

# A Quantum ESPRESSO Recipe for $Z_2$ Invariant of 2D Topological Material 1T'-WTe<sub>2</sub>

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# Motivation: The Quest for Dissipationless Electronics

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## The Bottleneck:

Modern electronics suffer from Joule heating and backscattering limits.

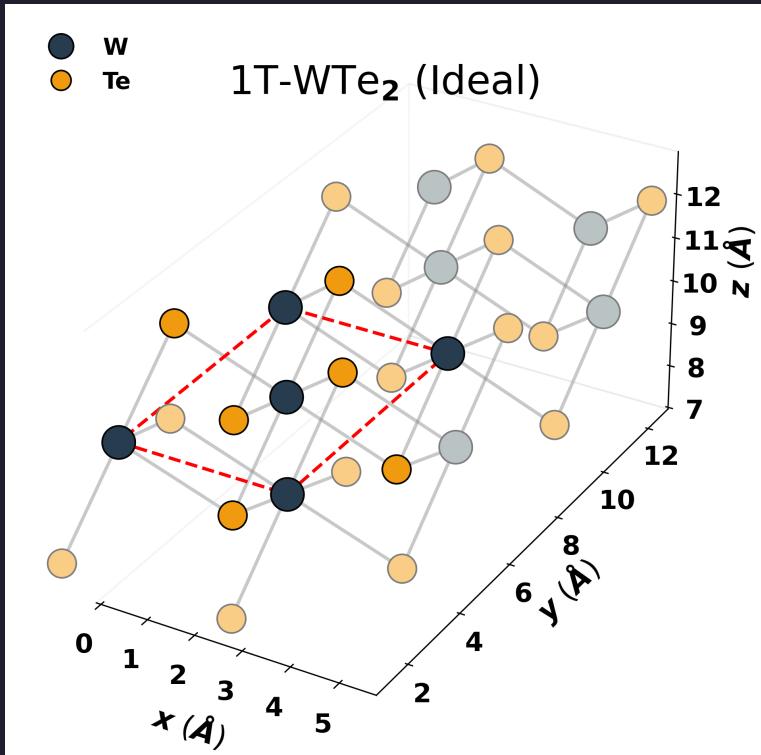
## The Solution:

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



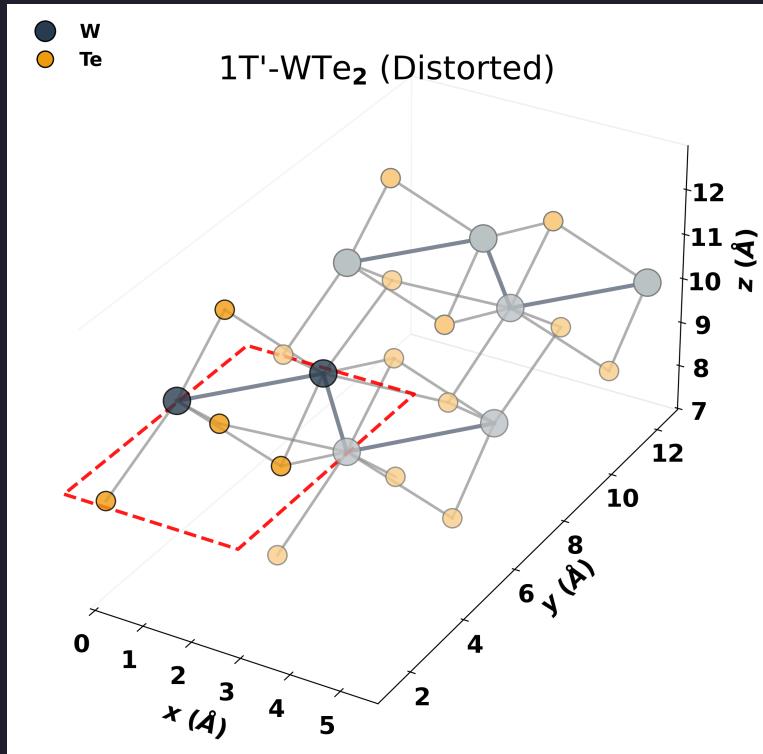
## The “Parent” Phase:

- **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

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## 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

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

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

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## The Foundation:

- **Structure:** Optimized via `vc-relax` (BFGS).
- **Vacuum:**  $> 15\text{\AA}$  isolation for monolayer physics.

