Today solid-state cooling technologies below liquid nitrogen boiling temperature (77 K), crucial to quantum information technology and probing quantum state of matter, are greatly limited due to the lack of good thermoelectric and/or thermomagnetic materials. Here, we report the discovery of colossal Nernst power factor of $3800 \times 10^{-4} \text{W m}^{-1} \text{K}^{-2}$ under 5 T at 25 K and high Nernst figure-of-merit of $71 \times 10^{-4} \text{K}^{-1}$ under 5 T at 20 K in topological semimetal NbSb$_2$ single crystals. The observed high thermomagnetic performance is attributed to large Nernst thermopower and longitudinal electrical conductivity, and relatively low transverse thermal conductivity. The large and unsaturated Nernst thermopower is the result of the combination of highly desirable electronic structures of NbSb$_2$ having compensated high mobility electrons and holes near Fermi level and strong phonon-drag effect. This discovery opens an avenue for exploring material option for the solid-state heat pumping below liquid nitrogen temperature.
thermopile structure, in which only the electrical contact is required at the colder side of the thermoelectric material that does not require compatible $p$- and $n$-type elements, and can reduce the thermal resistance. The Ettingshausen effect is shown in Fig. 1a. When a longitudinal current (along the $y$ direction) flows through a thermoelectric material under magnetic field, a transverse temperature gradient (along the $x$ direction) will be formed, yielding the reduction of temperature at the material’s transverse side surface. The cooling efficiency of Ettingshausen refrigeration is determined by the material’s electrical and thermal transport properties in orthogonal directions, which can be evaluated by a comprehensive parameter named as the Nernst figure-of-merit $z_N = \frac{S_y}{\kappa_x}$, where $S_y$ is the Nernst thermopower, $\kappa_x$ is the longitudinal electrical conductivity, $\kappa_{xx}$ is the transverse thermal conductivity, and magnetic field is along the $z$ direction, respectively. In contrast to the longitudinal TE power factor $PF = S_x \sigma_x$, where $S$ and $\sigma$ are the Seebeck thermopower and electrical conductivity along the same direction, respectively, the Nernst power factor $PF_N = S_y \sigma_y$ is used to determine the transverse pumping power. Electrons and holes moving in the opposite direction driven by the longitudinal current, can carry both charge and energy in the same transverse direction synergistically under magnetic field, resulting in a doubling of the transverse temperature gradient. Therefore, semimetals with zero bandgap or slight band overlap are particularly suitable for the Ettingshausen cooling at low temperatures below 77 K.

Although the Ettingshausen effect was discovered in 1886, Ettingshausen refrigeration has progressed far less than Peltier refrigeration. For a long time, the investigation is only limited in a few thermoelectric materials, such as Bi–Sb alloys and In–Sb alloys. The peak $z_N$ values of single-crystalline Bi$_2$Sb$_3$ and Bi$_9$Sb$_7$ are $55 \times 10^{-4}$ $\text{K}^{-1}$ under 1 T and $29 \times 10^{-4}$ $\text{K}^{-1}$ under 0.75 T at 115 K, respectively (Fig. 1b). Recently, the discovery of topological semimetals with high carrier mobility has rejuvenated the investigation of Ettingshausen effect. It is noted that the Dirac-like linear electronic band dispersion near Fermi level in topological semimetals can lead to an energy-independent electronic density of states that increases linearly with magnetic field, thus create huge electronic entropy. Indeed, the peak $z_N$ of Dirac semimetal ZrTe$_5$ was reported to reach $10.5 \times 10^{-4}$ $\text{K}^{-1}$ under 13 T at 120 K. Nodal-line semimetal PtSn$_4$ has a peak $z_N$ of $8 \times 10^{-4}$ $\text{K}^{-1}$ under 9 T at 10 K. Most recently, Pan et al. reported an ultrahigh $z_N$ of $265 \times 10^{-4}$ $\text{K}^{-1}$ under 9 T at 11.3 K in single-crystalline Weyl semimetal WTe$_2$. This value is already much higher than that of Bi–Sb alloys (Fig. 1b), which was recently shown to be also a topological semimetal in specific chemical composition range after all. These results motivate the discovery of new thermomagnetic materials with high $z_N$ below liquid nitrogen temperature from topological semimetals.

