

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

Shahriar Pollob<sup>1,\*</sup>, Apu Das<sup>2</sup>, Mohammad Dilwar Ali Alvee<sup>3</sup>, M. Shahnoor Rahman<sup>4</sup>

<sup>1</sup> Department of Physics, Shahjalal University of Science and Technology, Sylhet-3114, Bangladesh

<sup>2</sup> Department of Theoretical Physics, University of Dhaka, Dhaka-1000, Bangladesh

<sup>3</sup> Department of Materials Science & Engineering, Khulna University of Engineering & Technology, Khulna-9203, Bangladesh

<sup>4</sup> Department of Physics, University of Miami, Coral Gables, Florida 33124, USA

\* Presenter

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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.

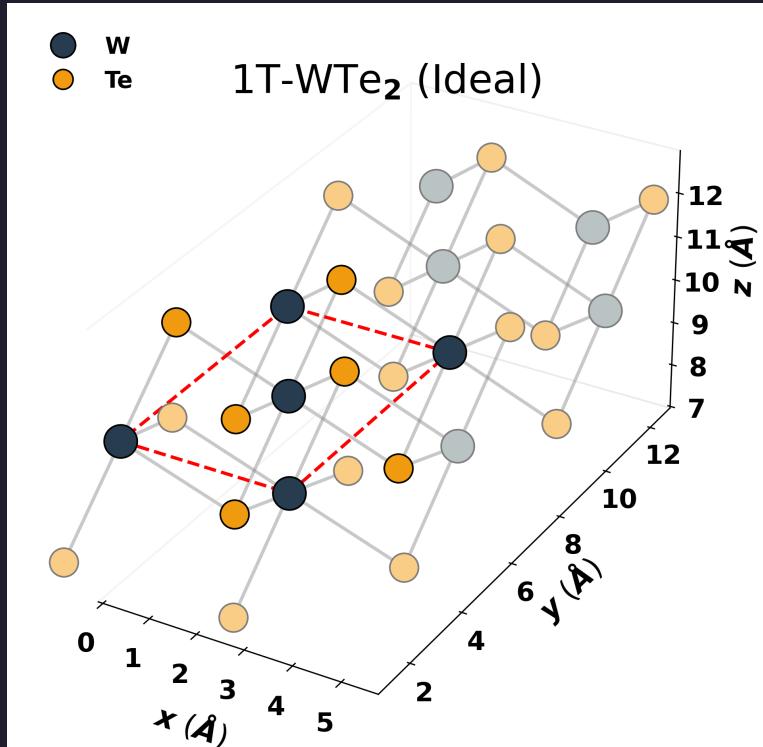
## The Solution:

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



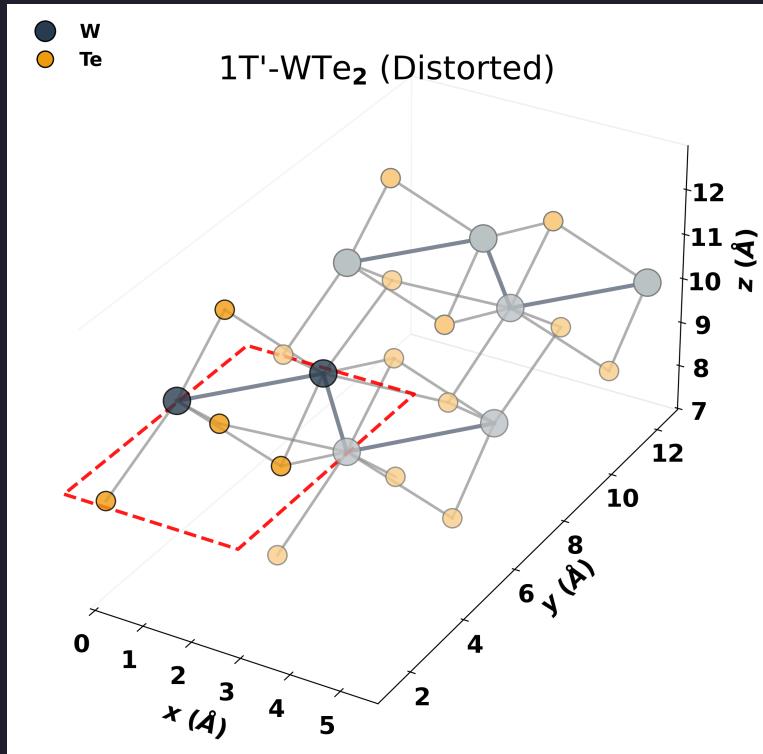
The “Parent” Structure:

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

Why it fails:

