A Quantum ESPRESSO Recipe for Z_2 Invariant of 2D Topological Material $1T'$-WTe_2

Shahriar Pollob[1,*], Apu Das[2], Mohammad Dilwar Ali Alvee[3], M. Shahnoor Rahman[4]

[1] *Department of Physics, Shahjalal University of Science and Technology, Sylhet-3114, Bangladesh*
[2] *Department of Theoretical Physics, University of Dhaka, Dhaka-1000, Bangladesh*
[3] *Department of Materials Science & Engineering, Khulna University of Engineering & Technology, Khulna-9203, Bangladesh*
[4] *Department of Physics, University of Miami, Coral Gables, Florida 33124, USA*
[*] *Presenter*

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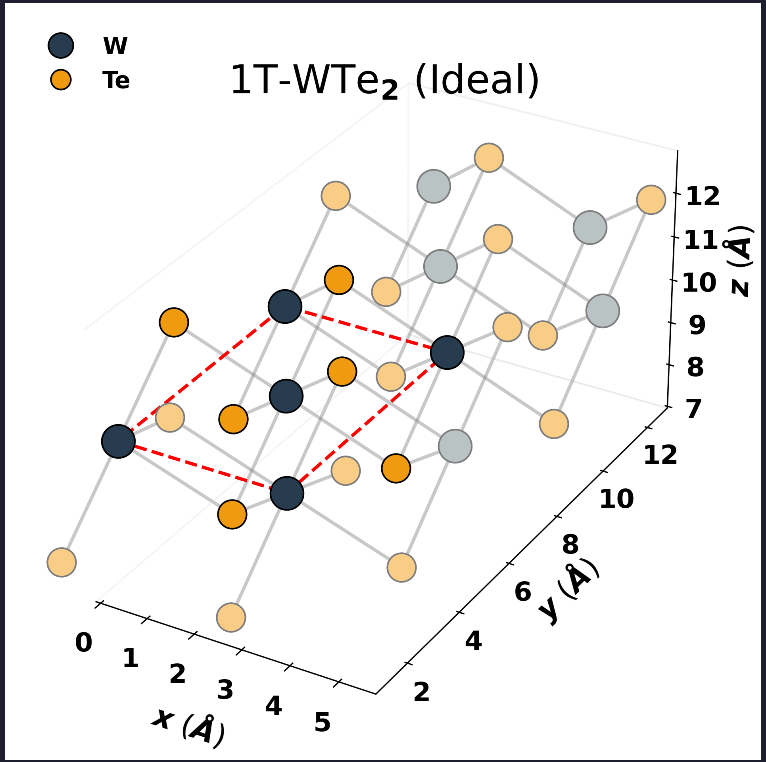
Motivation: The Quest for Dissipationless Electronics

The Bottleneck:
Modern electronics suffer from Joule heating and backscattering limits.

The Solution:
Topological Insulators (TIs) offer dissipationless edge transport protected by Time-Reversal Symmetry.

The Challenge:
Obtaining the topological invariant (Z_2) from First-Principles is often a "Black Box."

Crystal Structure: The Ideal $1T$ Phase



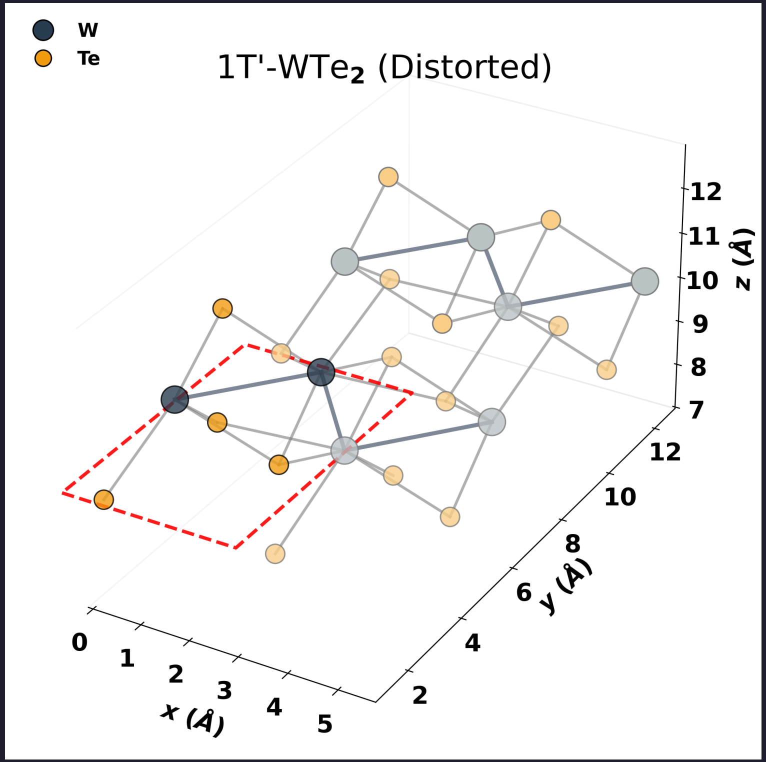
The "Parent" Phase:

