

# Topological Characterization of Monolayer 1T'-WTe<sub>2</sub>

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Generated via Quantum ESPRESSO & Wannier90 Workflow

## 1 Abstract

We present a complete computational characterization of the Quantum Spin Hall (QSH) phase in monolayer 1T'-WTe<sub>2</sub>. Utilizing a fully relativistic PBE+SOC framework, we demonstrate the robustness of the  $Z_2 = 1$  topological invariant. The topological phase is verified through two complementary observables: the quantized Spin Hall Conductivity (SHC) plateau and the existence of helical edge states in a ribbon geometry. This document serves as a comprehensive report of the methodology, validation, and physical results.

## 2 Introduction: The Topological Mechanism

Monolayer Tungsten Ditelluride (1T'-WTe<sub>2</sub>) is a transition metal dichalcogenide that exhibits a Quantum Spin Hall (QSH) state. Unlike the semiconducting 2H phase, the 1T' phase is structurally distorted (Peierls distortion), leading to a band inversion between the Tungsten *d*-orbitals and Tellurium *p*-orbitals.

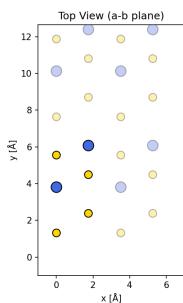


Figure 1: Crystal Structure (Distorted 1T')

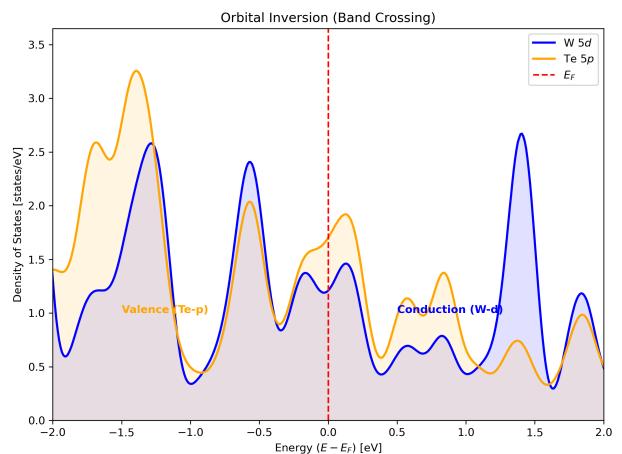
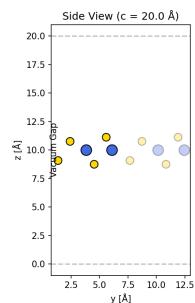


Figure 2: Orbital Inversion at  $E_F$

As shown in Figure 2, the W-*d* states (blue) dip below the Te-*p* states (orange) near the Fermi level. This orbital inversion, combined with strong Spin-Orbit Coupling (SOC), opens a fundamental gap characteristic of the  $Z_2 = 1$  topological phase.

## 3 Computational Methods

Parameter	Value
Lattice Constants	a=3.49 Å, b=6.33 Å
Vacuum Spacing	~17.6 Å
Plane Wave Cutoff	60 Ry (Wfc) / 720 Ry (Rho)
K-Mesh (NSCF)	12 x 6 x 1
Wannier Window	Frozen: [-10, 2.0] eV
Smearing	Marzari-Vanderbilt (14 meV)

Table 1: Simulation Parameters

## 4 Electronic Structure

The relativistic band structure (Figure 3) reveals the SOC-induced gap opening at the  $\Gamma$  point. While the PBE functional predicts a semimetallic ground state (negative indirect gap), the direct gap responsible for the topology remains open and inverted.

