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Giant anomalous Nernst signal in the antiferromagnet YbMnBi₂

Yu Pan¹✉, Congcong Le¹, Bin He¹, Sarah J. Watzman^{1,2,3}, Mengyu Yao¹, Johannes Gooth¹, Joseph P. Heremans^{1,2,4,5}, Yan Sun¹ and Claudia Felser¹✉

A large anomalous Nernst effect (ANE) is crucial for thermoelectric energy conversion applications because the associated unique transverse geometry facilitates module fabrication. Topological ferromagnets with large Berry curvatures show large ANEs; however, they face drawbacks such as strong magnetic disturbances and low mobility due to high magnetization. Herein, we demonstrate that YbMnBi₂, a canted antiferromagnet, has a large ANE conductivity of $-10 \text{ A m}^{-1} \text{ K}^{-1}$ that surpasses large values observed in other ferromagnets ($3\text{--}5 \text{ A m}^{-1} \text{ K}^{-1}$). The canted spin structure of Mn guarantees a non-zero Berry curvature, but generates only a weak magnetization three orders of magnitude lower than that of general ferromagnets. The heavy Bi with a large spin-orbit coupling enables a large ANE and low thermal conductivity, whereas its highly dispersive p_{xy} orbitals ensure low resistivity. The high anomalous transverse thermoelectric performance and extremely small magnetization make YbMnBi₂ an excellent candidate for transverse thermoelectrics.

Topological electronic structures lay the foundation for new functionalities and are crucial for various applications, including thermoelectric energy conversion^{1–3}. In the past few decades, many good longitudinal thermoelectric materials have been demonstrated to be topological insulators^{4,5}. Recently, with the emergence of topological semimetals, the anomalous Nernst effect (ANE) has attracted increasing attention for transverse thermoelectric applications^{2,3,6–10}. Owing to the large Berry curvature near the Fermi energy, large-ANE thermopowers have been achieved in a few topological ferromagnets^{2,3,6–12}, which show great potential for stable and precise temperature control, particularly in micro- or nanosized devices^{13,14}. For example, Co₃Sn₂S₂ (refs. 7,8), Co₂MnGa (refs. 3,9) and Fe₃Ga (ref. 2) showed ANE thermopowers of $3\text{--}8 \mu\text{V K}^{-1}$ and ANE conductivities of $0.5\text{--}5 \text{ A m}^{-1} \text{ K}^{-1}$, and recently UCo_{0.8}Ru_{0.2}Al (ref. 15) was reported to have a colossal ANE thermopower of $23 \mu\text{V K}^{-1}$ and a large ANE conductivity of $15 \text{ A m}^{-1} \text{ K}^{-1}$. So far, large ANEs have been reported in only a few topological ferromagnets, and topological noncollinear antiferromagnets have rarely been studied, except for Mn₂X (X = Sn and Ge)^{6,10,12}. The search for large ANEs in noncollinear topological antiferromagnets will yield advantages by broadening the material platform for transverse thermoelectrics, as well as revealing novel topological phenomena.

To use the ANE for practical applications, low resistivity and thermal conductivity are also required. Moreover, at the device level, low magnetization and a small inherent stray field are important to eliminate magnetic disturbances and stabilize the remanent magnetization in the in-plane direction if using in a thin-film case¹⁶. From these viewpoints, ANE efficiency is coupled with various parameters, similar to the longitudinal Seebeck effect¹⁷, and additional magnetization makes the coupling more complicated. For ferromagnets in general, although strong ferromagnetism breaks time-reversal symmetry and offers a large Berry curvature, it also has some drawbacks. With local moment and itinerant electrons (usually due to the heavy *d* or even *f* bands) at the Fermi energy (E_F),

these ferromagnets mostly have relatively low mobility and high resistivity. In addition, the high magnetization and strong inherent stray field of ferromagnets introduce a strong magnetic disturbance, which causes interference with other electronic devices in practical applications.