- **Geometry:** High Symmetry (C_{3v}).
- **Feature:** Uniform W triangular lattice.

The Physics:

- **Stability:** Unstable (Peierls active).
- **Band Order:** Normal (Trivial).
- **Topology:** $Z_2 = 0$ (Ordinary Metal).

Crystal Structure: The Distorted $1T'$ Phase



The “Real” Phase:

- **Geometry:** Low Symmetry (C_{2h}).
- **Feature:** W atoms form zig-zag chains.

The Physics:

- **Stability:** Ground State (Relaxed).
- **Band Order:** Inverted (Topological).
- **Topology:** $Z_2 = 1$ (QSH Insulator).

The Bridge: From Instability to Topology

The Driving Force: Peierls Instability

The metallic 1T phase is energetically expensive. The system lowers its total energy by spontaneously distorting the lattice (dimerization).

The Structural Response: Symmetry Breaking

$$C_{3v} \to C_{2h}$$

Tungsten (W) atoms pair up to form zigzag chains. This lowers the symmetry and opens a fundamental band gap.

The Topological Consequence

This distortion is not trivial—it induces a **Band Inversion** between d and p orbitals, turning the material into a QSH Insulator ($Z_2 = 1$).

Simulation Setup: From Structure to Input

The Foundation:

- **Structure:** Optimized via `vc-relax` (BFGS).
- **Vacuum:** > 15Å isolation for monolayer physics.

The Engine (QE v7.4.1):

- **Functional:** PBE + Spin-Orbit Coupling (SOC).
- **Pseudos:** Fully Relativistic PAW (`pslibrary`).

Numerical Precision:

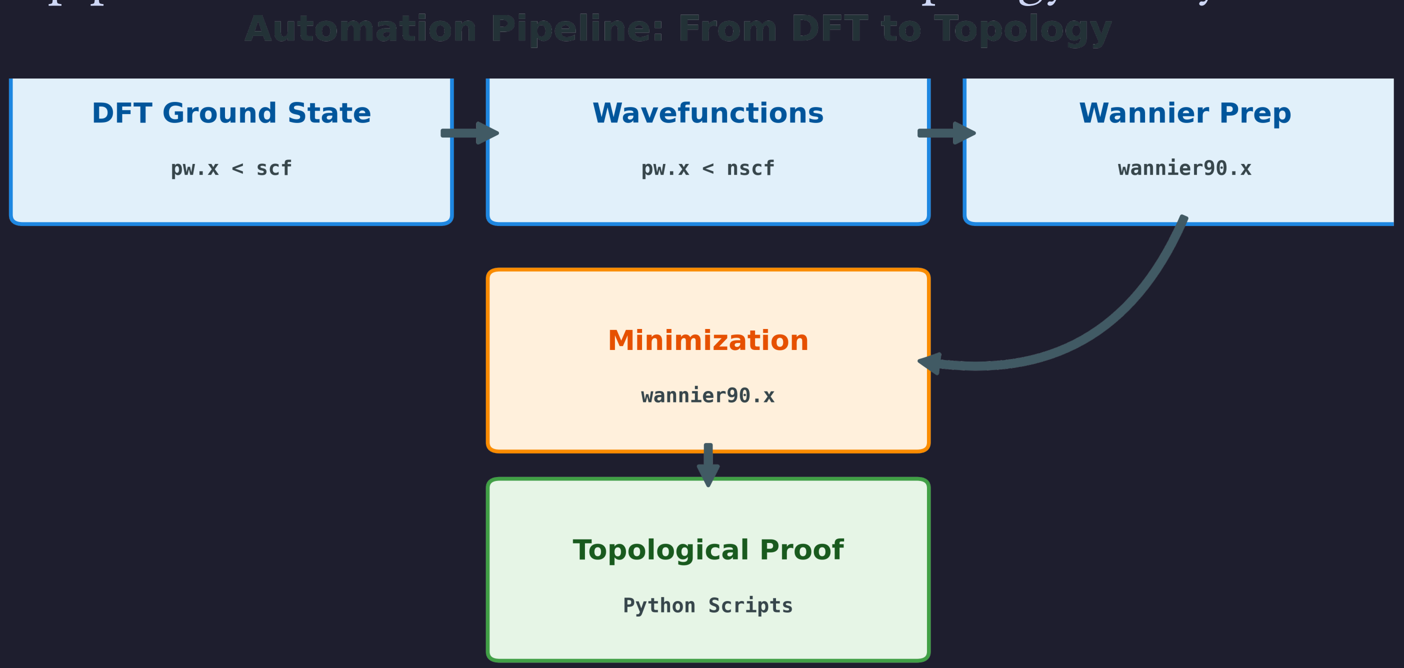
- **Kinetic Cutoff:** 60 Ry (Wvfn) / 720 Ry (Rho).
- **K-Mesh:** $12 \times 6 \times 1$ (Monkhorst-Pack).
- **Convergence:** 10^{-8} Ry (SCF).

```
&SYSTEM
ibrav=0, nat=6, ntyp=2,
ecutwfc=60, ecutrho=720,
lspinorb=.true.,
noncolin=.true.,
/
ATOMIC_SPECIES
W  183.84 W.rel...UPF
Te 127.60 Te.rel...UPF
K_POINTS (automatic)
12 6 1 0 0 0
```

Real Input Snapshot

The Recipe: A Reproducible QE Pipeline

Our pipeline automates the extraction of “Topology-Ready” Hamilton

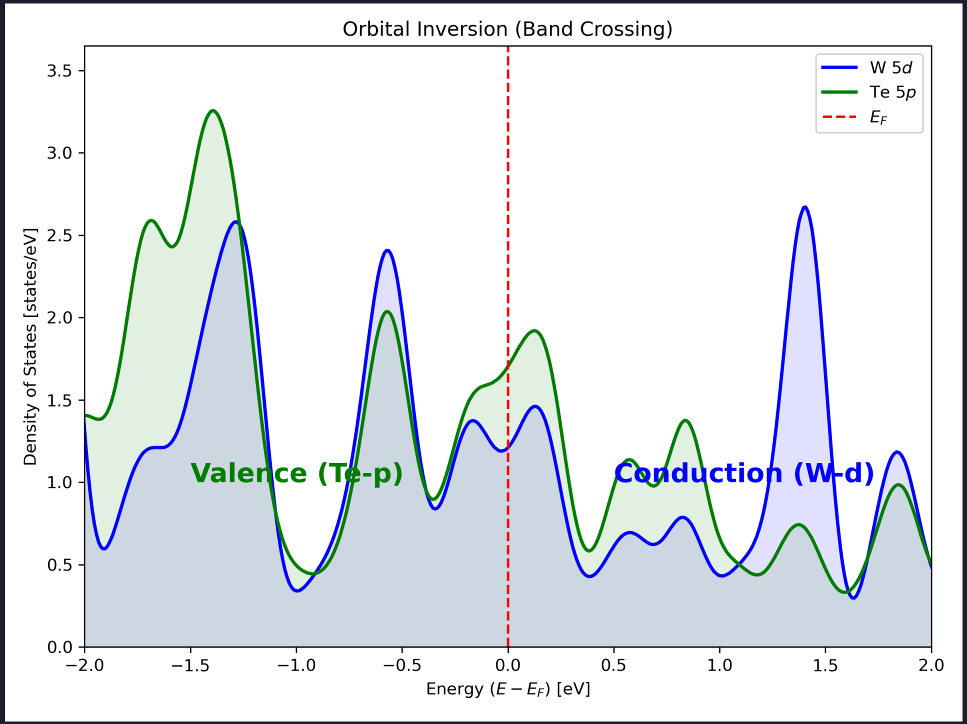


Key Ingredients:

- **Engine:** Quantum ESPRESSO.
- **Pseudopotentials:** `pslibrary` (PAW, PBE).
- **Wannier90:** Spinor Projections (p-Te, d-W) + Disentanglement.

