



Three-dimensional nature of anomalous Hall conductivity in $\text{YMn}_6\text{Sn}_{6-x}\text{Ga}_x$, $x \approx 0.55$



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The unique geometry of kagome lattices leads to topological features such as flat bands and Dirac cones. When paired with ferromagnetism and a Fermi level near Dirac points, they offer a platform for realizing topological Chern magnetotransport. This prospect recently drew interest in the ferrimagnetic kagome metal TbMn_6Sn_6 . However, density functional theory (DFT) calculations indicate that its 2D Chern gap lies well above the Fermi energy, raising questions about its role in anomalous Hall conductivity. Here, we study $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$, a structurally and electronically similar material, and find that its intrinsic anomalous Hall effect is three-dimensional. This demonstrates that the Hall response in such compounds does not originate from 2D Chern gaps. Additionally, we confirm that the newly proposed empirical scaling relation for extrinsic Hall conductivity is universally governed by spin fluctuations.

Kagome lattice magnets have attracted significant interest in condensed matter physics due to their high frustration in the case of antiferromagnetic interactions. Over the past decade, this interest has grown, as it has been shown that even unfrustrated ferromagnetic (or nonmagnetic) kagome planes can exhibit nontrivial electronic features, such as flat bands and Dirac cones^{1–7}. Recently, particular attention has been directed toward the so-called 166 family, the RMn_6Sn_6 compounds, where R represents a rare-earth element^{8–16}. In these compounds, Mn atoms form kagome planes, and the crystal structure provides a diverse material space for manipulating both electronic and magnetic properties (Fig. 1). Compounds with non-magnetic R atoms are simpler because magnetism arises solely from the Mn sublattice; however, they are also more complex due to frustrated interplanar magnetic interactions. As shown in Fig. 1, although all Mn planes are crystallographically equivalent, the exchange interactions are not; there are two distinct exchange paths: one (J_1) across the Sn layer and the other (J_2) across the RSn layer. In YMn_6Sn_6 (Y166), a R166 compound with non-magnetic R atom, $J_2 > 0$ (i.e., antiferromagnetic), while the dominant interaction is $J_1 < 0$. As in most metals, the exchange coupling decays relatively slowly with distance (roughly as $1/d^3$), so the minimal model Hamiltonian includes J_1 , J_2 , and J_3 . Notably, this Hamiltonian is frustrated if $J_2J_3 < 0$,

resulting in intriguing spin-spiral orders that exhibit phenomena such as the topological Hall effect^{17,18} and Lifshitz transitions¹⁹.

Replacing Y with a magnetic ion that strongly couples to the neighboring Mn planes introduces an additional indirect ferromagnetic coupling between these planes, which can overcome the direct antiferromagnetic J_2 and remove magnetic frustration. This occurs in Tb166 ^{15,20–25} and is now well understood^{12,16}. Additionally, due to well-understood reasons¹⁶, Tb has an easy axis anisotropy along the crystallographic c direction, making the material a collinear easy-axis ferrimagnet at low temperatures, leading to the observation of the anomalous Hall effect (AHE) (in contrast to Y166, which is an easy-plane spiral antiferromagnet). Er166 lies close to the critical boundary between collinear and noncollinear ordering due to thermal fluctuations of Er magnetic moments²⁶. Because of these specific characteristics, Tb166 recently garnered significant interest for various different properties^{12,20,22–24,27,28}, including a putative two-dimensional (2D) Chern gap around 130 meV above the Fermi energy, as inferred from scanning tunneling measurements²⁰. One of the consequences of a 2D Chern gap, when close to the Fermi energy, is large anomalous Hall effect. The intrinsic contribution to the anomalous Hall effect extracted from the scaling of the anomalous Hall resistivity matches the value expected from the Chern gap around 130 meV above the Fermi energy²⁰. However, density functional

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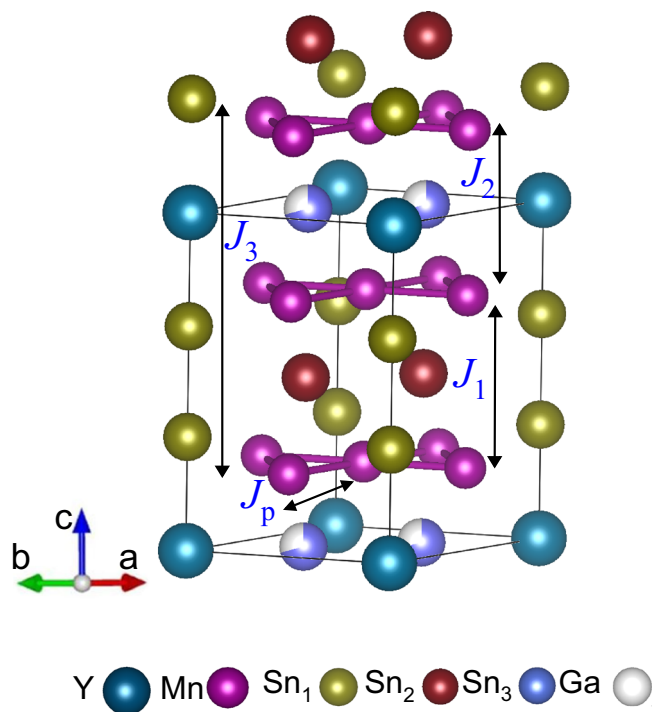


Fig. 1 | Crystal structure. Sketch of the crystal structure of $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$. J_i ($i = 1, 2, 3$) represent the exchange constants and J_p represents the in-plane exchange constant.

calculations^{12,16,29} consistently have shown that the 2D-Chern gap in Tb166 lies about 700 meV above the Fermi energy and does not contribute to the anomalous Hall conductivity (AHC). Instead, this AHC arises from several different regions in the Brillouin zone in ferrimagnetic Tb166¹². Additionally, an empirical scaling relation in the latter study suggested a potential contribution of spin fluctuations to the extrinsic anomalous Hall conductivity, an effect not previously investigated.

Regarding the latter, the standard method based on the theory by Crépieux and Bruno³⁰ for extracting the intrinsic (related to the Berry phases of conducting electron) and extrinsic (due to electron scattering) contributions to the AHC is to fit the temperature dependence of the AHC to a simple scaling relation,

$$\sigma_{xy} = a\sigma_{xx}^2 + c \quad (1)$$

where $c = \sigma_{xy}^A$ represents the intrinsic AHC, while the first term arises from defect scattering. This scaling relation has been widely used to extract the intrinsic AHC in various materials^{4,20,31}. However, Crépieux and Bruno's derivation did not account for scattering from thermally excited spin fluctuations, and currently a theoretical analysis of the effect of spin fluctuations on AHC is lacking.