In this work, we report that topological semimetal NbSb$_2$ single crystal is a promising high-performance thermomagnetic material with a colossal $PF_N$ of $3800 \times 10^{-4}$ W m$^{-1}$ K$^{-1}$ under 5 T at 25 K (Fig. 1c) and a high $z_N$ of $71 \times 10^{-4}$ $\text{K}^{-1}$ under 5 T at 20 K (Fig. 1b), much higher than most TE and thermomagnetic materials below 77 K. We found that the performance in NbSb$_2$ benefits from the combination of nearly identical electron and hole concentrations, high electron/hole carrier mobilities, and additional phonon-drag effect.

Results

Crystal structure

NbSb$_2$ is a topological semimetal. It crystallizes in centrosymmetric monoclinic structure with the space group of $C_{2/m}$. The schematics of its crystal structure is shown in Fig. 2a. The Nb atom is enclosed in a hendecahedron composed of Sb atoms. The hendecahedrons are connected with each other in the way of face-to-face along the $a$ axis and edge-to-edge along the $c$ axis, forming an atomic layer parallel to the $bc$ plane. The lattice parameters for NbSb$_2$ are $a = 10.239$ Å, $b = 3.632$ Å, $c = 8.333$ Å, and $\beta = 120.07^\circ$. Figure 2b shows the NbSb$_2$ single crystal grown by the chemical vapor transport method. The NbSb$_2$ single crystal has a bar-like shape with the length about 7 mm and the width about 1–2 mm. The X-ray characterization performed on the upper surface (Supplementary Fig. 1a) shows that strong (200), (400), and (600) diffraction peaks are observed, indicating the high quality of our NbSb$_2$ single crystal. Supplementary Fig. 1b shows that Nb and Sb are homogeneously distributed inside the matrix, consistent with the pure phase detected by XRD measurement.

Band structure

Figure 2c shows the calculated band structure of NbSb$_2$ with the inclusion of spin–orbit coupling (SOC) effect. The Fermi level crosses
the conduction band on the path from \( L \) to \( I \) and the valence band near \( L \), rendering it a typical semimetal. The energy overlap between conduction band and valence band is about 350 meV. From the Fermi surface (FS) plotted in Fig. 2d, we can identify one electron pocket (blue shell) and one hole pocket (red shell) in the first Brillouin zone. The calculated FS area on the ab plane is comparable to the experimentally measured area from the quantum oscillation measurement. A plot showing variation of the calculated FS area with chemical potential and comparison with the experimental value is shown in Supplementary Fig. 2, with the details shown in Supplementary Note 1. The similarity between the calculated and measured FS areas provides validity to the density functional theory (DFT)-predicted electronic structure. The electron pocket and the hole pocket have nearly the same volume leading to well-compensated electrons and holes near the Fermi level. Under orthogonal applied magnetic field, the electrons and holes in these pockets moving in the opposite direction along the longitudinal current are deflected in the same transverse direction, which can strengthen the Ettingshausen effect.

**Transport properties**

Supplementary Fig. 3a, b shows the temperature dependences of adiabatic transverse electrical resistivity \( \rho_{xx} \) and Hall resistivity \( \rho_{yx} \) of single-crystalline NbSb\(_2\) under different magnetic fields \( B \). When \( B = 0 \), the \( \rho_{xx} \) rises with increasing temperature, showing typical metal-like conduction behavior. The \( \rho_{xx} \) is \( \sim 2 \times 10^{-4} \) \( \Omega \) m at 5 K, which is about 3–4 orders of magnitude lower than those of typical TE materials for Peltier refrigeration. Upon applying magnetic field, the \( \rho_{xx} \) at temperatures below 100 K is greatly increased, a characteristic feature of topological semimetals. The magnetoresistance (MR) ratio of single-crystalline NbSb\(_2\) under 9 T at 5 K is 1.3 \( \times 10^2 \), comparable to those of extremely large magnetoresistance (XMR) materials reported before, such as MR = 8.5 \( \times 10^3 \) for NbP under 9 T at 1.85 K, 4.5 \( \times 10^3 \) for WTe\(_2\) under 14.7 T at 4.5 K, and 5 \( \times 10^3 \) for PtSn\(_4\) under 14 T at 1.8 K. Supplementary Fig. 3b shows that the absolute value of Hall resistivity \( |\rho_{yx}| \) firstly decreases with increasing temperature, reaches a minimum at about 100 K, and then increases at a higher temperature. Under the same magnetic field, the \( |\rho_{yx}| \) is much lower than the \( \rho_{xx} \).

