an upper critical field of ~ 0.41 T by means of resistivity, susceptibility, and specific heat measurements. These findings demonstrate that $\text{La}_3\text{Pt}_3\text{Bi}_4$ provides a material platform for studying novel superconductivity in the nodal-ring system.

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I. INTRODUCTION

Searching for topological superconductors (TSCs) with Majorana fermions has been one of the hottest topics in contemporary condensed-matter physics. The discovery of unconventional superconductivity [1–5] in the Cu-intercalated Bi_2Se_3 , a topological insulator, has initiated intense interest in TSCs. Although the p -wave superconductivity is considered to be an intrinsic TSC, in which the core of the vortex contains a localized quasiparticle with exactly zero energy [6], the properties of several experimental candidates remain debatable [7,8]. TSCs can also be realized at the interface of a heterostructure between a strong topological insulator and an s -wave superconductor due to the proximity effect [9–12], where the control of the chemical reaction and lattice mismatch at the interface remains challenging. The most promising candidates for TSCs are those in which fully gapped bulk superconductivity coexists with topologically protected gapless surface/edge states, such as $\text{FeTe}_{1-x}\text{Se}_x$ [13,14], β - PdBi_2 [15], and 2M-WS_2 [16]. Recently, nodal-line materials have received significant attention [17–19], because they have been predicted to exhibit several notable phenomena, including long-ranged Coulomb interaction, large surface polarization charge, etc. [20–23]. In particular, if superconductivity is induced in nodal-line materials [24] with torus-shaped Fermi surfaces derived from nodal

loops, then topological crystalline and second-order topological superconductivity can be realized [25]. Unfortunately, the nodal-line structure is difficult to realize in materials because it generally become gapped if the spin-orbit coupling (SOC) is considered [26–28]. So far, nodal-line materials are rarely reported in the presence of SOC [29–32], let alone the superconductors with such nodal lines [24,33].

Recently, a possible nontrivial band topology has been reported and enthusiastically discussed based on the strongly correlated $\text{Ce}_3(\text{Pt}_{1-x}\text{Pd}_x)_3\text{Bi}_4$ system [34,35], thereby resulting in renewed focus on the $\text{Ln}_3\text{T}_3\text{X}_4$ compounds (Ln = lanthanoid element, T = Cu, Au, Rh, Pd, and Pt, and X = Sb and Bi) [36]. As a member of the $\text{Ln}_3\text{T}_3\text{X}_4$ family, $\text{La}_3\text{Pt}_3\text{Bi}_4$ crystallizes in a cubic $\text{Y}_3\text{Au}_3\text{Sb}_4$ -type structure with space group $I\bar{4}3d$ (No. 220), which contains six gliding-mirror symmetry operations. To perform a comparison on the Kondo insulator $\text{Ce}_3\text{Pt}_3\text{Bi}_4$, measurements of resistivity, magnetic susceptibility, and specific heat of $\text{La}_3\text{Pt}_3\text{Bi}_4$ above 2 K were performed, and no superconductivity was reported [37–40]. In this Letter, we employed the density functional theory (DFT) to investigate the electronic band structure and its band topological properties of $\text{La}_3\text{Pt}_3\text{Bi}_4$. The results indicate that $\text{La}_3\text{Pt}_3\text{Bi}_4$ is a topologically nontrivial nodal-ring semimetal. Meanwhile, by performing resistivity, magnetic susceptibility, and specific heat measurements, we discover that $\text{La}_3\text{Pt}_3\text{Bi}_4$ crystals exhibit bulk superconductivity with a transition temperature of $T_C \sim 1.1$ K and an upper critical field of $\mu_0 H_{c2}(0) \sim 0.41$ T. These findings demonstrate that $\text{La}_3\text{Pt}_3\text{Bi}_4$ provides a material platform for studying novel superconductivity in the nodal-ring system.

II. EXPERIMENTAL AND COMPUTATIONAL METHODS

$\text{La}_3\text{Pt}_3\text{Bi}_4$ crystals were grown using the method described in Ref. [34], and the crystals with typical dimensions of $0.1 \times 0.1 \times 1$ mm³ were obtained [40], as shown in the

