

Disorder- and Topology-Enhanced Fully Spin-Polarized Currents in Nodal Chain Spin-Gapless Semimetals


Xiaodong Zhou^{1,2}, Run-Wu Zhang^{1,2}, Xiuxian Yang^{1,2}, Xiao-Ping Li^{1,2}, Wanxiang Feng^{1,2,*},
Yuriy Mokrousov^{3,4,†} and Yugui Yao^{1,2,‡}

¹Centre for Quantum Physics, Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement (MOE),
School of Physics, Beijing Institute of Technology, Beijing 100081, China

²Beijing Key Lab of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics,
Beijing Institute of Technology, Beijing 100081, China

³Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

⁴Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

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Recently discovered high-quality nodal chain spin-gapless semimetals MF_3 ($M = \text{Pd, Mn}$) feature an ultraclean 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 large values of respective conductivities. Our findings open a new material platform for exploring strong anomalous and spin transport properties in magnetic topological semimetals.

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Introduction.—After the discovery of magnetic topological insulators [1,2], different types of magnetic topological states ranging from insulators to semimetals have emerged [3–28]. 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_H^A 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) [29,30] and anomalous Nernst effect (ANE) [31,32]. 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 [33–49]. On the other hand, the Hall currents of spin J_H^S —i.e., the spin counterparts of J_H^A also known as the spin Hall effect (SHE) [50] and spin Nernst effect (SNE) [51]—are also largely driven by topological nodal features which give rise to large spin Hall conductivity (SHC) and spin Nernst conductivity (SNC) in nonmagnetic topological semimetals [52–65].

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 σ_{xy} and ANC α_{xy} can be decomposed into three different contributions (SHC σ_{xy}^s and SNC α_{xy}^s are also the case) [66–69]:

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

The first term is the so-called intrinsic (int) contribution, which can be well described by Berry phase theory [29,30], 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) [70,71] and side jump (sj) [72], respectively, and whose role in Hall effects of magnetic topological semimetals received very little attention so far, besides several very recent experimental [73–75] and model studies [76–81]. 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 ($M = \text{Pd, Mn}$) [17], which feature an ultraclean nodal chain residing right at the Fermi level, providing an ultrahigh Fermi velocity and 100% spin polarization simultaneously. This provides us with a perfect platform to clearly identify pure topological contributions to Hall transport. We show that such a remarkable electronic structure inevitably gives rise to large Hall effects. We further uncover the intrinsic mechanism as the main underlying physical origin of the large 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 Letter provides a foundation for educated design of large pure spin-polarized Hall currents for future “green” spintronics.

High-quality candidate hosting large 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 [7,17,82–84]. Among these, we select an outstanding example, the rhombohedral transition metal trifluorides MF_3 ($M = \text{Pd, Mn}$) [17,83] [Fig. 1(a)]. The ferromagnetic ground state is confirmed by performing a series of spin spiral calculations, as shown in Figs. S1 and S2 in Supplemental Material [85]. The high Curie temperature (≥ 450 K) is estimated from mean field approximation, Monte Carlo simulations, and Landau-Lifshitz-Gilbert spin dynamics (Fig. S3 [85]). MF_3 display a linear semimetallic band structure in the spin up channel, while exhibiting a large indirect band gap (2.46 eV for PdF_3 , 6.43 eV for MnF_3) in the spin down channel [Fig. 1(c) and Fig. S4 [85]], 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_1 , NL_2 , and NL_3) [see Figs. 3(c) and 3(d)], which are positioned in three mirror planes (\mathcal{M}_1 , \mathcal{M}_2 , and \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 ultraclean 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 [69]:

$$J_H^A = J^\uparrow + J^\downarrow = J^\uparrow, \quad (2)$$

$$J_H^S = (J^\uparrow - J^\downarrow) \frac{\hbar}{2e} = \frac{\hbar}{2e} J^\uparrow, \quad (3)$$