Analyzing the Tb166 data, we found¹² that Eq. (1) poorly describes σ_{xy} at higher temperatures, where scattering from spin fluctuations becomes increasingly important. At the same time, we found that the most fluctuating species in Tb166 is Tb, which fluctuates more strongly than Mn. We also found that the empirical formula,

$$\sigma_{xy} = a\sigma_{xx}^2 + d/\sigma_{xx} + c, \quad (2)$$

fits the experimental data exceptionally well (note that the additional contribution becomes significant when σ_{xx} is small, i.e., at higher temperatures). We tentatively attributed this term to spin fluctuations, primarily from Tb.

The role of magnons in intrinsic AHC was discussed by Yang et al.³². In particular, they argue that magnon scattering follows what they called “universality class C”, where the skew scattering can be neglected (albeit this

is in contradiction, for instance with refs. 33,34 and side jump contribution is a universal constant. While this paper makes a number of model assumptions (such as treating magnons in the “itinerant-s/localized-s model”, while our system is itinerant and the same electrons that ensure magnetism also carry transport), and its final formulas cannot be directly applied to experiment, their conclusions are qualitatively useful for us: they introduce a model parameter ξ , characterizing the relative strength of the magnon scattering, and show that AHC is increasing with this parameter, if it is sufficiently large. This is qualitatively the same behavior as in our empirical formula, Eq. (2), where this additional increase at high temperatures is absorbed in the d/σ_{xx} term. It is worth noting that the possibility that magnon scattering may be important for AHC has been brought up, previously, for instance in ref. 35.

A reliable protocol for extracting AHC from the experiment is crucial. The existing methods^{30,31,36} overlook spin fluctuations, and therefore rely on low-temperature data. An equation that accurately describes the AHC across the entire temperature range is of significant practical importance.

In this study, we address two key aspects concerning Tb166: first, whether the intrinsic contribution to the AHC is linked to the 2D Chern gap, and second, whether the component in the AHC scaling relation, attributed to spin fluctuations, can be observed in another R166 compound that does not contain Tb. This is particularly relevant as Tb was thought to be crucial for both the Chern-gap induced AHE²⁰ and the enhancement of spin fluctuations¹².

An ideal compound to investigate these properties would be a R166 compound with a non-magnetic R atom and a soft, and relatively isotropic ferromagnet. Such a compound would allow the access to the saturated ferromagnetic state in a standard laboratory setting, enabling measurements of anomalous Hall resistivity over a broad temperature range and in both in-plane and out-of-plane directions. We found that $\text{YMn}_6\text{Sn}_{6-x}\text{Ga}_x$, $0.30 \leq x \leq 0.61$ meet these criteria³⁷ and selected one particular composition $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ for the study. Our results show that the intrinsic AHC in this compound is comparable to that in Tb166 for the out-of-plane magnetic field (B), where the Chern gap is expected to contribute to the AHC. At the same time, we observed a similar AHC in the in-plane B , where the Chern gap contribution is not expected, confirming the 3D nature of the AHC. Furthermore, we verified the new AHC scaling introduced in ref. 12 and confirmed its spin-fluctuational origin.

Results and discussion

Crystallography

The crystal structure and atomic composition of $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ (Y166-Ga) were determined using single crystal X-ray diffraction. Similar to the parent compound YMn_6Sn_6 (Y166), Y166-Ga adopts a hexagonal $P6/mmm$ structure ($a = b = 5.4784$ Å, $c = 8.925$ Å), consisting of kagome planes $[\text{Mn}_3\text{Sn}]$ separated by two inequivalent layers Sn_2 and Sn_3YGa , as illustrated in Fig. 1.

The structure exhibits Sn-site doping with Ga, specifically at the Sn_3 site (Wyckoff position 2c). This was confirmed through modeling efforts for partial Ga occupancy at other Sn sites, which either resulted in poorer fits to the data or nonsensical Ga occupancy values. Refinement analysis determined the Sn:Ga site occupancy to be 0.725:0.175, corresponding to the full chemical formula noted above, i.e., ~ 0.55 Ga atoms per unit cell. Detailed crystallographic parameters from the single crystal X-ray diffraction experiment are summarized in Table 1.

Our DFT calculations, presented in Section “First principles calculations”, also reveal a significant energy advantage for Ga substitution at the Sn_3 site in the $[\text{Sn}_3\text{Y}]$ layer, rather than in the $[\text{Mn}_3\text{Sn}]$ or $[\text{Sn}_2]$ layers. $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ can thus be viewed as a moderately hole-doped (≈ 0.09 h/Mn) derivative of the parent compound Y166.

Magnetic properties

The temperature dependence of magnetic susceptibility ($\chi = M/B$) measured with a magnetic field $B = \mu_0 H$ of 0.1 T parallel to $[100]$ (χ_{100}) and along $[001]$ (χ_{001}) is shown in Fig. 2a. These susceptibility data indicate that Y166-Ga undergoes a paramagnetic-to-ferromagnetic ordering below 350 K, consistent with previous reports^{37,38}. Additionally, the easy-plane behavior is

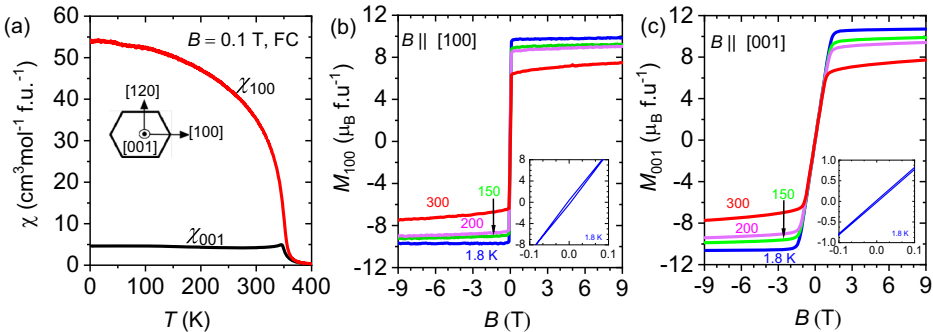
evident from the significantly larger χ_{100} compared to χ_{001} below the transition temperature (T_c), with an anisotropy ratio of $\chi_{100}/\chi_{001} = 5$ just below T_c . It is to be noted that parent compound Y166 orders with a commensurate antiferromagnetic helical structure below 345 K and exhibits an incommensurate double helical structure (DH) upon further cooling^{17,19,39}, while $\text{YMn}_6\text{Sn}_{1-x}\text{Ga}_x$ compounds show a ferromagnetic transition for doping concentrations $x > 0.30$ ³⁷.

