

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

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ICAP 2025 | SUST

International Conference on Advances in Physics

# 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.

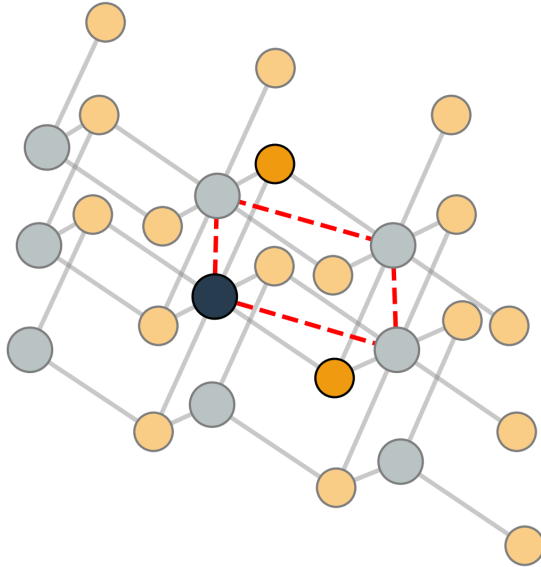
## The Challenge:

Obtaining the topological invariant ( $Z_2$ ) from First-Principles is often a “Black Box.”

# The Educational Journey: 1. The Ideal $1T$ Phase

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## 1T-WTe<sub>2</sub> (Ideal)



### The “Parent” Structure:

- Symmetry: Perfect Octahedral Coordination.
- Lattice: Hexagonal / Triangular W Lattice.

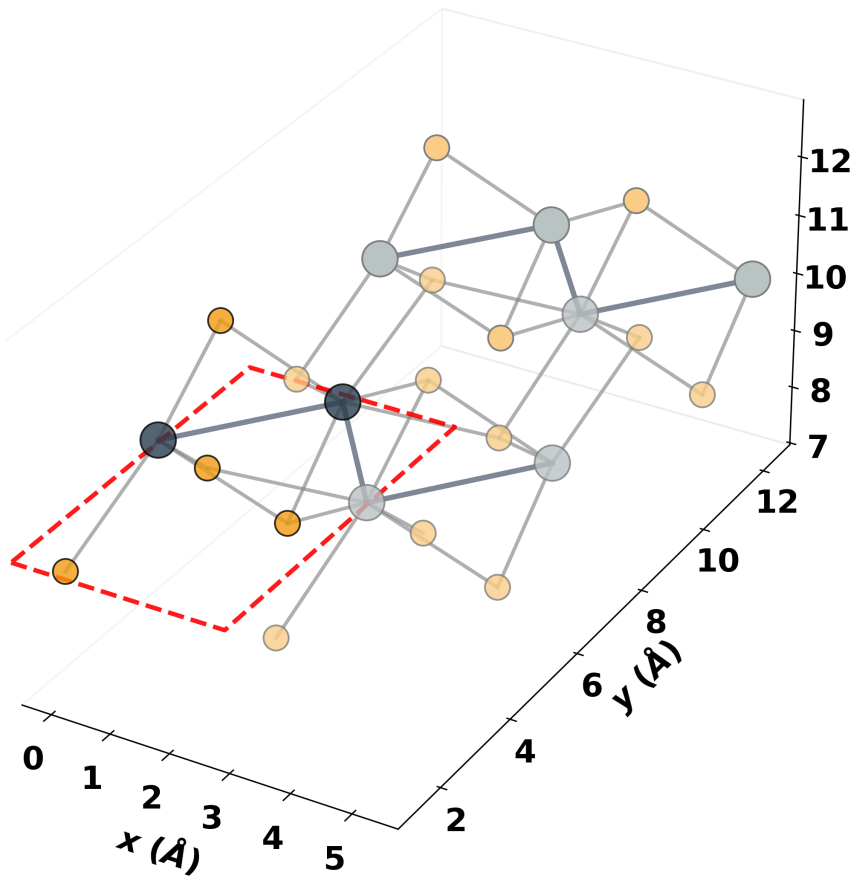
### Why it fails:

