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Large anomalous hall effect and negative magnetoresistance in half-topological semimetals

Reviewers' comments:

Reviewer #1 (Remarks to the Author):

Y. Zhu et al. presents detailed magneto-transport studies with theoretical support on TbPdBi Single crystals. Authors report giant field-induced AHE and claims it to be as consequence of the half-topological semimetal state along with canted AFM. The manuscript is overall interesting, but needs several clarifications before can be considered for publications:

1. Authors claim to prepare: "samples are high-quality single crystals". However no characterization evidence is presented. Authors must add crystal photo and results of structural characterization, like single crystal diffraction, or Laue etc. along with unit cell parameters. This also should verify how authors determined the 100 oriented face.

2. Authors has not performed any neutron diffraction or similar analysis to determine the actual spin structure of TbPdBi. So how authors knew the canted spin structure, or the AFM spin configuration of the grown crystals as extensively discussed in the manuscript? No ref also added regarding this.

3. From Fig.1a it is evident that the AHE peak value is increasing with temperature well beyond TN atleast until the shown temperature of 20 K. So, it is not clear how far the AHE signal increases with temperature? Again from Fig. 2b, ρxx sharply decreases with increasing temperature. So the ratio determining the Hall angle also should increase with temperature beyond 2%? So why the higher temperature Hall angles not shown in Fig.1c?

4. From Fig. 1b magnetization data, it is evident that the magnetization doesn't saturate above T_N. So thermal energy is too strong to polarize the spins. Then how the AHE signal can increase due to spin polarization effect (spin canting, exchange induced band splitting etc.) with increasing temperature? Besides, according to Fig. 2a/b, the -ve MR decreases more sharply with increasing temperature. But at 10 or 20 K, the increased thermal energy should induce more spin disorder. Then I am confused how the authors are claiming that the spin-scattering is the only/dominating origin for high AHE and negative MR.

5. Fig.S1 shows a peak in longitudinal resistivity around 50 K. What is the origin for that? Looks like it's independent from the magnetic behaviour and can this have something to do with the anomalous transport properties of TbPdBi?

6. Fig. 4e shows the theoretical calculation of the x-dependence of Hall conductivity and explains the effect of spin canting. But why the conductivity for xy, yz and zx are showing different behavior? In a cubic system x, y and z axes are equivalent directions. So why system shows such anisotropic behavior?

Reviewer #2 (Remarks to the Author):

General Comment: The manuscript entitled "Surprisingly large anomalous Hall effect and giant negative magnetoresistance in half-topological semimetals" by Yanglin Zhu et al. report the giant AHA and giant negative magnetoresistance in half-Heusler TbPdBi single crystals. And they contribute the exotic transport properties to the half-topological state. In overall, the giant AHA and large AHC are interesting. However, the manuscript needs more explanation on some points.
Comment 1: The band structure and density of states around Fermi level change in the canted AFM state. Thus, the carrier concentration changes may also contribute to Hall resistance. Is there any way for the author to separate this contribution?
Comment 3: You pointed out that the calculated AHC is an order of magnitude smaller than the experimental value. Is it possible that the extrinsic mechanism dominates the AHC?

Comment 4: The authors attribute the large negative MR effect to the half-topological state. However, specific theoretical analysis is lacking here. The topological insulator $MnBi_2Te_4$ also exhibits the half-topological semimetal state under magnetic field. Why does this alloy not show a large negative MR?

Response to reviewers' comments (COMMSPHYS-23-0072-T)

Reviewer #1:

Y. Zhu et al. presents detailed magneto-transport studies with theoretical support on TbPdBi Single crystals. Authors report giant field-induced AHE and claims it to be as consequence of the half-topological semimetal state along with canted AFM. The manuscript is overall interesting, but needs several clarifications before can be considered for publications:

1. Authors claim to prepare: "samples are high-quality single crystals". However no characterization evidence is presented. Authors must add crystal photo and results of structural characterization, like single crystal diffraction, or Laue etc. along with unit cell parameters. This also should verify how authors determined the 100 oriented face.

Response: We sincerely thank the reviewer for taking time to review our manuscript. We are glad to note that the reviewer finds our work interesting.

