The conception of topology\(^1\)\(^3\) has been known in condensed matter physics since 1980s. However, it is until recently that we have witnessed an exponential growth in the field of topological phases of matter in the last decade; thanks to the introduction of concept of topological insulators (TIs)\(^4\) and their proposition\(^5\) and confirmation\(^6\) in real material systems. This effective route to discovering TIs from theoretical conception to computational material proposition and to experimental confirmation has been followed by the discovery of other topological materials, such as topological crystalline insulator\(^1\)\(^4\)\(^6\), Dirac semimetal\(^10\)\(^11\), and most recently Weyl semimetal\(^14\)\(^17\). Depending on the geometry of Dirac cone, there are type-I and type-II Dirac/Weyl semimetals\(^18\)\(^22\). Interestingly, it has been shown that the interface or the “transition state” from type-I to type-II has distinctly different topological properties\(^23\)\(^27\), which we will call it a “type-III” semimetal. Both type-I and type-II Dirac/Weyl semimetals have been experimentally confirmed in real materials\(^11\)\(^13\)\(^17\)\(^19\)\(^21\); however, so far type-III Dirac/Weyl semimetal remains a theoretical conception. In this Letter, we will fill this outstanding gap by proposing a type-III semimetallic phase in a real material Zn\(_2\)In\(_2\)S\(_5\).

Topological semimetals host interesting new types of fermions as low-energy quasiparticles. They not only exhibit novel physical properties such as distinctive topological surface states\(^10\)\(^15\), large linear magnetoresistance\(^26\)\(^28\) and chiral anomaly\(^24\)\(^34\), but also offer a versatile platform for simulating relativistic particles of high-energy physics as well as “new particles” that have no counterparts in high-energy physics. The type-III Dirac semimetal has been theoretically proposed for realizing a solid-state analogue of block hole horizon\(^23\)\(^25\). To this end, we will again fill the gap by devising a material platform, an inhomogeneous Zn\(_2\)In\(_2\)S\(_5\), to simulate Hawking radiation at the black-hole horizon. Especially we suggest a high Hawking temperature associated with the analogous black-hole horizon in Zn\(_2\)In\(_2\)S\(_5\) to ease the experimental observation, in contrast to the low Hawking temperature in previously proposed black-hole horizon analogues, such as sound wave in flowing medium\(^35\), superfluid helium\(^36\)\(^37\) and Bose-Einstein condensates\(^38\)\(^39\).

We will first highlight the key features of the type-III Dirac semimetals, including their unique characteristics of Dirac-line Fermi surface with nontrivial topological invariant and critical chiral magnetic effect, in distinction from those of type-I and type-II Dirac semimetals. Then we will present evidence that Zn\(_2\)In\(_2\)S\(_5\) is the first candidate material for realizing the type-III Dirac fermions. Based on effective Hamiltonian analysis and first-principles calculations, we show novel properties of Zn\(_2\)In\(_2\)S\(_5\) including critical chiral magnetoresponse and Fermi arcs. Finally we will describe a solid-state realization of the black-hole-horizon analogue in inhomogeneous Zn\(_2\)In\(_2\)S\(_5\), to simulate black hole evaporation with a relatively high Hawking temperature. Our work not only enriches the fundamental physics of topological semimetals with new types of fermions but also provides an alternative route to studying black hole horizon, in real materials systems.

Topological Dirac and Weyl semimetals are characterized with fourfold and twofold linear band crossings at the Fermi level (the so-called Dirac and Weyl points), respectively. They can be further classified into two types by fermiology. One is the type-I Dirac/Weyl semimetals which have a typical conical dispersion and point-like Fermi surface\(^[\text{Fig. 1(a)}]\)\(^10\)\(^13\)\(^16\)\(^17\). The other is the type-II Dirac/Weyl semimetals which manifest in an overtilted cone-shape band structure, possessing both electron and hole pockets that contact at the type-II Dirac/Weyl point\(^[\text{Fig. 1(b)}]\)\(^13\)\(^22\). The type-III Dirac semimetal is distinct from both type-I and type-II semimetals. As illustrated in Fig. 1(c), the type-III Dirac point is also a protected band crossing point, but
connected by a line-like Fermi surface which is the Dirac line of the type-III Dirac semimetal. It is distinctively different from the type-I case of point-like Fermi surface or the type-II case of hyperbolic Fermi surface (coexistence of electron and hole pockets). The Dirac line is protected by the combination of topology and symmetry, and can be described by a topological invariant \[ N_2 = \frac{1}{4\pi i} \text{Tr}[K \oint_C dh(k)^{-1} \partial_h h(k)], \]

where \( C \) is a contour enclosing the Dirac line in momentum space. Here \( K \) is a proper symmetry operator, which commutes or anticommutes with the Hamiltonian (see Supplemental Material for more details [41]). The topological invariant is actually a winding number of phase around the line, and it stabilizes the Dirac line in the sense that the integral is integer, \( N_2 = 1 \) only for type-III semimetal. The Dirac line in momentum space with nonzero winding number is an analogue of the vortex line in superfluids [37].

