Giant Fully Spin-Polarized Currents Enhanced by Disorder in Nodal Chain Spin-Gapless Semimetals

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Recently discovered high-quality nodal chain spin-gapless semimetals $MF_3$ ($M = Pd, Mn$) feature an ultra-clean nodal chain in the spin up channel residing right at the Fermi level and displaying a large spin gap leading to a 100% spin-polarization of transport properties. Here, we investigate both intrinsic and extrinsic contributions to anomalous and spin transport in this class of materials. The dominant intrinsic origin is found to originate entirely from the gapped nodal chains without the entanglement of any other trivial bands. The side-jump mechanism is predicted to be negligibly small, but intrinsic skew-scattering enhances the intrinsic Hall and Nernst signals significantly, leading to giant values of respective conductivities. Our findings open a new material platform for exploring colossal anomalous and spin transport properties in magnetic topological semimetals.

Introduction.— After the discovery of magnetic topological insulators [1, 2], different types of magnetic topological states ranging from insulators to semimetals have emerged [2–16, 18–28]. This brings new vitality to the ideas evolving around the next generation of dissipationless spintronic devices benefiting from exotic anomalous and spin transport properties. The Hall currents of charge $J^A_H$ can be generated in magnetic materials either by an applied electric field $E$ or a thermal gradient $-\nabla T$, known correspondingly as the anomalous Hall effect (AHE) [5, 30] and anomalous Nernst effect (ANE) [6, 32]. Magnetic topological semimetals provide a prominent advantage to enhance anomalous Hall conductivity (AHC) and/or anomalous Nernst conductivity (ANC) driven by the divergent Berry curvature of gapped Weyl points or nodal lines (NLs), as reported previously for various systems theoretically and experimentally [33–47]. On the other hand, the Hall currents of spin $J^S_H$ — i.e., the spin counterparts of $J^A_H$ also known as the spin Hall effect (SHE) [48] and spin Nernst effect (SNE) [49] — are also largely driven by topological nodal features which give rise to large spin Hall conductivity (SHC) and spin Nernst conductivity (SNC) in non-magnetic topological semimetals [50–63].

In the realm of emergent anomalous and spin transport in topological semimetals, however, many issues still have to be addressed. One of the most prominent aspects is the role played by disorder-induced extrinsic mechanisms. It is well known that both AHC $\sigma_{xy}$ and ANC $\alpha_{xy}$ can be decomposed into three different contributions (SHC $\sigma_{xy}^s$ and SNC $\alpha_{xy}^s$ are also the case) [4, 64, 65, 67]:

$$\alpha_{xy}^{tot}(\sigma_{xy}^{tot}) = \alpha_{xy}^{int}(\sigma_{xy}^{int}) + \alpha_{xy}^{sk}(\sigma_{xy}^{sk}) + \alpha_{xy}^{sj}(\sigma_{xy}^{sj}) \quad (1)$$

The first term is the so-called intrinsic (int) contribution, which can be well described by Berry phase theory [5, 30], and which was the focus of previous studies on magnetic topological semimetals [33–47]. The second and the last terms are the disorder-driven extrinsic contributions referred to as the skew-scattering ($sk$) [68, 69] and side-jump ($sj$) [70], respectively, and whose role in Hall effects of magnetic topological semimetals received very little attention so far, besides several very recent experimental [71–73] and model studies [74–79]. Another challenge is to draw a clear correlation between the topological characterization and the magnitude of transport properties. Most of the previously reported materials suffer from a “contaminated” band dispersion around the Fermi level. Moreover, the situation is complicated by the fact that often the band topology is formed by fermions of opposite spin with parabolic dispersion, which greatly decreases the current spin-polarization and the carrier Fermi velocity in real spintronic devices.

In this Letter, we address the above two issues directly. Using first-principles calculations, we collect all contributions to the AHE and ANE as well as the SHE and SNE in the recently proposed novel nodal chain spin-gapless semimetals (NCSGSMs) $MF_3$ ($M = Pd, Mn$) [2], which feature an ultra-clean nodal chain residing right at the Fermi level, providing an ultrahigh Fermi velocity and 100% spin-polarization simultaneously. This provides us with a prefect platform to clearly identify pure topological contributions to Hall transport. We show that such a remarkable electronic structure inevitably gives rise to giant Hall effects. We further uncover the intrinsic mechanism as the main underlying physical origin of the giant AHC and ANC, resulting from the gapped nodal chain-
induced large Berry curvature. We find the side-jump to be negligibly small but discover that the intrinsic skew-scattering plays an important role for the overall signal. Our work provides a foundation for educated design of giant pure spin-polarized Hall currents for future "green" spintronics.