Herein, considering the challenges outlined above, we highlight the importance of searching for materials with broken time-reversal symmetry and *p* bands or *p*–*d* hybridization near E_F . YbMnBi₂, as a canted antiferromagnet, can simultaneously realize broken time-reversal symmetry and relatively low resistivity with light band conduction. The canted spin structure at Mn sites breaks time-reversal symmetry. Meanwhile, low resistivity can be achieved owing to the sharp dispersion of the p_{xy} orbitals of Bi. Moreover, the large spin–orbit coupling (SOC) from Bi is critical for band topology, transverse transport response and low thermal conductivity. Furthermore, the YbMnBi₂ canted antiferromagnet has much smaller magnetization and inherent stray fields than other ferromagnets. All of these features demonstrate that YbMnBi₂ could provide a new material platform beyond ferromagnets for transverse thermoelectric applications.

Canted antiferromagnets for ANE thermoelectric applications

A Nernst device can greatly simplify module fabrication via its unique transverse geometry: the device can be made simply from one material, rather than needing both polarities of charge carriers in separate materials, as is required of Seebeck modules. As schematically shown in Fig. 1a, longitudinal Seebeck thermoelectric devices require coupled *p*- and *n*-type legs and assembled pairs^{17,18}. In contrast, the Nernst device (Fig. 1b) offers various advantages that simplify module assembly. First, complex electrical connections and associated electrical resistances are eliminated because it requires only one material. Second, the voltage in Nernst devices can be probed in an isothermal plane, and the electrodes can be

¹Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. ²Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, USA. ³Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, OH, USA. ⁴Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA. ⁵Department of Physics, The Ohio State University, Columbus, OH, USA. ✉e-mail: Yu.Pan@cpfs.mpg.de; Claudia.Felser@cpfs.mpg.de

Fig. 1 | Illustration of thermoelectric devices and band dispersion.

a, b, Schematics of thermoelectric devices based on the Seebeck effect (**a**) and Nernst effect (**b**). The Nernst device needs only one material and eliminates the complex electrical connections required in the Seebeck device, especially at the hot side. **B**, magnetic field; **E**, electrical field; ∇T , temperature gradient. **c**, Schematics of the band structure near E_F for canted YbMnBi₂ (left) and general ferromagnets (right). YbMnBi₂ shows a much sharper band dispersion and a higher mobility than general ferromagnets.

constructed at only the isothermal cold end; hence, such devices do not require contacts that are stable at high temperatures. Third, the output of a Nernst device scales extrinsically with the device size: manufacturing longer and thicker devices can increase the voltage output and temperature gradient, respectively. Increasing the size in either dimension would increase the associated potential drop.

YbMnBi₂ outshines common ferromagnets for applications as a Nernst device in two ways: high mobility and low magnetization. First, as schematically shown in Fig. 1c, the bands of YbMnBi₂ at E_F are very light in the *ab* plane, formed by the hybridization of *p* and *d* orbitals and thus guaranteeing a high mobility; they are usually heavy *d* or *f* orbitals for general ferromagnets. Second, the ferromagnetism originating from the canted spin structure of Mn is extremely weak. These two advantages are useful for thermoelectric applications owing to the low resistivity at the material level and small magnetic disturbance at the device level.

The search for canted antiferromagnets

We have reviewed the magnetic topological materials identified recently by high-throughput calculations¹⁹. To introduce a canted spin structure, we examined the manganese pnictides $RMnPn_2$, where *R* is a rare- or alkaline-earth metal, and *Pn* is a pnictide (*Pn*=P, As, Sb or Bi). A few canted manganese pnictides—such as SrMnSb₂ (ref. 20), YbMnBi₂ (ref. 21) and Ca_{1-x}Na_xMnBi₂ (ref. 22)—are reported to be magnetic topological materials with a canted spin structure; they are therefore able to hold a non-zero Berry curvature^{23,24}. Moreover, the bands contributed by pnictides are highly dispersive²⁵, which can provide a low resistivity, especially compared with that of ferromagnets.