- Unstable: High energy state.
- Metallic: No band gap.
- **Not Topological.**

## The Educational Journey: 2. The Distorted $1T'$ Phase

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1T'-WTe<sub>2</sub> (Distorted)



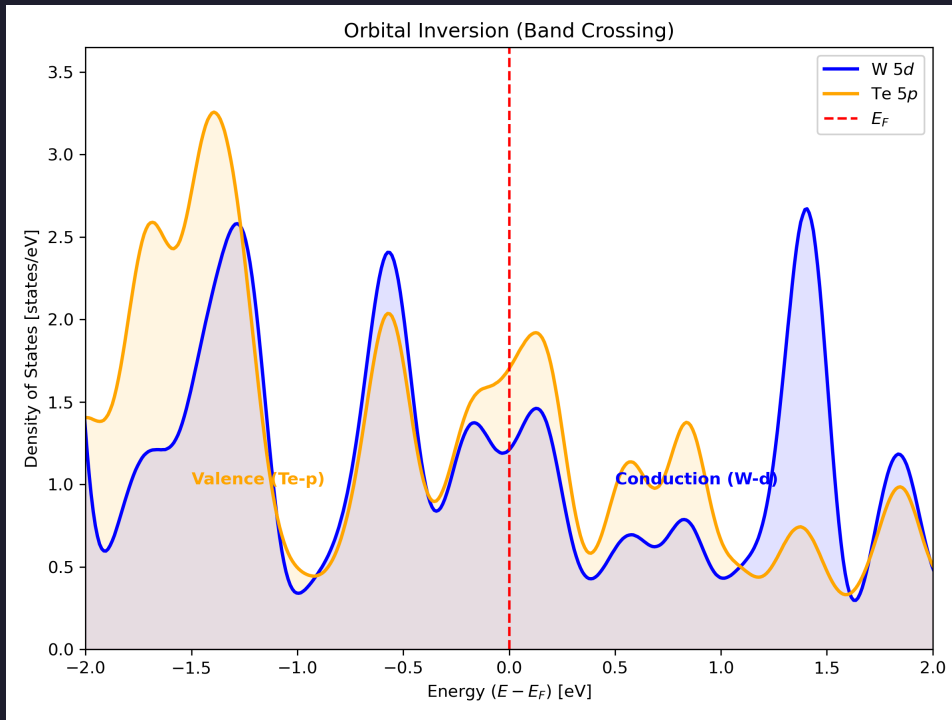
### The “Actual” Structure:

- Symmetry: Distorted (Peierls Instability).
- Action: W atoms dimerize along one axis.

### The Consequence:

- Stable: Energetically favorable.
- Insulating: Gap opens ( $E_g > 0$ ).
- Topological: Inverted Band Order ( $Z_2 = 1$ ).

# 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.

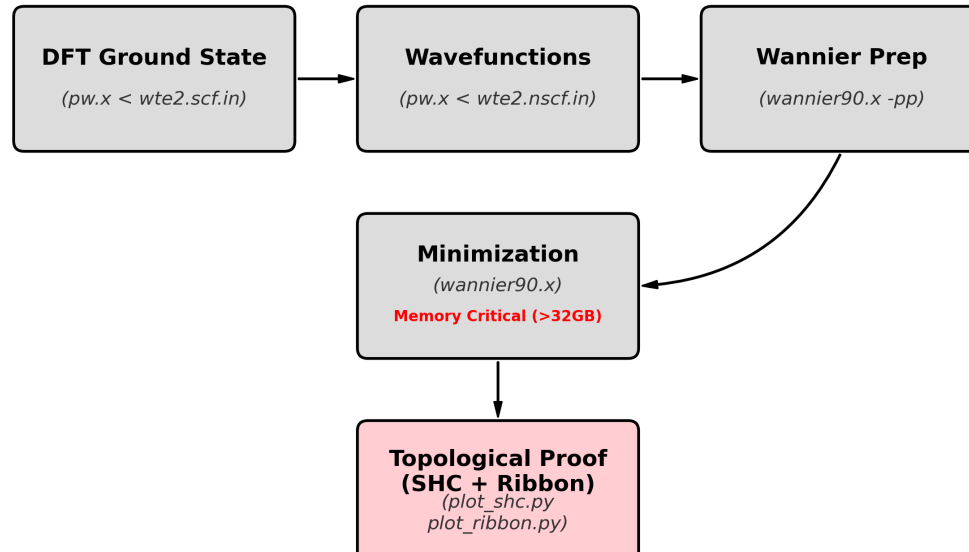
# The Recipe: A Reproducible QE Pipeline