To evaluate the Nernst figure-of-merit, we need to know the longitudinal conductivity \( \sigma_{yy} \), which can be calculated by the equation

\[
\sigma_{yy} = \frac{\rho_{xx} - \rho_{yx}\rho_{yy}}{\rho_{xx}\rho_{yy} - \rho_{yx}^2} = \frac{\rho_{xx}}{(\rho_{yy}/\rho_{xx})^2 + \rho_{yx}^2}
\]

where \( \rho_{yy} \) is the longitudinal electrical resistivity. The value of \( \rho_{yy}/\rho_{xx} \) is determined by measuring the electrical resistivity along the \( b \) axis (\( \rho_{xx} \)) and the electrical resistivity along the \( c \) axis (\( \rho_{yy} \)) of a thin square single-crystalline NbSb\(_2\) sample (Supplementary Figs. 4a, b). It seems that the electrical resistivities behavior of NbSb\(_2\) is more anisotropic at low temperatures, but less anisotropic at room temperature. Under the assumption that \( -\rho_{yx} \) is equal to \( \rho_{yx} \), the \( \sigma_{yy} \) under different magnetic fields is calculated and shown in Fig. 3a. The \( \sigma_{yy} \) first increases with increasing temperature, reaches a maximum, and then decreases with further increasing temperature. The temperature corresponding to the maximum \( \sigma_{yy} \) is gradually shifted from 35 K under \( B = 1 \) T to 85 K under \( B = 9 \) T.

The adiabatic Seebeck thermopower \( S_{xx} \) below 100 K is very small under \( B = 0 \) T (Fig. 3b), with the absolute value \(|S_{xx}|\) less than 5 \( \mu \)VK\(^{-1}\). Below 100 K, it increases modestly with increasing magnetic field, with the peak value around 20 \( \mu \) VK\(^{-1}\) even under \( B = 9 \) T. Above 100 K, the \(|S_{xx}|\) increases with increasing temperature, but the maximum is still much lower than those of conventional TE materials. Such low \( S_{xx} \) values are consistent with the semimetal feature of NbSb\(_2\) (Fig. 2c).

Figure 3c shows the temperature dependence of adiabatic Nernst thermopower \( S_{yx} \) of single-crystalline NbSb\(_2\). Under a magnetic field, the absolute value of \( S_{yx} \) initially increases with increasing temperature, reaches the maximum value of around 21 K, and then decreases at higher temperatures. Similar behavior is observed when the direction of the magnetic field is reversed, with the sign of \( S_{yx} \) is reversed accordingly. The maximum \( S_{yx} \) is about 616 \( \mu \)K\(^{-1}\) under 9 T at 21 K, about 30 times of the maximum \( S_{xx} \). Likewise, as shown in Supplementary Note 2, the thermal Hall effect has little influence on the \( S_{yx} \) measurement.

The adiabatic Nernst power factor \( PF_{xy} \) of single-crystalline NbSb\(_2\) under different magnetic fields is shown in Fig. 3d. The \( PF_{xy} \) firstly increases with increasing temperature, reaches a peak

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**Fig. 2 | Crystal structure and band structure of NbSb\(_2\). a** Crystal structure of NbSb\(_2\) from different perspectives. **b** Optical image of NbSb\(_2\) single crystal grown in this work. The inset shows the measurement direction of the Nernst thermopower. **c** Calculated band structure, density of states, and **d** Fermi surface with the spin–orbit coupling (SOC) for NbSb\(_2\). The red and blue pockets denote the hole and electron pockets, respectively.
around 24 W m\(^{-1}\)K\(^{-1}\) at 15.9 K\(^2\). As shown in Fig. 1c, this value is much higher than those of single-crystalline NbSb\(_2\). When the magnetic field is increased to 3 T, the \(\kappa_{xx}\) is further decreased. However, under a higher magnetic field, the \(\kappa_{xx}\) is almost unchanged. Such \(\kappa_{xx}\) reduction under magnetic field is caused by the suppression of the contribution of carriers in thermal transports. Moreover, as shown in Supplementary Fig. 6, the estimated isothermal \(\kappa_{xx}\) is slightly smaller than the measured adiabatic \(\kappa_{xx}\).

