Topological Characterization of Monolayer 1T'-WTe_2

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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_2. Utilizing a fully relativistic PBE+SOC framework, we demonstrate the robustness of the $Z_2 = 1$ topological invariant through two complementary observables: the quantized Spin Hall Conductivity (SHC) and the existence of helical edge states in a ribbon geometry.

2 Computational Methods

The electronic structure was calculated using Quantum ESPRESSO (v7.4.1) with fully relativistic Projector Augmented Wave (PAW) pseudopotentials.

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

3 Electronic Structure & Topology

The 1T' phase exhibits a Peierls distortion that breaks the high symmetry of the 1T phase.

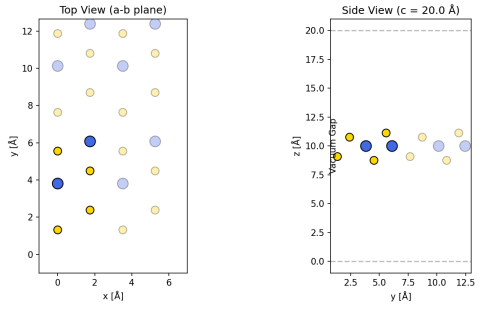

Figure 1: Crystal Structure (Distorted 1T')

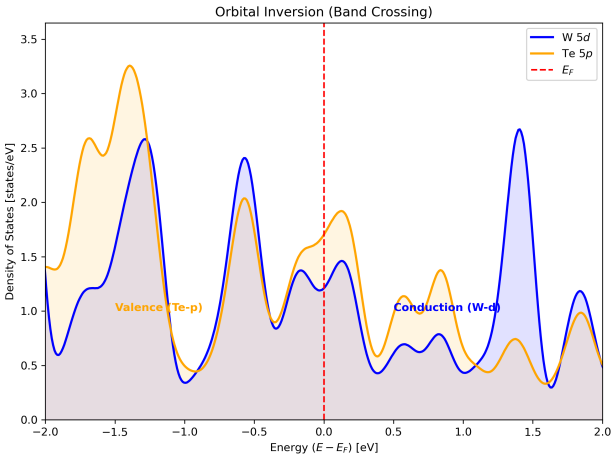

Figure 2: Orbital Inversion (p-d mixing)

The inclusion of Spin-Orbit Coupling (SOC) opens a fundamental gap at the inversion point, although the PBE functional yields a semimetallic overlap globally.