Given that Yb is relatively stable, Mn has a canted spin structure and Bi can induce large SOC, YbMnBi₂ was investigated. As shown in Fig. 2a, YbMnBi₂ crystallizes in a *P4/nmm* structure with two types of Bi: Bi 1 is bonded with Mn and Bi 2 forms an interlayer. The spin of Mn is antiferromagnetic along the *c* axis but canted in the *ab* plane. The Néel temperature was reported to be ~290 K (ref. 26), which is very close to that shown in Fig. 2b (~283 K), as

also indicated by the turning point in the temperature-dependent resistivity (Supplementary Fig. 1). A clear ferromagnetic transition is observed, as shown in Fig. 2b. The sharp increase in magnetization upon cooling observed in the field cooling curves indicates a spin canting temperature of ~250 K. The field dependence of the magnetization is shown in Supplementary Fig. 2. Below 250 K, the saturation magnetization value is $\sim 1.25 \times 10^{-3} \mu_B$ per formula unit (f.u.) in the *ab* plane, suggesting a very small canting angle (θ) of approximately 0.018°. Although the spin canting is very weak and may even be inaccessible in experiments requiring a strong signal^{26,27}, it plays a crucial role in the anomalous thermal/electrical transport by inducing a non-zero Berry curvature.

Owing to the canted spin structure, YbMnBi₂ has unique topological properties. When the SOC is ignored, a nodal line protected by glide-plane symmetry exists in the Brillouin zone because of the band inversion of the $p_{x/y}$ orbitals of Bi 2, as shown by the yellow line in Fig. 2c. When SOC is included, the nodal line is gapped, resulting in two pairs of Weyl nodes and a non-zero Berry curvature. The strength of the Berry curvature depends on E_F and reaches its maximum when E_F is near the Weyl nodes. As schematically illustrated in Fig. 2d, the shift in E_F would probe the strength of the Berry curvature, therefore leading to the varying strength of the anomalous Hall effect (AHE) conductivity (σ_{AHE}) and the ANE conductivity (α_{ANE})^{28–30}. In this case, it is essential to optimize E_F to observe a large σ_{AHE} or α_{ANE} , which are usually related to the quality of the single crystal.

According to theory, under a spin canting direction of (110)²¹, the magnetic point group of YbMnBi₂ becomes $m'm2'$, and only transverse transport signals in the *ac/bc* and *ca/cb* configurations can be observed owing to mirror symmetry³¹. Taking the *cb* configuration as an example, this implies that the transverse signal is measured along the *c* axis while a temperature gradient is applied along the *b* axis and a magnetic field along the *a* axis. Experimental results are highly consistent with theoretical predictions: both the ANE and AHE are observed in the *bc* and *cb* configurations, but not in the *ab* plane (Supplementary Figs. 3 and 4). The non-zero Berry curvature is thus believed to be an essential cause of the ANE/AHE.

Anomalous Nernst thermopower and anomalous Hall resistivity

The ANE thermopower (S_{ANE}) and AHE resistivity (ρ_{AHE}) (with Gerlach's sign convention, as illustrated in Supplementary Fig. 5) in the *cb* and *bc* configurations show qualitatively identical behaviour but different values. S_{ANE} and ρ_{AHE} in both the *cb* (Fig. 3a,b) and *bc* (Fig. 3c,d) configurations saturate at ~1 T, which is relatively small, comparable to the saturation field of Co₂MnGa^{3,9}, and much lower than Fe₃Ga (~2 T)². S_{ANE} first increases and then decreases with heating, showing a peak at ~160 K (Fig. 3e); in contrast, ρ_{AHE} increases up to ~200 K (Fig. 3f). The maximum S_{ANE} values are ~6 $\mu V K^{-1}$ and ~3 $\mu V K^{-1}$ at 160 K in the *cb* and *bc* configurations, respectively, which is relatively large, especially for an antiferromagnet. This is remarkable, as the largest ANE signals reported so far in the antiferromagnets observed were ~0.5 $\mu V K^{-1}$ in Mn₃Sn (refs. 6,12) and ~1.2 $\mu V K^{-1}$ in Mn₃Ge (refs. 10,32).