**High-quality candidate hosting giant fully spin-polarized current.** — A crucial issue for addressing topological contributions to anomalous transport is screening out the influence of trivial bands. To tackle this, we focus on a promising candidate platform — the recently proposed spin gapless semiconductors or semimetals [2, 7, 80, 85, 86]. Among these, we select an outstanding example, the rhombohedral transition metal trifluorides $MF_3$ ($M = \text{Pd, Mn}$) [2, 80] (Fig. 1(a)), which display a linear semimetallic band structure in the spin up channel, while exhibiting a large indirect band gap (2.46 eV for $\text{PdF}_3$, 6.43 eV for $\text{MnF}_3$) in the spin down channel (Fig. 1(c) and Fig. S1 in Supplemental Material [84]), thus enjoying a 100% spin-polarization of the states at the Fermi energy. The spin-up electronic structure around the Fermi level is formed by two types of cross-connection modes. The one mode comprises three accidentally formed NLs (NL$_0$, NL$_1$, NL$_3$) (see Fig. 3(c-d)), which are positioned in three mirror planes ($\mathcal{M}_1$, $\mathcal{M}_2$, $\mathcal{M}_3$) (see Fig. 1(a)) and are pinned at the two $Z$ points [[(0.5,0.5,0.5), (−0.5,−0.5,−0.5)]. The other mode, a "snakelike" structure with six corners at the $L$ points (NL$_4$), crosses the former three NLs transversely.

The ultra-clean topological nodal lines (NL$_{1-4}$) not only perfectly avoid the entanglement of trivial bands, but can generate the much desired fully spin-polarized Hall current based on AHE and ANE as well as their spin counterparts SHE and SNE (Fig. 1(d)). Accordingly, the anomalous and spin Hall currents can be written down as follows [67]:

$$J_H^A = J^+ + J^x = J^+,$$

$$J_H^S = (J^+ - J^x) \frac{\hbar}{2e} = \frac{\hbar}{2e} J^x,$$

since the spin-down bands reside far away from the Fermi level and do not contribute to the Hall effect. Respectively, the SHC and SNC are given by $\sigma_{xx} = \frac{\hbar}{2e} \sigma_{xy}$ and $\sigma_{xy} = \frac{\hbar}{2e} \sigma_{xy}$, as also confirmed by first-principles calculations (see Eqs. S2 [84]).

Next we proceed to explore these physical phenomena quantitatively. First, to confirm the leading mechanism of AHC in $MF_3$, the computed variation of $\sigma_{xy}$ (the superscript $\text{tot}$ is omitted in the following discussion) with $\sigma_{xx}$ at $E = E_f$ and $E = E_f - 0.04$ eV is plotted in Fig. 2(a) for the magnetization $M$ being along the $z$-axis ([111] direction) and $x$-axis ([110] direction), respectively. To do this, we use the implementation of uncorrelated disorder scattering formalism from the first-principles (see Eqs. (S5)-(S8) [84]). By analysing the dependency of $\sigma_{xy}$ on $\sigma_{xx}$, different scaling relations have been proposed for a variety of ferromagnets [81–83, 87, 88]: $\sigma_{xy} \propto \sigma_{xx}^{\alpha}$ in the dirty regime ($\sigma_{xx} < 10^4$ S/cm), nearly constant in the intrinsic regime ($\sigma_{xx} \sim 10^4 - 10^6$ S/cm), and $\sigma_{xy} \propto \sigma_{xx}^{\beta}$ or $\sigma_{xx}^{\gamma}$ in the clean regime ($\sigma_{xx} > 10^6$ S/cm). From Fig. 2(a), one can see that $MF_3$ is located within the intrinsic regime, and $\sigma_{xy}$ exhibits a nearly constant plateau for both $E = E_f$ and $E = E_f - 0.04$ eV for $10^5 < \sigma_{xx} < 10^6$ S/cm, in accordance with the above scaling relation. In other words, the AHC is dominated by the intrinsic mechanism. To reveal this observation more clearly, the component-resolved AHC of $\text{PdF}_3$ with

![FIG. 1. Nodal chain spin gapless semimetals (NCSGSMs) and their fully spin-polarized currents. (a) The crystal structure of $MF_3$ ($M = \text{Pt, Mn}$), and the view of (111) plane. The blue spheres are magnetic $M$ atoms, whereas yellow spheres are nonmagnetic F atoms. The red arrows label the spin magnetization aligned along [111] direction. The pink lines denote three mirror planes. The sketch of the Brillouin zone is shown in (b), and (c) shows spin-polarized band structure without SOC, where the inset is a zoom into the bands near the Z point. The horizontal violet dashed lines mark the con-