We agree with the reviewer that structure characterization data should be added to the manuscript. We apologize for overlooking to do so in the original manuscript. Indeed, we performed X-ray diffraction (XRD) experiments on the TbPdBi crystals used in this study. Fig. R1 below shows the XRD pattern measured on the (100) plane, from which two diffraction peaks. [(200) and (400)] can be observed. These two peaks match well the (200) and (400) peaks of the powder XRD pattern of YPdBi in the database, which is isostructural to TbPdBi. Like YPdBi, TbPdBi also has a cubic structure; its (100), (010) and (001) planes are equivalent. From the d-spacing of the (200) peak, the lattice parameter a is estimated to be ~ 6.6360 Å, consistent with the previously reported value (a ~ 6.65310 Å) [ref.37 in the manuscript]. The inset to Fig. R1 shows a typical crystal image of TbPdBi, on which we have denoted the (100) plane. We have added the structure characterization information in the "Single crystal growth" section in Methods and Fig. R1 as supplementary Fig. S1.

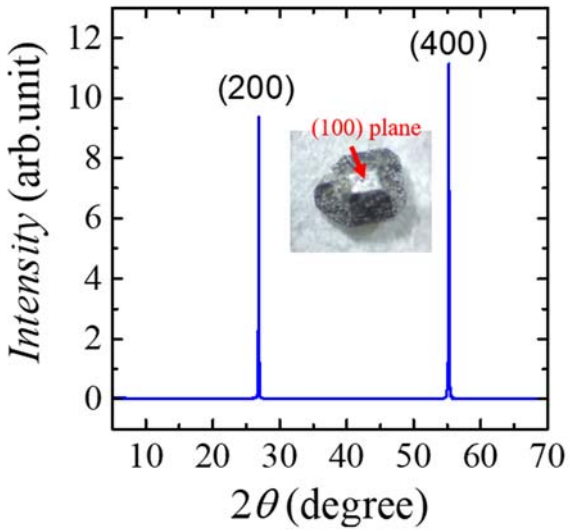

Fig. R1: X-ray diffraction pattern measured on the (100) plane of TbPdBi. Inset: mage of a TbPdBi crystal.

2. Authors has not performed any neutron diffraction or similar analysis to determine the actual spin structure of TbPdBi. So how authors knew the canted spin structure, or the AFM spin configuration of the grown crystals as extensively discussed in the manuscript? No ref also added regarding this

Response: We thank the reviewer for raising this important question. The magnetic structure of TbPdBi was determined by the neutron-diffraction experiments in a prior work by Pavlosiuk et al. [Physica B: Condensed Matter 536, 56 (2018)]. We are sorry for forgetting to cite this paper in the original manuscript. The neutron scattering experiment found its AFM state has the propagation vector of k = (1/2,1/2,1/2), which is identical to that of GdPtBi. In such an AFM state, the magnetic moments of Tb ions are aligned ferromagnetically within the (111) plane and antiferromagnetically between the (111) planes as shown in Fig. 3c in the manuscript. We have cited this paper in the revised manuscript (Ref. [46]). In general, antiparallel spins in AFM materials would be canted if an applied magnetic field is strong enough. Based on the measured magnetization shown in Fig. 1b, the polarized magnetization at 5 T is about 1/3 of the saturated magnetization above 15T, indicating that the canting angle of the magnetic moments of Tb is significantly larger near 5T where the anomalous Hall resistivity peaks below 10K.

3. From Fig.1a it is evident that the AHE peak value is increasing with temperature well beyond TN at least until the shown temperature of 20 K. So, it is not clear how far the AHE signal increases with temperature? (do you have data above 20K?