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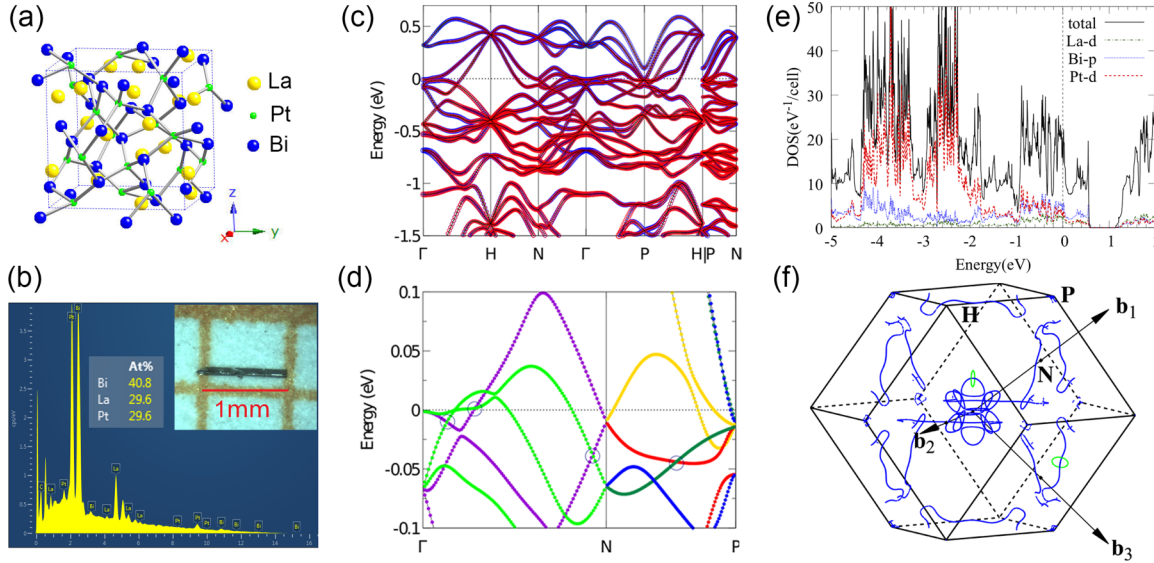


FIG. 1. (a) Crystal structure of $\text{La}_3\text{Pt}_3\text{Bi}_4$ with a $\text{Y}_3\text{Au}_3\text{Sb}_4$ -type structure (SG: $I\bar{4}3d$). (b) EDX spectrum of a $\text{La}_3\text{Pt}_3\text{Bi}_4$ single crystal. The inset is a photo of an $\text{La}_3\text{Pt}_3\text{Bi}_4$ crystal. (c) Electronic band structure of $\text{La}_3\text{Pt}_3\text{Bi}_4$ plotted with orbital characters along high-symmetry lines. Red and blue denote Pt-5d and Bi-6p orbitals, respectively, and the width of the lines is proportional to the weight of the orbital. (d) Electronic band structure plotted with irreducible representations of the little group along Γ -N and N-P. Along Γ -N, the dark violet (green) lines have eigenvalues of $-i$ ($+i$) for the gliding-mirror symmetry, while along N-P, the red lines have eigenvalues -1 and $-i$, gold lines have 1 and $-i$, dark green lines have 1 and $+i$, and blue lines have -1 and $+i$ for the screw and gliding-mirror symmetries, respectively. (e) PDOS of $\text{La}_3\text{Pt}_3\text{Bi}_4$ in the -5- to 2-eV energy range relative to the Fermi energy. (f) The first Brillouin zone showing the high-symmetry points and the nodal-ring structure (blue lines) of $\text{La}_3\text{Pt}_3\text{Bi}_4$. The green circles are the K path used to calculate the Berry phase.

inset of Fig. 1(b). Based on single-crystal x -ray diffraction (Rigaku Gemini A Ultra), the crystal structure was confirmed to be a cubic [see Fig. 1(a)], with lattice parameters $a = b = c = 10.175(5)$ Å, which agrees well with the results reported in Ref. [37]. Energy-dispersive x -ray spectroscopy measurements were performed using a Zeiss Supra 55 scanning electron microscope to verify the crystal composition of La:Pt:Bi = 3:3:4 [see Fig. 1(b)]. The resistivity, and specific heat were measured using a Quantum Design Physical Properties Measurement System (PPMS-9), with a ^3He refrigerator attachment down to 0.5 K. The dc magnetization of the crushed powders was measured using a commercial SQUID magnetometer (Quantum Design MPMS3).