![FIG. 1. Nodal chain spin gapless semimetals (NCSGSMs) and their fully spin-polarized currents. (a) The crystal structure of $MF_3$ ($M = \text{Pt, Mn}$), and the view of (111) plane. The blue spheres are magnetic $M$ atoms, whereas yellow spheres are nonmagnetic F atoms. The red arrows label the spin magnetization aligned along [111] direction. The pink lines denote three mirror planes. The sketch of the Brillouin zone is shown in (b), and (c) shows spin-polarized band structure without SOC, where the inset is a zoom into the bands near the Z point. The horizontal violet dashed lines mark the considered energy range of anomalous and spin transport. (d) Schematic illustration of fully spin-polarized Hall current induced by AHE (SHE) and ANE (SNE) in a NCSGSM (indicated with a hexagonal petal), when an electric field or a temperature gradient field is applied along the longitudinal direction.
FIG. 2. Giant spin-pure AHC and ANC. (a) AHC $\sigma_{xy}$ versus $\sigma_{xx}$ for PdF$_3$ at the true Fermi energy $E_f$ and at $E_f - 0.04$ eV, with the magnetization $M$ along the $z$ or $x$ direction, ranging across intrinsic from dirty to clean regimes. Note that when $M \parallel x$, the nonzero component of AHC is $\sigma_{yz}$. The data of MnF$_3$ for $M \parallel z$ is also plotted. In the plot, data for various ferromagnets are shown for comparison, as reported in previous works [81–83]. (b-c) Disorder-related contributions to the AHC ($\sigma_{int}^{xy}$, $\sigma_{isk}^{xy}$, $\sigma_{sj}^{xy}$, and the total $\sigma_{xy}$) as a function of $\sigma_{xx}$ (at $E_f$) and energy, respectively. In (c), the intrinsic AHC is calculated at the clean limit, while the extrinsic AHC is evaluated by incorporating a Gaussian disorder potential with a weak disorder parameter ($1.83$ eV$^2$bohr$^3$) [84], at where $\sigma_{xx}$ reaches $2.12 \times 10^5$ S/cm. (d-e) Disorder-related contributions to the ANC ($\alpha_{int}^{xy}$, $\alpha_{isk}^{xy}$, $\alpha_{sj}^{xy}$, and the total $\alpha_{xy}$) for various temperatures $T$ and energy, computed at $E_f$ and for $T = 200$ K, respectively.

$E = E_f$ and $E = E_f - 0.04$ eV when $M \parallel z$ are shown in Figs. 2(b) and S3 as $\sigma_{xx}$ is varied. The intrinsic part dominates the shape of AHC, while the intrinsic skew-scattering also plays an important role, contributing by about one-third of $\sigma_{xy}$. In contrast, we find the side-jump to be negligibly small.

The energy evolution of $\sigma_{xy}$, shown in Fig. 2(c), reveals considerable values in the range of $[-0.1, 0.1]$ eV, near the band crossing points, which can be easily accessed by current experimental techniques such as angle-resolved photoemission spectroscopy [12]. Another prominent feature of Fig. 2(c) is a large variation of $\sigma_{xy}$ with energy. According to the low-temperature Mott relation, which relates the ANC to the energy derivative of the AHC [6],

$$\alpha_{xy} = -\frac{\sigma_{xy}^2 k_B T}{3e} \left. \frac{d\sigma_{xy}}{dE} \right|_{E=E_f}$$

where $k_B$, $T$, and $e$ are Boltzmann constant, temperature, and elementary charge, respectively, one can expect a large ANC near the Fermi energy. Using the generalized Mott formula [84], we compute the ANC and show the component-resolved data in Figs. 2(d) and 2(e). The temperature dependence of ANC shows that the low-temperature Mott relation is valid up to about 40 K, and one can indeed observe an ANC which is much larger than that in traditional ferromagnets (typically $|\alpha_{xy}| = 0.01 - 1$ A/Km [35]) once $T \geq 50$ K. Remarkably, a giant $\alpha_{xy}$ of about 2 A/Km is observed at $T = 200$ K, which is by far larger than that in conventional ferromagnets. Another prominent advantage of PdF$_3$ is that the peak of $\alpha_{xy}$ is positioned right at the true $E_f$, as seen in Fig. 2(e), while the range of energies with large $\alpha_{xy}$ is wide enough for giant ANE to be easily detected experimentally.