Figure 2b, c shows the isothermal magnetization curves of Y166-Ga at some representative temperatures for $B \parallel [100]$ (M_{100}) and $[001]$ (M_{001}), respectively. In the entire temperature range measured M_{100} saturates below 0.5 T with a negligible hysteresis, while M_{001} saturates at slightly larger B . At 1.8 K M_{001} saturates at 2.2 T, which decreases with increasing temperature (1.7 T at 300 K), also with negligibly

Table 1 | Crystallographic data, atomic coordinates and equivalent displacement parameters for $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$

| | | | | | |
|---|--------------------------|-----------------|-----------------|-----------------|--------------------------|
| Crystal system | Hexagonal | | | | |
| Space group | <i>P</i> 6/ <i>mmm</i> | | | | |
| Temperature (K) | 120(2) | | | | |
| Wavelength (Å) | 0.71073 | | | | |
| Z formula units | 1 | | | | |
| 2θ _{min} | 4.564° | | | | |
| 2θ _{max} | 61.206° | | | | |
| Formula weight (g/mol) | 1103.76 | | | | |
| a,b (Å) | 5.4784(16) | | | | |
| c (Å) | 8.925(4) | | | | |
| Volume (Å) ³ | 231.97(17) | | | | |
| Density (calculated) (g/cm ³) | 7.901 | | | | |
| μ (MoK _α) mm ^{−1} | 29.896 | | | | |
| Goodness-of-fit on F ² | 1.186 | | | | |
| Final <i>R</i> indices [I≥2σ (<i>I</i>)] | R ₁ = 0.0172 | | | | |
| | wR ₂ = 0.0392 | | | | |
| <i>R</i> indices (all data) | R ₁ = 0.0183 | | | | |
| | wR ₂ = 0.0397 | | | | |
| Largest diff. peak & hole, e (Å ^{−3}) | 1.128 and −1.341 | | | | |
| Atom | Wyck | <i>x</i> | <i>y</i> | <i>z</i> | Ueq Å² |
| Y | 1a | 1.00000 | 1.00000 | 0.00000 | 0.007(1) |
| Sn(1) | 2e | 1.00000 | 1.00000 | 0.33674(8) | 0.004(1) |
| Sn(2) | 2d | 0.33333 | 0.66667 | 0.50000 | 0.006(1) |
| Sn(3) | 2c | 0.66667 | 0.33333 | 0.000000 | 0.005(1) |
| Ga(1) | 2c | 0.6667 | 0.33333 | 0.000000 | 0.005(1) |
| Mn(1) | 6i | 0.50000 | 0.50000 | 0.24504(9) | 0.005(1) |

Fig. 2 | Magnetic properties of $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$. **a** Magnetic susceptibility measured under an external magnetic field B of 0.1 T along the $[100]$ and $[001]$ directions using the field-cooled (FC) protocol. **b, c** Magnetization as a function of magnetic field $B \parallel [100]$ (**b**) and $B \parallel [001]$ (**c**) at selected temperatures ranging from 1.8 to 300 K. The insets in panels **b** and **c** show a magnified view of M vs B between ± 0.1 T at 1.8 K, revealing the presence of a very small hysteresis loop.



small hysteresis. At 1.8 K, saturation magnetization (M_{sat}) along $[100]$ is $9.85 \mu_B/\text{f.u.}$ while it is $10.7 \mu_B/\text{f.u.}$ along $[001]$. In either direction, M_{sat} gradually decreases with the increase in temperature, which attains a value of $7.5 \mu_B/\text{f.u.}$ along $[100]$ and $7.7 \mu_B/\text{f.u.}$ along $[001]$ at 300 K. The ratio of the saturated magnetization at 1.8–300 K ($M_{\text{sat},1.8\text{K}}/M_{\text{sat},300\text{K}}$) is 1.39 along the $[001]$ direction and 1.31 along the $[100]$ direction. For Tb166, the Mn moment shows the ratio of ~ 1.05 and the Tb moment exhibits the ratio of around 1.66 ^{12,40}. This suggests that the Mn moments in Y166-Ga experience more fluctuation between 1.8 and 300 K than in Tb166, where the Tb moments are the most fluctuating ones¹². This observation is consistent with the expectation, as the Curie temperature of Tb166 is about 70 K higher than that of Y166-Ga.

First principles calculations

To understand the doping-induced phase transition, we adopt the J_1 – J_3 effective model proposed in ref. 41. The spin Hamiltonian is expressed as follows

$$H = \sum_{\langle ij \rangle_1} J_1 S_i S_j + \sum_{\langle ij \rangle_2} J_2 S_i S_j + \sum_{\langle ij \rangle_3} J_3 S_i S_j \tag{3}$$

where J_i ($i = 1$ – 3) are the exchange interaction parameters as indicated in Fig. 1. The parameters were extracted using the least squared fitting of our DFT calculations into Eq. (3).

According to a thorough DFT-based analysis of the phase diagram for parent Y166 discussed in our earlier work¹⁷, we observed that $U = 0.6$ best reproduce the magnetic states for parent Y166 observed in the experiments. Therefore, in our study, we considered the same U parameter with one additional larger $U = 2$ for comparison.

The results along with those of Y166, taken from ref. 17, are summarized in Table 2. The fitting is achieved with excellent quality in all three cases, as all the relative energy differences between different magnetic states can be consistently and accurately reproduced by the model, especially in the case of $U = 0.6$ where the average error is less than 1 meV. This suggests that the minimal model adopted here is appropriate and reliable.

In Table 2, one can see that while J_1 and J_2 consistently favor ferromagnetic alignment regardless of different U values, the Hubbard U correction tends to stabilize the FM states further as J_3 shifts from positive to negative as U increases. According to the analytically determined phase diagram ref. 41, the spin model for all three U values yields the same correct FM ground state.

To assess the doping effect, we compare the results of the two compounds for the same $U = 0.6$ (i.e., columns 3 and 5). In Y166, J_1 dominates and has the same (opposite) sign as J_3 (J_2). This arrangement leads to a competition between J_2 and J_3 which results in the formation of a helical magnetic state^{17,41}. However, with Ga-doping, J_2 becomes ferromagnetic and now comparable to J_1 in strength. Although J_3 becomes antiferromagnetic, it is too weak to induce frustration.

