

A Quantum ESPRESSO Recipe for Z_2 Invariant of 2D Topological Material 1T'-WTe₂

Shahriar Pollob^{1,*}, Apu Das², Mohammad Dilwar Ali Alvee³, M. Shahnoor Rahman⁴

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.

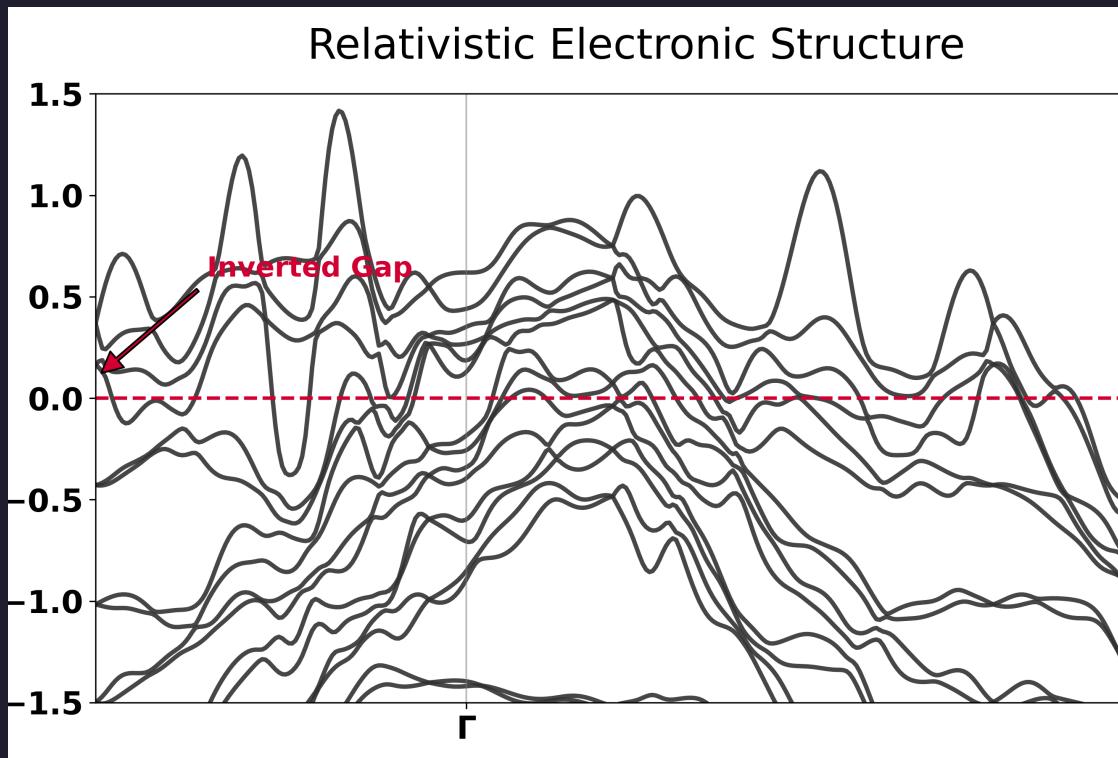
The Solution:

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.”

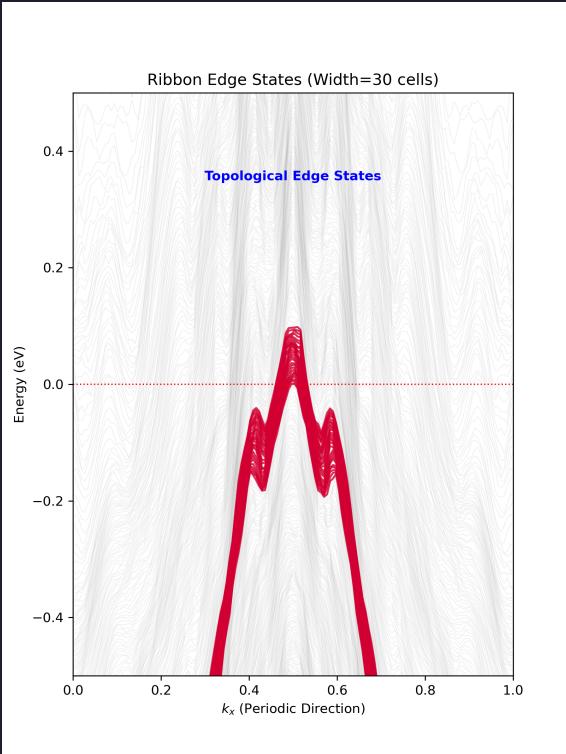
Electronic Structure: Band Inversion



Key Features:

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

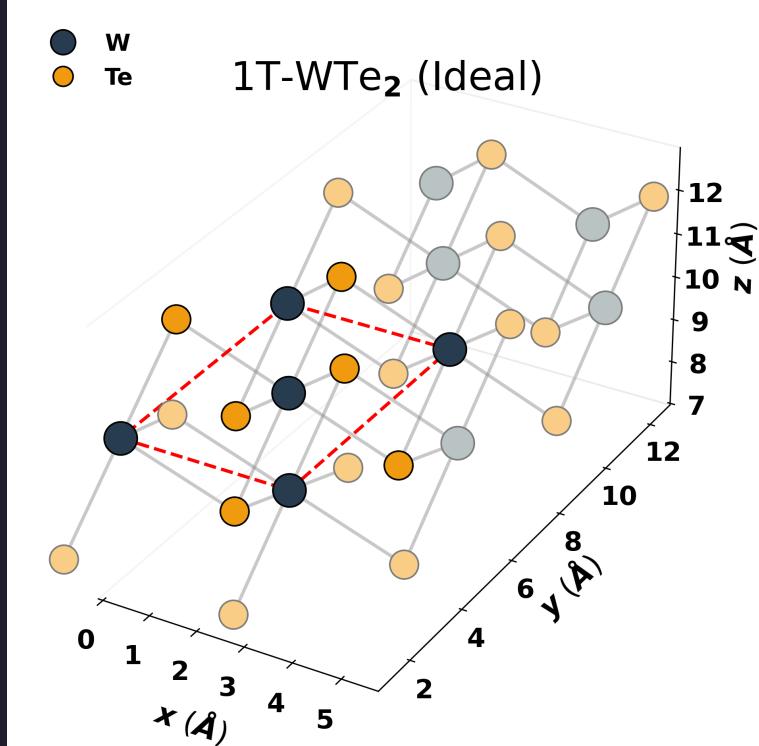
The Definitive Evidence: Edge States



Topological Protection:

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

Crystal Structure: The Ideal $1T$ Phase



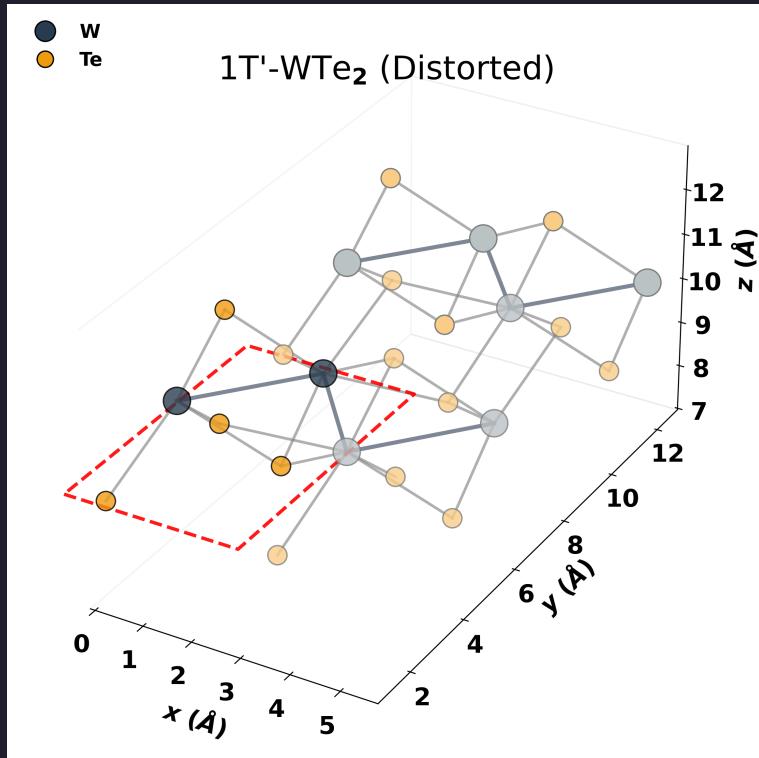
The “Parent” Structure:

- **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 $1T'$ -WTe₂ Phase



The “Real” Structure:

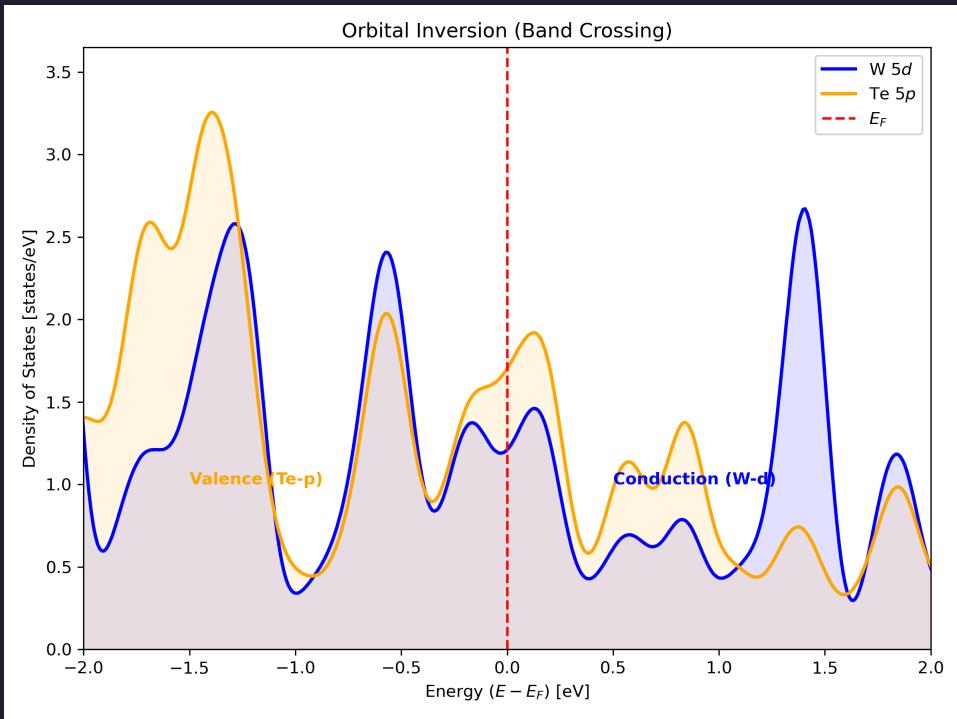
- **Symmetry:** Distorted (Peierls Instability).
- **Action:** W atoms dimerize along one axis.

The Magic:

- **Stable:** Energetically favorable.
- **Insulating:** Gap opens ($E_g > 0$).

- **Topological:** Inverted Band Order ($Z_2 = 1$).

The Mechanism: SOC-Driven Band Inversion



Orbital Physics:

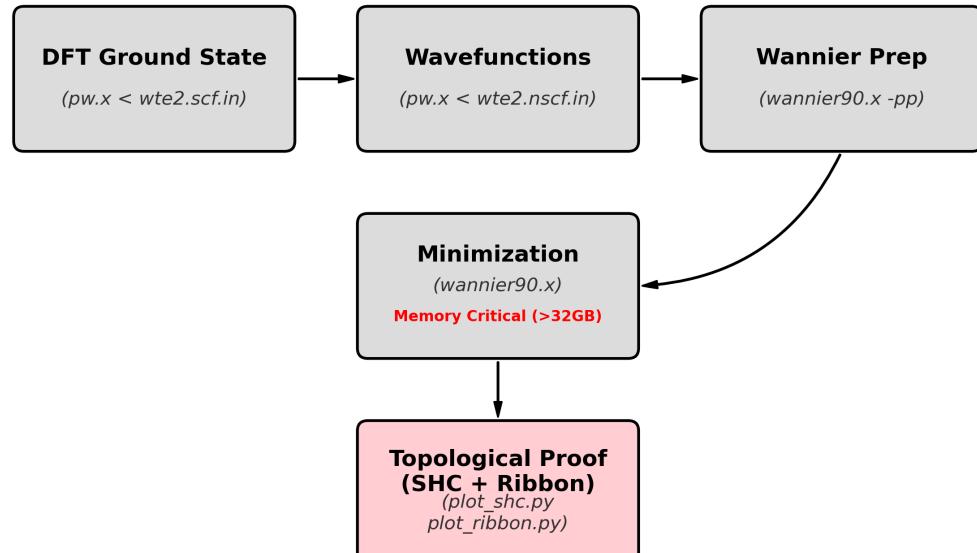
1. **Crystal Field:** Splits W-*d* orbitals.
2. **Spin-Orbit Coupling (SOC):** The heavy Tungsten core drives a relativistic energy shift.