The underlying physical origin of colossal transport properties.— Next, we uncover the underlying physical origin of the giant AHC and ANC in PdF$_3$ (similar analysis can be performed for SHC and SNC). The band structure of PdF$_3$ with SOC together with the Berry curvature $\Omega_{xy}$ along high symmetry lines is shown in
we integrate $\Omega_{xy}$ mainly distributed near the gapped nodal lines. Further, the Brillouin zone [Fig. 3(e)] indicates that the hot spots are at $\bar{Z}$-point, and an accidental degeneracy along the $\Gamma\bar{Z}$ direction. We stress that giant AHE and ANE predicted here differ from previous studies [35, 43], which require a simultaneous enhancement of the Berry curvature and density of states created by a large Fermi surface with Weyl points or a flat nodal line. In contrast, for NC-SGSMs, the density of states is nearly vanishing at the Fermi level. Hence the giant AHC and ANC predicted here are driven by pure topological characteristics.

Figs. 3(a-b). Clearly, the slightly gapped crossing points generate large $\Omega_{xy}$ with negligible contributions at other “trivial” regions. Specifically, a pronounced negative peak is found near the $Z(0.5, 0.5, 0.5)$ point, which is the rotation-invariant point of three glide mirrors ($M_1$, $M_2$, and $\tilde{M}_3$) – the combined symmetries of three mirrors, Fig. 1(a), with translational symmetry), and which hosts a fourfold degeneracy in the absence of SOC, ensured by three glide mirrors and $C_{3[111]}$ symmetry, Fig. 1(c) [2]. The SOC breaks three glide mirrors, and the fourfold degeneracy is split into a gapped group of states at $Z$ point, and an accidental degeneracy along the $\Gamma\bar{Z}$ direction. The former rather than the latter is responsible for the large $\Omega_{xy}$. Indeed, the distribution of $\Omega_{xy}$ in the Brillouin zone [Fig. 3(e)] indicates that the hot spots are mainly distributed near the gapped nodal lines. Further, we integrate $\Omega_{xy}$ along the $k_z$ direction (Fig. 3(f)), which shows prominent features near the $\bar{Z}, \bar{L}$ points and along the $\bar{Z}\bar{X}$ direction. We stress that giant AHE and ANE predicted here differ from previous studies [35, 43], which require a simultaneous enhancement of the Berry curvature and density of states created by a large Fermi surface with Weyl points or a flat nodal line. In contrast, for NC-SGSMs, the density of states is nearly vanishing at the Fermi level. Hence the giant AHC and ANC predicted here are driven by pure topological characteristics.

To further confirm the topological origin of transport in PdF$_3$, we also consider the case of the magnetization directed along other directions, e.g., $x$- and $y$-axes (see Figs. 4, S4, S5, and S6 [84]). The results show that the spectral features of the symmetry-allowed AHC and ANC are nearly the same as those for the case of magnetization oriented along the $z$-axis, while there is a large difference in magnitude, which indicates a strongly anisotropic anomalous and spin transverse transport in the $zx$ and $zy$ plane. Remarkably, a giant AHC of 646 S/cm and ANC of 2.8 A/Km are found (Fig. 4), among which the latter is particularly striking owing to the magnitude larger than that in the famous kagome magnet Co$_3$St$_2$S$_2$ [42] while approaching the largest recorded experimental values of about 4 A/Km in Co$_2$MnGa [35] and 5.2 A/Km in Fe$_3$Ga [43]. In Figs. S4 and S5, we present evidence that this enhancement originates from the intrinsic contribution, mediated by the reduction of magnetic symmetries from $R3c'$ for magnetization along $z$-axis to $C2'/c$ for $x$-axis ($C2'/c'$ for $y$-axis), that splits the nodal lines further and gives rise to Berry curvature’s amplification. In contrast, the change in extrinsic contributions is neglig-
able. This further supports the topological origin of large anomalous and spin transport in PdF₃.

Finally, we also investigated transverse transport in other NCSGSMs, in particular in MnF₃ [2, 80]. Large AHC (SHC) and ANC (SNC) are also found due to the similar topological band structure and Berry curvature distribution (see Figs. S1 and S2 [84]). We believe that giant fully spin-polarized currents can be also found in a large family of spin-gapless semimetals or semiconductors [2, 7, 80, 85, 86].