This qualitative shift aligns with expectations, considering the direct alteration of exchange pathways for J_2 and J_3 induced by the presence of doped-Ga. As a consequence of these changes, the frustration that was initially developed in the pure Y166 to promote the helical magnetic state is effectively mitigated. The system undergoes a transition, and the magnetic state collapses into a ferromagnetic (FM) order.

In addition to non-relativistic calculation producing Eq. (3), we performed separate calculations including SOC in order to address magnetic anisotropy (both single-ion and exchange anisotropies). Interestingly, while the calculated ground state is always ferromagnetic, regardless of the value of U , only $U = 2$ gives the correct easy-xy plane anisotropy and $U = 0$ and 0.6 give very small easy- z axis anisotropy.

Electrical resistivity and conductivity

The temperature dependence of electrical resistivity of Y166-Ga, measured with the electric current applied along the [100] direction (ρ_{100} , blue curve) and the [001] direction (ρ_{001} , red curve) over the temperature range 1.8–400 K, is shown in Fig. 3a. The resistivity decreases as temperature decreases, indicating the metallic behavior of the sample. Residual resistivity ratio (RRR), calculated as $\rho(400\text{K})/\rho(2\text{K})$, is 9 for $I \parallel [100]$ and is 18 for $I \parallel [001]$. These values are smaller than those in Y166^{17,19}, likely due to disorder induced by doping. Both ρ_{100} and ρ_{001} exhibit a kink at 350 K, indicative of the onset of a ferromagnetic transition, as observed in the susceptibility measurements [Fig. 2a]. Across the entire temperature range, ρ_{100} is greater than ρ_{001} . The conductivity anisotropy, $\sigma_{[001]}/\sigma_{[100]}$, is plotted in Fig. 3b, showing a value >2 , which suggests that the electronic transport in Y166-Ga is three dimensional, albeit moderately anisotropic. This behavior differs from that of the parent compound Y166, where the in-plane conductivity is greater than the out-of-plane conductivity¹⁹. The enhanced c -axis conductivity observed in Y166-Ga is similar to that found in Ge doped YMn₆Sn₆¹⁰.

The anisotropic transport behavior was further investigated by measuring the angular-dependent magnetoresistance (AMR). In this measurement, an electric current I was applied along the [100] direction, while the sample was rotated around the magnetic field within the crystallographic bc -plane, with $I \perp B$ held constant so that only transverse MR was measured. In this configuration, at $\theta = 0^\circ (90^\circ)$, $B \parallel [120] ([001])$. Since the largest magnetic saturation

field is below 2.5 T (see Fig. 2), the 9 T magnetic field aligns the magnetic moment M perpendicular to I at all times.

The AMR, defined as $[\rho_{xx}(\theta) - \rho_{xx}(\theta = 0)]/\rho_{xx}(\theta = 0) \times 100$, measured at 5 K is shown in Fig. 3c, with maximum value of -5.6% , indicating a substantial effect. To gain further insight into this large AMR, we compared the AMR with the ab initio calculated AMR using the GGA + U method. For this purpose, we used the all-electron WIEN2k package⁴², varying $U_{\text{eff}} = U - J$ from 1.2 to 2 eV. Assuming an isotropic transport scattering rate, the longitudinal conductivity $\sigma_{xx} \propto \omega_{pl}^2 \propto \sum_{\mathbf{k}} \delta(E - E_{\mathbf{k}}) v_{\mathbf{k}x}^2$, where v is the Fermi velocity. We calculated this quantity using the $19 \times 19 \times 11$ zone-centered k -point mesh and tetrahedron numerical integration, and an otherwise default setup. We found (Fig. 4) that AMR is very sensitive to correlation effects. The best agreement with the experiment occurs at $U_{\text{eff}} = 1.3$ eV, yielding a calculated value of 1.6% , which is over three times smaller than the experimental result but remains the same order of magnitude. This discrepancy may indicate the presence of an anisotropic scattering rate, or an underestimation of spin-orbit coupling (SOC) in the calculation, potentially related to the known underestimation of the AHC in TbMn₆Sn₆^{12,29}.

Anomalous Hall effect

Hall resistivity measured with $B \parallel [001]$ and the current $I \parallel [100]$ (ρ_{xy}) at representative temperatures is shown in Fig. 5a. The zero-field value of ρ_{xy} corresponds to the anomalous Hall resistivity ρ_{xy}^A . In Fig. 5b, we show the longitudinal conductivity, $\sigma_{xx} = 1/\rho_{xx}$, and the absolute value of the anomalous Hall conductivity, $(|\sigma_{xy}^A|) = -\rho_{xy}/\rho_{xx}$ (valid when $\rho_{yx} \ll \rho_{xx}^2$, and $\rho_{xx} = \rho_{yy}$), as a function of temperature between 1.8 and 300 K. This clearly indicates that $|\sigma_{xy}^A|$ varies with temperature across the entire temperature range. The scaling of the $|\sigma_{xy}^A|$, using the relation presented in Eq. (2), is shown in Fig. 5c. This scaling law effectively fits the high-temperature data, yielding the coefficients a , d , and c , as presented in Table 3 and compared to those from Tb166. The coefficient a , representing impurity scattering, is about an order of magnitude larger in Y166-Ga compared to Tb166, as expected due to increased disorder scattering in the doped sample. The intrinsic anomalous Hall conductivity of Y166-Ga (121 S/cm or $0.14 e^2/h$ per Mn layer) is comparable to that of Tb166 (140 S/cm). Interestingly, the magnitude of d is smaller in the Y166-Ga than in Tb166, consistent with the hypothesis that the term d/σ_{xx} in Eq. (2) is due to spin fluctuations¹². Notably, $d \neq 0$ in Y166-Ga despite the absence of highly fluctuating Tb atoms, likely because, as discussed in Section “Magnetic properties”, Mn in Y166-Ga fluctuates significantly more than in Tb166. This implies that the d/σ_{xx} is essential in the anomalous Hall scaling of RMn₆Sn₆ compounds due to the presence of Mermin–Wagner fluctuations¹⁷ involving either Mn or R atoms.