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

# Crystal Structure: The Distorted 1T' Phase



## The “Real” Structure:

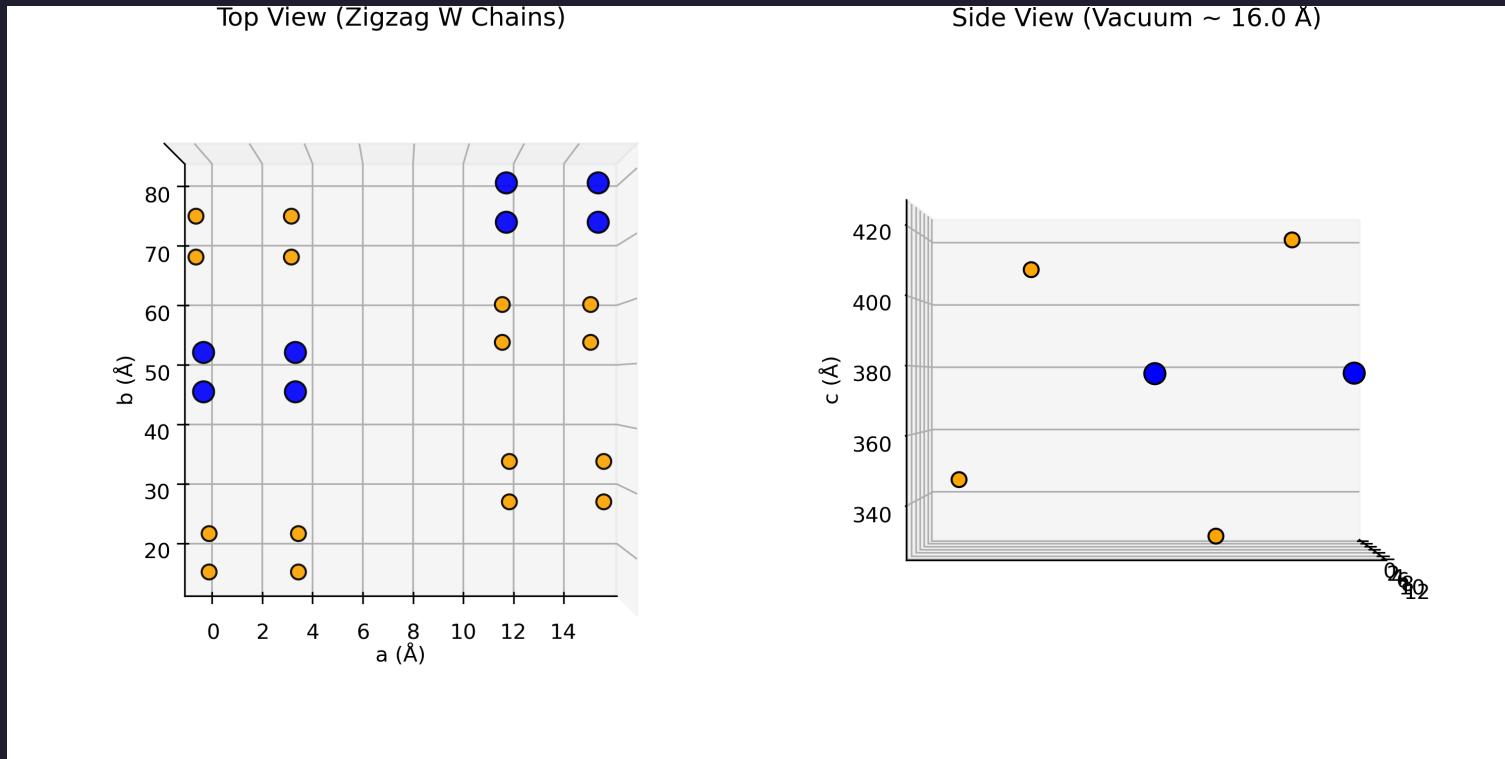
- **Symmetry:** Distorted (Peierls Instability).
- **Action:** W atoms dimerize along one axis.

## The Magic:

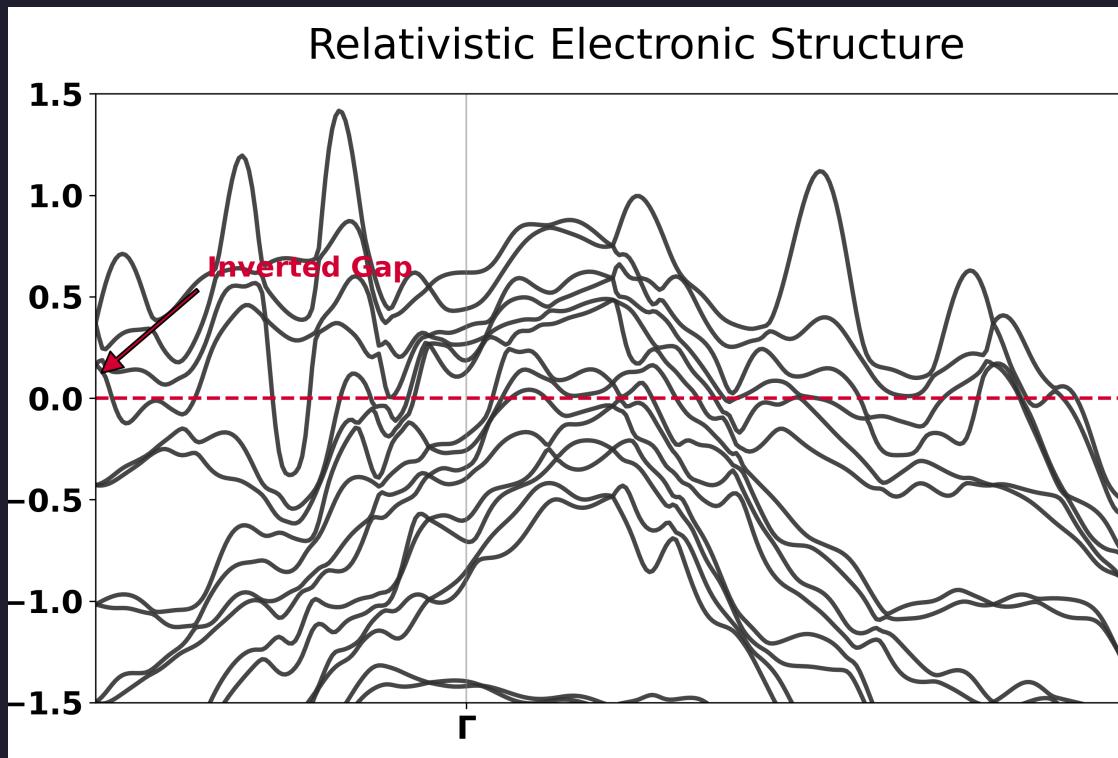
- **Stable:** Energetically favorable.
- **Insulating:** Gap opens ( $E_g > 0$ ).
- **Topological:** Inverted Band Order ( $Z_2 = 1$ ).