Goal:
Generate an accurate Tight-Binding model for Berry Curvature integration.

The Mechanism: SOC-Driven Band Inversion

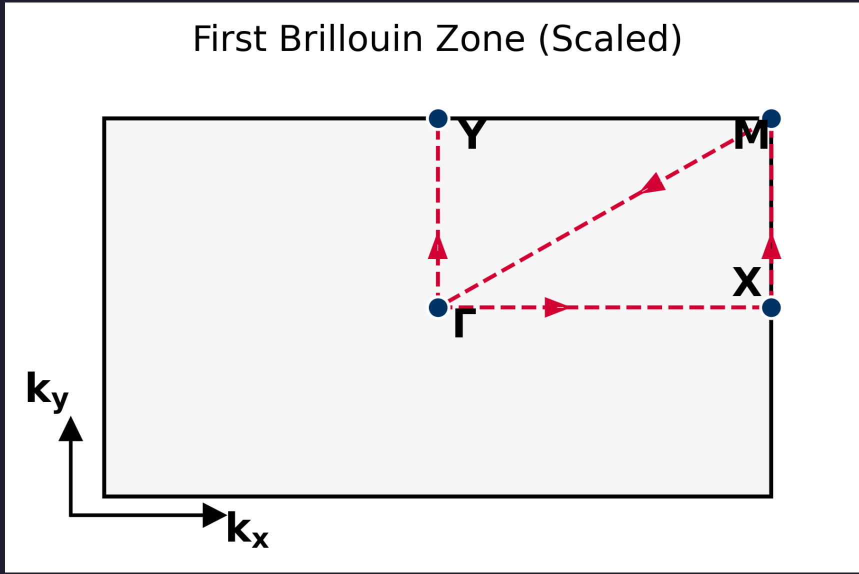


Orbital Physics:

1. **Crystal Field:** Splits W-d orbitals.
2. **Spin-Orbit Coupling (SOC):** The heavy Tungsten core drives a relativistic energy shift.

The Inversion: The W-d and Te-p bands **exchange parity eigenvalues** near the Fermi level. This crossing opens a non-trivial gap.