Figure 3e shows the adiabatic transverse thermal conductivity \(\kappa_{xx}\) of single-crystalline NbSb\(_2\) from 5 to 300 K measured by using the four-probe method. At \(B = 0\), the \(\kappa_{xx}\) increases with increasing temperature, reaches a peak of 90 W m\(^{-1}\)K\(^{-1}\) around 30 K, and then decreases with further increasing temperature. At 300 K, the \(\kappa_{xx}\) is around 24 W m\(^{-1}\)K\(^{-1}\), which is much higher than those of the TE materials for Peltier refrigeration, such as 1290 W m\(^{-1}\)K\(^{-1}\) for single-crystalline NbP under 8 T\(^3\), 1586 W m\(^{-1}\)K\(^{-1}\) for single-crystalline TaP under 9 T\(^2\), and 215 W m\(^{-1}\)K\(^{-1}\) for single-crystalline WTe\(_2\) under 9 T\(^2\). When the magnetic field is applied, the \(\kappa_{xx}\) of single-crystalline NbSb\(_2\) at low temperatures is significantly decreased. As shown in Supplementary Fig. 5, the \(\kappa_{xx}\) at 5 K is 35.9 W m\(^{-1}\)K\(^{-1}\) when \(B = 0\), but only 2.7 W m\(^{-1}\)K\(^{-1}\) when \(B = 1\) T. When the magnetic field is increased to 3 T, the \(\kappa_{xx}\) is further decreased. However, under a higher magnetic field, the \(\kappa_{xx}\) is almost unchanged. Such \(\kappa_{xx}\) reduction under magnetic field is caused by the suppression of the contribution of carriers in thermal transports. Moreover, as shown in Supplementary Fig. 6, the estimated isothermal \(\kappa_{xx}\) is slightly smaller than the measured adiabatic \(\kappa_{xx}\).

The measured \(\kappa_{xx}\) in Fig. 3e is mainly composed of the lattice thermal conductivity \(\kappa_l\) and carrier thermal conductivity \(\kappa_c\). Under magnetic field, their relationship can be expressed by the empirical formula\(^{10,12,14}\)

\[
\kappa_{xx}(B,T) = \kappa_l(T) + \kappa_c(B,T) = \kappa_l(T) + \frac{\kappa_{xx}(0,T)}{1 + \eta B^s}
\]

where \(\eta\) and \(s\) are the two factors related to the thermal mobility and scattering mechanism, respectively. The increase of \(B\) will suppress the contribution of carriers, which is responsible for the reduction of \(\kappa_{xx}\).
under high magnetic field (Fig. 3e). By using Eq. (2), the measured \( \kappa_{xx} \) data of NbSb\(_2\) under different \( B \) and \( T \) are fitted. The fitting results are shown in Supplementary Fig. 5a and Supplementary Table 1. The \( \kappa_{xx} \) increases with increasing temperature, reaching the maximum around 25 K, and then decreases at a higher temperature. The maximum is caused by the transition from the \( \kappa_{xx} - T^2 \) dependence at low temperature to \( \kappa_{xx} \) dependence at high temperature \(^{45}\). Based on the fitted \( \kappa_{xx} \), the Lorenz number \( L \) can be calculated from the Wiedemann–Franz law. As shown in Supplementary Fig. 5b, the \( L \) at low temperatures is significantly lower than the Sommerfeld value \( L_{ff} = 2.44 \times 10^{-4} \text{W K}^{-2} \), indicating the violation of Wiedemann–Franz law. The ratio of the Lorenz number to Sommerfeld value \( (L/L_{ff}) \) decreases from around 1 to near room temperature to the minimum value of 0.29 at \( T = 15 \) K, and then increases at a lower temperature, reaching 0.39 at 5 K. This trend is similar to the phenomenon found in WP2 by Jaoui et al.\(^{46}\). The violation of WF law might be caused by the inelastic scattering of carriers, while the upturn of \( L/L_{ff} \) at low temperatures can well satisfy the requirement of refrigeration below liquid nitrogen temperature.\(^{26}\)

Furthermore, the mechanical workability of NbSb\(_2\) single crystal is very high. Due to the enhanced magnetic field, the upturn of \( L/L_{ff} \) at low temperatures can well satisfy the requirement of refrigeration below liquid nitrogen temperature. In a two-carrier model with constant relaxation time approximation and under the ideal conditions of \( n_e = n_h \) and \( \mu_e = \mu_h = \mu \), the \( S_{yx} \) can be expressed as

\[
S_{yx} = \frac{\mu B}{2} \left( \frac{S_{xx}^h - S_{xx}^e}{S_{xx}^h} \right) \tag{5}
\]

where \( S_{xx}^h \) and \( S_{xx}^e \) are the Seebeck thermopower of electrons and holes under the magnetic field \( B \), respectively. The details about how Eq. (5) is obtained can be found in Supplementary Note 3. Different from the one-carrier model in which a saturated \( S_{yx} \) is observed under large magnetic field, the two-carrier model based on Eq. (5) gives an unsaturated \( S_{yx} \) when magnetic field increases, which is consistent with the measured \( S_{yx} \) vs. \( B \) behavior of single-crystalline NbSb\(_2\) shown in Fig. 4a.

