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

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Motivation: The Quest for Dissipationless Electronics

The Bottleneck:

Modern electronics suffer from Joule heating and backscattering limits.

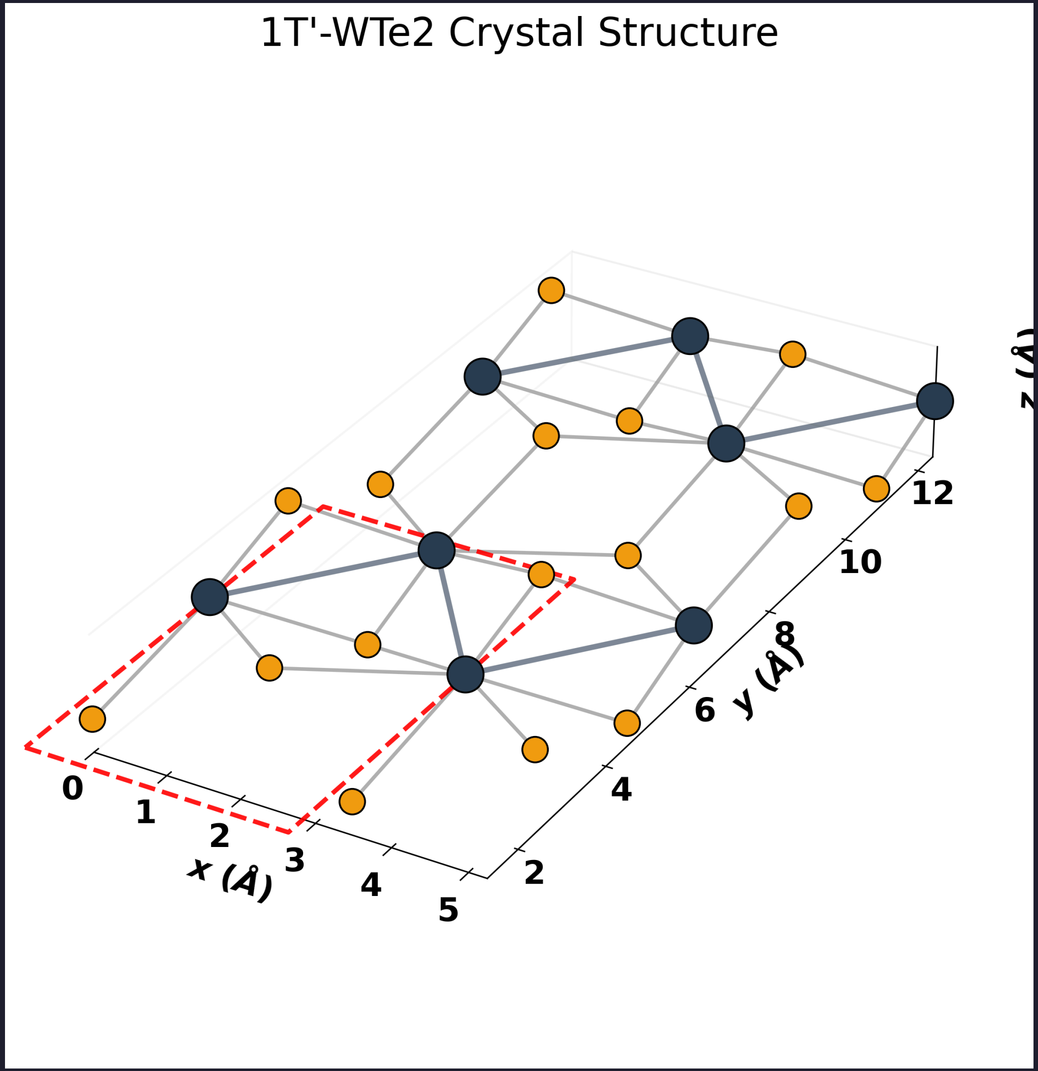
The Solution:

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."