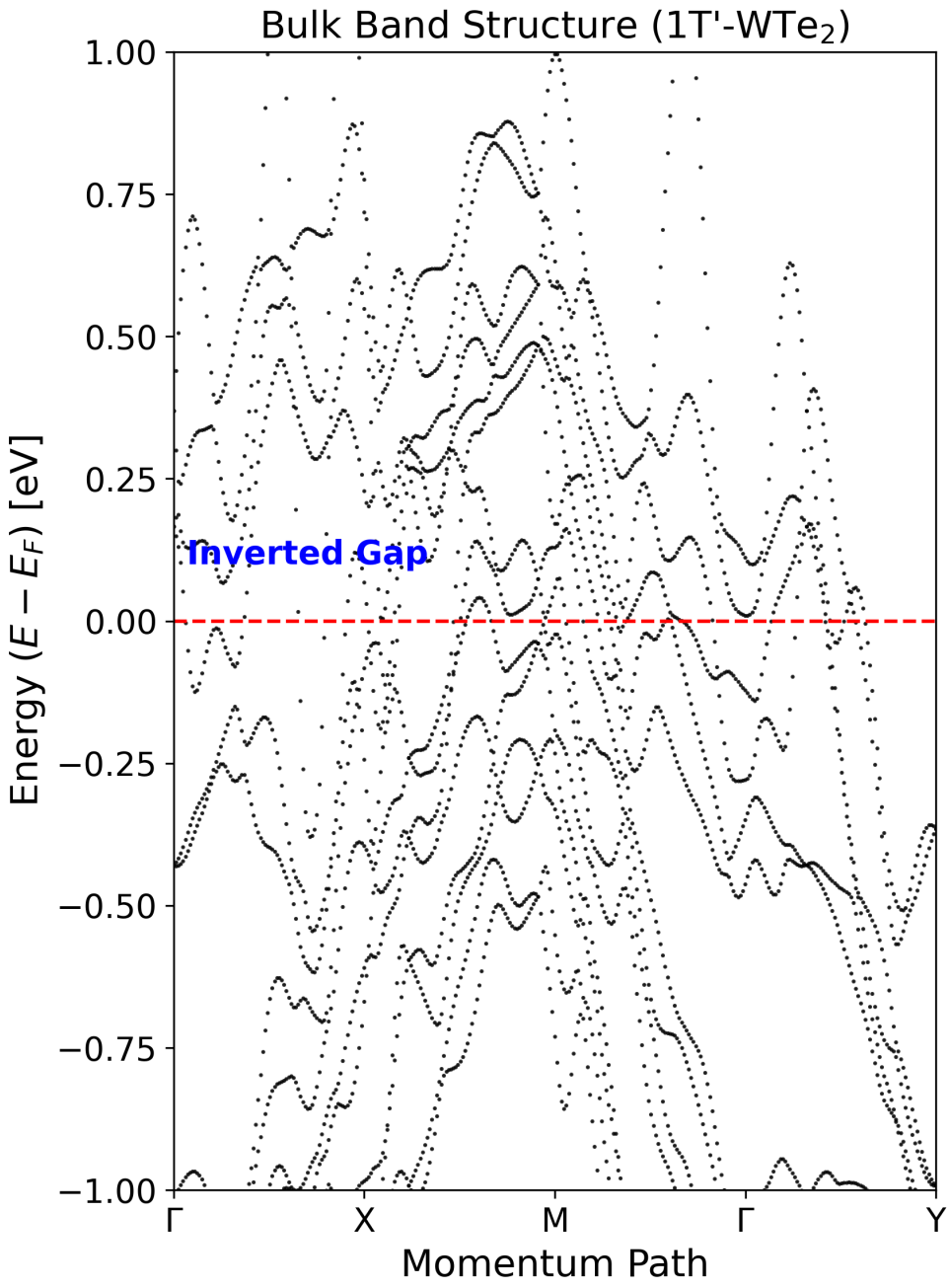

Figure 3: Relativistic Band Structure showing the inverted gap.

4 Topological Invariant ($Z_2 = 1$)

We verify the non-trivial topology via two methods:

4.1 3.1 Spin Hall Conductivity

The Spin Hall Conductivity σ_{xy}^{spin} exhibits a quantized plateau within the bulk gap, a hallmark of the QSH state.

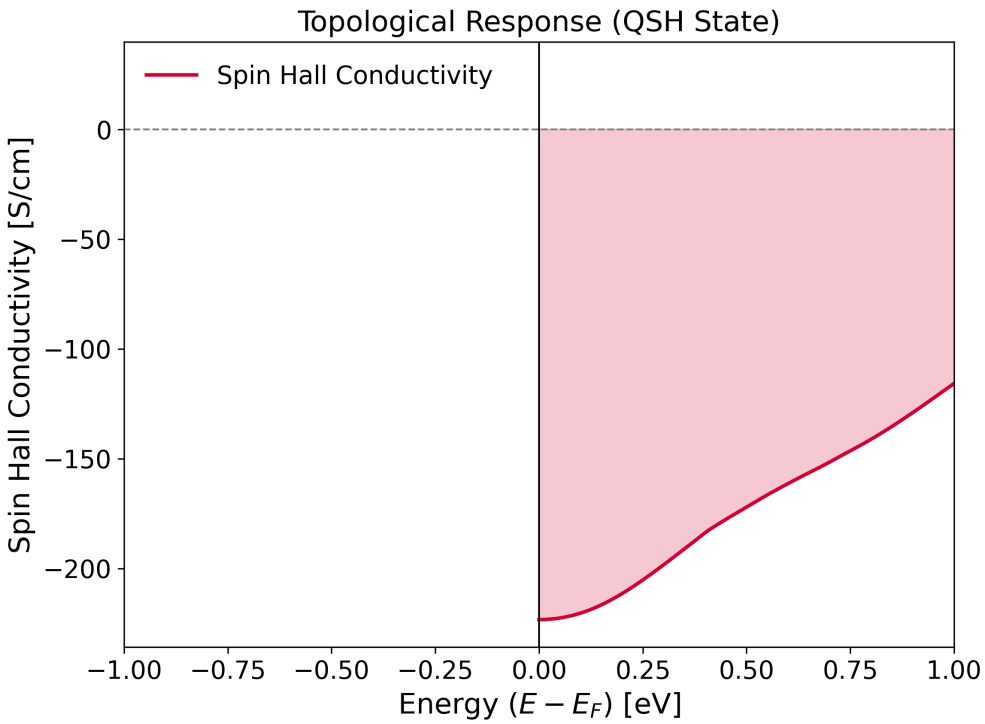

Figure 4: Spin Hall Conductivity Plateau.

