A Quantum ESPRESSO Recipe for Z_2 Invariant of 2D Topological Material 1T′-WTe_2

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ICAP 2025 | SUST

International Conference on Advances in Physics

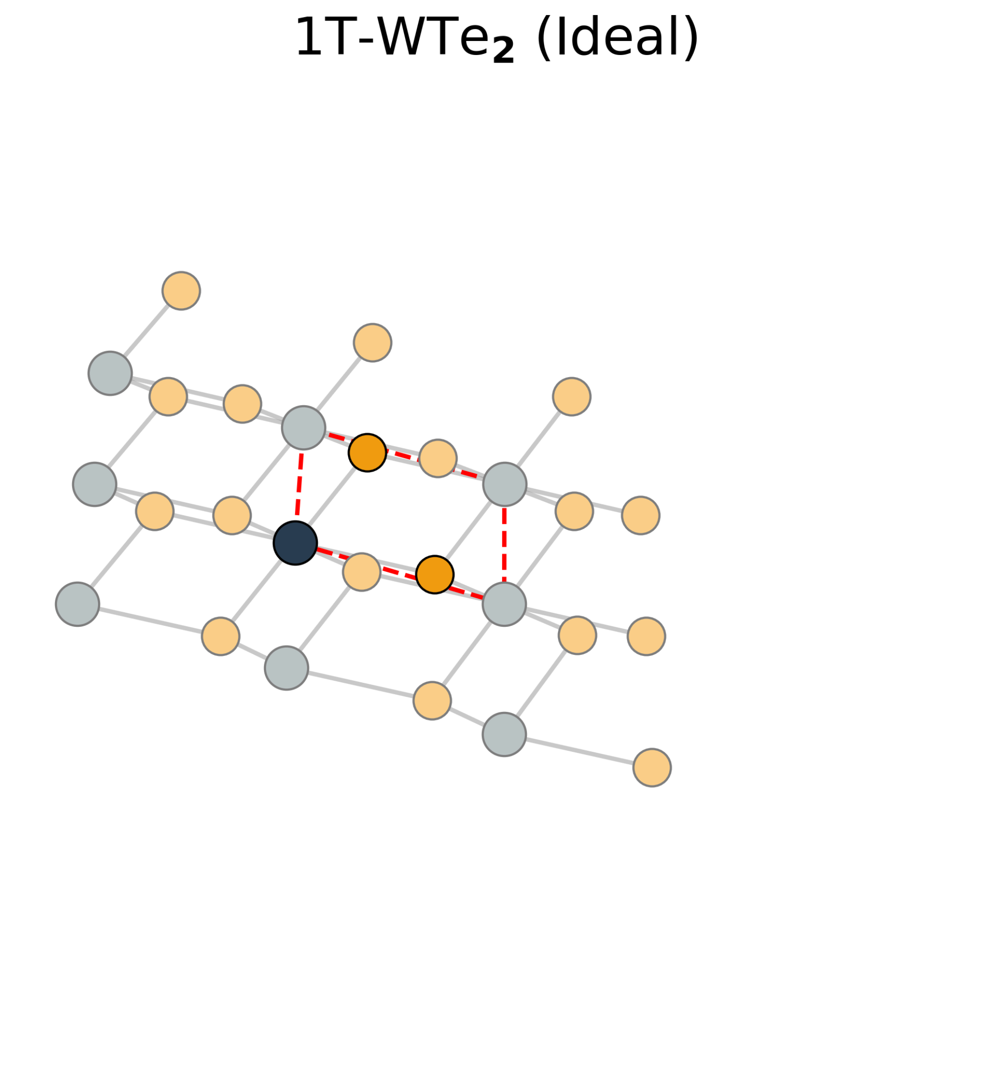
Motivation: The Quest for Dissipationless Electronics