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

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

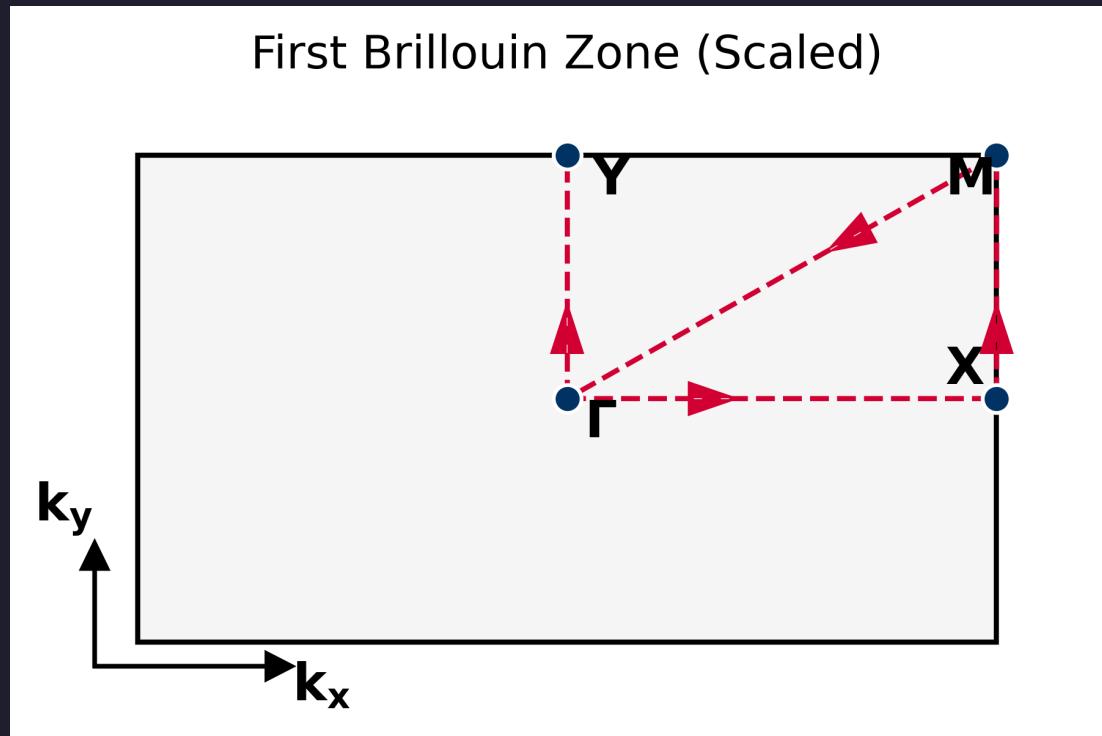
Goal:

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.