The Material: $1T'$-WTe_2 Structure

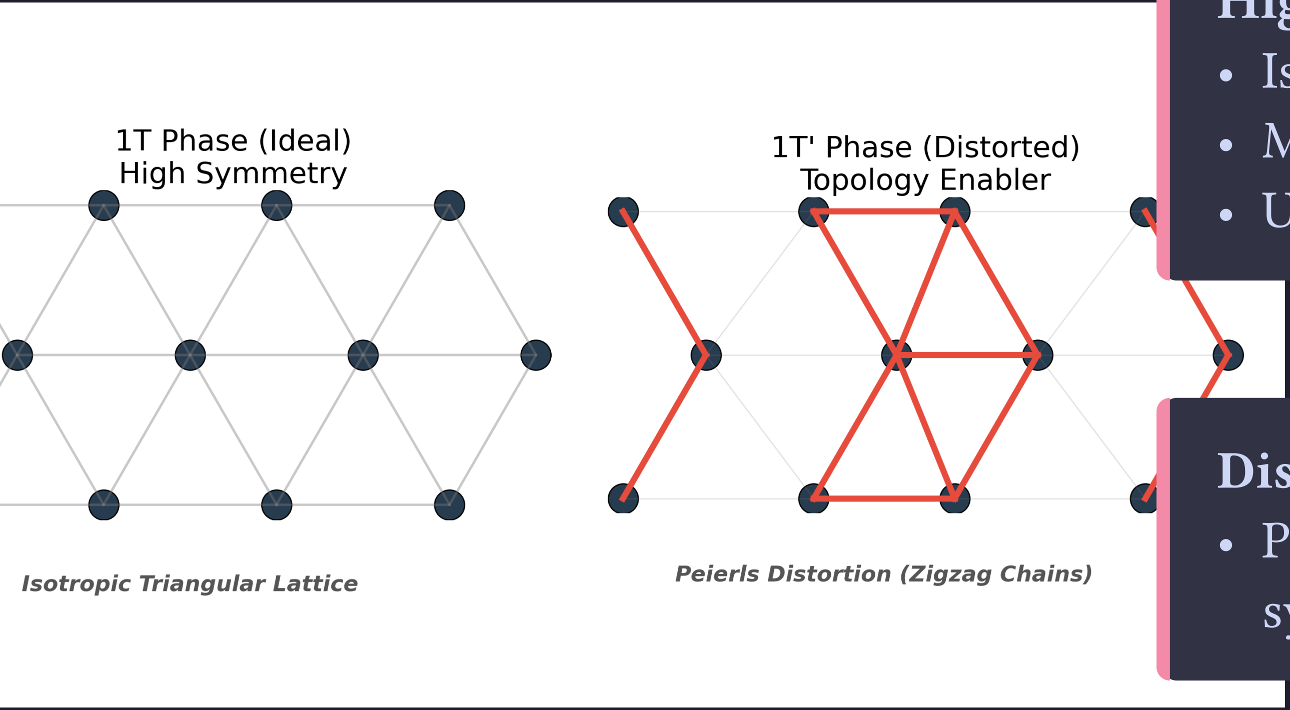


Crystal Symmetry:
Distorted Octahedral ($1T'$) phase.

Key Features:

- **Buckled Layers:** Atoms are not planar, creating local electric fields.
- **Zigzag Chains:** Tungsten (W) atoms form 1D chains along the a-axis.
- **Anisotropy:** distinct a and b lattice constants ($a \approx 3.49, b \approx 6.33$).

The Distinction: $1T$ vs $1T'$ Phase



High Symmetry ($1T$)

