$RRuB_2$ (R = Y, Lu), topological superconductor candidates with hourglass-type Dirac ring

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Topological properties and topological superconductivity in real materials have attracted intensive experimental and theoretical attention recently. Based on symmetry analysis and first-principles electronic structure calculations, we predict that $RRuB_2$ (R = Y, Lu) are not only topological superconductor (TSC) candidates but also own the hybrid hourglass-type Dirac ring which is protected by the nonsymmorphic space group symmetry. Due to the band inversion around the time-reversal invariant Γ point in the Brillouin zone, $RRuB_2$ also have Dirac topological surface states (TSSs). More importantly, their TSSs on the (010) surface are within the band gap of bulk and cross the Fermi level, which form single Fermi surfaces. Considering the fact that both YRuB₂ and LuRuB₂ are superconductors with respective superconducting transition temperatures (T_c) of 7.6 K and 10.2 K, the superconducting bulks will likely induce superconductivity in the TSSs via the proximity effect. The ternary borides $RRuB_2$ may thus provide a very promising platform for studying the properties of topological superconductivity and hourglass fermions in future experiments.

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I. INTRODUCTION

Topological superconductors (TSCs) with Majorana zero modes (MZMs) at boundaries and vortices have attracted intense interest due to their exotic physical phenomena and potential applications in topological quantum computation [1-3]. To well explore the exotic properties of MZMs, it is necessary to search for various TSCs, as many as possible, especially those with high superconducting transition temperature (T_c) as well as high sample quality. However, intrinsic spinless p + ip type TSCs are very scarce [4]. Instead, a feasible scheme that can achieve the equivalent $p_x + ip_y$ type superconductivity has been proposed by Fu and Kane [5], by which the topological superconductivity can be obtained in the topological surface states (TSSs) of a topological insulator (TI) via doping or proximity effect, such as Cu/Sr/Nbdoped Bi₂Se₃ [6–8], In-doped SnTe [9], Bi₂Se₃/NbSe₂, and Bi₂Se₃/Bi2212 heterostructures [10,11].

In order to avoid the complex interface effect and lattice mismatch between a superconductor and a TI or the disorder introduced by doping, a natural idea is to realize topological superconductivity in single compounds [12,13]. Although much effort has been devoted to searching for stoichiometric single-compound TSCs [14–16], for example, the existing superconductors Au₂Pb (1.18 K) [17], PdTe₂ (1.7 K) [18], PbTaSe₂ (3.8 K) [19,20], BiPd (3.8 K) [21,22], YD₃ (0.78 K to 4.72 K) [23], β -PdBi₂ (5.3 K) [24], all the known TSC candidates, are confronted with a very low T_c . As the energy spacing of the Caroli-de Gennes-Matricon (CdGM) bound

investigated based on the density functional theory (DFT) calculations using the projector augmented wave (PAW) method [27] as implemented in the VASP package [28]. The exchange-correlation functional was described by the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) type [29]. The kinetic energy cutoff of the plane wave basis was set to 500 eV. An $8 \times 8 \times 8$ Monkhorst-Pack *k*-point mesh [30] was taken for the Brillouin zone (BZ) sampling, and the Gaussian smearing method

states [25] is in the order of $\frac{\Delta^2}{\varepsilon_f}$ (the Δ and ε_f are the superconducting gap and the Fermi energy, respectively), increasing

the T_c is beneficial to the experimental observation of the

MZMs. An ideal stoichiometric single-compound TSC should

meet three criteria at the same time: (1) The stoichiometric

compound is an s-wave superconductor with relatively high

 T_c . (2) The compound possesses topological surface states

with spin-moment locking. (3) The TSSs remain separated

from the bulk states and across the Fermi level. Unfortunately,

the compounds that satisfy the criteria are still very rare so far.