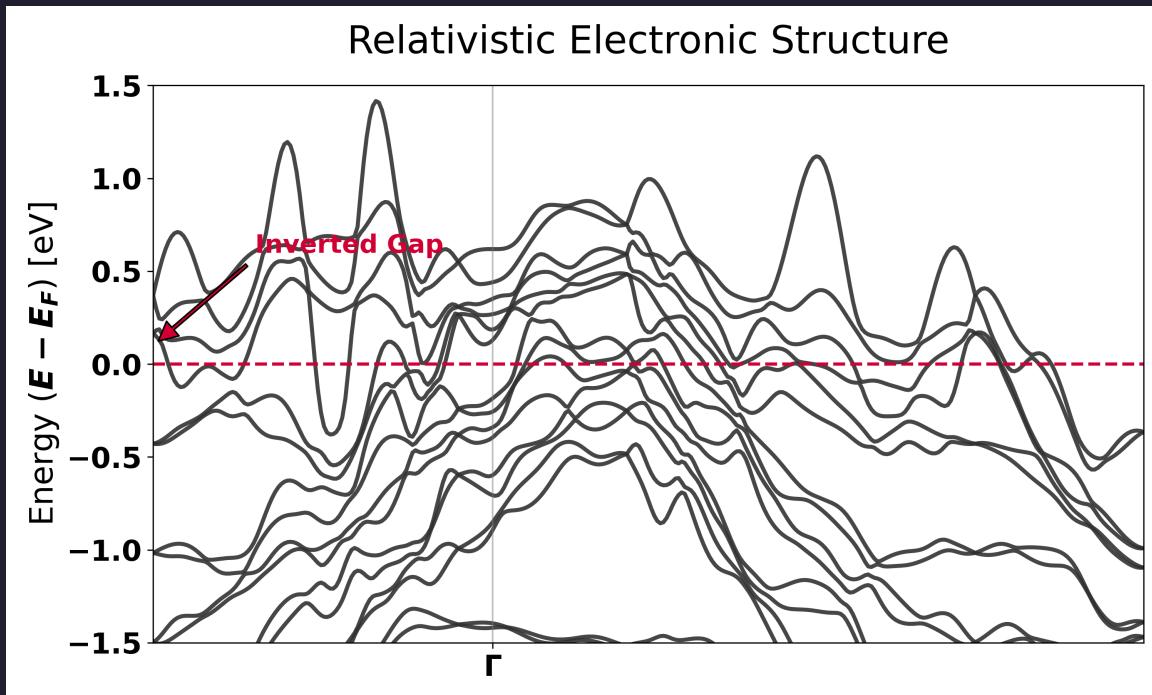
The Path:

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

Significance:

- The fundamental gap opens at Γ .
- 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 Γ .