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



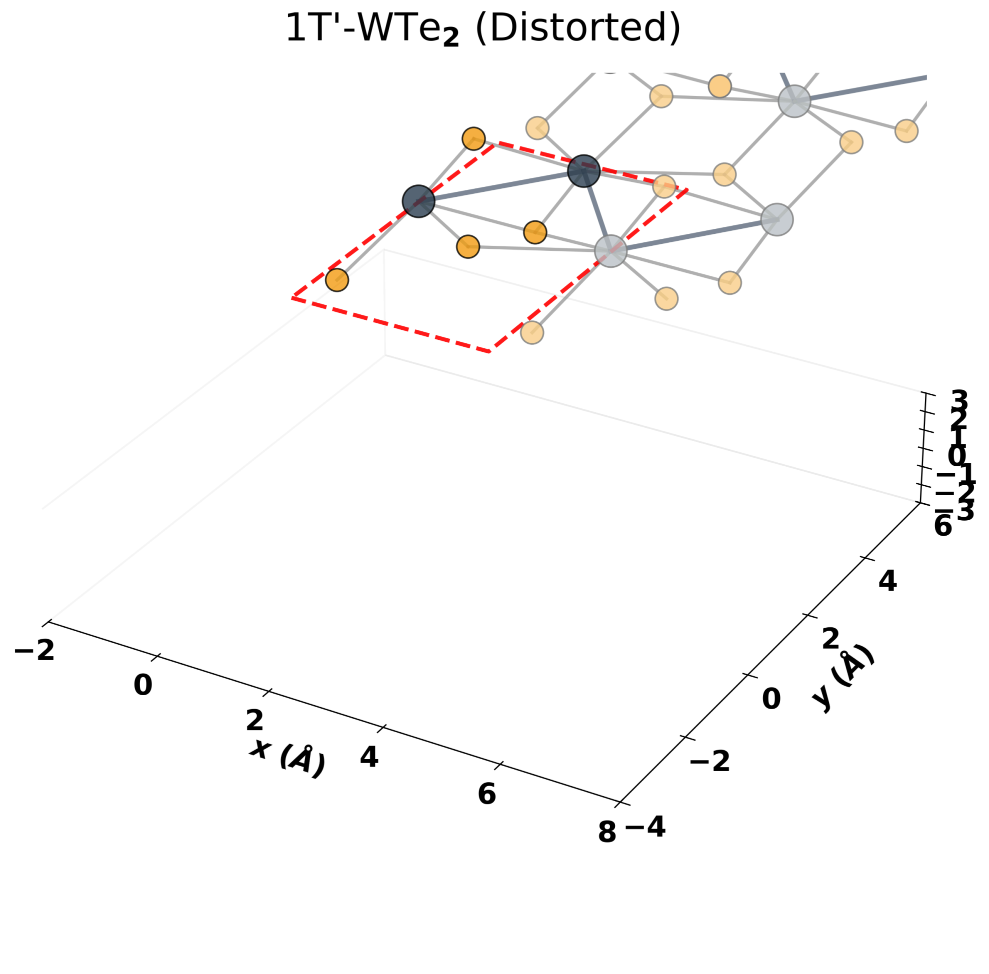
The "Parent" Structure:

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

Why it fails:

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

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



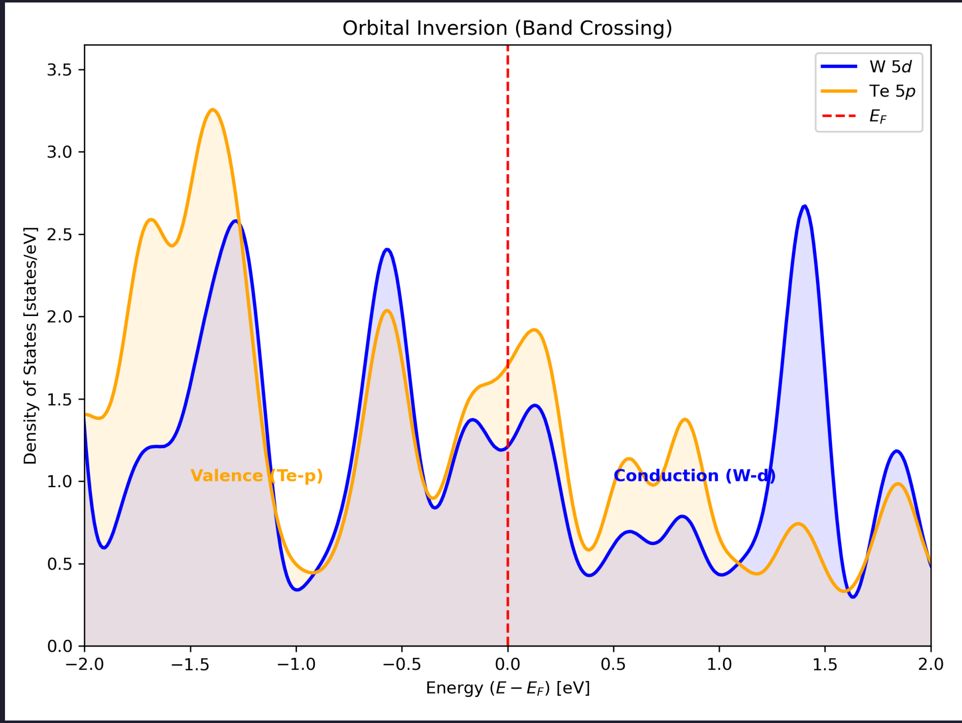
The "Actual" Structure:

- 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



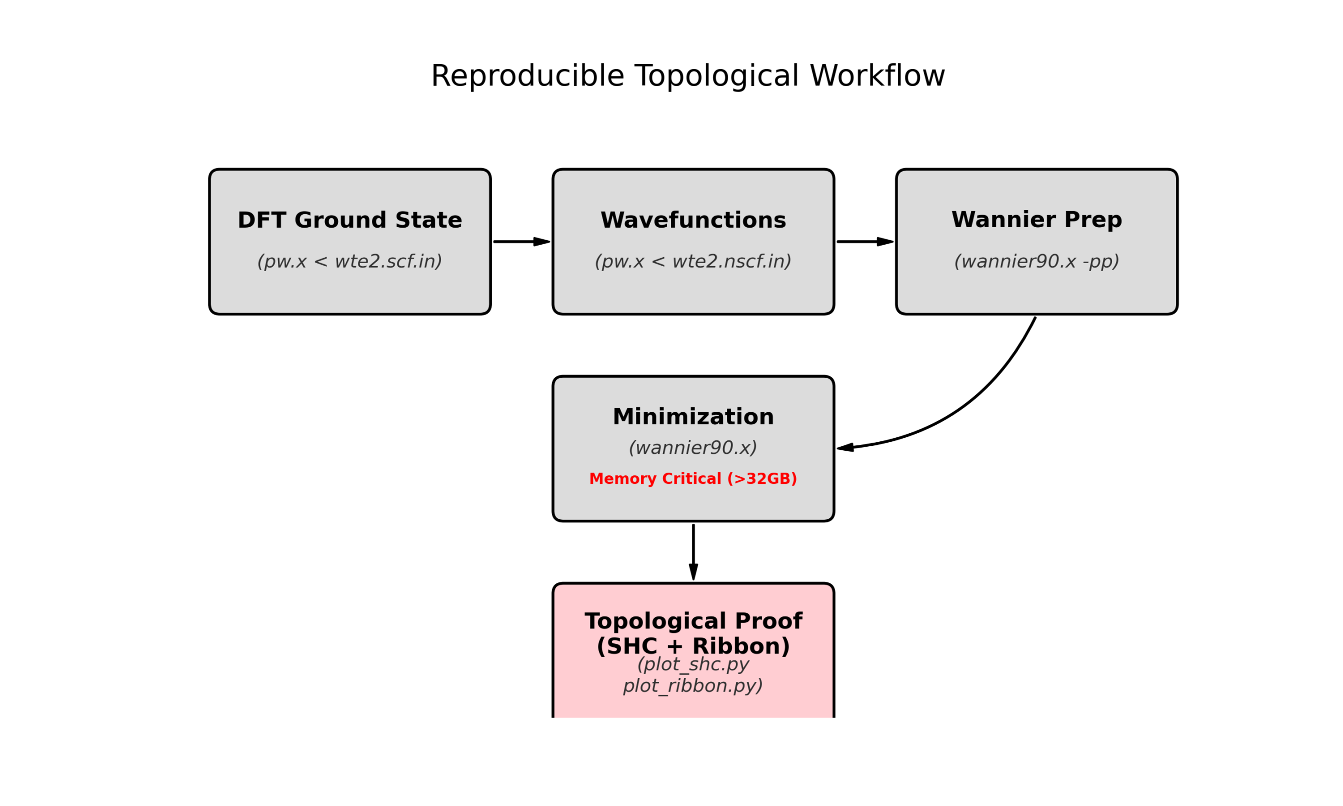
Orbital Physics:

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

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

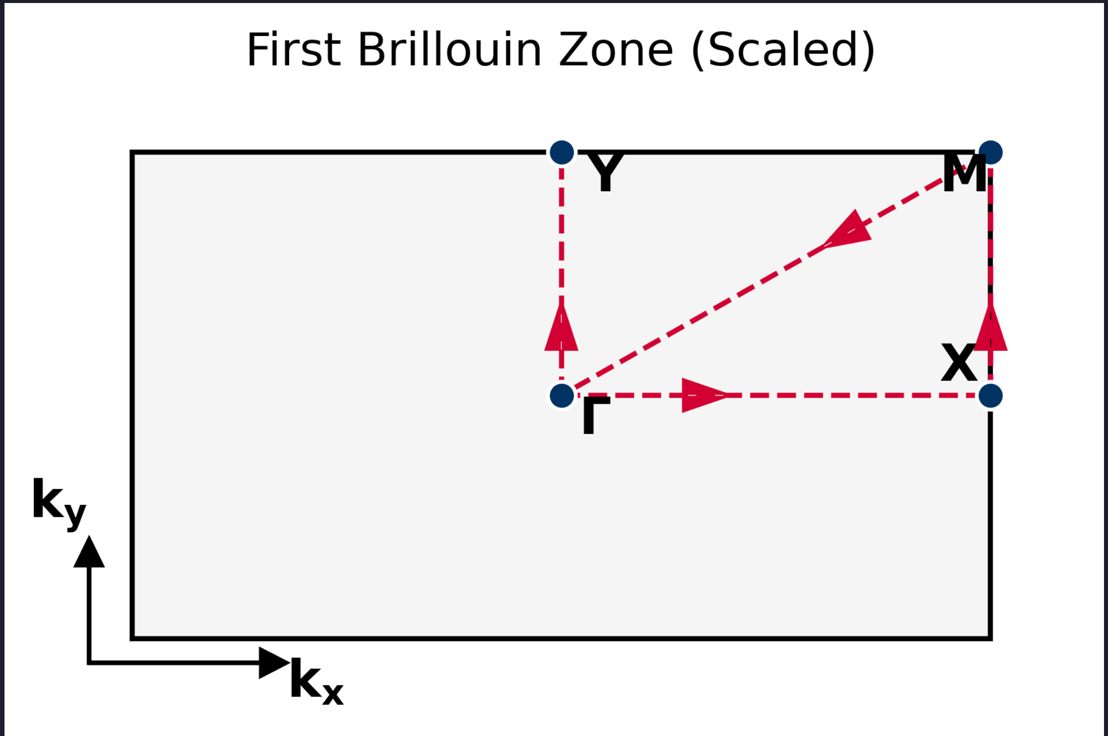
Goal:

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.