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Our pipeline automates the extraction of “Topology-Ready” Hamiltonians.



## Reproducible Topological Workflow



## Key Ingredients:

- **Engine:** Quantum ESPRESSO (`pw.x`) v7.4.1
- **Pseudopotentials:** `pslibrary` v1.0.0 (PAW, Fully Relativistic PBE)
- **Wannier90:** Spinor Projections (*p*-Te, *d*-W) + Disentanglement

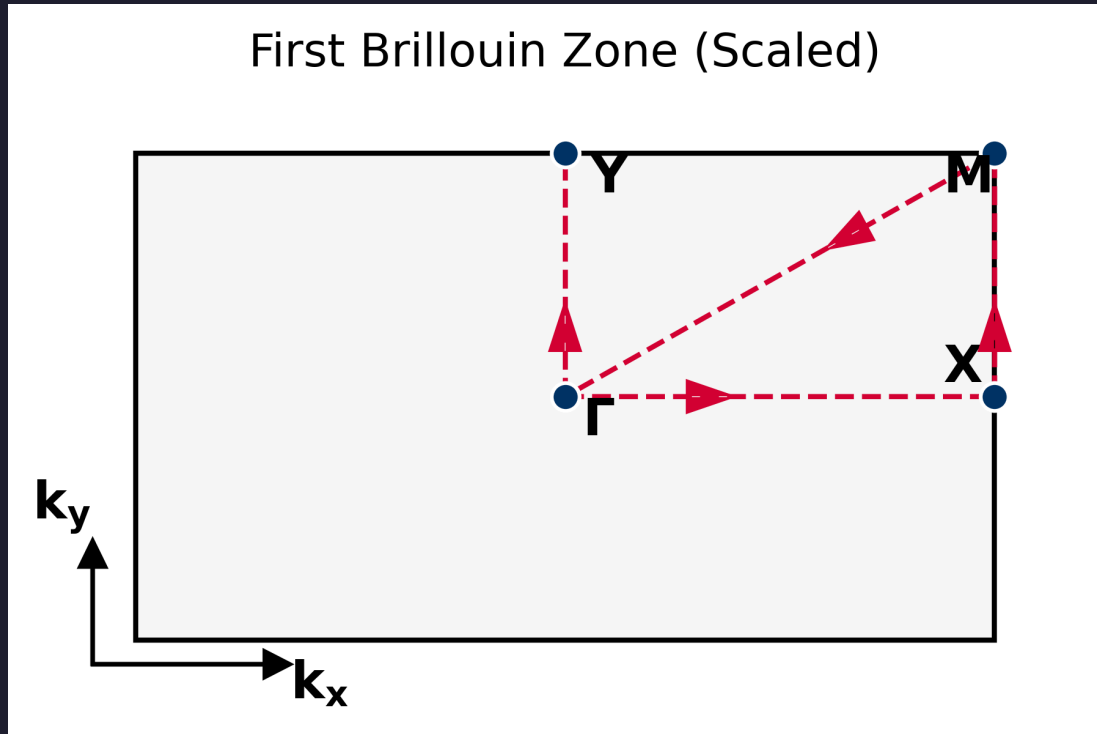
## Goal:

Generate an accurate Tight-Binding model for

Berry Curvature  
integration.