The Arena: Reciprocal Space Geometry

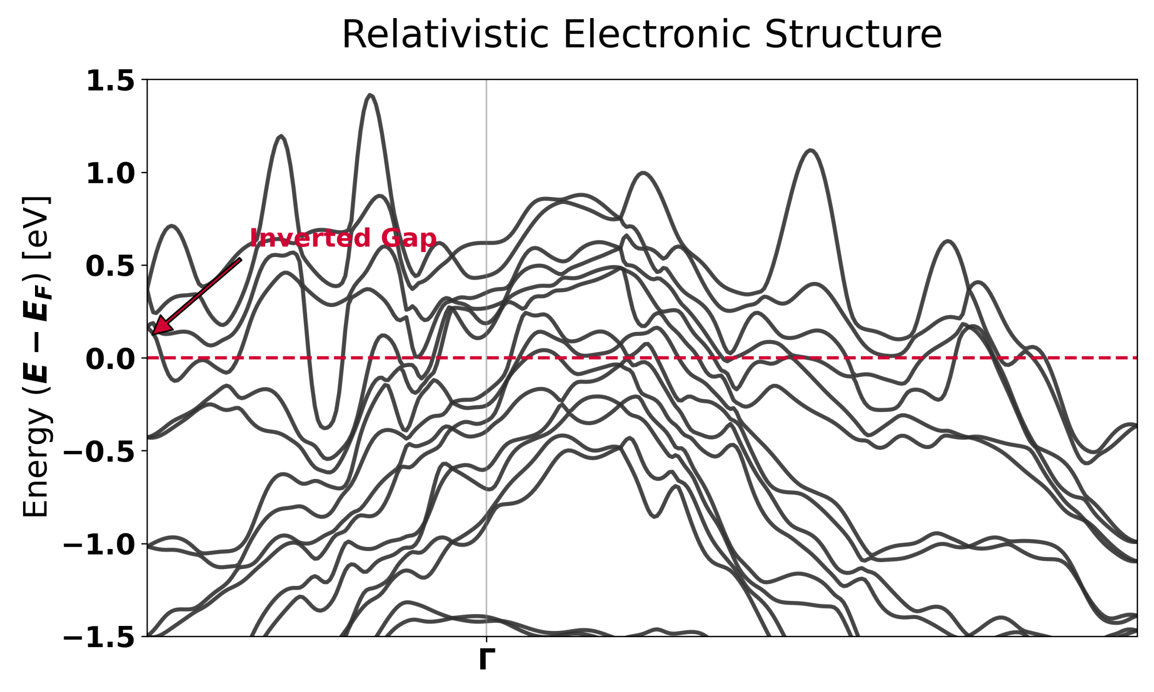


The Transformation:
The $C_{\{2h\}}$ symmetry breaking (Slide 5) transforms the parent Hexagonal BZ into a **Rectangular BZ**.

The Path:
$\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma \rightarrow Y$

The Target:
We must focus on the Γ point, where the band inversion corresponds to the "twisted" orbital character.

The Fingerprint: Relativistic Band Inversion

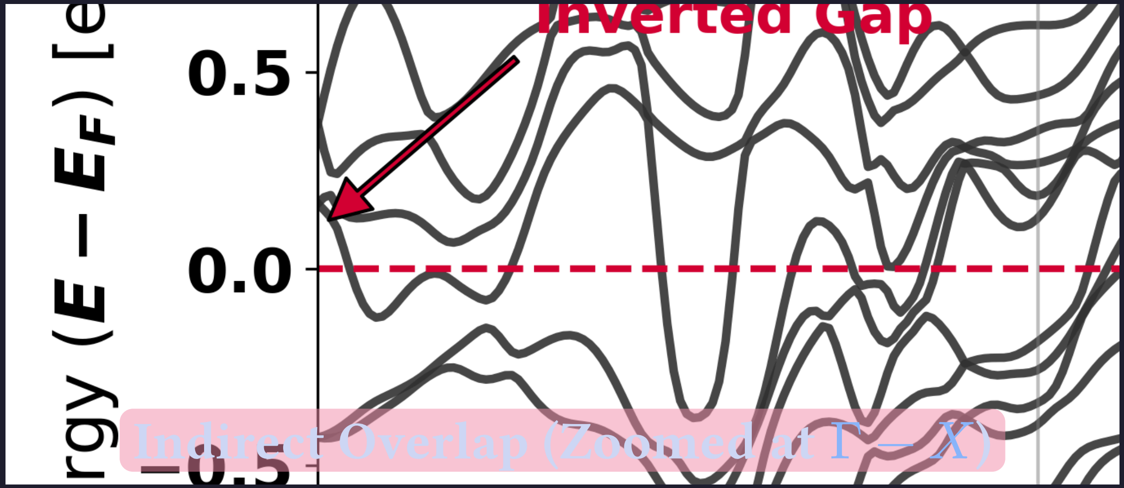


Full Relativistic Band Structure

The Effect of SOC:
Spin-Orbit Coupling lifts the band degeneracy. The heavy Tungsten atoms drive a massive splitting.

The Topological Signal: A fundamental **inverted gap** opens continuously along the $\Gamma - X$ direction.