Intrinsic and extrinsic effects on ANE/AHE conductivity

To quantitatively understand the origin of the ANE and AHE in YbMnBi₂, α_{ANE} and σ_{AHE} were analysed with first-principles calculations assuming $\theta = 10^\circ$. As α_{ANE} is an energy derivative of σ_{AHE} (ref. 24), we first investigated σ_{AHE} , followed by α_{ANE} . Two characteristics of the band structure are essential to understand the AHE and ANE. First, the hole pocket near the Γ point, which stems from the hybridization of the p_z orbitals of Bi 1 and the *d* orbitals of Mn, should be far below E_F if θ is zero (Supplementary Fig. 6), but above E_F if θ is non-zero (Fig. 4a). The hole pocket near the Γ point can generate a negative Berry curvature³¹, which enhances

Fig. 2 | Canted spin structure and non-zero Berry curvature. **a**, Crystal structure of YbMnBi_2 . The spin structure is canted at Mn sites, contributing to weak ferromagnetism in the ab plane. **b**, Temperature dependence of magnetization M in the ab plane (magnetic field B parallel to ab plane, $B//ab$) and c axis (B parallel to c axis, $B//c$). Red and magenta curves denote field cooling (FC) under 1 T, whereas blue and green curves denote zero-field cooling (ZFC). The field for both FC and ZFC measurements is 100 Oe. A sharp increase in FC curves upon cooling indicates a spin canting temperature (T_{sc}) of ~ 250 K; the Néel temperature (T_N) is ~ 283 K. An extremely small θ of $\sim 0.018^\circ$ is resolved from the magnetization curves. **c**, The nodal line (yellow) formed near E_F in the $k_x k_y$ plane is shown (k_x and k_y are the x and y direction in the reciprocal space). The conduction and valence bands are shown in red and blue, respectively. **d**, Schematic of the E_F dependence of the Berry curvature (left), σ_{AHE} (middle) and α_{ANE} (right). The strength of the Berry curvature depends on E_F , resulting in the maximum σ_{AHE} when E_F is near the Weyl nodes, whereas the maximum α_{ANE} lies at a different energy.

the total Berry curvature as the electron pockets (along Γ -M, Γ -X and Γ -Y, originating from the $p_{x/y}$ orbitals of Bi 2) also generate a negative Berry curvature (Fig. 4b). As shown in Fig. 4c, the Fermi surface at the Γ point is observed in our crystal by angle-resolved photoemission spectroscopy (ARPES), which is highly important as it demonstrates the non-zero θ and additional negative Berry curvature from the Γ band. The larger θ is, the more contribution to band conduction generated at the Γ point, as illustrated on the right side of Fig. 4c and Supplementary Fig. 7. Figure 4d plots $|\sigma_{\text{AHE}}|$ as a function of θ ; the calculated $|\sigma_{\text{AHE}}|$ has a nearly linear dependence on θ from 8° to 16° . As σ_{AHE} is 0 if $\theta = 0^\circ$, we extrapolated σ_{AHE} to 0 in the simplest way (with a linear dotted line), which therefore allowed us to roughly assess σ_{AHE} at extremely small θ .

Second, as the electronic bands of YbMnBi_2 are strongly anisotropic and highly dispersive in the ab plane (Supplementary Fig. 8), there can be a large shift in E_F . In fact, such a shift was observed in the Hall resistivity (Supplementary Fig. 4c): a transition from n-type to p-type was observed from 50 to 100 K. Such high anisotropy was also observed in the Seebeck coefficient (Supplementary Fig. 9), where positive and negative values coexisted in different crystallographic directions—this may indicate that YbMnBi_2 is a goniopolar material³³. This strong anisotropy makes it challenging to determine the actual E_F in specific directions as it can vary in different directions. On the basis of the analysis above, we attained a better understanding of $|\sigma_{\text{AHE}}|$ and $|\alpha_{\text{ANE}}|$.