## The Engine (QE v7.4.1):

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

## Numerical Precision:

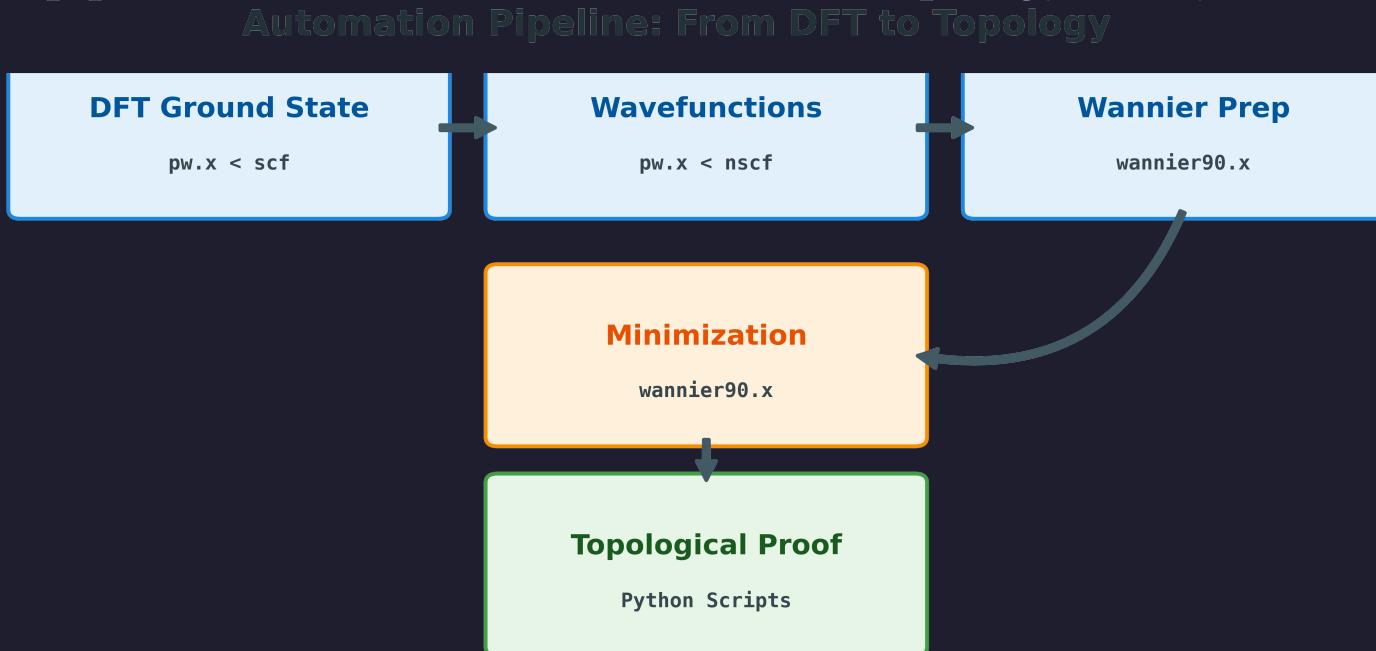
- **Kinetic Cutoff:** 60 Ry (Wvfn) / 720 Ry (Rho).
- **K-Mesh:**  $12 \times 6 \times 1$  (Monkhorst-Pack).
- **Convergence:**  $10^{-8}$  Ry (SCF).

```
&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” Hamiltonians.



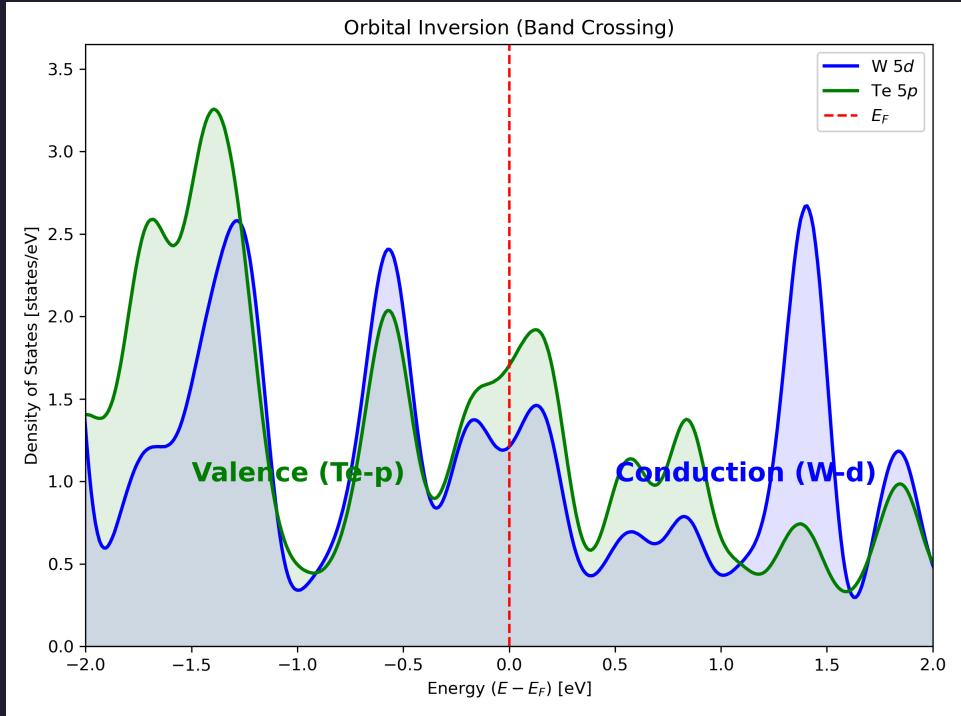
## Key Ingredients:

- **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