Response: We do not have data measured up to 30T beyond 20K. This is because our high field measurements were performed using the resistive magnet at the US National High Magnetic Lab facility and this system does not allow convenient field sweep measurements at high temperatures. If we heated the sample to high temperatures, it would take much longer time to cool down the sample to the base temperature for other measurements. With the limited magnet time available to us for this experiment in mind, we did not do measurements at temperatures above 20K. Nevertheless, we measured this sample to high temperatures in a PPMS with a 9T magnet. Although we conducted measurements only up to 9T, the AHE peak seems still observable at 30K and 50K but vanishes above 100K, see Fig. R2a below. Note that the field dependence of normal Hall resistivity at high temperatures significantly differs from that at low temperatures. As discussed in the manuscript, the normal Hall resistivity at low temperatures (<10K) exhibited a linear field dependence with a positive slope for fields above 15T (Fig. 1a in the manuscript), indicating that holes are the major carriers. However, at high temperatures, thermal excitations lead to the presence of excited electrons. That is, both electrons and holes contribute to transport such that the field dependence of normal Hall resistivity is not linear. The Hall resistivity data measured at 100 K and 200 K indeed show multi-band features. The data at 200K can be fitted quite well by the two-band model as shown by the dashed fitted curves in Fig. R2(a), while the fit for the 100K data show a clear deviation. The Hall resistivity data below 50K cannot be fitted at all with the two-band model. These results indicate that the AHE peak becomes weak and diminishes above 100K. The transport involving multiple band contributions at higher temperature is also evidenced by the temperature dependence of resistivity ρ_{xx} of TbPdBi shown in the supplementary materials (Fig. S1a) which exhibits a broad peak around 50K. The semiconducting-like behavior above 50K clearly shows that high temperature transport is dominated by excited charge carriers.

In order to further verify the above interpretation, we also measured another TbPdBi sample up to 18T and 100K using the same field and current configuration shown in Fig. 1a [i.e. I//(100) and B ⊥ (100)]. The data obtained on this sample (Fig. R2b) is consistent with the above interpretation. The two-band model fit is very good even at 100K for this sample but break down below 50K due to the presence of the AHE peak.

We have added these comments briefly under the supplementary materials (Note 1) and Fig. R2 to supplementary Figs. S2c&d.

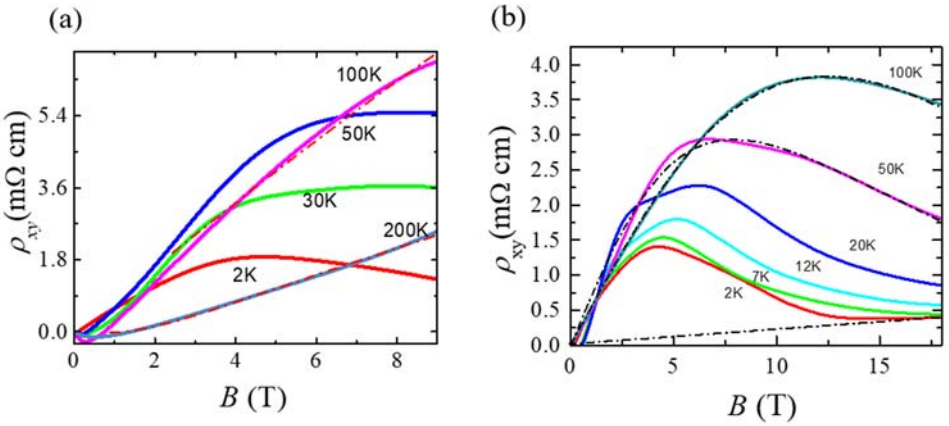

Fig. R2: (a) Hall resistivity ρ_{xy} measured up to 200K using PPMS for the TbPdBi sample used in this study. (b) Hall resistivity ρ_{xy} measured up to 100K and 18T for another TbPdBi sample.

Again from Fig. 2b, ρxx sharply decreases with increasing temperature. So, the ratio determining the Hall angle also should increase with temperature beyond 2%? So why the higher temperature Hall angles not shown in Fig.1c?