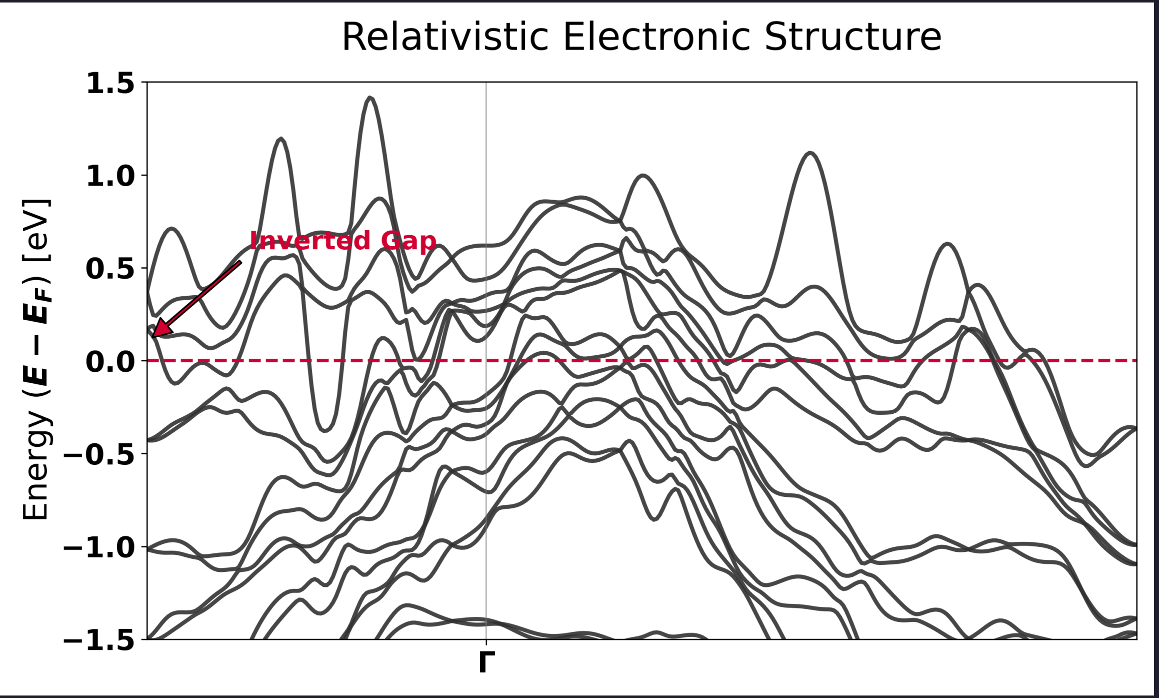
The Path:

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