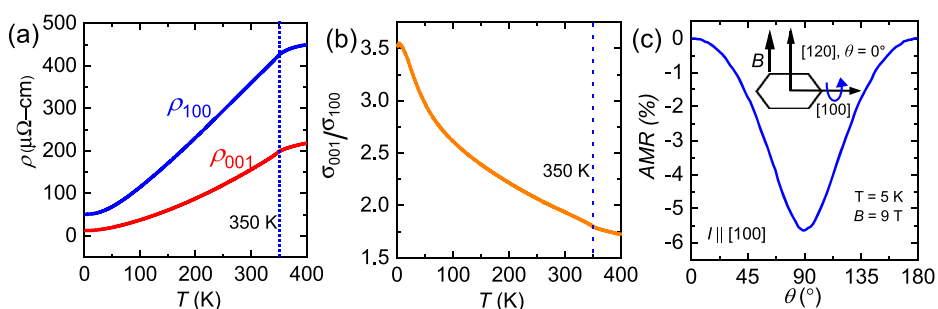
The similar magnitude of intrinsic AHC in Y166-Ga and Tb166 suggests that the intrinsic AHC in R166 compounds is a general property of ferrimagnetism rather than a result of exotic Chern physics, consistent with

Table 2 | Calculated exchange couplings J_1 , J_2 and J_3 in unit of meV

| U | $x = 1$ | | | $x = 0$ (Y166) |
|-------|---------|-------|-------|----------------|
| | 0 | 0.6 | 2 | 0.6 |
| J_1 | −14.5 | −11.9 | −17.3 | −12.86 |
| J_2 | −21.7 | −10.6 | −21.9 | 4.66 |
| J_3 | 1.8 | 1.5 | −4.0 | −2.20 |

The data for Y166 are taken from ref. 17.

Fig. 3 | Electrical transport properties of YMn₆Sn_{5.45}Ga_{0.55}. **a** Electrical resistivity as a function of temperature for current applied along the [100] and [001] directions. **b** Ratio of the conductivity along the [001] direction to that along [100]. **c** Angular magnetoresistance (AMR) as a function of angle θ , measured under a 9 T magnetic field, where the current (I) is along the [100] direction and θ is the angle between the magnetic field and [120] direction, as illustrated by the sketch in panel (c).



the conclusions drawn by Jones et al.¹². This interpretation is further supported by photoemission spectroscopy data from the parent compound Y166⁴³, which shows no such topological feature above the Fermi energy, with Ga doping shifting the Fermi energy even lower.

To further validate this interpretation, we measured the Hall conductivity of Y166-Ga by applying an in-plane magnetic field, ensuring that any 2D Chern gap contributions would be excluded if present. While measuring this in-plane configuration for Tb166 would require an exceptionally high magnetic field due to magnetic saturation constraints at low temperatures^{12,44}, Y166-Ga can be measured under standard lab conditions. For consistency with the ρ_{yx} measurement in Fig. 5, we applied the current along the [100] direction and applied the in-plane field along [120]. The Hall resistivity, ρ_{zx} , measured across a range of temperatures from 1.8 to 300 K, is shown in Fig. 6a.

In Fig. 6b, we plot $\sigma_{xx} = 1/\rho_{xx}$ alongside the absolute value of the anomalous Hall conductivity, $\sigma_{zx} = -\rho_{zx}/(\rho_{xx}\rho_{zz})$, which is valid when $\rho_{zx} \ll \rho_{xx}$ and ρ_{zz} . The scaling of σ_{zx} following the relation in Eq. (2), is presented in Fig. 6c, with the fitting coefficients a , d , and c presented in Table 3. Notably, the intrinsic AHC contribution, represented by coefficient c ($\sigma_{zx, \text{int}}^A$), is significantly larger than $\sigma_{yx, \text{int}}^A$, indicating that the AHC in Y166-Ga has a 3D nature and can be large without invoking the Chern physics. The coefficient $|d|$ is also larger in this measurement geometry, potentially pointing to enhanced spin-fluctuations, though this cannot be directly compared to Tb166 due to differing Hall geometries and remains a topic of future work on R166 compounds. However, it is noteworthy that the d/σ_{xx} term is also necessary in this case. Nevertheless, our findings reveal that the AHC in Y166-Ga displays 3D characteristics and supports theoretical

calculations that suggest the AHC arises from predominantly 3D bands¹², as further discussed in Section “Intrinsic AHC calculations for TbMn₆Sn₆ and YMn₆Sn₆”.

Intrinsic AHC calculations for TbMn₆Sn₆ and YMn₆Sn₆

The intrinsic AHC can be calculated by integrating the Berry curvature over the Brillouin zone (BZ)⁴⁵:

$$\sigma_{\alpha\beta} = -\frac{e^2}{\hbar} \int_{\text{BZ}} \frac{d\vec{k}}{(2\pi)^3} \sum_n f(E_n(\vec{k})) \Omega_{n,\alpha\beta}(\vec{k}) \quad (4)$$

where $f(E_n(\vec{k}))$ is the Fermi-Dirac distribution, $\Omega_{n,\alpha\beta}(\vec{k})$ is the contribution to the Berry curvature from state n , and $\alpha, \beta = \{x, y, z\}$.

A notable aspect of the calculation is the pronounced and rapid oscillation observed in the Berry curvature across the BZ, requiring a dense k mesh to ensure convergence. To accelerate the calculations, we implemented Eq. (4) in our recently-developed tight-binding (TB) code⁴⁶ and carried out the AHC calculations in RMn₆Sn₆ where $R = \text{Tb}$ and Y . A realistic TB Hamiltonian was constructed using the maximally localized Wannier functions (MLWFs) method^{47–49} implemented in WANNIER90⁵⁰ after the self-consistent density-functional-theory calculations performed using WIEN2K. A set of 118 Wannier functions (WFs) consisting of Y-4d (or Tb-5d), Mn-3d, and Sn- sp orbitals offers an effective representation of the electronic structure near the Fermi level (E_F). The self-consistent DFT calculations were carried out with out-of-plane magnetization in TbMn₆Sn₆ and both in- and out-of-plane magnetization in YMn₆Sn₆. For the in-plane YMn₆Sn₆ configuration, the moment is along lattice vector \mathbf{a} , as denoted in Fig. 7. A dense 256³ k -point mesh is used for the AHC calculations in TB.

Figure 7 presents the unit cell of YMn₆Sn₆ used in our calculation. The Cartesian coordinate system is chosen so that the lattice vector \mathbf{b} is along the y -axis, \mathbf{c} is along the z -axis, and \mathbf{a} is along the -30° direction off the x -axis. Lattice vectors \mathbf{a} and \mathbf{b} point along the nearest neighboring (NN) Mn–Mn bond direction. For the σ_{xy} calculations discussed below, the first subscript x denotes the current direction, and the second subscript y denotes the Hall-field direction.