# The Arena: Reciprocal Space Geometry

To capture the inversion, one must traverse specific high-symmetry points.



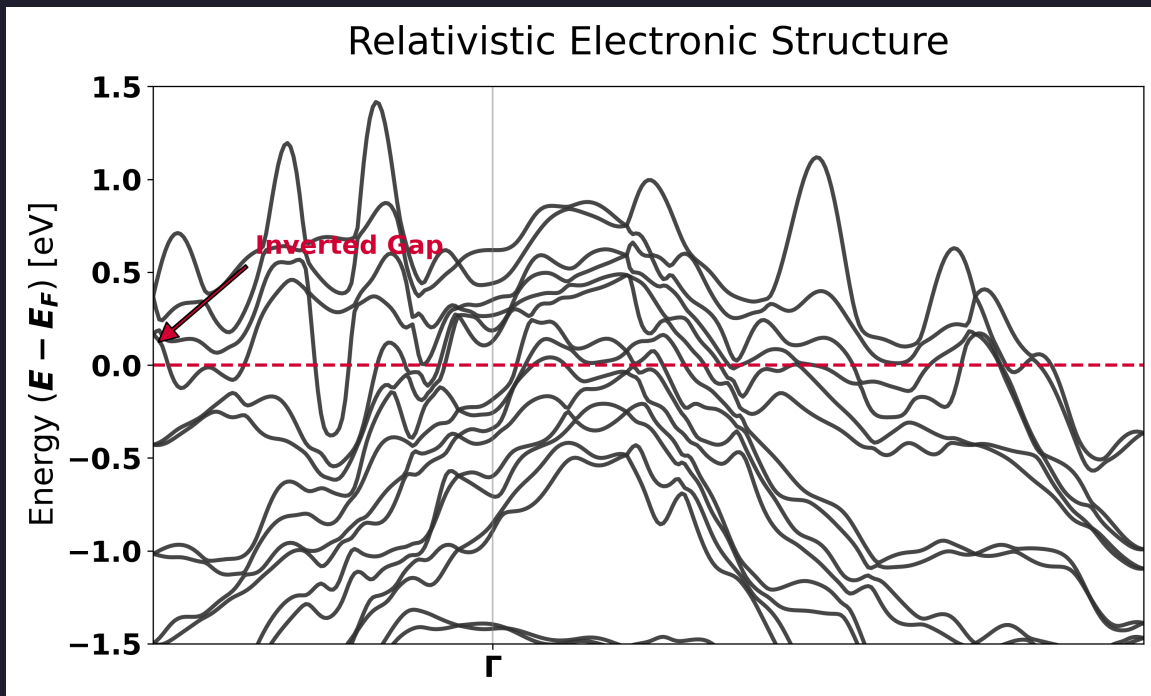
## The Path:

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

## Significance:

- The fundamental gap opens at  $\Gamma$ .
- The  $M \rightarrow \Gamma$  diagonal is critical for identifying background nodal lines.
- Rectangular BZ reflects the 1T' anisotropy.

