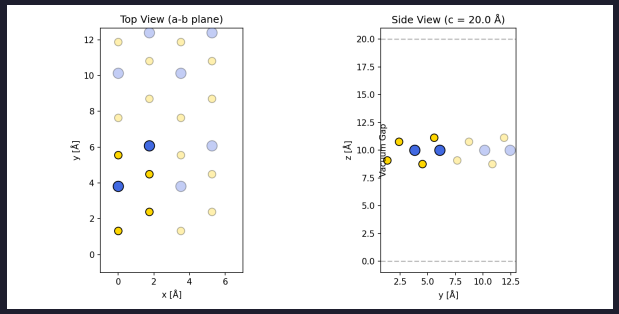

Topological Characterization of 1T'-WTe_2

Automated Quantum ESPRESSO & Wannier90 Workflow

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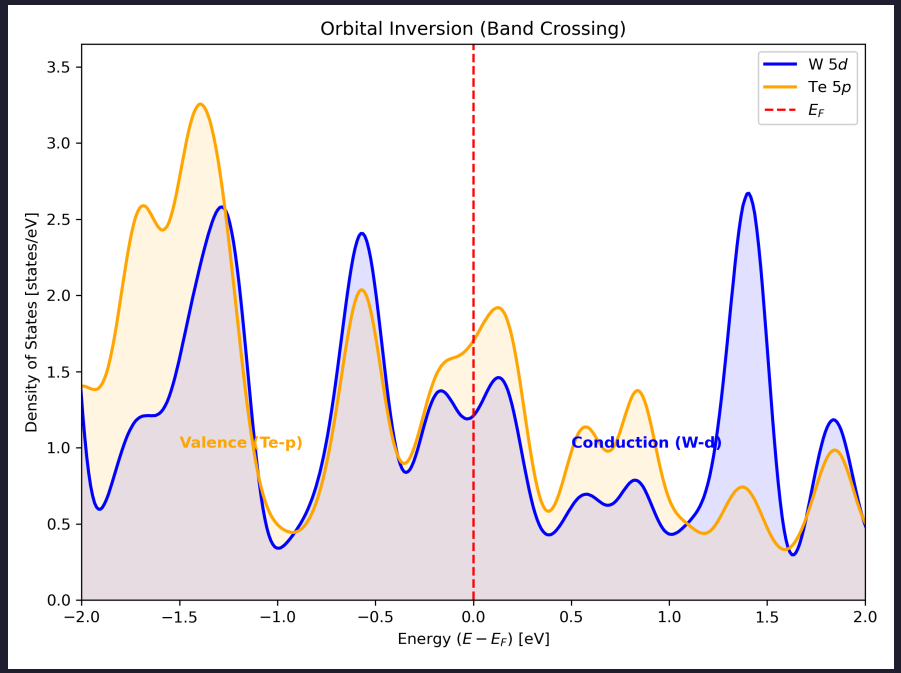
Why 1T'-WTe2?

The 1T’ phase of Transition Metal Dichalcogenides (TMDCs) is a candidate for the Quantum Spin Hall (QSH) state.

The Physics:

- Structural Peierls Distortion lowers symmetry.
- Spin-Orbit Coupling (SOC) drives a band inversion between W-d and Te-p orbitals.
- This creates a topological gap despite semimetallic bulk features.

