

Interaction-Driven Topological Transitions in Monolayer TaIrTe₄

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(Received 7 July 2025; revised 26 February 2026; accepted 18 May 2026; published 24 July 2026)

Discovering materials that combine topological phenomena with correlated electron behavior is a central pursuit in quantum materials research. Monolayer TaIrTe₄ has recently emerged as a promising platform in this context, hosting robust quantum spin Hall insulator (QSHI) phases both within a single-particle gap and within a correlation-induced gap arising from van Hove singularities (vHSs), accessed via electrostatic doping. Its intrinsic monolayer nature offers exceptional tunability and the potential to realize a rich variety of interaction-driven topological phases. In this work, we combine theory and experiment to map the phase landscape of monolayer TaIrTe₄. Using Hartree-Fock calculations, we investigate the interaction-driven phase diagram near the vHSs under commensurate filling conditions. By systematically tuning the dielectric screening and strain, we uncover a rich set of ground states—including QSHI, trivial insulator, higher-order topological insulator, and metallic phase—among which are interaction-driven topological phase transitions. Experimentally, we perform local and nonlocal transport measurements across a broad set of devices. Because of unavoidable strain variations during fabrication, the devices exhibit several distinct transport regimes, whose evolution is consistent with the theoretically predicted phase diagram. Finally, band-projected exact diagonalization together with insulating transport features at fractional fillings provide preliminary signatures consistent with a time-reversal-symmetric fractional QSHI in this system. Together, our results lay the groundwork for understanding correlation-driven topological phenomena in TaIrTe₄ and open new directions for engineering exotic quantum phases in low-dimensional materials beyond the limitations of moiré superlattices.

DOI: [10.1103/456g-q7bd](https://doi.org/10.1103/456g-q7bd)

Subject Areas: Condensed Matter Physics

I. INTRODUCTION

Enhanced electronic correlations, driven by high density of states (DOS) and suppressed kinetic energy, together

with nontrivial band topology, provide an ideal platform for realizing exotic quantum phases. Twisted and multilayer van der Waals systems—such as graphene and transition metal dichalcogenides (TMDs)—have emerged as leading platforms in this pursuit, enabling the realization of topological flat bands through stacking and twist-angle engineering. This approach has proven remarkably successful, giving rise to a wide range of correlated phases, including experimentally observed (fractional) topological insulators [1–8], (fractional) Chern insulators [9–13], and, theoretically, the potential realization of non-Abelian states [14–17].

On the other hand, there remains strong motivation to discover natural materials in which topology and correlated

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electrons are intrinsically intertwined—potentially offering enhanced energy scales and eliminating the need for fine-tuned twist angles or complex fabrication procedures. This raises a key question: are there alternative platforms beyond moiré for realizing interaction-driven topological phases? One promising route is to induce correlations through van Hove singularities (vHSs) or flat bands arising from geometric frustration in topological materials, as exemplified by kagome [18–23] and Lieb lattices [24–26], as well as systems like bismuth [27,28] and FeGe [29]. Monolayer TaIrTe₄ emerges as a compelling candidate in this landscape: a two-dimensional (2D) topological insulator with vHSs located near its single-particle topological gap. Initially predicted to be a quantum spin Hall insulator (QSHI) based on its band structure [30–32], recent experiments have not only confirmed this phase but also uncovered a correlated QSHI driven by electronic instabilities at the vHSs [4,8]. Compared to natural three-dimensional bulk systems, intrinsic monolayer TaIrTe₄ offers key advantages: its chemical potential can be precisely tuned to the vHSs via electrostatic gating—crucial for accessing correlation-driven electronic phases. Furthermore, its exposed surface allows for dielectric environment engineering, while its monolayer nature endows it with the capacity to sustain large strains, providing additional tunability. These features establish monolayer TaIrTe₄ as a uniquely versatile platform for exploring the interplay between topology and strong correlations. Unraveling this interplay is essential for uncovering new quantum phases and enabling next-generation electronic applications.

In this work, we systematically investigate the topological and correlated phase diagram in monolayer TaIrTe₄ combining theoretical, numerical, and experimental approaches. Starting with density functional theory (DFT) [33] and Lindhard susceptibility analysis, we identify a vHS-driven charge density wave (CDW) transition that leads to a 15×1 superlattice structure. To further explore the interaction-driven phases, we construct a minimal eight-band tight-binding model and apply a Hartree-Fock mean-field approach [34–36], focusing on the regime in which two additional electrons per supercell are introduced via electrostatic gating. Our calculations not only confirm the previously reported correlated QSHI near vHSs [4], but also predict an extended phase diagram featuring multiple electronic states. These include correlated metallic phases, trivial insulators, and higher-order topological insulators (HOTI), arising from topological phase transitions controlled by dielectric environment and onsite interactions.

To directly connect with experimentally accessible parameters, we further investigate uniaxial strain as an external tuning knob. Our theoretical results demonstrate that strain can induce topological phase transitions among the correlated states, offering a powerful route for experimentally engineering interaction-driven topological

phases [4,8,37–40]. Guided by these theoretical insights, we fabricated and studied over 100 monolayer TaIrTe₄ devices, performing both local and nonlocal transport measurements near vHSs. Interestingly, inherent strain variations introduced during device fabrication lead to distinct transport regimes that can be naturally interpreted within our theoretical phase diagram.

Our study bridges theoretical modeling and experimental observation, offering deep insights into the complex interplay of topology and electron interactions in TaIrTe₄. These findings position monolayer TaIrTe₄ as a compelling alternative platform to moiré systems for exploring interaction-driven quantum phases.

II. SINGLE PARTICLE PICTURE

A. Crystal structure and symmetries

As shown in Fig. 1(a), monolayer TaIrTe₄ has a space group of $P2_1/m$ (SG 11) according to Ref. [41]. Similar to monolayer 1T' WTe₂, Ta, and Ir atoms are aligned along the x direction, forming two one-dimensional metal chains. The key symmetries in TaIrTe₄ include lattice translations $t(\mathbf{R})$, with lattice vectors $\mathbf{R} = m\mathbf{a} + n\mathbf{b}$, where $\mathbf{a}$ and $\mathbf{b}$ are the primitive lattice vectors, mirror symmetry ($\mathcal{M}_x$), two-fold screw rotation $\tilde{C}_2 = t(\mathbf{R}_x/2)C_{2x}$ with a 180° rotation and a fractional lattice translation along $\mathbf{a}$, time-reversal symmetry $\mathcal{T}$, and spatial inversion symmetry $\mathcal{P}$. The

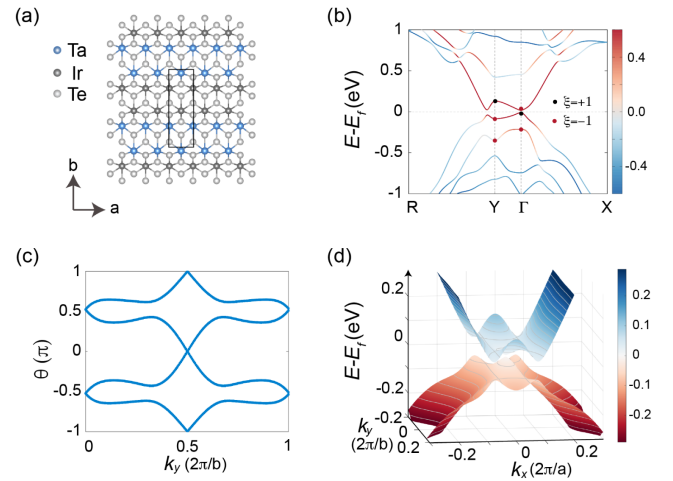


FIG. 1. Band structures and topological properties of monolayer TaIrTe₄ obtained from DFT calculations. (a) Schematic representation of the crystal structure, showing the arrangement of atomic sites. (b) DFT band structure along high-symmetry lines. The color gradient represents the weight differentiation between Ta and Ir + Te: red indicates a higher contribution from Ta, while blue signifies a dominant Ir and Te composition. The solid circles represent parities of bands around the Fermi level. (c) Wilson loop of four valence bands near the Fermi level along the k_y direction, indicating the topological nature of the bands. (d) Band structure of the lowest conduction and highest valence bands in the k_x - k_y plane.

presence of Ta chains suggests a strong electronic anisotropy, and the Ta atoms dominate the Fermi level, as further confirmed by our DFT analysis, making a significant contribution to the system's electronic susceptibility.

B. DFT band structure and topology

First, based on the above structural information, we perform DFT calculations of the lattice and electronic structures of 2D TaIrTe₄ using the Vienna *ab initio* simulation package (VASP). The relaxed lattice constants are $a = 3.816$, $b = 12.55$, and $c = 20$ Å (including vacuum), which agree well with experimental results [4] and other calculations [41]. Considering the effects of spin-orbit coupling (SOC), we calculate the band structure along the high-symmetry momenta with atom weights as shown in Fig. 1(b). The band gap is 21 meV at the Γ point, in agreement with experimental measurements [4].

To analyze the atomic and orbital contributions to the bands around the Fermi level, we define a weight differentiation between Ta and Ir + Te atoms as $w = w_{Ta} - (w_{Ir} + w_{Te})$, marked by color gradient, showing a higher contribution from Ta. By analyzing the orbital distribution, we find that Ta-5*d* orbitals dominate the orbital contributions around the Fermi level, specifically, the states of lowest conduction bands and highest valence bands are from the Ta's $d_{x^2-y^2}$, d_{yz} and d_{z^2} orbitals (see Appendix A for more details). Hence, we choose two *d* orbitals for our minimal tight-binding model in Sec. II C.

To determine the topological character of the bands, we calculate the parity eigenvalues (ξ) from the DFT wave functions at the time-reversal invariant momenta (TRIM), as indicated by the solid circles in Fig. 1(b). The number of inversion-odd Kramers pairs at the four TRIM Γ , X, Y, and R are 22, 22, 21 and 22, respectively. This leads to a QSHI with a $\mathbb{Z}_2$ invariant of $\nu_0 = 1$, indicating that the band inversion occurs at Y. As shown in Fig. 1(c), the Wannier center evolution of the four highest occupied valence bands is plotted over the full Brillouin zone ($0 \leq k_y \leq 2\pi$). Within the half Brillouin zone ($0 \leq k_y \leq \pi$), the Wannier centers exhibit an odd number of crossings at each phase θ , confirming the topological nature of the system with a $\mathbb{Z}_2$ invariant of 1. The vHS can be clearly seen in Fig. 1(d). Eight vHSs can be identified, with four in the conduction band and four in the valence band. These vHSs arise from the saddle points in the band structure, symmetrically distributed due to time-reversal symmetry $\mathcal{T}$ and mirror symmetry ($\mathcal{M}_x$).

C. Tight-binding band structure and topology

To enable subsequent many-body calculations in the CDW supercell, we construct a minimal tight-binding (TB) model guided by the DFT analysis above. Since our focus

lies on the low-energy physics near the vHS, we aim to develop a reduced model that faithfully captures the essential symmetries, topological features, and electronic structure of monolayer TaIrTe₄ near the Fermi level, while significantly reducing computational complexity. Based on the symmetry analysis in Sec. II A, we construct an eight-band tight-binding model from four orbitals. The general Hamiltonian is

$$\hat{H} = \sum_{\mathbf{R}_1, \mathbf{R}_2} \sum_{\alpha\beta s} t_{\alpha\beta}(\mathbf{R}_1 - \mathbf{R}_2) a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_2, \beta s} \quad (1)$$

where $\mathbf{R}_{1,2}$ are lattice vectors, and $t_{\alpha\beta}(\mathbf{R}_1 - \mathbf{R}_2)$ denotes the hopping amplitude (including the chemical-potential term). $a_{\mathbf{R}, \alpha s}^\dagger$ ($a_{\mathbf{R}, \beta s}$) is the creation (annihilation) operator at lattice site $\mathbf{R}$ with orbital index α and spin index s . Based on the crystal symmetry and DFT results reported above, we choose two *d* orbitals for each sublattice *A* and *B* [see Fig. 2(a)], where the basis is $(a_{Ad1s}, a_{Bd1s}, a_{Ad2s}, a_{Bd2s})$. In this basis, the matrix representations of the symmetry operations are $\Theta = is_y\tau_0\sigma_0\mathcal{K}$ for time-reversal symmetry, $P = s_0\tau_1\sigma_0$ for inversion symmetry, and $M_x = is_x\tau_0\sigma_0$ for mirror symmetry ($\mathcal{M}_x$). Therefore, the symmetry-allowed spin-orbital terms H_{SOC} are $\lambda_{\pm} \sin(ak_x)s_z\tau_3(\sigma_0 \pm \sigma_3)$. We use particle swarm optimization to get the hopping parameters by fitting to the DFT bands and have tabulated them in Appendix C.

Figure 2(b) shows the band structure along a high-symmetry line and the DOS of the tight-binding model. Because of the presence of both $\mathcal{P}$ and $\mathcal{T}$ symmetry, each band is twofold degenerate. Importantly, the model has a direct energy gap of $\Delta E = 23$ meV around the Γ point and a vHS (μ_{vHS}) 62 meV above the Fermi level, both of which agree well with the above DFT results and experiment [4]. To confirm the topological properties, we use the inversion operator $P = s_0\tau_1\sigma_0$ to get the parities of all bands, which have been marked as solid circles at time-reversal invariant momenta in Fig. 2(b). Compared with the DFT results in Fig. 1(b), the parities of our model exhibit the same order around the Fermi level, indicating the same band inversion mechanism at the Y point. The parity products of the occupied bands give us a $\mathbb{Z}_2$ invariant of $\nu_0 = 1$, as expected from DFT calculations. More details on the band inversion mechanism and the parities of the DFT bands can be found in Appendix C. Figure 2(c) shows the helical edge states along the high-symmetry line of the [010] edge. The helical edge states are degenerate at the $\bar{Y}$ point, connecting the conduction and valence bands and confirming the band inversion at the Y point and the QSHI phase at the charge neutral point (CNP).

Furthermore, we calculate the charge susceptibility as shown in Fig. 2(d). It exhibits a pronounced peak at $Q_a = 0.067 \cdot 2\pi/a$, indicating that the electronic instability is driven by scattering between adjacent vHSs. This

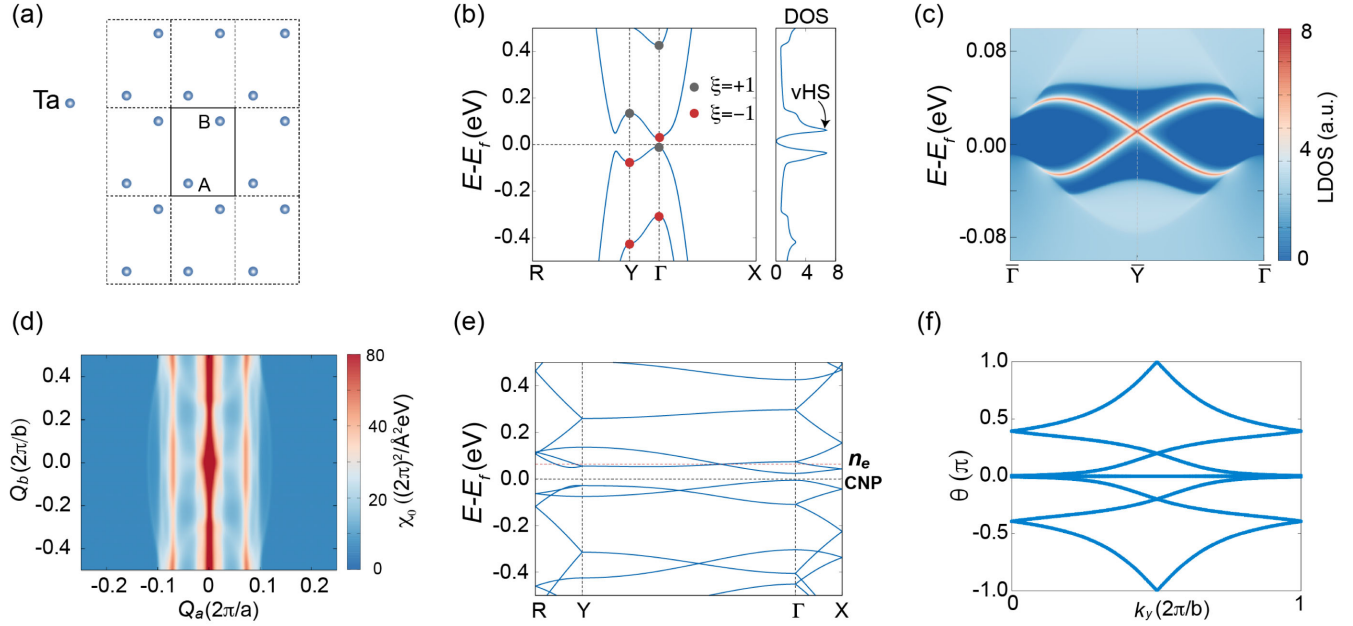


FIG. 2. Band structures and topological properties of monolayer TaIrTe₄ by TB model. (a) Orbital positions. (b) Band structure along high-symmetry lines and the corresponding density of states. (c) Topological edge states along the [010] edge, showing the helical edge features. (d) Calculated charge susceptibility (χ_0) of the conduction bands at the energy of the vHS. Two peaks emerge at $Q_a = \pm 0.067$ ($2\pi/a$), connecting two vHS. (e) Folded band structures for a 15×1 supercell configuration. (f) Wilson loop for the supercell, demonstrating the topological properties in the folded band structure.

suggests that the system favors a CDW state with a periodicity of approximately $15a$, directly linked to the nesting condition between vHSs. Guided by the DFT Lindhard susceptibility, we model the interaction-driven states in a 15×1 CDW supercell throughout, unless otherwise noted.

Therefore, the system can produce a 15×1 CDW state by gating [4]. Figure 2(e) shows the noninteracting folded band structure of a 15×1 supercell. Because of band folding, the band dispersion becomes much flatter around the Fermi level, especially at the vHS (marked with a red dashed line), where the density of states peaks and stronger electron interactions are expected. We also calculate the $\mathbb{Z}_2$ invariant and the Wannier center evolution along k_y of the supercell at CNP. As shown in Fig. 2(f), the topology at the charge neutral point is the same as that of the unfolded bands, exhibiting a $\nu_0 = 1$ topological gap.

III. CORRELATED ELECTRON STATES

A. Hartree-Fock mean-field calculations

Having established the framework to treat the vHS electronic instability at the single-particle level, we now consider how electron-electron correlations at the vHS further modify the phases. To do so, we perform Hartree-Fock mean-field (HFMF) calculations at the commensurate filling of 0.2 for the 15×1 supercell, i.e., two additional electrons per supercell relative to the CNP. We define this

filling level as n_e up front to connect with experimental observations later.

We incorporate local Coulomb interactions using the extended Hubbard model, which includes both on-site Hubbard U and density-density interaction V terms:

$$\hat{H}_{\text{int}} = U \sum_{\mathbf{R}\alpha} \hat{n}_{\mathbf{R},\alpha\uparrow} \hat{n}_{\mathbf{R},\alpha\downarrow} + \sum_{(\mathbf{R}_1\alpha) \neq (\mathbf{R}_2\beta)}^{3rdNN} \sum_{ss'} V_{\mathbf{R}_1\alpha, \mathbf{R}_2\beta} \hat{n}_{\mathbf{R}_1, \alpha s} \hat{n}_{\mathbf{R}_2, \beta s'}. \quad (2)$$

where subscript $\mathbf{R}$ labels a Bravais lattice site, α and β are composite sublattice and orbital indices, and s and s' are spin indices. $\hat{n}$ is the density operator, U is the strength of the onsite Hubbard interaction, and V is the amplitude of the density-density interaction between sites. A detailed derivation is given in Appendix D.

Given the large number of 120 orbitals per supercell, the self-consistent mean-field equations require efficient numerical methods for convergence. We employ a matrix-product approach to compute the order parameters, leveraging the correlation function:

$$\langle (\mathbf{a}^\dagger)^T \mathbf{a}^T \rangle = \bar{U}^* \text{diag}(n_F(\lambda_i)) \bar{U}^T, \quad (3)$$

where $\bar{U}$ represents the unitary matrix diagonalizing the mean-field Hamiltonian and $n_F(\lambda_i)$ is the Fermi-Dirac occupation function. This formulation enables rapid

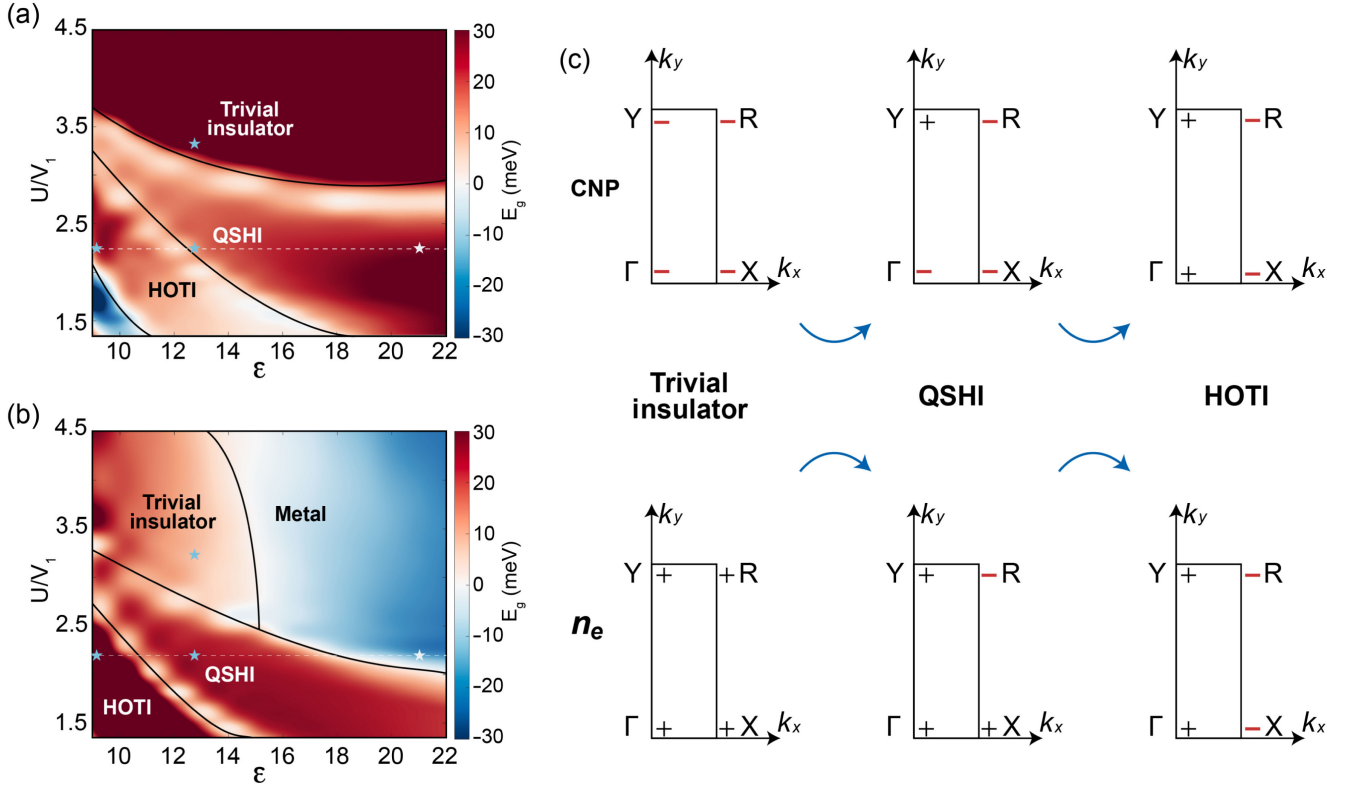


FIG. 3. The Hartree-Fock mean-field phase diagram and associated band topology at filling of 0.2. (a) Phase diagram of the CNP states inside the CDW phase, shown as a function of dielectric constant (ϵ) and the relative interaction ratio (U/V_1). This quantity is accessible to ARPES/STM at the doped state, not to CNP transport. The color scale represents the energy gap between the 60th and 61st bands in meV, where red indicates an insulating state with a finite gap, and blue denotes a metallic state without a fully global gap. The white regions indicate phase boundaries. (b) Phase diagram for the electron-doped states at $n = n_e$, with the gap defined between the 62nd and 63rd bands. White dashed line marks a reference value of $U/V_1 = 2.25$, while the solid black lines further outline the phase boundaries. Distinct phases are labeled: HOTI, QSHI, trivial insulator, and metal. (c) Parity products at the four time-reversal invariant momenta for the occupied bands: 1-60 for the CNP gap and 1-62 for the n_e gap. The transitions between trivial insulator, QSHI, and HOTI phases are identified by changes in the parity products. Panels (a) and (b) belong to different manifolds (CNP vs n_e); consequently, their gap closures or topological transitions need not coincide at the same (U/V_1 , ϵ).

evaluation of self-consistent fields by exploiting batched eigenvalue decomposition, significantly accelerating the iterative procedure. Additionally, a quasi-Newton acceleration method [42] is employed, which allows for efficient convergence of the large Hartree-Fock fixed-point equations. The result is a self-consistent solution for the correlated phases of TaIrTe₄, which we analyze in the following section through a determination of the phase diagram and topological characterization.

B. HFMF phase diagram

To explore the role of electron interactions on both the CNP ($n = 0$) and the doped states ($n = n_e$), we performed iterative self-consistent HFMF calculations for the 15×1 supercell at the filling of 0.2. The converged phase diagrams, shown in Figs. 3(a) and 3(b), are mapped as a function of the dielectric constant ϵ and the interaction ratio U/V_1 , where U and V_1 denote the on site and nearest-neighbor Coulomb repulsion, respectively. The formula

relating V_i and ϵ is given in the Appendix D 1. Although our calculations are carried out at a fixed filling of 0.2, corresponding to two extra electrons per supercell near the vHS, the resulting self-consistent mean-field potential affects the entire spectrum. As a result, both the CNP states and the n_e states are renormalized by interactions and thus serve as fingerprints of the underlying many-body phase. Figure 3(a) shows the phase diagram of the CNP gap, while Fig. 3(b) shows the same for the n_e gap. These results demonstrate that electron correlations significantly modify both the intrinsic and emergent gaps. Four distinct correlated electronic phases emerge in the phase diagram:

- (i) Quantum Spin Hall insulator: $\mathcal{PT}$ symmetric with nontrivial $\mathbb{Z}_2$ index $\nu_0 = 1$, featuring edge states.
- (ii) Higher-Order topological insulator: Identified by $\mathbb{Z}_4$ indicator $\kappa_1 = 2$, hosting corner states in real space.
- (iii) Trivial insulator: A trivial gapped state characterized by $\nu_0 = 0$ without band inversion, indicating the absence of topological edge or corner states.

- (iv) Metallic phase: A state where electron interactions fail to realize a fully gapped insulating phase, having nonzero DOS at the Fermi level.

