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

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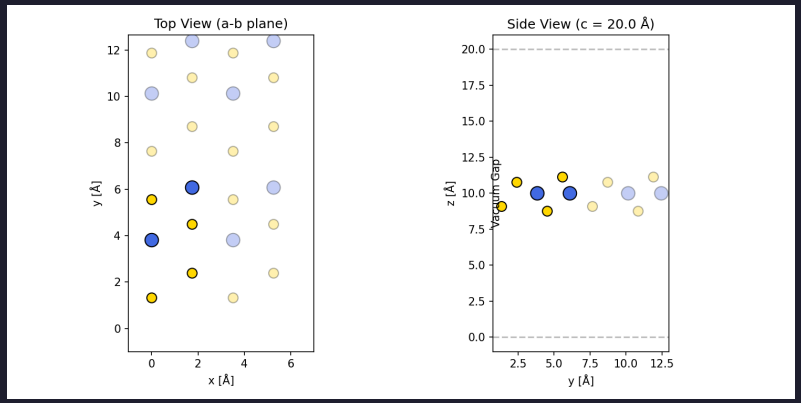
Motivation: The Reproducibility Gap

The Problem: Obtaining topological invariants (Z_2) from standard DFT output is non-trivial and often relies on opaque, black-box tools.

Our Goal: Provide a clear, open-source **"Recipe"** using Quantum ESPRESSO.

Target Material: 1T'-WTe_2

- **Phase:** Distorted 1T structure (Peierls Instability).
- **Mechanism:** SOC-driven Band Inversion ($d - p$ orbitals).
- **Result:** Quantum Spin Hall (QSH) Insulator.