# The Fingerprint: Relativistic Band Inversion



Full Relativistic Band Structure

## Global Profile:

Semimetallic overlap observed (typical for PBE), **BUT...**

**The Topological Signal:** A clear, direct gap opens at  $\Gamma$ .

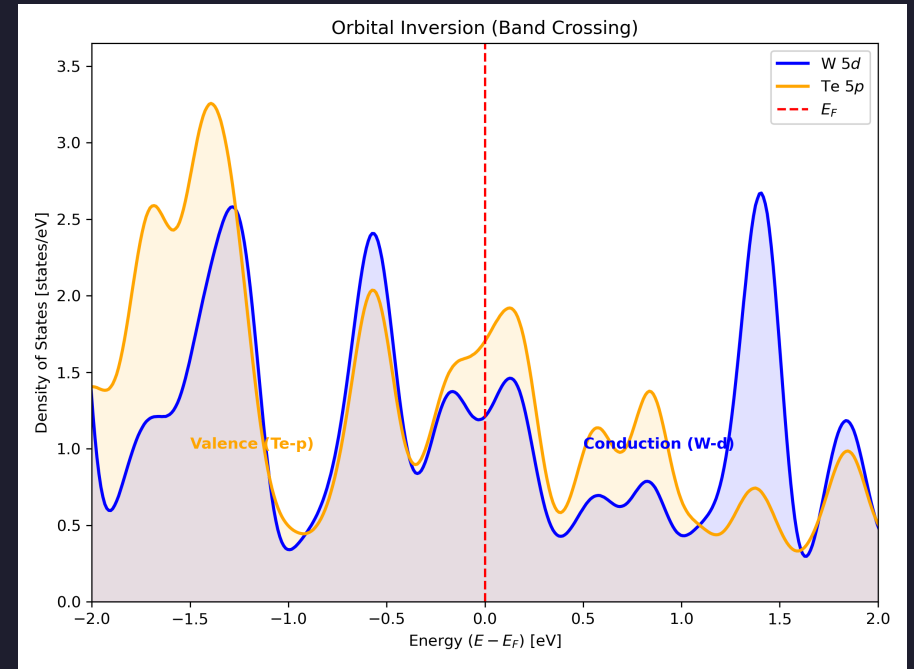
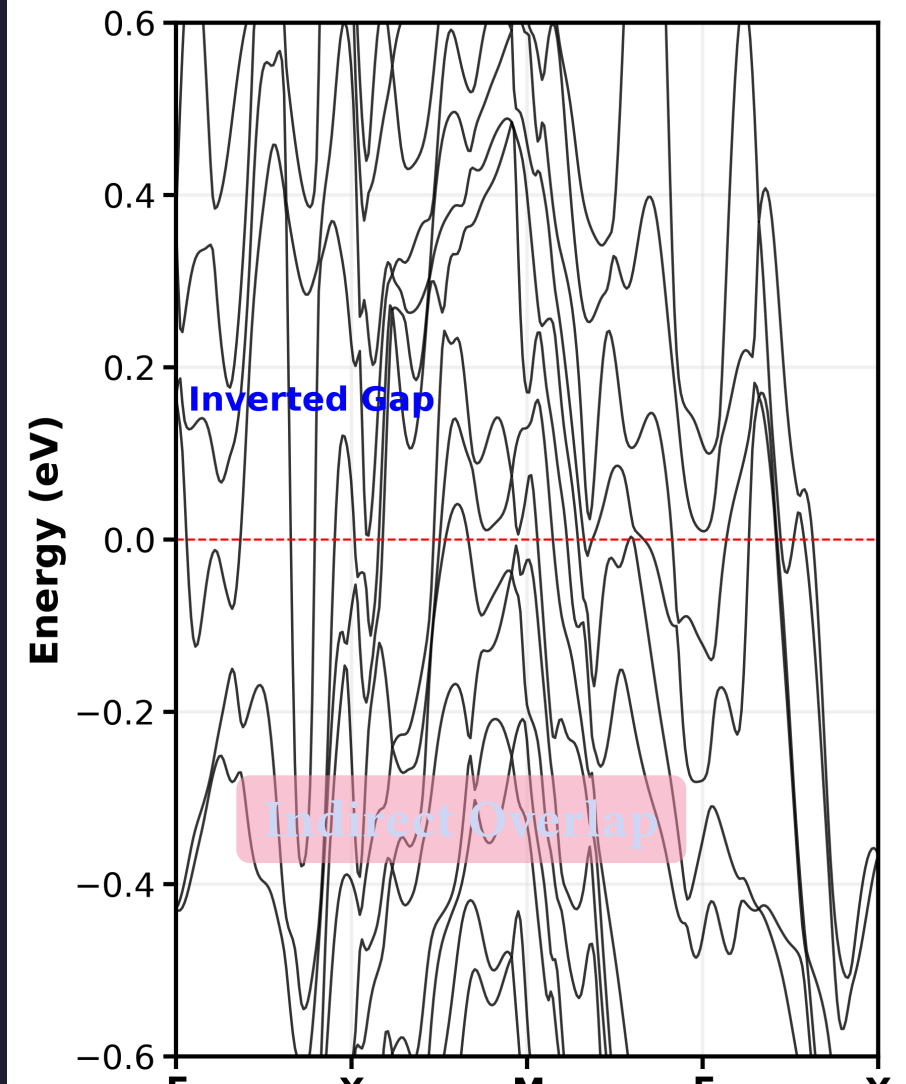