As shown in Fig. 3(c), different correlated phases can be analyzed by examining the parity products $\delta = \prod_{i=0}^n \xi_i$ of the n occupied bands at the four time-reversal invariant momenta. As the relative interaction ratio varies, changes in the parity products indicate topological phase transitions. The upper panel corresponds to the parity distribution for the CNP gap, while the lower panel represents that of the n_e gap.

Specifically, when $U \gg V_1$, the onsite interaction takes the dominant role, pushing the system toward the atomic (trivial) insulator state with a large band gap. As U/V_1 decreases, the system transitions from a trivial insulator to a QSHI, with the band closing at the Y (R) point for CNP (n_e) gap, indicative of a parity change there. Further decreasing the dielectric constant results in a transition from the QSHI to a HOTI, accompanied by a band gap closing and reopening at the Γ (X) point for CNP (n_e) gap, signifying a parity change at Γ (X). Simultaneous band inversion at both R and X identifies the HOTI phase, characterized by the $\mathbb{Z}_4$ invariant $\kappa_1 = 2$.

These transitions demonstrate that electron correlation plays a fundamental role in modifying the topological properties of the system. Furthermore, our Hartree-Fock calculations at $\nu = 0.2$ filling reveal that combined topological phases emerge depending on the topological nature of CNP and n_e gaps as shown in Table I. Because the CNP and n_e gaps originate from distinct band manifolds, their self-consistent evolutions under interactions may occur at different values of U/V_1 for a given ε .

To further characterize these phases, we analyze the associated band structures and topological nature at representative parameter points, as shown in Figs. 3(a) and 3(b).

1. Dual QSHI

To describe the dual QSHI phase, we take as a representative point $U/V_1 = 2.25$, $\varepsilon = 13$. As shown in

TABLE I. Classification of correlated phases based on the CNP and n_e states. The system belongs to class AII of the Altland-Zirnbauer tenfold symmetry classification [43]. For insulating phases, we use the $\mathbb{Z}_2$ index ν_0 and, the $\mathbb{Z}_4$ index κ_1 : trivial insulator ($\nu_0 = 0$, $\kappa_1 = 0$), QSHI ($\nu_0 = 1$), and HOTI ($\nu_0 = 0$, $\kappa_1 = 2$). Metal denotes the absence of a global gap.

Phase	$n = 0$	$n = n_e$
Dual QSHI	$\nu_0 = 1$	$\nu_0 = 1$
Dual HOTI	$\kappa_1 = 2$	$\kappa_1 = 2$
Dual trivial insulator	$\nu_0 = 0$	$\nu_0 = 0$
HOTI + QSHI	$\kappa_1 = 2$	$\nu_0 = 1$
QSHI + trivial insulator	$\nu_0 = 1$	$\nu_0 = 0$
QSHI + metal	$\nu_0 = 1$	Metal
Trivial insulator + metal	$\nu_0 = 0$	Metal

Fig. 4(a), the dual QSHI phase emerges when both the CNP gap and the n_e gap exhibit a nontrivial $\mathbb{Z}_2$ topology. The parity products at the TRIMs are shown in the middle panel of Fig. 3(c). Although the band inversion occurs at different momenta, both the CNP gap and the n_e gap share the same $\mathbb{Z}_2$ topological invariant $\nu = 1$. Figure 4(b) shows the evolution of the Wannier centers of all occupied bands along the k_x direction for the n_e gap. The Wannier bands exhibit a π -phase difference at $k_x = \pi$, consistent with opposite parity at R and X. The Wannier bands along the k_y direction exhibit the same behavior, as shown in Fig. 14(c) in the Appendix D 2, together indicating a clearly defined QSHI feature. For the CNP gap, the Wannier band phases exhibit distinct phase jumps along different momentum directions, occurring at $k_x = 0$ along k_x and at $k_y = \pi$ along k_y , as illustrated in Fig. 14 of Appendix D 2. As shown in Fig. 4(c), two distinctive helical edge states emerge in both the n_e gap and CNP gap, confirming the topological properties of a dual QSHI. The gapless edge states are degenerate at $\bar{X}$ for the n_e gap and $\bar{\Gamma}$ for the CNP gap, in agreement with the Wilson loop and parity product distributions. This phase is consistent with previously observed dual QSHI in experiments [4], further validating our theoretical approach.

2. Dual HOTI

As for the dual HOTI phase, we take the representative parameter point $U/V_1 = 2.25$, $\varepsilon = 9$ as an example. Figure 4(d) illustrates the dual HOTI phase, where both the CNP and n_e gaps carry a higher-order topology characterized by the $\mathbb{Z}_4$ invariant $\kappa_1 = 2$. As shown in Fig. 3(c), the parity product distribution is the same for both gaps, where the band inversion occurs at both R and X momenta. Furthermore, the Wilson loop [Fig. 4(e)] along the k_y direction shows a feature of a HOTI, with two bands at $\pm\pi$ emerging at the boundary, indicating that the average Wannier center is located at the boundary in real space. Meanwhile, the Wilson loop phases along the k_x direction remain zero, in agreement with the parity distributions (see Appendix D 3 for details). To further confirm this phase, we construct a 10×8 rectangular superlattice with open boundary conditions and calculate the density distribution of the degenerate states in the n_e gap as shown in Fig. 4(f). Two degenerate corner states are observed, obeying C_{2z} symmetry. These corner states confirm the nontrivial topology associated with the HOTI phase, distinct from the conventional edge topology of QSHI phases.

3. Trivial insulator and metal

Beyond the above exotic topological phases, Fig. 5 illustrates the dual trivial insulator and metallic states. As shown in Figs. 5(a)–5(c), the dual trivial insulator phase arises when both the CNP and n_e gaps are topologically trivial ($\nu = 0$), leading to two correlated insulating gaps

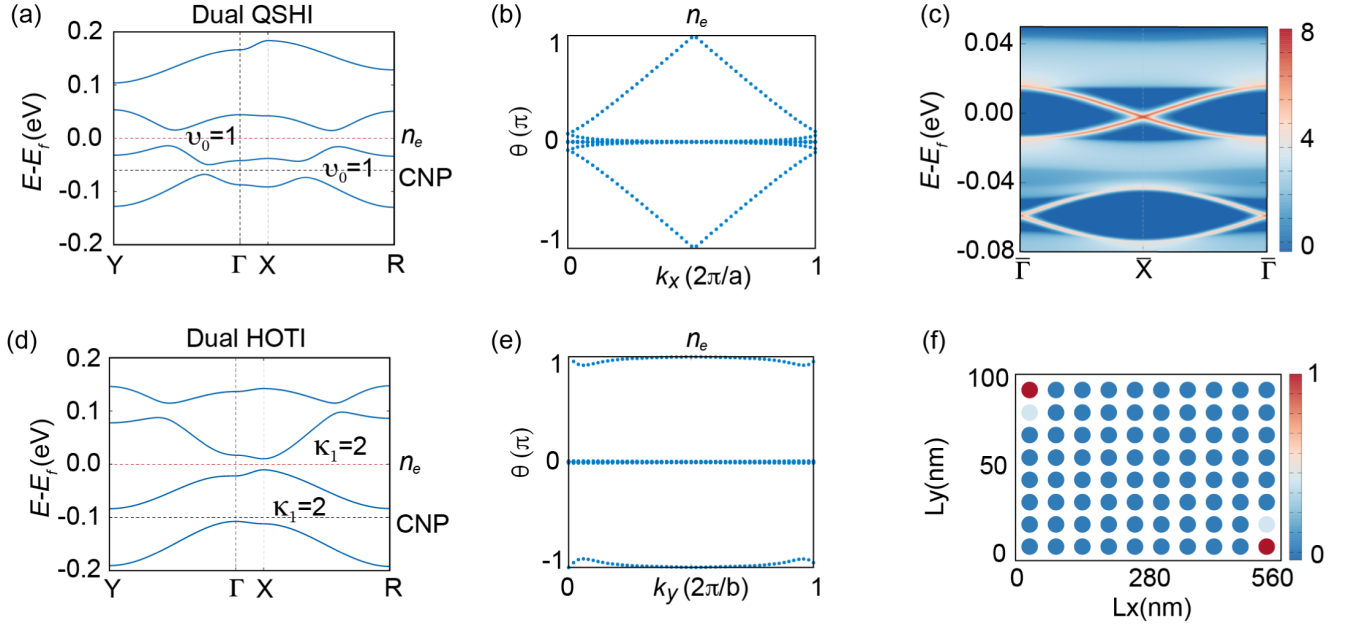


FIG. 4. Topological characterization of the dual QSHI and dual HOTI phases. (a)–(c) Band structure, Wilson loop evolution along k_x for n_e gap, and [100] edge states for the dual QSHI phase, showing two $\mathbb{Z}_2$ topological gaps at the n_e and CNP levels. The color scale in (c) indicates the local density of states at the edge. (d)–(f) The band structures along high-symmetry lines, evolution of the Wannier centers for n_e gap, and spatial density profile of corner states for the HOTI phase, with both gaps exhibiting $\kappa_1 = 2$ higher-order topology. The color scale in (f) represents the real-space density distribution of the corner states.

without protected edge states. The parity products, shown in the left panel of Fig. 3(c), indicate the absence of band inversions for both CNP and n_e gaps. As the dielectric constant increases, the system transitions into a QSHI + metal phase [Figs. 5(d)–5(f)], where the n_e gap collapses. However, the CNP gap remains finite and retains its nontrivial topological character despite the metallic behavior in the doping region. This demonstrates the crucial role of electron interactions in stabilizing correlated insulating phases, as the weakening of correlated effects leads to the emergence of metallic states (see Appendix D 4 for details).

These findings emphasize that the introduction of electron correlations not only stabilizes topological insulating states but also introduces new phases where different topological gaps coexist. Our results thus provide a theoretical framework to explain the experimentally observed dual QSHI and predict new correlated insulating and metallic phases in TaIrTe₄.

C. Strain effects

Thus far, our theoretical analysis has demonstrated a rich variety of correlated phases by tuning the interaction strength and dielectric screening. However, these parameters are not directly tunable in experiments. A more accessible experimental tuning parameter is uniaxial strain, which can influence both the single-particle electronic structure and the effective interaction in the system. Therefore, to systematically explore how strain modulates the correlated electronic phase diagram, we incorporate

strain effects into our tight-binding model via the relation

$$t'_{ij} = t_{ij} e^{-\beta(\delta/l)}, \quad (4)$$

where t'_{ij} represents the modified hopping parameter under strain, t_{ij} is the unstrained hopping amplitude, δ/l denotes the relative change in bond length due to strain, and β is an empirical parameter that quantifies how sensitive the hopping amplitude is to lattice deformations.

To determine a suitable value for β , we apply uniaxial strain in our DFT calculations and extract the evolution of the energy gap at the CNP under strain. As shown in Fig. 6(a), when compressive strain is applied, the system remains a $\mathbb{Z}_2$ topological insulator, with an increasing band gap as the strain magnitude increases. In contrast, under tensile strain, a gap-closing and reopening transition occurs around 1% strain, leading to the emergence of a HOTI phase (for more details on topological phase transitions by DFT see Appendix E).

By fitting the tight-binding model parameters to match the strain-dependent DFT gap closure, we obtain the blue curve in Fig. 6(a), with $\beta = 1.5$, which reproduces the topological transition in the DFT results. Furthermore, to confirm the HOTI phase in our DFT calculations, we evaluate the parity products at the four time-reversal invariant momenta, namely Γ , X, Y, and R. The computed parity products at these points are $(- + - +)$, confirming a nontrivial $\mathbb{Z}_4$ invariant of $\kappa_1 = 2$. This result indicates that

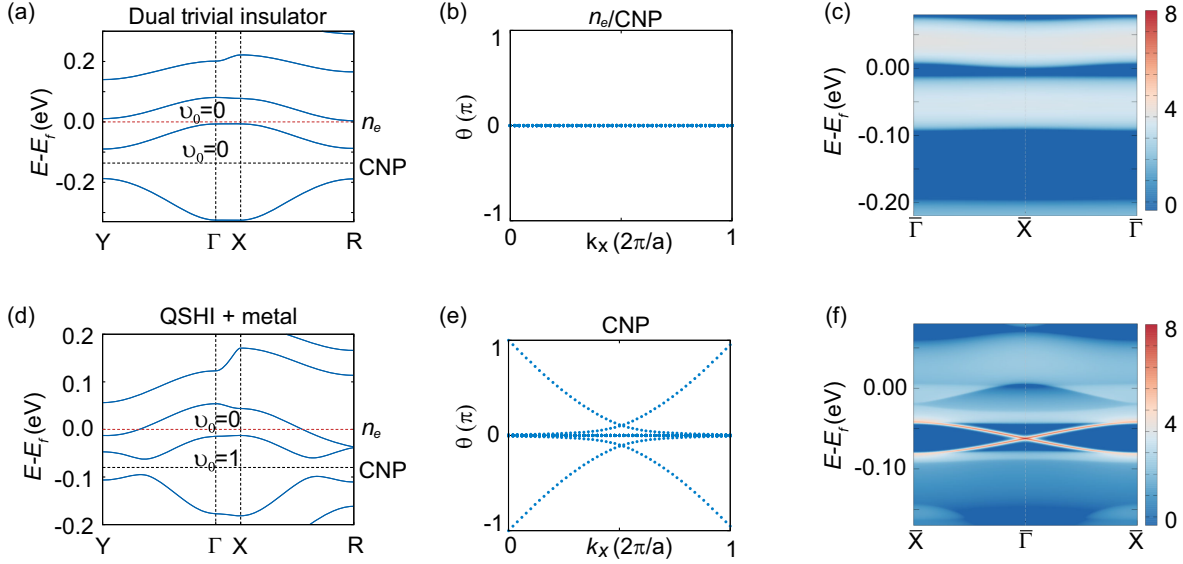


FIG. 5. Topological band features of the dual trivial insulator and QSHI + metal phases. (a)–(c) Band structure along high-symmetry lines, Wilson loop evolution, and edge spectrum for the dual trivial insulator phase. Both the CNP and n_e gaps are topologically trivial with $\nu_0 = 0$, and no gapless edge states are observed. (d)–(f) Band structure, Wilson loop along k_x , and [100] edge states for the QSHI + metal phase. The CNP gap shows a nontrivial $\mathbb{Z}_2$ topology, while the doping gap remains metallic without a global gap. The color scales in (c) and (f) indicate the local density of states at the edge.

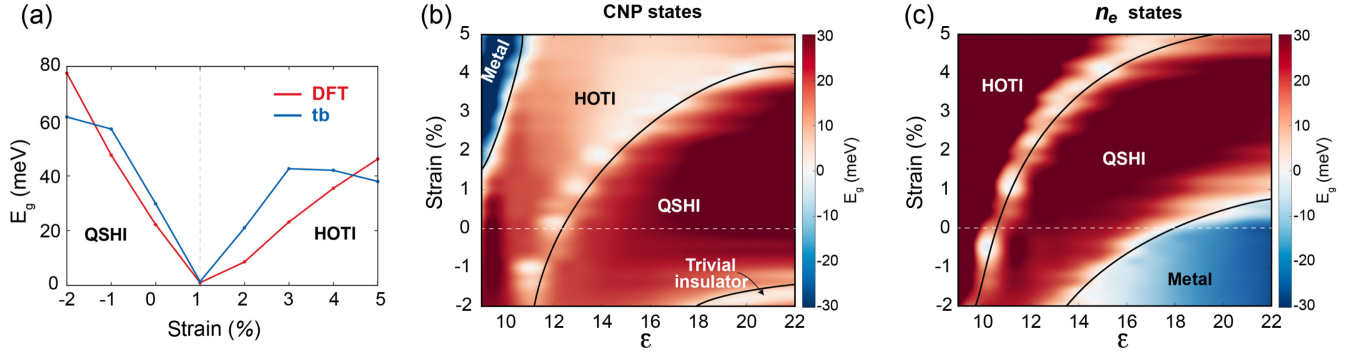


FIG. 6. The phase transitions under strain. (a) The energy gap at different strains. The red lines represent the data from DFT calculations, while the blue lines are derived from the tight-binding model. (b) The HFMF phase diagram at filling $\nu = 0.2$ as a function of the dielectric constant and the strain for the CNP states. Note that the dashed line in this figure matches the dashed line in Figs. 3(a) and 3(b). (c) The same diagram for the gaps between bands 62 and 63 for n_e states.

the system undergoes two band inversions, specifically at the Γ and Y points, leading to the higher-order topology.

Using this strain-tuned tight-binding model, we compute the HFMF phase diagrams as a function of strain and dielectric constant, fixing $U/V_1 = 2.25$. The results are presented in Figs. 6(b) and 6(c), showing the strain-dependent phase evolution of the CNP gap and n_e gap.

As shown in Fig. 6(b), the CNP gap exhibits multiple strain-induced phase transitions, including transitions between metal, HOTI, QSHI, and trivial insulator phases. Compared to the strain-induced effects on the n_e states, strain has a broader impact on the CNP gap, significantly expanding the QSHI and HOTI phase regions. The trivial insulator phase is characterized by parity

products (---), while the QSHI phase has (---+-), indicating that band inversion occurs at the Y point, identical to the DFT results. Thus, interactions do not modify the band inversion mechanism within the QSHI sector, even though they can drive transitions to HOTI or trivial phases by closing and reopening the gap.

For the n_e gap, increasing tensile strain ($\delta > 0$) leads to a transition from a QSHI to a HOTI phase. The parity products at Γ , X , Y , and R change from (++++-) to (+-+-), indicating that the band inversion reoccurs at the X point. This transition causes the system's $\mathbb{Z}_2$ index ν_0 to change from 1 to 0, while the $\mathbb{Z}_4$ invariant becomes $\kappa_1 = 2$, confirming the HOTI phase. Under compressive strain ($\delta < 0$), the n_e gap increases for small ϵ , reinforcing the

QSHI phase [Fig. 6(b)]. Additionally, for sufficiently large ϵ , the QSHI phase transitions into a metallic state due to strong screening effects that suppress electron interactions. The interplay between strain, dielectric screening, and electron-electron interactions thus provides a powerful means of tuning topological phase transitions. Here, we also choose two representative phases to exhibit the strain effect on the correlated phase transitions. Further analyses for representative strain values are provided in Appendices E 4 and E 5.

These results indicate that strain provides an effective tool for engineering correlated topological phases in TaIrTe₄, offering a pathway to control the emergence of QSHI, HOTI, and trivial insulating states through lattice deformation.

IV. EXPERIMENTAL ASSESSMENT OF PHASES

Uniaxial strain is, in principle, a controllable parameter in experiments, and monolayers can typically withstand substantial strain before mechanical failure. However, applying continuous and precisely controlled strain to small, fragile monolayer flakes remains experimentally challenging, requiring the careful selection of stretchable substrates and the development of compatible fabrication techniques. To date, only limited experimental work has demonstrated controllable and continuous strain tuning in thin layers [44–48]. While direct strain control represents a promising avenue for future studies, here we adopt a statistical approach to evaluate strain effects. During sample fabrications, TaIrTe₄ is picked up and transferred using flexible polymers (see Appendix H) as part of the boron nitride encapsulation process. This procedure inevitably introduces unintentional, sample-dependent strain, which is difficult to control but expected to vary randomly across devices. By fabricating and characterizing a broad set of samples, we effectively probe a range of strain conditions. As we show below, this strategy enables access to multiple distinct regions of the phase diagram.

We fabricated dual-gated monolayer TaIrTe₄ devices and probed their electronic states using both local and nonlocal transport measurements, while continuously tuning the Fermi level from charge neutrality to the vicinity of vHSs. We note that in our dual-gate geometry, the perpendicular electric field $E_{\perp}$ produces negligible changes to the low-energy band topology and does not shift the phase boundaries of our HFMF phase diagrams (see Appendices F and H 6). Although DFT calculations identify vHSs in both the conduction and valence bands, recent experiments [4] indicate that only the conduction-band vHSs are fully accessible via electrostatic doping, leading to a correlated insulating gap at a doping density $n = n_e$. On the valence side, an onset of increasing resistance is observed at the highest accessible hole doping, suggesting that vHSs may also be present in the valence band but require stronger hole doping to reach. Therefore, our analysis focuses primarily

on the charge neutrality point ($n = 0$) and the conduction-band vHS regime ($n = n_e$). Note that transport at the CNP probes the ungated electronic structure ($n = 0$), far from the vHSs and without CDW order.

The experimental evaluation strategy proceeds as follows: (i) We first measure the temperature dependence of the longitudinal resistance to distinguish between insulating and metallic behaviors. (ii) For samples exhibiting insulating behavior—indicative of a bulk gap—we perform nonlocal transport measurements to determine whether the nonlocal response is enhanced within the gap. Such enhancement suggests the presence of edge transport, consistent with QSHI regime. (iii) Definitive confirmation of the QSHI requires the observation of a quantized longitudinal conductance of $2e^2/h$. However, as widely recognized in the community, achieving such quantization is experimentally challenging and requires ultra-short channel devices with nearly ideal contacts—conditions that are not practical for large-scale statistical studies. Therefore, we rely primarily on criteria (i) and (ii) for statistical evaluation, while providing representative examples of quantized conductance from short-channel devices, with which the long-channel samples assigned to host QSHI states exhibit empirically consistent transport characteristics.

Based on our DFT and HFMF calculations, the theoretically predicted phase diagram contains several possible correlated phases, including QSHI, HOTI, trivial insulator, and metallic phases. Experimentally, we can distinguish metallic from insulating phases directly through the temperature dependence of the longitudinal resistance $R_{xx}(T)$. Among insulating phases, QSHI states exhibit distinct quantized edge conductance, providing a clear transport signature. However, both HOTI and trivial insulator phases lack quantized edge transport, making them difficult to distinguish using standard transport measurements alone. Therefore, in our experimental analysis, we conservatively group these two transport-indistinguishable possibilities under the category of *insulators*. Based on the above phase-classification strategy and by simultaneously considering the states at both the CNP and at n_e doping level, we identify three distinct experimental phases, as summarized in Table II: (i) Dual QSHI, (ii) QSHI + metal, and (iii) Dual insulator. These experimentally observed states

TABLE II. Classification of correlated phases based on edge transport behaviors at $n = 0$ for CNP phase and $n = n_e$ for n_e phase.

Phase	$n = 0$	$n = n_e$
Dual QSHI	QSHI	QSHI
QSHI + metal	QSHI	Metal
Dual insulator	HOTI or Trivial insulator	HOTI or Trivial insulator

align closely with our theoretical predictions, and each regime is described in detail in the following sections.

A. Transport characteristics of dual QSHI

We first describe the dual QSHI behavior, which is consistent with previous experimental reports [4]. Among the 105 measured devices, approximately 35% exhibit this qualitative behavior. The characteristic features of this type are as follows: at charge neutrality ($n = 0$), a resistance peak is observed, corresponding to the single-particle gap; at finite electron doping near $n_e \approx 6.5 \times 10^{12} \text{ cm}^{-2}$, a second resistance peak emerges, attributed to a vHS-induced electronic instability. These two resistance peaks are typically of comparable magnitude, on the order of 10 to 100 k Ω , depending on the channel length. Temperature-dependent resistance maps reveal that both peaks correspond to insulating states, separated by a narrow metallic region, as illustrated in a representative device in Fig. 7(a). In this device, thermal activation fitting yields an estimated charge-neutral gap of approximately 6.1 meV and an electron-doped gap of around 4.6 meV (see Appendix H 4). The thermal-activation gap extracted

from transport represents a global, device-averaged energy gap rather than the intrinsic local single-particle gap [49]. Because the channel is relatively long ($L_{\text{CH}} = 5 \text{ }\mu\text{m}$), spatial inhomogeneities create lower-gap regions that dominate carrier transport. Consequently, the measured activation gap is reduced (see more details in Appendix H 4).

In this type of device, we can further identify signatures of edge transport through nonlocal responses in a multi-terminal geometry. As shown in Fig. 7(b), the system exhibits enhanced nonlocal signals—defined as the ratio between nonlocal and local voltage drops—within both gap regions. This behavior is consistent with dominant edge conduction, which confines current flow along the sample boundaries, resulting in enhanced nonlocal signals relative to local ones. To definitively confirm the topological nature of QSHI by the edge transport, short-channel devices (with channel lengths on the order of 100 nm) are required, as previously demonstrated for monolayer QSHI [4,5]. This is because a short-channel device with a small size can effectively suppress bulk conduction arising from inhomogeneity and operate in a regime where the edge mean free path exceeds the channel length—that is, the edge ballistic

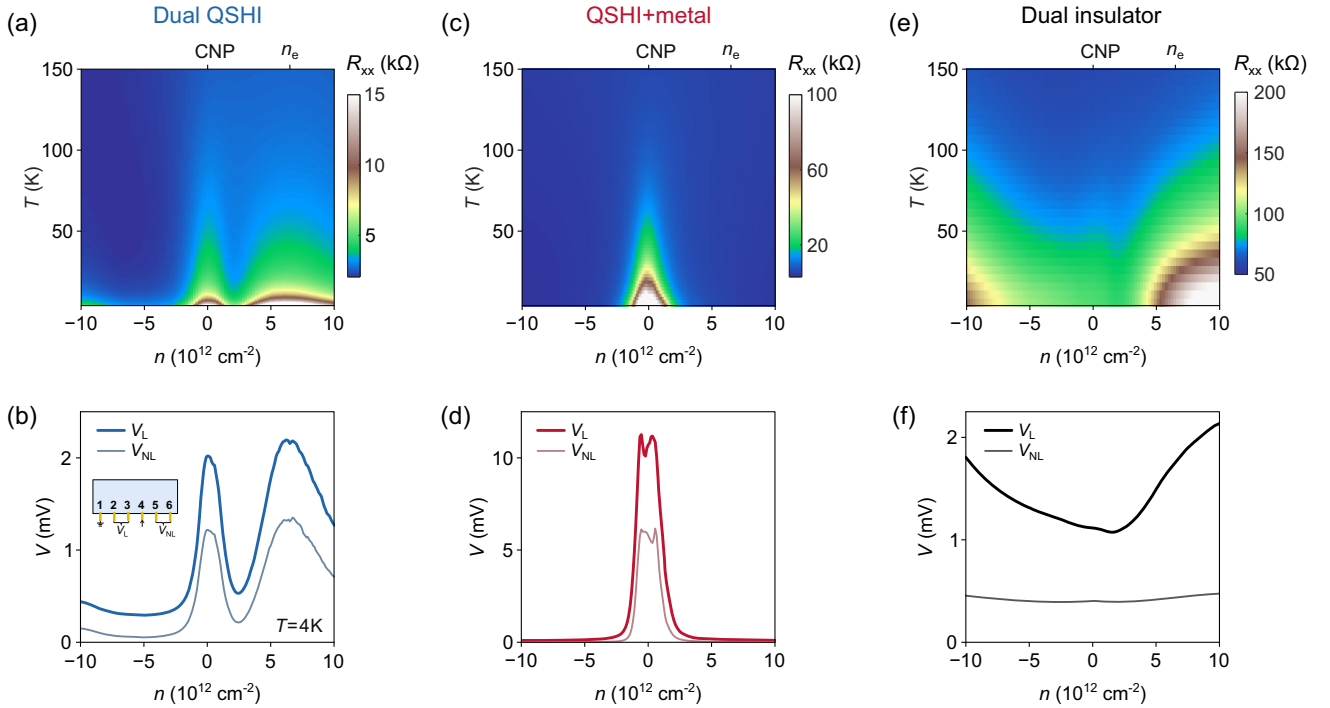


FIG. 7. Three representative transport behaviors of monolayer TaIrTe₄ devices. (a) Dual QSHI: Temperature (T)-dependent longitudinal resistance R_{xx} map as a function of carrier density (n), showing two pronounced peaks at the CNP and at electron doping near $n_e = 6.5 \times 10^{12} \text{ cm}^{-2}$. (b) Local and nonlocal voltage responses versus n at $T = 4 \text{ K}$. Inset: schematic of the measurement setup, where current (I_{xx}) is applied between pins 4 and 1 (grounded), local voltage (V_L) is measured between pins 3 and 2, and nonlocal voltage (V_{NL}) between pins 5 and 6. Enhanced nonlocal signals are observed at both the CNP and the n_e gap. (c) QSHI + metal: R_{xx} map as a function of n and T , showing a single peak at the CNP. Resistance decreases upon electron or hole doping. (d) Corresponding local and nonlocal responses at $T = 4 \text{ K}$, with strong nonlocal enhancement at the CNP gap. (e) Dual insulator: R_{xx} map as a function of n and T , displaying a weak peak at the CNP. Resistance increases with both electron and hole doping. (f) Corresponding local and nonlocal responses at $T = 4 \text{ K}$, where the nonlocal response is suppressed across the entire doping range.