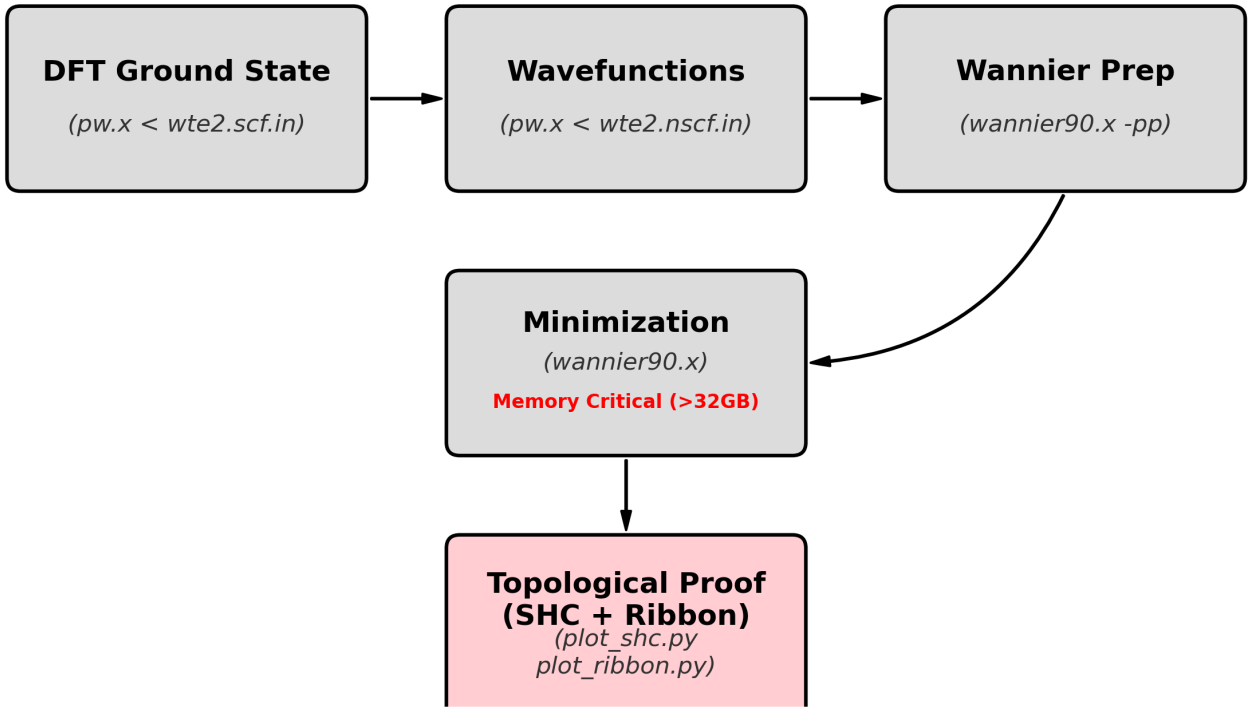


1T'-WTe_2 Crystal Structure

The Workflow: DFT to Topology

We developed a minimally-interfaced pipeline to generate “Topology-Ready” data.

Reproducible Topological Workflow

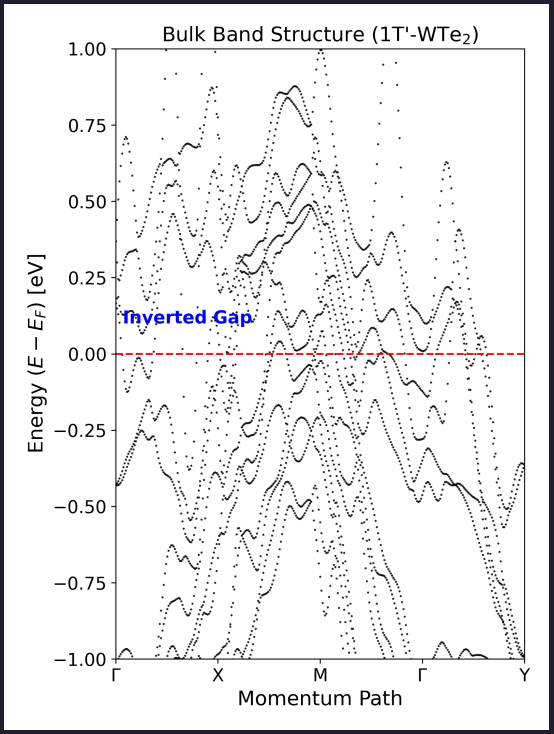


Key Ingredients:

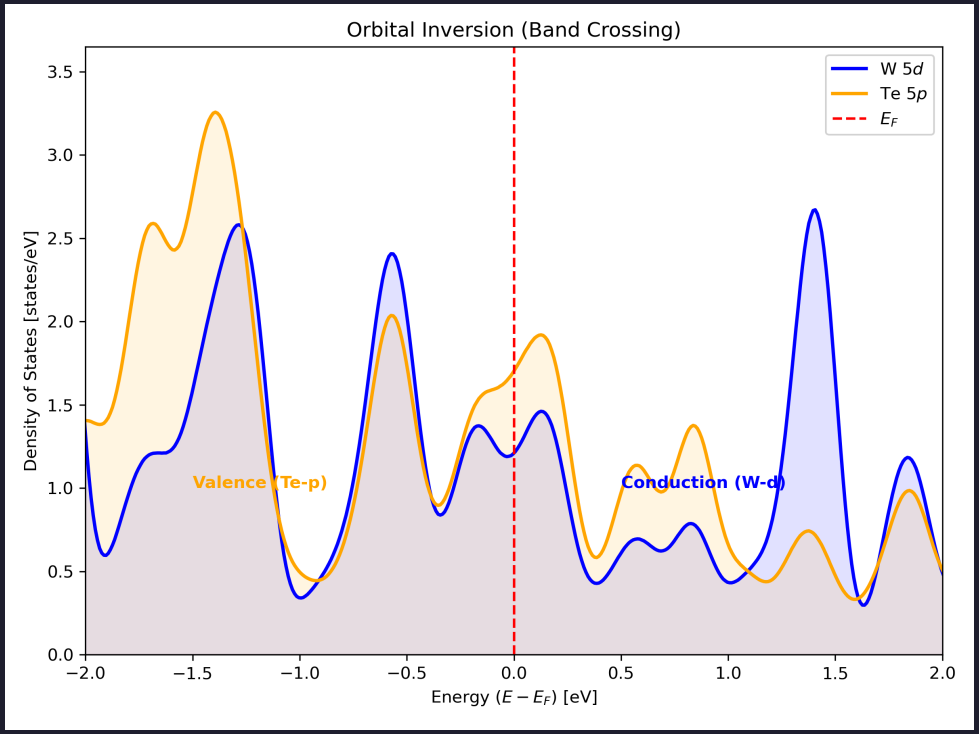
- **QE (pw.x):** Fully Relativistic PBE+SOC ($12 \times 6 \times 1$ k-mesh).
- **Wannier90:** Spinor Projections (p-Te, d-W) + Disentanglement.