Electronic structure calculations of $\text{La}_3\text{Pt}_3\text{Bi}_4$ were carried out using plane-wave basis DFT as implemented in the Vienna *ab initio* Simulation Package (VASP) [41,42]. The valence-ion interactions were approximated using the projected augmented-wave method [43], and the exchange-correlation functional was approximated using the Perdew, Burke, and Ernzerhoff flavor of the general gradient approximation [44]. The SOC was considered throughout the calculation as a second variation to the total energy. The plane-wave basis energy cutoff was chosen to be 370 eV, and a $6 \times 6 \times 6$ Γ -centered K -mesh was used for Brillouin zone integration to ensure the convergence of the total energy to 1 meV/atom. The geometry was fully relaxed to all forces < 1 meV/Å and internal stress < 0.1 kbar. Finally, the electronic structure obtained from VASP was fitted to a tight-binding Hamiltonian formed by the La 5d, Pt 5d, and Bi 6p orbitals using the Wannier projection method [45,46]. The symmetrization of the resulting Hamiltonian and the symmetry analysis of the band structure were performed using

the WANNYSYMM code [47]. The symmetrized Hamiltonian was then employed to calculate the nodal structure and relevant topological invariants using the WANNIERTOOLS code [48].

III. RESULTS AND DISCUSSION

First, we discuss the electronic band structure and its topological nature based on the DFT calculations. Figures 1(c) and 1(d) show the electronic band structure of $\text{La}_3\text{Pt}_3\text{Bi}_4$ with SOC. The electronic states near the Fermi level are dominated by the Pt 5d and Bi 6p orbitals, as shown by the projected density of states (PDOS) in Fig. 1(e). The total density of states (DOS) is $n(E_F) = 6.55$ states/eV/f.u. or, equivalently, $\gamma_b = 15.45$ mJ/(mol K²). By comparing to the experimentally observed value (please refer to the experimental results), we conclude that the electronic correlation is well described at the DFT level. Large SOC splitting is expected and observed in the resulting band structure. The band structure is similar to that of $\text{Ce}_3\text{Pt}_3\text{Bi}_4$ at higher temperatures (assuming local Ce 4f states) [35]. At Γ , the highest occupied states are doubly degenerate Γ_7 , which are extremely close to the Fermi level, and the next highest occupied states are quarterly degenerate Γ_8 around $E_F - 70$ meV. All the states in the Γ -N-P plane can be classified using the eigenstates of the gliding-mirror symmetry. The Γ_7 state consists of a pair of states with opposite eigenvalues ($\pm i$) of the gliding-mirror symmetry, whereas the Γ_8 state consists of two pairs. Meanwhile, at point N, all the states are doubly degenerate because the system preserves the time-reversal symmetry. These two states bear equal eigenvalues under the gliding-mirror symmetry. Therefore, between Γ and N, an odd number of band crossings must be formed by states with opposite eigenvalues of the gliding-

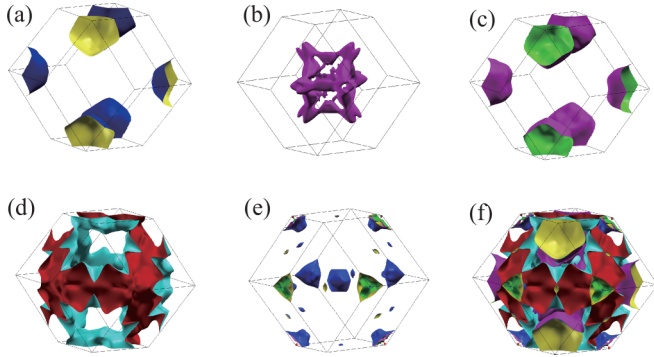


FIG. 2. Fermi surface of La₃Pt₃Bi₄. (a)–(e) Separated Fermi surface sheets. Three of the Fermi surface sheets around *P* are too small, so we plot them together in panel (e). (f) Full Fermi surface plot.

mirror symmetry. A similar argument can also be applied to *N*-*P*. Furthermore, since these states can be classified using the gliding-mirror symmetry, they must form a loop in the Γ -*N*-*P* gliding-mirror plane. Hence, the DFT band-structure calculations show that La₃Pt₃Bi₄ is a nodal-ring semimetal protected by the gliding-mirror symmetry, as discussed for the isostructure Ce₃Pd₃Bi₄ in Ref. [35]. However, we must point out that the nodal rings in La₃Pt₃Bi₄ are different from those in Ce₃Pd₃Bi₄ at low temperatures [35]. The symmetry-protected nodal rings in Ce₃Pt₃Bi₄ are located near the *P* point, whereas they are located around the *N* point and the Γ point in La₃Pt₃Bi₄. Such difference is related with the partially localized nature of the Ce 4*f* states in Ce₃Pd₃Bi₄, effectively corresponding to different electron fillings.