ternary borides $RRuB_2$ (R = Y, Lu) are ideal topological superconductor candidates that meet the above criteria. More-

over, they also own hourglass-type nodal rings protected by

the nonsymmorphic space group symmetries. Considering the

fact that the experimental T_c of YRuB₂ and LuRuB₂ are 7.6 K

In this work, we propose that the rare-earth transition-metal

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FIG. 1. (a) Crystal structure of $RRuB_2$ (R = Y, Lu). The blue, red, and golden balls represent R, Ru, and B atoms, respectively. (b) Bulk Brillouin zone (BZ) and projected two-dimensional (2D) BZ of the (010) surface. The red dots and blue lines represent the high-symmetry points and paths in the BZ, respectively.

with a width of 0.05 eV was adopted. The energy and force convergence criteria were set to 10^{-6} eV and 0.001 eV/Å, respectively. The optimized lattice parameters for YRuB₂ are a = 5.914 Å, b = 5.320 Å, and c = 6.357 Å, and for LuRuB₂ are a = 5.818 Å, b = 5.252 Å, and c = 6.282 Å, in good agreement with their experimental values (a = 5.910 Å, b = 5.229 Å, and c = 6.363 Å for YRuB₂ and a = 5.809 Å, b = 5.229 Å, and c = 6.284 Å for LuRuB₂) [31]. The surface states and spin textures of a semi-infinite *R*RuB₂ (R = Y, Lu) surface were calculated with the surface Green's function method by using the WannierTools [32] package.

III. RESULTS

As shown in Fig. 1(a), the ternary borides $RRuB_2$ (R = Y, Lu) own a nonsymmorphic space group No. 62 (*Pnma*) with the corresponding D_{2h} point group symmetry, which can be generated by the following three symmetry elements: The inversion \mathcal{P} , the mirror \mathcal{M}_y : $(x, y, z) \rightarrow (x, -y + \frac{1}{2}, z)$, and glide mirror $\widetilde{\mathcal{M}}_x$: $(x, y, z) \rightarrow (-x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2})$. Based on the combination of these three symmetry operations, we can obtain another glide mirror: $\widetilde{\mathcal{M}}_z$: $(x, y, z) \rightarrow (x + \frac{1}{2}, y, -z + \frac{1}{2})$. Here the tilde represents a nonsymmorphic operation, which includes a translation with fractional lattice parameters. Moreover, the *R*RuB₂ are nonmagnetic, indicating that the time-reversal symmetry \mathcal{T} is preserved [33]. Their three-dimensional (3D) bulk Brillouin zone (BZ) with the projected two-dimensional (2D) BZ of the (010) surface are plotted in Fig. 1(b).

The calculated band structures of YRuB₂ and LuRuB₂ without the spin-orbit coupling (SOC) are shown in Figs. 2(a) and 2(c), respectively. One can see that YRuB₂ and LuRuB₂ have similar electronic band structures, in which the band crossing points (red circles) along the high-symmetry Γ -Y and Γ -Z paths indicate that there is a nodal ring around the Γ point in the $k_x = 0$ plane protected by the M_x symmetry (see Supplemental Material (SM) Fig. S1 [34]). Since the symmorphic and nonsymmorphic space groups have the same irreducible representations in the interior of BZ and the highest rotation symmetry is of twofold axis for YRuB₂ and LuRuB₂, the nodal ring around the Γ point in the $k_x = 0$ plane



FIG. 2. Band structures of YRuB₂ and LuRuB₂ calculated without and with the spin-orbit coupling (SOC) along the high-symmetry paths in the BZ, respectively.



FIG. 3. The hourglass-type band dispersions of (a)–(c) YRuB₂ and (d)–(f) LuRuB₂ along paths S-X, S-R, and S-K in the presence of SOC. Here *K* is an arbitrary point on path T-R; we take the midpoint between T and R for illustration as shown in (c) and (f). The red numbers and signs in the figures represent the eigenvalues g_x of $\widetilde{\mathcal{M}}_x$, and the numbers in brackets show the degeneracy of the eigenvalues. (g) The schematic figure of the fourfold degenerate Dirac ring formed by the neck points (red dots) of the hybrid hourglass dispersion on the $k_x = \pi$ plane. (h), (i) The distribution of the hourglass Dirac ring (the white colored rings) surrounding point S for YRuB₂ and LuRuB₂, respectively. The color bar shows the local gap between the two crossing bands.

will open a complete gap with the inclusion of SOC. Thus both YRuB₂ and LuRuB₂ have the band inversion around the Γ point [Figs. 2(b) and 2(d)], which is crucial for the appearance of their topological surface states (TSSs) (We will discuss this point in detail later). We have also examined the correlation effect in the 4*d* electrons of Ru atoms with different Hubbard U values, in which no substantial change is found for the band structure near the Fermi level (see Fig. S2 in the SM [34]).