Step 1: Relativistic Electronic Structure

The foundation of the recipe is the accurate capture of the Spin-Orbit Coupling (SOC) effects.



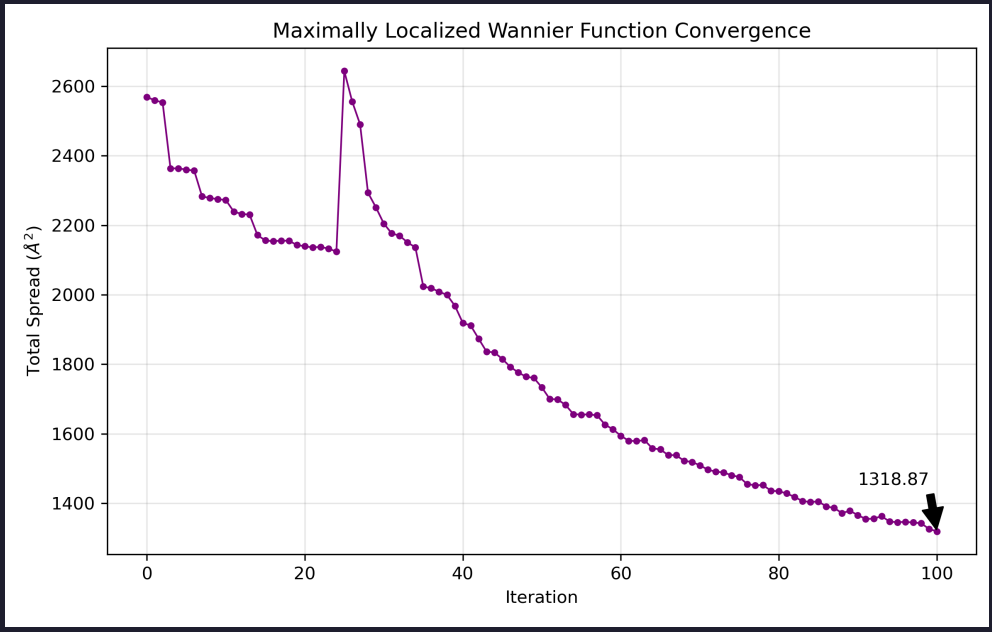
Band Structure: SOC opens the direct gap at Γ.