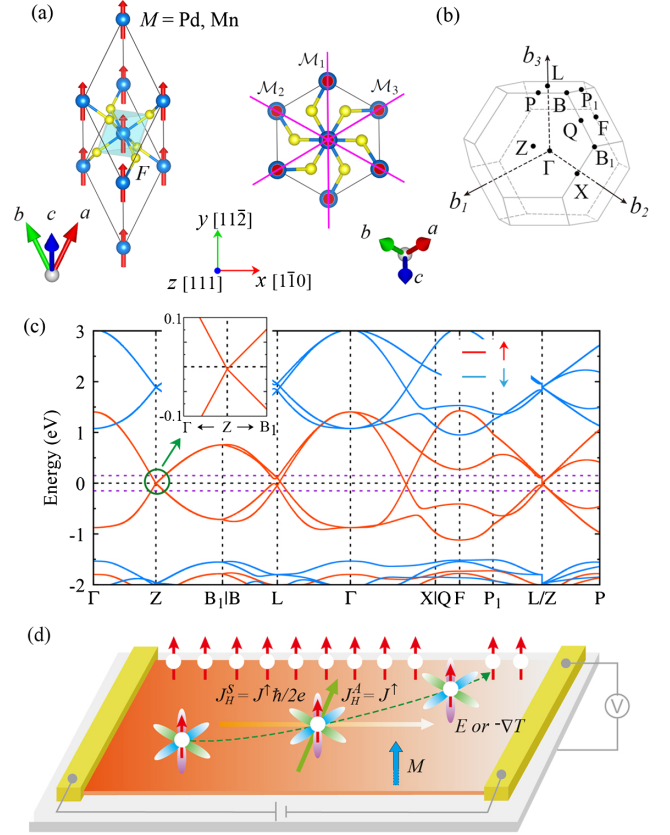


FIG. 1. Nodal chain spin gapless semimetals (NCSGSMs) and their fully spin-polarized currents. (a) The crystal structure of MF_3 ($M = \text{Pd, Mn}$), and the view of (111) plane. The blue spheres are magnetic M atoms, whereas yellow spheres are nonmagnetic F atoms. The red arrows label the spin magnetization 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 close-up of 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.

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 $\sigma_{xy}^s = (\hbar/2e)\sigma_{xy}$ and $\alpha_{xy}^s = (\hbar/2e)\alpha_{xy}$, as also confirmed by first-principles calculations (see Fig. S5 [85]).

Next, we proceed to explore these physical phenomena quantitatively. First, to confirm the leading mechanism of AHC in MF_3 , the computed variation of σ_{xy} (the superscript tot is omitted in the following discussion) with σ_{xx} at $E = E_f$ and $E = E_f - 0.04$ eV is plotted in Fig. 2(a) for the magnetization \mathbf{M} being along the z axis ([111] direction) and x axis ([1 $\bar{1}$ 0] direction), respectively. To do this, we use the implementation of uncorrelated disorder scattering