On the other hand, the hourglass-type fermions protected by nonsymmorphic symmetry have been proposed in recent works [35–37]. Interestingly, YRuB₂ and LuRuB₂ display an hourglass-type dispersion in a large energy range from -0.17 eV to 0.42 eV along the S-X path as shown in Figs. 2(b) and 2(d) [the corresponding enlargements shown in Figs. 3(a) and 3(d)]. Let's first consider the hourglass-type dispersion along path S-X: $(\pi, k_y, 0)$, where $-\pi < k_y \leq \pi$. This path locates in the $k_x = \pi$ plane which is invariant under $\widetilde{\mathcal{M}}_x$, so that each Bloch state $|\Phi_n\rangle$ at the path is also an eigenstate of $\widetilde{\mathcal{M}}_x$. Since the rotation or mirror operations under the SOC not only act on the spatial coordinates but also on the spin degrees of freedom, we have

$$(\widetilde{\mathcal{M}}_x)^2 = \mathcal{T}_{011}\bar{E} = -e^{-ik_y},\tag{1}$$

in the S-X path, where \overline{E} denotes the 2π spin rotation and $\mathcal{T}_{011}: (x, y, z) \rightarrow (x, y + b, z + c)$ is the lattice translation operator. Hence the eigenvalue g_x of $\widetilde{\mathcal{M}}_x$ must be $\pm i e^{-ik_y/2}$. For a state $|\Phi_n\rangle$ with an eigenvalue g_x of $\widetilde{\mathcal{M}}_x$, it has a Kramers partner $\mathcal{PT}|\Phi_n\rangle$ satisfying

$$\mathcal{M}_{x}(\mathcal{PT}|\Phi_{n}\rangle) = g_{x}(\mathcal{PT}|\Phi_{n}\rangle).$$
(2)

This demonstrates that the Kramers partners $|\Phi_n\rangle$ and $\mathcal{PT}|\Phi_n\rangle$ in the S-X path share the same eigenvalue g_x .

At the same time, the S and X points are the time-reversal invariant momenta (TRIM). At the S point: $(\pi, \pi, 0)$, we can get $g_x = \pm 1$ (we further obtain that the eigenvalue of lower energy is $g_x = -1$ and the higher one is $g_x = +1$ by computing the traces of the corresponding matrix representations [38]) and

$$\widetilde{\mathcal{M}}_{x}(\mathcal{T}|\Phi_{n}\rangle) = g_{x}(\mathcal{T}|\Phi_{n}\rangle),$$
 (3)

hence each Kramers partner $|\Phi_n\rangle$ and $\mathcal{T}|\Phi_n\rangle$ at the S point must have the same eigenvalue g_x . Meanwhile,

$$\widetilde{\mathcal{M}}_{x}(\mathcal{P}|\Phi_{n}\rangle) = g_{x}(\mathcal{P}|\Phi_{n}\rangle), \qquad (4)$$

thus we may choose $|\Phi_n\rangle$, $\mathcal{T}|\Phi_n\rangle$, $\mathcal{P}|\Phi_n\rangle$, and $\mathcal{PT}|\Phi_n\rangle$ as a degenerate quartet at the S point, which must have the same g_x .