Response: As noted above, thermally excited carriers dominate transport at temperature above 50K, and the normal Hall resistivity ρ_{xy}^{N} exhibits nonlinear field dependence due to the contribution of multiple bands. As discussed above, our Hall resistivity data can be fitted using the two-band model, and the anomalous Hall resistivity diminishes at temperatures above 100K. Thus, the anomalous Hall angle should be zero above 100K. Even though a small anomalous Hall resistivity component remains between 20K and 100K, it is nearly impossible for us to separate it from the normal Hall contribution due to the multiple-band effects in the normal Hall contribution. This is the reason why we did not include high-temperature Hall angle data in Fig. 1c. Moreover, we see from our magnetic susceptibility (χ) data in supplementary Fig. S1b that 1/χ precisely follows the Curie-Weiss law above 100K, indicating absence of short-range magnetic order above 100 K. For these reasons, our Hall resistivity data above 100K is not expected to involve an anomalous Hall resistivity component, which is consistent with fact that the Hall resistivity data above 100 K can be fitted by the two-band model of the normal Hall contribution.

4. From Fig. 1b magnetization data, it is evident that the magnetization doesn't saturate above T_N. So thermal energy is too strong to polarize the spins. Then how the AHE signal can increase due to

spin polarization effect (spin canting, exchange induced band splitting etc.) with increasing temperature?

Response: We thank the referee for raising this insightful question. We agree with the referee that at temperatures above T_N, thermal energy is strong so that the magnetic polarization is weakened. Indeed, this is manifested in our isothermal magnetization data measured at 20 K (Fig. 1b in the main text). Although the AHE peaks at 10-20K (Fig. 1a) are seemingly higher than those at temperatures below T_N, there exist multiple band normal Hall contributions to this peak. As noted above, the normal Hall contribution due to thermal excitation leads to multiple band effects in Hall resistivity, which could result in a broad normal Hall resistivity peak overlapping with the AHE peak. The broad peaks seen at 30K and 50K (Fig. 2Ra) are most likely dominated by multiple band normal Hall contributions. As the referee indicated, the AHE peak should decrease as the temperature is increased above T_N due to the weakened exchange-induced band splitting. The increase of the ρ_{xy} peak above T_N should arise from normal Hall contributions from multiple bands. This interpretation is supported by the following observations. At temperatures below T_N (e.g. 1.7 K and 4.0 K), the AHE peak remains sharp and hardly changes with temperature; its normal Hall contribution can be described by a single band scenario, as manifested by the linear field dependence of ρ_{xy} above 15 T below T_N. However, when at temperatures well above T_N (i.e. 10 -20 K), the ρ_{xy} peak involves contributions not only from AHE but also from multiple-band normal Hall, which is manifested by the clear deviation from nonlinear field dependence of ρ_{xy} in the high-field limit. However, it is hard to separate the anomalous Hall resistivity from the multiple-band normal Hall contribution.

In our original manuscript, for the ρ_{xy} data above T_N (i.e. 7 K, 10K, 15K & 20K), we approximately treated the normal Hall contribution as a single-band normal Hall contribution and extracted the anomalous Hall resistivity by subtracting the linear normal Hall contribution from ρ_{xy}. The anomalous Hall resistivity obtained through this approach is somewhat overestimated since there are multiple-band normal Hall contributions to the peak of ρ_{xy} above T_N as discussed above. To avoid confusion, in the revised manuscript we have removed the anomalous Hall-angle data at 7K and 10 K from Fig. 1c, and also removed the anomalous Hall resistivity and conductivity at these temperatures from the supplementary Figs. S2a and 2b. We have also briefly added the preceding discussion under the supplementary Note 1 in the revised manuscript.

Besides, according to Fig. 2a/b, the -ve MR decreases more sharply with increasing temperature. But at 10 or 20 K, the increased thermal energy should induce more spin disorder. Then I am confused how the authors are claiming that the spin-scattering is the only/dominating origin for high AHE and negative MR

Response: This is a good question. The referee's understanding would be correct if the magnetic polarization (transition from an AFM state to a field-forced FM state) did not lead to an electronic transition. The temperature independence of both the transverse and longitudinal MR below 20K seen in TbPdBi implies that it involves a unique mechanism. Our DFT calculations indeed suggest it to be the case. As shown in Figs. 3e and 3f, the calculated electronic band structure of TbPdBi exhibits a topological phase transition from an AFM to a FM state. In the AFM state, it is a semimetal with band inversion in both the spin channels, and the bands crossing the Fermi level are hardly spin polarized.