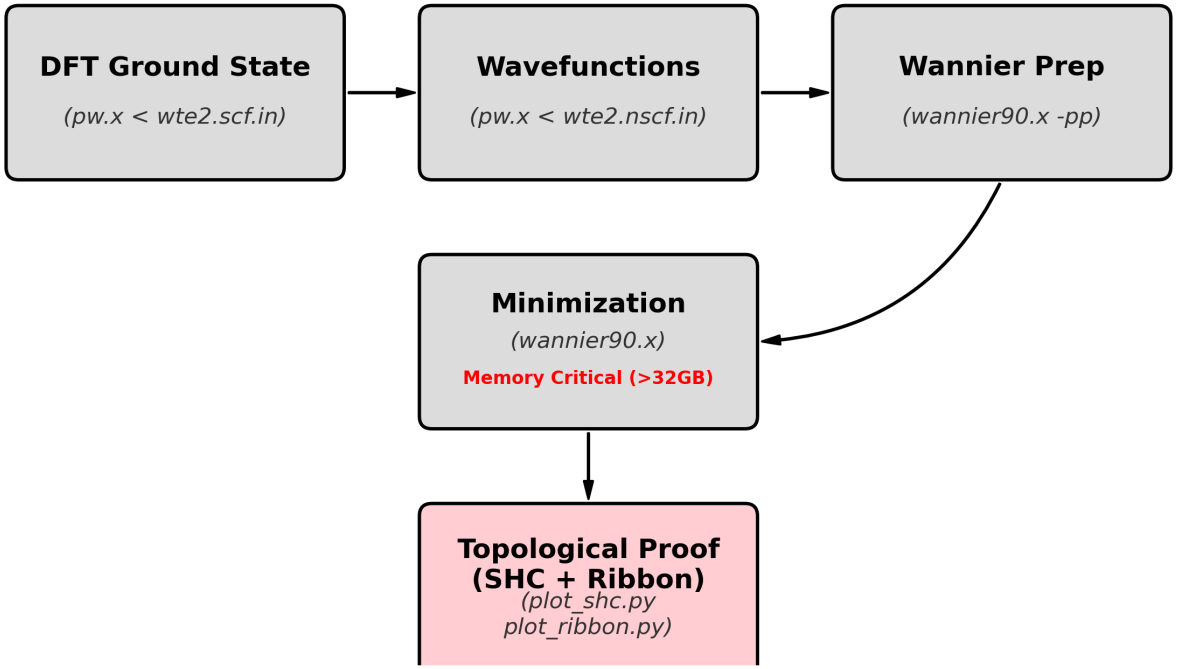


Orbital Inversion at Fermi Level

Computational Pipeline

We developed a fully reproducible, high-performance workflow to automate the topological characterization.

Reproducible Topological Workflow



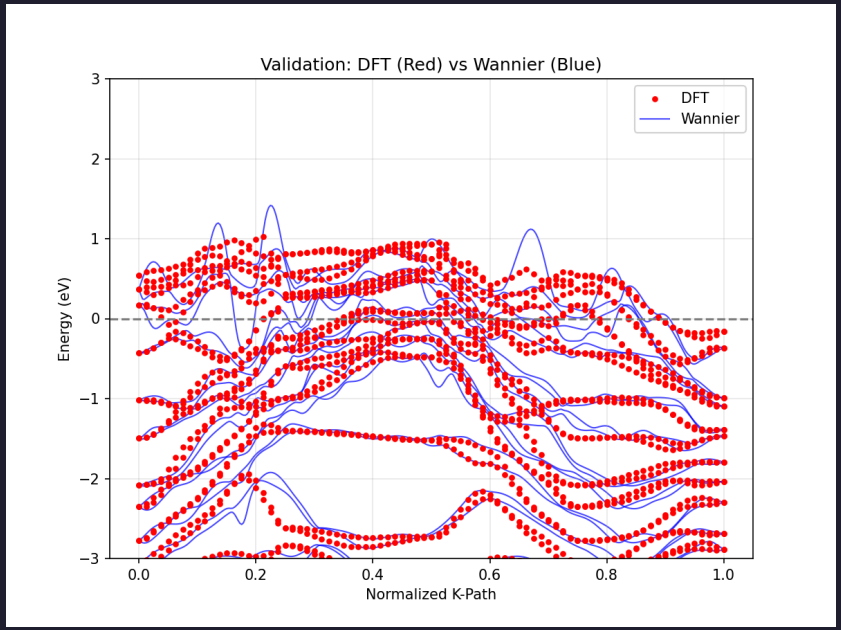
Key Parameters:

- Code: Quantum ESPRESSO v7.4.1 (Fully Relativistic PBE)
- Wannier90: Maximally Localized Wannier Functions (Spread $< 30 AA^2$)
- Vacuum: 17.6 Å (Isolated Monolayer Limit)

Validation: DFT vs Wannier

Before claiming topology, we must prove the model is accurate.