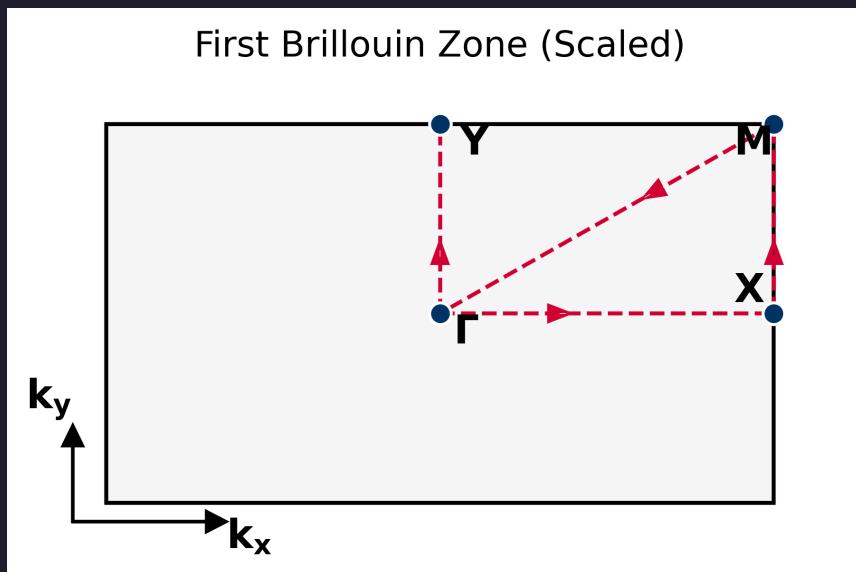


## Orbital Physics:

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**.

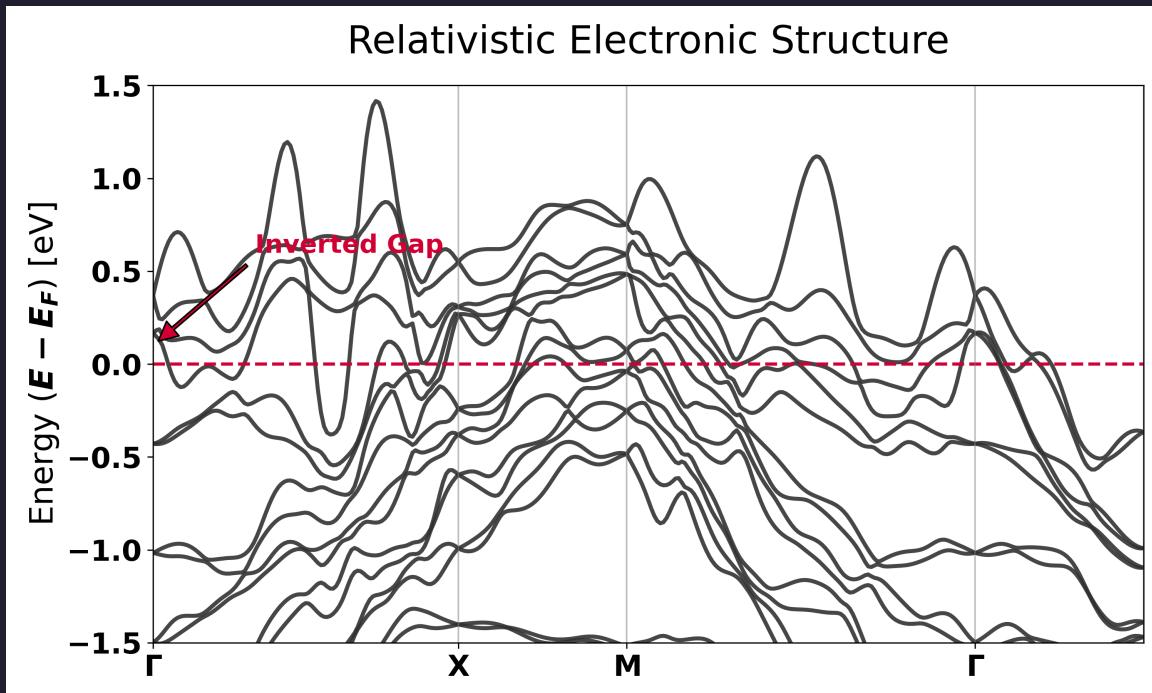
## The Path:

$\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma \rightarrow Y$

## The Target:

We must focus on the  $\Gamma$  point, where the band inversion corresponds to the “twisted” orbital character.

# The Fingerprint: Relativistic Band Inversion



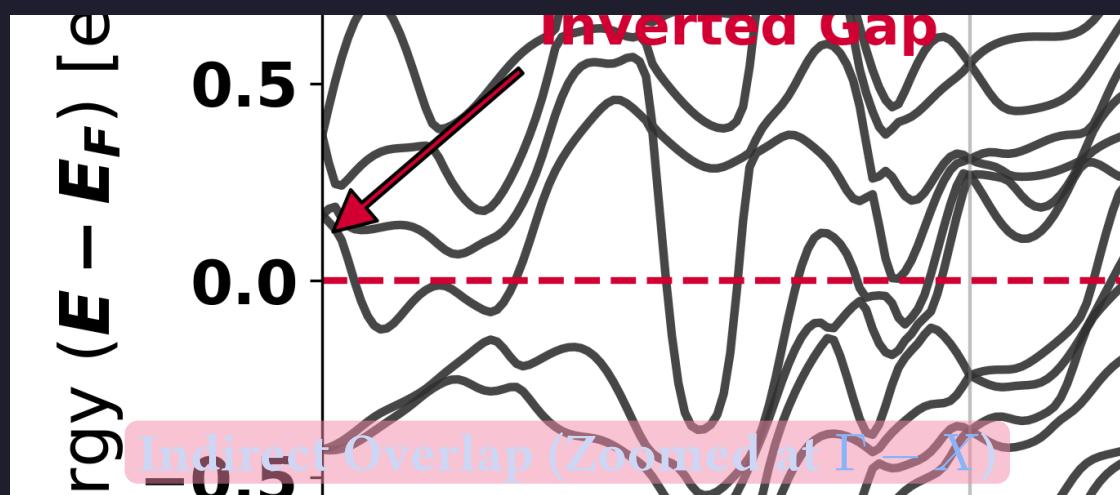
Full Relativistic Band Structure