In contrast, as the AFM state is driven to a FM state by magnetic fields above 15T, the system evolves into a half-topological semimetal state with a single-spin-channel band inversion; that is, the spin-down bands cross the Fermi level, while the spin-up bands are pushed away from the Fermi level. In other words, the AFM-to-FM transition leads to a half-topological semimetal (HTS) state with high spin polarization, which results in reduced spin scattering and thus produces a giant negative MR. At temperatures that are not far above T_N, (e.g. 10 K and 20 K), although the long-range AFM order is suppressed, a short-range AFM order can exist. This AFM order could also be polarized to an FM state under strong magnetic fields even though the net spin polarization would be reduced due to increased thermal excitations. This scenario is supported by the observation that the magnetization at 20 K exhibits a sublinear field dependence (Fig. 1b). Our observation of the temperature independence of MR below 20K suggests that the spin scattering in the HTS state is very weakly dependent on temperature once the system assumes the HTS.

Note that the spin polarization here refers to the band spin polarization, rather than the polarization of Tb^{3+} local moments driven by the magnetic field. If the AFM-to-FM transition did not cause an electronic structural transition and the giant negative MR purely originated from the suppression of magnetic scattering by the local moments of Tb^{3+}, the MR would be strongly temperature dependent. This is clearly not the case in our observations. We have now embedded the preceding discussion briefly in the revised manuscript on page 11.

5. Fig.S1 shows a peak in longitudinal resistivity around 50 K. What is the origin for that? Looks like it's independent from the magnetic behavior and can this have something to do with the anomalous transport properties of TbPdBi?

Response: Such a broad peak in the temperature dependence of resistivity is a common signature seen in Bi-based half-Heusler compounds RePtBi (Re = Gd, Nd,Tb) (Ref. [10,11,12] in the manuscript). This can be understood as follows: In semimetals with small Fermi pockets and in narrow-gap semiconductors, high-temperature transport is primarily governed by excited carriers, resulting in behavior resembling that of semiconductors. In contrast, at low temperatures, excited charge carriers are substantially suppressed, and transport is metallic dominated by the electrons/holes hosted by small Fermi pockets. We have added the preceding discussion in the revised manuscript.

6. Fig. 4e shows the theoretical calculation of the *x*-dependence of Hall conductivity and explains the effect of spin canting. But why the conductivity for xy, yz and zx are showing different behavior? In a cubic system x, y and z axes are equivalent directions. So why system shows such anisotropic behavior?

Response: We thank the reviewer for this insightful comment. Note first that the system transitions from AFM to FM when *x* increases from 0 to 1. The crucial preserved symmetry in AFM (FM) phase is the rotational symmetry C_3 about the [111] direction ($\bar{S}_4$ about the [100] direction). There is a cyclic relation x→y→z→x when C_3 is preserved. Therefore, the AHC obeys the relation of $\sigma_{xy} = \sigma_{yz} = \sigma_{zx}$. On the other hand, there is only a cyclic relation y→ z→ -y→ -z →y while x→-x is self-related if $\bar{S}_4$ is preserved. The AHC should, therefore, only follow the constraint $\sigma_{xy} = \sigma_{xz} = \sigma_{x-y} = -\sigma_{xy}$, so that $\sigma_{xy} = \sigma_{xz} = 0$. However, since $\sigma_{yz} = \sigma_{z-y} = -\sigma_{zy}$, σ_{yz} can be nonzero. As seen in Fig. 4e, when *x* varies from 0 to 1, $\sigma_{xy} = \sigma_{yz} = \sigma_{zx} = 0$ due to Berry curvature cancellation in the beginning and then σ_{yz} grows dramatically while σ_{xy} and σ_{zx} are close to zero. Because there are residual numerical errors and there are no preserved symmetries in the canted state, σ_{xy} and σ_{zx} are not

exactly zero in our calculations. We have now briefly added the preceding discussion to supplementary Note 4.

Response to Reviewer #2:

General Comment: The manuscript entitled "Surprisingly large anomalous Hall effect and giant negative magnetoresistance in half-topological semimetals" by Yanglin Zhu et al. report the giant AHA and giant negative magnetoresistance in half-Heusler TbPdBi single crystals. And they contribute the exotic transport properties to the half-topological state. In overall, the giant AHA and large AHC are interesting.