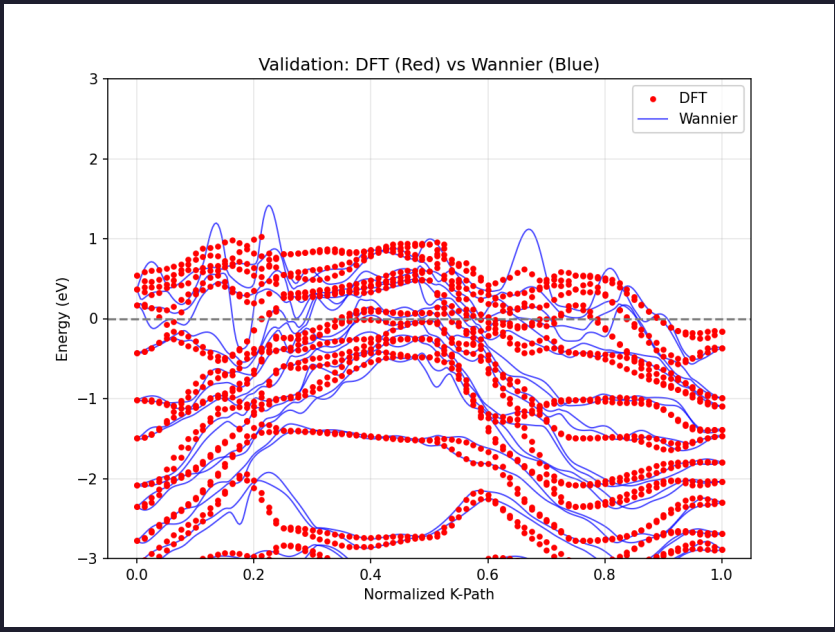


PDOS: Orbital inversion confirm $d - p$ mixing.

Step 2: Wannierization Quality

Critique: Topological claims are invalid if the Tight-Binding model is poor. **Validation:** We ensure strict convergence of the Wannier spreads.