## 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  $\Gamma$ ).

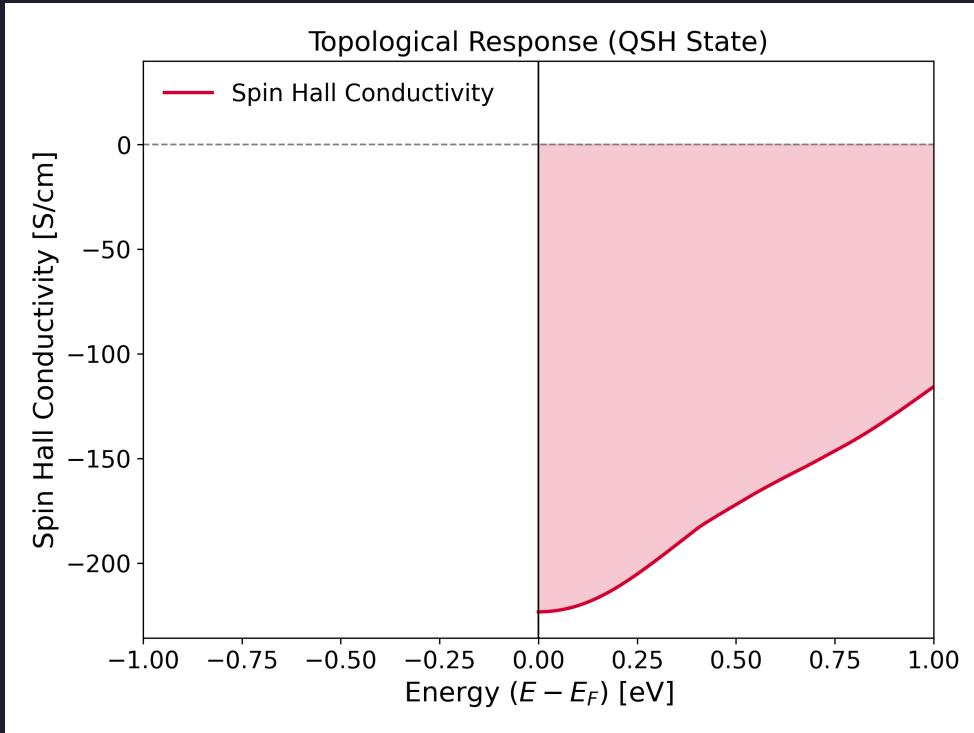
## The Cause:

Standard PBE underestimates gaps. This “Semimetallic” state is a known simulation feature of  $1T'$  – WTe<sub>2</sub>.

## Why Topology Survives:

$Z_2$  depends on **Local Parity Exchange**. Size of the global gap is irrelevant as long as the direct gap at  $\Gamma$  is inverted.

# Definitive Evidence I: Quantized Transport



## The Observable:

Spin Hall Conductivity ( $\sigma_{xy}^{\text{spin}}$ ).