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SUPPLEMENTAL MATERIAL FOR “GIANT FULLY SPIN-POLARIZED CURRENTS ENHANCED BY DISORDER IN NODAL CHAIN SPIN-GAPLESS SEMIMETALS”

Details of first-principles calculations

Electronic structure calculations.—The electronic structure calculations were performed by employing the full-potential linearized augmented plane-wave (FP-LAPW) method as implemented in the FLEUR code [1]. The GGA-PBE functional was used in all calculations. The primitive lattice constants of α = β = γ = 52.480° (55.223°) for PdF₃ (MnF₃) were adopted [2]. The energy cut-off of plane wave was chosen as 4.5 a₀⁻¹ (4.8 a₀⁻¹) for PdF₃ (MnF₃), where a₀ is Bohr’s radius, and a k-mesh of 10 × 10 × 10 was used. The effective Hubbard parameter for the d-orbitals of Pd and Mn atoms was set to be 4.0 eV [2]. The 56 Wannier functions including the d-orbitals of Pd (Mn) atoms and the p-orbitals of F atoms on a k-mesh of 8 × 8 × 8 were constructed using WANNIER90 package [3].

Anomalous Hall and anomalous Nernst effects.—The anomalous Hall conductivity (σₓᵧ) and Fermi-sea (σₓᵧ) terms. The intrinsic contribution σₓᵧ was calculated using the Kubo formalism with a constant Γ approximation [4],

\[ \sigma_{ij}^{I} = \frac{-e^2 \hbar}{2\pi} \int \frac{d^3k}{(2\pi)^3} \sum_{m,n,m\neq n} \text{Im} \left[ v_{im}^t(k)v_{jm}^j(k) \right] \times \frac{(E_{mk} - E_{nk})}{(E_f - E_{mk} + \Gamma^2)((E_f - E_{nk})^2 + \Gamma^2)^2} \]

(5)

\[ \sigma_{ij}^{II} = \frac{e^2 \hbar}{\pi} \int \frac{d^3k}{(2\pi)^3} \sum_{m,n,m\neq n} \text{Im} \left[ v_{im}^t(k)v_{jm}^j(k) \right] \times \frac{1}{(E_{mk} - E_{nk})[(E_f - E_{mk})^2 + \Gamma^2]} \text{Im} \left[ \ln \frac{E_f - E_{mk} + \Gamma}{E_f - E_{nk} + \Gamma} \right] \}

(6)

where \( e, \hbar, v, k, E_{mk}, E_f, \) and Γ are the elementary charge, reduced Planck constant, velocity operator, Cartesian coordinates, eigenenergy at band index \( n \) and momentum \( k \), Fermi energy, and constant band broadening, respectively. The bold font \( i \) represents the imaginary unit. To model the variation of \( \sigma_{ij}^{int} \) against \( \sigma_{xx} \) (at \( E_f \)) [see Fig. 2(b) in the main text], Γ was altered in the range of 0 ~ 0.25 eV. On the other hand, to analyze the variation of \( \sigma_{ij}^{int} \) versus energy [see Fig. 2(c) in the main text], Γ was fixed at 0 eV (i.e., clean limit). To ensure the convergence, a ultra-dense k-mesh of 451 × 451 × 451 was used to calculate the intrinsic anomalous Hall effect.

In the case of clean limit, \( \sigma_{ij} \) can be reduced to the well-known Berry curvature expression [5],

\[ \sigma_{ij} = \frac{-e^2}{\hbar} \sum_n \int \frac{d^3k}{(2\pi)^3} \Omega_{ij}^n(k) f_n(k), \]

(7)

where \( f_n(k) = 1/\exp((E_{mk} - E_f)/k_B T) + 1 \) is the Fermi-Dirac distribution function, \( \Omega_{ij}^n(k) \) is the band- and momentum-resolved Berry curvature.

\[ \Omega_{ij}^n(k) = -\sum_{m\neq n} \frac{2\text{Im} \left[ v_{im}^t(k)v_{jm}^j(k) \right]}{(\omega_{mk} - \omega_{nk})^2}. \]

(8)

In our calculations, the extrinsic contribution of \( \sigma_{ij} \) has two parts, side-jump \( \sigma_{ij}^{sk} \) and intrinsic skew-scattering \( \sigma_{ij}^{sk} \), which are simulated by incorporating a Gaussian disorder potential. It should be noted that the intrinsic skew-scattered calculation here differs from the conventional skew-scattering, which contains more than two powers of disorder potential of vertex correlations. The formalism and first-principles code were developed by Czaja et al. [4] in terms of the retarded and advanced Green functions \( G^R/A \),

\[ \sigma_{ij}^{I} = \frac{e^2 \hbar}{4\pi} \int \frac{d^3k}{(2\pi)^3} \text{Tr} \left[ \Gamma^i(E_f,k)G^R(E_f,k)v^jG^A(E_f,k) - (i \leftrightarrow j) \right], \]

