The study on quantum spin Hall effect and topological insulators formed the prologue to the surge of research activities in topological materials in the past decade. Compared to intricately engineered quantum wells, three-dimensional weak topological insulators provide a natural route to the quantum spin Hall effect, due to the adiabatic connection between them and a stack of quantum spin Hall insulators, and the convenience in exfoliation of samples associated with their van der Waals-type structure. Despite these advantages, both theoretical prediction and experimental identification of weak topological insulators remain scarce. Here, based on first-principles calculations, we show that AuTe$_2$Br locates at the boundary between a strong and a weak topological semimetal state. We identify the key structural parameter that dictates the traversal of the topological transition, which can be easily realized in experiments. More interestingly, the critical topology of AuTe$_2$Br persists up to an applied pressure of ~15.4 GPa before a structural phase transition accompanied by a change of electronic topology and the onset of superconductivity. Our results establish AuTe$_2$Br as a new candidate for an effective tuning between weak and strong topological phases in a single material, with the potential to realize various other topological phases of matter.

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WTI state. Despite its sensitivity to structural variations, the critical topology is found to persist up to an applied pressure of ~15.4 GPa, where a pressure-induced structural phase transition from \textit{Cmc2} to \textit{Pmmm} occurs. The low-pressure TI phase emerges from a topological nodal-line metal (TNLM) protected by mirror symmetry when the spin-orbit coupling (SOC) is ignored. In contrast, the high-pressure phase in the absence of SOC is a TNLM stabilized by a distinct mechanism due to the combination of the mirror-reflection and space-time-inversion symmetry. Furthermore, superconductivity is observed in a wide pressure range in the high-pressure phase. By a scrutinization on the structural parameters that dictate the topological transition between the strong and weak topological phases, our results add another candidate to the list of WTI and hence QSH insulators via proper tuning. Our work also provides a fertile playground for the exploration of topological phase transitions and topological superconductivity.

**RESULTS**

**Critical topology at ambient pressure**

\textit{AuTe}_2\textit{X} (\textit{X} = \textit{Cl}, \textit{Br}) crystallize in an orthorhombic structure, consisting of halogen atoms inserted between layers of \textit{AuTe}_2 networks stacking along the \textit{b} axis (Fig. 1a), despite their space groups differing from each other—\textit{Cmcm} (No. 63) and \textit{Cmc2} (No. 36) for \textit{Cl}, and \textit{Br}, respectively\textsuperscript{26–29}. The topological properties of \textit{AuTe}_2\textit{X} remained unexplored until recently\textsuperscript{29,30}. Transport measurements revealed the compensated semimetal nature of \textit{AuTe}_2\textit{Br} with ultrahigh carrier mobility of \textit{~105 cm}^2\textit{V}^{-1}\textit{s}^{-1} and a nonsaturated magnetoresistance reaching \textit{~3 × 105} at 4.2 K and 58 T\textsuperscript{29}. More interestingly, it was proposed that the QSH effect can be realized in monolayer \textit{AuTe}_2\textit{Cl} through the confinement effect\textsuperscript{30}. Our calculations on the band structure of bulk \textit{AuTe}_2\textit{Cl} (Supplementary Fig. 1) give unanimously a topological nontrivial gap along the \textit{\Gamma–Y} direction and a \textit{Z2} of (1; 110), regardless of whether Expt. or Opt. structural parameters are used, confirming the STI nature of \textit{AuTe}_2\textit{Cl}. Note that such an STI is topologically