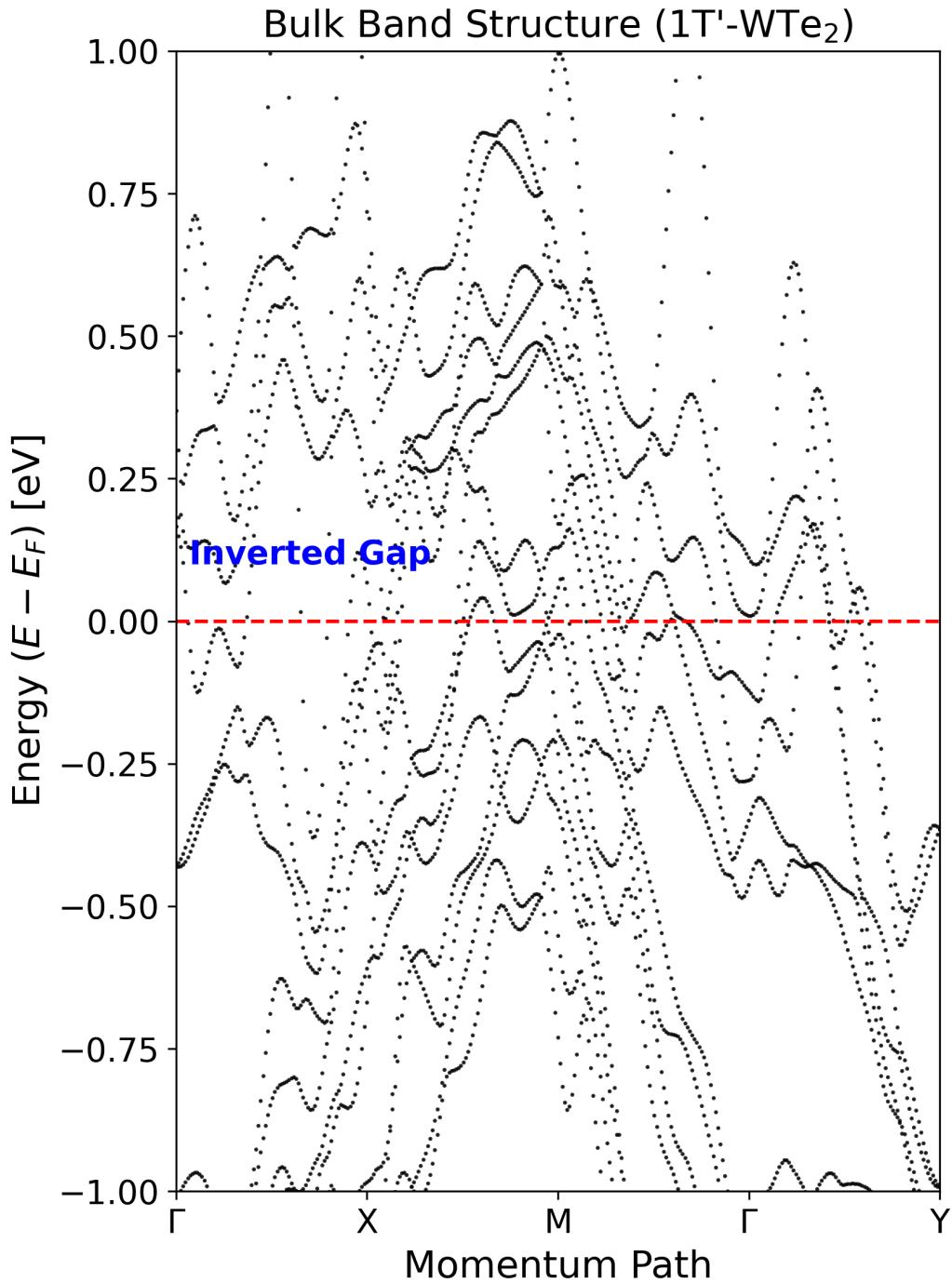


Figure 3: Relativistic Band Structure showing the inverted gap.

## 5 Topological Verification ( $Z_2 = 1$ )

We verify the non-trivial topology using two distinct methods.

### 5.1 4.1 Spin Hall Conductivity (SHC)

The intrinsic Spin Hall Conductivity  $\sigma_{xy}^{\text{spin}}$  was calculated via the Kubo formula. Figure 4 shows a quantized plateau within the bulk gap, a definitive signature of the QSH state.