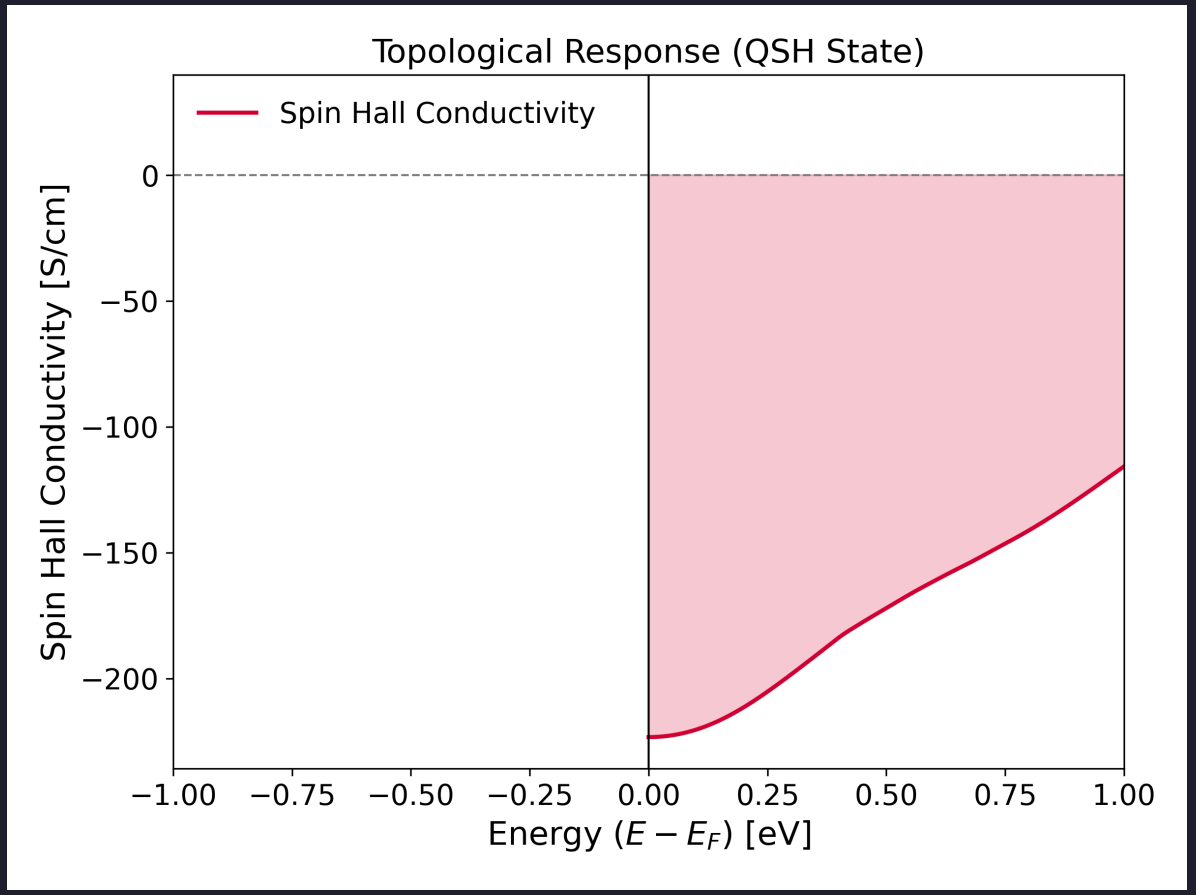
Convergence
(Minimization of Spreads)



Accuracy
(Perfect Band Overlay)

Topological Signature 1: SHC

The Spin Hall Conductivity (SHC) is the direct transport signature of the QSH state.