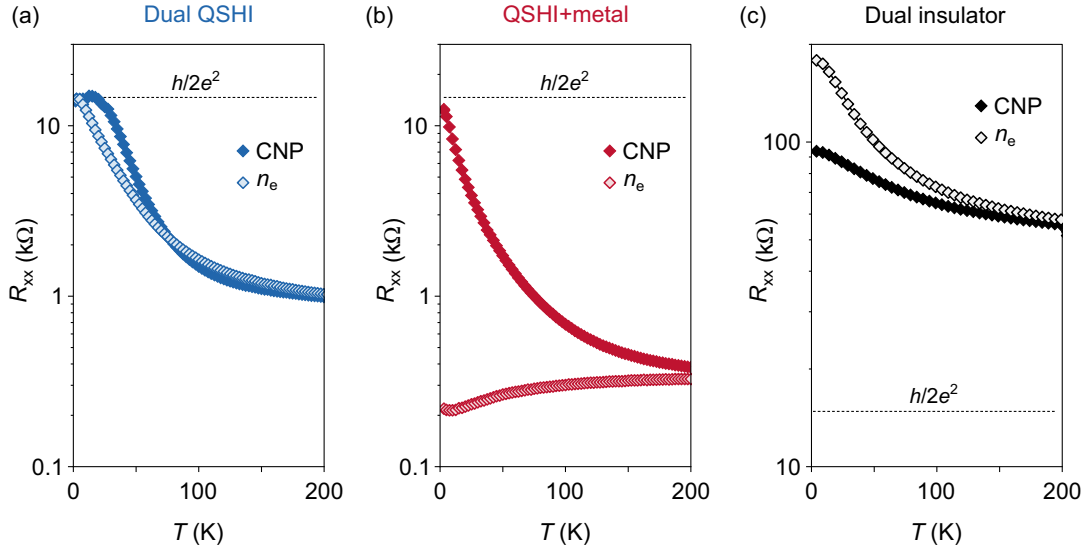


FIG. 8. Temperature-dependent resistance of the CNP and n_e phases in short-channel devices. (a) Dual QSHI: Both the CNP and the n_e phase exhibit insulating behavior, with resistance saturating to the quantized value of $h/2e^2$ at low temperatures. Solid rhombus, CNP phase; hollow rhombus, n_e phase. (b) QSHI + metal: The CNP phase shows insulating behavior with resistance approaching $h/2e^2$, while the n_e phase displays metallic behavior. (c) Dual insulator: Both phases are insulating, but their resistances deviate significantly from the quantized value.

transport regime. In one such device with a channel length of $L_{\text{ch}} = 140$ nm, both resistance peaks saturate to the quantized value of $h/2e^2$ at low temperatures, as shown in Fig. 8(a). At the same time, as shown explicitly in Fig. 32 of Appendix H 8, when plotted on a linear scale the longitudinal resistance R_{xx} in both QSH plateaus exhibits clear low-temperature saturation (onsets at ~ 25 K for QSH-I and ~ 10 K for QSH-II). These results indicate that both the CNP and n_e gaps correspond to QSHI.

B. Transport characteristics of QSHI + metal

Among the 105 measured devices, approximately 7% exhibit the qualitative behavior of QSHI + metal, in which the CNP gap corresponds to a QSHI, while the n_e state remains metallic rather than insulating. Results from a representative device displaying this behavior, which—unlike the previously discussed dual QSHI—exhibits a resistance peak only at the CNP, with no corresponding peak at $n = n_e$. Temperature-dependent measurements further confirm this distinction, revealing insulating behavior at the CNP and metallic behavior at n_e , as shown in Fig. 7(c). For this device, thermal activation fitting yields a charge-neutral gap of approximately 28.0 meV, as estimated from the temperature-dependent resistivity at the CNP [Fig. 28(a) in the Appendix H 6], consistent with our DFT calculations (21 meV) in Sec. II B. The QSHI nature of the CNP is further supported by nonlocal transport measurements [Fig. 7(d)] and the observation of quantized conductance in a short-channel device [Fig. 8(b)], similar to the previously discussed case.

These experimental observations are in good agreement with the predictions from our HFMF phase diagram. The appearance of the QSHI + metal phase may be attributed to the screening-induced suppression of many-body electron-electron interactions at large dielectric constants. Under such conditions, the weakened correlations are insufficient to induce a global gap at this doping level, resulting in a metallic behavior consistent with a Fermi-liquid-like state. These results underscore the crucial role of electron interactions and dielectric screening in tuning the correlated topological phases in monolayer TaIrTe₄.

C. Transport characteristics of dual insulator

Interestingly, among the 105 measured devices, the majority (58%) exhibit a dual insulator phase. In these monolayer TaIrTe₄ devices, the resistance peak at the CNP becomes less prominent compared to the steadily increasing resistance observed on both the electron- and hole-doped sides, as shown in Figs. 7(e) and 7(f). Notably, no resistance peak is observed at $n = n_e$; instead, the resistance continues to rise throughout the accessible electron-doping range. Temperature-dependent measurements confirm that the entire doping range remains insulating [Fig. 7(e)]. Moreover, no significant enhancement of non-local response is detected at either the CNP or $n = n_e$. In addition, in the short-channel limit, the resistance values [black curves in Fig. 8(c)] deviate significantly from the expected quantized edge conductance. Therefore, in this type of device, our observations suggest the absence of QSHI behavior at both $n = 0$ and $n = n_e$, despite the presence of insulating behavior at both doping levels.

Comparison with the theoretical phase diagram (Figs. 3 and 6) suggests two plausible scenarios for the experimentally observed dual insulator phase. Using the dual QSHI phase at $\varepsilon = 13$ and $U/V_1 = 2.25$ as a reference point, we identify (i) Increasing the interaction ratio to $U/V_1 \gtrsim 3.25$ at fixed $\varepsilon = 13$ drives both the CNP and n_e gaps into a trivial insulating phase [see Fig. 3(b)]. (ii) Alternatively, applying tensile strain beyond $\sim 3\%$ under moderate interaction strengths (still with $\varepsilon = 13$, $U/V_1 = 2.25$) drives both gaps into the HOTI phase, as shown in Fig. 6. While HOTIs are topologically nontrivial, their hallmark corner states cannot be directly resolved by conventional edge-transport measurements. Since our transport measurements cannot distinguish a HOTI from a trivial insulator, we characterize this regime as a dual-insulator phase, defined experimentally by the absence of robust quantized edge transport at both $n = 0$ and $n = n_e$.

To exclude artifacts from bulk defects or impurity-assisted bulk conduction, we fabricated control devices in which one edge of the TaIrTe₄ flake was covered by an insulating BN flake while the opposite edge remained contacted. In the QSHI regimes, the nonlocal response V_{NL} is strong when an edge contributes, but is strongly suppressed when that edge is capped by BN; outside the QSHI gap, V_{NL} is weak in both cases. These results demonstrate that the enhanced nonlocal response originates predominantly from edge channels rather than bulk conduction (see Fig. 31 in Appendix H 7).

Despite consistent fabrication and measurement conditions, the three distinct transport behaviors in Fig. 7 appear relatively randomly. Actually, the unavoidable strain in monolayer samples—arising from substrate interactions, device fabrication, or transfer processes—may naturally induce the transitions between the dual QSHI, QSHI + metal, and dual insulator phases observed in our experiments. This is further supported by the observation that a single device can exhibit different behaviors in different regions as shown in Fig. 34 of Appendix H 10.

V. POSSIBLE FRACTIONAL QSHI

Motivated by the robust QSHI regimes in our phase diagrams, we ask whether fractionalized, time-reversal-invariant topological order [7,50,51] can emerge in monolayer TaIrTe₄. To this end, we project the electron-electron interaction onto the isolated bands relevant to the dual-QSHI window (one well separated band per spin) and perform band-projected exact diagonalization (ED), keeping density-density interactions up to nearest neighbors (see more details in Appendix G 1).

First, we focus on the spin-polarized case (Fig. 26 in Appendix G 2). At filling $\nu = 1/3$, we find a threefold quasidegenerate ground-state manifold, clearly separated from excited states by a many-body gap [Fig. 26(b)]. The momenta of these ground states, the smooth many-body Berry curvature that integrates to $1/3$ per state [yielding the

many-body Chern number $C = 1/3$ for each state, as shown in Fig. 26(c)], and the particle-entanglement spectrum [Fig. 26(d)] with the expected quasihole counting together provide the standard, strict diagnostics of a fractional Chern insulator (FCI). Second, it's expected that FCI and its time-reversal partner can form a FQSHI/FTI. Combining two time-reversed copies of the above $\nu = 1/3$ FCI, we then study the spinful problem. The ED spectrum [Fig. 26(a)] exhibits a ninefold quasi-degenerate ground-state manifold at $\nu = 2/3$, consistent with a fractional quantum spin Hall insulator formed by two counterpropagating FCIs.

Finally, we also get some preliminary signatures from the transport experiment. Once a CDW is established in high-quality devices, in addition to the CNP and n_e gaps we observe extra resistance features at fractional fillings without magnetic hysteresis, consistent with time-reversal-preserved correlated states (Fig. 39 in Appendix H 14). While preliminary, these observations, taken together with the ED diagnostics above, strongly suggest that monolayer TaIrTe₄ is a viable platform for realizing a FQSHI.

VI. CONCLUSION AND DISCUSSION

To summarize, this work integrates theoretical approaches with experimental measurements to investigate interaction-driven phase diagram in monolayer TaIrTe₄ that arise from the interplay between its QSHI topology and vHSS-induced correlations. Our theoretical framework includes DFT, tight-binding modeling, and Hartree-Fock mean-field calculations, which together reveal a rich landscape of phases—including HOTIs, trivial insulators, and metallic states—extending beyond the previously reported correlated QSHI near the vHSSs. More importantly, we performed ED calculations that reveal a possible fractional QSHI, with convincing signatures including a quasi-degenerate ground-state manifold, many-body Chern number, and particle-entanglement spectrum. Notably, our theory predicts that when the Fermi level is tuned to the vHSSs, electronic correlations can influence not only the correlated phase itself but also modify the topological character of the charge-neutral gap—a feature that is, in principle, not detectable through transport measurements, and calls for future spectroscopy investigation such as scanning tunneling microscopy.

On the experimental side, we investigate over 100 monolayer TaIrTe₄ devices using both local and nonlocal transport measurements. Unavoidable sample-to-sample strain variations and different dielectric screening introduced during fabrication, while unintentional, interestingly enable access to multiple interaction-driven phases. In addition to the correlated QSHI, we observe metallic and other insulating states near the vHSSs. It should be noted that transport measurements alone cannot unambiguously distinguish a HOTI from a trivial insulator; further experiments, such as local probes of corner-localized states, will

be needed to directly verify the HOTI scenario. We also observed the additional insulating features at fractional fillings that persist to elevated temperatures, consistent with fractional physics. Each of these distinct regimes presents a promising avenue for future exploration. Our large-scale datasets enable a statistical classification of the observed behaviors—a level of experimental rigor and breadth that is unprecedented among monolayer systems, offering valuable guidance for ongoing and future investigations.

Overall, our findings establish a unified theoretical and experimental framework for correlated topological phenomena in TaIrTe₄ and related two-dimensional systems. The demonstrated tunability of topological states via electron interactions and strain offers exciting prospects for engineering quantum topological properties in van der Waals materials—beyond the constraints of moiré superlattices.

Looking ahead, the interaction-induced strong superlattice potential provides a promising avenue for realizing exotic fractionalized phases—most notably, the elusive fractional topological insulator protected by time-reversal symmetry [50,51], which has yet to be observed experimentally. Moreover, when the charge density wave instability associated with van Hove singularity is suppressed—via lattice strain, applied pressure, or enhanced Coulomb screening—superconductivity can emerge as a competing ground state [52]. This continuous evolution from a correlated topological insulator to an intrinsic superconductor opens a novel path toward achieving topological superconductivity. Taken together, there are exciting opportunities for device architectures that harness the gate-tunable interplay of correlation, topology, and superconductivity—laying the foundation for integrated non-Abelian quantum platforms and superconducting quantum circuits [53].

ACKNOWLEDGMENTS

We gratefully acknowledge Su-Yang Xu and Kenneth S. Burch for generously providing access to their facilities for fabricating the devices used in the statistical analysis presented in this work. We thank Peitao Liu and Ning Mao for helpful discussions. J. L., L. P., A. D., and Y. Z. acknowledge support from the National Science Foundation Materials Research Science and Engineering Center program through the UT Knoxville Center for Advanced Materials and Manufacturing (DMR-2309083). The work done at Boston College was supported by the Air Force Office of Scientific Research (Grants No. FA9550-22-1-0270 and No. FA9550-24-1-0117) and the Alfred P. Sloan Foundation. The single crystal growth and characterization of TaIrTe₄ at U. C. L. A. were supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences under Award No. DE-SC0021117. K. W. and T. T. acknowledge support from the JSPS KAKENHI (Grants No. 21H05233 and No. 23H02052), the CREST (JPMJCR24A5), JST and

World Premier International Research Center Initiative (WPI), MEXT, Japan.

DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: DFT CALCULATIONS

1. Methods

To characterize the electronic structure and topological properties of monolayer TaIrTe₄, we perform first-principles calculations based on density functional theory using the VASP with the projector augmented wave (PAW) method. Exchange-correlation effects are treated within the generalized gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) functional. A plane-wave cutoff energy of 500 eV is employed throughout the calculations. The Brillouin zone (BZ) is sampled using a $16 \times 8 \times 1$ Monkhorst-Pack k -point mesh, and a vacuum layer of 20 Å is created along the c direction to eliminate interlayer coupling. Structural relaxation is performed with convergence criterion of 10^{-6} eV for the total energy and 10^{-3} eV/Å for the ionic forces. The optimized in-plane lattice constants are $a = 3.816$ and $b = 12.55$ Å, agreeing well with previous experimental and calculations.

2. Band structure

Based on the relaxed structure, we compute the electronic band structures with and without spin-orbit coupling to understand the role of SOC in determining the topological band inversions. As shown in Fig. 9(a), in the absence of SOC, the valence and conduction bands show band inversions at both Γ and Y points, as the parity eigenvalues of the three relevant bands near the Fermi level are $(- - +)$ at both momenta, indicating double band inversion. This configuration leads to trivial topological phase with $\mathbb{Z}_2$ invariant $\nu_0 = 0$. Upon inclusion of SOC [Fig. 9(b)], the parity ordering at the Γ point changes to $(-, +, -)$, while the Y point remains unchanged. This parity reordering removes the inversion at Γ , leaving only a single inversion at Y , and leads to a nontrivial $\mathbb{Z}_2$ topological index $\nu_0 = 1$, confirming that monolayer TaIrTe₄ is a quantum spin Hall insulator.

To provide an accurate Wannier representation of the DFT-calculated bands, we constructed maximally localized Wannier functions (MLWFs). Specifically, we projected the Bloch wave functions onto the Ta (s, p, d orbitals), Ir (s, d orbitals), and Te (s, p orbitals), totaling 124 orbitals. These orbitals well-capture the character of the states around the Fermi level, including all relevant electronic states within the energy range of interest. Among these 124 orbitals, 88 are occupied valence orbitals. The resulting

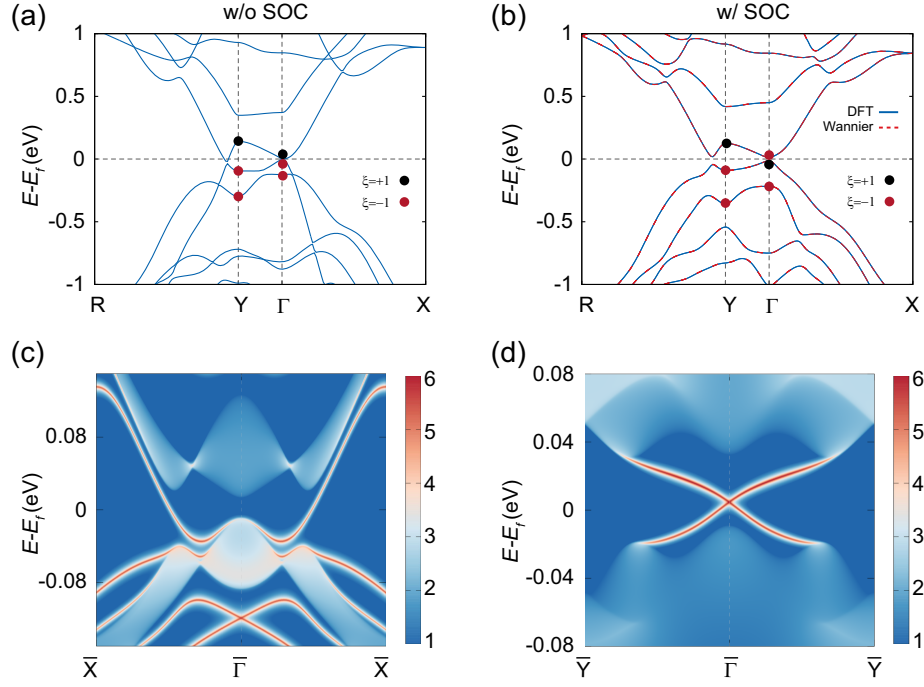


FIG. 9. DFT band structures and topological edge states of monolayer TaIrTe₄. (a) DFT band structure without SOC. Parity eigenvalues ($\xi = \pm 1$) at the TRIM points Γ and Y indicate identical band inversion pattern $(-, -, +)$, resulting in a trivial $\mathbb{Z}_2$ topological phase. (b) DFT band structure with SOC. The parity eigenvalues at Γ change to $(-, +, -)$, resulting in a single band inversion and a nontrivial $\mathbb{Z}_2$ invariant $\nu_0 = 1$. The Wannier-interpolated bands (red dashed lines) closely reproduce the DFT results (blue lines), confirming the accuracy of the Wannier projection. (c),(d) Topological edge states along [100] and [010] directions calculated from the Wannier-based tight-binding model, clearly showing the gapless helical edge states features of QSHI.

Wannier-interpolated band structure (red dashed lines) exhibits excellent agreement with the DFT bands, especially near the Fermi level, confirming the reliability and accuracy of our Wannier representation.

Furthermore, we calculate the topological edge states by iterative Green's function method [54] along the [100] and [010] crystallographic directions. As shown in Figs. 9(c) and 9(d), well-defined helical edge states emerge in both directions, traversing the bulk gap and confirming the nontrivial topology and bulk-edge correspondence of TaIrTe₄.

3. Atom and orbital contributions to electronic bands

In the following, we analyze the atomic and orbital characteristics of the electronic bands near the Fermi level obtained from DFT calculations to prepare for the construction of the effective minimal tight-binding model. Figure 10 shows the fat-band analysis including atomic contributions from Ta, Ir, and Te atoms. The results reveal that the electronic states around the Fermi level are predominantly contributed by Ta atoms, as evidenced by the strong intensity near the Fermi level. Thus, the low-energy

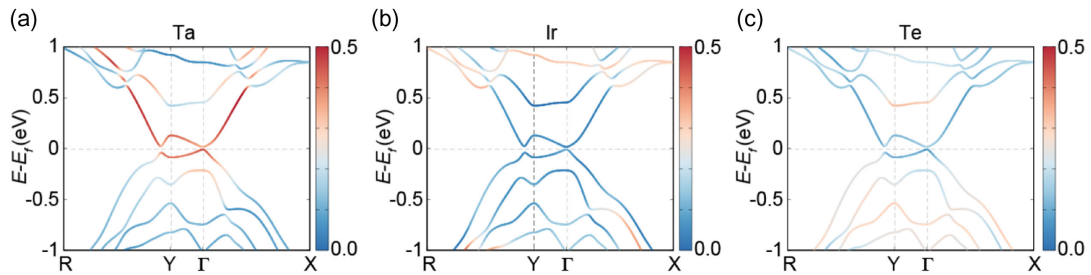


FIG. 10. Atomic contribution to the electronic bands of TaIrTe₄. (a) Fat-band plot showing the dominant orbital contributions from Ta atoms. (b)–(c) Fat-band plots for Ir and Te atoms, respectively. The color scale represents the magnitude of atomic contribution, clearly indicating the states near the Fermi level are predominantly from Ta atoms.

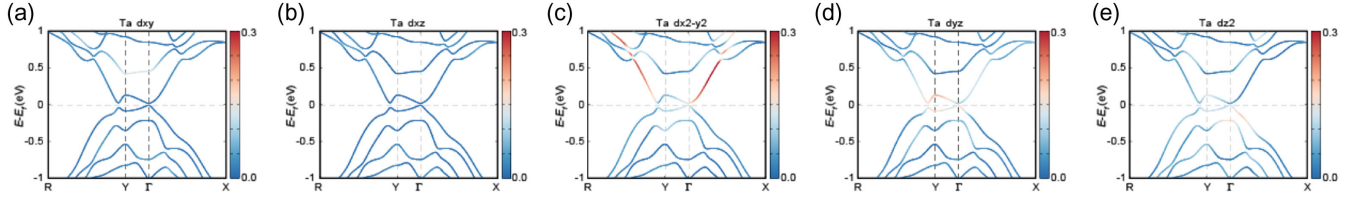


FIG. 11. Orbital decomposition of Ta-5d orbitals near the Fermi level. (a)–(e) Orbital-resolved fat-band plot for the Ta 5d orbitals, including d_{xy} , d_{xz} , $d_{x^2-y^2}$, d_{yz} , d_{z^2} . The bands near the Fermi energy are dominated by the Ta $d_{x^2-y^2}$ and d_{yz} orbitals, with minor contributions from d_{z^2} . The orbitals d_{xy} and d_{xz} have negligible contributions.

electronic physics of TaIrTe₄ is primarily dictated by the Ta atoms. Therefore, we will focus on Ta atoms in the following analysis.

To further clarify the orbital character of the Ta-dominated bands near the Fermi level, we decomposed these bands into five Ta 5d orbitals: d_{xy} , d_{xz} , $d_{x^2-y^2}$, d_{yz} , and d_{z^2} , as shown in Figs. 11(a)–11(e).

The orbital decomposition clearly illustrates that the valence and conduction bands near the Fermi level mainly originate from the Ta $d_{x^2-y^2}$ [Fig. 11(c)] and Ta d_{yz} [Fig. 11(d)] orbitals, with a smaller but noticeable contribution from the Ta d_{z^2} orbital [Fig. 11(e)]. In contrast, the Ta d_{xy} and d_{xz} orbitals show essentially no significant contribution to these bands [Figs. 11(a) and 11(b)]. This indicates that the bands relevant to low-energy physics are predominately governed by the $d_{x^2-y^2}$ and d_{yz} orbitals, both of which exhibit significant dispersion and thus dominate the electronic structure near the Fermi level. Consequently, our minimal effective tight-binding model focuses primarily on these two active orbitals to accurately capture their dispersion characteristics.

APPENDIX B: COMPUTATIONAL METHODS FOR $\mathbb{Z}_2$ AND $\mathbb{Z}_4$ INVARIANTS

The characterization of topological phases in TaIrTe₄ requires a precise determination of its topological invariants. In this study, we compute both the $\mathbb{Z}_2$ and $\mathbb{Z}_4$ topological indices using Wilson loop methods and symmetry indicators based on density functional theory and tight-binding model calculations.

1. Wilson loop calculation of the $\mathbb{Z}_2$ invariant

The Wilson-loop method [55,56] is a widely used method for topological classification of band structures. Here, we define the Berry connection matrix for $\mathcal{N}$ occupied states for a small segment $[k_{x,i}, k_{x,i+1}]$,

$$F_{i,i+1}^{n,m}(k_y) = \langle u_n(k_{x,i}, k_y) | u_m(k_{x,i+1}, k_y) \rangle, \quad (\text{B1})$$

where u_{n,k_x,k_y} is the periodic part of Bloch function $\psi_{n,\mathbf{k}}$ and $k_{x,i} = [(2\pi i)/(N_x a_x)]$. The band indices m and n go over all occupied bands. Then, we can use a product of

$F_{i,i+1}^{n,m}(k_y)$ to get the Berry phase matrix for a loop in discretized formula as

$$\mathcal{W}(k_y) = \prod_{i=0}^{N_x-1} F_{i,i+1}. \quad (\text{B2})$$

The Berry phase associated with the eigenvalues of above matrix, also known as Wilson bands, can be given by

$$\theta_n = -\text{Im} \log(w_n), \quad (\text{B3})$$

where w_n is the n th eigenvalue of Matrix $\mathcal{W}$ and θ_{n,k_y} is the Berry phase for the n th band along the k_x loop for a fixed k_y . The topological invariant can be obtained by the gauge-invariant winding number of the Wilson-loop evolution along k_y for both the time-reversal broken and time-reversal invariant systems. A nontrivial $\mathbb{Z}_2$ invariant is characterized by a spectral flow of the Wilson bands across the Brillouin zone.

To compute $\mathbb{Z}_2$, we use the Fu-Kane formula, which expresses the strong TI index $\nu_0 \in \mathbb{Z}_2$ as

$$(-1)^{\nu_0} = \prod_{K \in \text{TRIMs}} (+1)^{\frac{1}{2}n_K^+} (-1)^{\frac{1}{2}n_K^-} = (-1)^{\frac{1}{2} \sum_{K \in \text{TRIMs}} n_K^\pm}, \quad (\text{B4})$$

where n_K^+ (n_K^-) denotes the number of occupied bands with even (odd) parity at each time-reversal invariant momenta (TRIMs) K . Because of Kramers pairing, $n_K^\pm$ is always even. This formulation enables an efficient determination of the topological phase.