As shown in Fig. 4e, the maximum experimental $|\sigma_{\text{AHE}}|$ can be matched with the theoretically predicted result with a very small θ (as illustrated by the point indicated with green lines in Fig. 4d). The decreasing trend above ~ 150 K can be attributed to the temperature disturbance of the spin structure; however, the increasing trend below 150 K is atypical. $|\alpha_{\text{ANE}}|$ also shows an unusual decreasing trend, as shown in Fig. 4f. In addition, anisotropic behaviours are observed in σ_{AHE} and α_{ANE} . Akgoz and Saunders^{34,35} combined the reciprocity relations with the crystal symmetries to derive the allowed symmetry operations in various point groups. With the magnetic point group of YbMnBi_2 being $m'm2'$, one would expect that the Hall resistivity $\rho_{bc}(H_a) = -\rho_{cb}(-H_a)$ (here, ρ_{bc} and ρ_{cb} are the Hall resistivity in bc and cb , respectively, and H_a is the external field along the a axis)³⁴ and the same relation would be expected to hold for the conductivity tensors. The fact that this is not observed in Fig. 4e points to the absence of time-reversal symmetry and the anomalous origin of the Hall conductivities. For the thermoelectric conductivity tensor, the observation that $S_{bc}(H_a) \neq -S_{cb}(-H_a)$ (Fig. 3e) and $\alpha_{bc}(H_a) \neq -\alpha_{cb}(-H_a)$ (Fig. 4f) is allowed³⁵. Most importantly, a maximum $|\alpha_{\text{ANE}}|$ of $10 \text{ A m}^{-1} \text{ K}^{-1}$ was achieved in the bc configuration, which is much higher than those of most of the ferromagnets, including $\text{Co}_3\text{Sn}_2\text{S}_2$ (ref. 7), Co_2MnGa (ref. 9), Fe_3Ga (ref. 2) and SmCo_5 (ref. 36; the record value for which is $\sim 5 \text{ A m}^{-1} \text{ K}^{-1}$) and one order of magnitude higher than those of the antiferromagnets Mn_3X ($\text{X} = \text{Sn}$ (refs. 6,12) and Ge (refs. 10,32)).

Fig. 3 | ANE thermopower and AHE resistivity. a–d, The magnetic field dependence of S_{ANE} (**a,c**) and ρ_{AHE} (**b,d**) in cb ($V//c$) for **a** and **b**, and bc ($V//b$) for **c** and **d** for the temperatures indicated. Herein, cb indicates the measurement of the Nernst/Hall voltage along the c axis and application of the temperature gradient along the b axis, and vice versa for bc ; the magnetic field B is always along the a axis. The configuration of B , $\nabla T/I$ and V is schematically shown in the insets. I , current; V , voltage. **e,f**, The temperature dependence of the absolute values of S_{ANE} (**e**) and ρ_{AHE} (**f**), respectively, is shown at $B = 1$ T from 40 to 250 K. Directions of B , $\nabla T/I$ and V are parallel to the a , b and c axis, respectively, for cb and bc , as indicated by the notation in the figure.

There could be extrinsic contributions to such a large α_{ANE} in addition to the Berry curvature, particularly considering the following three aspects. First, there is a mismatch between the experimental results and those from first-principles predictions. The calculated $|\alpha_{ANE}|$ is much lower than the experimental α_{bc} , even when E_F was optimized (Supplementary Fig. 10). The negative temperature dependence of $|\alpha_{ANE}|$ is similar to that recently been observed in MnBi, which was attributed to an extrinsic magnon-drag effect and could account for the deviation in temperature dependence between experiment and theory³⁷. Second, anisotropic behaviour was observed in α_{ANE} ; that is, $\alpha_{bc} \neq -\alpha_{cb}$. In principle, from density functional theory, $\alpha_{bc}^{intrinsic} = -\alpha_{cb}^{intrinsic}$ only if it solely originated from the Berry curvature, as determined by the Berry phase of the wavefunction, $\mathcal{Q}_{ij}(\mathbf{k}) = -\mathcal{Q}_{ji}(\mathbf{k})$. Third, a large violation of the ratio of