Figure 8 shows the AHC values calculated at $T = 0 = \text{K}$ as functions of Fermi energy using Eq. (4). In the out-of-plane orientation of both TbMn₆Sn₆ and YMn₆Sn₆, only σ_{xy} exhibits substantial values, while σ_{yz} and σ_{zx} remain negligible, as illustrated in the top and middle panels of Fig. 8. Conversely, with in-plane magnetization in YMn₆Sn₆, both σ_{yz} and σ_{zx} demonstrate appreciable values, while σ_{xy} remains negligible, as depicted in the bottom panel of Fig. 8. The band-filling calculation indicates that when doping YMn₆Sn₆ by 0.09 hole/Mn, corresponding to a Fermi energy shift of -0.037 eV , $\sigma_{xy} = 77.62 \text{ S/cm}$, and $\sigma_{zx} = 36.76 \text{ S/cm}$. While the former closely aligns with the experimental value, the latter is approximately 10 times smaller than the experiment. These comparison has to be taken

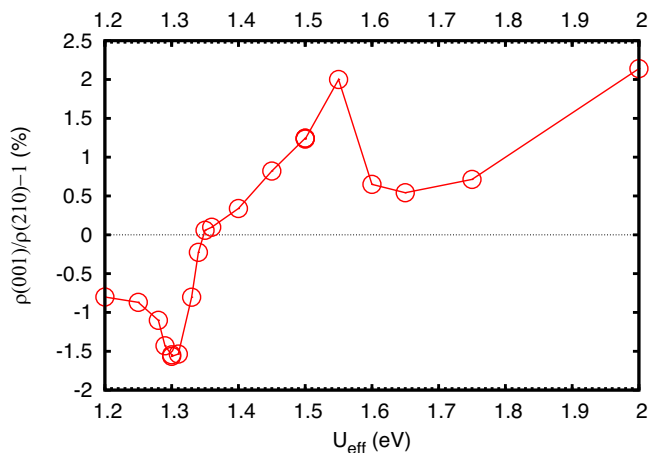
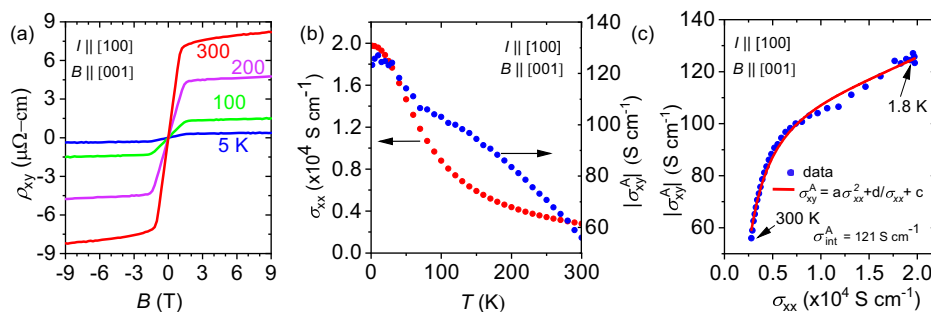


Fig. 4 | Calculated angular magnetoresistance. Angular magnetoresistance between the full polarization along the crystallographic [001] and [120] axes, as a function of the effective Hubbard interaction, calculated for YMn₆Sn₅Ga.

Fig. 5 | Anomalous Hall effect of YMn₆Sn_{5.45}Ga_{0.55} measured with $\mathbf{B} \parallel [001]$ and $\mathbf{I} \parallel [100]$.

a Anomalous Hall resistivity ρ_{xy} as a function of magnetic field at selected temperatures. **b** Longitudinal conductivity (σ_{xx} , red spheres), and anomalous Hall conductivity ($|\sigma_{xy}^A|$, blue spheres) as a function of temperature. **c** $|\sigma_{xy}^A|$ (blue spheres) plotted as a function of σ_{xx} in the temperature range 1.8–300 K. The solid represents a fit to Eq. (2).



with caution, as random substitution of 0.55 Ga likely affects the electronic structure beyond a simple rigid Fermi energy shift. Nevertheless, our theoretical calculations predict that the Hall transport in R166 is 3D, consistent with the experimental findings.

We reported results of magnetic and electrical transport measurements of $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ in two different geometries, supported by first-principles and DFT calculations. Our magnetotransport measurements across these two geometries confirm a more reliable scaling law that not only extracts the intrinsic AHC, but also accounts for contributions from spin fluctuations. These measurements revealed the 3D nature of the intrinsic AHC, which we attribute to the ferromagnetic properties of the material. The excellent agreement of the AHE with the empirical scaling law over the entire temperature suggests that this scaling relation may be important for not only for the large family of RMn_6Sn_6 ferro/ferromagnetic compounds, but also for other systems with strong spin fluctuations.

Methods

Crystal growth and structural characterization

Single crystals of $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ were grown by using Sn as a flux by the molten flux method. Y pieces (Alfa Aesar 99.9%), Mn pieces (Alfa Aesar 99.95%), Sn shots (Alfa Aesar 99.999%) and Ga pieces (Alfa Aesar 99.9999%) were added into a 2-mL aluminum oxide crucible in molar ratio of 1.6:18:2. The crucible was then sealed in a fused silica ampule under vacuum. The sealed ampule was heated to 1150 °C over 10 h, homogenized at 1150 °C for 24 h, and then cooled down to 600 °C with a rate of 5 °C/h. Once the furnace reached 600 °C, the molten flux was separated from the crystals by using a centrifuge. Upon opening the crucible, nice hexagonal-looking crystals up to 20 mg were obtained.

The crystal structure and the atomic composition were verified from a single crystal X-ray diffraction experiment. An arbitrary sphere of data was collected on a silver block-like crystal, having appropriate dimensions of $0.073 \times 0.068 \times 0.026$, on a Bruker D8 diffractometer equipped with a Bruker APEX-II detector using a combination of ω - and ϕ -scans of 0.5° ⁵¹. Data were corrected for absorption and polarization effects and analyzed for space group determination⁵². The structure was solved by dual-space methods and expanded routinely⁵³. The model was refined by full-matrix least-squares analysis of F^2 against all reflections⁵⁴.