(9)

\[ \sigma_{ij}^{II} = \frac{e^2 \hbar}{2\pi} \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{E_f} dE \text{Re} \left[ \text{Tr} \left[ \Gamma^i(E,k)G^R(E,k)\gamma(E,k)G^R(E,k)\Gamma^j(E,k)G^R(E,k) - (i \leftrightarrow j) \right] \right], \]

(10)
in which the vector vertex function $\Gamma(E, k)$ and scalar vertex function $\gamma(E, k)$ can be solved iteratively,

$$\Gamma(E, k) = \mathbf{v}(k) + V \int \frac{d^3k'}{(2\pi)^3} O_{kk'} G^A(E, k') \Gamma(E, k') G^R(E, k') O_{kk'},$$

$$\gamma(E, k) = I + V \int \frac{d^3k'}{(2\pi)^3} O_{kk'} G^R(E, k') \gamma(E, k') G^R(E, k') O_{kk'},$$

where $\mathbf{v}(k)$ is the vector velocity operator, $I$ is the identity matrix, $O_{kk'}$ is the overlap matrix, $V = U^2 n_{\text{imp}}$ is the disorder parameter ($U$ and $n_{\text{imp}}$ are disorder strength and disorder concentration, respectively). To model the variation of $\sigma_{ij}^{sk}$ and $\sigma_{ij}^{sj}$ against $\sigma_{xx}$ (at $E_f$) [see Fig. 2(b) in the main text], $V$ was altered in the range of $0 \sim 80$ eV$^2 a_0^3$ ($a_0$ is Bohr’s radius). On the other hand, to analyze the variation of $\sigma_{ij}^{sk}$ and $\sigma_{ij}^{sj}$ versus energy [see Fig. 2(c) in the main text], $V$ was fixed at a weak disorder value of 1.83 eV$^2 a_0^3$. To ensure the convergence, a ultra-dense $k$-mesh of $350 \times 350 \times 350$ was used to calculate the extrinsic anomalous Hall effect.

After calculated the anomalous Hall conductivity, the component-resolved anomalous Nernst conductivity $\alpha_{ij}$ can be obtained by using the generalized Mott formula [6]:

$$\alpha_{ij} = -\frac{1}{e} \int dE (\frac{\partial f}{\partial E}) \sigma_{ij} E - E_f \frac{T}{},$$

here, $f$ is the Fermi-Dirac distribution function and $T$ is temperature. To converge the anomalous Nernst conductivity, the anomalous Hall conductivity was initially calculated with an energy interval of 0.01 eV and then was interpolated to 0.1 meV.

**Spin Hall and spin Nernst effects.**—The intrinsic spin Hall and spin Nernst conductivities can be calculated from the Berry phase theory [7–11]. Nevertheless, because the bands near the Fermi energy are fully single-spin component, both the intrinsic and extrinsic contributions of spin Hall ($\sigma_{ij}^{sk}$) and spin Nernst ($\alpha_{ij}^{sk}$) conductivities can be calculated through the anomalous Hall ($\sigma_{ij}^{sk}$) and anomalous Nernst ($\alpha_{ij}^{sk}$) conductivities, i.e., $\sigma_{ij}^{sk} = \frac{\hbar}{2\pi} \sigma_{ij}$ and $\alpha_{ij}^{sk} = \frac{\hbar}{2\pi} \alpha_{ij}$, respectively.

### Supplemental Figures of MnF$_3$

**The giant anomalous and spin transport of MnF$_3$.**—Besides PdF$_3$, we have also investigated the electronic properties as well as the spin and transport of MnF$_3$. Similarly to PdF$_3$, MnF$_3$ has a similar fully spin-polarized band structure (Fig. S1). The small band gap induced by spin-orbit coupling (Fig. S2(a)) gives rise to large Berry curvature $\Omega_{xy}$ near the $Z$ and $L$ points as well as along the $\Gamma - X$ direction (Fig. S2(b)). Figures S2(e) and S2(f) display the distribution of $\Omega_{xy}$ in the first Brillouin zone and its integral along the $k_y$ direction, respectively, from which one can see that the large hot pots are located near the gapped nodal lines. This leads to a giant intrinsic anomalous Hall conductivity (close to 400 S/cm) and anomalous Nernst conductivity (above 1 A/Km) near the Fermi level. Moreover, the spin Hall and spin Nernst conductivities are displayed in Figs. S2(c) and S2(d).