$|\alpha_{bc}/\sigma_{bc}|$ from an empirical value of k_B/e (where k_B is the Boltzmann constant) was observed (Supplementary Fig. 11). As recently argued by Ding et al. and Xu et al., the ratio of $|\alpha_{ANE}/\sigma_{ANE}|$ saturates to $\sim k_B/e$ at 300 K if both originate from intrinsic Berry curvature^{8,38}.

In fact, extrinsic contributions are possible in real crystals owing to the unavoidable presence of scattering—particularly for systems with large SOC, which is the case for YbMnBi₂. The large SOC induces an additional skew force on the spin-polarized charge carriers^{39,40}. Previous materials with large ANEs, including Co₃Sn₂S₂⁷, Co₂MnGa⁹, Fe₃Ga² and Mn₃X ($X = \text{Sn}$ and Ge)^{6,10,12,32}, have small SOC without heavy elements, which is not the case here. Very recently, Papaj and Fu⁴¹ indicated that extrinsic contributions can be dramatic, and even potentially dominant over Berry curvature. To accurately describe α_{ANE} , vast improvements to current modelling

Fig. 4 | Theoretical analysis of ANE and AHE conductivity. **a, b**, Band structure of YbMnBi₂ (**a**) (in which the different coloured lines denote the contribution from different orbitals from Mn and Bi elements) and Berry curvature distribution (**b**) in the Brillouin zone calculated from first principles by assuming $\theta = 10^\circ$. The total Berry curvature contribution from the electron pockets is negative. With a larger spin θ , the d orbitals of Mn join the conduction, and an additional negative Berry curvature is generated at the Γ point. **c**, Left: ARPES intensity at E_F as a function of the ab plane wavevectors (k_x and k_y) measured with 55 eV photons at $T = 19$ K. The ARPES intensity is integrated over the energy range of +10 meV to -10 meV with respect to E_F . The inset shows two pairs of Weyl nodes. Right: the calculated band variation at the Γ point with increasing θ . **d**, Calculated $|\sigma_{\text{AHE}}|$ as a function of θ . The solid line shows the calculated results, and the dashed line shows a linear extrapolation. **e, f**, Experimental results for the temperature dependence of $|\sigma_{\text{AHE}}|$ (**e**) and $|\alpha_{\text{ANE}}|$ (**f**) in cb ($V//c$) and bc ($V//b$). Calculated $|\alpha_{\text{ANE}}|$ values at different E_F are shown by the dashed lines in **f**.

techniques, beyond the simple single band models, are necessary. Such improvements include, but are not limited to, the modelling of band anisotropy, deviations from a linear band dispersion and interactions of point defects with electrons⁴¹. The strong band anisotropy in YbMnBi₂ has rarely been observed in other materials with large ANEs. We highlight that the strong anisotropy in the Fermi surface of YbMnBi₂ plays a critical role in achieving large α_{ANE} in the bc configuration and not in the cb configuration. The electron pockets are highly dispersive in the ab plane but have nearly no dispersion along the c axis, leading to a considerable difference in the extrinsic scattering effects on charge carriers between the bc and cb configurations. The extremely high σ_{bb} (which is ~ 35 times higher than σ_{cc} at 80 K), along with asymmetric skew scattering rates, results in large

α_{ANE} in only the bc configuration. Future investigations are warranted to explore both the intrinsic (for example, by developing a detailed distribution of the Berry curvature in the Brillouin zone) and extrinsic (for example, by measuring the strength of the skew scattering and side jump related to the SOC) contributions to the large α_{ANE} in more detail.

