Robust Quantum Spin Hall State in Monolayer 1T'-WTe_2

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Presented at **ICAP 2025**
International Conference on Advances in Physics
Shahjalal University of Science and Technology (SUST)

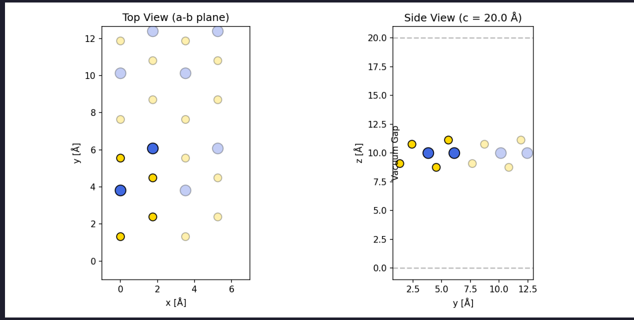
What is a Topological Insulator?

Standard insulators have a global energy gap. **Topological Insulators (TIs)** are distinct: they are insulating in the bulk but conducting at the edges.

The Mechanism: Band Inversion Driven by strong **Spin-Orbit Coupling (SOC)**, the conduction and valence bands swap character (parity).

The Hamiltonian:

$$H = H_0 + \underbrace{\lambda_{\mathrm{SOC}}(L) \cdot (S)}_{\text{Topological Driver}}$$



1T'-WTe2 Crystal Structure

This inversion creates a non-trivial winding number ($Z_2 = 1$), necessitating gapless edge states.

Computational Framework

We characterize the topology using **Density Functional Theory (DFT)** and **Wannier Interpolation**.

1. First-Principles Hamiltonian (DFT): Solving the Kohn-Sham equations with relativistic pseudopotentials (PBE + SOC): **1. First-Principles Hamiltonian (DFT):** Solving the Kohn-Sham equations with relativistic pseudopotentials (PBE + SOC):

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}((r))\right]\psi_i = \varepsilon_i \psi_i$$

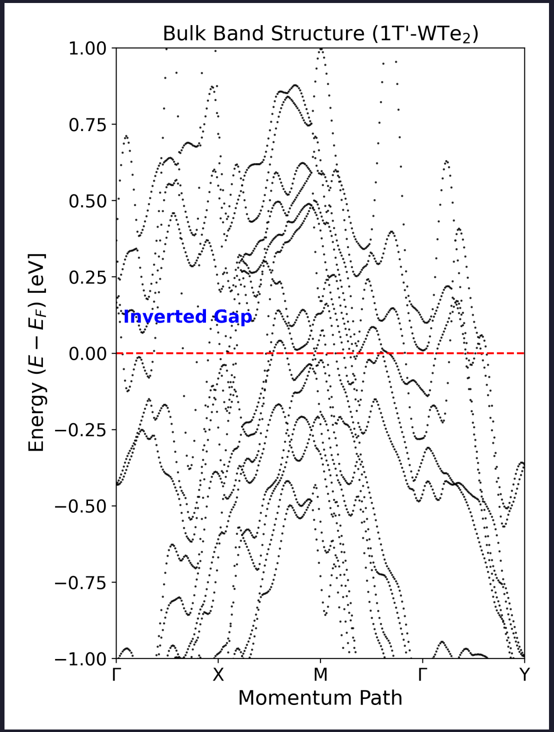
2. Topological Invariant (Kubo Formula): The Spin Hall Conductivity (SHC) is calculated via the Berry Curvature $\Omega_{\{n\}}((k))$:

$$\sigma_{\mathrm{xy}}^{\mathrm{spin}} = \frac{e^2}{\hbar} \sum_n \int_{\mathrm{BZ}} \frac{d^2 k}{(2\pi)^2} f_{n((k))} \Omega_{n,\mathrm{xy}}^{\mathrm{spin}}((k))$$