# Phase Transition Mechanism

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# Electronic Structure: Band Inversion

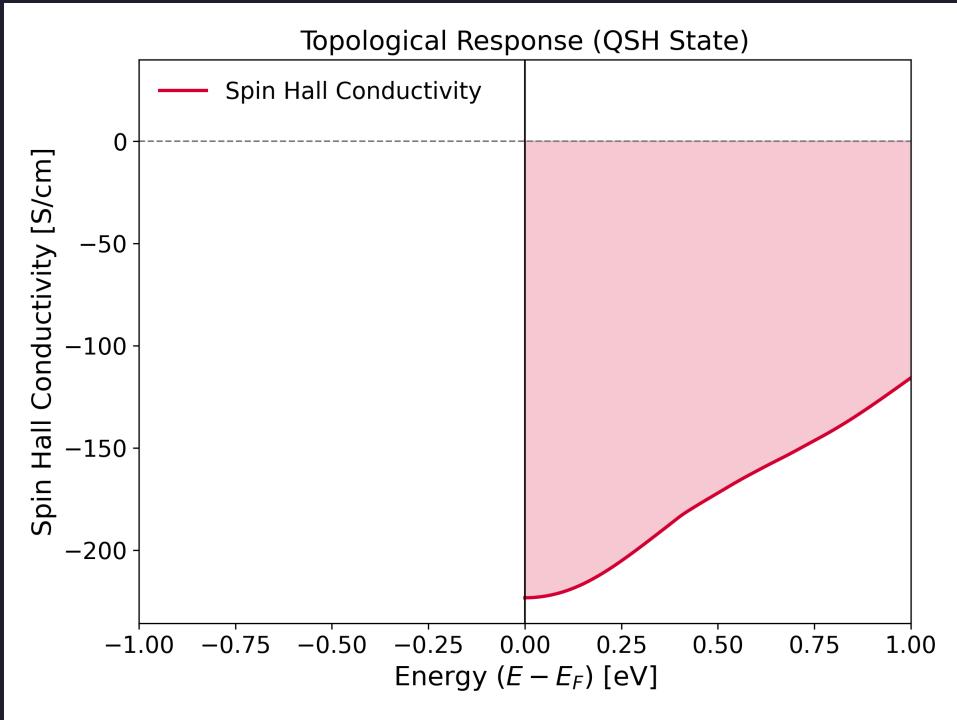


## Key Features:

- **Band Inversion:**  $p$ -orbital bands swap parity near  $\Gamma$ .
- **Spin-Orbit Coupling:** Essential for opening the gap ( $E_g \approx 50$  meV).
- **Direct Gap:** Located at  $Q$  point (monolayer feature).

# Spin Texture & Berry Curvature

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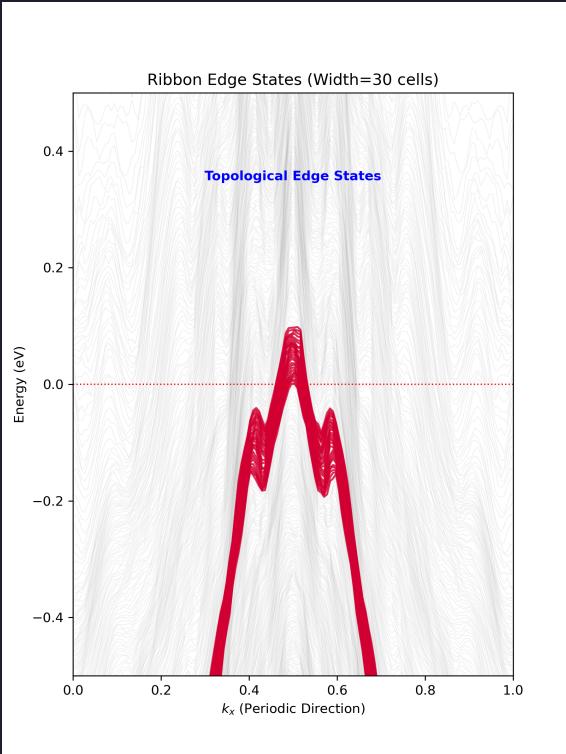


## Spin-Momentum Locking:

- Spins are locked to momentum  $k$ .
- Signatures of topological surface states.
- **Result:** Suppression of backscattering.

