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Unconventional superconducting pairing in a B20 multifold Weyl fermion semimetal

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Topological superconductors present an ideal platform for exploring nontrivial superconductivity and realizing the Majorana boundary modes. However, finding a single-phase topological material with nontrivial superconducting states has been a challenge. Here, we predict nontrivial superconductivity in the pristine chiral metal RhGe with a transition temperature of 5.8 K. Chiral symmetries in RhGe enforce multifold Weyl fermions at high-symmetry momentum points and spin-polarized Fermi arc states that span the entire surface Brillouin zone. These bulk and surface chiral states support multiple type-II van Hove singularities that enhance superconductivity in RhGe. Our analysis of superconducting pairing symmetries involving Chiral Fermi pockets in RhGe indicates the presence of nontrivial superconducting pairing. Our study establishes RhGe as a promising candidate material for hosting mixed-parity pairing and topological superconductivity.

The quest for Majorana zero modes (MZMs) which are key for the development of fault-tolerant quantum computation devices has spurred interest in search for topological superconductors [1–3]. Recent efforts have focused on characterizing MZMs in theoretical models and experiments on complex heterostructures [4–7]. Unfortunately, the observation of isolated MZMs still remains inconclusive. In their simplest form, the MZMs have been predicted to exist at the boundary of a two-dimensional chiral p -wave superconductor [8–10]. However, the scarcity of such superconductors necessitates the exploration of alternative avenues for realizing MZMs.

A significant breakthrough is the prediction of MZMs at the vortex core of the gapped surface states of three-dimensional (3D) topological insulators via the proximity effect of an s -wave superconductor [11, 12]. This has ignited efforts to look for superconductivity in topological insulators and semimetals employing chemical doping, external pressure, and reduced dimensionality [13–22]. Noteworthy examples are the iron-based superconductors with Dirac-type inverted band crossings, which show the signature of topological superconductivity with MZMs at the vortex core [23–25]. Alternately, the momentum-dependent odd-parity pairing can originate from the large spin-orbit coupling (SOC) in non-centrosymmetric superconductors [26–32]. However, most superconductors reported to date are inversion symmetric. The Pauli exclusion principle and parity conservation dictate that a superconductor with even parity must be a spin singlet, while an odd parity superconductor must be spin-triplet [33, 34]. A material that lacks inversion symmetry and has parity-breaking SOC can thus support an admixture of spin-singlet and spin-triplet pairings [27–32].

Here we show that the CoSi family of materials are ideal

candidates for hosting topological superconductivity. These materials form chiral crystal structures and support unconventional Kramers-Weyl fermions [35–41]. They host the longest possible Fermi-arc surface states spanning the entire surface Brillouin zone (BZ) and feature intriguing optoelectronic and spintronic properties, including helicity-dependent photocurrent [42], a large circular photogalvanic effect [43], a spin Nernst effect [44], and exciting plasmons [45]. Here, we demonstrate that RhGe exhibits an electron-phonon-coupling (EPC) mediated superconductivity driven by multiple type-II van Hove singularities (VHSs) associated with its chiral bands. The superconducting state, nontrivial electronic topology, and the chiral crystal symmetries offer all the crucial prerequisites for hosting mixed-parity topological superconductivity in RhGe [46–49]. By characterizing possible pairing symmetries in the Fermi pockets around the multifold Weyl nodes at the Γ and R points, we demonstrate a time-reversal-symmetry broken topological superconducting state in RhGe.

RhGe assumes a B20-type chiral cubic lattice with space group $P2_13$ (Fig. 1(a)) [50, 51]. The B20 structure emerges due to a pair sublattice distortion along the $[111]$ direction (chiral axis), which dimerizes the bonds and breaks (roto)-inversion symmetries [Figs. 1(a)-(b)]. It preserves a three-fold rotation $\{C_{3,111}|000\}$ symmetry along the $[111]$ direction and three $\frac{2\pi}{3}$ screw rotation symmetries with a non-primitive translation ($\{S_{2,100}|\frac{1}{2}\frac{1}{2}0\}$, $\{S_{2,010}|\frac{1}{2}0\frac{1}{2}\}$, and $\{S_{2,001}|\frac{1}{2}0\frac{1}{2}\}$). The fully relaxed lattice parameter of RhGe is $a = 4.79$ Å and internal parameters are $u_{Rh} = 0.134$ and $u_{Ge} = 0.838$ (both Rh and Ge occupy the Wyckoff position $4a \rightarrow \{u_x, u_x, u_x\}$, x is Rh or Ge), see Supplementary Materials (SMs) for details [52].