Table 3 | Comparison of intrinsic anomalous Hall conductivity between TbMn_6Sn_6 ¹² and $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$

| Compound | c (S/cm) | a (S/cm) ⁻¹ | d (S/cm) ² |
|--|------------|--------------------------|-------------------------|
| TbMn_6Sn_6 ($\ \sigma_{xy}\ $) | 140 | 8.69×10^{-9} | -2.47×10^5 |
| $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ ($\ \sigma_{xy}\ $) | 121 | 3.25×10^{-8} | -1.75×10^5 |
| $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ ($\ \sigma_{xz}\ $) | 310 | 1.89×10^{-7} | -5.41×10^5 |

Magnetic property measurements

DC magnetization, resistivity, and magnetoresistance measurements were performed in a Quantum Design Dynacool Physical Property Measurement System (PPMS) with a 9 T magnet. ACMS II option was used in the same PPMS for DC magnetization measurements. Single crystals of $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ were polished to adequate dimensions for electrical transport measurements. Crystals were oriented with the [001] and [100] directions parallel to the applied field for the c -axis and ab -plane measurements.

Resistivity and magnetotransport measurements

Resistivity and Hall measurements were done using the 4-probe method. Pt wires of 25 μm were used for electrical contacts with contact resistances $<30 \Omega$. Contacts were affixed with Epotek H20E silver epoxy. An electric current of 4 mA was used for the electrical transport measurements.

The samples were polished to dimensions of $\sim 1.00 \times 0.40 \times 0.15$ mm, with the long axis oriented along either the [100], [120] or [001] crystallographic direction.

The longitudinal resistivity, ρ_{ii} , was calculated from the measured longitudinal resistance, R_{ii} , using the relation: $\rho_{ii} = R_{ii}A/l$, where $A = td$ is the cross-sectional area (t is the thickness, and d is the width of the sample), and l is the length of the sample between the two voltage contacts.

The Hall resistivity was calculated using the relation: $\rho_{ij} = R_{ij}t$, where $R_{ij} = V_i/I_j$ and t represent the measured Hall resistance and the sample thickness, respectively. Here, V_i is the transverse voltage developed along the i -direction in the presence of a magnetic field along k , with current I_j in the j -direction. The indices i , j , and k are mutually orthogonal, representing x , y , or z directions in different measurement geometries.

To account for the contact misalignment, the antisymmetric (Hall) and symmetric (magnetoresistance) contributions to the resistivity and Hall data, respectively were corrected using symmetrization and anti-symmetrization techniques as follows:

$$\rho_{ii} = \frac{\rho_{ii}(+B) + \rho_{ii}(-B)}{2}, \quad \rho_{ij} = \frac{\rho_{ij}(+B) - \rho_{ij}(-B)}{2}.$$

The longitudinal resistivity and Hall resistivity data were acquired in a four-loop sequence: the magnetic field B was swept from $+B_{\text{max}}$ to $-B_{\text{max}}$, and then back from $-B_{\text{max}}$ to $+B_{\text{max}}$. Symmetrization and antisymmetrization were applied to data obtained during B -field sweeps from $+B_{\text{max}}$ to 0 and from $-B_{\text{max}}$ to 0, as well as from 0 to $+B_{\text{max}}$ and from 0 to $-B_{\text{max}}$.

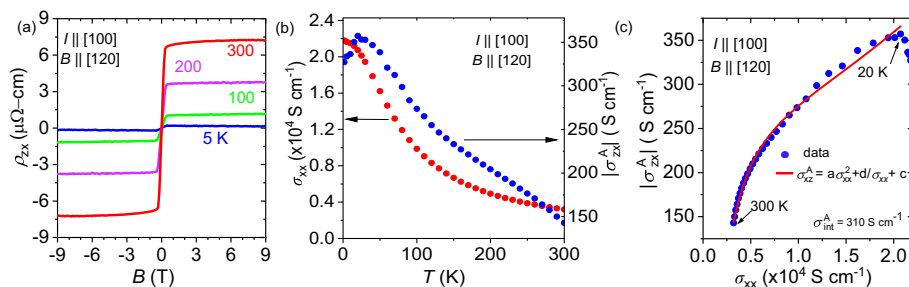
Hall conductivity for various directions was calculated using the following relations:

$$\sigma_{xy} = \frac{-\rho_{xy}}{\rho_{xx}^2}, \quad \sigma_{zx} = \frac{-\rho_{zx}}{\rho_{xx}\rho_{zz}}.$$

Fig. 6 | Anomalous Hall effect of $\text{YMn}_6\text{Sn}_{5.45}\text{Ga}_{0.55}$ measured with $B \parallel [120]$ and $I \parallel [100]$.

a Anomalous Hall resistivity ρ_{zx} as a function of magnetic field at selected temperatures.

b Longitudinal conductivity (σ_{xx} , red spheres), and anomalous Hall conductivity ($|\sigma_{xz}^A|$, blue spheres) as a function of temperature. **c** $|\sigma_{xz}^A|$ (blue spheres) plotted as a function of σ_{xx} in the temperature range 1.8–300 K. The solid represents a fit to Eq. (2).



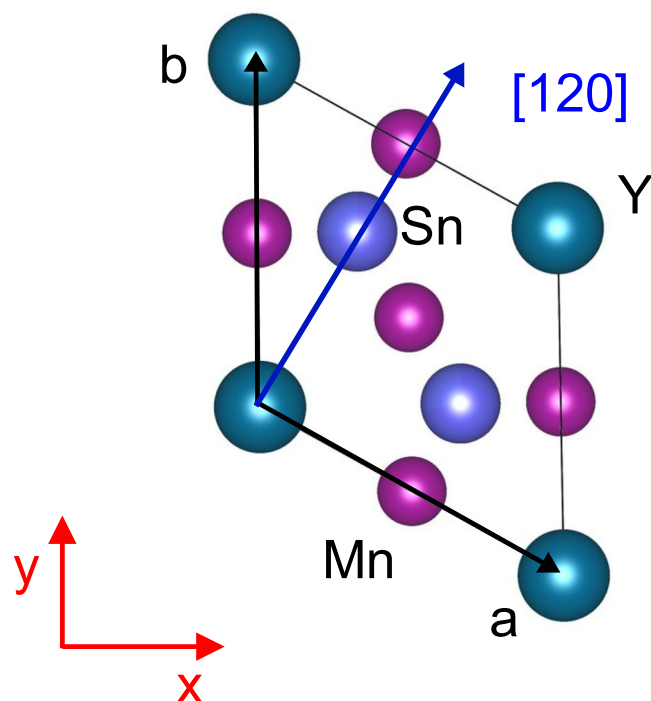


Fig. 7 | Primitive unit cell used in AHC calculations. The top view of the YMn_6Sn_6 primitive unit cell. The x - and y -axes are highlighted in red, while the $[120]$ direction is denoted in blue. The z -axis is perpendicular to the plane.