Interestingly, the type-III Dirac semimetal can also be viewed as the critical state of Lifshitz transition between type-I and type-II Dirac semimetals [24]. The Lifshitz transition was investigated recently and a solid-state realization of black-hole-horizon analogue based on inhomogeneous topological semimetals was proposed [23,25]. It is hoped that topological semimetals will provide an alternative way to observe black hole horizon in condensed matter systems. So far, however, no material system is known to be a type-III Dirac semimetal. Next, we will fill this gap by demonstrating \( \text{Zn}_2\text{In}_2\text{S}_5 \) to be the first type-III Dirac semimetal, and how to realize its black-hole-horizon analogue.

\( \text{Zn}_2\text{In}_2\text{S}_5 \) has a layered structure consisting of nonuple layers stacked together along the \( z \)-direction (see Supplemental Material [41]). Each nonuple layer consists of two \( \text{In} \) and two \( \text{Zn} \) layers which are sandwiched by \( \text{S} \) layers alternately, and every \( \text{In} \) or \( \text{Zn} \) atom lies in the center of a terahedron or octahedron of \( \text{S} \) atoms. The coupling is strong between atomic layers within the nonuple layer but much weaker between adjacent nonuple layers. Due to different stacking of these basic building blocks, two kinds of structures of \( \text{Zn}_2\text{In}_2\text{S}_5 \) arise, i.e., AB-stacked hexagonal structure with \( \text{P6}_3\text{mc} \) symmetry and ABC-stacked rhombohedral structure with \( \text{R3m} \) symmetry.

\( \begin{array}{cccc}
\text{Dispersion} & \text{Type-I} & \text{Type-II} & \text{Type-III} \\
& \text{Dirac cone} & \text{Overtilted Dirac cone} & \text{Critical Dirac cone} \\
& \text{Fermi surface} & \text{Point-like} & \text{Electron \& hole pockets} & \text{Dirac line (with } N_2 = 1 \text{)} \\
& \text{DOS} (E_F) & \text{Vanishing} & \text{Parabolic peak} & \text{Finite} \\
& \text{Surface Fermi Arc} & \checkmark & \checkmark & \checkmark \\
& \text{Chiral anomaly} & \text{Along all direction} & \text{Anisotropic, inside a cone region} [40] & \text{Except for the critical plane} [41] \\
& \text{Black hole analogue} & \text{Outside} & \text{Inside} & \text{Horizon} \\
& \text{Typical materials} & \text{Na}_3\text{Bi} [10], \text{Cd}_4\text{As}_2 [12] & \text{PtTe}_2 [20, 21], \text{VAI}_3 [22] & \text{Zn}_2\text{In}_2\text{S}_5 \text{ (this work)}
\end{array} \)
and (0 actually two flat $\Delta$ since neither energy difference of 1 meV. This is an unique feature of Zn$_2$In$_2$S$_5$. This is an unique feature of Zn$_2$In$_2$S$_5$. (b) and (e) The zoom-in band structures along $\Gamma$-$\Lambda$ of Zn$_2$In$_2$S$_5$($R3m$) and Zn$_2$In$_2$S$_5$($P6_3mc$), respectively. (c) and (f) The in-plane band dispersions around the Fermi level of Zn$_2$In$_2$S$_5$($R3m$) and Zn$_2$In$_2$S$_5$($P6_3mc$), respectively.