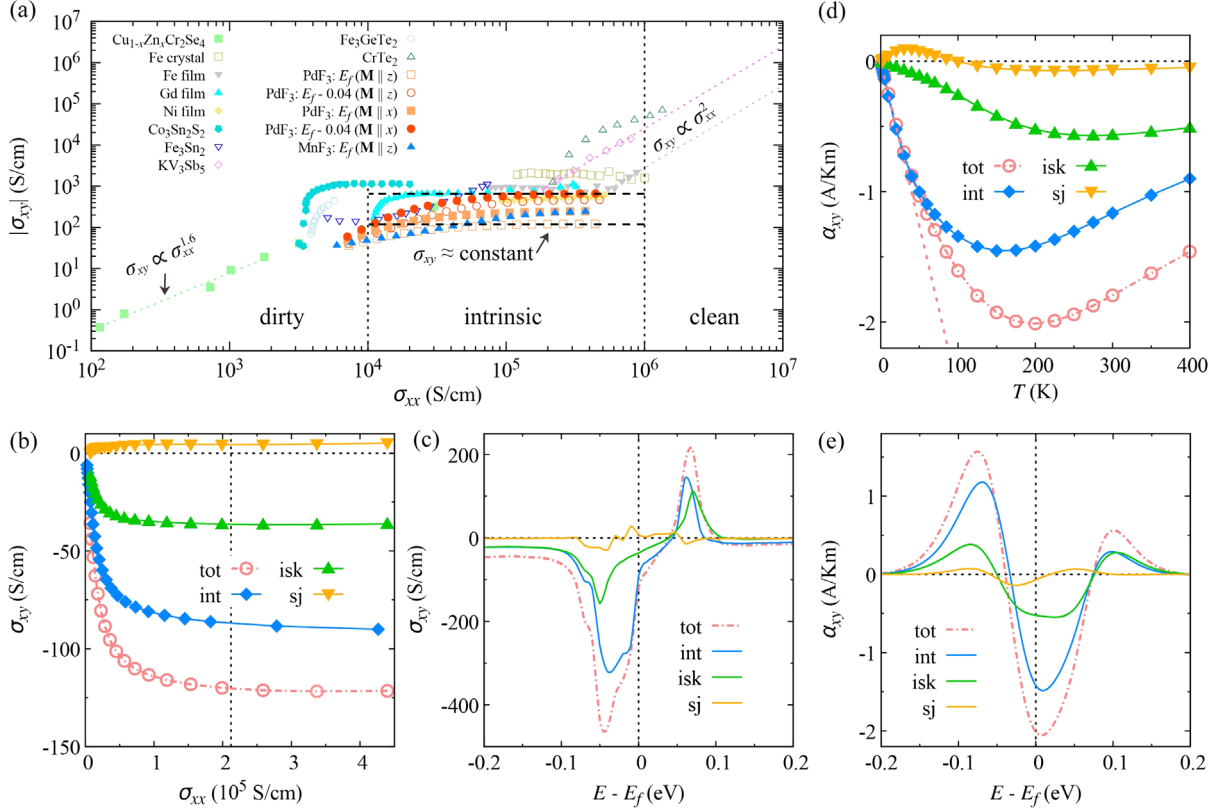


FIG. 2. Large spin-pure AHC and ANC. (a) AHC σ_{xy} versus σ_{xx} for PdF₃ at the true Fermi energy E_f and at $E_f - 0.04$ eV, with the magnetization \mathbf{M} along the z or x direction, ranging across intrinsic from dirty to clean regimes. Note that when $\mathbf{M} \parallel x$, the nonzero component of AHC is σ_{yz} . The data of MnF₃ for $\mathbf{M} \parallel z$ are also plotted. In the plot, data for various ferromagnets are shown for comparison, as reported in previous works [108–110]. (b), (c) Disorder-related contributions to the AHC (σ_{xy}^{int} , σ_{xy}^{isk} , σ_{xy}^{sj} , and the total σ_{xy}) as a function of σ_{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 ($1.83 \text{ eV}^2 \text{ bohr}^3$) [85], corresponding to $\sigma_{xx} = 2.12 \times 10^5 \text{ S/cm}$, where the extrinsic σ_{xy} reaches a plateau, indicated by a vertical dashed line in (b). (d), (e) Disorder-related contributions to the ANC (α_{xy}^{int} , α_{xy}^{isk} , α_{xy}^{sj} , and the total α_{xy}) for various temperatures T and energy, computed at E_f and for $T = 200 \text{ K}$, respectively.