# The Definitive Evidence: Edge States

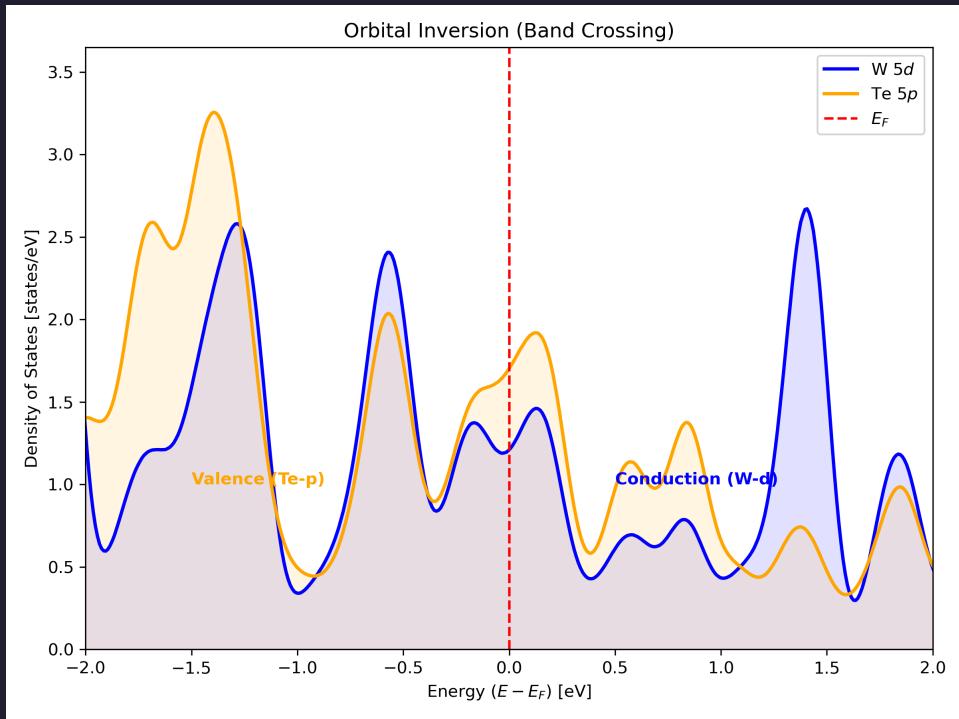
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## Topological Protection:

- **Gapless States:** Crossing the bulk gap.
- **Conducting Channels:** Located physically at the edges.
- **Robustness:** Immune to non-magnetic disorder.

# 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.

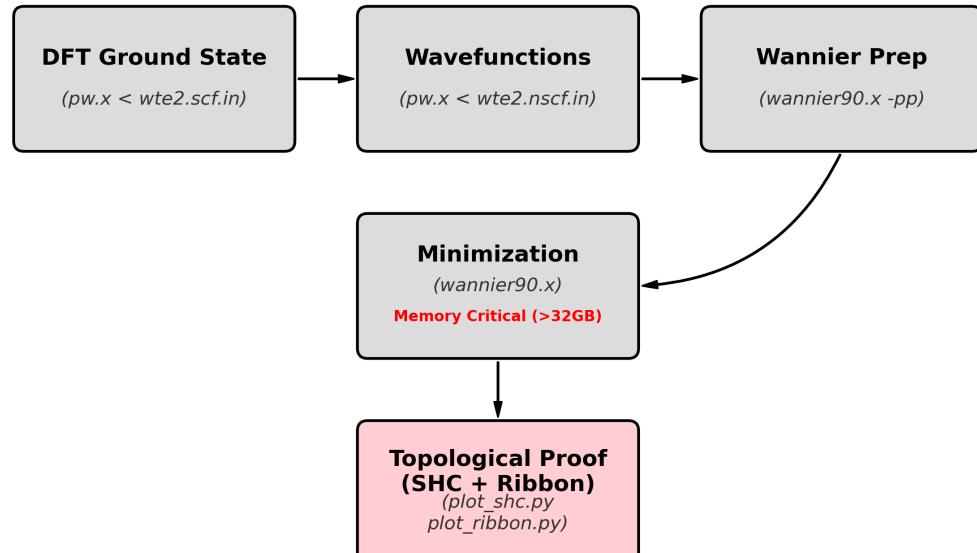
**The Inversion:** The W-*d* and Te-*p* bands exchange parity eigenvalues near the Fermi level. This crossing opens a non-trivial gap.