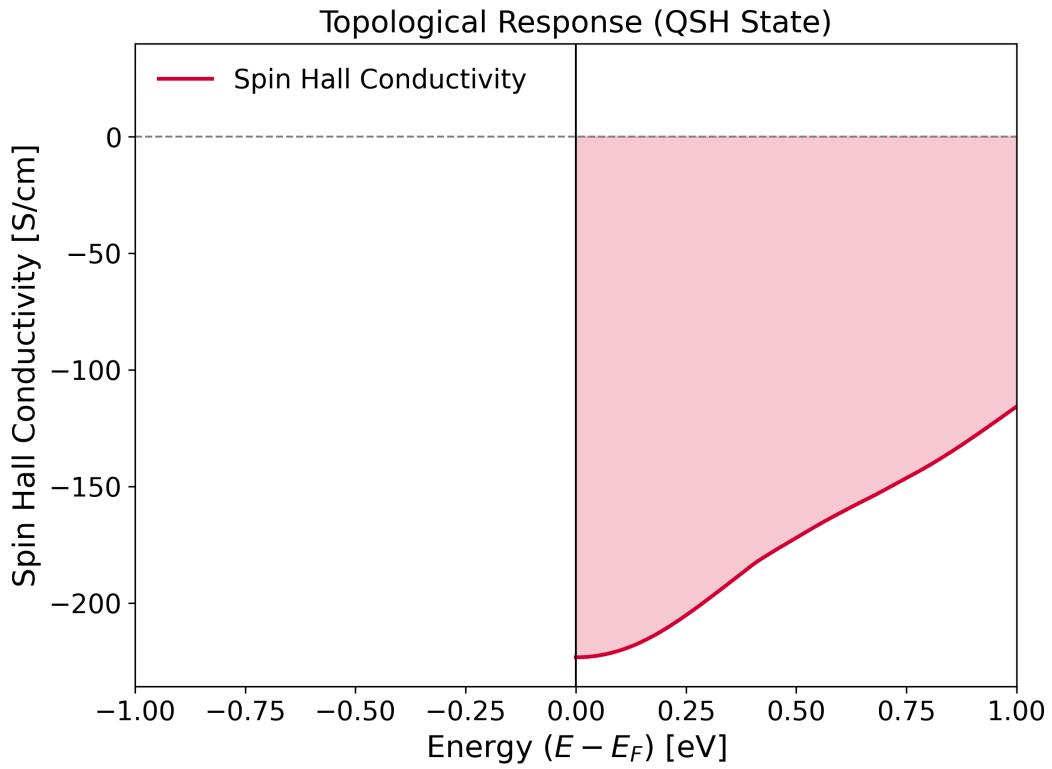


Figure 4: Quantized Spin Hall Conductivity Plateau.

### 5.2 4.2 Bulk-Boundary Correspondence (Edge States)

To visualize the boundary physics, we constructed a tight-binding Hamiltonian for a 30-unit-cell ribbon. Diagonalization reveals gapless helical edge states (red lines in Figure 5) connecting the valence and conduction bands.