Response: We thank the reviewer for taking time to review our manuscript and finding work interesting.

However, the manuscript needs more explanation on some points.

Comment 1: The band structure and density of states around Fermi level change in the canted AFM state. Thus, the carrier concentration changes may also contribute to Hall resistance. Is there any way for the author to separate this contribution?

Response: The referee raised a good question. We agree with the referee that the band structure and the density of states near the Fermi level should change in the canted AFM state. As shown in Fig. 1b, TbPdBi undergoes an AFM-to-FM transition around 15T below T_N. Our DFT calculations indicate that this magnetic transition is accompanied by an electronic structure transition. As shown in Figs. 3e and 3f, the AFM state is a semimetal with band inversion in both the spin channels, and the bands crossing the Fermi level are hardly spin polarized. In contrast, as the AFM state is driven to a FM state by magnetic fields above 15T, the system evolves into a half-topological semimetal state with a single-spin-channel band inversion; that is, the spin-down bands cross the Fermi level, while the spin-up bands are pushed away from the Fermi level. In other words, the AFM-to-FM transition leads to a half-topological semimetal (HTS) with high spin polarization. Such an electronic structure transition driven by a magnetic transition can be expected to lead to changes in carrier concentration.

In the FM phase above 15T for $T < T_N$, the Hall resistivity ρ_{xy} exhibits a linear field dependence (Fig. 1a), which can be attributed to normal Hall contributions. From the slope of ρ_{xy} above 15T in the FM phase at 4K, the carrier density is estimated to be ~ 5.19×10^{19} cm^{-3}. However, in the canted AFM state below 15T, the anomalous Hall resistivity is mixed with the normal Hall resistivity and varies with magnetic field. Since there is an electronic structure transition involved in the AFM-to-FM transition, we expect the normal Hall contribution to change across the magnetic transition. Although we can separate the normal Hall resistivity ρ_{xy}^N from the anomalous Hall resistivity $\Delta\rho_{xy}^{AH}$ for the FM phase, where ρ_{xy}^N is linearly proportional to the field and $\Delta\rho_{xy}^{AH}$ remains constant, we cannot separate ρ_{xy}^N from $\Delta\rho_{xy}^{AH}$ for the canted AFM phase since $\Delta\rho_{xy}^{AH}$ varies with magnetic field. In our analyses of $\Delta\rho_{xy}^{AH}$ (supplementary Fig. S2a), we approximately assumed that the normal Hall resistivity ρ_{xy}^N in the canted AFM state follows the same linear field dependence as the FM phase (dashed line in Fig. 1a). From the calculated AFM (Fig. 3f) as well as FM (Fig. 3e) band structures, the carrier density in the AFM phase is expected to be lower than that in the FM phase, since the FM phase hosts larger

Fermi pockets. This implies that our extracted $\Delta\rho_{xy}^{AH}$ is slightly underestimated so that the anomalous Hall angle of TbPdBi shown in Fig. 1d is also slightly underestimated. We have briefly added the preceding discussion to the supplementary Note 2.

Comment 3: You pointed out that the calculated AHC is an order of magnitude smaller than the experimental value. Is it possible that the extrinsic mechanism dominates the AHC?