2. Symmetry indicators and the $\mathbb{Z}_4$ invariant

To determine the higher-order topology of the system, we compute the $\mathbb{Z}_4$ invariant using symmetry indicators derived from the inversion eigenvalues at TRIMs. The $\mathbb{Z}_4$ invariant is defined as

$$\kappa_1 \equiv \sum_{K \in \text{TRIMs}} (n_K^-)/2 \mod 4 \in \mathbb{Z}. \quad (\text{B5})$$

This index corresponds to the sum of the number of Kramers pairs with -1 parity eigenvalues of occupied

bands at each TRIM point, modulo 4, distinguishing between different topological phases:

- (i) $\kappa_1 = 0$: Trivial insulator.
- (ii) $\kappa_1 = 1, 3$: Topological insulator (TI) with $\nu_0 = 1$.
- (iii) $\kappa_1 = 2$: Higher-order topological insulator.

To extract the $\mathbb{Z}_4$ invariant, we utilize the eigenvalues of the inversion symmetry operator applied to the occupied bands at TRIMs, computed from the DFT-derived tight-binding Hamiltonian. This approach allows us to classify the topological character of different interaction-induced phases. By applying these computational methods, we establish the topological phase diagram of TaIrTe₄ under different interaction and strain conditions, confirming the emergence of nontrivial QSHI, HOTI, and trivial insulating states. Inversion is a convenient diagnostic for identifying HOTI (via the $\mathbb{Z}_4$ indicator), and that when inversion is broken the HOTI can still be established and tracked using Wilson loop method.

3. Bulk indices, Wilson loops, and edge states

For 2D time-reversal invariant (TRI) band insulators, the QSHI phase is characterized by a $\mathbb{Z}_2$ invariant ν [57]. With

inversion symmetry, ν is obtained from the products of parity eigenvalues of occupied bands at the TRIMs [58]. A band inversion at any TRIM flips the local parity product and can toggle ν .

Bulk-boundary correspondence implies that $\nu = 1$ enforces an *odd* number of helical edge crossings between the two edge TRIMs, whereas $\nu = 0$ allows a fully gapped edge spectrum [57,58]. Equivalently, the Wilson loop (Wannier charge centers, WCC) over half the Brillouin zone provides a gauge-invariant diagnosis of ν [56]: an *odd* spectral flow (odd crossings of a reference line) yields $\nu = 1$, an even number yields $\nu = 0$. The WCC spectral flow is in one-to-one correspondence with the presence (absence) of gapless helical edge modes.

In the HOTI regions ($\mathbb{Z}_4 = \kappa = 2$), the Wilson loop is flat along one reciprocal direction but shows $\pm\pi$ jumps along the orthogonal direction, consistent with gapped edges and corner-localized states in finite geometries. Figure 12 shows (i) parity products at TRIMs, (ii) Wilson-loop spectra, and (iii) edge spectral functions to make this correspondence explicit in each phase.

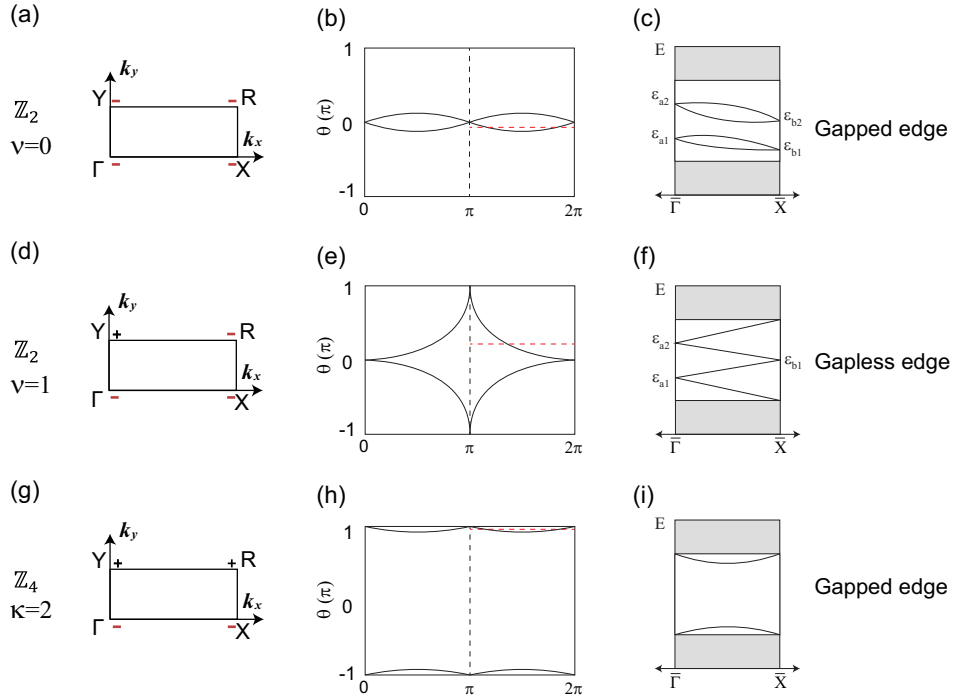


FIG. 12. Bulk–edge correspondence for three representative insulating phases. Left column: parity products at the four TRIMs; middle column: Wilson-loop evolution; right column: edge spectrum (for a symmetry-preserving [100] edge). (a)–(c) Trivial insulator ($\nu_0 = 0$, $\kappa_1 = 0$)—No parity inversion; trivial Wilson-loop evolution with no π winding; gapped edge spectrum without boundary modes. (d)–(f) QSHI ($\nu_0 = 1$)—An odd number of parity inversions yields nontrivial $\mathbb{Z}_2$; the Wilson loop exhibits partner switching (the flow crosses the red reference line an odd number of times over half the BZ); the edge spectrum shows a single Kramers pair traversing the bulk gap (gapless helical edge). (g)–(i) HOTI ($\nu_0 = 0$, $\kappa_1 = 2$)—Even $\mathbb{Z}_2$ but nontrivial $\mathbb{Z}_4$; the Wilson loop displays two π -pinned Wannier bands or flows characteristic of higher-order topology; the edge spectrum is fully gapped (no helical crossing), consistent with corner—rather than edge—modes. In the Wilson-loop panels the red dashed line marks the reference for counting crossings over half of the Brillouin zone; in the edge panels the shaded region indicates the bulk gap.

TABLE III. Summary of three phases in terms of topological indices, Wilson-loop and edge-state signatures. Here ν_0 denotes the parity product of occupied bands, and κ_1 is the $\mathbb{Z}_4$ indicator for 2D systems.

Phase	$\mathbb{Z}_2$ (ν_0)	$\mathbb{Z}_4$ (κ_1)	Wilson loop	Helical edge states
QSHI	1	1 or 3	Odd partner switching (helical)	Present (quantized edge conductance)
HOTI	0	2	Wannier bands pinned at π	Absent (gapped edges; corner modes)
Trivial insulator	0	0	No crossing/no pinning	Absent (fully insulating)

APPENDIX C: EIGHT-BAND TIGHT-BINDING MODEL

To establish an effective low-energy Hamiltonian for TaIrTe₄, we start from the electronic structure analysis near the Fermi level. The DFT orbital decomposition indicates that the dominant orbitals contributing around the Fermi energy are $d_{x^2-y^2}$ and d_{yz} from the two Ta atoms. Hence, we construct a minimal 8-band model based on these orbitals, incorporating spin degrees of freedom.

The general form of the 8-band Hamiltonian is given by

$$H(\mathbf{k}) = H_0(\mathbf{k}) + H_{\text{SOC}}(\mathbf{k}), \quad (\text{C1})$$

where $H_0(\mathbf{k})$ captures orbital hopping, and $H_{\text{SOC}}(\mathbf{k})$ introduces spin-orbit coupling.

1. Optimized Wannier fit (hopping terms)

Considering crystal symmetries and nearest-neighbor hopping processes, the noninteracting Hamiltonian $H_0(\mathbf{k})$ is expressed as

$$H_0(\mathbf{k}) = [\mu_1 + t_1 \cos(ak_x)]\Gamma_1^+ + [\mu_2 + d_1 \cos(ak_x)]\Gamma_1^- + [(t_2 + t_3 e^{ibk_y})(1 + e^{iak_x})]\Gamma_2^+ + [(d_2 + d_3 e^{ibk_y})(1 + e^{iak_x})]\Gamma_2^- \\ + h_1 \cos(ak_x)\Gamma_3 + [(h_2 + h_3 e^{ibk_y})(1 + e^{iak_x})]\Gamma_4^+ + [(h_2 + h_3 e^{-ibk_y})(1 + e^{-iak_x})]\Gamma_4^- + \text{H.c.}, \quad (\text{C2})$$

where t_i , d_i represent intra-orbital hoppings within $d_{x^2-y^2}$ and d_{yz} orbitals, respectively, and h_i describe interorbital couplings between these orbitals. Potentials for different orbitals are denoted by μ_1 and μ_2 .

The Hamiltonian matrices Γ_i are linear combinations of Pauli matrices acting in the orbital and sublattice basis:

$$(a_{\mathbf{k},Ad_{x^2-y^2}s}, a_{\mathbf{k},Bd_{x^2-y^2}s}, a_{\mathbf{k},Ad_{yz}s}, a_{\mathbf{k},Bd_{yz}s}),$$

where A, B denote two Ta atoms, and $s = \uparrow, \downarrow$ is the spin.

Explicitly, these matrices are defined as

$$\Gamma_1^\pm = \frac{1}{4}\tau_0(\sigma_0 \pm \sigma_3), \quad \Gamma_2^\pm = \frac{1}{4}(\tau_1 + i\tau_2)(\sigma_0 \pm \sigma_3), \\ \Gamma_3 = \frac{1}{2}\tau_0(\sigma_1 + i\sigma_2), \quad \Gamma_4^\pm = \frac{1}{4}(\tau_1 \pm i\tau_2)(\sigma_1 + i\sigma_2),$$

with σ_i acting on orbital space, and τ_i on sublattice degrees of freedom.

2. Spin-orbit coupling from symmetry

Considering symmetry constraints—translation symmetry $T(\mathbf{R})$, inversion symmetry $\mathcal{P}$, time-reversal symmetry Θ , and mirror symmetry ($\mathcal{M}_x$)—we introduce SOC into the Hamiltonian. In our chosen basis, these symmetries are represented by

$$\Theta = is_y\tau_0\sigma_0\mathcal{K}, \quad \mathcal{P} = s_0\tau_1\sigma_0, \quad \mathcal{M}_x = is_x\tau_0\sigma_0.$$

These symmetry operations enforce constraints:

$$OH(\mathbf{k})O^{-1} = H(O\mathbf{k}),$$

where O represents symmetry operations. The resulting symmetry-allowed SOC terms (up to nearest neighbors) are simplified as

$$H_{\text{SOC}}(\mathbf{k}) = \lambda_1 \sin(ak_x)s_z\Gamma_5^+ + \lambda_2 \sin(ak_x)s_z\Gamma_5^-, \quad (\text{C3})$$

with the matrices

$$\Gamma_5^\pm = \frac{1}{4}\tau_3(\sigma_0 \pm \sigma_3)$$

and parameters λ_1 and λ_2 quantify SOC strength for $d_{x^2-y^2}$ and d_{yz} orbitals, respectively.

3. Band structure and parity eigenvalues

Figure 13 illustrates the band structures and parity eigenvalues (ξ) obtained from our optimized tight-binding model, elucidating the underlying band inversion mechanisms. Figure 13(a) schematically depicts the evolution of bands under different symmetry conditions: initially, screw symmetry protects the degeneracies at $k_x = \pi$ (X, R points). Without spin-orbit coupling, the degeneracies at X and R are robust due to the screw symmetry, and these degenerate bands have opposite parity eigenvalues ($\xi = \pm 1$), originating from sublattice

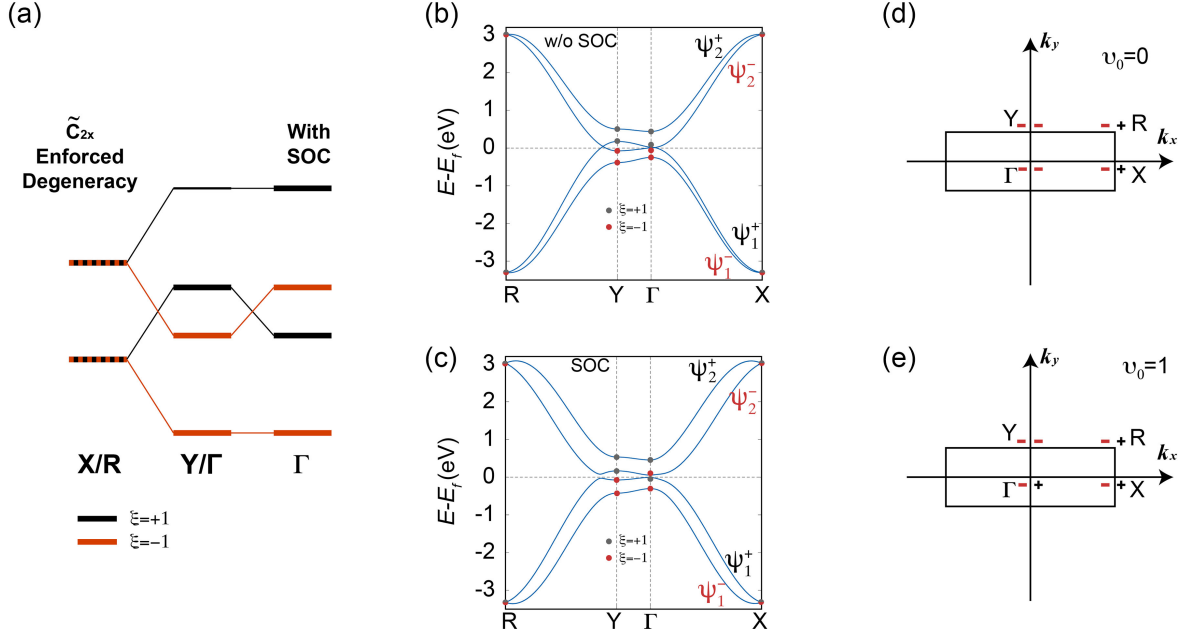


FIG. 13. Mechanism of band inversion and parity eigenvalues from tight-binding model. (a) Schematic illustration of the band inversion mechanism, showing the evolution of bands under screw symmetry and spin-orbit coupling. The black and orange lines denote states with positive ($\xi = +1$) and negative ($\xi = -1$) parity eigenvalues, respectively. (b),(c) Band structures obtained from the tight-binding model (b) without SOC and (c) with SOC, respectively. Bands near the Fermi level are labeled as ψ_1^+ and ψ_2^+ , and the parity eigenvalues at the time-reversal invariant momenta are explicitly indicated by solid circles. (d),(e) Schematic distribution of parity eigenvalues at the TRIM points (Γ , X, Y, R) without and with SOC, respectively. The parity eigenvalue switching at the Γ point leads to a topological transition from a trivial insulator ($\nu_0 = 0$) to a quantum spin Hall insulator phase ($\nu_0 = 1$), indicating a single band inversion occurring at the Y point when SOC is included.

symmetry. However, at the (Γ) and (Y) points, the screw symmetry does not enforce band degeneracy, allowing bands with different orbital characters to split. Consequently, the bands at these points undergo simultaneous parity inversion, resulting in identical parity configurations ($- - +$), as explicitly shown in Fig. 13(b). This scenario yields a trivial topological invariant ($\nu_0 = 0$), consistent with our DFT calculations without SOC.

Upon incorporating SOC, the parity inversion at the Γ point is reversed to a normal state, whereas the inversion at the Y point persists. Thus, as depicted in Fig. 13(c), the parity eigenvalues at Γ become ($- + -$), while at Y remain ($- - +$). This single band inversion at the Y point gives rise to a nontrivial topological phase characterized by a $\mathbb{Z}_2$ invariant $\nu_0 = 1$. The resulting quantum spin Hall insulator phase is further confirmed by the presence of robust helical edge states along both [100] and [010] edges, as demonstrated in Fig. 9 of Sec. A and Fig. 2 in Sec. IIC of the main text.

Figures 13(d) and 13(e) explicitly show the parity eigenvalue distributions at the four time-reversal invariant momenta, clearly highlighting the transition from a trivial to a nontrivial $\mathbb{Z}_2$ topological phase induced by SOC. Collectively, these results not only accurately reproduce the band eigenvalues near the Fermi level but also consistently

capture the topology evolution revealed by our DFT calculations, validating the accuracy and robustness of our tight-binding model. All fitted model parameters are summarized explicitly in Table IV.

4. Calculation of the charge susceptibility

To analyze the electronic instabilities induced by Fermi surface nesting and vHS, we compute the static Lindhard charge susceptibility $\chi_0(\mathbf{q})$ based on the non-interacting 8-band tight-binding model. The susceptibility is evaluated using the following expression:

TABLE IV. Tight-binding model parameters of the eight-band model for monolayer TaIrTe₄. The model parameters correspond to Eqs. (C2) and (C3).

Parameter	Value (meV)	Parameter	Value (meV)
μ_1	1610	h_1	-45
μ_2	-1700	h_2	10
t_1	-700	h_3	10
t_2	130	λ_1	200
t_3	-15	λ_2	-150
d_1	800		
d_2	100		
d_3	-40		

$$\chi_0(\mathbf{q}) = -\frac{1}{N_k} \sum_{\mathbf{k}, n, m} \frac{f(\epsilon_{n\mathbf{k}}) - f(\epsilon_{m\mathbf{k}+\mathbf{q}})}{\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}+\mathbf{q}} + i\eta}, \quad (\text{C4})$$

where $f(\epsilon)$ is the Fermi-Dirac distribution, $\epsilon_{n\mathbf{k}}$ is the eigenvalue of the n th band at momentum $\mathbf{k}$, and η is a small broadening factor introduced to regularize the denominator. The summation runs over all band indices n, m and discrete momentum points $\mathbf{k}$ in the Brillouin zone.

We performed this calculation on a dense k -mesh (typically 300×300) to ensure convergence near sharp features such as vHSSs. The resulting $\chi_0(\mathbf{q})$ characterizes the momentum-resolved charge response of the system and can be used to identify possible nesting vectors or ordering wave vectors associated with CDW instabilities.

APPENDIX D: HARTREE-FOCK MEAN FIELD CALCULATIONS

1. Methods

Here, we consider general Coulomb interactions in TaIrTe₄,

$$\hat{V} = \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' \sum_{s, s'} \hat{c}_s^\dagger(\mathbf{r}) \hat{c}_{s'}^\dagger(\mathbf{r}') V_{\text{int}}(|\mathbf{r} - \mathbf{r}'|) \hat{c}_{s'}(\mathbf{r}') \hat{c}_s(\mathbf{r}),$$

where $\hat{c}_s(\mathbf{r})$ is electron annihilation operator at continuous coordinate $\mathbf{r}$ with spin s . It can be projected to the Wannier lattice basis as

$$\hat{c}_s^\dagger(\mathbf{r}) = \sum_{\mathbf{R}, \alpha} w_{\mathbf{R}, \alpha}^*(\mathbf{r}) a_{\mathbf{R}, \alpha s}^\dagger, \quad (\text{D1})$$

where subscript $\mathbf{R}$ labels a Bravais lattice site, α is a sublattice or orbital index, and s is a spin index. The interaction can be expressed as

$$\begin{aligned} \hat{V}_{\text{int}} = & \frac{1}{2} \sum_{\mathbf{R}_1 \mathbf{R}_2 \mathbf{R}_3 \mathbf{R}_4} \sum_{\alpha \beta \beta' \alpha'} \sum_{s s'} \hat{a}_{\mathbf{R}_1, \alpha s}^\dagger \hat{a}_{\mathbf{R}_2, \beta s'}^\dagger \\ & \times V_{\mathbf{R}_1 \mathbf{R}_4, \mathbf{R}_2 \mathbf{R}_3}^{\alpha \alpha' s, \beta \beta' s'} \hat{a}_{\mathbf{R}_3, \beta' s'} \hat{a}_{\mathbf{R}_4, \alpha' s}, \end{aligned} \quad (\text{D2})$$

where

$$\begin{aligned} V_{\mathbf{R}_1 \mathbf{R}_4, \mathbf{R}_2 \mathbf{R}_3}^{\alpha \alpha' s, \beta \beta' s'} = & \iint d\mathbf{r} d\mathbf{r}' V_{\text{int}}(|\mathbf{r} - \mathbf{r}'|) w_{\mathbf{R}_1, \alpha}^*(\mathbf{r}) w_{\mathbf{R}_2, \beta}^*(\mathbf{r}') \\ & \times w_{\mathbf{R}_3, \beta'}(\mathbf{r}') w_{\mathbf{R}_4, \alpha'}(\mathbf{r}). \end{aligned} \quad (\text{D3})$$

Here, we assume that the “density-density” interaction takes an important role in the system, $V_{\mathbf{R}_1 \mathbf{R}_4, \mathbf{R}_2 \mathbf{R}_3}^{\alpha \alpha' s, \beta \beta' s'} \approx V_{\mathbf{R}_1 \mathbf{R}_4, \mathbf{R}_2 \mathbf{R}_3}^{\alpha \alpha s, \beta \beta s'} \equiv V_{\mathbf{R}_1 \alpha s, \mathbf{R}_2 \beta s'}$. Then the Coulomb interaction can be written as

$$\begin{aligned} \hat{V}_{\text{int}} = & \frac{1}{2} \sum_{\mathbf{R}_1 \mathbf{R}_2} \sum_{\alpha \beta} \sum_{s s'} \hat{a}_{\mathbf{R}_1, \alpha s}^\dagger \hat{a}_{\mathbf{R}_2, \beta s'}^\dagger V_{\mathbf{R}_1 \alpha s, \mathbf{R}_2 \beta s'} \hat{a}_{\mathbf{R}_2, \beta s'} \hat{a}_{\mathbf{R}_1, \alpha s} \\ = & \frac{1}{2} \sum_{\mathbf{R}_1 \alpha \neq \mathbf{R}_2 \beta} \sum_{s s'} \hat{a}_{\mathbf{R}_1, \alpha s}^\dagger \hat{a}_{\mathbf{R}_2, \beta s'}^\dagger V_{\mathbf{R}_1 \alpha, \mathbf{R}_2 \beta} \hat{a}_{\mathbf{R}_2, \beta s'} \hat{a}_{\mathbf{R}_1, \alpha s} \\ & + \sum_{\mathbf{R} \alpha} U \hat{a}_{\mathbf{R}, \alpha \uparrow}^\dagger \hat{a}_{\mathbf{R}, \alpha \downarrow}^\dagger a_{\mathbf{R}, \alpha \downarrow} a_{\mathbf{R}, \alpha \uparrow}, \end{aligned} \quad (\text{D4})$$

where we separate off the on-site Hubbard term with coefficient U . In our approximation, the hopping process of electrons getting through the lattice is modified by the Coulomb interaction. In our main text, we focus on the density-density interaction as

$$\begin{aligned} \hat{H}_{\text{int}} = & U \sum_{\mathbf{R} \alpha} \hat{n}_{\mathbf{R}, \alpha \uparrow} \hat{n}_{\mathbf{R}, \alpha \downarrow} \\ & + \frac{1}{2} \sum_{\mathbf{R}_1 \alpha \neq \mathbf{R}_2 \beta} \sum_{s s'} V_{\mathbf{R}_1 \alpha, \mathbf{R}_2 \beta} \hat{n}_{\mathbf{R}_1, \alpha s} \hat{n}_{\mathbf{R}_2, \beta s'}, \end{aligned} \quad (\text{D5})$$

where $\hat{n}$ is the density operator, U is the strength of the onsite Hubbard interaction, and V is the amplitude of the density-density interaction between sites.

We use a double-gate method to model screening effects and get the values of U and V . A general Coulomb interaction $V(r)$ is screened by a pair of metallic gates, each a distance $\pm d$ from the 2D TaIrTe₄. The gates are assumed to be perfect conductors so that the screened Coulomb interaction can be expressed as

$$V(r) = \frac{e^2}{4\pi\epsilon_0\epsilon_r} \sum_{z \in \mathbb{Z}} \frac{(-1)^z}{\sqrt{r^2 + (2dz)^2}}, \quad (\text{D6})$$

where ϵ_r is a background dielectric constant and the distance between two gates is $d = 100$ Å. We have checked the influence of the distance d for our results. The Hartree-Fock mean field (HFMF) phase diagram of $d = 200$ Å is similar to $d = 100$ Å. To simulate the onsite screening, we vary U by considering r in a range of 0.8 to 2.0 Å.