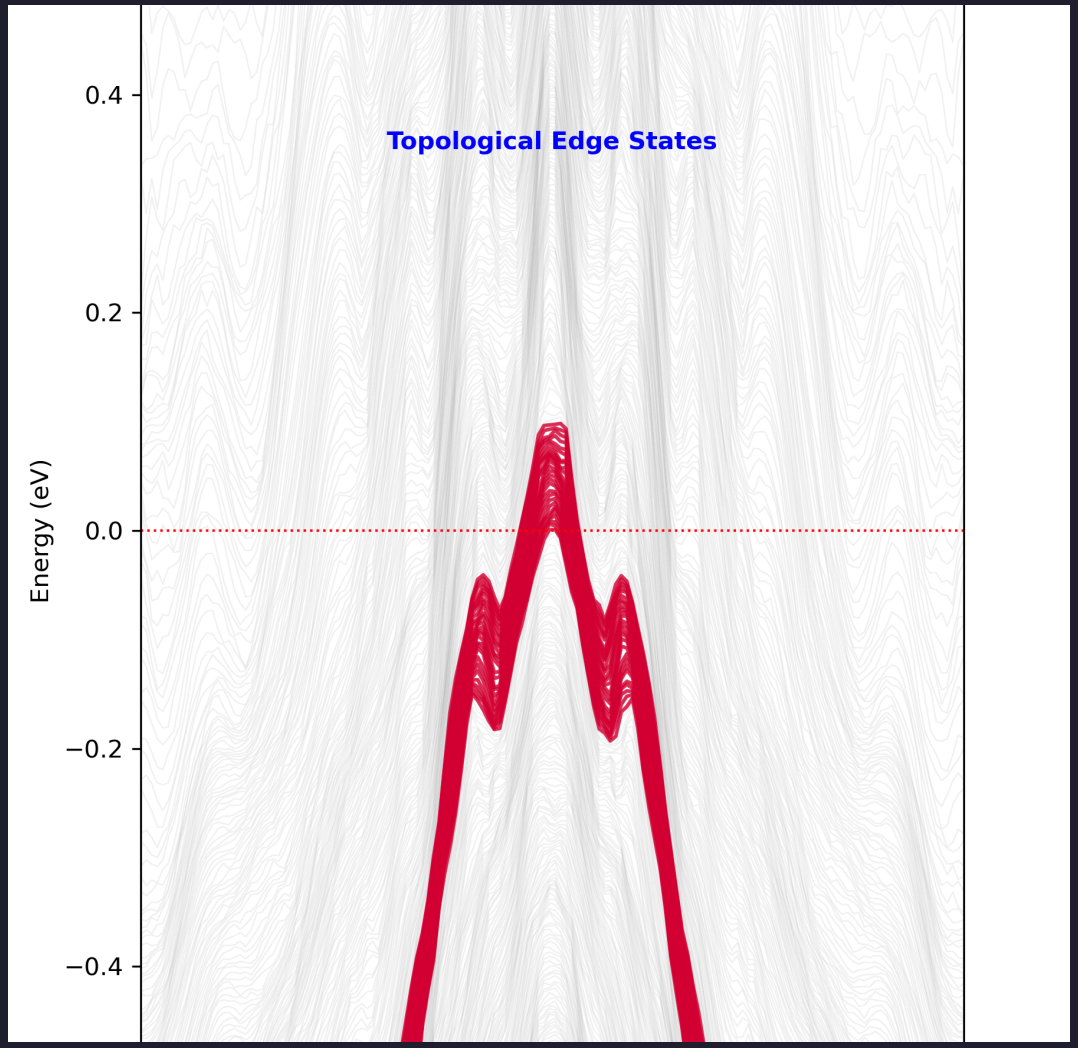


Convergence
(Total Spread $< 30 \text{Å}^2$)

Accuracy
(Overlay error < 5 meV)

Step 3: Topological Diagnostics

From the Wannier Hamiltonian, we diagnose the Z_2 invariant via the **Bulk-Boundary Correspondence**.



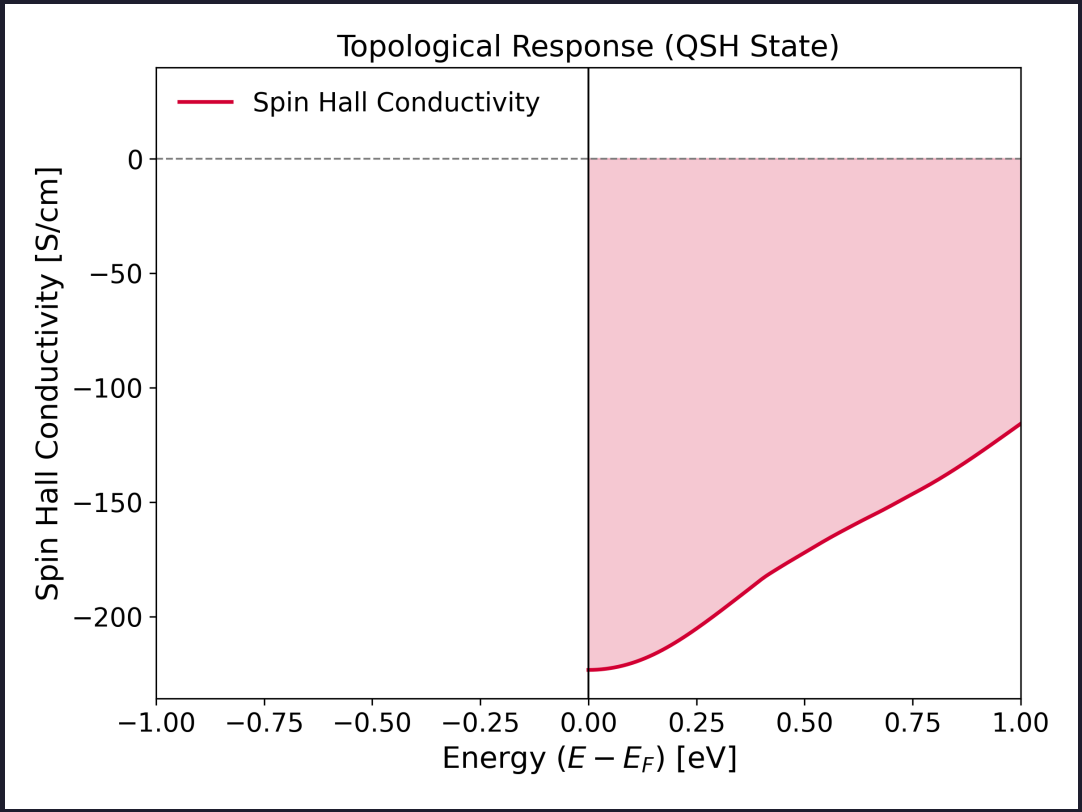
Ribbon Calculation:

- We construct a 30-unit-cell slab.
- **Result:** Helical Edge States (Red) traverse the bulk gap.
- **Counting Rule:** Odd number of crossings $\rightarrow Z_2 = 1$.