The similar analysis also applies to the X point. At X: $(\pi, 0, 0)$, since $g_x = \pm i$, each Kramers partner $|\Phi_n\rangle$ and $\mathcal{T}|\Phi_n\rangle$ should have opposite eigenvalues g_x , and the degenerate quartet must be composed of two states with $g_x = +i$ and two other states with $g_x = -i$. Therefore, there must be a pair switching when going from S to X, which gives rise to an hourglass-type dispersion [see Fig. 3(a)]. In particular, the neck point (red dot) of hourglass-type dispersion is a fourfold degenerate point for YRuB₂, which is formed by the enforced band crossing of two degenerate bands with the opposite eigenvalues g_x . In contrast, it is not completely an hourglass-type dispersion along the S-X path for LuRuB₂ [see Fig. 3(d)], which is caused by the increasing band dispersion due to the strengthened SOC. In addition to the hourglasstype Dirac fermion (red dot), there is a type-II Dirac fermion (blue dot) derived from the two degenerate bands with the opposite eigenvalues g_x [shown in the inset of Fig. 3(d)]. Here the hourglass-type fermion accompanying the type-II Dirac fermion is termed as a hybrid hourglass-type fermion, and the nodal line composed of hybrid hourglass-type fermions as the hybrid hourglass-type nodal line. To our knowledge, the hybrid hourglass-type Dirac fermion found here has not been discussed before.

Likewise, for path S-R: (π, π, k_z) , we have

$$(\widetilde{\mathcal{M}}_x)^2 = \mathcal{T}_{011}\bar{E} = e^{-ik_z},\tag{5}$$

on S-R. Thus the eigenvalue g_x of $\widetilde{\mathcal{M}}_x$ must be $\pm e^{-ik_z/2}$. For a state $|\Phi_n\rangle$, it has a Kramers partner $\mathcal{PT}|\Phi_n\rangle$ that satisfies Eq. (2). Therefore, the Kramers partners $|\Phi_n\rangle$ and $\mathcal{PT}|\Phi_n\rangle$ on S-R share the same eigenvalue g_x . At R: (π, π, π) , we can also get $g_x = \pm i$. Hence at R each Kramers partner $|\Phi_n\rangle$ and $\mathcal{T}|\Phi_n\rangle$ should have the opposite eigenvalues g_x , and the degenerate quartet must be composed of two states with $g_x = +i$ and two other states with $g_x = -i$. Thus, there must be also a pair switching when going from S to R. But, different from the case with the S-X path, the band dispersion of YRuB2 and LuRuB₂ changes dramatically along path S-R [see Figs. 3(b) and 3(e)]. This gives rise to multiple band inversions as well as the emergence of the type-I Dirac fermion (red dot) or type-II Dirac fermion (marked by the blue dots). Here we remind that the band-crossing points (green dots) have the same eigenvalue g_x of $\widetilde{\mathcal{M}}_x$. Thus they will be gapped by a perturbation, except for the one with the protection by a screw axis C_{2z} . Here we will not discuss it in detail, because our main concern is about the hourglass-type Dirac ring formed by the neck points (red dots) of the hourglass-type dispersion.

The above analysis can be further generalized to any one path connecting S to a point on the boundary lines T-R or X-T in the $k_x = \pi$ plane [see Fig. 3(g)]. The degeneracies on paths T-R or X-T can be explained in a similar way. Here we take an arbitrary K point on path T-R for analysis. At $K: (\pi, k_v, \pi)$,

we have

$$(\widetilde{\mathcal{M}}_x)^2 = \mathcal{T}_{011}\bar{E} = e^{-ik_y},\tag{6}$$

hence the eigenvalue g_x of $\widetilde{\mathcal{M}}_x$ must be $\pm e^{-ik_y/2}$. For a state $|\Phi_n\rangle$, it has a Kramers partner $\mathcal{PT}|\Phi_n\rangle$ satisfying Eq. (2). Thus, the Kramers partners $|\Phi_n\rangle$ and $\mathcal{PT}|\Phi_n\rangle$ at the *K* point share the same eigenvalue g_x . Meanwhile, path T-R keeps invariant with respect to the \mathcal{M}_z operation. The commutation relation between $\widetilde{\mathcal{M}}_x$ and $\widetilde{\mathcal{M}}_z$ is

$$\widetilde{\mathcal{M}}_{x}\widetilde{\mathcal{M}}_{z} = -\mathcal{T}_{\overline{1}01}\widetilde{\mathcal{M}}_{z}\widetilde{\mathcal{M}}_{x},\tag{7}$$

where the negative sign is the result of these operations on spin, i.e., from $\{\sigma_x, \sigma_z\} = 0$, so that $\{\widetilde{\mathcal{M}}_x, \widetilde{\mathcal{M}}_z\} = 0$ on path T-R. Then we can get