### Supplemental Figures of PdF$_3$

The component-resolved anomalous Hall conductivity ($\sigma_{xy}^{int}, \sigma_{xy}^{sk}, \sigma_{xy}^{sj}$, and the total $\sigma_{xy}$) versus $\sigma_{xx}$ at $E = E_f - 0.04$ eV is plotted in Fig. S3. Clearly, all the components are enhanced by shifting $E_f$ downward 0.04 eV, comparing to the results at $E_f$ (see Fig. 2(b) in the main text). Nevertheless, the key features are remained, i.e., the shape of anomalous Hall conductivity is dominated by $\sigma_{xy}^{int}$, and the magnitude is amplified by the contribution from $\sigma_{xy}^{sk}$. Note that $\sigma_{xy}$ reaches a nearly constant plateau for $E = E_f$ and $E = E_f - 0.04$ eV when $\sigma_{xx} > 1 \times 10^5$ S/cm and $\sigma_{xx} > 2 \times 10^5$ S/cm, respectively. The side-jump contribution $\sigma_{xy}^{sj}$ is also small at $E = E_f - 0.04$ eV but interestingly exhibits a sign change at $\sigma_{xx} \sim 0.7 \times 10^5$ S/cm.

We have also investigated the anisotropy of anomalous Hall and anomalous Nernst effects when the magnetization is along $x$-axis ([110]) and $y$-axis ([112]) (refer to Fig. 1(a) in the main text), as shown in Figs. S4 and S5. Firstly, we discuss the intrinsic contribution. Apparently, both anomalous Hall and anomalous Nernst conductivities are enhanced when magnetization $\mathbf{M}$ rotates from $z$ axis ([111] direction) to $xy$ plane ([111] plane), indicating a strong anisotropy within the $zx$ and $yz$ planes. In addition, if $\mathbf{M}$ is along the $x$ and $y$ axes, the sizes of the intrinsic contribution are nearly the same, indicating the isotropy of the anomalous Hall and anomalous Nernst effects within the $xy$ plane. The
anisotropy of anomalous transport on the $zx$ and $yz$ plane as well as the isotropy on the $xy$ plane are in accordance with the change of magnetocrystalline anisotropy energy [2]. The close relationship between anomalous transport and magnetocrystalline anisotropy energy has been well discussed in our previous works [12, 13].

Moreover, one can see that the symmetry-allowed tensor elements of anomalous Hall and anomalous Nernst conductivities are changed. When $\mathbf{M}$ is along the $z$ axis, the magnetic space group of the system is $R\bar{3}c'$, which has one three-fold rotation axis $C_{3[111]}$, and three combined operations of time-reversal $\bar{T}$ and glide mirrors $\bar{M}$ ($T\bar{M}_1$, $T\bar{M}_2$, $T\bar{M}_3$). With respect to $\bar{M}_1$, $\Omega_{zx}$ and $\Omega_{xy}$ are odd, while $\Omega_{yz}$ is even. With respect to $\bar{T}$, all components of $\Omega_{ij}$ are odd. Thus, $\Omega_{zx}$ and $\Omega_{xy}$ are even, while $\Omega_{yz}$ is odd under the combined symmetry $T\bar{M}_1$. After integrating the Berry curvature in the first Brillouin zone, the $zx$ and $xy$ components of anomalous Hall and anomalous Nernst conductivities are nonvanishing. Another two $T\bar{M}$ symmetries are related to $T\bar{M}_1$ by $C_{3[111]}$, which further force $zx$ component to be zero. Therefore, only the $xy$ component of anomalous Hall and anomalous Nernst conductivities can exist for $R\bar{3}c'$ group. In the same way, when $\mathbf{M}$ is along $x$ axis ($y$ axis), the $\sigma_{yz}$ ($\sigma_{zx}$ and $\sigma_{xy}$) are nonvanishing due to the symmetry $\bar{M}_1$ ($T\bar{M}_1$) in the magnetic space group $C2/c$ ($C2'/c'$).