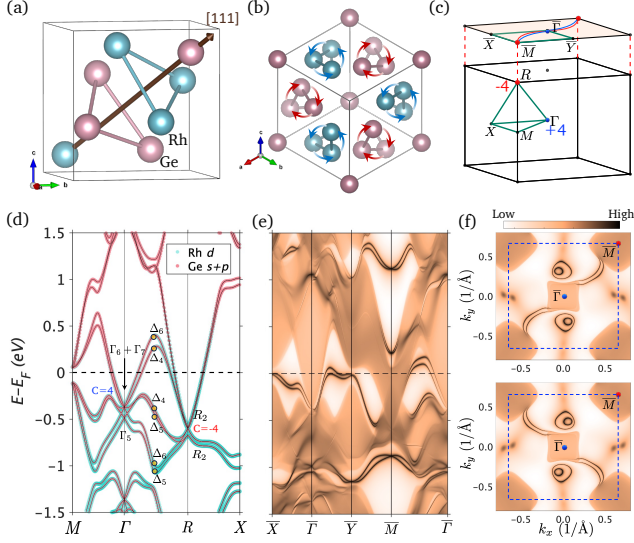


FIG. 1. (a)-(b) Chiral crystal structure of RhGe with a pair distortion along the $[111]$ chiral axis. (c) Bulk Brillouin zone (BZ) and the projected (001) surface BZ. High-symmetry k points, chiral charges, and the Fermi-arc surface states are highlighted. (d) Bulk band structure of RhGe with spin-orbit coupling. The Rh- d and Ge- (s,p) orbital contributions and band representations are shown. (e) (001)-surface spectral function along the high-symmetry directions in the surface BZ. Sharp black lines show the chiral surface states. (f) Calculated band contours at the Fermi level. The Fermi-arc surface states connect the $+4$ chiral-charge Weyl node at the BZ center $\bar{\Gamma}$ with the -4 chiral-charge node at the BZ corner $\bar{M}$. Top and bottom panels depict the opposite connectivity of the Fermi-arc states at the top (Rh termination) and bottom (Ge termination) surfaces.

Bulk band structure of RhGe is shown in Fig. 1(d). The presence of time-reversal and non-symmorphic symmetries enforces multiple band degeneracies to generate a unique semi-metallic phase with unconventional multifold Weyl fermions. In the absence of SOC, the band structure realizes a three-fold (spin-1 fermion) and a four-fold degenerate band-crossing (double Weyl fermion) pinned at the high-symmetry Γ and R points with chiral charges of $+2$ and -2 , respectively. Inclusion of the SOC splits the three-fold node at Γ into a Kramers Weyl node (spin-1/2 fermion) at -0.48 eV and a four-fold degenerate unconventional RSW Weyl node (spin-3/2 fermion) at -0.37 eV. At the R point, a six-fold degenerate chiral node (double spin-1 fermion) is formed at -0.58 eV. The chiral charges of the nodes at the Γ and R points are $+4$ and -4 , respectively. The surface state spectrum in Fig. 1(e) shows four topological surface states connecting the projection of the bulk chiral nodes at the $\bar{\Gamma}$ and $\bar{R}$ points. At the Fermi energy, these states form the Fermi arcs spanning the entire BZ. Unlike the surface states of generic-point Weyl semimetals, the surface states in RhGe originate from the symmetry-enforced bulk Weyl nodes, making them robust against local perturbations and disorder. The chiral nature of these surface states is depicted in the electronic structure of the top and bottom surface terminations, where the Fermi-arc connectivity is seen to

switch between the pockets at the center and the corners of the surface BZ [Fig. 1(f)].