Figure 1: Zoom at  $\Gamma$ : Parity Exchange

# A Complication: The Semimetallic Ground State

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## 1.1 W12 Band Structure (PBE-PSC)



### The Observation:

The Conduction Band Minimum (CBM) dips below the Valence Band Maximum (VBM) at different k-points ( $Q$  vs  $\Gamma$ ).

### The Explanation:

PBE functionals notoriously underestimate gaps.

### The Crucial Insight:

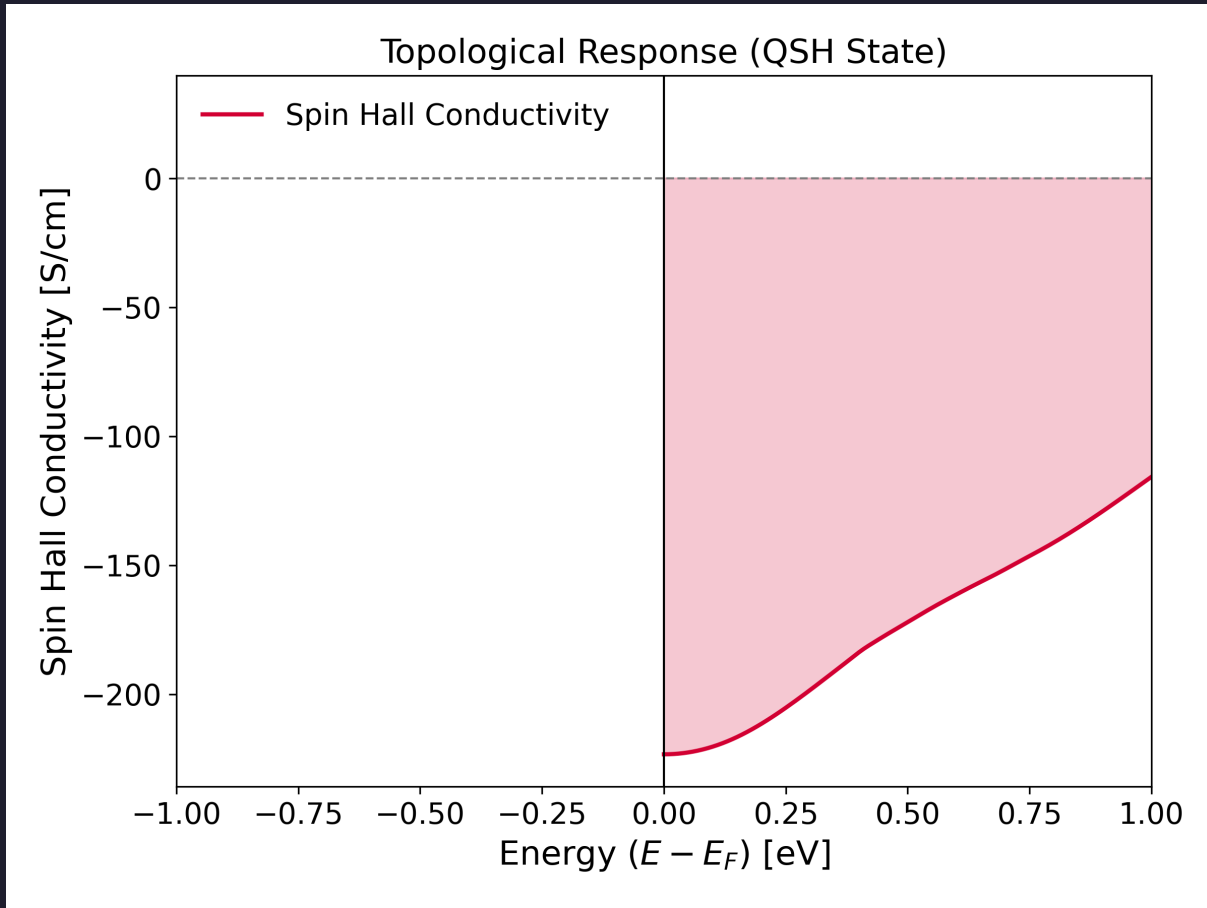
Topology is defined by the **Inverted Direct Gap**. As long as the direct gap at  $\Gamma$  is non-zero and inverted, the  $Z_2$  invariant is robust.