Using the symmetrized tight-binding Hamiltonian obtained with Wannier functions, we identified the nodal-ring structure of La₃Pt₃Bi₄ and calculated the Berry phase around the nodal rings [see Fig. 1(f)]. The nodes of La₃Pt₃Bi₄ can be generally classified into four sets: 12 symmetrically equivalent small nodal rings around Γ (type A), 12 symmetrically equivalent large nodal rings across the border of Brillouin zones around *N* points (type B), 12 symmetrically equivalent small nodal rings around *P* points, and individual high-symmetry nodal points. Among them, only type B is protected by the crystal symmetries, which are ~ 30 meV below the Fermi level. Type A nodal rings are not protected by the crystal symmetries, but are even closer (within 10 meV) to *E_F* and large in the *K* space, and are more relevant to transport properties in the undoped case. Nevertheless, it can be estimated from DOS calculations that the Fermi level would be brought down 35 meV with 0.3 hole/f.u. doping. Therefore, we primarily discuss these two types of nodal rings herein. Using the Wilson loop method, we calculated the Berry phase around both the type A and the type B nodal rings using the *K* path, as shown by the green circles in Fig. 1(f). Both nodal rings yield a Berry phase of π , suggesting that both are topologically nontrivial. We note that the bands crossing *E_F* lead to eight Fermi surface sheets (Fig. 2), among which the four pockets around *P* [Fig. 2(e)] and two pockets around *H* [Figs. 2(a) and 2(c)] are not related with the nodal rings. The other two pockets [Figs. 2(b) and 2(d)] are associated with nodal rings around Γ and *N*, respectively.

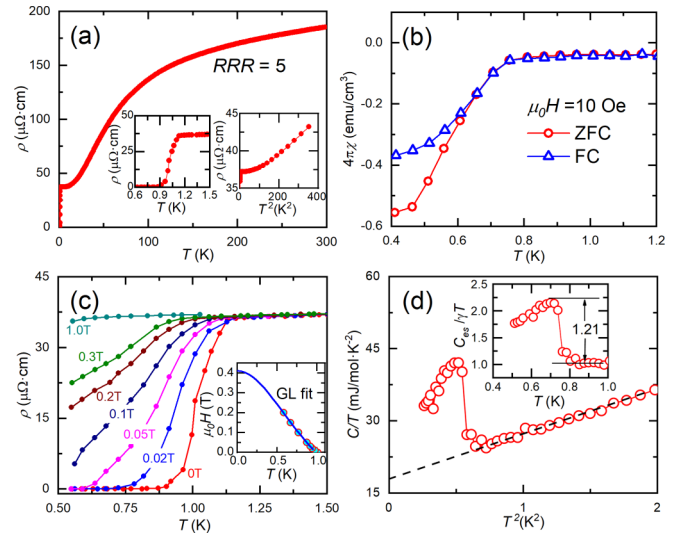


FIG. 3. (a) Temperature dependence of the resistivity of La₃Pt₃Bi₄. Left inset: The detail of the superconducting transition. Right inset: Temperature square dependence of the resistivity below 20 K. (b) $\chi(T)$ near the superconducting transition, measured at 10 Oe field with both ZFC and FC processes. (c) Temperature dependence of the resistivity of the La₃Pt₃Bi₄ single crystal measured under various magnetic fields up to 1.0 T. Inset: Temperature dependence of the upper critical field $\mu_0 H_{c2}$. (d) Specific heat divided by temperature, C/T , as a function of T^2 , measured at zero field. The dashed straight line is a guide to the eyes. Inset: Temperature dependence of $C_{es}/\gamma T$ in the superconducting state at zero field, where $C_{es} = C - \beta T^3$.