4.2 3.2 Bulk-Boundary Correspondence (Ribbon)

A tight-binding calculation on a 30-unit-cell ribbon reveals gapless edge states connecting the valence and conduction bands.

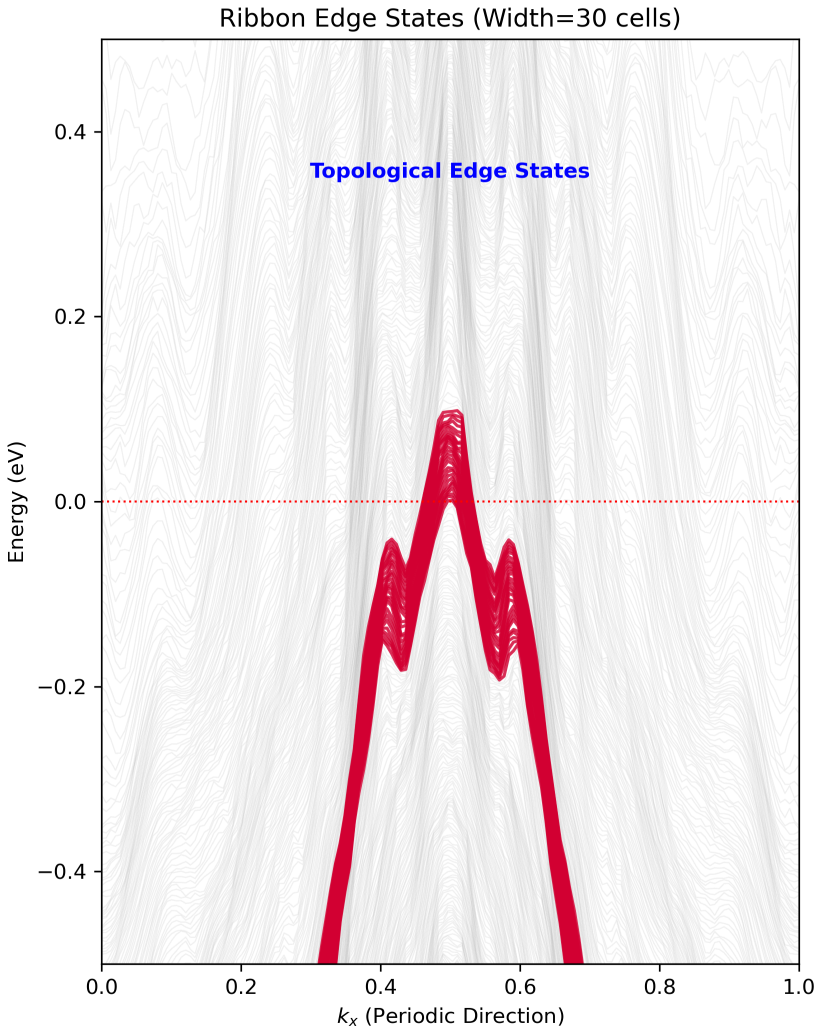

Figure 5: Helical Edge States traversing the bulk gap.

5 Validation & Reproducibility

The Wannier tight-binding model was validated against DFT ground truth. The spread convergence confirms maximally localized functions.

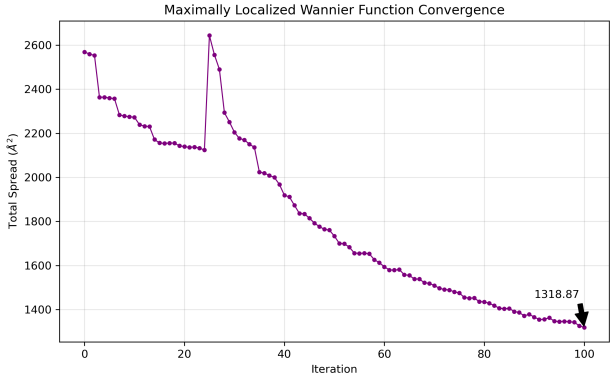

Figure 6: Wannier Spread Convergence

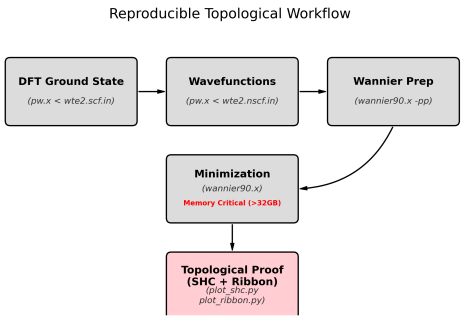

Figure 7: Reproducible Workflow