![Fig. 1 Band structure calculations for AuTe2Br without spin-orbit coupling (SOC). a Crystal structure of AuTe2Br with the Cmc2 space group. \textit{h}_{layer}, \textit{d}_{layer}, and \textit{h}_{layer} = \textit{d}_{layer} + \textit{h}_{layer} represent the height of an Au–Te layer (i.e., the vertical distance along \textit{b} between the top and bottom Te atoms in the same Au–Te layer), the vertical distance between the top Te atom in one Au–Te layer and the bottom Te atom in the Au–Te layer above the previous one, and the vertical distance between two adjacent AuTe2Br layers, respectively. b The 3D bulk Brillouin zone (BZ). c–e are the calculated band structure, orbital-projected band structures along the \textit{\Gamma–Y–K} directions, and the energy difference map between the Au \textit{d}_{xz+yz} and Te \textit{p}_z bands in the \textit{\Gamma–Y–K} plane of the BZ for AuTe2Br with experimental (Expt.) structural parameters, respectively. f–h are those results with fully optimized (Opt.) structural parameters. The contour of the nodal ring is shown by the red line in (e) and (h). The background color represents the magnitude of the gap between the Au \textit{d}_{xz+yz} and Te \textit{p}_z bands. With the gap increasing, the color changes from white to blue. Red ellipse highlights the zero gap.](image-url)
equivalent to the topological semimetal suggested by previous studies, if a curved chemical potential between valence and conduction bands is defined. Considering that some bands in AuTe2Br intersect the Fermi level, in the following we adopt the terms strong topological semimetal (STSMT) and weak topological semimetal (WTSM) to avoid ambiguity. The topological properties are not affected by the semimetallic nature, and the approaches in the study of STI and WTI can be naturally utilized in our case.

Our calculation results for AuTe2Br in the monolayer limit are presented in Supplementary Fig. 2. Fully optimized structure parameters are adopted for the monolayer, giving relaxed lattice constants close to the experimental values for the bulk counterpart. Similar to the case of monolayer AuTe2Cl, monolayer AuTe2Br is shown to be a 2D TI, rendering it a candidate platform for the study of QSH effect.

Turning to the bulk AuTe2Br, the calculation results in the absence of SOC are shown in Fig. 1c–h for Expt. and Opt. structural parameters, respectively. The results are similar for the two sets of parameters. We find a metallic ground state with electron pockets at the X and M points and hole pockets at the Γ and Y points. The bands exhibit crossing points in the high symmetry directions Γ–Y and Y–K that are tied to the ΓYKZ plane of the bulk Brillouin zone. By projecting the states onto atomic orbitals, we find that the two bands forming the crossing points are contributed by the Au d_{xy} + Te p_y orbital and Te p_z orbital, respectively, as shown in Fig. 1d, g. The band order is inverted around the Y point, indicating a nontrivial topology. Due to the presence of mirror symmetry associated with the ΓYKZ plane, the crossing points actually form a nodal line in this plane centering around Y, as depicted in Fig. 1e, h.

The calculation results for the band structure of bulk AuTe2Br with SOC included are shown in Fig. 2a, h for Expt. and Opt. structural parameters, respectively. The nodal line is gapped for both cases. Surprisingly, however, topologically distinct results are found for the two sets of parameters. Before structural optimization, there is a gapped Dirac cone arising from the band hybridizations between Au d_{xy}, Te p_y orbitals along Γ–Z, resulting in inverted bands at the Y point (Fig. 2b). With structural optimization, the band order at Γ is inverted as well (Fig. 2f). To further characterize the band topology, the Wannier charge centers (WCC) evolution on the time-reversal invariant planes is calculated using the Wilson loop method, as shown in Fig. 2c. In a WCC plot, the Z indices can be obtained by counting the number of times the WCC curves intersect with any arbitrary horizontal reference line. For example, for the k_z = 0 plane, no intersection is found so that the associated Z = 0 [the top left panel in Fig. 2c], while for the k_z = 0.5 plane, one intersection is found so that the associated Z = 1 [the top right panel in Fig. 2c]. For a 3D TI, Z is determined by the parity of the sum of the Z indices associated with all the k_i = 0 (i = x, y, z) planes. For the Expt. and Opt. case, respectively, we get Z = 1 (1:110) and Z = 0 (0:110) and, thus, an STI (STSM) state and a WTI (WTSM) state. This is also reflected in the calculated surface states on the (001) projected surface (note that this is a side surface): one Dirac point is pinned at Y for the Expt. case (Fig. 2d), while two Dirac points are pinned at Γ and Y for the Opt. case (Fig. 2h).