For the HFMF loop, we again write the extended Hubbard Hamiltonian defined on a tight-binding basis:

$$\begin{aligned} \hat{H} = & \hat{H}_0 + \hat{H}_{\text{int}} \\ = & \sum_{\mathbf{R}_1 \mathbf{R}_2} \sum_{\alpha \beta s} t_{\mathbf{R}_1 - \mathbf{R}_2, \alpha \beta} a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_2, \beta s} + U \sum_{\mathbf{R} \alpha} \hat{n}_{\mathbf{R}, \alpha \uparrow} \hat{n}_{\mathbf{R}, \alpha \downarrow} \\ & + \frac{1}{2} \sum_{(\mathbf{R}_1 \alpha) \neq (\mathbf{R}_2 \beta)} \sum_{s s'} V_{\mathbf{R}_1 \alpha, \mathbf{R}_2 \beta} \hat{n}_{\mathbf{R}_1, \alpha s} \hat{n}_{\mathbf{R}_2, \beta s'}, \end{aligned}$$

where $\mathbf{R}_1$ and $\mathbf{R}_2$ label a lattice sites, α, β are composite sublattice-orbital indices, and s, s' are spin indices. The matrix of correlation functions of a generic bilinear Hamiltonian are obtained by eigendecomposition:

$$\begin{aligned} \mathbf{c}^\dagger H \mathbf{c} &= \mathbf{c}^\dagger U \Lambda U^\dagger \mathbf{c} = \boldsymbol{\gamma}^\dagger \Lambda \boldsymbol{\gamma} \\ &\Rightarrow \langle (\mathbf{c}^\dagger)^T (\mathbf{c})^T \rangle = \langle (\boldsymbol{\gamma}^\dagger U^\dagger)^T (U \boldsymbol{\gamma})^T \rangle = \langle U^* (\boldsymbol{\gamma}^\dagger)^T \boldsymbol{\gamma}^T U^T \rangle = U^* \langle (\boldsymbol{\gamma}^\dagger)^T \boldsymbol{\gamma}^T \rangle U^T = U^* \text{diag}(n_F(\lambda_i)) U^T, \end{aligned} \quad (\text{D7})$$

where $\mathbf{c}$ is a vector of annihilation operators. The Hartree-Fock approximation to the density-density interaction term yields such a bilinear:

$$\begin{aligned} \hat{n}_{\mathbf{R}_1, \alpha s} \hat{n}_{\mathbf{R}_2, \beta s'} &= a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_1, \alpha s} a_{\mathbf{R}_2, \beta s'}^\dagger a_{\mathbf{R}_2, \beta s'} \\ &\approx \langle a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_1, \alpha s} \rangle a_{\mathbf{R}_2, \beta s'}^\dagger a_{\mathbf{R}_2, \beta s'} + \langle a_{\mathbf{R}_2, \beta s'}^\dagger a_{\mathbf{R}_2, \beta s'} \rangle a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_1, \alpha s} \quad \text{Hartree} \\ &\quad - \langle a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_2, \beta s'} \rangle a_{\mathbf{R}_2, \beta s'}^\dagger a_{\mathbf{R}_1, \alpha s} - \langle a_{\mathbf{R}_2, \beta s'}^\dagger a_{\mathbf{R}_1, \alpha s} \rangle a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_2, \beta s'}. \quad \text{Fock} \end{aligned}$$

We demand translational invariance by picking a preferred origin and forcing all other correlation functions to match, i.e.,

$$\langle a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_2, \beta s'} \rangle = \langle a_{\mathbf{R}_1 - \mathbf{R}_2, \alpha s}^\dagger a_{\mathbf{0}, \beta s'} \rangle, \quad (\text{D8})$$

which means the correlation functions depend only on the difference in coordinates. This yields a new, also translationally invariant, bilinear Hamiltonian

$$\hat{H}_{\text{HF}} = \sum_{\substack{\mathbf{R}_1 \mathbf{R}_2, \\ \alpha \beta s s'}} h_{\mathbf{R}_1 - \mathbf{R}_2, \alpha \beta s s'} a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_2, \beta s'}$$

with

$$\begin{aligned} h_{\mathbf{R}_1 - \mathbf{R}_2, \alpha \beta s s'} &= t_{\mathbf{R}_1 - \mathbf{R}_2, \alpha \beta} \delta_{ss'} + U \delta_{\mathbf{R}_1 - \mathbf{R}_2, \mathbf{0}} \delta_{\alpha \beta} \begin{bmatrix} \langle a_{\mathbf{R}_1 \alpha \downarrow}^\dagger a_{\mathbf{R}_1 \alpha \downarrow} \rangle & -\langle a_{\mathbf{R}_1 \alpha \downarrow}^\dagger a_{\mathbf{R}_1 \alpha \uparrow} \rangle \\ -\langle a_{\mathbf{R}_1 \alpha \uparrow}^\dagger a_{\mathbf{R}_1 \alpha \downarrow} \rangle & \langle a_{\mathbf{R}_1 \alpha \uparrow}^\dagger a_{\mathbf{R}_1 \alpha \uparrow} \rangle \end{bmatrix}_{ss'} \\ &\quad + \delta_{\mathbf{R}_1 - \mathbf{R}_2, \mathbf{0}} \delta_{\alpha \beta} \delta_{ss'} \sum_{\mathbf{R} \neq \mathbf{0}, \gamma, s''} V_{0\alpha, R\gamma} \langle a_{\mathbf{R}\gamma s''}^\dagger a_{\mathbf{R}\gamma s''} \rangle - V_{R1\alpha, R2\beta} \langle a_{\mathbf{R}_2 \beta s'}^\dagger a_{\mathbf{R}_1 \alpha s} \rangle, \end{aligned}$$

which leads to a fixed-point equation for the correlation functions. Our relatively large Hartree-Fock problem is tractable for the following reasons. First, translational invariance simplifies the calculation of correlation functions. The Fourier transform of H_{HF} is block diagonal in $\mathbf{k}$:

$$\begin{aligned} \hat{H}_{\text{HF}} &= \frac{1}{N_k} \sum_{\mathbf{k}} \left[\sum_{\mathbf{R}_1 - \mathbf{R}_2} h_{\mathbf{R}_1 - \mathbf{R}_2, \alpha \beta s s'} e^{-i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \right] a_{\mathbf{k}, \alpha s}^\dagger a_{\mathbf{k}, \beta s'} \\ &= \frac{1}{N_k} \sum_{\mathbf{k}} h_{\mathbf{k}, \alpha \beta s s'} a_{\mathbf{k}, \alpha s}^\dagger a_{\mathbf{k}, \beta s'}, \end{aligned}$$

yielding correlation functions $\langle c_{\mathbf{k}, \alpha s}^\dagger c_{\mathbf{k}, \beta s'} \rangle$ by the above derivation. N_k is the number of points in the k -space mesh. The small block matrices can be diagonalized in parallel on a GPU. The real space correlation functions are of course given by the inverse transform

$$\langle a_{\mathbf{R}_1, \alpha s}^\dagger a_{\mathbf{R}_2, \beta s'} \rangle = \frac{1}{N_k} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_1 - \mathbf{R}_2)} \langle a_{\mathbf{k}, \alpha s}^\dagger a_{\mathbf{k}, \beta s'} \rangle,$$

which are plugged back into the real-space Hamiltonian to construct the next Hartree-Fock iterate. The second

acceleration is to use a direct quasi-Newton method [42], which allows us to converge the large Hartree-Fock fixed point equations, converging 120 orbital problems in relatively few iterations. Self-consistent tests starting from nearby single-Q (14×1 , 16×1), rational approximants (e.g, 29×1), multi-Q (Q and 2Q), and random seeds all relax to the 15×1 solution or remain higher in energy.

2. Topological properties of dual QSHI phase

Figure 14 provides details of the topological properties associated with the dual QSHI phase discussed in the main text. In this phase, both the n_e gap (between the 62nd and 63rd bands) and the CNP gap (between the 60th and 61st bands) exhibit identical nontrivial $\mathbb{Z}_2$ topological invariants ($\nu_0 = 1$). Specifically, at the representative parameter point $U/V_1 = 2.25$, $\varepsilon = 13$, the correlated insulating state belongs to the dual QSHI phase. The band inversions for n_e gap occurs at the R point in momentum space, as indicated by the parity product distributions in panels (a). In contrast, for the CNP gap [Fig. 14(d)], the band inversion occurs at the Y point, as reflected in the parity configuration. The topological character of each gap is further confirmed by the evolution of the Wannier centers. For the

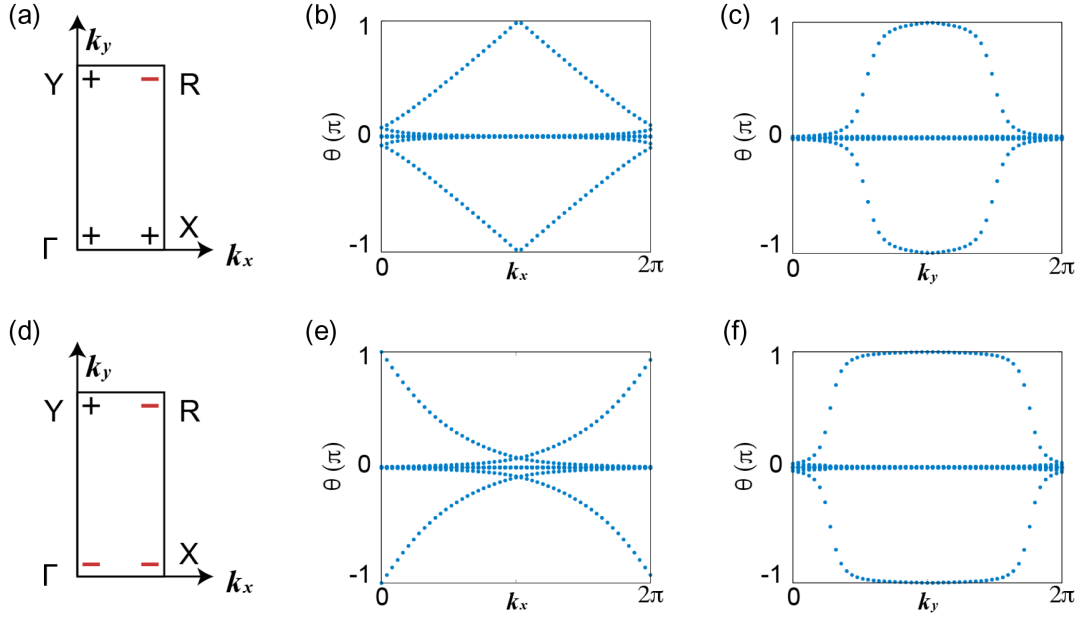


FIG. 14. Topological properties for the dual QSHI phase at $U/V_1 = 2.25$, $\varepsilon = 13$. (a)–(c) Parity eigenvalues and Wilson loop evolutions along k_x and k_y for the n_e gap, indicating a nontrivial topology with band inversion at the R point. (d)–(f) Corresponding results for the CNP gap, demonstrating the identical topological nature and confirming the dual QSHI state.

n_e gap [panels (b) and (c)], the Wannier center evolution shows nontrivial windings along both k_x and k_y directions, characterized by phase jumps at $\pm\pi$, indicating clearly defined QSHI behavior. Similar topological features are observed at the CNP gap, as shown in panels (e) and (f). Despite the difference in inversion momenta, both gaps

yield a nontrivial $\mathbb{Z}_2$ gap, constituting the dual QSHI phase. These features also explain the presence of helical edge states in both gaps, as described in the main text. These findings fully reproduce and support the existence of the dual QSHI state, confirming that electron interactions stabilize robust topological insulating phases at both n_e and CNP gaps.

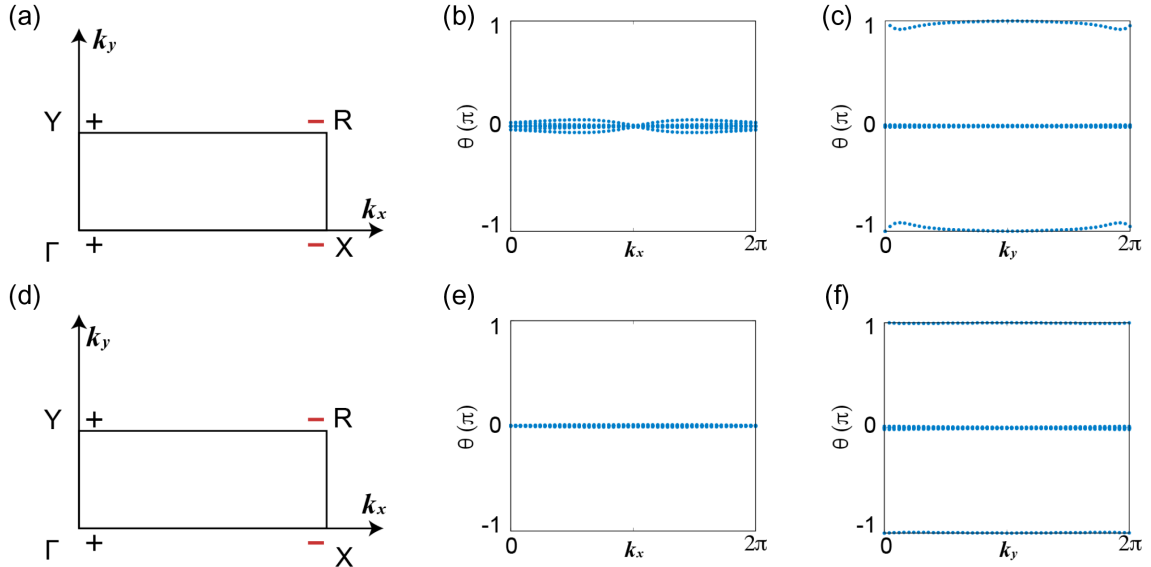


FIG. 15. Topological properties for the dual HOTI phase. (a),(d) Parity products at the four time-reversal invariant momenta for the occupied bands at the n_e gap (a) and the CNP gap (d), both showing the same pattern (+, −, +, −), indicating a $\mathbb{Z}_2$ index $\nu = 0$ and a $\mathbb{Z}_4$ invariant $\kappa_1 = 2$. (b),(e) Wilson loop spectra along the k_x direction for the n_e and CNP gaps, respectively, both showing trivial winding (flat phases). (c),(f) Wilson loop spectra along the k_y direction for the n_e and CNP gaps, respectively, showing two branches pinned at $\pm\pi$, confirming the higher-order topology.

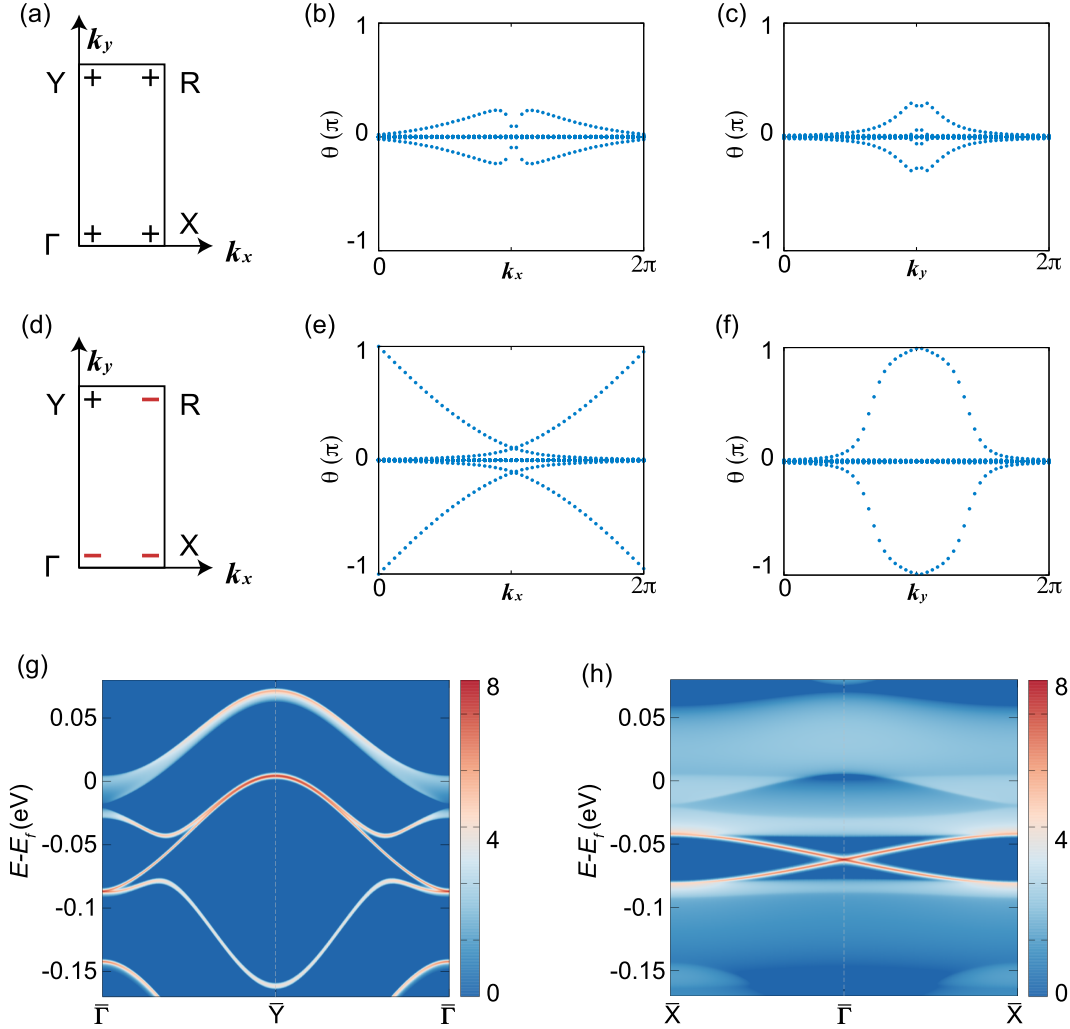


FIG. 16. Topological properties for the QSHI + Metal phase. (a),(d) Parity eigenvalues of the occupied bands at the n_e gap (a) and the CNP gap (d), respectively. The n_e bands have $\nu_0 = 0$ with trivial parity configuration, while the CNP bands exhibit a nontrivial $\nu_0 = 1$ index due to band inversion at the Y point. (b),(e) Wilson loop along k_x direction for the n_e and CNP bands. Flat phases indicate no winding for the n_e bands, while the CNP bands exhibit a nontrivial flow. (c),(f) Wilson loop along k_y , confirming the $\mathbb{Z}_2$ index change only in the CNP gap. (g),(h) Edge spectra along [010] and [100] directions. Helical edge states appear only at the CNP gap (h), while no clear topological edge modes are found at the n_e gap (g), due to the absence of a nontrivial gap.

3. Topological properties of the dual HOTI phase

In Fig. 15, we further characterize the topological properties of the dual HOTI phase. At both the n_e gap and CNP gap, the parity product distributions of the occupied bands are identical, as shown in Fig. 15. Specifically, the parity eigenvalues at the four TRIMs follow the pattern $(+, -, +, -)$, leading to a $\mathbb{Z}_2$ topological index $\nu_0 = 0$. However, the system exhibits a higher-order topology captured by the $\mathbb{Z}_4$ invariant $\kappa_1 = 2$.

The Wilson loop spectra further confirm this higher-order topological nature. Along the k_x direction, the Wilson loop phases remain zero across the Brillouin zone, indicating a trivial winding [Figs. 15(b) and 15(e)]. In contrast, along the k_y direction, the Wilson loop exhibits two branches pinned at $\pm\pi$, as shown in Figs. 15(c) and 15(f).

This behavior is consistent with a quantized polarization localized at the edges, confirming the presence of higher-order topology in both the n_e and CNP gaps. These topological features directly lead to the emergence of corner states, as observed in the main text, further validating the existence of the dual HOTI phase.

4. Topological characterization of the QSHI + metal phase

In the regime of weak electron-electron interactions, particularly at large dielectric constants (e.g., $\epsilon = 20$), our Hartree-Fock mean-field calculations reveal a distinct phase in which the system exhibits a metallic state at the n_e gap while preserving a nontrivial topological insulator at

the charge neutrality point. This coexistence defines the QSHI + metal phase.

As shown in Figs. 16(a)–16(c), the n_e gap does not develop a global insulating gap across the Brillouin zone. Instead, it remains partially gapless, indicating a metallic character. Nevertheless, we can still compute the parity eigenvalues of the occupied states at the four time-reversal invariant momenta, which yield a trivial configuration $\nu_0 = 0$. This is further supported by the Wilson loop calculations along both k_x and k_y directions [Figs. 16(b) and 16(c)], where no winding or flow in the Wannier phases is observed. This metallic character stems from insufficient electron correlations, as strong dielectric screening effectively weakens both onsite and intersite interactions. Consequently, the system remains in a Fermi-liquid-like state near the doping level, with no topological protection.

In contrast, the CNP gap remains robust and topologically nontrivial, even in the presence of reduced interactions. As shown in Figs. 16(d)–16(f), the parity products indicate a band inversion occurring at the Y point, leading to a nontrivial $\mathbb{Z}_2$ index $\nu_0 = 1$. This conclusion is verified by the Wilson loop spectra, where a characteristic gapless flow emerges in the k_x direction [Fig. 16(e)], confirming the persistence of a QSHI state at charge neutrality.

The topological distinction between these two energy gaps is further revealed by the calculated edge states. As shown in Figs. 16(g) and 16(h), the CNP gap supports well-defined helical edge states connecting conduction and valence bands, consistent with the presence of a QSHI phase. In contrast, no clear edge states are observed within the n_e gap region, demonstrating the absence of a full gap and a topologically trivial metallic character.

These results establish that under weak interaction conditions, the system undergoes a topological differentiation between the n_e and CNP gaps: the n_e gap becomes metallic, while the CNP retains a correlated QSHI character. This QSHI + metal phase highlights the critical role of interaction strength in stabilizing different topological phases and provides a concrete example of gap-selective topological behavior within a single correlated system.

APPENDIX E: STRAIN EFFECT

1. Strain dependence of the CNP topology from DFT

To quantify how uniaxial strain modifies the topology at the CNP, we performed DFT calculations under tensile strain η applied along [100]. For each η , we extract a global energy gap,

$$E_{\text{gap}}(\eta) \equiv E_c(\eta) - E_v(\eta),$$

where E_c and E_v denote, respectively, the conduction-band minimum and valence-band maximum that define the CNP gap in the primitive cell. By convention, Fig. 17 plots $E_{\text{gap}}(\eta)$ as a function of η and shows

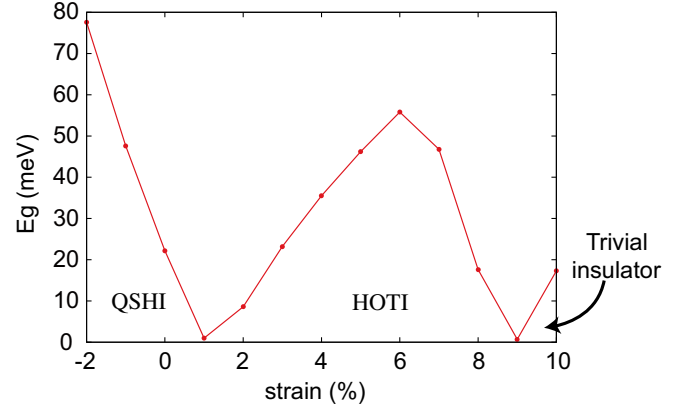


FIG. 17. DFT calculation of strain effect on the CNP gap in monolayer TaIrTe₄. Single-particle band gap at the CNP as a function of uniaxial strain η (along [100]). The gap closes and reopens near $\eta \approx 1\%$, indicating a transition from QSHI ($\nu_0 = 1$) to a HOTI regime ($\kappa_1 = 2$). For larger strain, the gap decreases again and becomes topologically trivial beyond $\eta \approx 9\%$.

- (i) QSHI $\rightarrow$ HOTI at small strain. The first zero crossing appears at $\eta \approx 1\%$, signaling a band inversion at Y. At this point the parity products at the four TRIMs give $\nu_0 = 0$ and the symmetry indicator yields $\kappa_1 = 2$, while the Wilson-loop spectrum shows Wannier bands pinned at π , identifying a HOTI at the CNP.
- (ii) HOTI $\rightarrow$ trivial requires much larger strain. Only when $\eta \gtrsim 9\%$ does the system evolve toward a trivial regime ($\nu_0 = 0$, $\kappa_1 = 0$). Such large strain is typically beyond realistic device windows, explaining why transport at the CNP most commonly observes either QSHI (no or very small strain) or HOTI (modest strain), rather than a trivial insulator.

2. Topological properties of QSHI under compressive strain

To confirm the strain-induced topological response in monolayer TaIrTe₄, we perform first-principles calculations under -1% uniaxial compressive strain. As shown in Fig. 18(a), the DFT-calculated band structure (blue) and Wannier-interpolated bands (red dashed) match well, revealing a significantly enhanced energy gap of approximately 38 meV. This enlarged gap is advantageous for observing robust edge-state transport in experiments.

We further evaluate the topological nature of the system by computing the parity eigenvalues of the occupied bands at the four time-reversal invariant momenta: Γ , X, Y, and R. The resulting parity products are $(+, +, -, +)$, which match the unstrained case and confirm that the system remains in the quantum spin Hall insulator phase under compressive strain.

Figure 18(b) presents the Wilson loop evolution of the Wannier centers along the k_x direction. The Wannier phases exhibit a gapless flow and cross $\theta = \pm\pi$ at $k_x = 0$,

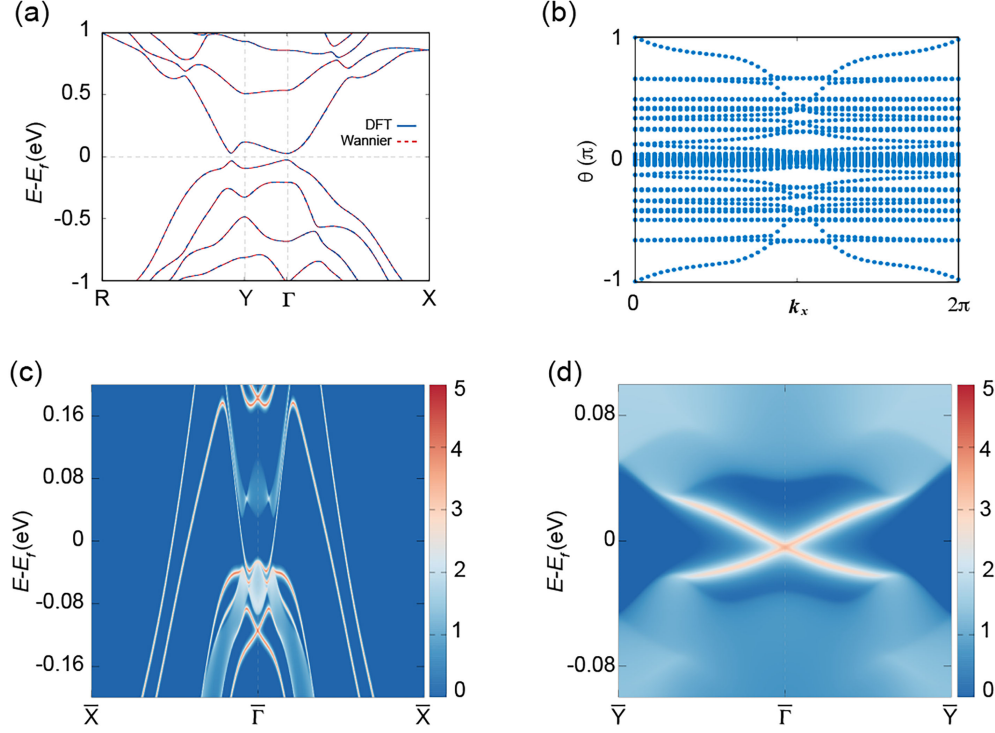


FIG. 18. Topological properties for QSHI under -1% strain. (a) DFT band structure (blue) and Wannier interpolation (red dashed) under -1% uniaxial strain. The band gap increases to approximately 38 meV. (b) Wilson loop evolution of the occupied bands along the k_x direction, showing a nontrivial winding with $\pm\pi$ phase jump at $k_x = 0$, confirming the $\mathbb{Z}_2$ invariant $\nu_0 = 1$. (c) Topological edge states along the $[100]$ direction, showing gapless helical edge modes. (d) Topological edge states along the $[010]$ direction, also showing helical edge modes protected by time-reversal symmetry.

indicating a nontrivial $\mathbb{Z}_2$ index $\nu_0 = 1$. This agrees well with the parity product analysis. Figures 18(c) and 18(d) show the edge state spectra along the $[100]$ and $[010]$ directions, respectively. In both cases, a pair of gapless helical edge modes traverse the bulk gap, further confirming the nontrivial topological character. These edge states are protected by time-reversal symmetry and are a hallmark of QSHI.

In summary, our results demonstrate that the QSHI phase in TaIrTe_4 is robust against moderate compressive strain.

The enlarged band gap improves the experimental accessibility of the edge states, offering a promising route for realizing strain-enhanced topological transport in correlated 2D materials.