Next, we focus on the discovery of superconductivity in La₃Pt₃Bi₄. Figure 3(a) shows the temperature dependence of the resistivity between 0.5 and 300 K for a La₃Pt₃Bi₄ crystal. At *T* = 300 K, the resistivity is about 185 $\mu\Omega$ cm. Upon cooling down from 300 K, the resistivity exhibits metallic characteristics with a continuous change in the slope. The residual resistivity ratio [RRR = $\rho(300 \text{ K})/\rho(2 \text{ K})$] is about 5, larger than that reported previously [38], indicating the high quality of our crystal. At $T_C^{\text{onset}} \sim 1.1$ K, the resistivity starts to drop abruptly, and then at $T_C^{\text{onset}} \sim 0.86$ K, it reaches zero, which is consistent with the onset of a diamagnetic transition [see Fig. 3(b)], indicating the occurrence of a superconducting transition. As shown in the right inset of Fig. 3(a), the *T*-square dependence of the resistivity in the normal state (*T* $\leq$ 20 K) shows nonlinear behavior, indicating that the electron-phonon scattering may play an important role here. Figure 3(b) presents the temperature dependence of the susceptibility, $\chi(T)$, below 1.2 K, measured with both zero-field cooling (ZFC) and field cooling (FC) processes. The superconducting volume fraction at 0.4 K is about 37%, indicating that bulk superconductivity emerges below *T_C* in La₃Pt₃Bi₄. It is worth noting that La₃Pt₃Bi₄ is the first reported superconductor in the Ln₃T₃X₄ (Ln = lanthanoid element, *T* = Cu, Au, Rh, Pd, and Pt, and *X* = Sb and Bi) family, implying that other members may be superconductors as well; however, this must be confirmed through further investigations. We also note that the half-Heusler LaPtBi compound was found to be a noncentrosymmetric superconductor with a *T_C* of ~ 0.9 K,

$\mu_0 H_{c2}(0) = 1.5$ T and to be another candidate for a TSC [49]; however, the superconducting properties, such as $\mu_0 H_{c2}(0)$, the specific heat jump at T_C , and the properties in the normal state, such as the $\rho(T)$ behavior, differ from those exhibited by $\text{La}_3\text{Pt}_3\text{Bi}_4$ reported herein.

Figure 3(c) shows the temperature dependence of the resistivity, $\rho(T, H)$, around the superconducting transition measured at various magnetic fields applied perpendicular to the current. With increasing magnetic field, the superconducting transition gradually shifts to a lower temperature. We estimated the H_{c2} using the middle temperature of the superconducting transition (T_C^{mid}) and plotted $H_{c2}(T)$, as shown in the inset of Fig. 3(c). According to the Ginzburg-Landau theory, $H_{c2}(T)$ can be fitted using the formula $H_{c2}(T) = H_{c2}(0)(1 - t^2)/(1 + t^2)$ to get the zero-temperature upper critical field $\mu_0 H_{c2}(0) \simeq 0.41$ T, where t is the reduced temperature ($t = T/T_C$), as shown by the blue line in the inset of Fig. 3(c). The estimated $H_{c2}(0)$ is much lower than that of the half-Heusler LaPtBi compound (≈ 1.5 T) [49]. Furthermore, the superconducting coherence length ξ_0 for the $\text{La}_3\text{Pt}_3\text{Bi}_4$ compound was estimated to be ~ 28.4 nm using the formula $H_{c2}(0) = \Phi_0/2\pi\xi_0^2$, where Φ_0 (2.071×10^{-15} Wb) is the fluxoid quantum.

To measure the specific heat $C(T)$, we arranged several needlelike crystals on the measurement puck. $C(T)/T$ as a function of T^2 , measured at zero magnetic field, is shown in Fig. 3(d). A significant specific heat jump was observed at approximately 0.8 K, thereby confirming again that $\text{La}_3\text{Pt}_3\text{Bi}_4$ exhibits bulk superconductivity. We used the formula $C/T = \gamma + \beta T^2$ to fit the $C(T)$ data (1.1–2 K) in the normal state to obtain the Sommerfeld coefficient $\gamma = 17.3$ mJ/(mol K²) and the Debye constant $\beta = 9.9$ mJ/(mol K⁴), corresponding

to the Debye temperature $\Theta_D = 125$ K. We note that the γ value here is somehow smaller than that reported previously [38], which may be due to different temperature ranges used for fitting. The electronic specific heat $C_{\text{es}}(T)$ in the superconducting state was obtained by subtracting the phonon contribution term βT^3 from the total $C(T)$, as shown in the inset of Fig. 3(d). The normalized specific heat jump $\Delta C/(\gamma T_C)$ at T_C was estimated to be 1.21, which is smaller than the well-known BCS theory value (~ 1.43).

IV. CONCLUSIONS

In summary, by combining resistivity, susceptibility, and specific heat measurements, we discovered bulk superconductivity with $T_C^{\text{onset}} = 1.1$ K and $\mu_0 H_{c2}(0) = 0.41$ T in the $\text{La}_3\text{Pt}_3\text{Bi}_4$ compound. The first-principles calculations demonstrate that $\text{La}_3\text{Pt}_3\text{Bi}_4$ is a nodal-ring semimetal protected by the gliding-mirror symmetry. These results indicate that $\text{La}_3\text{Pt}_3\text{Bi}_4$ provides a material platform for studying novel superconductivity in the nodal-ring system.

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