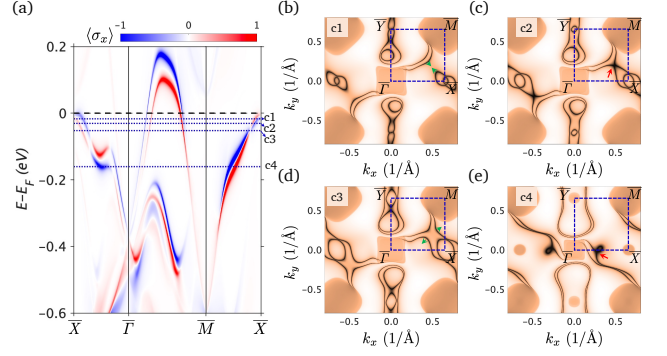


FIG. 2. (a) Spin-polarized surface states of RhGe on the (001) surface along $\bar{X} - \bar{\Gamma} - \bar{M} - \bar{X}$. The dashed blue lines c1 (17 meV), c2 (30 meV), c3 (50 meV), and c4 (160 meV) below the Fermi level show constant energy cuts in (b)-(e). The chiral fermi-arc states exchange connectivity from c1 to c4. Red arrows in c2 and c4 locate the generic k -points type II VHSs that appear as a crossing between the chiral surface states.

Fig. 2 demonstrates the evolution of surface Fermi arcs as a function of band energy and reveal the presence of type-II VHSs as seen experimentally in CoSi and RhSi [53]. Note that the position of the VHS at a generic k point dictates the nature of the VHS as type II. Figure 2(a) illustrates the calculated spin-polarized surface states along $\bar{X} - \bar{\Gamma} - \bar{M} - \bar{X}$. A large SOC-driven spin-splitting in the chiral surface states is evident with high spin polarization at the Fermi energy. Evolution of the associated Fermi arcs is shown in Figs. 2(b)-(e) through successive energy cuts, where the VHSs appear as crossing points of different pockets. In the constant-energy cut c1 ($E = 17$ meV), one interband and one intraband crossing appears around the $\bar{X}$ and $\bar{Y}$ points, respectively. As we lower energy to 30 meV (cut c2), the two helicoid arc states move toward each other and touch at the generic momentum points $(\pm 0.49, \pm 0.19) \text{ \AA}^{-1}$ to form type-II VHSs. Further lowering the energy to 50 meV (cut c3) captures the intermediate stage of the chirality exchange between the helicoid states, where the inner state along $\bar{\Gamma} - \bar{Y}$ crosses at $(0, \pm 0.52) \text{ \AA}^{-1}$. Finally, at 160 meV (cut c4), another intraband crossing appears at the symmetry-equivalent generic momentum point $(\pm 0.26, \mp 0.02) \text{ \AA}^{-1}$. These multiple type-II VHSs in the surface state spectrum could induce an electronic surface instability and lead to unconventional superconductivity in RhGe.

Since RhGe exhibits a superconducting state below ~ 4.3 K [50], its surface states can become superconducting via the proximity effect. Accordingly, we now investigate the possibility of superconductivity in the bulk states and discuss the associated pairing symmetries. Figure 3(a) shows the bulk band structure along the chiral axis ($\Gamma - R$ line) and the density of states (DOS) of RhGe. A careful analysis reveals that a large DOS at 0.4 eV above the Fermi energy is associated with the VHS. In Fig. 3(b), we illustrate constant energy contours on the $k_z = 0.62 \text{ \AA}^{-1}$ plane. The crossing of constant energy