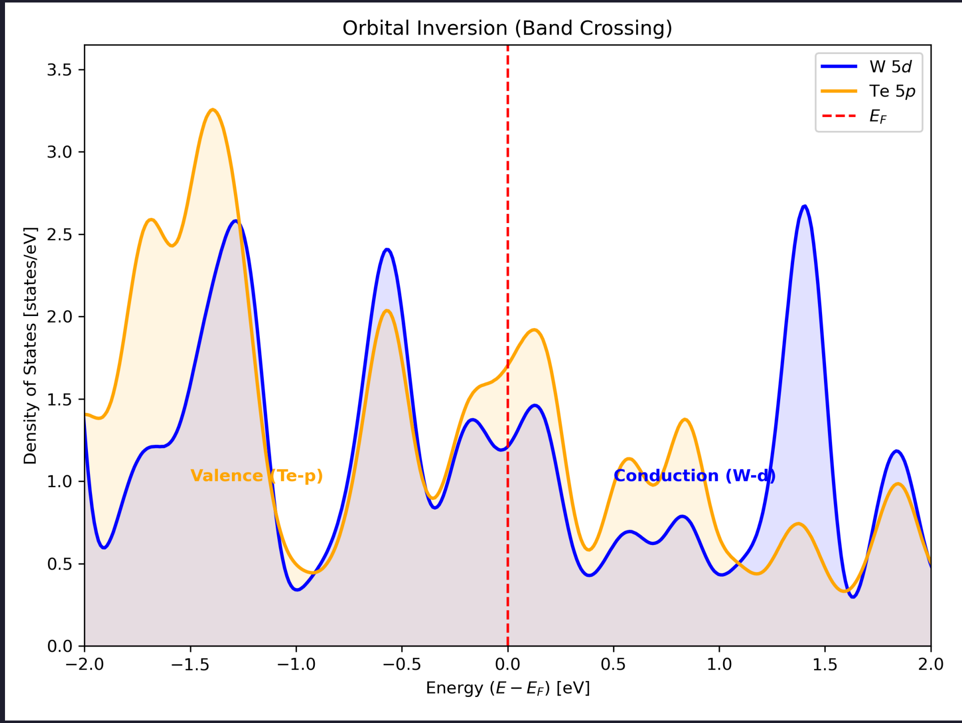
- Isotropic Triangular Lattice.
- Metallic or Trivial Insulator.
- Unstable in WTe_2.

Distorted ($1T'$)

- Peierls Instability: Spontaneous symmetry breaking.

- Zigzag Chains: Formation of W-W dimers (Red lines).
- Topology: This distortion, combined with SOC, inverts the bands.

The Mechanism: SOC-Driven Band Inversion



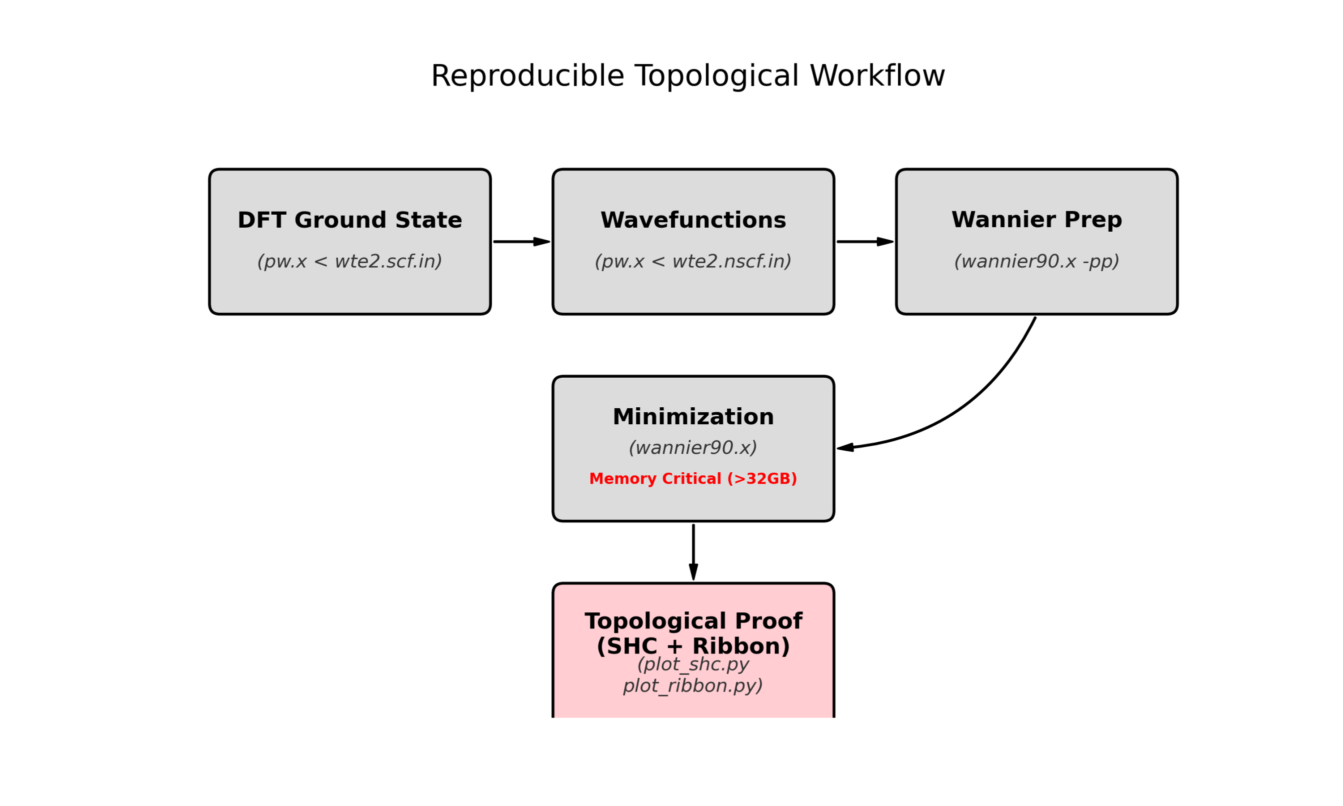
Orbital Physics:

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.



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

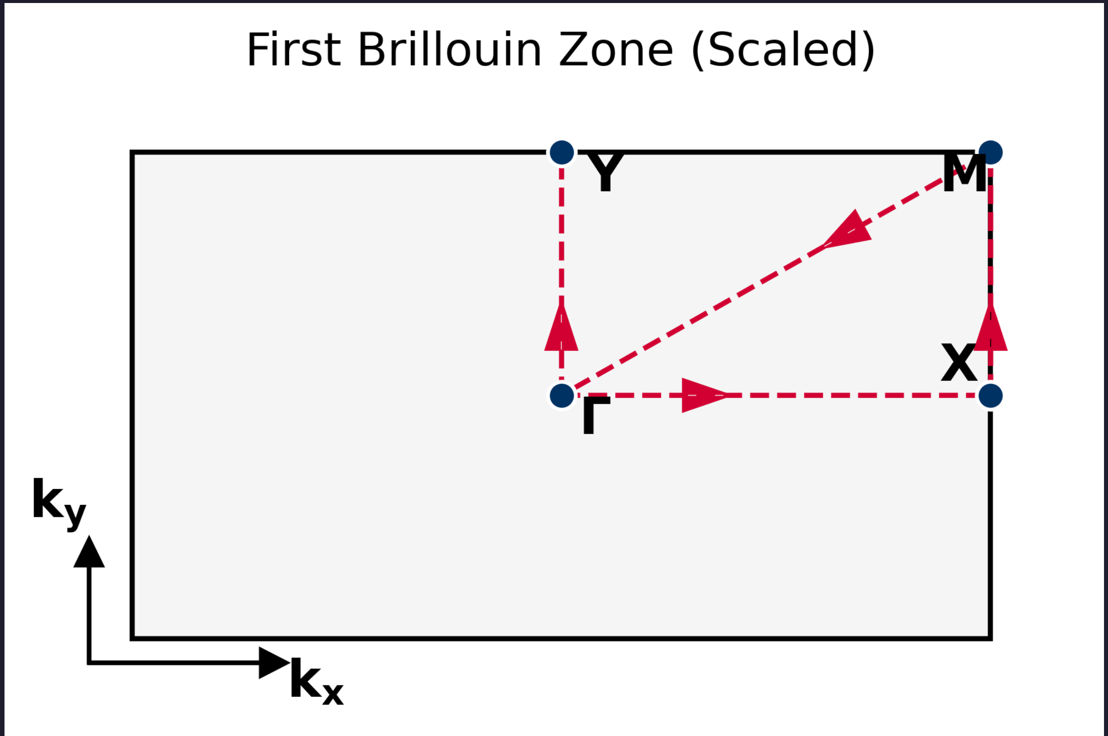
Goal:

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.