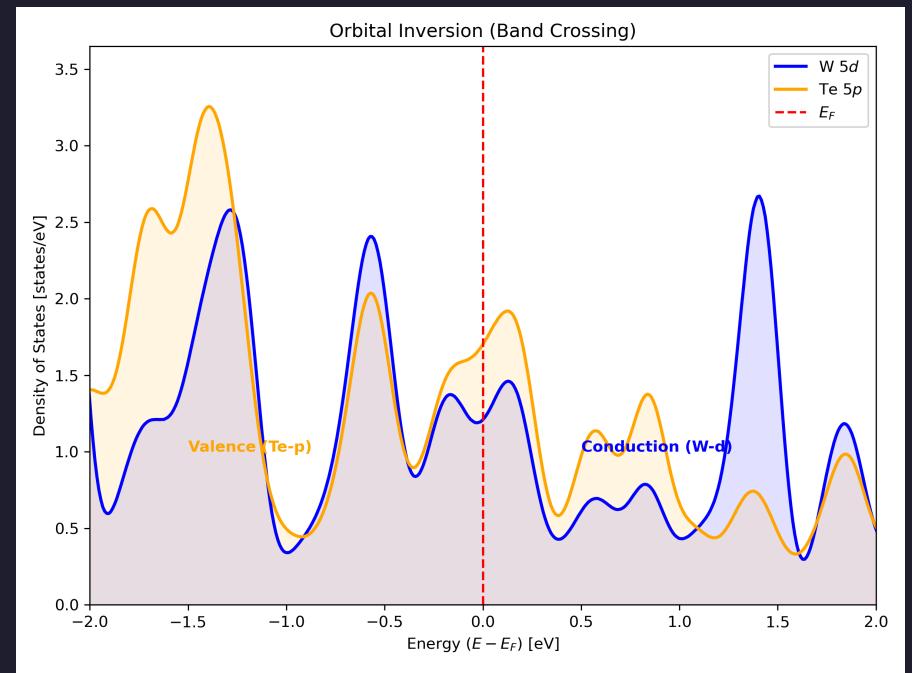
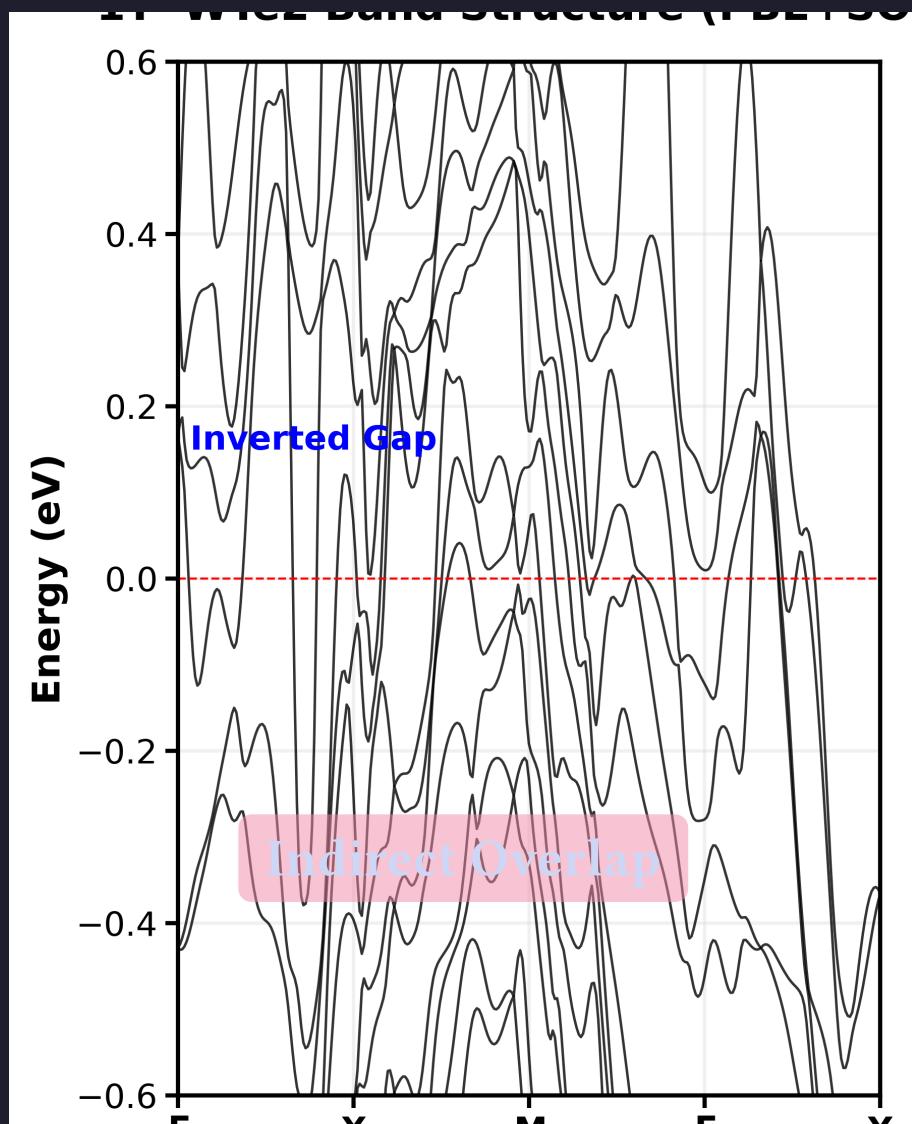


Figure 1: Zoom at Γ : Parity Exchange

A Complication: The Semimetallic Ground State



The Observation:

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

The Explanation:

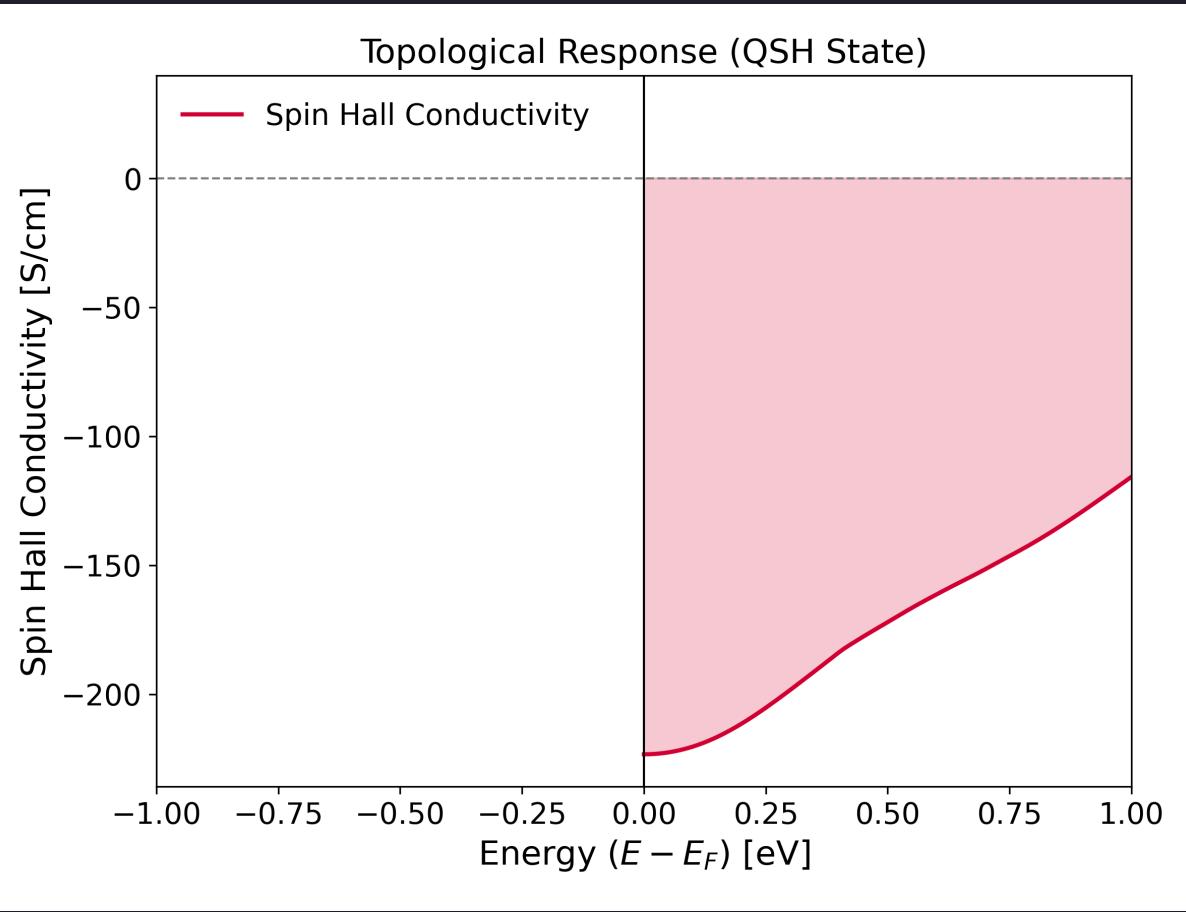
PBE functionals notoriously underestimate gaps.

The Crucial Insight:

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

Definitive Evidence I: Quantized Transport

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:

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

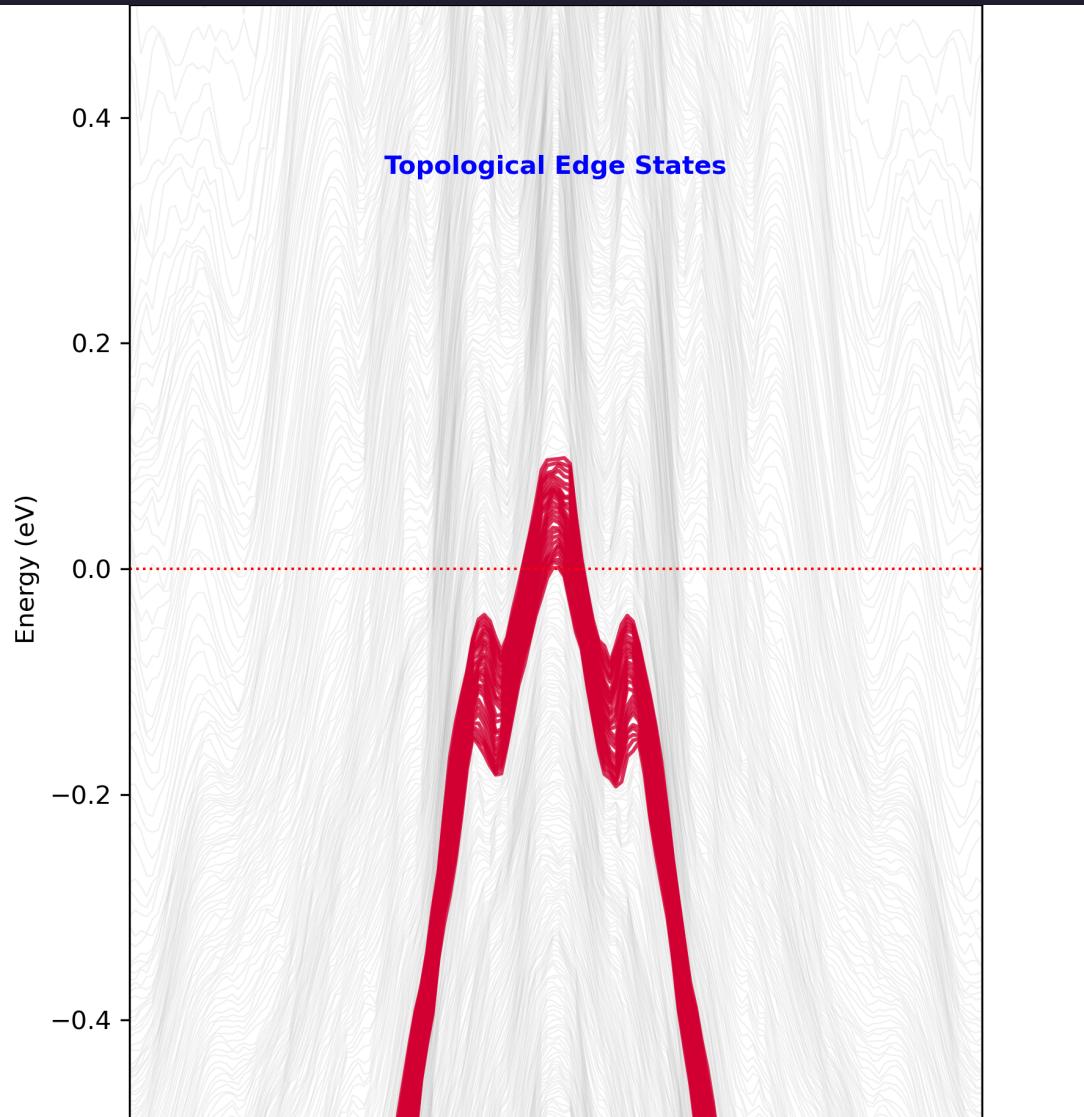
Implication:

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

against non-magnetic perturbations.

Definitive Evidence II: Visualizing Edge Highways

Bulk-Boundary Correspondence guarantees conductive states at the interface.



Calculation:

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

Observation:

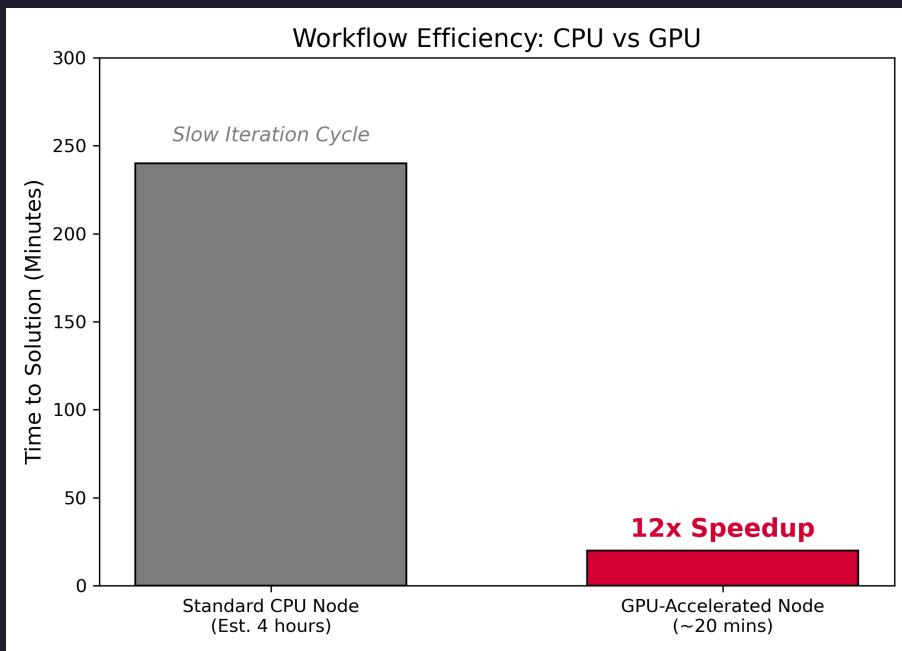
Helical edge states (Red) traverse the bulk gap, connecting valence and conduction bands.

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

Our “Recipe” successfully characterizes 1T'-WTe₂.

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'-WTe₂ 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)