# 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

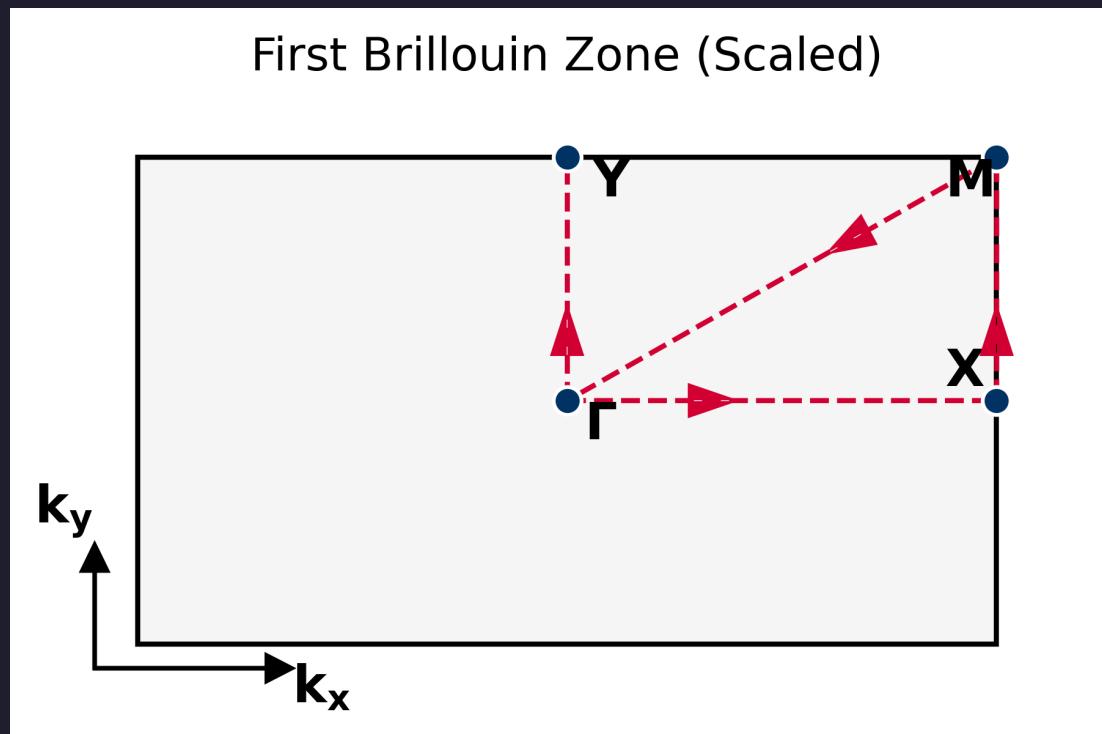
## Goal:

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.



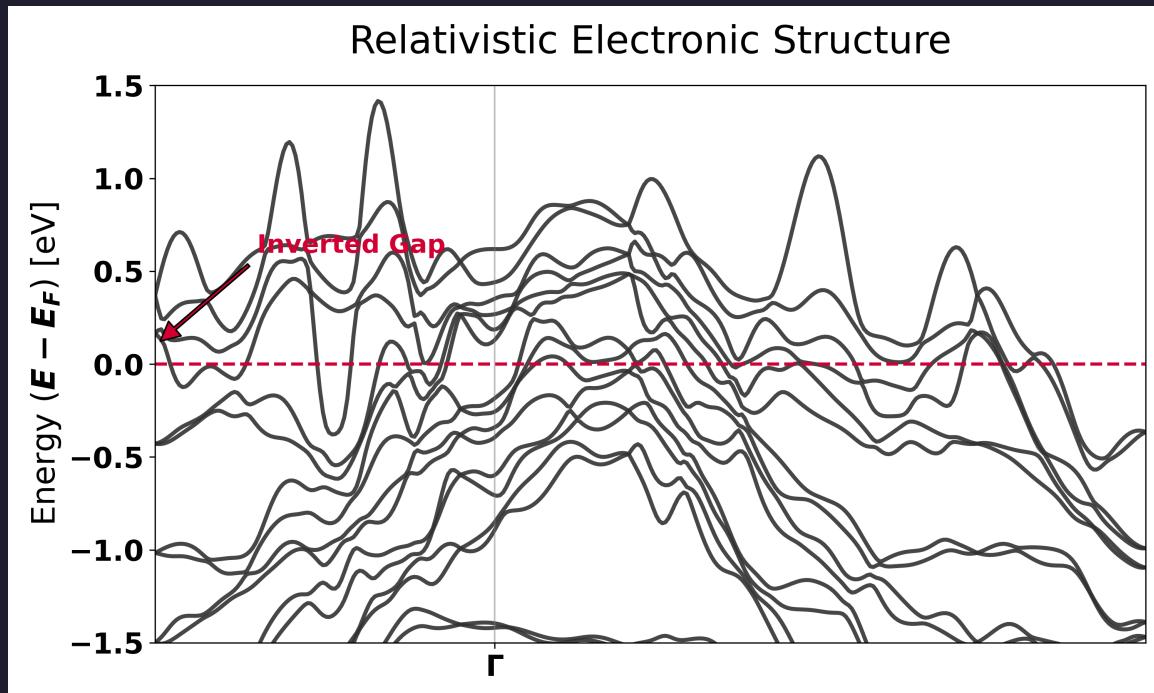
## The Path:

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

## 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



**Global Profile:**

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

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

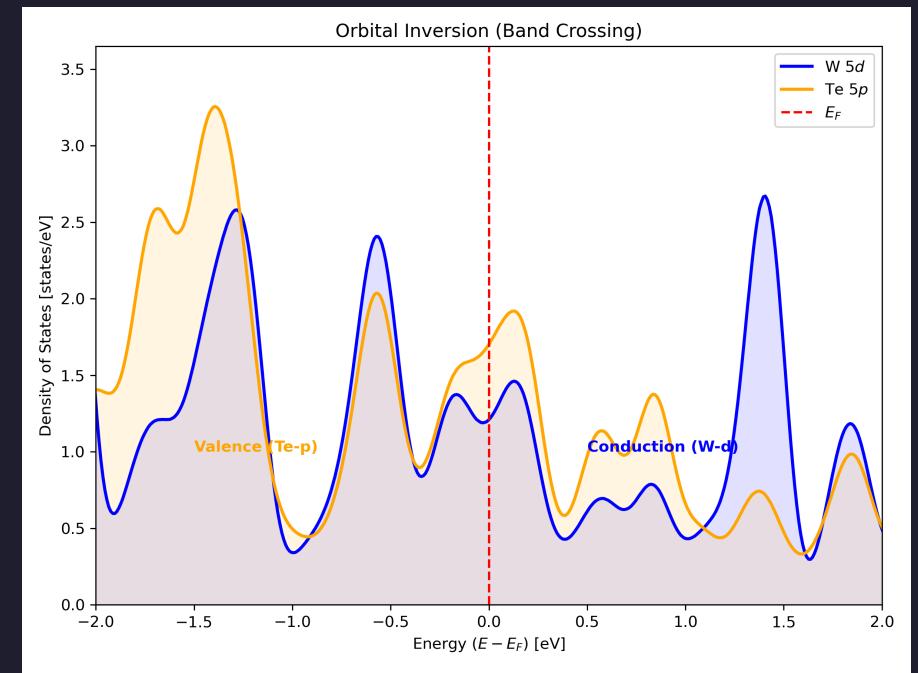
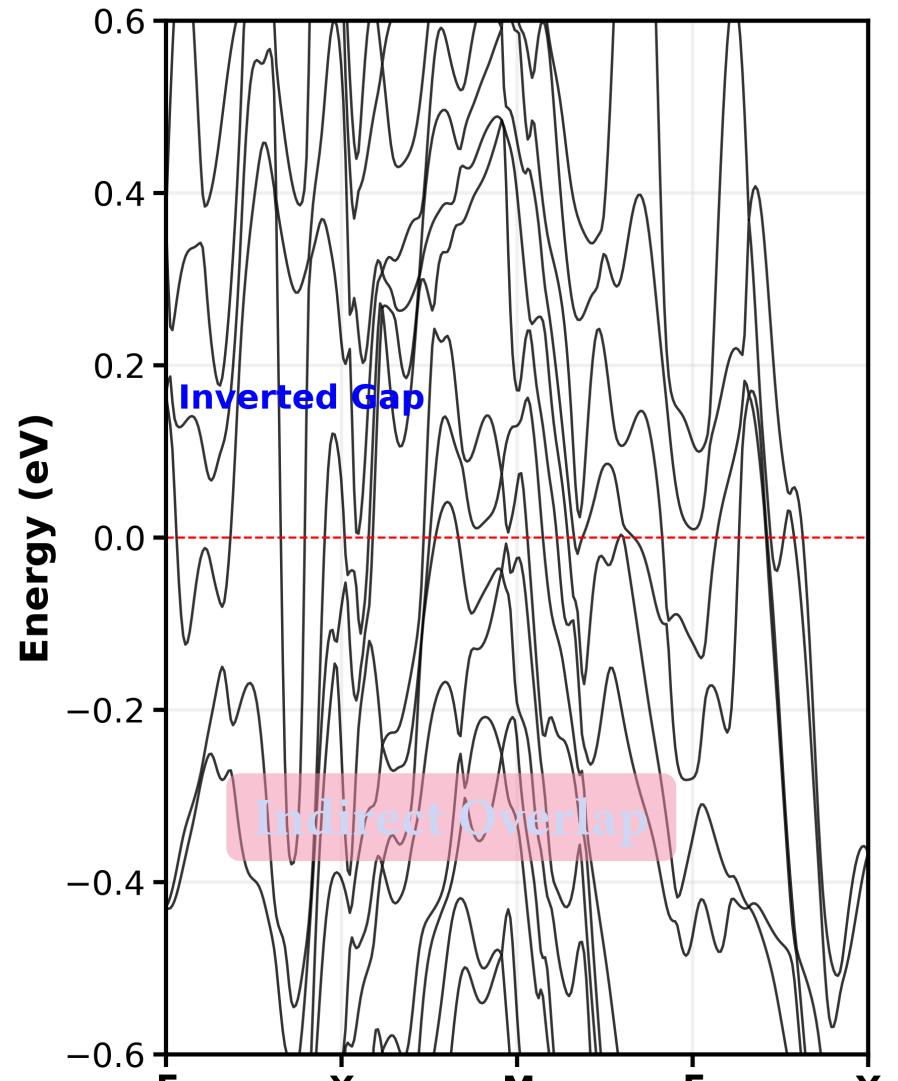