$$\widetilde{\mathcal{M}}_{x}(\widetilde{\mathcal{M}}_{z}|\Phi_{n}\rangle) = -g_{x}(\widetilde{\mathcal{M}}_{z}|\Phi_{n}\rangle), \qquad (8)$$

indicating the two states $\widetilde{\mathcal{M}}_z | \Phi_n \rangle$ and $| \Phi_n \rangle$ have the opposite eigenvalues on path T-R. Likewise, at each k point on path T-R, the degenerate quartet of $|\Phi_n\rangle$, $\mathcal{PT}|\Phi_n\rangle$, $\widetilde{\mathcal{M}}_z|\Phi_n\rangle$, and $\mathcal{M}_{z}\mathcal{PT}|\Phi_{n}\rangle$ must be composed of two states $(|\Phi_{n}\rangle)$ and $\mathcal{PT}|\Phi_n\rangle$) with $+e^{-ik_y/2}$ and two other states $(\widetilde{\mathcal{M}}_z|\Phi_n\rangle$ and $\widetilde{\mathcal{M}}_z\mathcal{PT}|\Phi_n\rangle$) with $-e^{-ik_y/2}$. Therefore, there must be a pair switching when going from S to the arbitrary K point on path T-R (similar for path X-T). Figure 3(c) shows the hourglasstype band dispersion accompanying an extra Dirac fermion (purple dot) for YRuB₂, derived from the path connecting S to the point K on T-R. One notes that there is another type-II Dirac fermion (blue dot) along path S-K for LuRuB₂ in addition to the hourglass-type fermion [see Fig. 3(f)]. As a result, the neck points (red dots) of the hourglass-type dispersion of YRuB₂ and LuRuB₂ are guaranteed and meanwhile there forms a continuous nodal ring encircling point S in the $k_x = \pi$ plane [see Fig. 3(g)]. This is further confirmed by our DFT calculations, as shown in Figs. 3(h) and 3(i) for YRuB₂ and LuRuB₂, respectively. Thus this hybrid hourglasstype Dirac ring is essentially and entirely determined by the nonsymmorphic space group symmetry. At the same time, this also provides various pair switchings of glide-reflection eigenvalues for the hybrid hourglass-type fermions to form robust Dirac points. In addition, these Dirac points are 80 to 150 meV below the Fermi level, which can be observed by angle-resolved photoemission spectroscopy (ARPES) measurements.

As shown above, both YRuB₂ and LuRuB₂ have the band inversions around the Γ point. Due to the anticommutation relation of inversion and mirror symmetries, a Bloch state at the TRIM points except for the Γ and T points is in quadruple degeneracy with two double degeneracies marked simultaneously by plus and minus parities. Although RRuB₂ does not have a global band gap in the entire BZ when including the SOC, the topological Z_2 invariant [39] can still be well defined on the $k_v = 0$ plane by the product of the parities of all occupied states at the four time-reversal invariant momentum (TRIM) points (Γ , Z, T, and X) as listed in Table I. Our calculation shows that $Z_2 = 1$, indicating the existence of nontrivial TSSs on the (010) surface in Fig. 4. On the other hand, if the nonsymmorphic symmetry above is broken, the hourglass-type Dirac ring will open a band gap, and the band inversion around the Γ point will result in a strong topological insulator phase for YRuB₂ and LuRuB₂ (see Table I).

TABLE I. Parity products of all occupied band eigenstates at eight TRIM points in the BZs and the Z_2 indices of YRuB₂ and LuRuB₂.