Response: We appreciate the referee raising this insightful question. Note that intrinsic anomalous Hall conductivity (AHC) can be much larger than extrinsic AHC in some cases. As far as we know, the anomalous Hall angles due to extrinsic AHE usually fall into the range of 0.1-1% [Wang et al., Nanomaterials 11, 854 (2021)], which are two orders of magnitude smaller than in TbPdBi. Further, the intrinsic vs extrinsic origin of AHE can also be distinguished by the scaling behavior of the AHE. The intrinsic anomalous Hall conductivity σ_{yx}^{AHE} is independent of the longitudinal conductivity σ_{xx} for moderately clean systems, and it is proportional to $\sigma_{xx}^{1.6}$ for multiband disordered metals (Branford et al., PRL 102, 227201(09)). In contrast, for the extrinsic AHC, σ_{yx}^{AHE} in the clean region is proportional to σ_{xx}. To determine whether the AHE of TbPdBi is dominated by intrinsic or extrinsic origin, we plotted the anomalous Hall conductivity σ_{yx}^{AHE}(obtained via tensor conversion from the anomalous Hall resistivity and longitudinal Hall resistivity) as a function of the longitudinal conductivity σ_{xx} on a semi-log scale (Fig. R3). The data in Fig. R3 can be fitted by $\sigma_{xy}^{AHE} \propto \sigma_{xx}^{\alpha}$ with $\alpha = 0.6$. The σ_{xx} of TbPdBi is within the range of 600-750 Ω^{-1}cm^{-1}, indicating that our sample is near the boundary between the disordered metal and the moderately clean regimes. Thus, the scaling behavior of $\sigma_{xy}^{AHE} \propto \sigma_{xx}^{0.6}$ seen in TbPdBi can be attributed to be of intrinsic origin. Therefore, even if an extrinsic AHE is present in TbPdBi, it is not dominant. We have added the preceding discussion briefly in the supplementary Note 3.

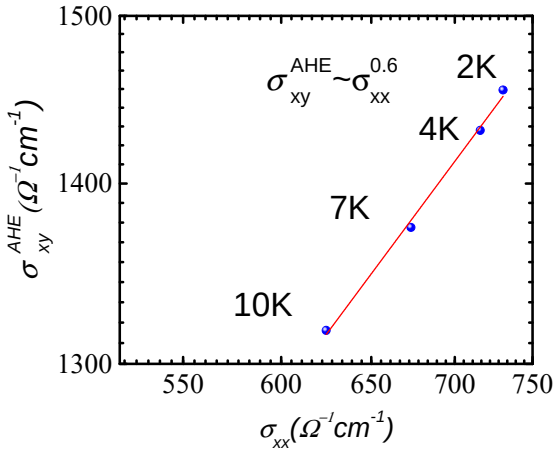

Fig. R3: Anomalous Hall conductivity σ_{yx}^{AHE}as a function of the longitudinal conductivity $\sigma_{xx}$for TbPdBi.

Comment 4: The authors attribute the large negative MR effect to the half-topological state. However, specific theoretical analysis is lacking here. The topological insulator MnBi2Te4 also exhibits the half-topological semimetal state under magnetic field. Why does this alloy not show a large negative MR?

Response: As shown in Fig. 3e and 3f in the main text, our calculated electronic band structure of TbPdBi shows a topological phase transition from the AFM to the FM state. In the AFM state, it is a semimetal with band inversion in both the spin channels, and the bands crossing the Fermi level are hardly spin polarized (Fig. 3f). In contrast, as the AFM state is driven to a FM state by the magnetic field, the system evolves into a half-topological semimetal state with a single-spin-channel band inversion (Fig. 3e); that is, the spin-down bands cross the Fermi level, while the spin-up bands are pushed away from the Fermi level. In other words, the AFM-to-FM transition leads to a half topological semimetal (HTS) state with high spin polarization, which results in reduced spin scattering, and thus a giant negative MR above 15T. We have added the preceding discussion briefly in the revised manuscript.

Regarding $MnBi_2Te_4$, we noted a reference which claims that $MnBi_2Te_4$ is a half-magnetic topological insulator (TI) [Lu et al., PRX 11, 011039 (2021)], which is quite different from our half-topological semimetal state. In the half-magnetic TI state, the magnetization exists only on the $MnBi_2Te_4$ terminated surface and opens a massive Dirac gap, while the opposite surface terminated at Bi_2Te_3 remains nonmagnetic and thus gapless. [Here the term "half-magnetic" refers to the presence of magnetism on the $MnBi_2Te_4$ termination layer, but not on the Bi_2Te_3 termination layer.] The bulk bands maintain non-trivial band topology for both spin up and spin down channels. As such, this electronic state cannot be called a half-semimetal state. In contrast, our half-topological semimetal state in the field-driven FM phase of TbPdBi maintains a non-trivial band topology only in the spin-down channel, while the spin-up channel becomes trivial and opens a gap.

We hope that we have satisfactorily addressed all the questions raised by the reviewers, and they will find our revised manuscript suitable for publication.