# Definitive Evidence I: Quantized Transport

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The Spin Hall Conductivity (SHC) provides a measurable order parameter.





### The Observable:

$\sigma_{xy}^{\text{spin}}$  calculated via Kubo-Greenwood formula.

### The Result:

A quantized plateau exists at exactly:

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

### Implication:

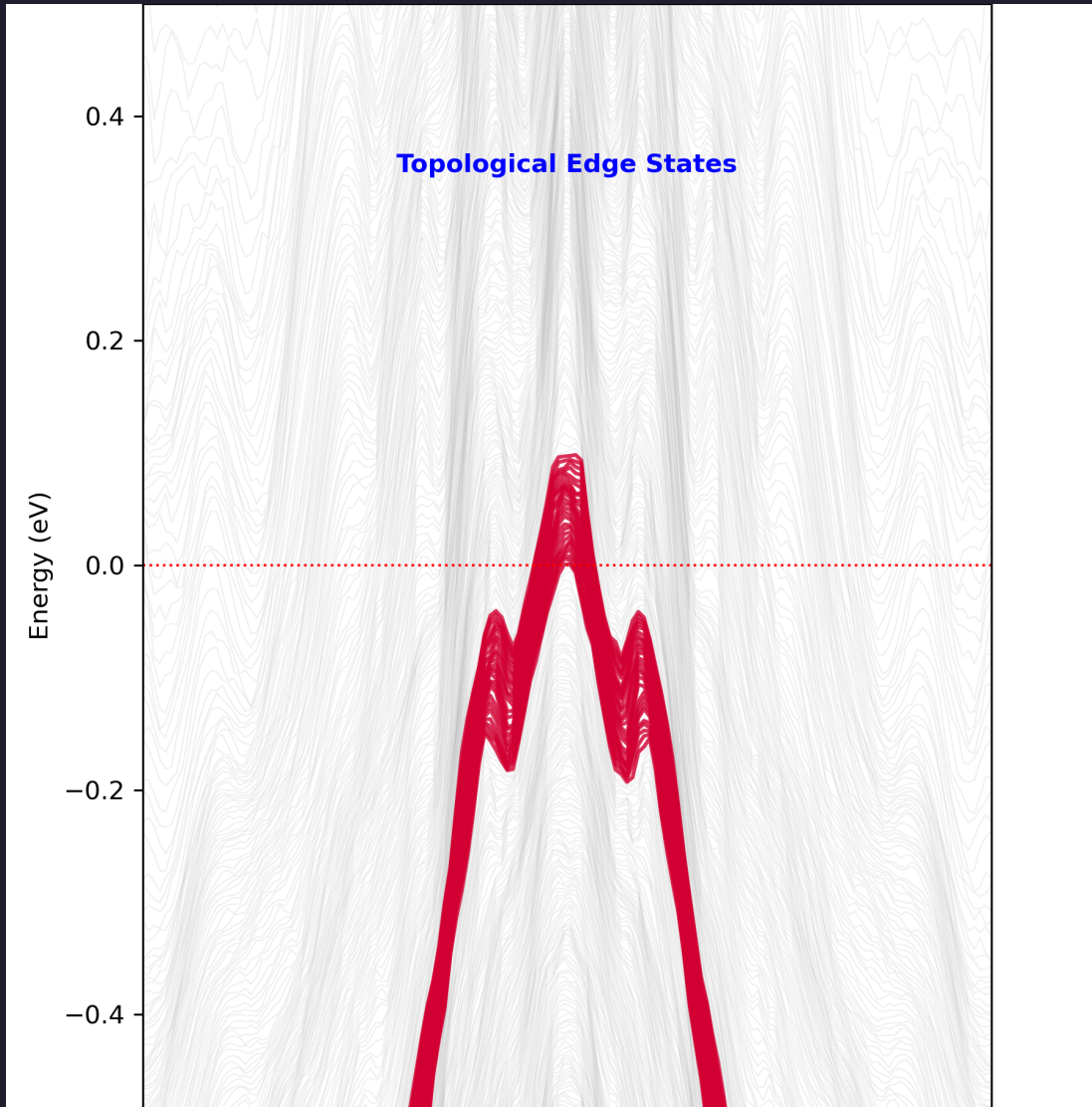
This quantization is the hallmark of the Quantum Spin Hall (QSH) state, protected