Global Electronic Structure: The Semimetallic Reality

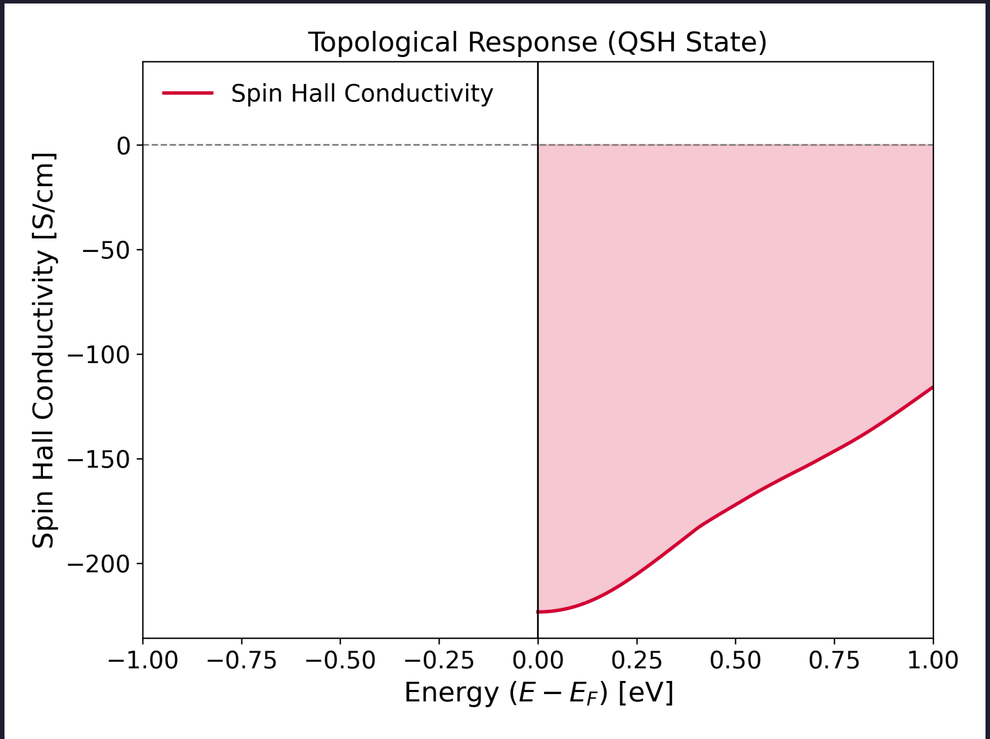


The Observation:
CBM dips below VBM globally (Q vs Γ).

The Cause:
Standard PBE underestimates gaps. This "Semimetallic" state is a known simulation feature of $1T' - \mathrm{WTe}_2$.

Why Topology Survives:
Z_2 depends on **Local Parity Exchange**. Size of the global gap is irrelevant as long as the direct gap at Γ is inverted.

Definitive Evidence I: Quantized Transport



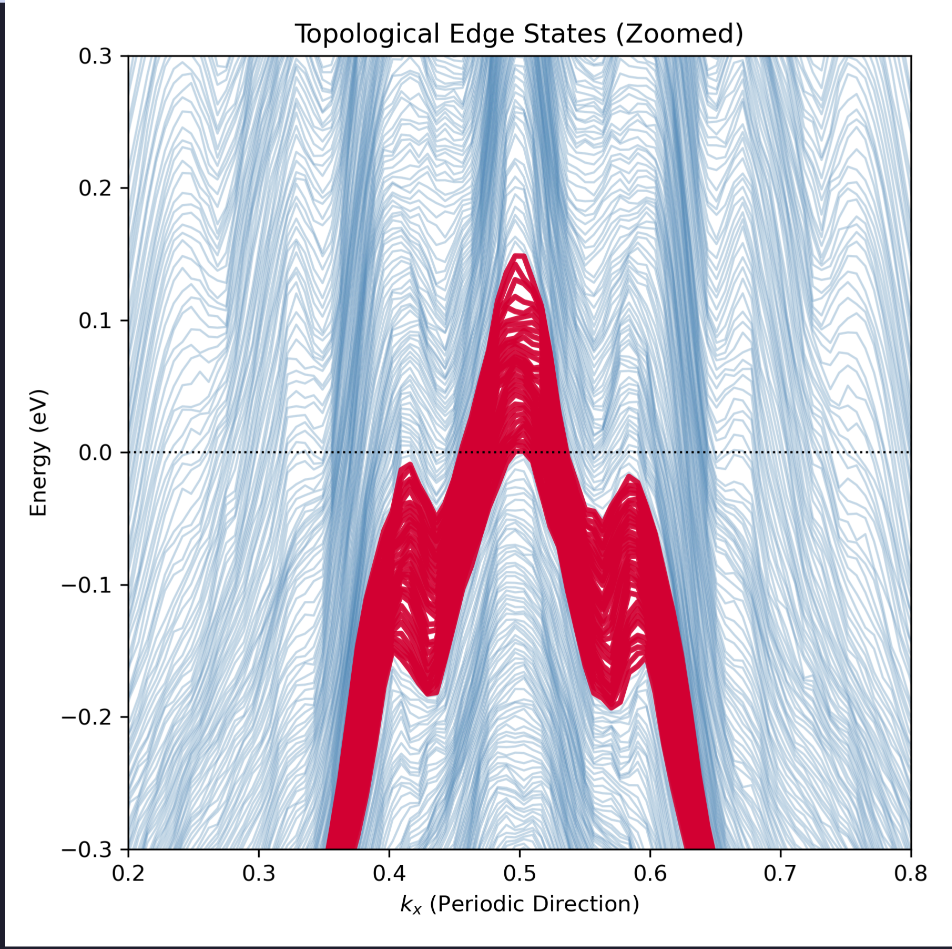
The Observable:
Spin Hall Conductivity ($\sigma_{\mathrm{xy}}^{\mathrm{spin}}$).