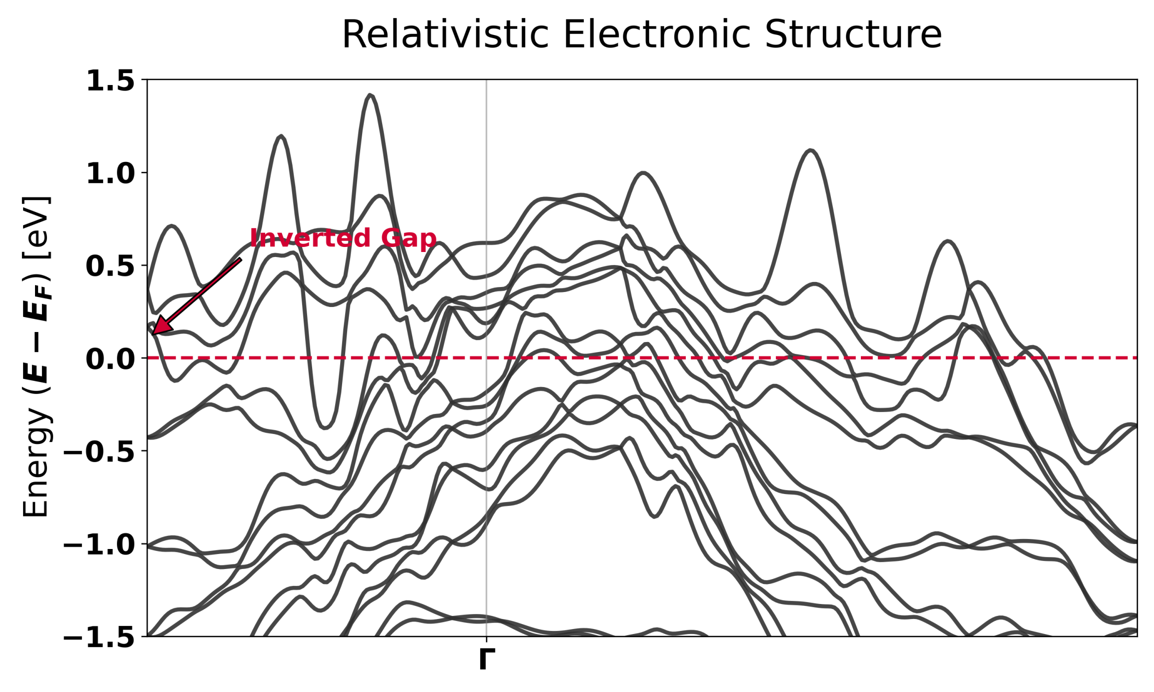
The Path:

$\Gamma \to X \to M \to \Gamma \to Y$

Significance:

- The fundamental gap opens at Γ.
- The $M \to \Gamma$ 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 Γ.