3. Topological properties under tensile strain

To illustrate the strain-driven topological phase transition from a QSHI to a HOTI phase, we perform first-principles calculations at $+5\%$ tensile strain. As shown in Fig. 19(a), the DFT and Wannier-interpolated bands reveal a clear

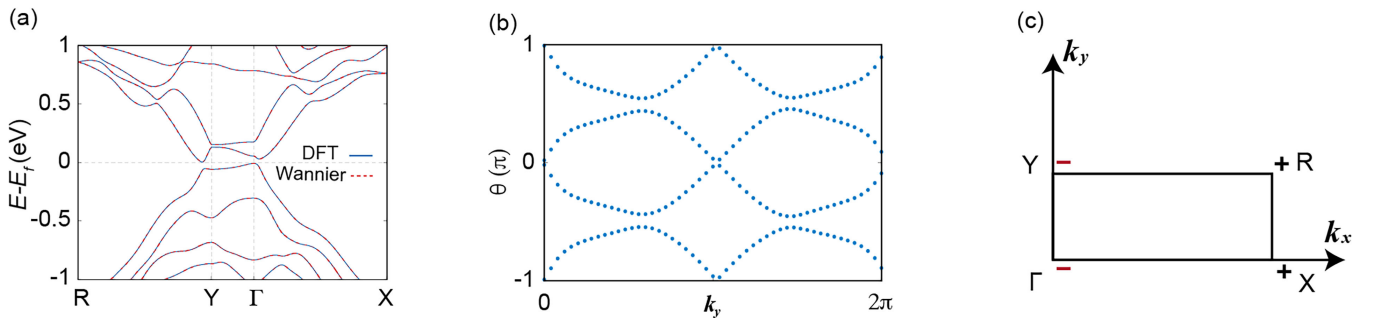


FIG. 19. Topological properties of TaIrTe_4 under $+5\%$ tensile strain. (a) DFT band structure (blue) and Wannier interpolation (red dashed) under strain, showing a new band inversion at the Γ point. (b) Wilson loop evolution along the k_y direction. The appearance of $\pm\pi$ flow signals higher-order topology. (c) Parity products at the four TRIM points (Γ , X , Y , R), yielding the pattern $(-, +, -, +)$. This corresponds to a trivial $\mathbb{Z}_2$ index $\nu_0 = 0$ and nontrivial $\mathbb{Z}_4$ index $\kappa_1 = 2$, indicative of a HOTI phase.

band inversion at the Γ point, which is absent under zero strain. This inversion accompanies the one already present at Y, leading to a double band inversion scenario.

The Wilson loop calculation along the k_y direction [Fig. 19(b)] exhibits two Wannier bands crossing $\theta = \pm\pi$, indicating a nontrivial higher-order topology. Consistently, the parity products at the four time-reversal invariant momenta (Γ, X, Y, R) are $(-, +, -, +)$ [Fig. 19(c)], confirming that the system's $\mathbb{Z}_2$ invariant becomes $\nu_0 = 0$, while the $\mathbb{Z}_4$ invariant $\kappa_1 = 2$, characteristic of a HOTI phase.

These results validate our main-text phase diagram and demonstrate that under sufficient tensile strain, the system transitions into a HOTI state with double parity inversions and boundary-localized topological corner modes.

4. QSHI + HOTI phase under 2% tensile strain

To further illustrate the impact of strain on correlated topological phases, we present a representative example of

the QSHI + HOTI phase at 2% tensile strain, with fixed interaction strength $U/V_1 = 2.25$ and dielectric constant $\varepsilon = 13$. As shown in Fig. 20(a), the band structure reveals two distinct insulating gaps: one at the n_e level and the other at the charge neutrality point. The system thus enters a hybrid phase, where the n_e gap hosts a quantum spin Hall insulator, while the CNP gap transitions into a higher-order topological insulator.

This distinction is confirmed by detailed topological analyses. For the n_e gap, the parity products at the four TRIMs (Γ, X, Y, R) follow the pattern $(+ + + -)$, as shown in Fig. 20(c), corresponding to a $\mathbb{Z}_2$ index $\nu_0 = 1$. The Wilson loop evolution further supports this assignment: along k_x , we observe nontrivial winding with a pair of phases crossing at π [Fig. 20(d)], and a gapless flow of Wannier centers along k_y [Fig. 20(e)]. These features are characteristic of the QSHI phase. Moreover, the helical edge states remain clearly visible within the n_e gap, as shown in Fig. 20(b).

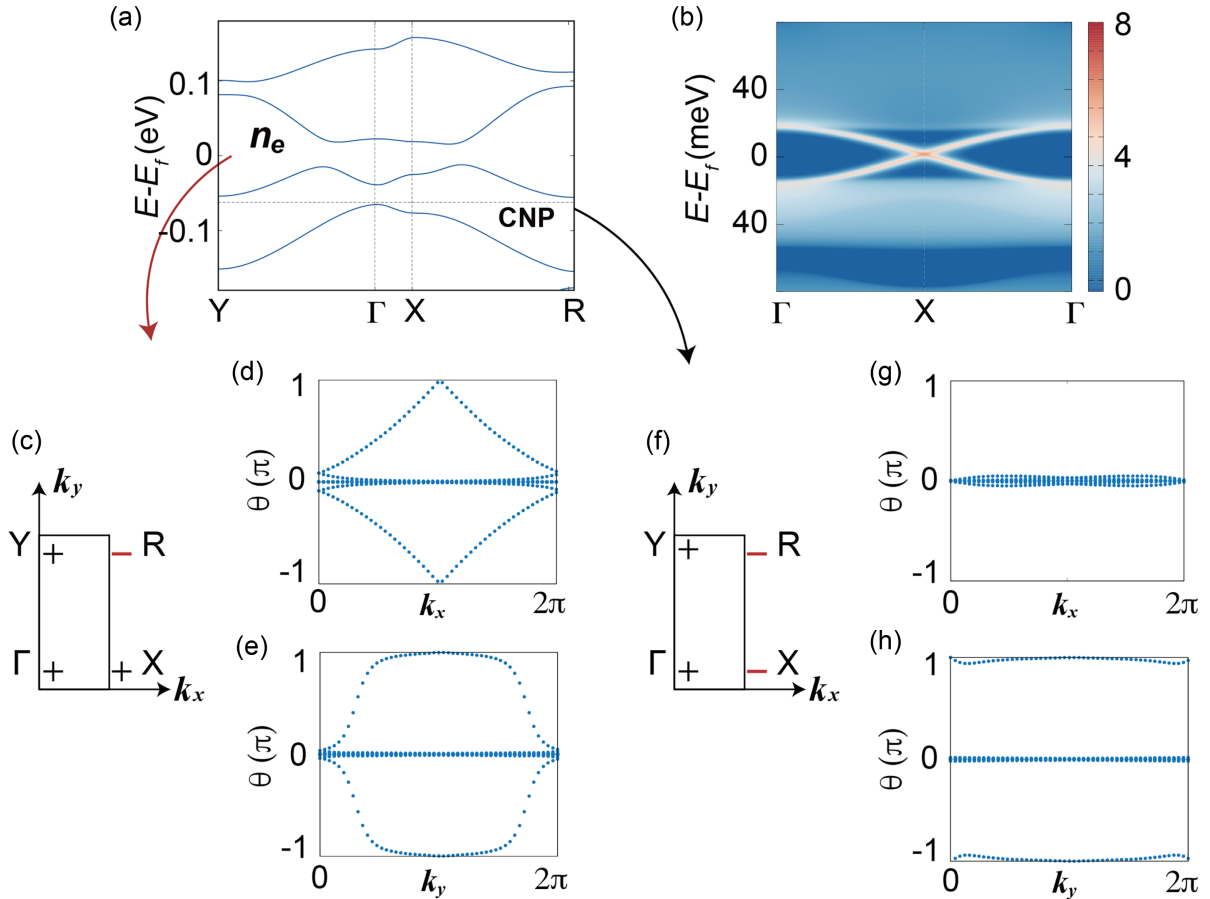


FIG. 20. Topological properties for the QSHI + HOTI phase under 2% tensile strain. (a) Band structure showing two distinct gaps at the n_e level and CNP. (b) Edge spectral function along the $[100]$ edge, showing helical edge states only at the n_e gap. (c) Parity products at four TRIMs for occupied bands up to the n_e gap, giving $\nu_0 = 1$. (d)–(e) Wilson loop of occupied bands up to the n_e gap along k_x and k_y , respectively. (f) Parity products for bands up to the CNP, giving $\nu_0 = 0$, $\kappa_1 = 2$. (g)–(h) Wilson loop evolution for CNP gap, showing trivial $\mathbb{Z}_2$ but nontrivial $\mathbb{Z}_4$ topology.

By contrast, the CNP gap exhibits a different topological structure. The parity products follow the distribution $(+ - + -)$, indicating that the system undergoes band inversions at both the X and R points. This leads to a trivial $\mathbb{Z}_2$ index ($\nu_0 = 0$), but a nontrivial $\mathbb{Z}_4$ index $\kappa_1 = 2$, confirming the HOTI character. The Wilson loops along both directions [Figs. 20(g) and 20(h)] show flat and gapped phases, with a phase shift of $\pm\pi$ emerging only along k_x , consistent with boundary-localized Wannier centers typical of HOTIs. No helical edge states are observed in the CNP gap, as expected for a second-order topological insulator.

This result demonstrates that under the same interaction conditions ($U/V_1 = 2.25$, $\varepsilon = 13$), varying the strain alone can induce a topological phase transition from the previously observed dual QSHI state into a mixed QSHI + HOTI configuration. It also highlights that the CNP gap is more sensitive to strain modulation than the n_e gap, which retains its QSHI topology under small tensile strains.

5. Dual HOTI phase under 4% tensile strain

By further increasing the tensile strain to 4%, while keeping the interaction parameters fixed at $U/V_1 = 2.25$ and dielectric constant $\varepsilon = 13$, we observe a clear transition from the QSHI + HOTI coexistence at 2% strain into a robust dual HOTI phase, as summarized in Fig. 21.

In this dual HOTI state, both the n_e gap and the CNP gap exhibit trivial $\mathbb{Z}_2$ invariants ($\nu_0 = 0$), yet share identical, nontrivial $\mathbb{Z}_4$ topology characterized by $\kappa_1 = 2$. Specifically, the parity products at the four TRIM points (Γ , X, Y, R) indicate band inversions occurring simultaneously at both the X and R points for both n_e and CNP gaps, reflecting double band inversions that stabilize higher-order topological insulator phases.

Further confirmation is provided by Wilson loop analyses. As shown in Figs. 21(d), 21(e), 21(g), and 21(h), Wilson loop evolutions along k_x exhibit trivial phases without crossings, whereas along k_y direction, nontrivial

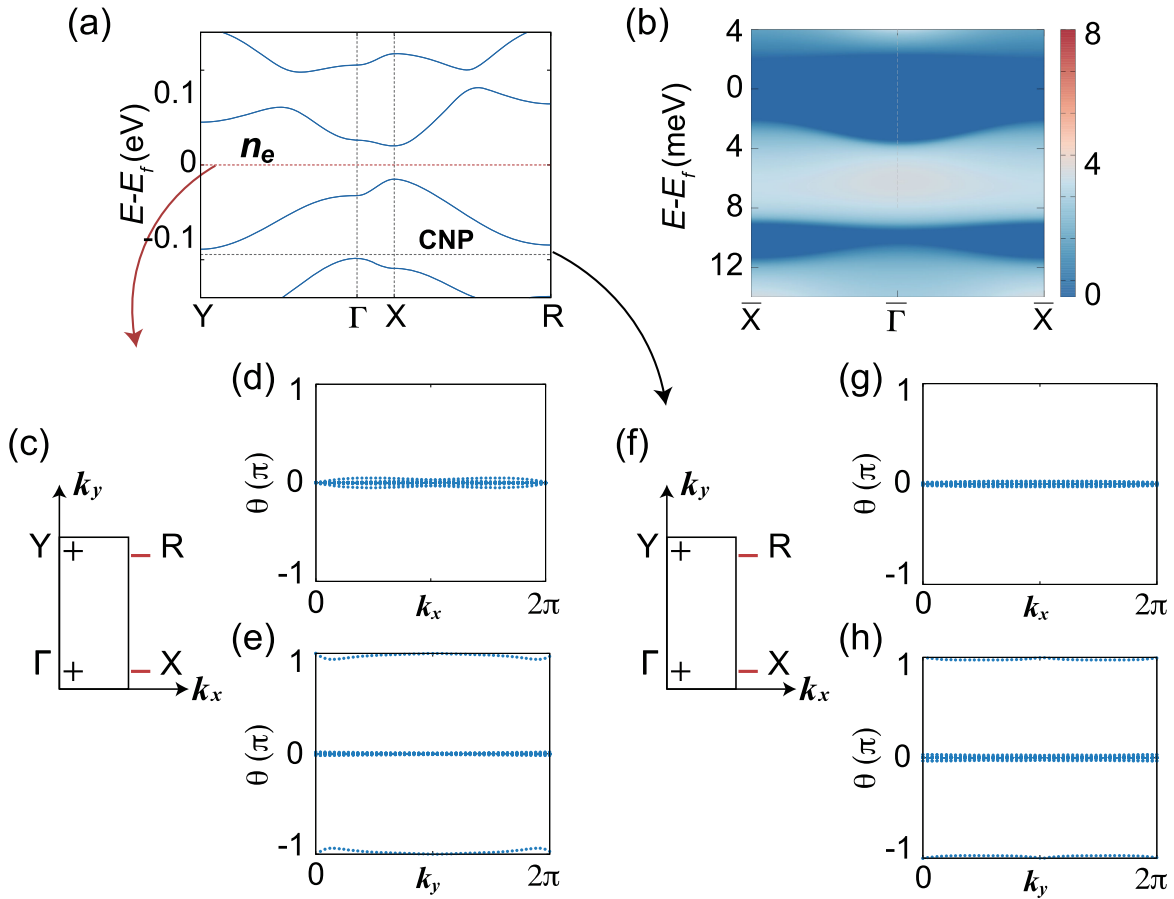


FIG. 21. Topological characterization of the dual HOTI phase under 4% tensile strain. (a) Band structure for the correlated insulating phases at the n_e and CNP gaps under tensile strain. (b) Calculated edge spectral function along the [100] direction, confirming the absence of helical edge states. (c) Parity products at four TRIM points (Γ , X, Y, R) for the occupied bands up to the n_e gap, giving a trivial $\mathbb{Z}_2$ invariant $\nu_0 = 0$ but a nontrivial $\mathbb{Z}_4$ invariant $\kappa_1 = 2$. (d)–(e) Wilson loop evolutions along k_x and k_y directions for the n_e gap, showing nontrivial topology only along the k_y direction. (f) Parity products at TRIM points for occupied bands up to the CNP gap, also giving $\nu_0 = 0$ and nontrivial $\kappa_1 = 2$. (g)–(h) Wilson loop evolutions along k_x and k_y directions at the CNP gap, demonstrating a similar topological behavior as in the n_e gap, thus confirming the presence of a dual HOTI phase.

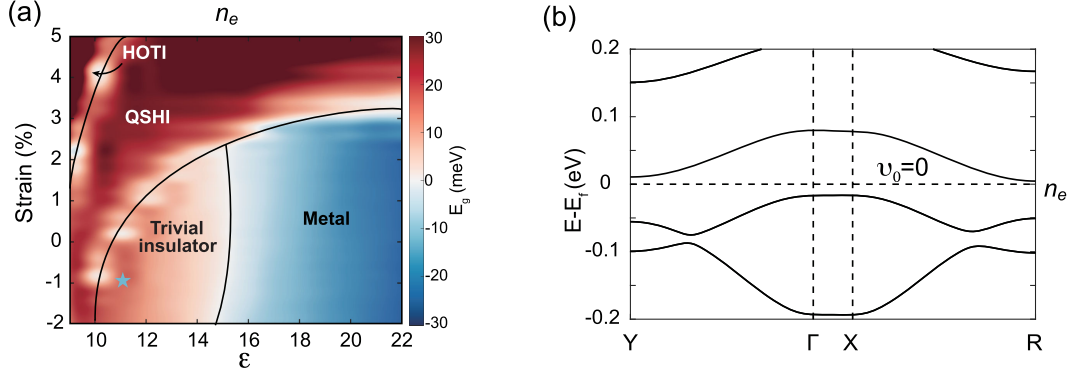


FIG. 22. Trivial region at the doped gap ($n = n_e$) revealed under strain. (a) HFMF phase diagram at fixed interaction ratio $U/V_1 = 3.2$ as a function of dielectric constant ϵ and uniaxial strain. The color scale denotes the doped-gap magnitude E_g (meV): red indicates an insulating state with a finite gap, whereas blue corresponds to a metallic state without a global gap. Black lines mark phase boundaries. A clear trivial-insulator dome appears between the QSHI and metallic regions. (b) Representative bulk bands along a high-symmetry line for a point inside the dome in (a), showing a gapped spectrum with $\nu_0 = 0$ at $n = n_e$.

$\pm\pi$ phase shifts occur consistently in both gaps. Such anisotropic Wannier center evolutions precisely match the parity products analysis, verifying the Z_4 topology. Moreover, the edge spectral function along the $[100]$ edge [Fig. 21(b)] clearly shows the absence of gapless helical edge states, consistent with the HOTI classification.

Thus, the 4% tensile strain scenario provides clear evidence that mechanical strain acts as an effective tuning parameter, driving the system from QSHI or mixed phases into stable, purely HOTI phases, further enriching the topological phase diagram of correlated TaIrTe₄.

6. Trivial-insulator region at the doped gap ($n = n_e$)

To clarify where a trivial insulator appears at the doped gap, we computed the HFMF phase diagram at a fixed interaction ratio $U/V_1 = 3.2$ while sweeping the dielectric constant ϵ and uniaxial strain. A distinct trivial-insulator dome emerges between the QSHI and metallic regions in the $(\epsilon, \text{strain})$ plane. Inside this dome the doped gap remains finite and the Z_2 index of the $n = n_e$ manifold is trivial, $\nu_0 = 0$.

APPENDIX F: WEAK INFLUENCE OF A PERPENDICULAR ELECTRIC FIELD ON BAND TOPOLOGY AND HFMF PHASES

Dual gating in our devices also tunes a vertical electric displacement field D (perpendicular electric field $E_\perp$). Here we assess its impact on the single-particle bands and on the interaction-driven phase diagrams.

DFT level. DFT calculations with a uniform $E_\perp$ up to 1 V/nm—well beyond the experimentally accessible range—show negligible changes to the low-energy dispersions near the CNP gap. The overall band shapes remain intact, with only minor band splittings (Fig. 23). This weak response is consistent with the dominant Ta orbital character at E_F and the tiny out-of-plane displacement of Ta sites in the monolayer, which together suppress the field's dipolar coupling to the relevant states.

van Hove region. Band-structure linecuts across the conduction-band van Hove saddle [path A–B in Fig. 24(a)] further confirm that both the momentum position and energy of the VHS are essentially unchanged for $E_\perp \leq 1$ V/nm [Figs. 24(b)–24(f)].

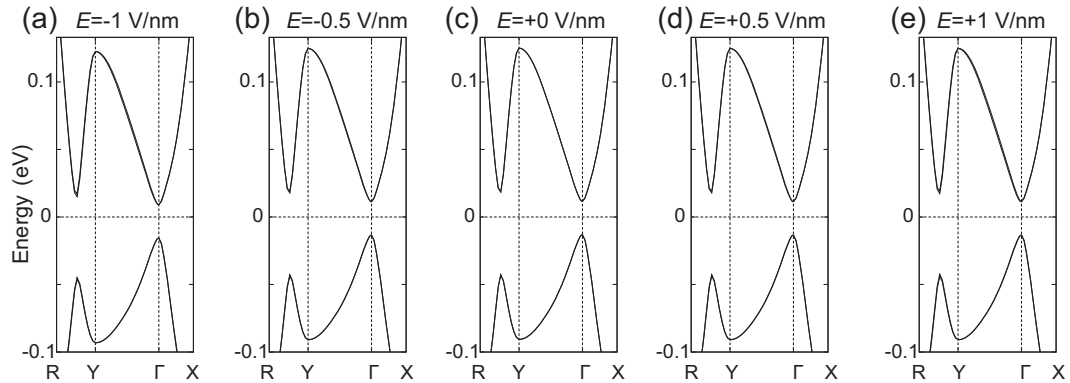


FIG. 23. DFT bands under perpendicular field. DFT-calculated band structures in the CNP window for several $E_\perp$ values (up to ± 1 V/nm). The overall dispersions remain nearly unchanged; only small band splittings appear at finite field.

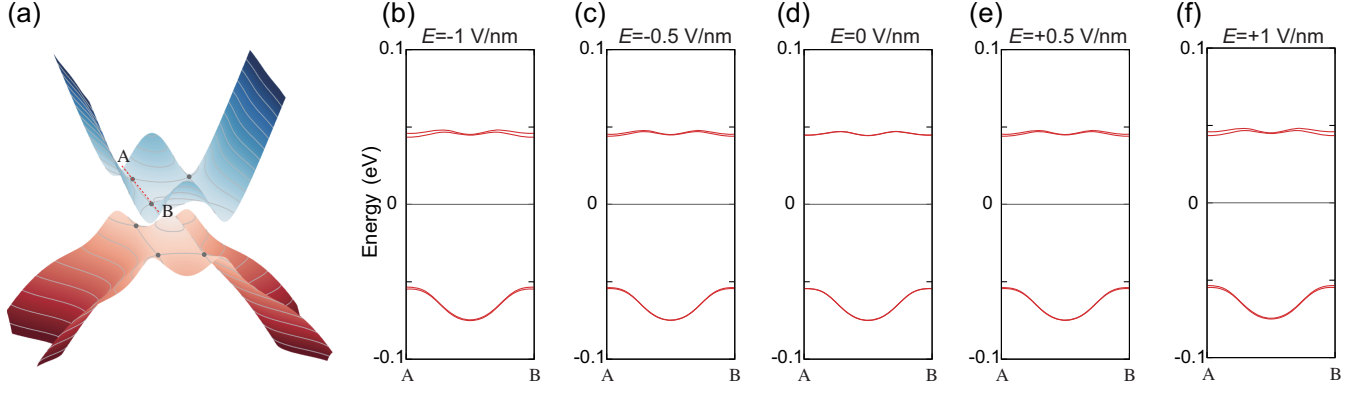


FIG. 24. vHS linecuts vs $E_{\perp}$. (a) Schematic 3D view and A-B linecut through the conduction-band vHS. (b)–(f) Energy-momentum cuts for $E_{\perp} = 0, \pm 0.5$, and ± 1.0 V/nm (as labeled), showing essentially unchanged saddle-point momentum and energy across the field range.

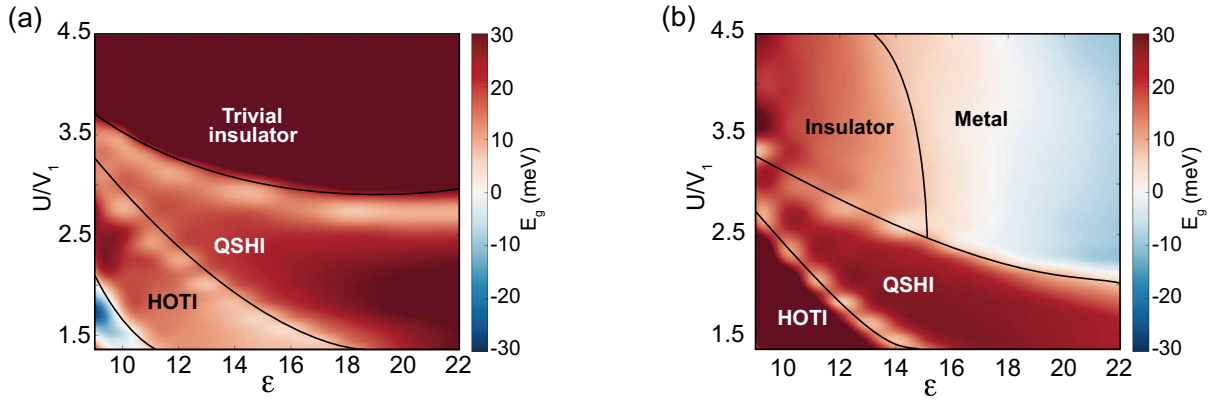


FIG. 25. HFMF robustness to $E_{\perp}$. HFMF phase diagrams in the 15×1 CDW supercell with $E_{\perp} = 1$ V/nm for the CNP gap (left) and n_e gap (right). Color encodes gap magnitude E_g (red: insulating; blue: metallic). Phase sectors (QSHI/HOTI/trivial/metal) and boundaries remain essentially unchanged by the perpendicular field.

Many-body level. To test any residual effect on interactions, we incorporated $E_{\perp}$ as a layer-asymmetric on-site potential in the 15×1 CDW supercell and calculated the HFMF phase diagrams. Comparing $E_{\perp} = 0$ and $E_{\perp} = 1$ V/nm for both the CNP gap and the n_e gap reveals only minor quantitative shifts; the phase regions (QSHI/HOTI/trivial insulator/metal) and their boundaries are essentially unchanged [Figs. 25(a) and 25(b)].

Taken together, these results demonstrate that a perpendicular electric field has only a weak effect on the relevant band topology and on the correlated HFMF phases in monolayer TaIrTe₄ within (and beyond) the experimental field window.

APPENDIX G: POSSIBLE FRACTIONAL TOPOLOGICAL INSULATOR

1. Band projected exact diagonalization

With the Hartree-Fock method, we obtain a renormalized tight-binding model:

$$H_0 = \sum_{ia\sigma s j b \sigma' s'} t_{ia\sigma s j b \sigma' s'} c_{ia\sigma s}^{\dagger} c_{j b \sigma' s'} + \text{H.c.} \quad (\text{G1})$$

Here, i, j label unit cells, a, b label sublattices, σ, σ' distinguish orbitals centered on the same sublattice, and s, s' are spin indices.