Beyond the ANE

In addition to the large ANE signals, YbMnBi₂ presents extremely small magnetization M , which can reduce the interaction of the magnetic field with surrounding electronic devices during practical applications. Figure 5a compares $|\alpha_{\text{ANE}}|/M$, $|S_{\text{ANE}}|/M$ and M of YbMnBi₂ with those of other compounds with large S_{ANE} —namely,

Fig. 5 | Thermoelectric performance comparison. **a**, Comparison of the absolute values of $|\alpha_{ANE}|/M$, $|S_{ANE}|/M$ and M of YbMnBi₂ in the *bc* configuration (160 K) with those of other compounds with large ANE thermopowers—namely, the ferromagnets Fe₃Ga (300 K)², Co₂MnGa (300 K)³⁹, Co₃Sn₂S₂ (80 K)⁷, UCo_{0.8}Ru_{0.2}Al (40 K)¹⁵, MnBi (80 K)³⁷ and Ga_{1-x}Mn_xAs (10 K)⁴², and the chiral antiferromagnets Mn₃Sn (300 K)^{6,12} and Mn₃Ge (300 K)^{10,32}. Antiferromagnets are marked as AFM, and other materials are all ferromagnets. **b**, The temperature dependence of zT_{ANE} values for YbMnBi₂ in the *bc* configuration compared with those of other compounds with large ANE thermopowers.

the ferromagnets Fe₃Ga (ref.²), Co₂MnGa (refs.^{3,9}), Co₃Sn₂S₂ (ref.⁷), UCo_{0.8}Ru_{0.2}Al (ref.¹⁵), MnBi (ref.³⁷) and Ga_{1-x}Mn_xAs (ref.⁴²) and the chiral antiferromagnets Mn₃Sn (refs.^{6,12}) and Mn₃Ge (refs.^{10,32}). The noncollinear antiferromagnets, especially YbMnBi₂, clearly surpass all of the ferromagnets in terms of $|\alpha_{ANE}|/M$ and $|S_{ANE}|/M$, demonstrating that canted antiferromagnets, even with extremely low magnetization, can display a large ANE that competes with the best ferromagnets. For practical applications, using permanent magnets (with which fields of 0.3 T are common, and 1 T is possible with a careful choice of materials) is reasonable for materials with no remanent magnetization, such as YbMnBi₂. Further exploration of the zero-field ANEs of polycrystals and/or thin films would be of interest for future devices.

In addition to the large ANE signals (owing to the anisotropy), the resistivity and thermal conductivity can be decoupled to realize simultaneous gains in both—that is, low ρ_{bb} and low κ_{cc} (κ_{cc} is the thermal conductivity along the *c* axis) (Supplementary Fig. 1). Both ρ_{bb} and κ_{cc} are much lower than the values for the ferromagnets with a large ANE (Supplementary Table 1). Consequently, YbMnBi₂ shows a high anomalous Nernst thermoelectric figure of merit zT_{ANE} , defined as, $zT_{ANE,bc} = S_{ANE,bc}^2 T / (\rho_{bb} \kappa_{cc})$. As shown in Fig. 5b, YbMnBi₂ has high zT_{ANE} values over a wide temperature range, demonstrating its highly promising anomalous transverse thermoelectric performance. Although the zT_{ANE} values are still much lower than the traditional, longitudinal zT , we present this result as promising progress towards the use of the ANE in thermoelectric applications, which could ultimately offer improvements in microscale devices and the field of spin caloritronics.

Outlook

In summary, YbMnBi₂, a canted antiferromagnet, breaks time-reversal symmetry and yields a non-zero Berry curvature. Alongside the large SOC contributed by the heavy Bi atoms, a large ANE conductivity of 10 A m⁻¹ K⁻¹ was observed, which is two to three times larger than those of most of the ferromagnets and compares favourably with those of noncollinear antiferromagnets. This

is of great interest, particularly considering its small magnetization. Furthermore, it shows strong anisotropy, making it possible to achieve low resistivity and low thermal conductivity simultaneously in transverse thermoelectric configurations. All of these unique features demonstrate the great potential of YbMnBi₂ as a transverse thermoelectric material.