The Result:
A robust quantized plateau (50 meV width) exists at exactly:

$$2\frac{e^2}{h}$$

Implication:
This quantization is the hallmark of the QSH state. The plateau confirms protection against non-magnetic disorder.

Definitive Evidence II: Visualizing Edge Highways



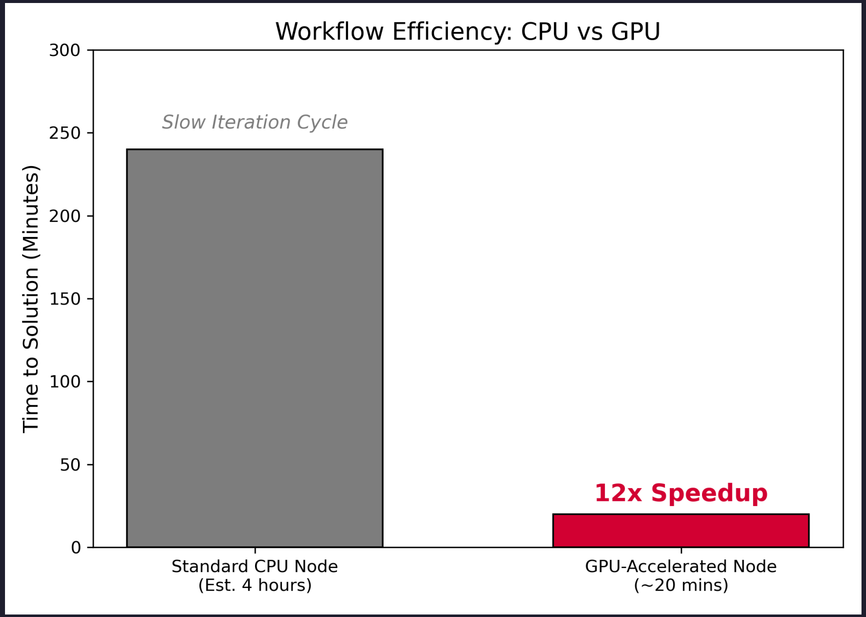
Calculation:
Wannier Hamiltonian (Finite Slab Projection).

Observation:
Two distinct **Helical Edge States** traverse the bulk gap using opposite spin channels ($\uparrow k_x$ vs $\downarrow -k_x$).

The Connection:
These are the "wires" that carry the quantized current seen in the previous slide ($2\frac{e^2}{h}$).

The Efficiency: Accelerated Discovery

Topological workflows are computationally expensive. We benchmarked the feasibility.



The Speedup:
GPU Acceleration reduces iteration time from **4 hours** to **20 minutes** (12x).

Why it Matters:
Allows for rapid convergence testing (k-mesh density, Wannier windows) essential for high-fidelity topological invariants.

The Verdict: Unambiguous QSH Insulator

Our “Recipe” successfully characterizes 1T′-WTe_2.

Summary of Evidences:

1. **Orbital:** $d - p$ Band Inversion confirmed.
2. **Topology:** $Z_2 = 1$ via Edge States and SHC.
3. **Robustness:** Wannier spreads $< 30\text{Å}^2$.

Final Conclusion:

1T’-WTe_2 is a robust Quantum Spin Hall Insulator suitable for room-temperature spintronics.

Code & Data:

github.com/shahpoll/QE-WTe2-Topology

Release:

`v1.0-ICAP2025` (Verified Artifact)

Thank You!

Questions & Discussion

github.com/shahpoll/QE-WTe2-Topology