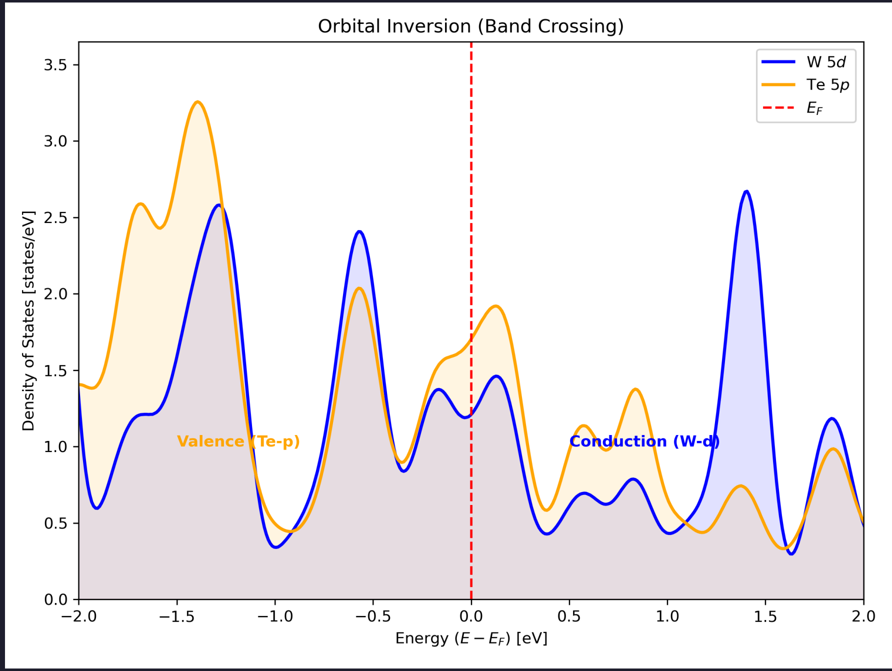
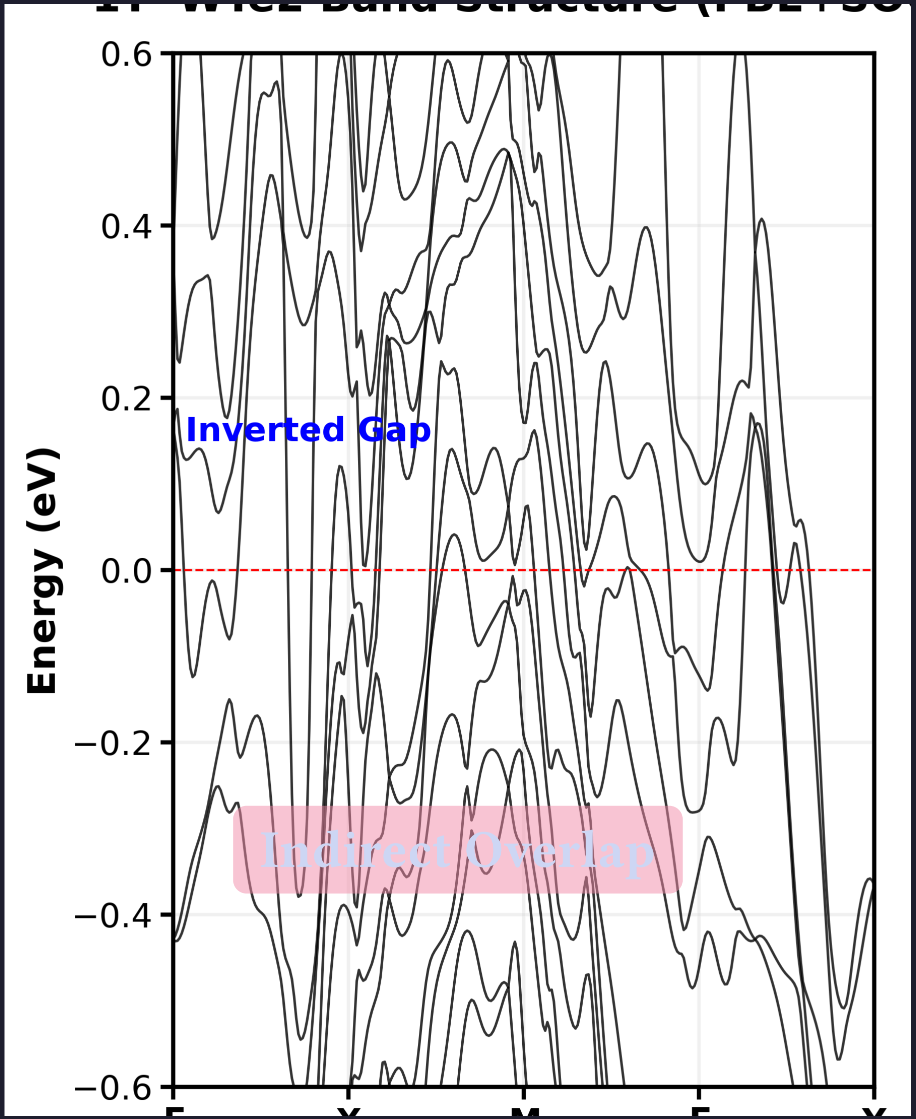