formalism from the first principles [see Eqs. (S5)–(S8) Ref. [85]]. By analyzing the dependency of σ_{xy} on σ_{xx} , different scaling relations have been proposed for a variety of ferromagnets [108–112]: $\sigma_{xy} \propto \sigma_{xx}^{1.6}$ in the dirty regime ($\sigma_{xx} < 10^4 \text{ S/cm}$), nearly constant in the intrinsic regime ($\sigma_{xx} \sim 10^4\text{--}10^6 \text{ S/cm}$), and $\sigma_{xy} \propto \sigma_{xx}^2$ or σ_{xx}^1 in the clean regime ($\sigma_{xx} > 10^6 \text{ S/cm}$). From Fig. 2(a), one can see that MF_3 is located within the intrinsic regime, and σ_{xy} exhibits a nearly constant plateau for both $E = E_f$ and $E = E_f - 0.04 \text{ eV}$ for $10^5 < \sigma_{xx} < 10^6 \text{ S/cm}$, 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 PdF₃ with $E = E_f$ and $E = E_f - 0.04 \text{ eV}$ when $\mathbf{M} \parallel z$ are shown in Fig. 2(b) and Supplemental Material Fig. S6 as σ_{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 σ_{xy} .

In contrast, we find the side jump to be negligibly small. Note that although the density of states for semimetals is usually small at the Fermi level, the longitudinal conductivity σ_{xx} can reach up to $10^3\text{--}10^4 \text{ S/cm}$ for WTe₂ [113–115] and Co₃Sn₂S₂ [36,37], $10^4\text{--}10^7 \text{ S/cm}$ for ZrSiS [116], and $10^4\text{--}10^6 \text{ S/cm}$ for our cases MF_3 .

The energy evolution of σ_{xy} , shown in Fig. 2(c), reveals considerable values in the range of $[-0.1, 0.1] \text{ eV}$, 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 σ_{xy} with energy. According to the low-temperature Mott relation, which relates the ANC to the energy derivative of the AHC [31],

$$\alpha_{xy} = -\frac{\pi^2 k_B^2 T}{3e} \left. \frac{d\sigma_{xy}}{dE} \right|_{E=E_f}, \quad (4)$$