We first calculated the band structure of Zn$_2$In$_2$S$_5$. As shown in Fig. 2(a) and 2(d), there are flat bands along the $\Gamma$-$A$ direction near the Fermi level. Meanwhile, another band disperses upward crossing the flat bands in between $\Gamma$ and A. As shown in the zoom-in figures [Fig. 2(b) and 2(e)], the upward dispersive band crosses with the upper flat band but avoids crossing with the lower flat band. The band crossings are unavoidable in both materials, because the two crossed bands belong to different representations of the crystal symmetry group. Take Zn$_2$In$_2$S$_5$($R3m$) as an example, the two bands belong to 2D $\Lambda_6$ and 1D $\Delta_5$/$\Lambda_6$ representations, respectively, as distinguished by $C_{3v}$ rotational symmetry around the $k_z$ axis. The different representation prohibits hybridization between them, resulting in a pair of 3D Dirac points at $\pm(0.254, 0.254, 0.254)$ (in units of $2\pi/a$). For Zn$_2$In$_2$S$_5$($P6_3mc$), the upper flat band and the upward dispersive band belong to 2D irreducible representation $\Delta_9$ and $\Delta_7$, respectively, of the $C_{6v}$ symmetry. One unique feature of the $P6_3mc$ structure is that there are actually adjacent double Dirac points $(0, 0, \pm 0.306)$ and $(0, 0, \pm 0.308)$ (in units of $(2\pi/a, 2\pi/a, 2\pi/c)$) with an energy difference of 1.0 meV. This is because there are actually two flat $\Delta_9$ bands that are close to each other but not exactly degenerate [see the inset of Fig. 2(e)]. Since neither $R3m$ nor $P6_3mc$ structure has inversion symmetry, these Dirac semimetal states have fourfold degenerate Dirac points, but with splitting of in-plane band dispersions away from Dirac points [Fig. 2(c) and 2(f)]. This is an unique feature of Zn$_2$In$_2$S$_5$, which is different from other Dirac semimetals that require both time-reversal and inversion symmetries. Additionally, we also investigate the strain effect on the electronic structure and found that the position of type-III Dirac points in the $k_z$ axis can be effectively tuned by external strain.

To further reveal the nature of the type-III Dirac points, we fit the energy spectrum from first-principles calculations to a low-energy effective model [41]. If neglecting the tiny splitting induced by inversion symmetry breaking which is insignificant to the main conclusion, the quasiparticles are described by a pair of Weyl Hamiltonian in the vicinity of one Dirac point,

$$h^c_{\pm} = c_\perp(k_x\sigma_x \pm k_y\sigma_y) + c_\parallel k_z\sigma_z + v\delta k_z\sigma_0,$$

where $\delta k_z = k_z - k^c_z$, with $k^c_z = 0.102$ Å$^{-1}$. The parameters $c_\perp = 2.29$ and $v = -c_\parallel = 1.36$ eVÅ, indicate that there exists a flat band along $k_z$ direction. It is straightforward to derive the topological invariant using $K = \pm\sigma_z$ in Eq. 3 and find that $N_2 = 1$. We thus conclude that Zn$_2$In$_2$S$_5$ is a type-III Dirac semimetal.

The topological nature of the type-III Dirac point in Zn$_2$In$_2$S$_5$ is also confirmed by calculating the $Z_2$ topological invariants which are well-defined in both the $k_z = 0$ and the $k_z = \pi$ planes. Taking Zn$_2$In$_2$S$_5$($R3m$) as an example, the $k_z = 0$ plane is found topologically nontrivial with $Z_2 = 1$; while the $k_z = \pi$ plane is topologically trivial with $Z_2 = 0$. Therefore, a band ordering inversion between $\Gamma_4$ and $\Gamma_5 + \Gamma_6$ bands should occur along the $k_z$ direction [see Fig. 2(b)], resulting in a band gap closure at the Dirac point.

Topological surface states and Fermi arcs are expected to appear on side surfaces of Zn$_2$In$_2$S$_5$. Figure 3 shows the projected surface DOS for the (100) surface of a semi-infinite Zn$_2$In$_2$S$_5$($R3m$) system, from which we have an
intuitive visualization of topological surface state and Fermi arcs. It is seen that the topological surface state emanates from one projection of bulk Dirac point on the (100) surface, as shown in Fig. 3(a). The Fermi surface contains two pieces of half-circle Fermi arcs, as shown in Fig. 3(b), touching at two singularity points where the surface projections of bulk Dirac points appear. Due to the flat Dirac-line Fermi surface, the shape of electron and hole pockets varies rapidly with the increasing chemical potential. All these characteristics, in sharp contrast to conventional metals and topological insulators, should be experimentally observable by modern angle-resolved photoemission spectroscopy technique.

We have shown the existence of type-III Dirac semimetal Zn$_2$In$_2$S$_5$. Now we discuss the possibility of realizing a solid-state analogue of black-hole horizon in Zn$_2$In$_2$S$_5$. So far, various black-hole analogues based on different systems have been proposed [12]. For example, Unruh proposed a sonic black hole for sound wave propagating in flowing liquid [32], while Volovik suggested a black-hole/white-hole pair in superfluid Helium with a moving vierbein domain well [32] [33]. In the theoretical model Eq. (1), the last term is the same as the Doppler shift for quasiparticles under a Galilean transformation to a moving frame of reference with a velocity $v$, which is similar to the case of sonic black hole analogue where the sound wave propagates in moving fluid. In general relativity, a relativistic quasiparticle in 3+1 dimensional spacetime can be described by the line element $ds^2 = g_{\mu\nu} dx^\mu dx^\nu$, where $g_{\mu\nu}$ is the inverse (covariant) metric describing an effective curved spacetime in which the relativistic quasiparticles propagate [42]. To obtain a spacetime interpretation, we derive the effective covariant metric $g_{\mu\nu}$ according to Eq. (4) [41]:

$$g_{\mu\nu} = 
\begin{pmatrix}
-1 - v^2/c^2_\parallel & 0 & -v/c_\parallel^2 \\
0 & 1/c_\perp^2 & 0 \\
-v/c_\parallel^2 & 0 & 1/c_\perp^2
\end{pmatrix},$$

(5)

which has a similar form of the acoustic metric of Unruh’s sonic black hole [32] [12].

Now let’s assume that the dragging velocity $v = v(z)$ depends on the spacial $z$ coordinate in an inhomogeneous Zn$_2$In$_2$S$_5$ system, which can, in principle, be realized by controllable (tunable) structural distortion. As the metric has translation invariance in the $x$- and $y$-direction, for simplicity we make a dimension reduction to the 1+1 dimensional spacetime by ignoring the coordinates $x$ and $y$. As a result, the corresponding linear element becomes

$$ds^2 = - \left(1 - \frac{v^2(z)}{c_\parallel^2}\right) d\tau^2 + \frac{dz^2}{c_\parallel^2 - v^2(z)},$$

(6)

By performing a coordinate transformation: $\tau = t + \int^z dz v(z)/(c_\parallel^2 - v^2(z))$, we obtain an effective line element that shares the same form of the radial part of the Schwarzschild line element for gravitational black holes [43]. Similar to the Schwarzschild metric which has a singularity at the Schwarzschild radius corresponding to an event horizon, the above metric also has a horizon ($z_h$), where the dragging velocity equals to the local “speed of light” for quasiparticles: $v(z_h) = \pm c_\parallel$. The corresponding “Newtonian gravitational field” at horizons is given by: $E_g(z_h) = \frac{v(z_h)}{c_\parallel^2} \frac{dv}{dz} |_{z_h}$. According to the fitted parameters of Eq. (4), assuming $v(z) > c_\parallel$ ($v(z) < -c_\parallel$) in the region $z > z_h$ ($z < z_h$), an inhomogeneous Zn$_2$In$_2$S$_5$ system can be derived (see Fig. 4). Hence all quasiparticles in the upper region ($z > z_h$) move upward, and cannot cross the plane $z = z_h$, which indicates that this plane is the black-hole horizon. Consequently, the inner observers living in the lower region ($z < z_h$) cannot obtain any information from the upper region ($z > z_h$) if they can only use the relativistic quasiparticles for communication.

A black hole can slowly radiate away its mass by emitting a thermal flux at the horizon, as pointed out by Hawking [44]. The analogous model presented above not only suggests a new route to simulating an event horizon, but also facilitates the realization of the Hawking radiation analogue in inhomogeneous type-III Dirac semimetals. Although this model is static in equilibrium, the dissipation process right after the creation of the black hole horizon analogue is similar to the process of the Hawking radiation [23] [24]. The corresponding Hawking temperature can be directly determined by the “surface gravity” at the horizon $E_g(z_h)$ [37] [42]:

$$T_H = \frac{\hbar c_\parallel}{2\pi k_B E_g(z_h)} = \frac{\hbar}{2\pi k_B} \frac{dv}{dz} |_{z_h},$$

(7)

where $k_B$ and $\hbar$ are the Boltzmann and the reduced Planck constants, respectively. Obviously, $T_H$ may reach high temperature as long as the gradient of the drag-
ging velocity is sufficiently large across the horizon. As the dragging velocity $v$ is a material-dependent parameter which can be effectively tuned by strain and chemical doping [45–47], it is expected to reach a high value of $T_H$ in inhomogeneous $\text{Zn}_2\text{H}_2\text{S}_5$.

In addition to simulating event horizons and Black hole evaporation, other novel astrophysical phenomena such as gravitational lensing effect [40], gravity wave [47], and cosmological constant problem [46] can also be explored in type-III Dirac semimetals. In future work we will investigate possible strain engineering of the black-hole horizon analogue in inhomogeneous $\text{In}_2\text{Zn}_2\text{S}_5$. Other interesting directions for future research including the realization of other topological states, such as type-III Weyl semimetal by breaking time-reversal symmetry via magnetic doping, the interplay between different topological states in $\text{Zn}_2\text{H}_2\text{S}_5$, and the analytical estimation of transport and optical behaviors of type-III topological semimetals.

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