Here, ρ_{xx} and ρ_{zz} represent the longitudinal resistivities for current along the $[100]$, and $[001]$ crystallographic directions, respectively, with the magnetic field applied perpendicularly. For the calculation of σ_{yx} both ρ_{xy} and ρ_{xx} were measured simultaneously in the same sample. For the calculation of σ_{zx} , ρ_{zx} and ρ_{xx} were measured simultaneously in the sample, and ρ_{zz} was measured on a separate crystal of the same growth batch. The term $\rho_{xx}\rho_{zz}$ in the denominator of σ_{xz} accounts for the resistivity anisotropy in the hexagonal system. For σ_{xy} , $\rho_{xx} = \rho_{yy}$ is used due to the isotropic in-plane resistivity. The conductivity relations used here are valid under the condition: $\rho_{ii}\rho_{jj} \gg \rho_{ij}\rho_{ji}$.

First-principles calculations

The first-principles calculations were performed using Vienna ab initio Simulation Package (VASP)⁵⁵ within projector augmented wave (PAW) method^{56,57}. The Perdew–Burke–Erzerhof (PBE)⁵⁸ generalized gradient approximation was employed to describe exchange–correlation effects. The on-site Coulomb interactions are taken into account using LDA + U ⁵⁹ to improve the description of the interactions between localized 3d-electrons of Mn and an effective $U_{\text{eff}} = U - J = 0, 0.6$ and 2 are considered.

The experimental values were used for the lattice parameters and kept fixed for all the calculations, including the geometry optimization, where only internal coordinates were relaxed. To properly determine the structure, we performed geometry optimization for 2d, 2e, and 2c three different Ga substitution sites. The 2c site, consistent with the experimental analysis, gives the lowest energy which is then considered as the magnetic ground state.

Data availability

The authors declare that the main data supporting the findings of this study are available within the article. Extra data are available from the corresponding author upon request.

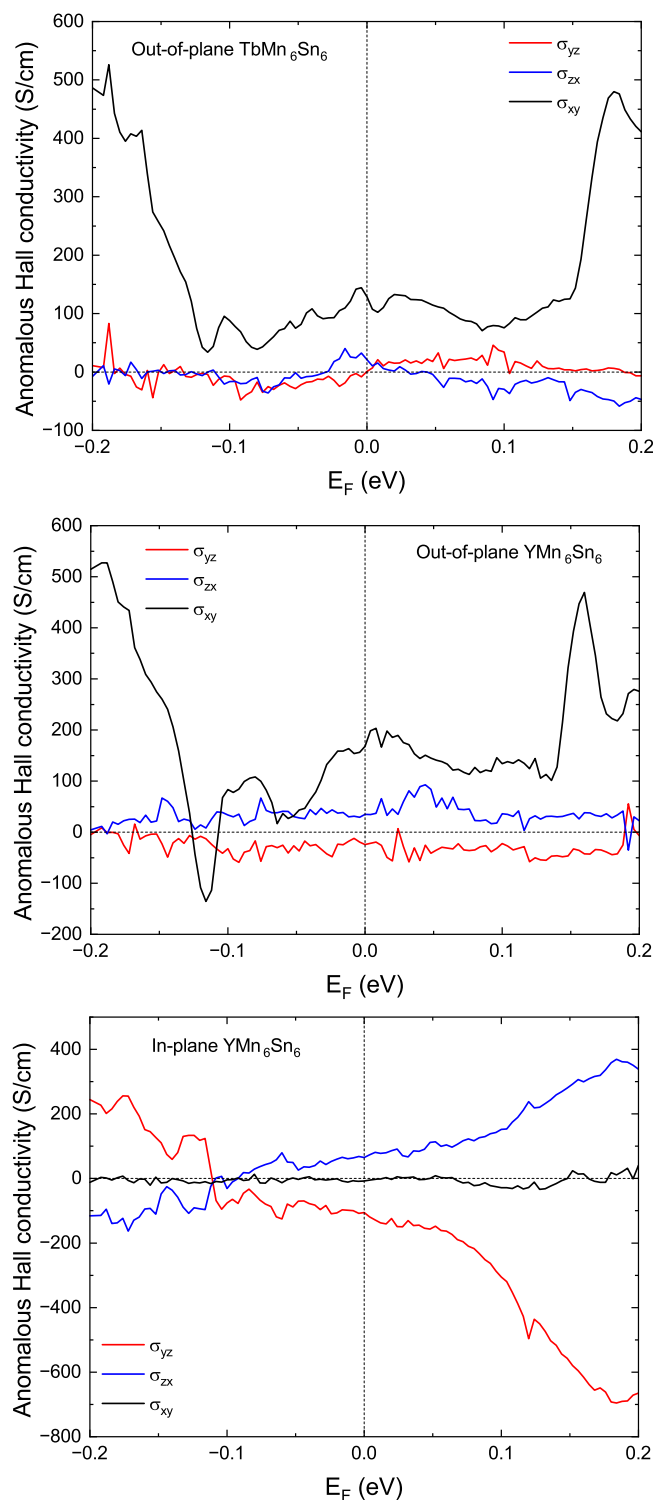


Fig. 8 | Calculated intrinsic anomalous Hall conductivity (AHC) of TbMn_6Sn_6 and YMn_6Sn_6 as a function of Fermi energy (E_F). The intrinsic AHC of TbMn_6Sn_6 (Top) was calculated with an out-of-plane magnetization configuration, while that of YMn_6Sn_6 was calculated with both out-of-plane magnetization (Middle) and in-plane magnetization configurations (Bottom).

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Author contributions

N.J.G. and H.B. conceived the idea and coordinated the project. H.B. grew single crystals. R.B.R. and M.E.G. helped in the crystal growth. H.B., A.G.O., and A.D. characterized the structural and chemical composition of the

samples. H.B. performed magnetic and magnetotransport measurements. P.E.S. helped in some magnetotransport measurements. H.B. carried out the data analysis. I.I.M. and P.H.C. contributed to the DFT calculations. Z.N. and L.K. contributed to the AHC calculations. H.B. and N.J.G. wrote the manuscript with inputs from I.I.M., and L.K. All authors contributed to the discussion of the results.

Competing interests

The authors declare no Competing Financial or Non-Financial Interests.

Additional information

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