**Tuning between the strong and weak topological phases**

The dichotomy between the two cases indicates that AuTe2Br exhibits a critical topology, where the balance is tipped towards an STSM or a WTSM state by a small variation in the crystal structure. It is therefore interesting to study how the band topology evolves under hydrostatic pressure. To obtain the structural parameters under pressure, high-pressure x-ray diffraction (XRD) measurements were performed, and the results are displayed in Fig. 3a. With increasing pressure, the Cmc2_1 phase persists up to ~18.8 GPa. Upon further compression, new diffraction peaks emerge, indicative of a structural phase transition. Enthalpy calculations show that above 15 GPa, the
Pmmm symmetry is favored (Fig. 3b, c). No imaginary modes are found in the phonon calculations above 20 GPa (Supplementary Fig. 4), confirming the robust dynamic stability of this Pmmm phase under high pressure. The lattice constants extracted from Rietveld refinements are displayed in Fig. 3d, showing a drastic drop of b across the structural transition.

The band structure under pressure before the structural transition is shown in Supplementary Fig. 5. With increasing pressure, the band dispersion along Γ–Y increases. However, for both Expt. and Opt. structural parameters, the band order at Γ and Y is maintained. In other words, the critical topology of AuTe2Br between an STSM and WTSM is robust against pressure, provided the space group stays the same.

At first glance, this seems to be inconsistent with the fact that the band topology is sensitive to variations in structural parameters. To solve this apparent discrepancy, we investigate the relation between the critical topology and the structural parameters. As discussed above and schematically shown in Fig. 2b, f, the key difference between an STI and WTI state is the band order at Γ. We plot for AuTe2Cl and AuTe2Br the dependence of the energy difference of the two bands at Γ, \[ \Delta E_\Gamma \equiv E(\text{Au } d_{xz/yz}) - E(\text{Te } p_z) \], on representative structural parameters (Fig. 4, see Fig. 1a).
for the definition of these parameters]. AuTe₂Cl being an STSM is robust against structural variations. For AuTe₂Br, with Expt structural parameters, the pressure-induced decreasing of $h_{\text{layer}}$ pushes the data points under pressure to the left of the ambient pressure data point Br (Expt.) (Fig. 4a), meaning that AuTe₂Br is always an STSM.

However, for the Opt. case, as shown in Fig. 4a, one would expect a transition from WTS to STSM with the considerable pressure-induced decreasing of $h_{\text{layer}}$ since the ambient pressure data point Br (Opt.) is already very close to the boundary. Such a transition is not observed in our calculations (Supplementary Fig. 5). This may be explained by the counteracting effect of the pressure evolution of another parameter, namely, $d_{\text{layer}}$. As shown in the inset to Fig. 4(b), $\Delta E_{\text{f}}$ evolves with $d_{\text{layer}}$ in a similar fashion to the case of $h_{\text{layer}}$, but $d_{\text{layer}}$ itself increases with pressure.

To allow for a more direct comparison with future experiments that utilize the tuning of structural parameters to traverse the boundary between the strong and weak topological phases, we define a more experimentally-relevant parameter $L_{\text{layer}} = d_{\text{layer}} + h_{\text{layer}}$. As shown in Fig. 4c, starting from Br (Expt.), a WTS state may be achieved by increasing $L_{\text{layer}}$, which can be realized by, e.g., tensile strain along $b$, or intercalation between the Au and Te layers. This adds AuTe₂Br as another example of readily achievable topological transition between strong and weak phases to the existing case of ZrTe₅.

Topology and superconductivity in the high-pressure phase
We now turn to the band topology of the high-pressure $Pnmm$ phase. In the absence of SOC, the band structure exhibits a 3D metallic nature with some bands featuring large energy dispersion across the Fermi level (Fig. 5a). The 3D Brillouin zone is shown in Fig. 5b. There are two band crossings along two paths in the $k_z = 0$ plane, $\Gamma-Z$ and $\Gamma-T$ (Fig. 5c). The crossings are attributed mainly to the Te-$p_z$ and $p_x$ orbitals. At $\Gamma$, the $p_x$ band lies above $p_y$, which is a signature of band inversion, implying the nontrivial band topology of the $Pnmm$ phase. Moreover, due to the recovery of the inversion symmetry in this phase, a mechanism different from the ambient pressure one dictates the presence of a nodal line in the $k_z = 0$ plane and centering around $\Gamma$ (Fig. 5d). Here, the nodal line is protected by the combination of the space-time-inversion symmetry and mirror-reflection symmetry$^{34,35}$. With the inclusion of SOC, the nodal line is fully gapped with a gap size of ~0.02 eV, as shown in Fig. 5a. The (100) surface band structures are shown in Fig. 5e. Outside the projection of the nodal line crossings, the surface bands disperse upwards when SOC is ignored. Taking SOC into account, there is a metallic surface band connecting the projected bulk valence and conduction bands. This surface band exhibits spin-momentum-locked spin textures, as displayed in Fig. 5f. To further characterize the band topology, the WCC evolution on the time-reversal invariant planes is calculated (Supplementary Fig. 6), and the $Z_2$ index is determined to be (1;001), indicative of strong topological nature of high-pressure $Pnmm$ phase of AuTe₂Br.