	Г	R	S	U	Т	Х	Y	Ζ	$(v_0; v_1v_2v_3)$
YRuB ₂	_	_	_	_	+	_	_	_	(1; 101)
LuRuB ₂	-	-	—	_	+	_	-	—	(1; 101)

Thus, both YRuB₂ and LuRuB₂ have robust TSSs on their surfaces. The calculated TSSs on (010) surfaces of YRuB₂ and LuRuB₂ are shown in Figs. 4(a) and 4(b), respectively. One can note that YRuB₂ has the Dirac TSSs around the $\bar{\Gamma}$ point on the (010) surface protected by the time-reversal symmetry, while for LuRuB₂ the Dirac point of surface states at the $\bar{\Gamma}$ point overlaps with the bulk states. Interestingly, both of their TSSs on the (010) surfaces cross the Fermi level and are within the bulk gaps, especially forming single Fermi surfaces [Figs. 4(c) and 4(d)]. Meanwhile, previous experiments found that both YRuB₂ and LuRuB₂ are superconductors [26]. The superconducting bulks of YRuB₂ and LuRuB₂ may induce the equivalent p + ip superconductivity in the single TSSs on the (010) surface, which support the Majorana zero modes in the vortex cores. Thus, YRuB₂ and LuRuB₂ may be single-compound TSCs satisfying the aforementioned three criteria. Note that if the chemical potential of $RRuB_2$ moves to 50 meV (μ_2) below the Fermi level as shown in Figs. 4(a) and 4(b), their TSSs will merge into the bulk states (see Fig. S3 in the SM [34]), which could cause the disappearance of the topological superconducting state. This makes the surface topological superconductivity sensitive to the position of the chemical potential [40]. However, we also investigate the surface states of $YRuB_2$ on the (100) and (001) surfaces, as shown in the SM Fig. S4 [34]. We find that the surface states on the (100) and (001) planes are rather complex and these surface states across the Fermi level form double Fermi surfaces, thus we do not discuss them here.

IV. DISCUSSION AND SUMMARY

As a new class of topological superconductor candidates with hourglass-type nodal rings, $RRuB_2$ (R = Y, Lu) have many advantages. First, $RRuB_2$ are such a class of stoichiometric single-compound superconductors (SCs), compared



FIG. 4. Surface energy bands of (a) YRuB₂ and (b) LuRuB₂ along the high-symmetry paths in the projected 2D BZ of the (010) surface. The chemical potentials at the Fermi level $E_f(\mu_1)$ and 50 meV below the Fermi level (μ_2). Surface spectrum of (c) YRuB₂ and (d) LuRuB₂ at a fixed energy E_f . Here the black arrows represent the directions of spins.

with the doped TIs [41], the TI/SC heterostructures [42], or the pressurized TIs [43,44], that RRuB₂ can avoid the disorder effect, lattice mismatch, and interface reaction issues. Second, the T_c 's of YRuB₂ (7.6 K) and LuRuB₂ (10.2 K) are higher than those of the existing SCs with TSSs, such as Au₂Pb (1.18 K) [17], PdTe₂ (1.7 K) [18], PbTaSe₂ (3.8 K) [19,20], BiPd (3.8 K) [21,22], YD₃ (0.78 K to 4.72 K) [23], β -PdBi₂ (5.3 K) [24]. The higher T_c is helpful for the experimental observation of the MZMs. In addition, the hourglass-type Dirac ring has the drumheadlike surface states [36], giving rise to interesting phenomena such as the anomalous Landau level spectrum [45], the possible surface magnetism/superconductivity [46,47], the unusual optical response [48], and the anisotropic electron transport [49]. Importantly, unlike a general nodal line that can be removed by the spin-orbit coupling (SOC), the hourglass-type nodal ring is guaranteed by the nonsymmorphic symmetries and cannot be removed by the SOC.

In summary, based on symmetry analysis and firstprinciples electronic structure calculations, we predict that $RRuB_2$ (R = Y, Lu) are not only topological superconductors but also own the hybrid hourglass-type Dirac ring which is protected by the nonsymmorphic space group symmetry. Especially, their topological Dirac surface states remain separated from the bulk states, cross the Fermi level, and preserve single helical spin textures. The superconductivity in bulk YRuB₂ (7.6 K) and bulk LuRuB₂ (10.2 K) may further give rise to superconductivity in the topological surface states by the proximity effect. To the best of our knowledge, LuRuB₂ has the highest T_c among the stoichiometric single-compound TSC candidates. Thus the *R*RuB₂ (R = Y, Lu) materials may provide a very promising platform for the realization of topological superconductivity and hourglass fermions in future experiments.

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