We further include density-density interactions of the form

$$H_I = \sum_{ijab\sigma\sigma's's'} V_{ia\sigma s j b \sigma' s'} n_{ia\sigma s} n_{j b \sigma' s'}, \quad (\text{G2})$$

where $V_{ia\sigma s j b \sigma' s'}$ denotes the interaction matrix element. We now transform the fermionic operators to momentum space:

$$c_{ia\sigma s}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_i} c_{\mathbf{k} a \sigma s}^{\dagger}, \quad (\text{G3})$$

where $c_{\mathbf{k} a \sigma s}^{\dagger}$ is the Fourier component of the localized Wannier orbital. In this basis, the interaction becomes

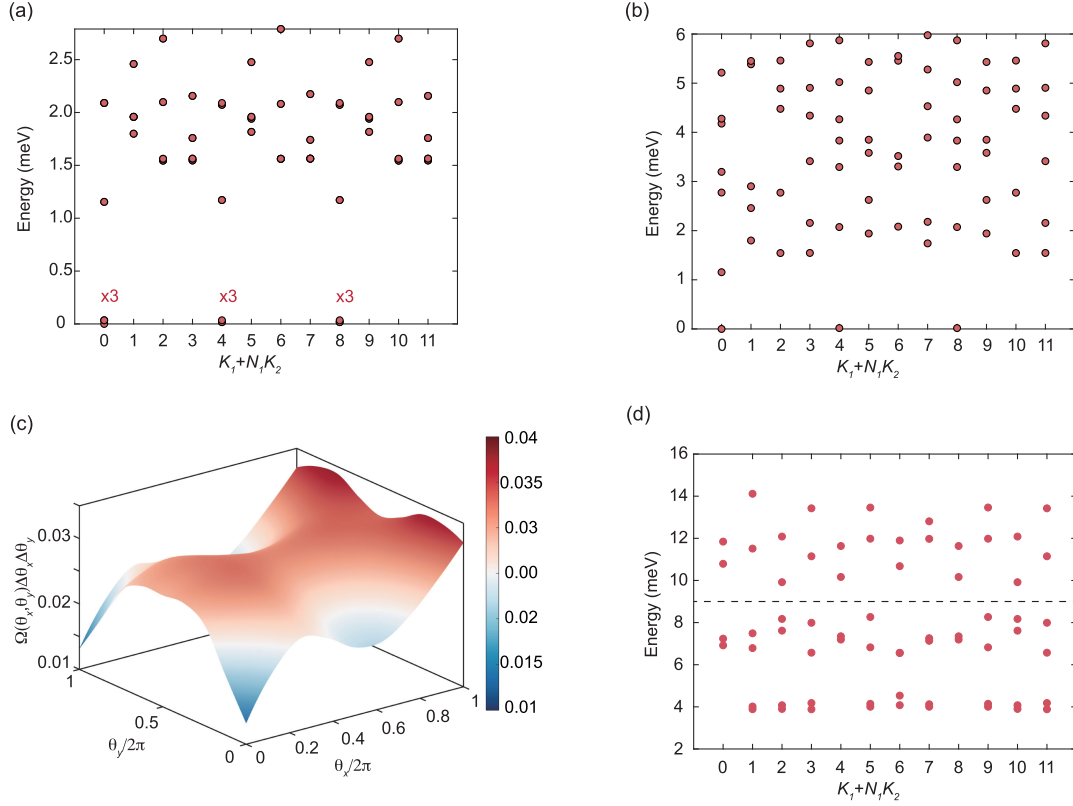


FIG. 26. Fractionalized states in monolayer TaIrTe₄ from ED. (a) The many-body spectrum for the spinful case with $n_{\uparrow} = n_{\downarrow} = 4$ on a 12-site momentum mesh. (b) The many-body spectrum for the spin-polarized case with $n_{\uparrow} = 4$ on the same 12-site momentum mesh. (c) The distribution of the many-body Berry curvature for the ground state at $k = 0$ on the 12-site momentum mesh. The parameters θ_x and θ_y denote the twisted boundary conditions. (d) The particle entanglement spectrum of the ground-state manifold in (b), where the system is partitioned into subsystems with $N_A = 2$ and $N_B = N_e - N_A$. The dashed line indicates the entanglement gap, and 42 levels are found below the gap.

$$\begin{aligned}
 H_I &= \sum_{ijab\sigma\sigma's's'} V_{ia\sigma s j b \sigma' s'} n_{ia\sigma s} n_{j b \sigma' s'} \\
 &= \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \sum_{\sigma\sigma's's'} \sum_{a, \Delta} \frac{V_{ia\sigma s j b \sigma' s'}}{N} e^{i(\mathbf{k}_1 - \mathbf{k}_4) \cdot \Delta} \delta_{\mathbf{k}_1 - \mathbf{k}_4, \mathbf{k}_3 - \mathbf{k}_2} \\
 &\quad \times c_{\mathbf{k}_1 b \sigma' s'}^\dagger c_{\mathbf{k}_2 a \sigma s}^\dagger c_{\mathbf{k}_3 a \sigma s} c_{\mathbf{k}_4 b \sigma' s'}. \quad (\text{G4})
 \end{aligned}$$

For the tight-binding model H_0 , we diagonalize it to obtain Bloch eigenstates (note that spin is a good quantum number in our model):

$$\begin{aligned}
 H_0 &= \sum_{n\mathbf{k}s} \epsilon_{n\mathbf{k}s} \gamma_{n\mathbf{k}s}^\dagger \gamma_{n\mathbf{k}s}, \\
 \gamma_{n\mathbf{k}s}^\dagger &= \sum_{a\sigma s} U_{na\sigma s}(\mathbf{k}) c_{\mathbf{k}a\sigma s}^\dagger, \\
 U^\dagger(\mathbf{k})U(\mathbf{k}) &= I. \quad (\text{G5})
 \end{aligned}$$

Thus, the Fourier component of a Wannier orbital can be expanded in the Bloch basis as

$$c_{\mathbf{k}a\sigma s}^\dagger = \sum_n U_{na\sigma s}^*(\mathbf{k}) \gamma_{n\mathbf{k}s}^\dagger. \quad (\text{G6})$$

Expressed in the Bloch basis, the interaction Hamiltonian becomes

$$\begin{aligned}
 H_I &= \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \sum_{\sigma\sigma's's'} \sum_{a, \Delta_{NN}} \frac{V_{ia\sigma s j b \sigma' s'}}{N} e^{i(\mathbf{k}_1 - \mathbf{k}_4) \cdot \Delta} \delta_{\mathbf{k}_1 - \mathbf{k}_4, \mathbf{k}_3 - \mathbf{k}_2} \\
 &\quad \times \sum_{n_1, n_2, n_3, n_4} U_{n_1 b \sigma' s'}^*(\mathbf{k}_1) U_{n_2 a \sigma s}^*(\mathbf{k}_2) U_{n_3 a \sigma s}(\mathbf{k}_3) \\
 &\quad \times U_{n_4 b \sigma' s'}(\mathbf{k}_4) \gamma_{n_1 \mathbf{k}_1 s'}^\dagger \gamma_{n_2 \mathbf{k}_2 s}^\dagger \gamma_{n_3 \mathbf{k}_3 s} \gamma_{n_4 \mathbf{k}_4 s'}. \quad (\text{G7})
 \end{aligned}$$

Here, Δ denotes the displacement vector connecting the two sites that participate in the density-density interaction.

2. The fractional Chern insulator and fractional topological insulator

For simplicity, in all of our calculations, we keep the density-density interaction up to the nearest-neighbor sites, and choose $V_0 = 0.7$ and $V_1 = 0.4$ eV. The parameters V_0 and V_1 denote the on site and nearest-neighbor

density-density interactions, respectively. In the following, we projected onto the target band and ignore the band dispersion within the flat-band approximations. We first focus on the spin-polarized case. At the filling factor $\nu = 1/3$, a fractional Chern insulator (FCI) state is obtained, as shown in Fig. 26(b). Three nearly degenerate ground states appear at momenta $k = 0, 4$, and 8 , consistent with the generalized Pauli principle, and are well separated from the excited states by a clear energy gap. Figure 26(c) displays the many-body Berry curvature of the ground states at $k = 0$, which exhibits a smooth distribution and integrates to a fractional value of $1/3$ per state. This indicates that the many-body Chern number of the ground-state manifold is $C = 1/3$. Furthermore, the particle entanglement spectrum shown in Fig. 26(d) exhibits a distinct entanglement gap. The number of levels below the gap, indicated by the dashed line, is 42, matching the expected counting of quasi-hole excitations for a fractional quantum Hall state. Taken together, these results provide compelling evidence that the system realizes a robust fractional Chern insulator at $\nu = 1/3$. We now turn to the spinful case. As shown in Fig. 26(a), the ground states form a ninefold quasidegenerate manifold, consistent with the expected degeneracy of a *fractional topological insulator* (FTI). We note that our Hartree-Fock plus exact diagonalization (HF + ED) approach has limited accuracy due to the double-counting issue inherent to this method. Nevertheless, our results suggest the possible realization of a fractional topological insulator in this system. A more detailed investigation will be left for future work.

APPENDIX H: EXPERIMENTAL DETAILS

1. TaIrTe₄ crystal growth process

TaIrTe₄ crystals were synthesized using the Te-flux method with a molar ratio of Ta:Ir:Te (>99.99% purity) of 3:3:94. The elements were placed in an alumina crucible, sealed in a vacuum quartz tube, and gradually heated to 1373 K, where they were held for 10 h. The mixture was then slowly cooled to 873 K at a rate of 2 K/h. The resulting TaIrTe₄ crystals were separated from the excess Te flux via centrifugation.

2. TaIrTe₄ exfoliation and device fabrication

TaIrTe₄ flakes were exfoliated onto oxygen plasma-cleaned SiO₂ chips using the scotch-tape method inside an Ar-filled glovebox to solve the air sensitivity nature of thin flakes. The layer thickness was determined through optical microscopy [Fig. 27(a) shows a monolayer TaIrTe₄ flake]. Target flake regions were patterned using a tip-scratching and cleaning process. For subsequent short-channel device fabrication, stripe-shaped TaIrTe₄ flakes with naturally exfoliated boundaries were preferentially selected.

We designed a bottom-contact, dual-gated device structure to encapsulate the monolayer TaIrTe₄ flake and

enhance gate tunability. First, few-layer graphene (FLG) and boron nitride (BN) flakes were sequentially picked up using a PDMS/PC stamp to serve as the top gate and dielectric layer, respectively [Fig. 27(b)]. Next, the monolayer TaIrTe₄ flake was picked up by the stack [Fig. 27(c)]. Subsequently, bottom-contact electrodes (Ti 2 nm/Pt 10 nm) were patterned onto the BN and metal back-gate surface [Fig. 27(d)], with the channel length defined by the spacing between adjacent electrodes. The bottom-contact structure was then thermally annealed in a forming gas atmosphere (Ar:H₂ = 1:1) at 350 °C for 3 h to remove polymer residues and surface contaminants. Finally, the FLG/BN/TaIrTe₄ stack was precisely aligned and transferred onto the bottom-contact structure using a transfer stage, ensuring that the FLG was in contact with the pre-patterned top-gate electrode. The final device structure is shown in Fig. 27(e).

3. Electrical measurements of TaIrTe₄ devices

Electrical measurements were performed using Montana and Cryomagnetics cryostats. The electrical transport properties of TaIrTe₄ devices were characterized using standard lock-in techniques, and gate voltages were applied via Keithley source meters. In dual-gated devices, the carrier density (n) and electric field (E) were controlled through a combination of the top-gate voltage (V_{tg}) and bottom-gate voltage (V_{bg}).

$$n = \frac{\epsilon_0 \epsilon_{\text{BN}} V_{\text{bg}}}{e d_{\text{b}}} + \frac{\epsilon_0 \epsilon_{\text{BN}} V_{\text{tg}}}{e d_{\text{t}}}, \quad (\text{H1})$$

$$E = \frac{1}{2} \left(\frac{V_{\text{bg}}}{d_{\text{b}}} - \frac{V_{\text{tg}}}{d_{\text{t}}} \right), \quad (\text{H2})$$

Here, ϵ_0 is the vacuum permittivity, ϵ_{BN} is the BN dielectric constant ($\epsilon_{\text{BN}} \approx 3$) and d_{b} (d_{t}) is the dielectric thickness of the bottom (top) BN.

4. Thermal activation gap analysis

To quantitatively evaluate the insulating behavior observed at the charge neutrality point and on the electron-doped side, we perform thermal activation analysis on the longitudinal conductance $G_{xx}(T)$ for three representative monolayer TaIrTe₄ devices. As shown in Fig. 28, the temperature dependence of G_{xx} (extracted from the data shown in Fig. 7) is fitted using the Arrhenius relation:

$$G_{xx}(T) \propto \exp(-\Delta/2k_B T), \quad (\text{H3})$$

where Δ denotes the activation energy gap, T is the temperature, and k_B is the Boltzmann constant. Upper panel of Fig. 28 shows G_{xx} at the CNP for three distinct device types. The extracted thermal gaps are: $\Delta_{\text{CNP}} = 6.1$ meV

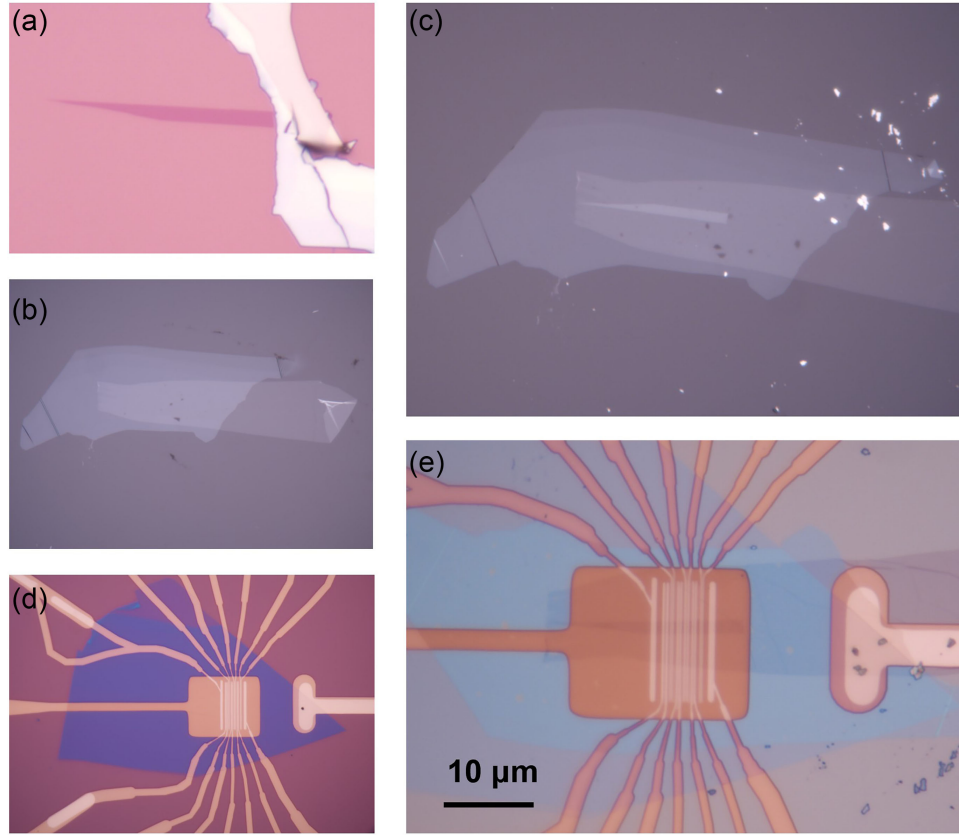


FIG. 27. Device fabrication process of monolayer TaIrTe₄ device. (a) Optical image of an exfoliated monolayer TaIrTe₄ flake with a ribbonlike shape on a SiO₂ substrate. The exfoliation was performed in a glovebox under an inert atmosphere. (b) A stack consisting of few-layer graphene (FLG, serving as the top gate) and boron nitride (BN) is prepared on a PC/PDMS stamp. (c) The monolayer TaIrTe₄ flake is picked up using the FLG/BN stack. (d) Optical image of the bottom-contact structure, where a metal pad serves as the back gate, and BN acts as the dielectric layer. Contact electrodes are patterned on the surface, with a small gap between adjacent electrodes to define the channel length. (e) Optical image of the final device structures.

(dual-QSHI); $\Delta_{\text{CNP}} = 28.0$ meV (metal + QSHI); $\Delta_{\text{CNP}} = 6.1$ meV (dual-insulator). Lower panel shows the thermal activation behavior on the electron-doped side at $n = n_e$: $\Delta_{n_e} = 4.6$ meV (dual-QSHI); $\Delta_{n_e} = 8.8$ meV (dual insulator).

These results support our classification of correlated phases based on edge transport, and confirm that dual-QSHI and metal + QSHI phases are associated with larger, robust gaps, while the dual-insulator phase shows a much weaker insulating behavior consistent with non-topological or higher-order insulating states.

5. Activation gap in long-channel devices

In Arrhenius analysis, the extracted activation gap reflects a *global*, device-averaged energy gap. In our measurements, the channel length is relatively long ($L_{\text{ch}} \approx 1\text{--}5$ μm), so spatial inhomogeneity across the whole flake will reduce the global gap size. This mechanism is sketched in Fig. 29, where the single particle QSHI gap (~ 30 meV) is reduced to a global activation gap < 10 meV. Similarly, for the dual-QSHI state we obtain

an activation gap of ~ 6.1 meV at CNP and a correlated gap of ~ 4.6 meV at n_e [Figs. 28(a) and 28(b)].

6. Robustness against vertical electric field

Here, we examine the effect of a vertical electric field on the electronic properties of monolayer TaIrTe₄. Experimentally, we find that the system is largely insensitive to an applied vertical electric field within the experimentally accessible range.

Figure 30 shows the dual-gate resistance maps under a vertical electric field E for three representative devices: (a) dual QSHI, (b) QSHI + metal, and (c) dual insulator. In all cases, the resistance peaks remain nearly unchanged along the direction of the applied electric field E (indicated by the white arrows), demonstrating that the transport characteristics are robust against vertical electrical field.

This observation indicates that the vertical electric field does not significantly modify the phase boundaries or alter the overall topological features of the phase diagram. The experimental results therefore support the claim in the main text that the vertical electric field plays a minor role in

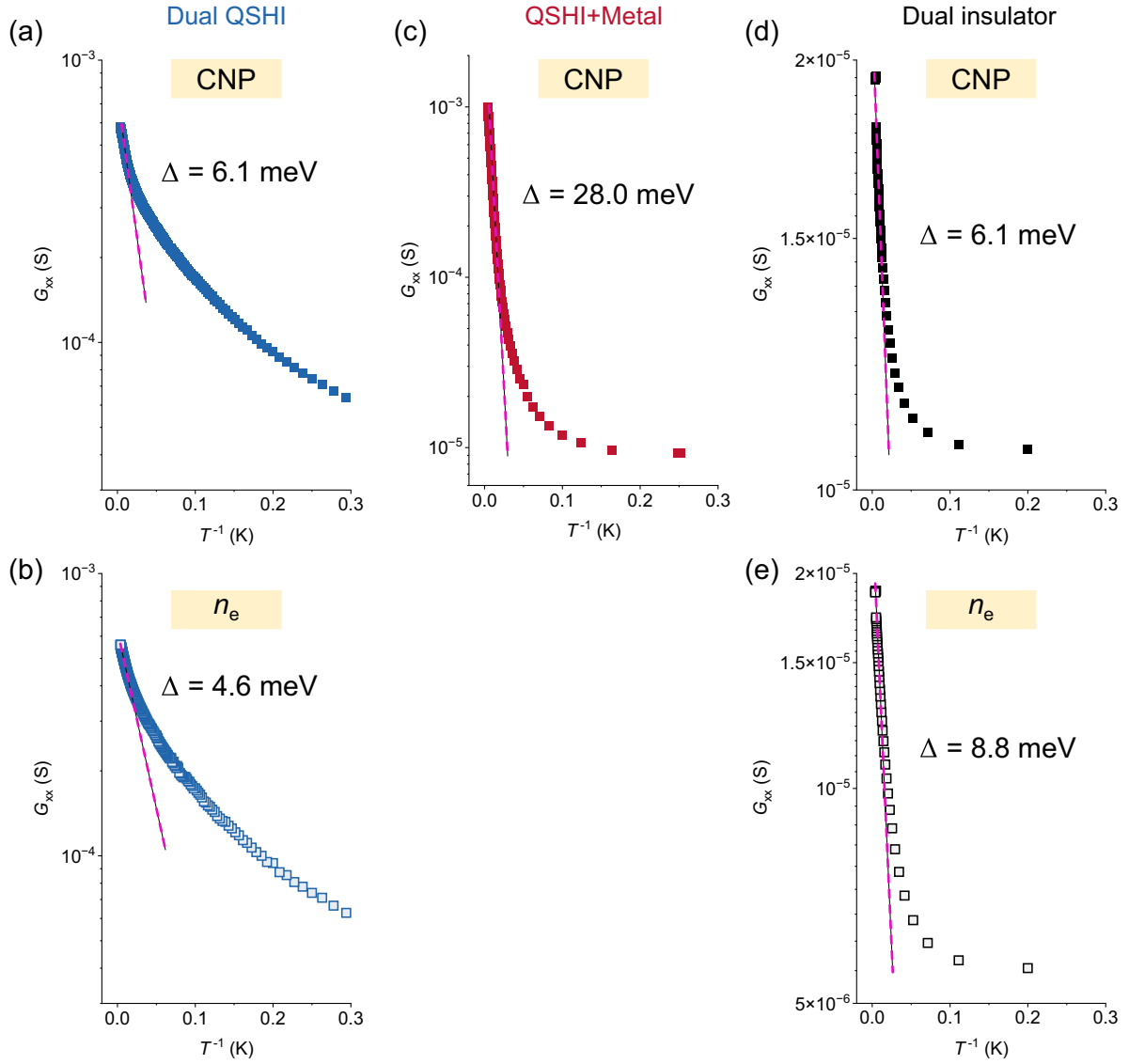


FIG. 28. Band gap extraction via thermal activation fitting. The activation gaps are extracted based on the temperature-dependent conductance G_{xx} by using the Arrhenius relation $G_{xx} \propto \exp(-\Delta/2k_B T)$. (i) dual QSHI: (a) $\Delta_{\text{CNP}} = 6.1$ meV; (b) $\Delta_{n_e} = 4.6$ meV; (ii) QSHI+metal: (c) $\Delta_{\text{CNP}} = 28.0$ meV; (iii) dual Insulator: (d) $\Delta_{\text{CNP}} = 6.1$ meV; (e) $\Delta_{n_e} = 8.8$ meV.

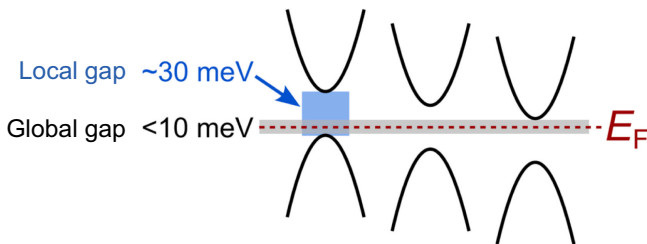


FIG. 29. Schematic of global band-gap reduction by spatial inhomogeneity in long-channel devices. Local regions (blue) can host a large gap (~ 30 meV), but the effective *global* gap across the whole sample is reduced to < 10 meV.

determining the correlated and topological phases in monolayer TaIrTe₄.

7. Controlled nonlocal experiment: Eliminating bulk-defect artifacts

To verify that the enhanced nonlocal response originates from edge channels, we fabricated a control device in which one half of the sample edge was capped by a BN flake while the opposite edge remained exposed (Fig. 31). When the edge is exposed, the nonlocal voltage V_{NL} is strongly enhanced as the chemical potential enters the QSHI gap and is suppressed outside the gap. In contrast,

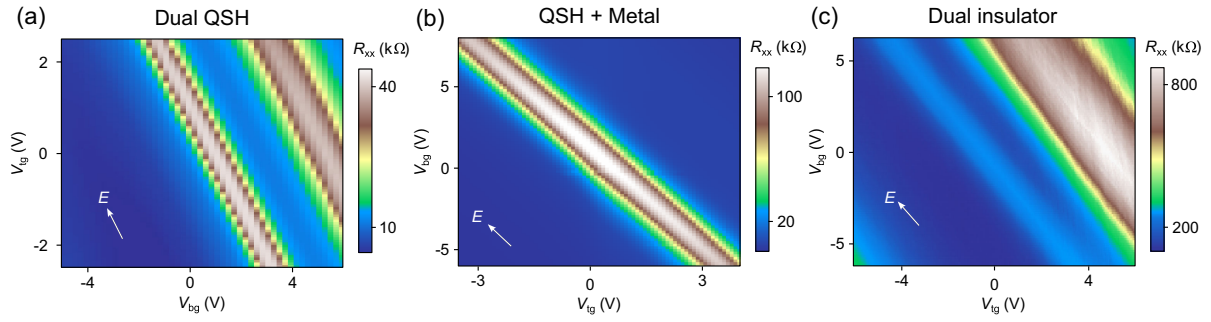


FIG. 30. Electrical characteristics of monolayer TaIrTe₄ under a vertical electric field. Dual-gate resistance maps for (a) dual-QSHI, (b) QSHI + metal, and (c) dual-insulator regimes. In all cases, the resistance peaks remain essentially unchanged along the electric-field direction, demonstrating the robustness of the observed phases against vertical electric fields.

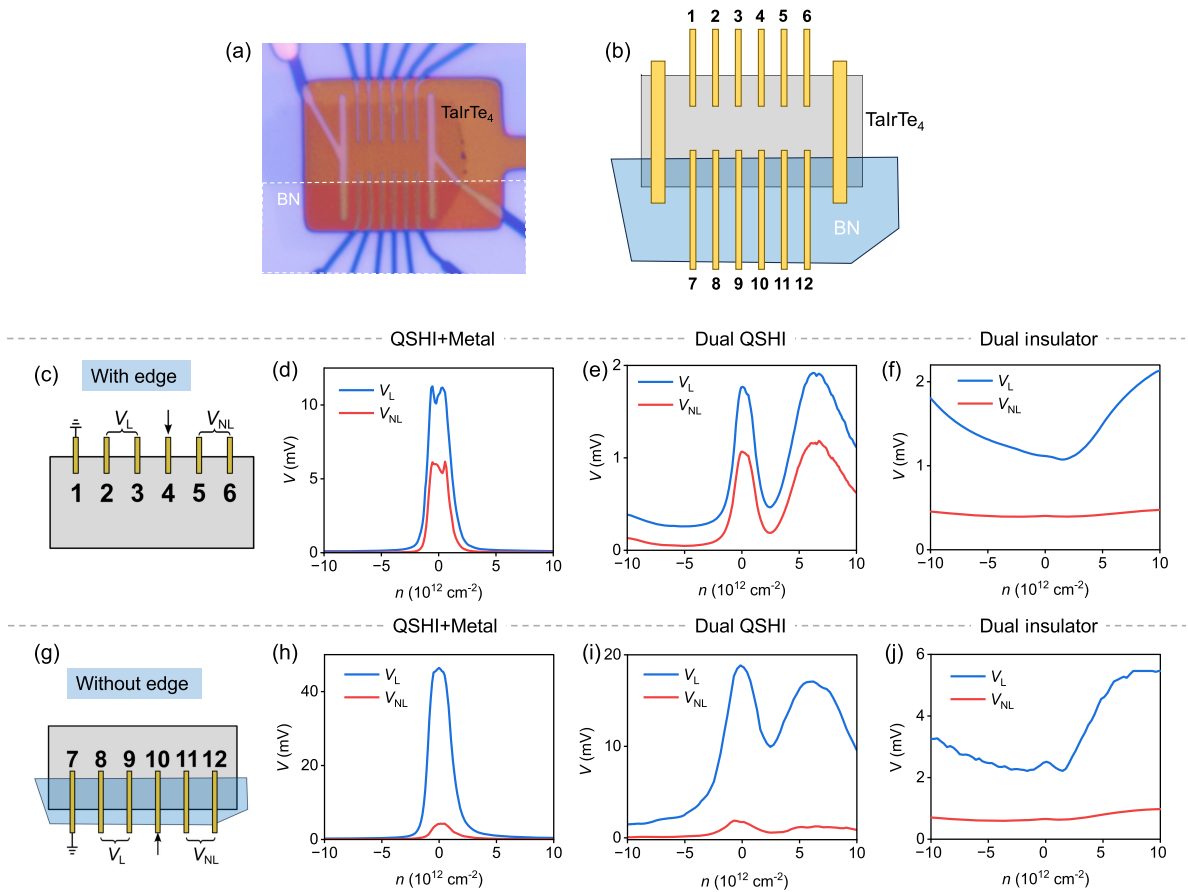


FIG. 31. Nonlocal transport with and without edge contribution. (a)–(b) Optical image and schematic of a representative device, where the bottom half of the sample edge was capped with a BN flake, and the top edge remained exposed. (c) Illustration of the edge-dominated nonlocal measurement setup (current $I_{xx} = 100 \text{ nA}$; local and nonlocal voltages recorded simultaneously). (d)–(f) Local and nonlocal responses for (d) QSHI + metal, (e) dual-QSHI, and (f) dual-insulator devices with edge contribution. (g) Illustration of the inner bulk dominated nonlocal measurement setup (edge capped by BN). (h)–(j) Local and nonlocal responses: the nonlocal voltage V_{NL} remains suppressed in all three cases. These results confirm that the enhanced nonlocal signal in QSHI regimes arises from edge contribution rather than bulk-defect or impurity pathways.

capping edge eliminates the enhancement of nonlocal response within the QSHI gap. Devices in the dual-insulator regime exhibit only weak nonlocal signals, independent of edge capping. Together, these results rule out bulk-defect-driven artifacts and confirm the edge dominated nonlocal response.