Figure 1: Zoom at  $\Gamma$ : Parity Exchange

# A Complication: The Semimetallic Ground State

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## 2) W<sub>2</sub>C Band Structure (PBE+SC)



### 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.

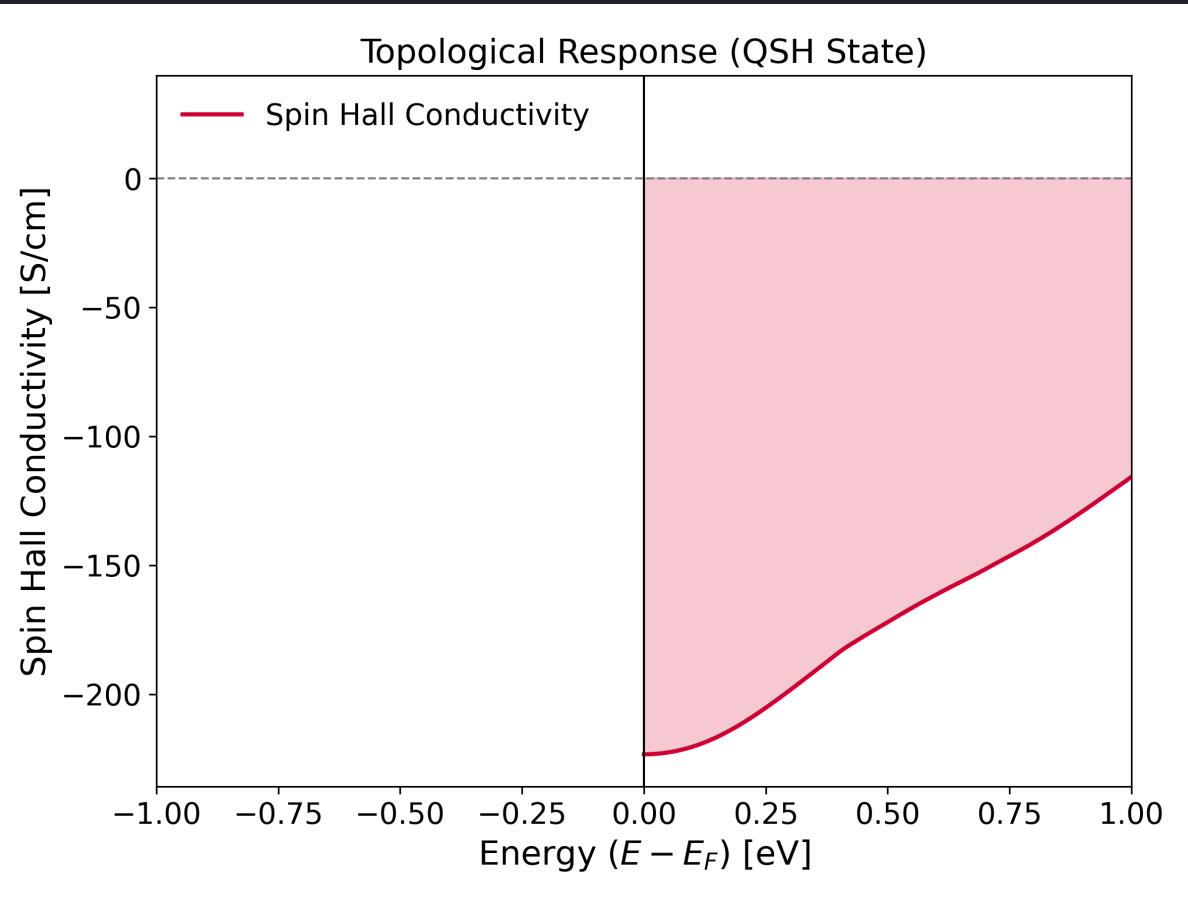
### The Crucial Insight:

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:**

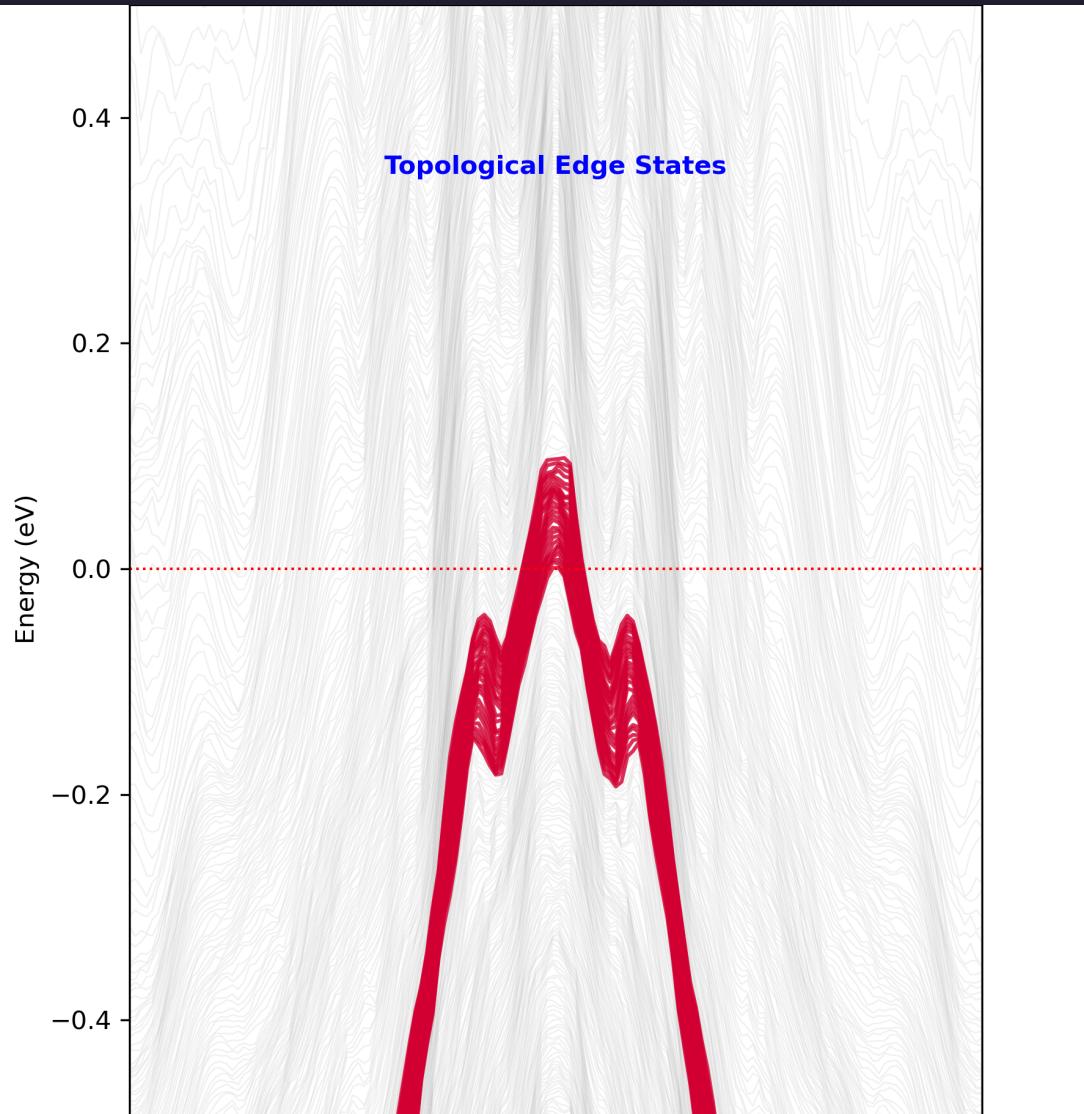
This quantization is the hallmark of the Quantum Spin Hall (QSH) state, protected

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:**

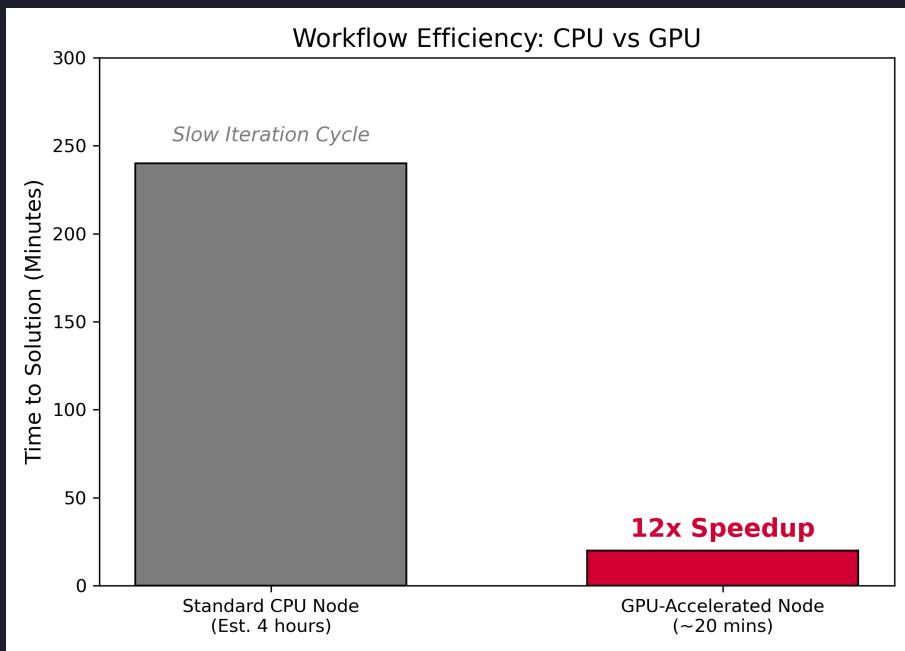
Helical edge states (Red) traverse the bulk gap, connecting valence and conduction bands.

**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)