The giant anomalous transport is dominated by the intrinsic mechanism, which originates from the large Berry curvature around gapped nodal lines. When $\mathbf{M}$ is along the $z$ direction, the large Berry curvature is mainly lying on the $\bar{M}_1$, $\bar{M}_2$, and $\bar{M}_3$ planes, at where four nodal lines ($\text{NL}_1$, $\text{NL}_2$, $\text{NL}_3$, and $\text{NL}_4$) are broken (see Fig. 3(e,f) in the main text). When the $\mathbf{M}$ is along the $x$ or $y$ axis, the symmetry is further reduced, for example, the absence of $C_{3[111]}$. Hence, the nodal lines are further split at more nodes, giving rising to the enhanced Berry curvature in more regions (Figs. S4(c) and S4(d)). Specially, when $\mathbf{M}$ is along the $x$ direction, $\text{NL}_1$ is still survived even including spin-orbit coupling because the glide mirror symmetry $\bar{M}_1$ that is vertical to the magnetization direction is preserved [2], and thus it contributes a small Berry curvature on $\alpha_{yz}$ plane (compare Fig. S4(c) with Fig. 3(f) in the main text). It further reveals that the origin of large anomalous and spin transport in PdF$_3$ result from the gapped nodal lines.

Next, we discuss the intrinsic mechanism of anomalous transport when $\mathbf{M}$ is along the $z$ and $x$ axes, as shown in Fig. S5. Clearly, the $isk$ contribution plays an important role and the trends for both magnetized directions are remained. On the other hand, the $sj$ contribution is negligible small. In contrast to the strong anisotropy of the $int$ contribution relevant to band topology, the $isk$ and $sj$ contributions do not display obvious enhancement when $\mathbf{M}$ rotates from $z$ axis to $x$ axis even with more gapped topological nodes.

The temperature-dependence of the component-resolved anomalous Nernst conductivity ($\alpha_{yz}^{int}$, $\alpha_{yz}^{isk}$, $\alpha_{yz}^{sj}$, and the total $\alpha_{yz}$) when $\mathbf{M}$ is along the $x$ axis is plotted in Fig. S6. Similarly, the main features of anomalous Nernst conductivity remain unchanged expect for the enhanced magnitude, comparing to the case of $\mathbf{M}\parallel z$ (see Fig. 2(d) in the main text). In the entire temperature range, the $int$ mechanism plays the leading role, and the $isk$ contribution is much stronger than the negligible $sj$ contribution. Specially, in the low temperature region of $T < 50$ K, the total Nernst conductivity is almost equivalent to the intrinsic one due to the cancel between $isk$ and $sj$ contributions.
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FIG. S1. Spin-polarized band structure of MnF$_3$ without SOC.

FIG. S2. Giant anomalous and spin transport of MnF$_3$. (a,b) The relativistic band structure and Berry curvature along high symmetry lines. (c,d) The intrinsic anomalous Hall ($\sigma_{xy}$) and anomalous Nernst ($\alpha_{xy}$ at $T = 300$ K) conductivities as well as the intrinsic spin Hall ($\sigma^s_{xy}$) and spin Nernst ($\alpha^s_{xy}$ at $T = 300$ K) conductivities as a function of energy. The spin Hall and spin Nernst conductivities are in units of $\hbar/2e$ S/cm and $\hbar/2e$ A/Km, respectively. (e) The distribution of Berry curvature $\Omega_{xy}$ in the first Brillouin zone and (f) the projection of Berry curvature onto the $k_x$-$k_y$ plane by integrating $\Omega_{xy}$ along the $k_z$ direction. To observe the main features of $\Omega_{xy}$, the values of less than 200 bohr$^2$ are not shown.
FIG. S3. Component-resolved anomalous Hall conductivity ($\sigma_{xy}^{int}$, $\sigma_{xy}^{isk}$, $\sigma_{xy}^{sj}$, and the total $\sigma_{xy}$) versus $\sigma_{xx}$ at $E = E_f - 0.04$ eV for PdF$_3$ when the magnetization is along the $z$ direction ($M \parallel z$).
FIG. S4. (a,b) The intrinsic anomalous Hall and anomalous Nernst conductivities ($T = 200$ K) of PdF$_3$ when the magnetization $M$ is along the $z$, $x$, and $y$ axes. (c,d) The Berry curvature $\Omega_{yz}$ and $\Omega_{zx}$ integrated along the $k_z$ direction with $M$ being along the $x$ and $y$ axes, respectively. The black lines draw the nodal lines. To observe the main features of Berry curvature, the values of less than 200 bohr$^2$ are not shown.
FIG. S5. The extrinsic anomalous Hall (a,c) and anomalous Nernst (b,d) conductivities of PdF$_3$ when the magnetization $\mathbf{M}$ is along the $z$ and $x$ axes.
FIG. S6. Component-resolved anomalous Nernst conductivity ($\alpha_{yz}$, $\alpha_{isk}$, $\alpha_{sj}$, and the total $\alpha_{yz}$) as a function of temperature $T$ for PdF$_3$ when the magnetization $\mathbf{M}$ is along the $x$ axis.