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.

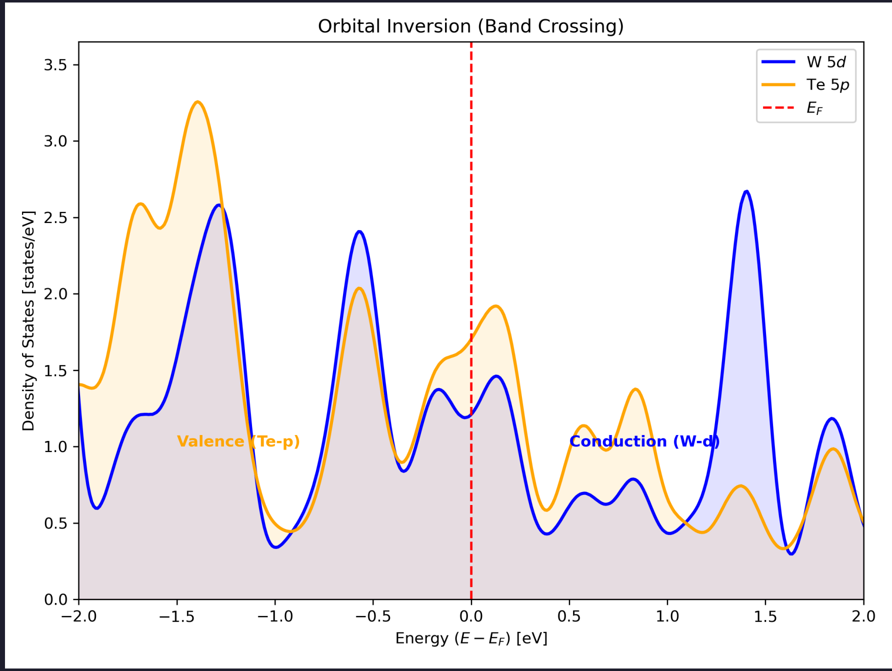
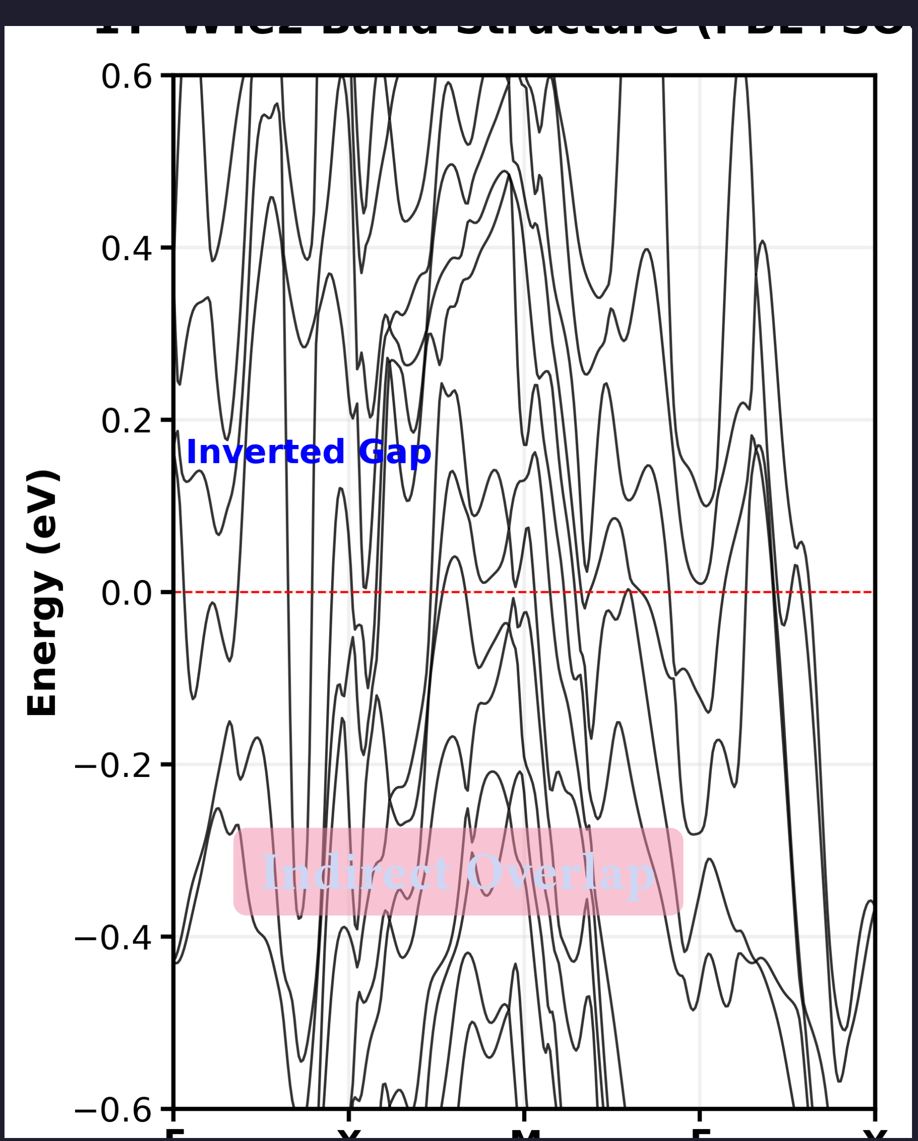