Reviewers' comments:

Reviewer #1 (Remarks to the Author):

Authors have satisfactorily addressed to all my concerns, except the last point, regarding the anisotropic Hall conductivity value illustrated in Fig. 4. Whatever is authors' argument that the anisotropic effect is due to spin canting etc., but the general crystal structure is unchanged. The half-Heusler TbPdBi compound having a cubic structure, all the x, y and z axes are equivalent and must have symmetric properties. Even if we agree that the Sigma_yz is having significantly high value compare to the other direction, how one can experimentally find out the y-z direction independent of the origin or selected coordinate system? Therefore authors must resolve this issue in their theoretical calculation, so that it doesn't violate the general norms of basic crystallography.

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Response: We sincerely thank the reviewer for reading our revised manuscript and finding our response satisfactory.

Regarding the technical question of anisotropic Hall conductivity calculations, the Hall conductivity depicted in Figure 4 is the intrinsic anomalous Hall conductivity (AHC). In contrast to extrinsic anomalous Hall conductivity, the intrinsic AHC solely depends on the band structure, as expressed by the following equation:

$$\sigma_{ij} = -e^2\hbar \int_{Bz} \frac{d^3k}{8\pi^3} \Omega_{ij}(k)$$

Here, $\Omega_{ij}(k)$ represents the Brillouin zone (BZ) integral of the k-dependent Berry curvature tensor Ω. **The key point is that the Berry curvature tensor Ω exhibits the spin-symmetry and NOT the lattice symmetry of the crystal lattice in magnetic materials**. The magnetic lattice of TbPdBi, of course, thus possesses symmetry that is lower than the cubic symmetry of the lattice. This point and the dependence of the AHC on the magnetic state has been discussed extensively in the literature [*A. A. Hirsch and Y. Weissman, Phys. Lett. A 44, 239 (1973)*; *N. V. Volkenshtein, et al., Sov. Phys. JETP 11, 48 (1960)*; *Hongbin Zhang et al., Physical Review B 84, 024401 (2011)*]. For example, first-principles calculations show that the intrinsic AHC of hcp Co could decrease by a factor of 4 as the magnetization M_s is tilled off the easy axis (c-axis) [*E. Roman, Y. Mokrousov, and I. Souza, Phys. Rev. Lett. 103, 097203 (2009)*].

In our work, TbPdBi initially displays the antiferromagnetic (AFM) ground state, which is indeed found to preserve the C3 rotational symmetry about the [111] direction and obeys $\sigma_{xy} = \sigma_{yz} = \sigma_{zx} = 0$ due to Berry curvature cancellation. Note that for the [100] direction, the preserved symmetry is $\bar{S}_4$, and the resulting AHC conforms to the relationships: $\sigma_{xy} = \sigma_{xz} = \sigma_{x-y} = -\sigma_{xy}$, implying that $\sigma_{xy} = \sigma_{xz} = 0$. Also, $\sigma_{yz} = \sigma_{z-y} = -\sigma_{zy}$, which suggests that σ_{yz} could be nonzero. However, initial AFM state where the magnetization is zero (x =0 of Figure 4), $\sigma_{yz} = 0$.

After the application of an external magnetic field along [100] direction, the system transitions into a spin-canted state (0<x<1in Figure 4) in which no symmetries are preserved, leading to the emergence of the net Berry curvature Ω_{yz}, and consequently, σ_{yz} exhibits a significant increase, as depicted in Figure 4.

From an experimental perspective, the referee correctly points out that we would not be able to distinguish between the equivalent *a*, *b* and *c* axis. Note that we initially denote the field direction as the [100] direction (*x* direction in our theoretical modeling), resulting in the observed magnetization M_{100}, which yields a nonzero computed Hall conductivity (σ_{yz}). However, if we applied the initial field along [001] (*z* direction in theoretical calculations), the nonzero AHC term would be σ_{xy}.

We have briefly incorporated the preceding discussion into supplementary Note 4 of the revised manuscript.

REVIEWERS' COMMENTS:

Reviewer #1 (Remarks to the Author):

Authors have satisfactorily addressed all my previous concerns. I have no further comments on this.