In addition to the nontrivial band topology, we observed superconductivity in a wide pressure range in the $Pnmm$ phase. Temperature-dependent resistance data for AuTe₂Br single crystals are shown in Fig. 6a. A superconducting transition emerges at ~19 GPa and persists to the highest pressure of ~51 GPa we measured. We then check the superconducting transition under magnetic field (Fig. 6b) and obtain the upper critical field $H_{c2}$ at various pressures (Fig. 6c). The pressure dependence of the superconducting transition temperature $T_c$ is summarized in Fig. 6d. Nevertheless, the nontrivial band topology of AuTe₂Br leaves the possibility of topological superconductivity an interesting topic for future studies.

**DISCUSSION**
In summary, AuTe₂Br is proposed as a new platform for the exploration of WTI states based on our first-principles calculations.
Nontrivial topology was found both for the ambient pressure phase and the phase after a pressure-induced structural phase transition, the latter accompanied by superconductivity observed in our measurements. Importantly, our calculations also demonstrate the promising possibility of investigating QSH effect in monolayer AuTe$_2$Br, which can be readily obtained due to the van der Waals-type structure.

The fact that AuTe$_2$Br lies in close proximity to the topological transition between an STSM and WTSM state holds substantial potential in the continuous tuning of such a transition. Although we have shown that pressure may not be the ideal tuning knob, probably as a result of an opposite trend in the pressure evolution of structural parameters determining the electronic topology, we demonstrate that specifically designed variation of a key parameter, i.e., the distance between adjacent Au-Te layers, can serve this purpose. This may be achieved by intercalation, strain, etc. It would then be more interesting to see how superconductivity is affected when the topological transition is traversed.

**METHODS**

Sample synthesis and magneto-resistivity measurements

AuTe$_2$Br single crystals were synthesized, as described in ref. 30. The as-grown single crystals are soft, silver flakes with high quality, and the biggest natural plane is (010) plane (see Supplementary Fig. 3a). Magneto-resistivity measurements under ambient pressure were performed in a physical property measurement system (PPMS; Quantum Design).

Resistance measurements under pressure

High-pressure resistance measurements were performed on AuTe$_2$Br single crystals with silicone oil as the pressure transmitting medium (denoted as S1, S2, and S3 for different runs) by using a diamond anvil cell (DAC). The experimental pressures were determined by the pressure-induced fluorescence shift of ruby at room temperature before and after each experiment. A direct current four-probe technique was adopted. Resistance measurements were performed with a PPMS.

**XRD measurements under pressure**

AuTe$_2$Br single crystals were ground into powder by using a mortar for use in the high-pressure synchrotron angle-dispersive X-ray diffraction measurement. The high-pressure synchrotron XRD experiments were carried out using a symmetric diamond anvil cell (DAC) with a 300-micron cuvet diamond. A rhenum gasket was drilled by laser with a 90-micron diameter hole as the sample chamber. The sample chamber was filled with a mixture of the sample, a ruby ball, and silicone oil as the pressure transmitting medium. The experimental pressures were determined by the pressure-induced fluorescence shift of ruby. Synchrotron angle-dispersive XRD measurements were carried out at beamline BL15U1 of the Shanghai Synchrotron Radiation Facility (SSRF) using a monochromatic beam of 0.6199 Å. The diffraction patterns were integrated by using the Dioptas software, and Rietveld refinement was performed by using the GSAS software.