Figure 1: Zoom at Γ: Parity Exchange

A Complication: The Semimetallic Ground State



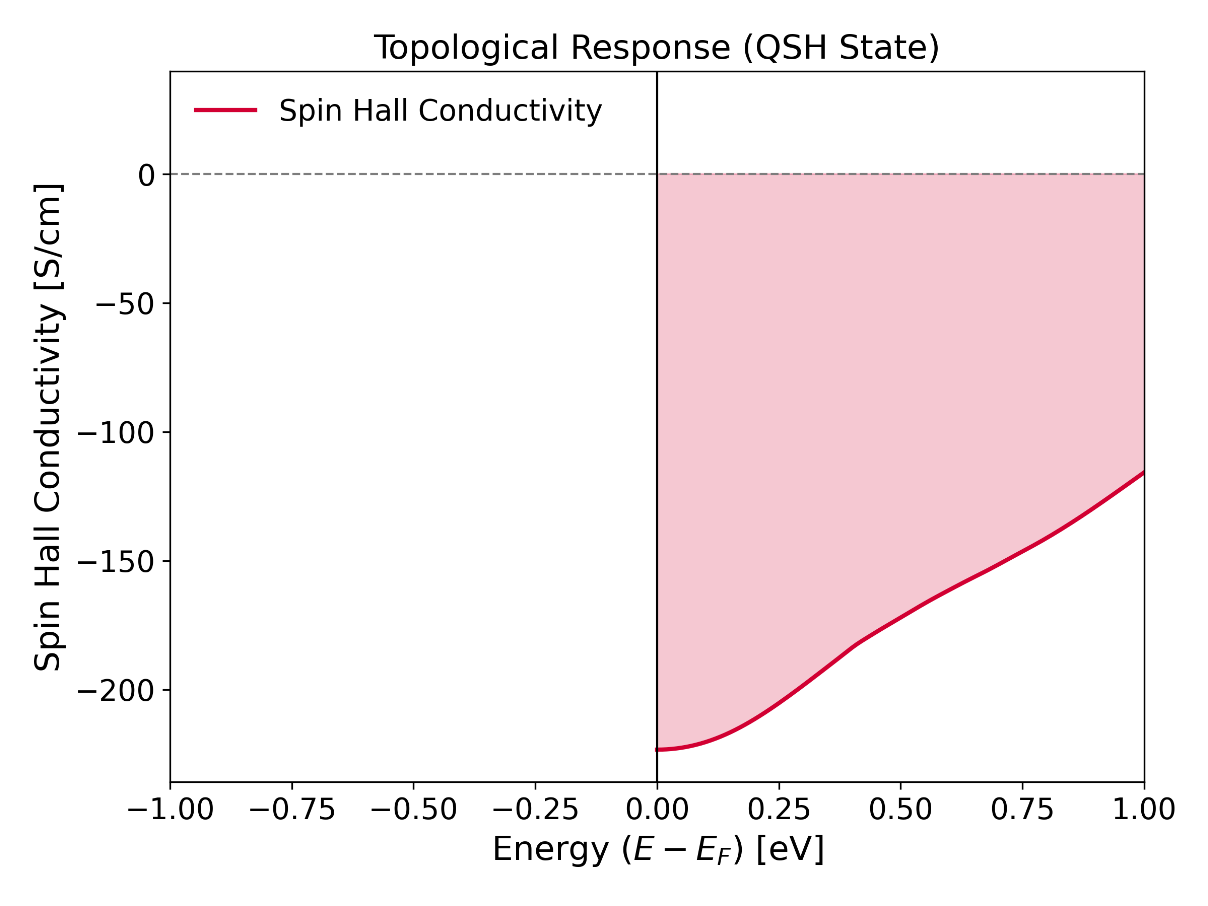
The Observation:
The Conduction Band Minimum (CBM) dips below the Valence Band Maximum (VBM) at different k-points (Q vs Γ).

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:

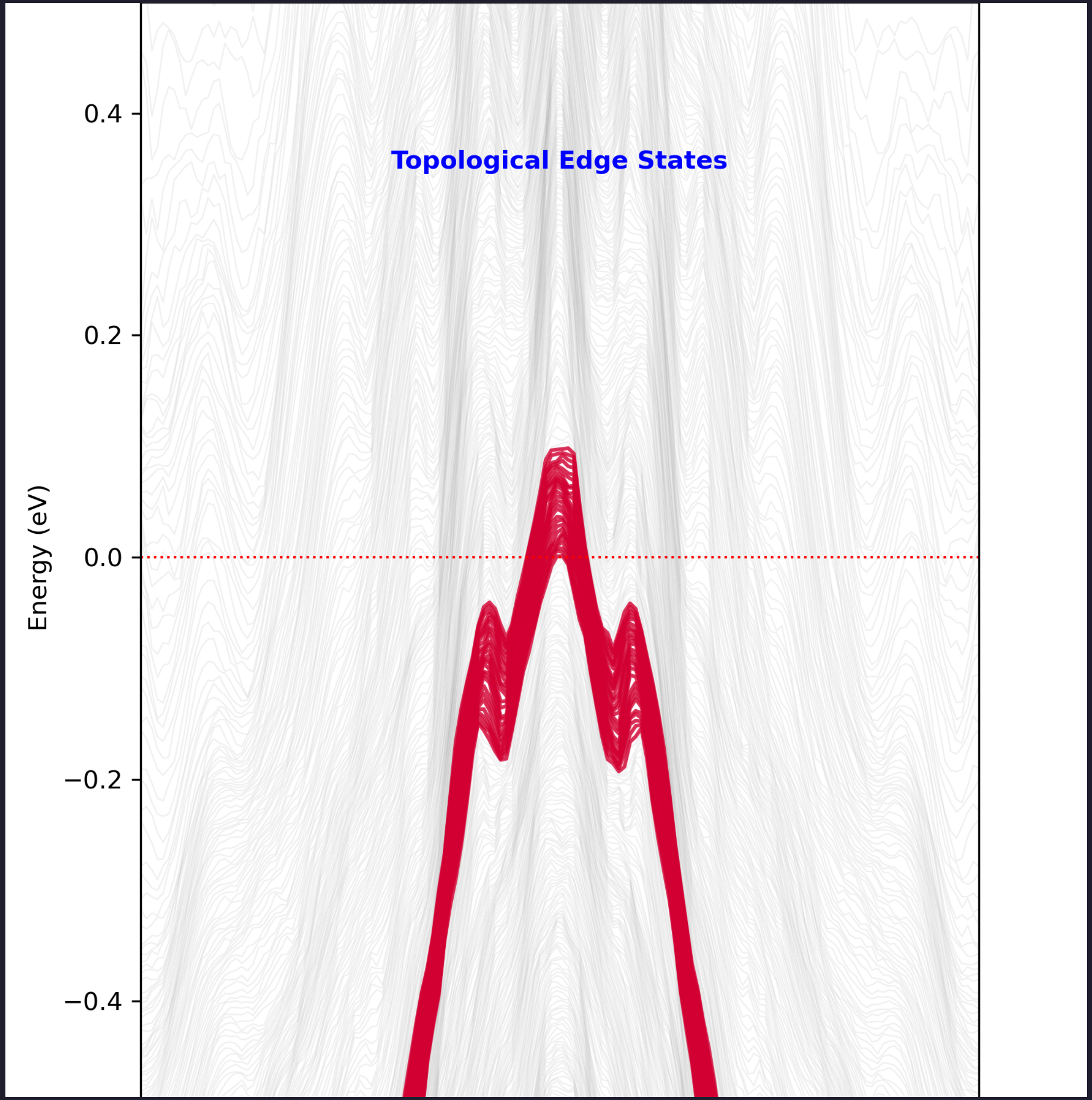
$$2\frac{e^2}{h}$$

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.



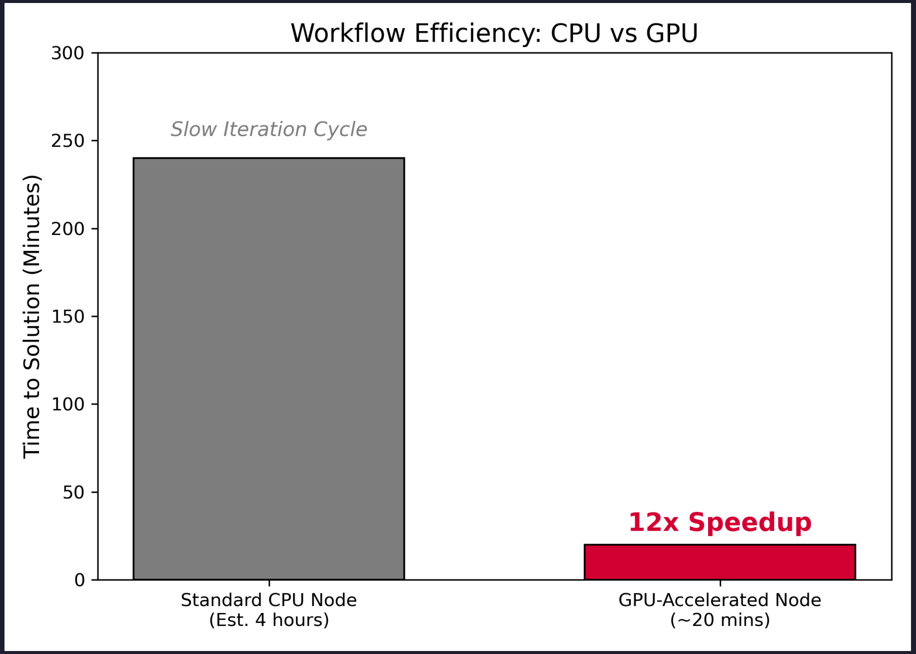
Calculation:
Wannier Hamiltonian projected onto a 30-unit-cell finite slab.

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 $< 30 Å^2$.

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)