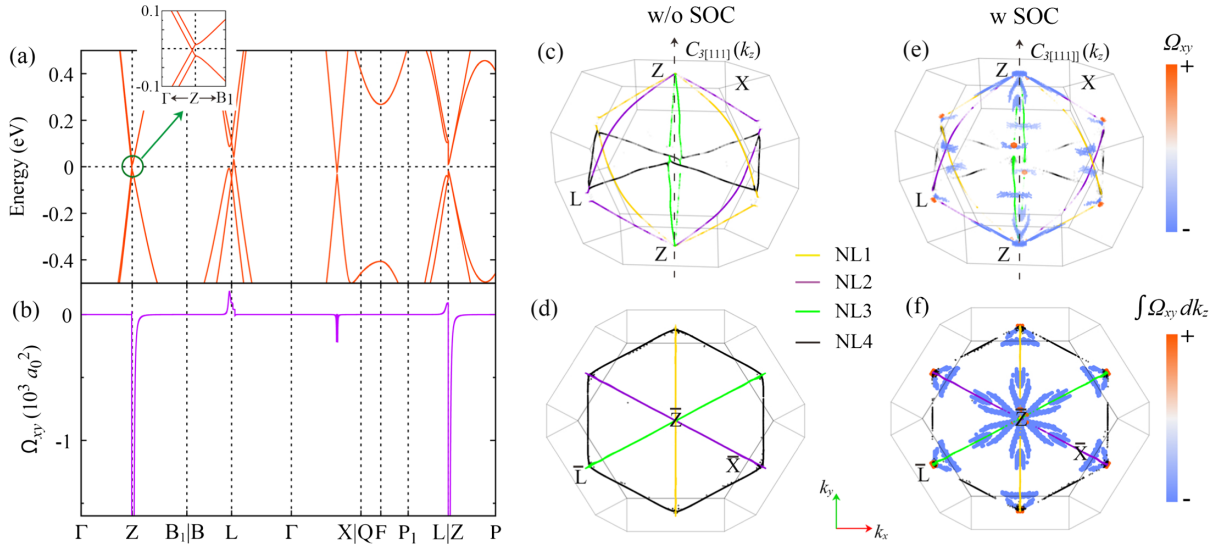


FIG. 3. The underlying physical origin of large AHC and ANC. (a) The band structure of PdF₃ with SOC, with the inset zooming into the bands near the Z point. (b) Berry curvature Ω_{xy} along high symmetry lines (singular value at Z point reaches 0.46×10^5 bohr²). (c) The distribution of nodal lines in the Brillouin zone, and (d) projected on k_x - k_y plane. (e) Ω_{xy} and nodal lines in the Brillouin zone, and (f) projected to the k_x - k_y plane where Ω_{xy} is integrated along the k_z direction, i.e., $\int \Omega_{xy}(k_x, k_y, k_z) dk_z$. To present main features in the distribution of Ω_{xy} , the values of less than 200 bohr² are not shown.

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 [85], 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 large α_{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 PdF₃ is that the peak of α_{xy} is positioned right at the true E_f , as seen in Fig. 2(e), while the range of energies with large α_{xy} is wide enough for large ANE to be easily detected experimentally.

The underlying physical origin of strong transport properties.—Next, we uncover the underlying physical origin of the large AHC and ANC in PdF₃ (similar analysis can be performed for SHC and SNC). The band structure of PdF₃ with SOC together with the Berry curvature Ω_{xy} along high symmetry lines is shown in Figs. 3(a)–3(b). Clearly, the slightly gapped crossing points generate large Ω_{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 [\tilde{M}_1 , \tilde{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) [17]. 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 Γ Z direction. The former rather than the latter is responsible for the large Ω_{xy} . Indeed, the distribution of Ω_{xy} in the Brillouin zone [Fig. 3(e)] indicates that the hot spots are mainly distributed near the gapped nodal lines. Further, we integrate Ω_{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 large 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 NCSGSMs, the density of states is nearly vanishing at the Fermi level. Hence, the large AHC and ANC predicted here are driven by pure topological characteristics.

To further confirm the topological origin of transport in PdF₃, we also consider the case of the magnetization directed along other directions, e.g., x and y axes (see Fig. 4 and Supplemental Material Figs. S7–S9 [85]). 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 or zy plane. Remarkably, a large 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

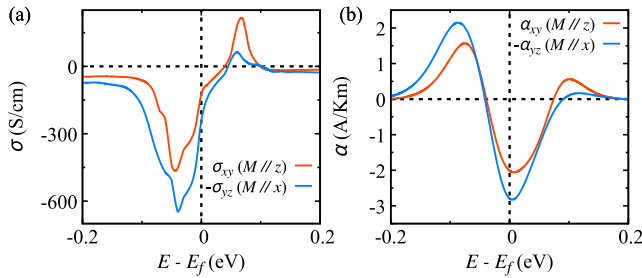


FIG. 4. Anisotropic AHC and ANC. (a),(b) Total AHC and ANC ($T = 200$ K) for PdF₃ when the magnetization \mathbf{M} is aligned along the z and x axes.

Co₃Sn₂S₂ [42] while approaching the largest recorded experimental values of about 4 A/Km in Co₂MnGa [35] and 5.2 A/Km in Fe₃Ga [43]. In Figs. S7 and S9, we present evidence that this enhancement originates from the intrinsic contribution, mediated by the reduction of magnetic symmetries from $R\bar{3}c'$ 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 negligible. 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 [17,83]. Large AHC (SHC) and ANC (SNC) are also found due to the similar topological band structure and Berry curvature distribution (see Figs. S4 and S5 Ref. [85]). We believe that large fully spin-polarized currents can be also found in a large family of spin-gapless semimetals or semiconductors [7,17,82–84].

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* wxfeng@bit.edu.cn

† y.mokrousov@fz-juelich.de

‡ ygyao@bit.edu.cn

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