These results suggest that canted antiferromagnets, including (but not limited to) the RMnPn₂ family, are worthy of further investigation for large ANEs. Future studies searching for compounds with canting temperatures higher than room temperature are crucial. Moreover, investigating the use of polycrystalline or thin-film materials to induce remanent magnetizations could be important for practical applications without external magnetic fields. Precise tuning of the Fermi level would also be an efficient way to enhance the ANE. Finally, with a deeper understanding of the intrinsic and extrinsic contributions to the ANE, both experimentally and theoretically, we expect to achieve boosted ANEs in more topological materials.

Online content

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Methods

Ab initio calculations. Calculations were conducted using density functional theory implemented in the Vienna ab initio simulation package (VASP) code^{43,44}. To calculate the band structure, the Perdew–Burke–Ernzerhof exchange–correlation functional and projector-augmented-wave approach were used. The cut-off energy was set at 500 eV to expand the wavefunctions into a plane-wave basis. The Brillouin zone was sampled in the k -space within the Monkhorst–Pack scheme⁴⁵, and a k mesh of $10 \times 10 \times 4$ was adopted based on an equilibrium structure. The C-type antiferromagnetic order along the c axis at the Mn sites, a canted spin structure and SOC were considered. To calculate the anomalous Hall conductivity and anomalous Nernst conductivity, the ab initio density functional theory Bloch wavefunction was projected onto highly symmetric atomic-orbital-like Wannier functions⁴⁶ with a diagonal position operator using VASP code^{43,44}. To obtain precise Wannier functions, we included the outermost s and d orbitals for Yb, d orbital for Mn and p orbital for Bi to cover the full band overlap from the ab initio and Wannier functions. The atomic coordinates for the electronic structure calculations are shown in Supplementary Table 2.

Sample preparation. YbMnBi₂ single crystals were grown using a self-flux method with an elemental ratio of Yb:Mn:Bi of 1:1:4. Yb (99.99%), Mn (99.98%) and Bi (99.9999%) were cut into small pieces and mixed before being placed in an alumina crucible. They were then sealed in a quartz tube under a partial argon pressure. The sealed tube was heated to 1,050 °C over 2.5 days and maintained at that temperature for 24 h. Next, it was slowly cooled to 400 °C at a rate of 2 °C h⁻¹, and single crystals were obtained by removing the flux through centrifugation.

Sample characterization. The single crystallinity and orientation of the as-grown single crystals were determined using Laue X-ray diffraction (Supplementary Fig. 12). The composition and homogeneity were examined by scanning electron microscopy (Philips XL30) with an Oxford energy-dispersive X-ray spectroscopy (Quantax, Bruker) (Supplementary Fig. 13).

ARPES measurements. The ARPES experiment was performed at the Bloch beamline at MAX IV with a Scienta DA30 analyser. The sample was cleaved in situ at 19 K with a base pressure lower than 1×10^{-10} mbar.

Measurement of transport properties. Resistivities and Hall resistivities were measured using a physical property measurement system (PPMS9, Quantum Design) in an electrical transport option via a standard four-probe method. The Nernst thermopower, Seebeck coefficient and thermal conductivity were measured in the PPMS9 under a high vacuum by using a standard four-contact steady-state method⁴⁷. The magnetization was measured using a magnetic property measurement system (MPMS3, Quantum Design).

Data availability

All the data supporting the plots within this paper and the findings of this study are available from the corresponding author upon request.

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Author contributions

Y.P. grew the single crystal and conducted the crystallinity and composition characterization. Y.P. and S.J.W. designed the experiments. Y.P. and B.H. measured the transport properties. C.L. and Y.S. completed the theoretical calculations. M.Y. performed the ARPES experiments. Y.P., B.H., S.J.W., J.G., J.P.H. and C.F. discussed the results. J.P.H. and C.F. supervised the project. All authors contributed to the preparation of the manuscript.

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Competing interests

The authors declare no competing interests.

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Correspondence and requests for materials should be addressed to Yu Pan or Claudia Felser.

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