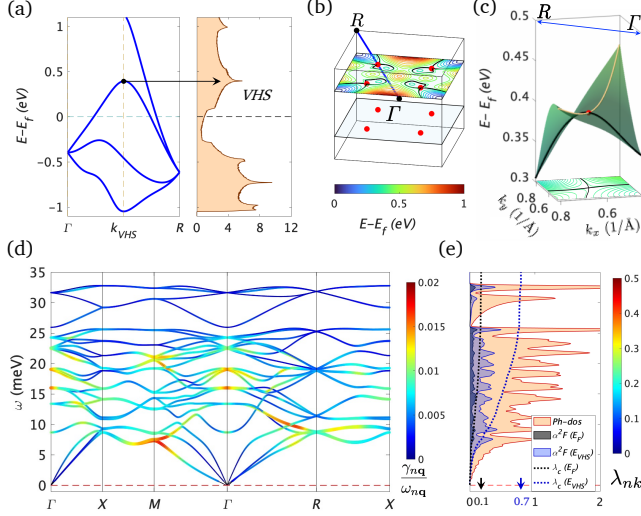


FIG. 3. (a) Bulk band structure of RhGe connecting unconventional Weyl fermions at the Γ and R points (left panel) and electronic density of states (right panel). Location of bulk VHSs on the $\Gamma - R$ line is marked. (b) Constant energy surface at $k_z = 0.62$ Å⁻¹. Locations of VHSs in the bulk BZ are marked with red circles. (c) Three-dimensional dispersion around a VHS point on the $k_x - k_y$ plane at $k_z = 0.62$ Å⁻¹. (d) Phonon dispersion along the high symmetry directions in the bulk BZ. The size and color of markers are proportional to γ_{nq}/ω_{nq} , where γ_{nq} gives the phonon linewidth and ω_{nq} is the phonon frequency (see text for details). (e) Eliashberg spectral function and cumulative EPC at the Fermi energy (E_F) and the VHS energy ($E_{VHS} = 0.4$ eV). Enhancement of electron-phonon interaction due to the peaked DOS at VHS is visible in the Eliashberg spectral function and EPC.

lines reveals saddle points at the symmetry-equivalent generic momentum point $k_{VHS} = (0.62, 0.62, 0.62)$ Å⁻¹ on the $\Gamma - R$ line. The associated saddle-like energy dispersion is shown in Fig. 3(c). Importantly, unlike the usual saddle points, the saddle points here lie on the chiral axis and on the bands forming the multifold Weyl cones. Considering the symmetry of the lattice, there are eight such saddle points in the whole BZ.

Novel electronic phenomena originating from the saddle-point VHSs can be probed by tuning the binding energy at the $E_{VHS} = 0.4$ eV. This can be achieved by electron doping as reported in recent experiments [53]. In Fig. 3(d), we present the phonon spectrum weighted by the dimensionless quantity γ_{nq}/ω_{nq} , where γ_{nq} is phonon linewidth, ω_{nq} is the phonon frequency, $\mathbf{q}$ is the wavevector, and n is the phonon band index. The quantity γ_{nq}/ω_{nq} gives the measure of a phonon branch's contribution to the superconductivity, see SM for details. The phonon branches over an extended frequency and momentum region contribute to the superconductivity in RhGe. Moreover, the phonon DOS, Eliashberg spectral function, and the cumulative EPC display an enhanced EPI strength from $\lambda_{E_F} = 0.17$ to $\lambda_{E_{VHS}} = 0.78$ as one tunes the energy from the Fermi level to the VHS. This enhancement of the EPC strengthens the BCS superconducting state in RhGe. An estimate of the superconduct-

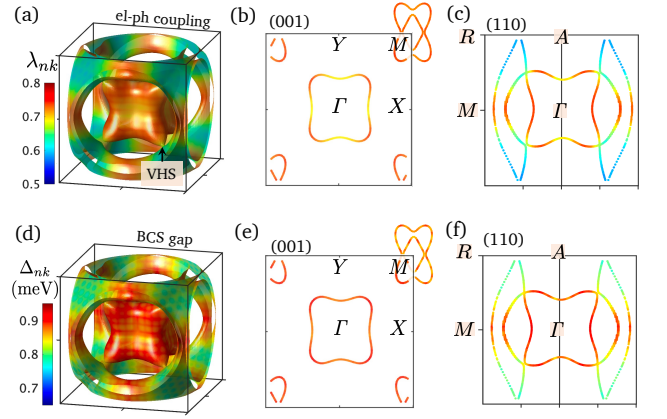


FIG. 4. (a) Constant energy surface (CES) of RhGe at $E_{VHS} = 0.4$ eV. The color scale represents the strength of electron-phonon coupling. The VHS located at the $[111]$ chiral axis is marked with a black-red arrow. (b-c) Electronic-phonon-coupling weighted CES on (001) and (110) planes. Major contribution to the EPC comes from the pockets around the Γ point. (d) Distribution of superconducting gap over the CES. (e-f) Superconducting gap distribution on (001) and (110) plane cuts of the CES. Anisotropic distribution of the EPC and the superconducting gap is evident.

ing transition temperature based on the Allen-Dynes equation, $T_c = \frac{\omega_{\log}}{1.2} \exp \left[\frac{-1.04(1+\lambda)}{\lambda(1-0.62\mu^*)-\mu^*} \right]$, with $\lambda_{E_{VHS}} = 0.78$ and the screened Coulomb interaction parameter $\mu^* = 0.1$, is ≈ 5.98 K, close to the experimentally reported T_c [50]. Here $\omega_{\log}$ is the logarithmic average of the phonon frequency.