The inset in Fig. 4d shows that the \( S_{yx} \) and \( \mu \) of single-crystalline NbSb\(_2\) are very low at low temperature, reaching \( \mu_e = 2.1 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) and \( \mu_h = 1.2 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) at 5 K. These values are comparable with the high mobility found in the extremely large magnetoresistance materials, such as Cd\(_3\)As\(_2\) (\( \mu_e = 6.5 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) and \( \mu_h = 0.5 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) at 10 K)\(^{10}\), PtSn\(_4\) (\( \mu_e = 7.6 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) and \( \mu_h = 7.6 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) at 2 K)\(^{22}\), LaBi (\( \mu_e = 2.6 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) and \( \mu_h = 3.3 \text{m}^2 \text{V}^{-1} \text{s}^{-1} \) at 2 K)\(^{22}\). The observed high \( \mu_e \) and \( \mu_h \) are also consistent with the Dirac-like band dispersion of NbSb\(_2\) near the Fermi level (Fig. 2c). The large \( \mu_e \) and \( \mu_h \) are one important reason for the large \( S_{yx} \) of single-crystalline NbSb\(_2\).

In addition, it is instructive to plot \( (S_{xx}^h - S_{xx}^e) \) of single-crystalline NbSb\(_2\) under different temperatures and magnetic fields. In Fig. 4e, \( (S_{xx}^h - S_{xx}^e) \) shows a local peak at 25 K, which is believed to have a consequence for the observed colossal Nernst power factor. In thermoelectrics, such extra-large thermopower peak at low temperature is usually caused by the phonon-drag effect\(^{15}\). With increasing temperature, the phonons with higher momentum are excited. When the momentum of the long-wave acoustic phonons is similar with that of the carriers on the Fermi surface, the phonon-drag effect occurs, leading to the appearance of a peak in the Seebeck thermopower curve at low temperature. The Seebeck thermopower of a material can be written as \( S_{xx} = S_{xx}^e + S_{xx}^p \), where \( S_{xx}^p \) is related to the charge carrier diffusion processes and \( S_{xx}^e \) is related to phonons. In a degenerate limit, the \( S_{xx} \) usually has linear temperature dependence\(^1\). The estimation details of \( S_{xx}^e \) and \( S_{xx}^p \) are shown in Supplementary Note 4. However, as presented in Supplementary Fig. 9, both \( S_{xx}^e \) and \( S_{xx}^p \) deviate off the linear temperature dependence below 100 K, indicating the non-negligible \( S_{xx}^e \) in single-crystalline NbSb\(_2\) at low temperatures. By subtracting the \( S_{xx}^e \) from the \( S_{xx} \), the \( S_{xx}^p \) can be estimated, with the details shown in Supplementary Note 5. As shown in Fig. 4f, the absolute values of \( S_{xx}^e \) and \( S_{xx}^p \) show the maxima of value at 75 K and 193 K at 25 K, much larger than the \( S_{xx}^p \) (5.4 mK V\(^{-1}\)) and \( S_{xx}^p \) (3.6 mK V\(^{-1}\)) at the same
temperature, respectively. Consequently, the synergistic effect of $S_{e}$ and $S_{h}$ greatly improves the total Ettingshausen effect in the single-crystalline NbSb$_2$. At higher temperature, the phonon-drag effect is quickly weakened since the significantly excited high-frequency phonons lead to the reduction of the relaxation time of long-wave acoustic phonons. Thus, the $S_{e}$ and $S_{h}$ are quickly decreased after reaching the maxima values. Above 125 K, the electrical transports are mainly determined by the carrier diffusion process. At this time, the measured $\rho_{yx}$ is comparable with the theoretical value of $283 \mu^2/\Omega\cdot m$ (Supplementary Fig. 10), where $\mu = 1200$ K is derived from the relation $E_F = \frac{1}{2m}(3\pi^2n)^{2/3}$ (see ref. 55), with the carrier concentration $n$ equaling to $1.5 \times 10^{20}$ cm$^{-3}$ and $m$ equalling to the free electron mass $m_0$. These prove that the fitted $\mu$ and $n$ in Fig. 4d are reasonable.