## The Result:

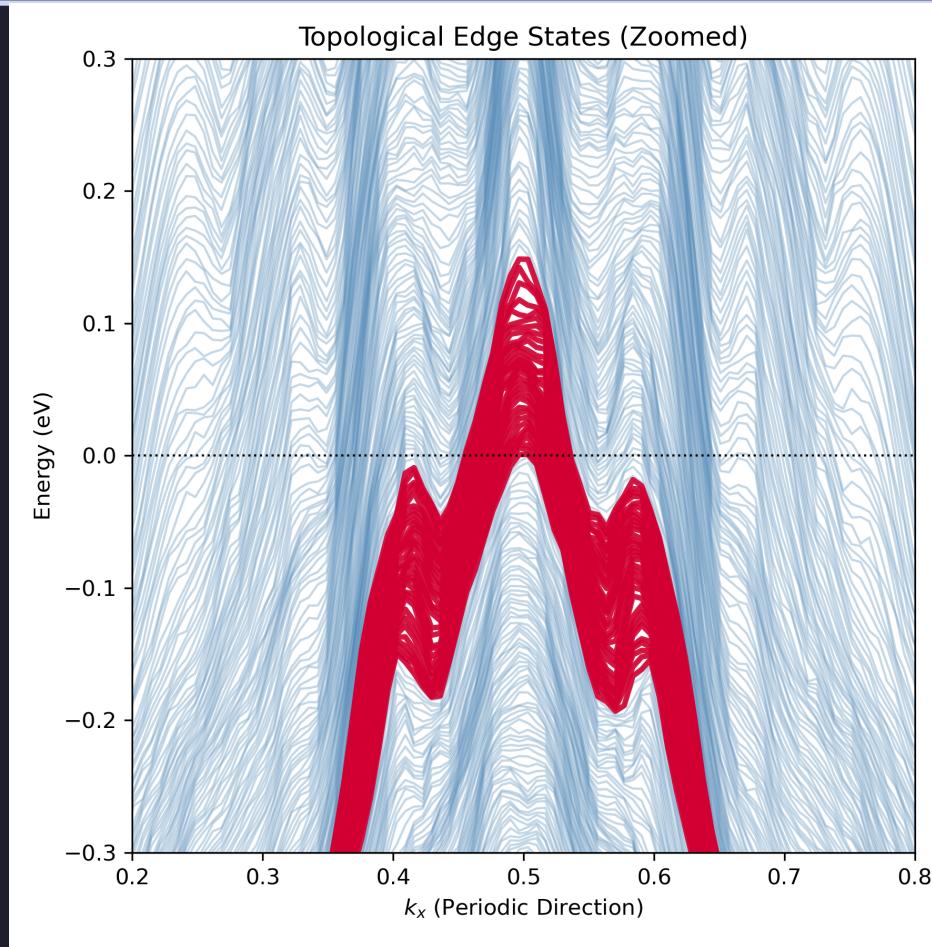
A robust quantized plateau ( 50 meV width) exists at exactly:

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

## 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:

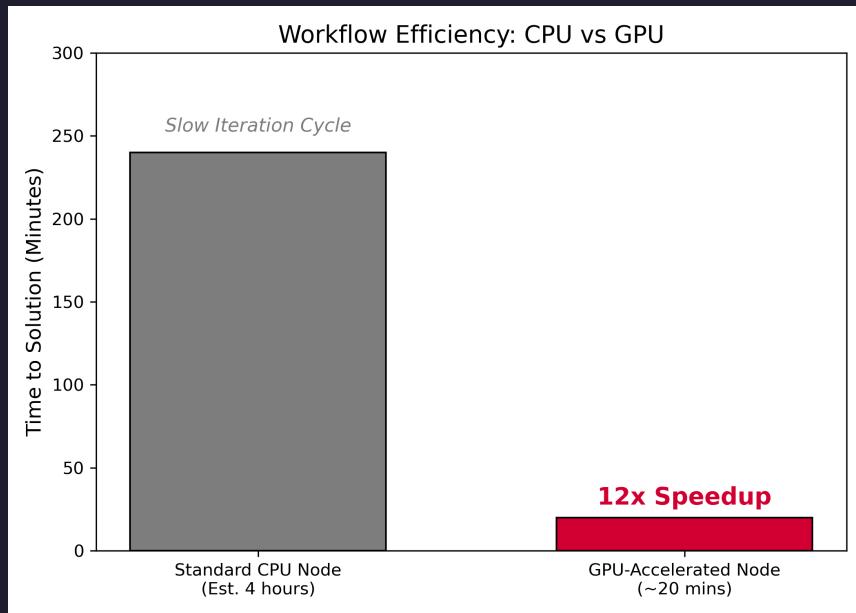
Two distinct **Helical Edge States** traverse the bulk gap using opposite spin channels ( $\uparrow k_x$  vs  $\downarrow -k_x$ ).

## 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

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Our “Recipe” successfully characterizes 1T'-WTe<sub>2</sub>.

## Summary of Evidences:

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

## Final Conclusion:

1T'-WTe<sub>2</sub> is a robust Quantum Spin Hall Insulator suitable for room-temperature spintronics.



## Code & Data:

[github.com/shahpoll/QE-WTe2-Topology](https://github.com/shahpoll/QE-WTe2-Topology)

## Release:

v1.0 - ICAP2025 (Verified Artifact)

# Thank You!

Questions & Discussion