8. Low-temperature saturation of longitudinal resistance in the QSH plateaus

Figure 32 replots the data of Fig. 8(a) on a linear resistance scale. The longitudinal resistance R_{xx} within both the charge-neutral (CNP, $n = 0$) and electron-doped ($n_e = 6.5 \times 10^{12} \text{ cm}^{-2}$) QSHI gaps clearly shows low-temperature saturation behavior, consistent with edge-dominated QSH transport. Quantitatively, the QSH-I edge resistance saturates below $\sim 25 \text{ K}$, while the QSH-II edge resistance saturates below $\sim 10 \text{ K}$.

9. Statistical significance and experimental reproducibility

To systematically assess the reproducibility and universality of the observed correlated topological phases, we performed transport measurements across a large number of monolayer TaIrTe₄ devices. A total of 105 high-quality devices were investigated, allowing robust statistical analysis of the observed transport behaviors.

Based on the characteristic $R_{xx}(n, T)$ profiles, we identified three representative device categories:

- (1) Type-I (dual QSHI): Comprising about 35% of measured devices, these samples exhibit quantized edge conductance at both the CNP and an electron-doped correlated insulating state, consistent with the theoretically predicted dual QSHI phase arising from significant electron-electron interactions near the vHS.
- (2) Type-II (QSHI + metal): Representing approximately 7% of the devices, these samples exhibit

well-quantized edge conductance only at the CNP and metallic behavior at finite doping, indicative of relatively weak electron correlations insufficient to stabilize correlated insulating phases at the van Hove singularities.

- (3) Type-III (dual insulator): The majority (58%) of measured devices demonstrate insulating transport throughout the doping range, without clear edge conductance quantization. This category likely encompasses trivial insulating or higher-order topological insulating phases, both characterized by the absence of gapless helical edge modes. The prevalence of this category suggests that minor variations in sample quality, device disorder, gating uniformity, or local strain conditions significantly affect the electronic structure, potentially suppressing or obscuring clear quantization.

The experimental distribution highlights two key insights. First, the considerable proportion (35%) of type-I devices confirms that the interaction-induced dual QSHI phase is robustly reproducible and experimentally accessible. However, the dominance of type-III devices underscores practical challenges in reliably achieving ideal topological phases, indicating a strong sensitivity of the correlated states to disorder, gating uniformity, and subtle variations in fabrication process.

Overall, the comprehensive device statistics validate the experimental realization of theoretically predicted correlated topological phases and emphasize the critical importance of precise control over material quality and device conditions for future investigations and applications of correlated topological materials.

10. Spatial inhomogeneity and strain-induced phase variations

To assess whether device-to-device and region-to-region variations in our transport data can be attributed to local

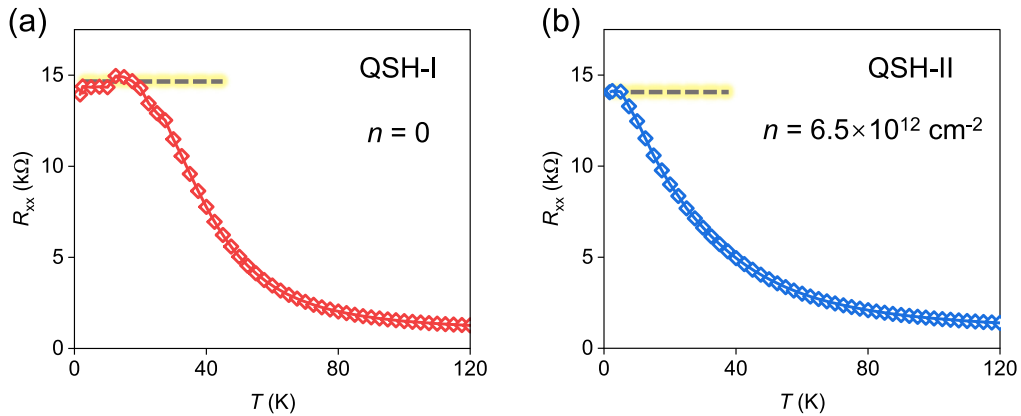


FIG. 32. The saturation of longitudinal resistance at low temperature. R_{xx} vs T plotted on a linear scale for (a) CNP gap ($n = 0$) and (b) the electron-doped gap at $n_e = 6.5 \times 10^{12} \text{ cm}^{-2}$. In both cases, R_{xx} exhibits clear low-temperature saturation behavior. The saturation onsets at $\sim 25 \text{ K}$ for QSH-I and $\sim 10 \text{ K}$ for QSH-II. Data are replotted from the measurements shown in Fig. 8(a).

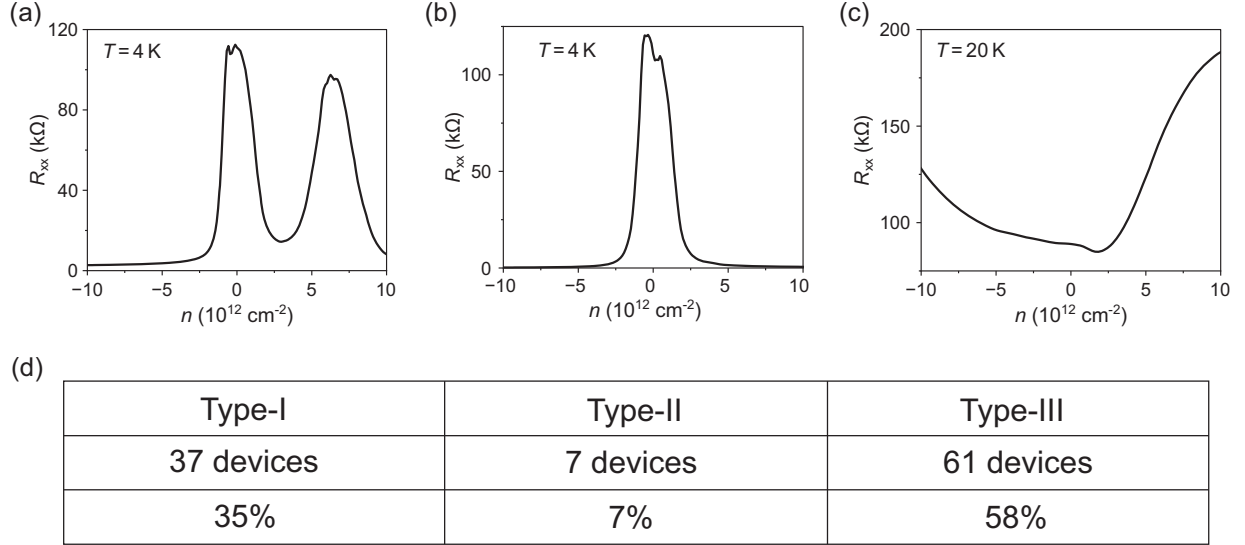


FIG. 33. Statistical classification of monolayer TaIrTe₄ devices based on transport signatures. Out of 105 high-quality devices, three distinct types are identified based on the resistance behavior $R_{xx}(n, T)$ as a function of carrier density n and temperature T . Top panels: Representative R_{xx} - n curves at low temperature ($T = 4$ – 40 K) for each device type. Bottom: Summary table listing the number and percentage of devices in each category: Type-I (dual QSHI), type-II (QSHI + metal), and type-III (dual insulator).

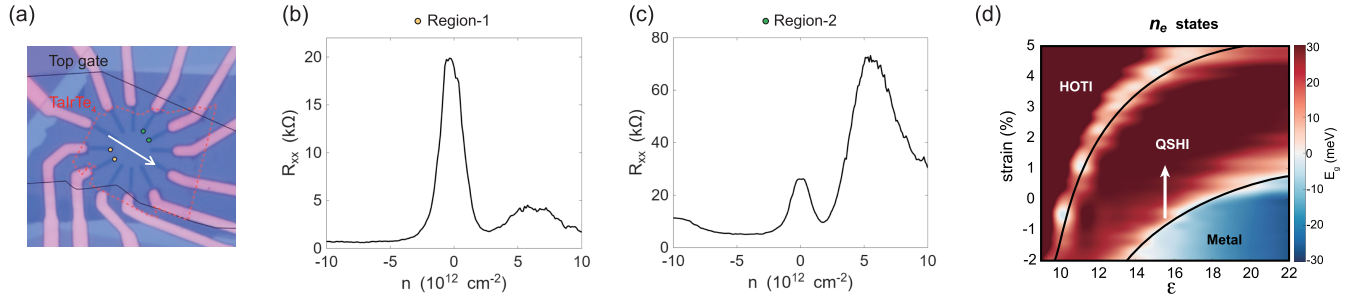


FIG. 34. Spatially inhomogeneous strain of a large TaIrTe₄ device. (a) Optical micrograph of the measured device. (b)–(c) Four-probe R_{xx} versus carrier density n from two distinct regions of the same flake (region-1 and region-2). Both regions show comparable CNP resistance peaks, the correlated resistance peak near $n_e = 6.5 \times 10^{12} \text{ cm}^{-2}$ differs substantially, indicating that local strain variations drive region-dependent correlated phases. (d) HFMF phase diagram versus dielectric constant and uniaxial strain for the n_e states [same as Fig. 6(c)]. The variation from region-1 to region-2 likely follows the white arrow.

strain, we performed spatially resolved measurements on a large-area monolayer TaIrTe₄ device (flake size $> 15 \times 15 \mu\text{m}^2$) fabricated on pre-patterned bottom electrodes. Two regions of the same flake (denoted region-1 and region-2) are measured in the same condition.

Figure 34 compares four-probe longitudinal resistance R_{xx} versus carrier density n taken from these two regions. Both traces display a comparable peak at the CNP. By contrast, the correlated resistance peak near the electron-doped $n_e = 6.5 \times 10^{12} \text{ cm}^{-2}$ differs markedly in magnitude between these two regions. This contrast implies spatial inhomogeneity that strongly modulates the correlated state.

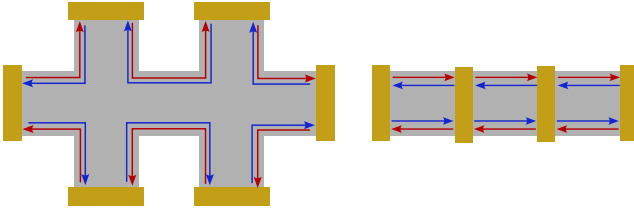
These observations are naturally explained by local strain variations introduced during assembly on prepatterned electrodes. Within our theory, modest tensile uniaxial strain

($\sim 1\%$) can tune the CNP between QSHI and HOTI, whereas a much larger strain ($\gtrsim 9\%$) is required to render the CNP trivial (Fig. 17). In the doped window, the same strain variations modify the effective interaction and band folding, shifting the HFMF phase boundaries between QSHI, HOTI, trivial insulator, and metal (Figs. 3 and 6).

11. Clarification on R_{xx} measurements and edge quantization in a four-probe geometry

In this work, we employ four-probe local resistance measurements to identify quantized edge transport in the QSH regime. As schematically illustrated in Fig. 35, quantized transport can in principle be observed in both two-probe and four-probe configurations. However, the experimental requirements are fundamentally different for

QSH edge: equilibrate chemical potential



QAH edge: NO local equilibration

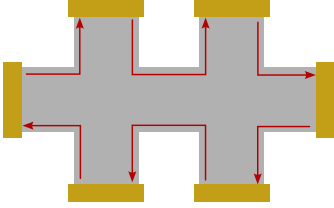


FIG. 35. Comparison between helical QSH and chiral QH/Chern edge transport in different measurement geometries. Top: QSH edge channels are helical, consisting of two counter-propagating modes with opposite spin, which can locally equilibrate the chemical potential along the edge. Bottom: QH/Chern edge channels are chiral and unidirectional, where local equilibration is not required for quantized transport. In two-probe measurements, QSH quantization is highly sensitive to contact transparency and spin mixing, whereas chiral edge transport is comparatively insensitive to imperfect contacts. This motivates the use of four-probe local resistance measurements to establish QSH edge quantization.

helical QSH edges compared to chiral edges in the QH or Chern-insulator case.

For QH/Chern insulators, the edge states are chiral and unidirectional, which makes the measured conductance relatively insensitive to contact transparency. In contrast, a QSH insulator hosts helical edge channels consisting of two counter-propagating modes with opposite spin. As a consequence, observing an ideal two-probe quantized conductance in the QSH regime requires nearly perfectly Ohmic contacts with close to unity transmission for *both* spin channels. In practice, even weak spin mixing, partial reflection, or imperfect mode matching at the contacts can substantially degrade the two-probe signal and obscure quantization.

For these reasons, QSH quantization is typically established using a four-probe geometry, where voltage probes minimally perturb the current-carrying edge channels and contact resistances are largely eliminated from the measured signal. In our local R_{xx} measurements, the voltage electrodes span both the top and bottom edges, such that the two opposite edges contribute symmetrically as series edge resistances. This symmetric current distribution enables the extracted edge conductance to approach the quantized value of $2e^2/h$ in the short-channel limit, consistent with helical edge transport in the QSH regime.

12. Reciprocity test in local transport

We performed an explicit reciprocity test of the local transport response in the QSH regime. In our measurements, we apply a dc bias current I_{dc} together with a small ac excitation dI , and measure the differential resistance dV/dI using lock-in detection.

Reciprocity at $B = 0$. We first examine the dependence of dV/dI (equivalently, R_{xx} at a fixed I_{dc}) on the dc current polarity at zero magnetic field. As shown in Fig. 36 for two representative dual-QSH states (QSH-I and QSH-II), the measured dV/dI remains essentially unchanged upon reversing I_{dc} , indicating that the local resistance is largely independent of current polarity in the experimentally relevant bias range. This behavior is consistent with reciprocal transport mediated by helical edge channels: opposite current directions are carried by opposite spin channels related by time-reversal symmetry, such that the linear-response resistance satisfies the expected reciprocity at $B = 0$.

Reciprocity under small magnetic fields. Under a finite but small out-of-plane magnetic field, time-reversal symmetry is broken and the two helical channels become, in principle, nondegenerate. Nevertheless, Onsager reciprocity implies that reversing both the magnetic field and the current direction maps the transport back onto an equivalent configuration, and therefore the measured resistance is expected to remain unchanged to leading order. To test

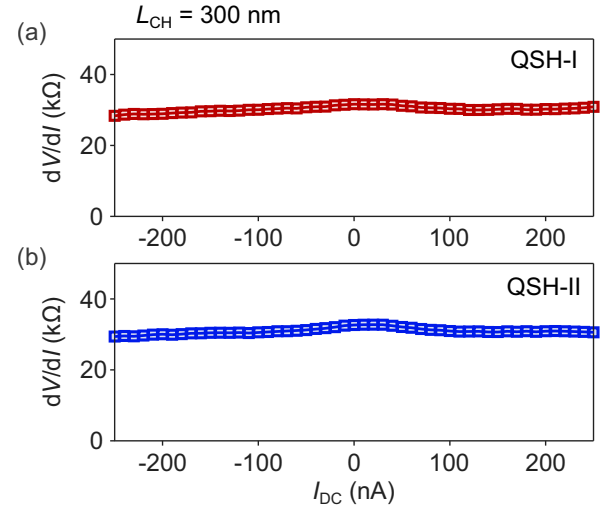


FIG. 36. Local differential resistance under reversed current polarity at $B = 0$. Differential resistance dV/dI measured as a function of dc bias current I_{dc} (with a small ac excitation and lock-in detection) for two representative dual-QSH states: (a) QSH-I and (b) QSH-II. The differential resistance remains essentially unchanged upon reversing I_{dc} , indicating that the local resistance is largely independent of current polarity within the measured bias range, consistent with reciprocal transport in the QSH regime.

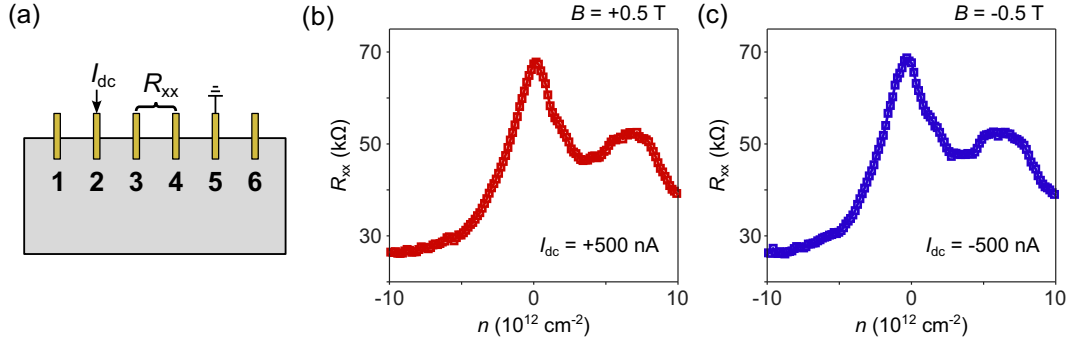


FIG. 37. Reciprocity test of local transport under small magnetic fields. (a) Schematic of the measurement configuration for R_{xx} : a dc current I_{dc} is applied between contacts 2 and 5, and the local voltage is measured between contacts 3 and 4. (b) R_{xx} measured at $B = +0.5 \text{ T}$ with $I_{dc} = +500 \text{ nA}$. (c) R_{xx} measured at $B = -0.5 \text{ T}$ with $I_{dc} = -500 \text{ nA}$. The close agreement between (b) and (c) demonstrates the expected reciprocity upon simultaneous reversal of B and current polarity.

this expectation experimentally, we fabricated an additional device with a slightly longer channel length (so that the conductance is not fully quantized), which provides an improved dynamic range for comparing resistance traces. As shown in Fig. 37, we find that the local resistance satisfies

$$R_{xx}(B = +0.5 \text{ T}, I_{dc} = +500 \text{ nA}) \approx R_{xx}(B = -0.5 \text{ T}, I_{dc} = -500 \text{ nA}), \quad (\text{H4})$$

consistent with the expected reciprocity relation for edge-dominated transport in the linear-response regime.

13. Nonlocal transport measurements

Measurement geometry. In a nonlocal configuration, the “through electrodes” used in our local R_{xx} measurements (which span both the top and bottom edges) are not applicable. Instead, we employ multi-terminal devices in a Hall-bar geometry, as shown in Fig. 38(a). When the chemical potential lies inside the bulk gap of an ideal QSHI, bulk conduction is suppressed and the injected current is predominantly carried by helical edge channels along the sample boundary, leading to a strongly enhanced nonlocal voltage signal [schematically illustrated in

Fig. 38(b)]. In contrast, when bulk conduction dominates, current mainly traverses the interior between the source and drain, producing only a weak nonlocal response [Fig. 38(c)].

Nonlocal signatures across the phase diagram. As shown in the main text [Figs. 7(b), 7(d), and 7(f)], we simultaneously measure the local and nonlocal voltages as a function of carrier density n . In the dual QSHI and QSHI + metal regimes, the nonlocal voltage V_{NL} is strongly enhanced within the CNP gap, consistent with edge-dominated transport. Moreover, in the Dual QSHI regime, V_{NL} also exhibits a pronounced enhancement within the correlated QSH gap. By contrast, V_{NL} is strongly suppressed in the dual-insulator regime, consistent with the absence of robust edge transport.

Why nonlocal signals are not generally quantized and why length scaling is challenging. We emphasize that, even though an ideal helical edge has a quantized two-terminal conductance of e^2/h per edge, the *nonlocal* voltage (or nonlocal resistance) is not generically expected to be quantized. This is because the nonlocal response depends sensitively on current partitioning between multiple edge paths, contact transparency, and equilibration at the voltage probes. Furthermore, systematic length dependence is difficult to establish in a nonlocal geometry: the injected

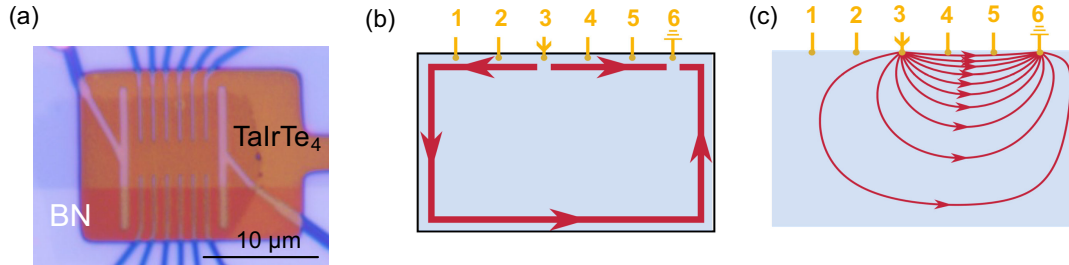


FIG. 38. Nonlocal measurement setup and schematic current distributions. (a) Optical micrograph of a multiterminal monolayer TaIrTe₄ device in a Hall-bar geometry. (b) Edge-dominated transport in the QSH regime yields a strong nonlocal response. (c) Bulk-dominated transport produces only a weak nonlocal signal. Adapted from Ref. [4].

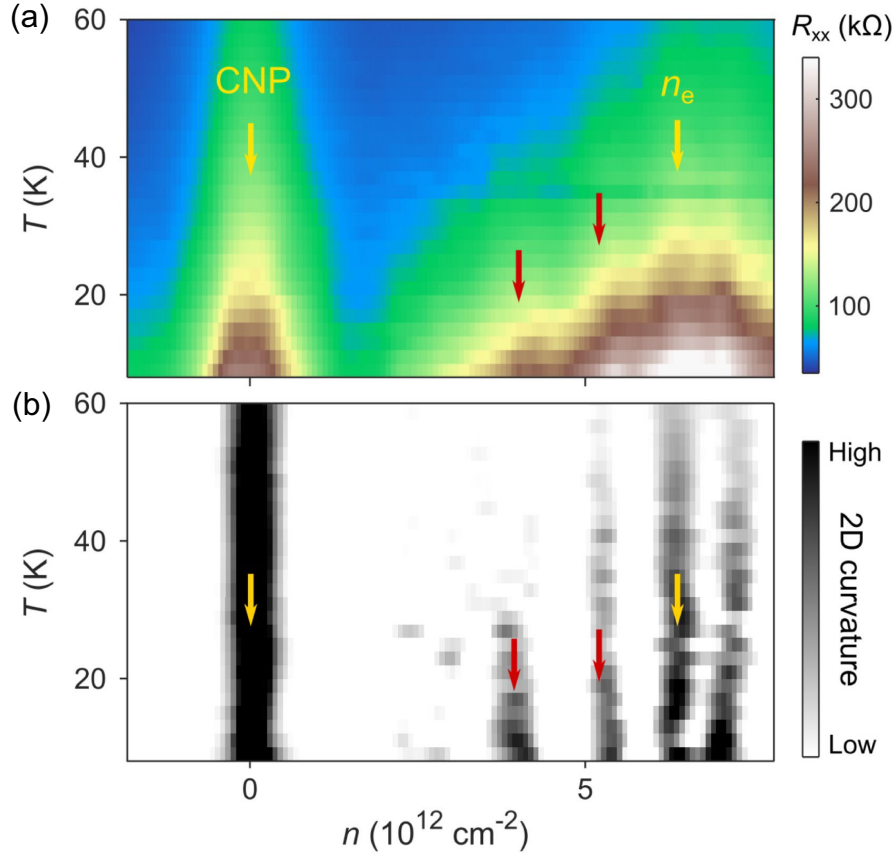


FIG. 39. Possible fractional-filling states in monolayer TaIrTe₄. (a) Four-probe longitudinal resistance R_{xx} versus carrier density n and temperature T . (b) Two-dimensional curvature (second-derivative) map of panel (a) that enhances weak structures. Robust insulating features are observed at the CNP and on the electron-doped side near $n_e = 6.5 \times 10^{12} \text{ cm}^{-2}$. In addition, extra ridges or peaks appear at fractional fillings (red arrows), persisting over tens of kelvin and suggesting incipient interaction-driven incompressible states.

current naturally splits between distinct boundary paths that can differ greatly in length. For example, in Fig. 38(b), current injected between contacts 3 and 6 can follow both a shorter path along the inner edge and a much longer path along the outer boundary. Unless the entire device is patterned into a uniformly small perimeter, the outer-edge path is inevitably long. For monolayer TaIrTe₄, such aggressive nanofabrication is additionally challenging due to air sensitivity, and similar practical limitations apply to many other materials. As a result, observing quantized nonlocal signals or extracting clean length scaling is generally difficult in nonlocal measurements, even when edge-dominated transport is present.

14. Fractional-filling features in transport

To search for possible fractional QSHI states, we measured the four-probe longitudinal resistance R_{xx} in a dual-gated monolayer TaIrTe₄ device after the CDW is established. Besides the prominent insulating peaks at the CNP and at the electron-doped vHS ($n_e \approx 6.5 \times 10^{12} \text{ cm}^{-2}$), the data reveal additional, insulating features at fractional fillings. These show up more clearly

in the two-dimensional curvature (second-derivative) map of $R_{xx}(n, T)$ [59], where multiple ridges persist over a broad temperature range. While a full identification requires future Hall or nonlinear probes, these fractional-filling signatures are consistent with the emergence of interaction-driven fractional gapped states and provide experimental motivation for the FQSHI regimes discussed in Appendix G.

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