By solving the anisotropic Migdal-Eliashberg equation on the imaginary axis with 0.25 eV cut-off over the Matsubara frequencies, we further obtain the EPC and superconducting gap structure over the constant energy surface (CES) at E_{VHS} (Fig. 4). The calculated EPC and superconducting gap function over the CES are shown in Figs. 4(a) and 4(c), respectively. Both the EPC and the superconducting gap function show anisotropic distribution over the CES in the momentum space. This is more evident from the (001) and (110) cuts presented in Figs. 4(d)-4(f) and Fig. 4(i)-4(k) for the EPC and the superconducting gap function, respectively. Note that without the SOC, EPC is the largest for the pockets centered at the Γ point with an anisotropic s-wave-like BCS superconducting gap distribution on the $k_x - k_y$ plane and along the k_z direction. A more realistic description of the gap function over the Fermi surface may require calculations with SOC, which is not practical within the first-principles methods.

Therefore, to gain a deeper understanding of the gap function and the potential pairing symmetries influenced by the SOC for the Fermi pockets near the Γ point, we employ the kinetic model introduced in Ref. [46] (see SM for details [52]). The projected electronic states near the Fermi surface are described by $\hat{\psi}_{m,\mathbf{k}}$ ($m = 3/2, 1/2$). These two Fermi pockets are associated with the multifold fermionic excitations described by the total angular momentum $S = 3/2$ near the Γ point. Ignoring inter-pocket pairings, the

intra-pocket Cooper pairings between the electrons at $\mathbf{k}$ and $-\mathbf{k}$ are described by the condensate $b_{m,\mathbf{k}} = \langle \hat{\psi}_{m,\mathbf{k}} \hat{\psi}_{m,\mathbf{k}}^\dagger \rangle$. Here, $\hat{\psi}_{m,\mathbf{k}}$ is the time-reversal partner of the electron states at $\mathbf{k}$: $\hat{\psi}_{m,\mathbf{k}} = \eta_{m,\mathbf{k}} \hat{\psi}_{m,-\mathbf{k}}$ with $\eta_{m,\mathbf{k}} = e^{2im\phi_{\mathbf{k}}}$, where $\phi_{\mathbf{k}}$ is the azimuthal angle of $\mathbf{k}$. Note that the condensate is an even function of momentum $b_{m,-\mathbf{k}} = b_{m,\mathbf{k}}$ for half-integers $m = 3/2, 1/2$, forcing the gap function $\Delta_m(\mathbf{k}) = -\sum_{\mathbf{p}} \sum_{m'} U_{mm'}(\mathbf{k}, \mathbf{p}) b_{m',\mathbf{p}}$ to be even. This can be seen by considering the mean-field theory to decouple the interactions in the Cooper channel as $H_{\text{pairing}} = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{p}} \sum_{m, m'} U_{mm'}(\mathbf{k}, \mathbf{p}) (\hat{\psi}_{m,\mathbf{k}}^\dagger \hat{\psi}_{m,\mathbf{k}}^\dagger b_{m',\mathbf{p}} + \hat{\psi}_{m',\mathbf{p}} \hat{\psi}_{m',\mathbf{p}}^\dagger b_{m,\mathbf{k}}^* - b_{m',\mathbf{p}} b_{m,\mathbf{k}}^*)$ with $U_{mm'}(\mathbf{k}, \mathbf{p}) = U_{mm'}(\mathbf{k}, -\mathbf{p})$. The superconducting gap function $\Delta_m(\mathbf{k}) = -\sum_{\mathbf{p}} \sum_{m'} U_{mm'}(\mathbf{k}, \mathbf{p}) b_{m',\mathbf{p}}$ is clearly even $\Delta_m(-\mathbf{k}) = \Delta_m(\mathbf{k})$. Thus, for the superconducting pairing symmetry, L is an even integer which at the lowest angular momentum is s -wave ($L = 0$) and d -wave ($L = 2$). The nature of superconducting gap symmetry is determined by the most attractive channel in expanding the interaction $U_{mm'}(\mathbf{k}, \mathbf{p})$ in terms of the basis functions. The s -wave pairing is the most symmetric where the gap function preserves the time-reversal symmetry and yields a trivial superconducting state. Higher-angular momentum pairings can break the time-reversal symmetry and give rise to nontrivial superconductivity characterized by the topological charge ν . Different possible pairing symmetries and topological states are summarized in Table I. These results indicate that RhGe would realize topological superconductivity, whose properties are robust to weak and intermediate disorder strengths [54] (see Sec. VI of SMs [52]).