Electronic band structure of AuTe$_2$X ($X = \text{Cl, Br}$)

We carried out first-principles calculations within the framework of the projector augmented-wave (PAW) method$^{36}$, as implemented in the Vienna Ab initio Simulation Package (VASP)$^{37,38}$. A kinetic energy cutoff of 500 eV and a Γ-centered k mesh of $11 \times 11 \times 7$ were selected in all calculations. The energy and force convergence criterion were defined as $10^{-6}$ eV and 0.01 eV/Å for self-consistent convergence. The van der Waals (vdW) corrections$^{39,40}$ and spin-orbit coupling (SOC) effect are considered for all calculations. The electronic band structure for AuTe$_2$X ($X = \text{Cl, Br}$) were calculated with experimental structure and fully optimized lattice parameters (PBE + D2). PBE + D2 represents Perdew–Burke–Ernzerhof (PBE)$^{41}$, generalized gradient approximation (GGA) functional with D2 empirical vdW corrections$^{41}$. The WANNIER90 package$^{42-44}$ was adopted to construct Wannier functions from the first-principles results without an iterative maximal-localization procedure. The

**Fig. 6** Pressure-induced superconductivity in AuTe$_2$Br. a Temperature dependence of the resistance of AuTe$_2$Br single crystals with silicone oil as the pressure transmitting medium. S1, S2 and S3 represent different runs. b Magnetic field dependence of the superconducting transition of AuTe$_2$Br single crystal (S2) at 27.8 GPa. The superconducting transition temperatures $T_c$ are defined as shown in the panel. c Temperature dependence of the upper critical field $B_{c2}$. Solid lines are a guide to the eye. d Pressure dependence of $T_c$. 

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High-pressure structure calculations for AuTe₂Br

Beyond the pressure where a pressure-induced structural phase transition takes place, we performed a high-pressure crystal structure searching of AuTe₂Br by using an in-house program called MAGUS (machine learning and graph theory assisted universal structure searcher), which is accelerated by the employment of Bayesian optimization and graph theory. This method has been successfully applied in many systems under high pressure, such as compounds inside plants and layered materials [46-49]. The structural optimization and electronic structure calculations were carried out within density functional theory using the projector augmented-wave method as implemented in the VASP. We chose $\text{s}^1\text{p}^2$, $\text{s}^2\text{p}^4$ and $\text{s}^2\text{p}^6$ as the valence electrons for Au, Te and Br respectively while using the GGA in the PBE exchange-correlation functional. The plane-wave cutoff was set as 340 eV and the Brillouin zone (BZ) was meshed choosing the gamma-centered functional. The cell parameters of AuTe₂Br under lower pressure (Expt.) and fully optimized lattice parameters (Opt.), respectively. The cell parameters of AuTe₂Br and AuTe₂I demonstrated a slight decrease in the lattice parameters under pressure. The lattice constants of AuTe₂Br are 5.37 × 0.025 Å⁻¹ and 5.44 × 0.025 Å⁻¹ respectively. The cell volume of AuTe₂Br decreased from 309 Å³ at 0 GPa to 293 Å³ at 15 GPa.

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DATA AVAILABILITY

Source data that support the plots within the paper and other findings of this study are available from the corresponding authors upon reasonable request.

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AUTHOR CONTRIBUTIONS
E.J.C. conceived the idea and designed the experiments. E.J.C. and L.M.Y. were responsible for electrical transport experiments under high pressure. X.B.S. and W.W.Z. performed the electronic band calculations for topology. T.H.H. and J.S. conducted the DFT calculations for high-pressure structure searching. L.M.Y., F.L.L. and W.G.Y. performed XRD measurements under high pressure. W.L.M., Z.J.W. and S.J. grew single crystals. E.J.C., X.B.S. and Y.X. analyzed the data and wrote the paper. X.B.S., Y.X., W.G.Y. and S.Y.L. supervised the project. E.J.C., X.B.S. and L.M.Y. contributed equally to this work. All authors discussed the results and commented on the manuscript.

COMPETING INTERESTS
The authors declare no competing interests.

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