against non-magnetic  
perturbations.

# Definitive Evidence II: Visualizing Edge Highways

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Bulk-Boundary Correspondence guarantees conductive states at the interface.



### Calculation:

Wannier Hamiltonian projected onto a 30-unit-cell finite slab.

### Observation:

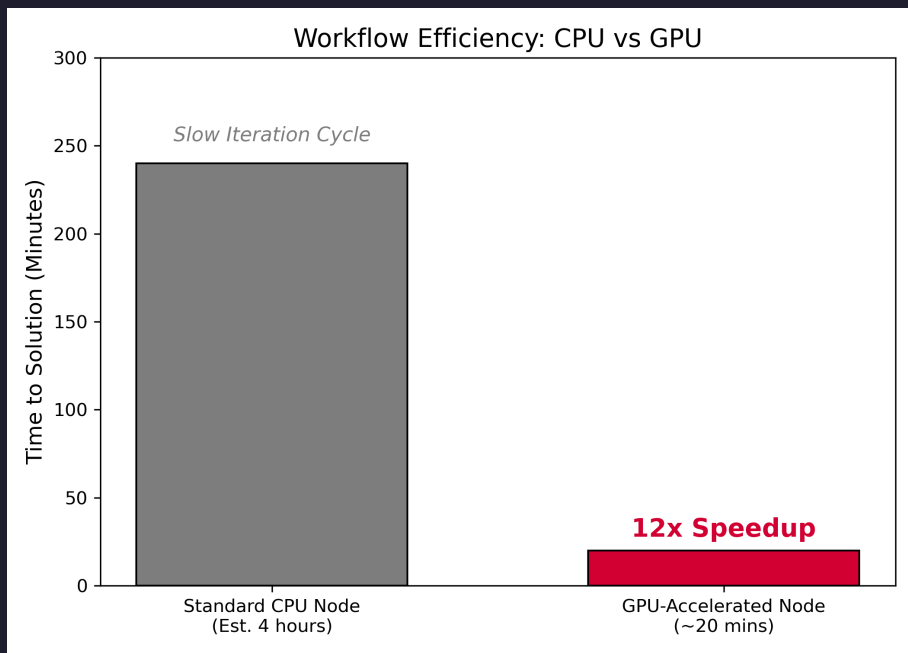
Helical edge states (Red) traverse the bulk gap, connecting valence and conduction bands.

### Verdict:

Odd number of crossings  $\rightarrow Z_2 = 1$ .

# 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/Quantum-ESPRESSO-WTe2-Topology](https://github.com/shahpoll/Quantum-ESPRESSO-WTe2-Topology)

## Release:

v1.0 - ICAP2025 (Verified Artifact)