TABLE I. Possible superconducting pairing symmetries around Γ and the associated topological states.

(L, M)	Gap function	Nature of superconducting state	Time-reversal symmetry	Topological charge
(0, 0)	s -wave	Trivial	Preserved	$\nu = 0$
(2, 2)	$k_x^2 - k_y^2 + 2ik_x k_y$	Weyl	Broken	$\nu = +2$
(2, 1)	$(k_x + ik_y) k_z$	Weyl+nodal loop	Broken	$\nu = +1$
(2, 0)	$3k_z^2 - k^2$	nodal loop	Preserved	$\nu = 0$
(2, -1)	$(k_x - ik_y) k_z$	Weyl+nodal loop	Broken	$\nu = -1$
(2, -2)	$k_x^2 - k_y^2 - 2ik_x k_y$	Weyl	Broken	$\nu = -2$

We emphasize that for the pairing symmetries listed in Table I, we employed a rotational-symmetric effective model. In an actual crystal, however, the pairing functions follow point-group symmetries, so that the effective interaction in the pairing channel should be expanded in terms of the basis functions of the corresponding irreducible representations (Fig. 1(d)). The point-group symmetry at Γ is described by the double group T . The normal group admits conjugate representations, E , with even basis functions ($d_{z^2} \equiv 2z^2 - x^2 - y^2, d_{x^2-y^2} \equiv x^2 - y^2$). Both pairings would yield nodal-line superconductors. Due to the conjugate nature of the representation, a phase-locking between them leads to pairings of types $d_{z^2} \pm id_{x^2-y^2}$, which break the time-reversal symmetry. Since such complex pairings replace the nodal pairings with nodes, they are energetically favored over d_{z^2} and $d_{x^2-y^2}$ due to the gain in the condensation energy.

TABLE II. Possible superconducting pairing symmetries around R and the associated topological states.

(L, M)	Gap function	Nature of superconducting state	Time-reversal symmetry	Topological charge
(1, 1)	$k_x + ik_y$	Weyl	Broken	$\nu = +1$
(1, 0)	k_z	Nodal loop	Preserved	$\nu = 0$
(1, -1)	$k_x - ik_y$	Weyl	Broken	$\nu = -1$

Unlike the Γ pocket, the condensate is odd around the R pocket. The excitations around R are described by a multifold fermion with $S = 1$, and hence $m = 1$ for the states near the Fermi surface. The phase factor $\eta_{m,\mathbf{k}} = \eta_{m,-\mathbf{k}}$ is even and gives rise to an odd condensate $b_{m,\mathbf{k}} = -b_{m,-\mathbf{k}}$. Therefore, only odd angular momenta will survive in the expansion of the pairing interaction $U_{mm'}(\mathbf{k}, \mathbf{p})$. The possible pairing symmetries are provided in SMs [52]. The point-group symmetry of R is described by the double group C_3 . The normal group has a one-dimensional representation with the basis $p_z \equiv z$. The corresponding pairing symmetry leads to a nodal-loop superconductor. The symmetry group also admits a conjugate representation with basis functions ($p_x \equiv x, p_y \equiv y$). The pairing symmetry could be $p_x \pm ip_y$, *i.e.*, the Weyl superconductors, see Table II. In recent experiments, RhGe was reported to show superconductivity with the coexistence of weak ferromagnetism [50], which can substantiate the topologically non-trivial nature of the superconductivity.

We have demonstrated RhGe to be a strong candidate for realizing topological superconductivity. Owing to its structural chirality, RhGe possesses multifold Weyl fermions located at the Γ and R momentum points on the chiral axis. The bands connecting these momentum points feature type-II saddle-point VHSs with enhanced EPI and superconductivity. By performing the anisotropic Eliashberg analysis, we demonstrate that both the EPC and the BCS gap exhibit pronounced anisotropy across the Fermi surface. On characterizing the pairing symmetries around the Γ and R points using a low-energy model, we establish the nontrivial superconducting state in RhGe. Moreover, the lack of inversion symmetry in RhGe can allow the development of an admixture of pairing symmetries and strengthen the unconventional superconducting state. The presence of time-reversal-symmetry broken topological superconductivity can be verified via future magnetic optical Kerr and μ -SR experiments. Our study establishes RhGe to be a promising B20 Weyl semimetal for exploring topological superconductivity and Majorana fermions.

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