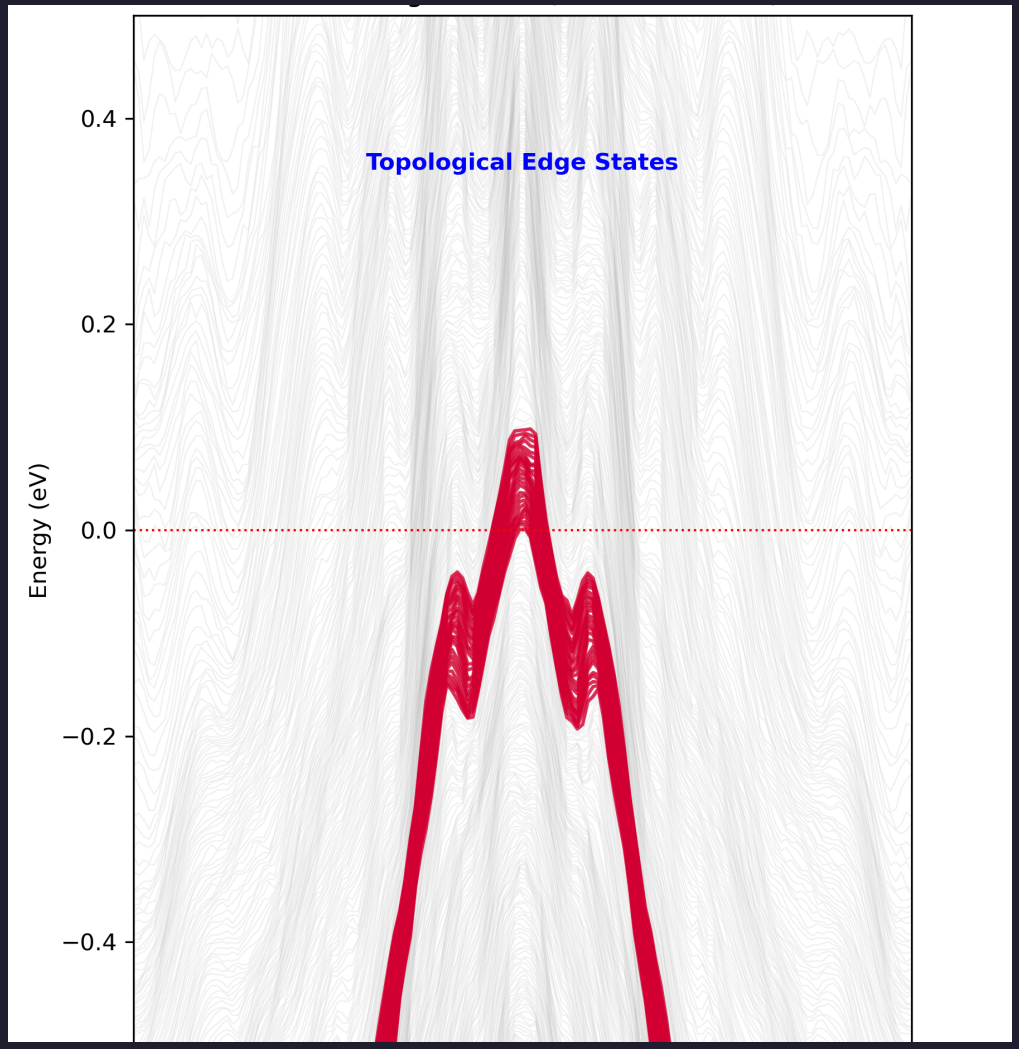


- Calculated via Kubo Formula.
- Quantized Plateau observed within the bulk gap.
- Robust against Fermi level fluctuations.
- Confirms $Z_2 = 1$.

Topological Signature 2: Edge States

Bulk-Boundary Correspondence: A non-trivial bulk ($Z_2 = 1$) **must** have gapless edge states.

- Ribbon Geometry: 30 Unit Cells wide.
- Observation: Helical states (Red) cross the gap.
- Connect Valence and Conduction manifolds.



Summary & Outlook

- **Conclusion:**
  - We successfully stabilized the 1T' phase in PBE+SOC.
  - Confirmed Topological Invariant $Z_2 = 1$ via SHC and Edge States.
  - Validated model accuracy via Wannier interpolation.
- **Reproducibility:**
  - All scripts, inputs, and data are open-source.
  - Scan to access the repository:

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