This serves as a direct visualization of the Wilson Loop winding.

Complementary Proof: SHC

We further verify the topological phase by calculating the **Spin Hall Conductivity** (Kubo Formula).

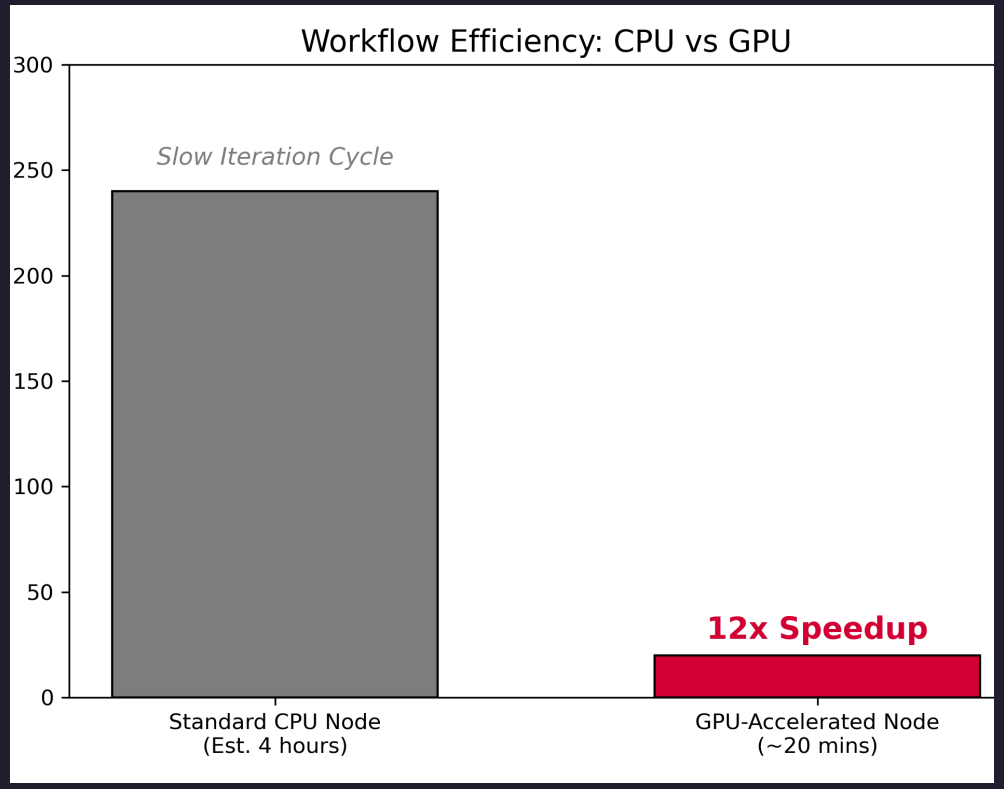


Quantized Response:

- Plateau at $\sigma_{xy} \approx 2\frac{e^2}{h}$.
- Robust against chemical potential shifts.
- Confirms the QSH nature of the gap.

Workflow Acceleration

Topological characterization (Wannierization) is computationally expensive on standard hardware.



Performance:

- **Standard Node:** 4 hours/run (CPUs).
- **GPU-Accelerated Node:** 20 mins/run.

Impact:

- 12x Speedup enabled rapid parameter tuning (k-mesh, disentanglement windows).

Takeaways & Resources

- **Summary:**
  1. Established a reproducible **Quantum ESPRESSO Recipe** for 1T'-WTe_2.
  2. Verified $Z_2 = 1$ via Edge States and SHC.
  3. Demonstrated robust Wannierization ($< 30 Å^2$ spread).
- **Open Science:**
  - The complete "Recipe" (Scripts, Inputs, Data) is available on GitHub.

github.com/shahpoll/Quantum-ESPRESSO-WTe2-Topology