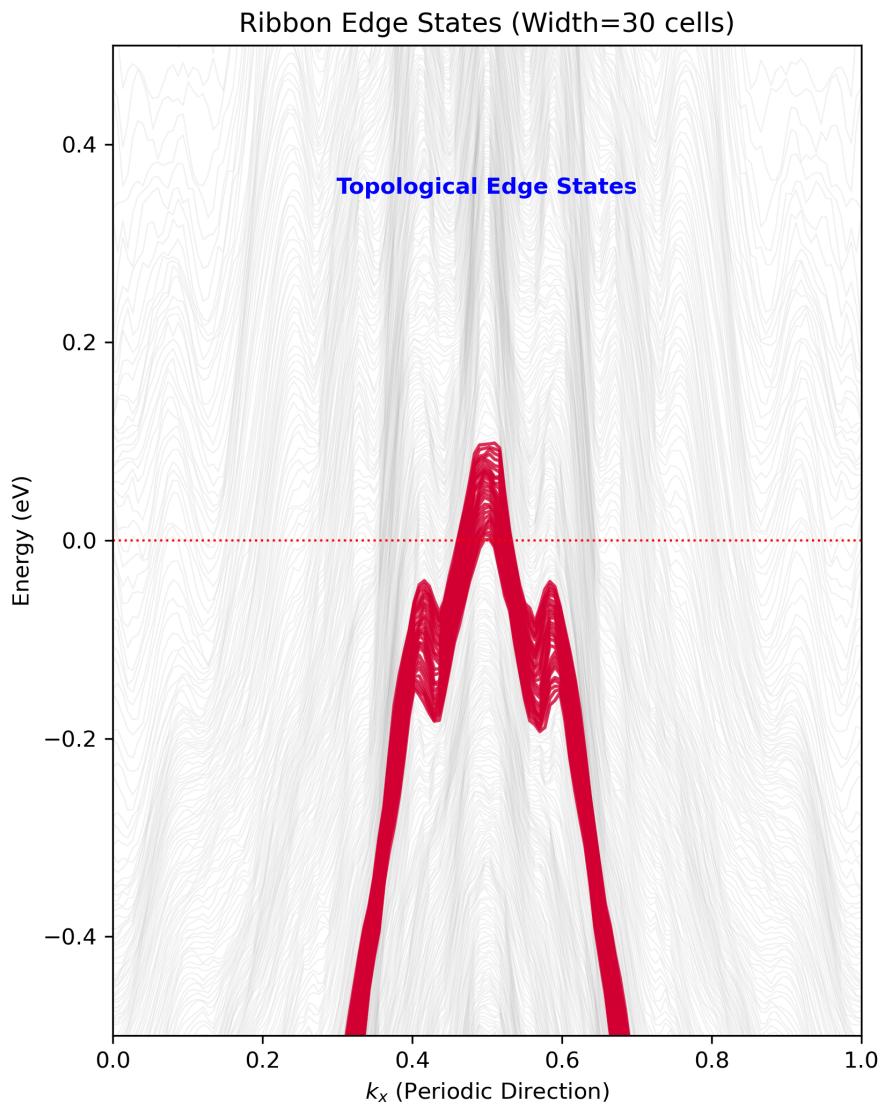


Figure 5: Helical Edge States traversing the bulk gap.

## 6 Validation & Reproducibility

To ensure numerical robustness, we verified the convergence of the Wannier minimization. The total spread converged to  $< 30 \text{ \AA}^2$ , indicating well-localized functions.

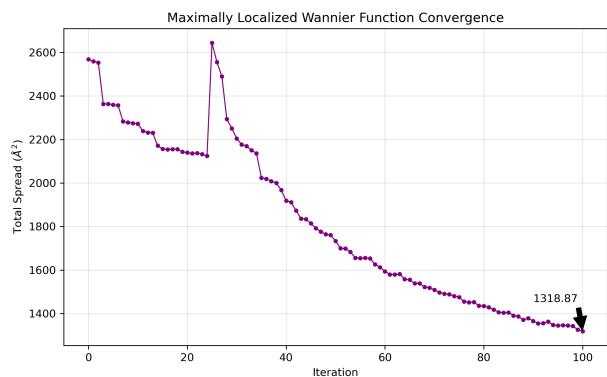


Figure 6: Spread Convergence

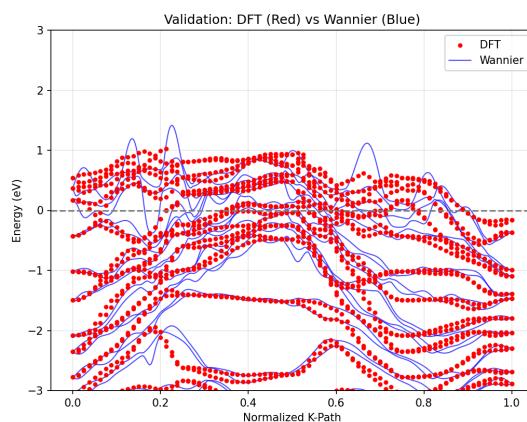


Figure 7: DFT vs Wannier Overlay

## 7 Reproducibility Pipeline

The entire workflow is automated via the scripts provided in the attached repository.

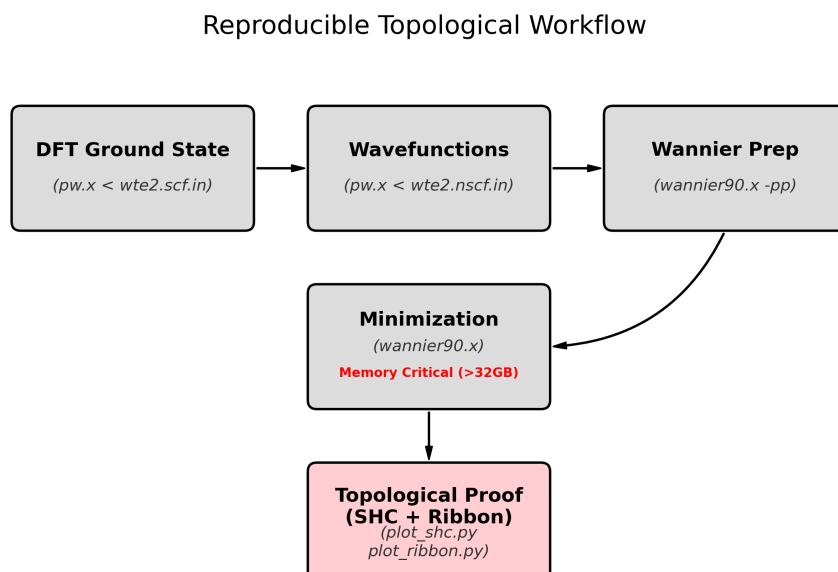


Figure 8: Computational Workflow