Figure 1: Zoom at Γ: Parity Exchange

A Complication: The Semimetallic Ground State



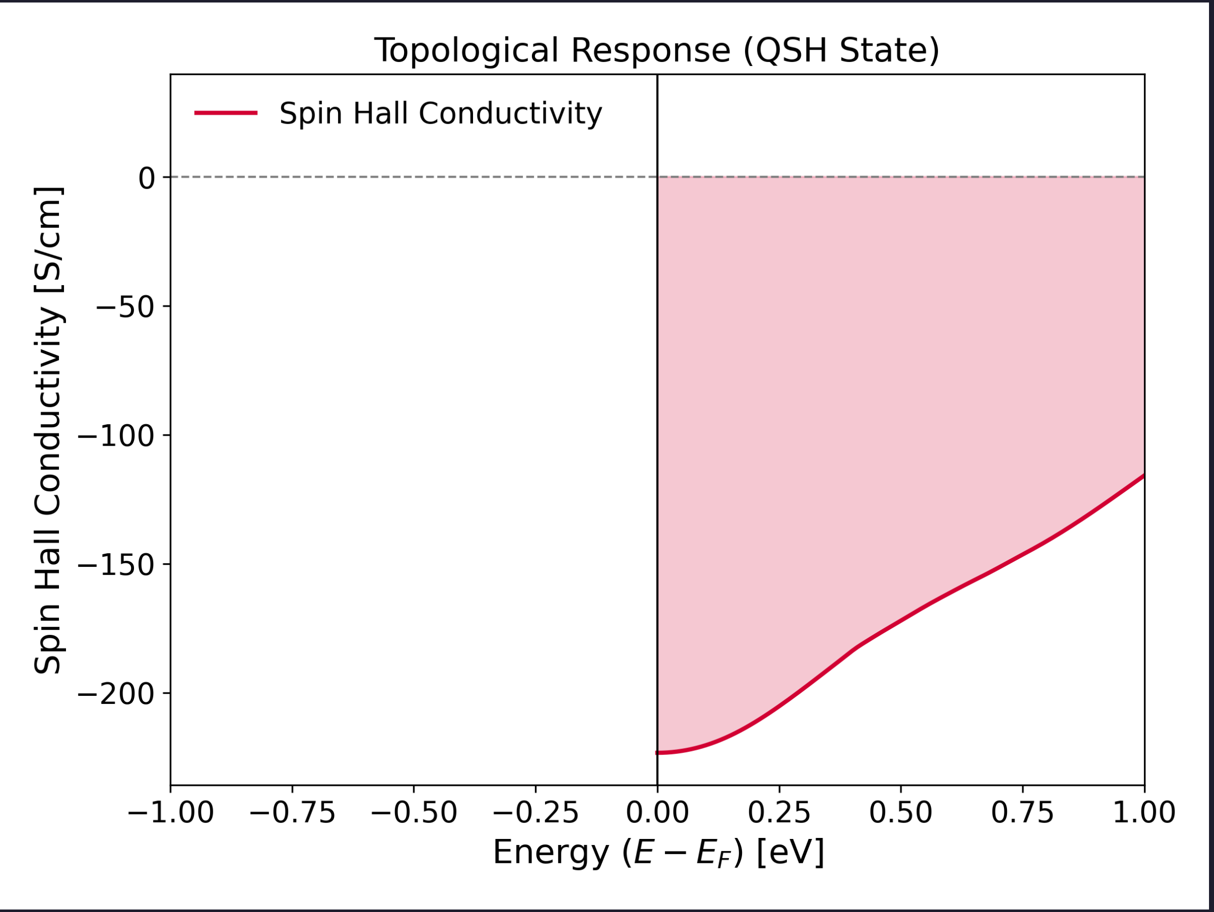
The Observation:
The Conduction Band Minimum (CBM) dips below the Valence Band Maximum (VBM) at different k-points (Q vs Γ).

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

The Result:
A quantized plateau exists at exactly:

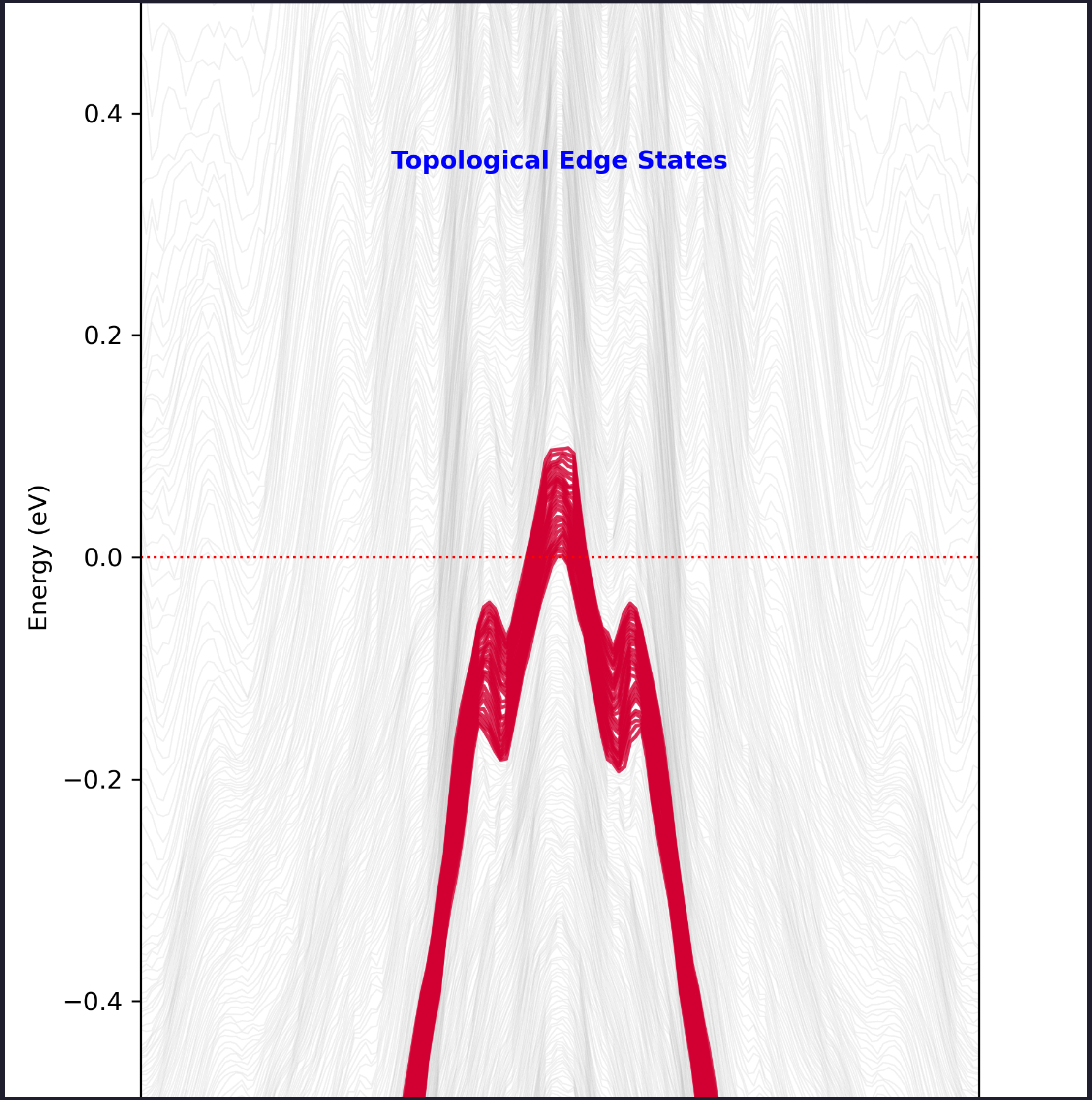
$$2\frac{e^2}{h}$$

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:

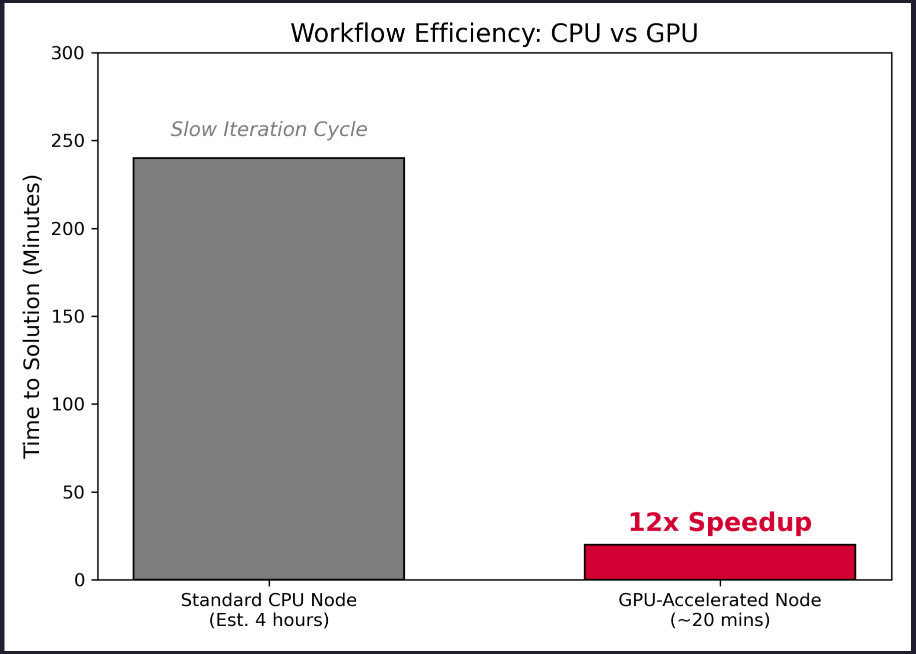
Helical edge states (Red) traverse the bulk gap, connecting valence and conduction bands.

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′-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/Quantum-ESPRESSO-WTe2-Topology

Release:

`v1.0-ICAP2025` (Verified Artifact)