**Discussion**

In summary, we report a colossal Nernst power factor of $3800 \times 10^{-4}$ W m$^{-1}$ K$^{-2}$ under 5 T at 25 K and a high Nernst figure-of-merit $z_n$ with of $71 \times 10^{-4}$ K$^{-1}$ under 5 T at 20 K in single-crystalline NbSb$_2$. There are a number of factors synergistically contributed to the large and unsaturated Nernst thermopower $S_{yx}$ under magnetic field: (1) a favorable band structure providing nearly identical electron and hole concentrations at Fermi level, (2) extraordinary high electron and hole mobilities benefiting from the Dirac-like dispersion of low energy excitations common to several well-known topological semimetals, and (3) strong phonon-drag effect. The phonon-drag effect derived from our data analysis suggests phonon can play an important role in the transport process of Dirac fermions, which is another interesting phenomenon worth of further investigation. This work provides a new material option for the solid-state heat pumping below liquid nitrogen temperature.

**Methods**

**Sample synthesis**

NbSb$_2$ single crystal was synthesized by the chemical vapor transport method in two steps. First, the polycrystalline powder was synthesized by solid-state reaction. The niobium powder (alfa, 99.99%) and antimony shot (alfa, 99.9999%) with stoichiometry 1:2 was encapsulated in a vacuum quartz tube and reacted at 1023 K for 48 h. Next, the polycrystalline NbSb$_2$ powders and 0.3 g iodine were sealed in another vacuum quartz tube. The quartz tube was placed in a horizontal furnace with a temperature gradient for 2 weeks. The hot end temperature and cold end temperature of the quartz tube are 1373 K and 1273 K, respectively. Finally, shiny and bar-like single crystals appear in the cold end of the quartz tube.
Characterization and transport property measurements

The phase composition of the single-crystalline NbSb2 was characterized by X-ray diffraction (XRD, D/max-2550 V, Rigaku, Japan) and scanning electron microscopy (SEM, ZEISS supra-55, Germany) with energy-dispersive X-ray spectroscopy (EDS, Oxford, UK). The electrical and thermal transport properties of single-crystalline NbSb2 were measured under the magnetic field by using physical property measurement system (PPMS, Quantum design, USA). The alternating current was used in the electrical conductivity measurement with the purpose to eliminate the thermal Hall effect. The transverse resistivity and Hall resistivity were measured by the four-probe method and the measurement system (PPMS, Quantum design, USA). The alternating current was measured under the magnetic field was applied in the z direction perpendicular to the bc plane. In addition, comparing with the thermal conductivity of the sample with and without adhering Cu wires (Supplementary Fig. 12), it is concluded that the Cu wires have little influence on the measurement.

Calculation

First-principles calculations were carried out using Quantum espresso software package with the lattice parameters given in the materials project[25] Perdew-Burke-Emzerhof (PBE) exchange-correlation functional[26] within the generalized gradient approximation (GGA) and fully relativistic norm-conserving pseudopotentials generated using the optimized norm-conserving Vanderbilt pseudopotentials[27] were used in the calculations. The primitive Brillouin zone was sampled by using a 10 × 10 × 10 Monkhorst–Pack k mesh, and a plane-wave energy cut-off of 900 eV was used. The Fermi surface calculation was performed on a dense k mesh of 41 × 41 × 41 and was visualized by using Xcrysd software[28]. The QE calculations were also verified using the projector-augmented wave (PAW)[29] method as implemented in the Vienna ab initio simulation package (VASP)[30] which gave similar results.

Data availability

The data generated in this study are provided in the Source Data file. Source data are provided with this paper.

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Author contributions
P.L., P.Q., and X.S. designed the experiment. P.L. synthesized the samples and performed the transport property measurements, with the help of Q.X. and J.X., and N.A. provided band structure calculations. P.L., Q.X., J.X., and Y. X. analyzed the transport properties based on the two-carrier model. P.L., P.Q., Q.L., L.C., and X.S. analyzed the data and wrote the manuscript.

Competing interests
The authors declare no competing interests.

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Correspondence and requests for materials should be addressed to Pengfei Qiu or Xun Shi.

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