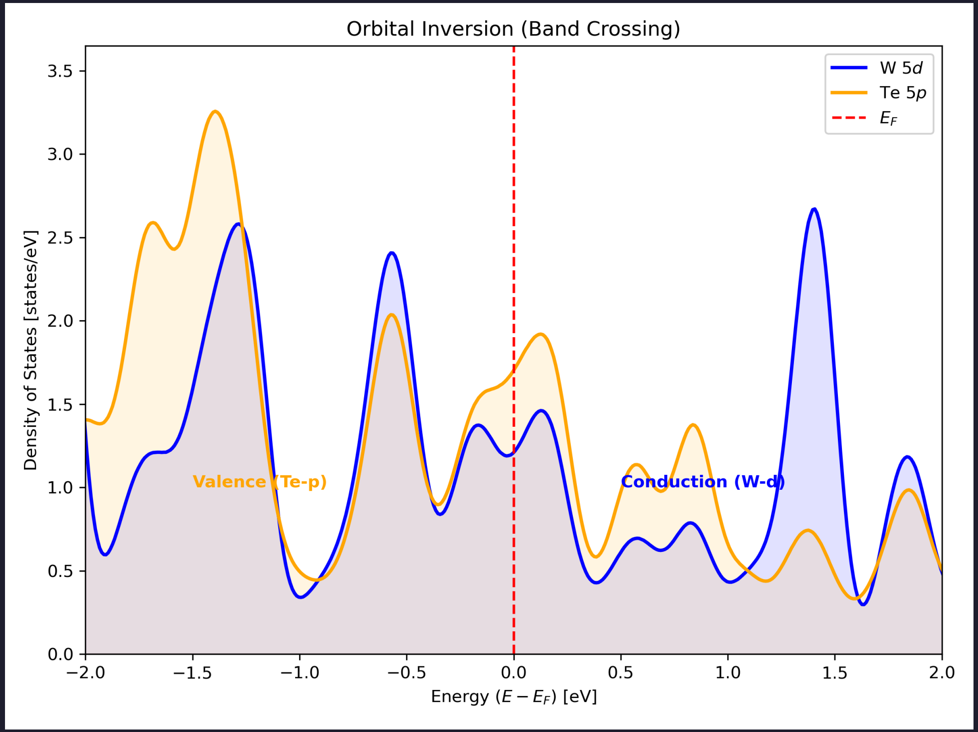
Tools: Quantum ESPRESSO → Wannier90 → PostW90

Results: Band Inversion

The 1T’ structural distortion induces a semimetallic ground state, but the **direct gap** opens due to SOC.



Relativistic Band Structure

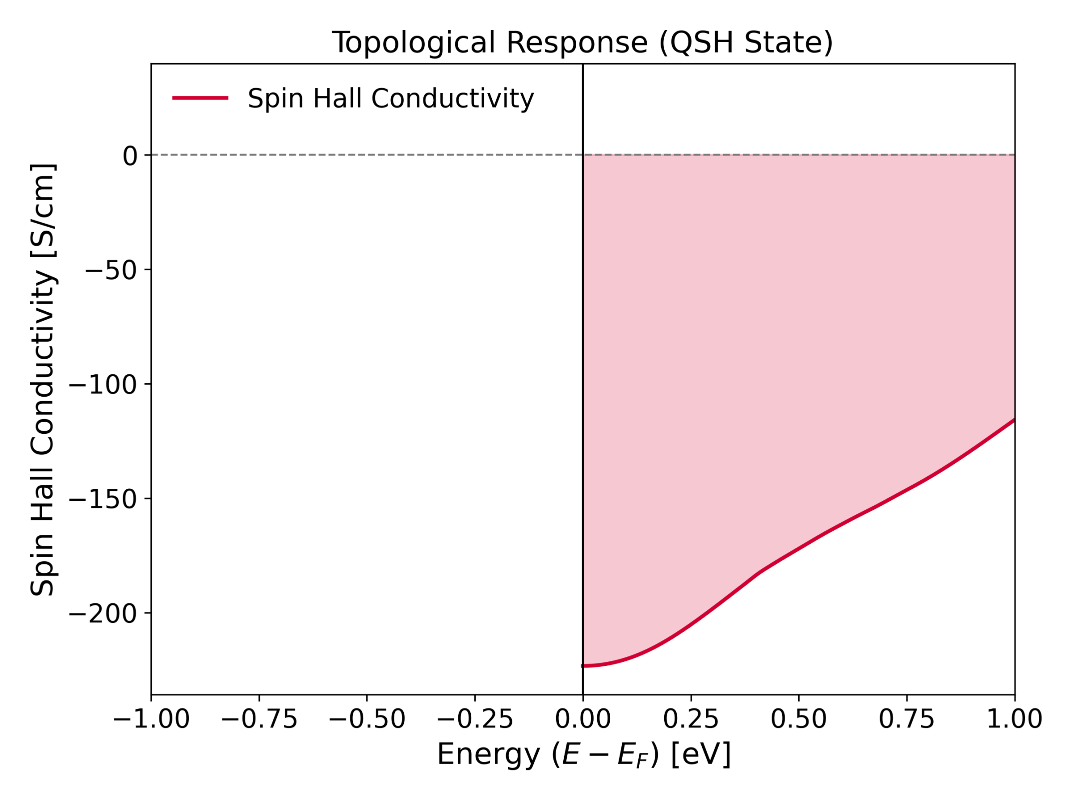


Orbital Mixing ($d - p$ Inversion)

Observation: The W-d and Te-p bands invert near Γ, a signature of the QSH phase.

Proof 1: Spin Hall Conductivity

We calculate the intrinsic SHC using the Kubo-Greenwood formula.



The Result:

- A quantized plateau appears in the bulk gap.
- Value: $\sigma_{\text{xy}} \approx 2\frac{e^2}{h}$ (Conductance Quantum).

Implication: This non-zero invariant confirms the **Quantum Spin Hall** state ($Z_2 = 1$).

Proof 2: Helical Edge States

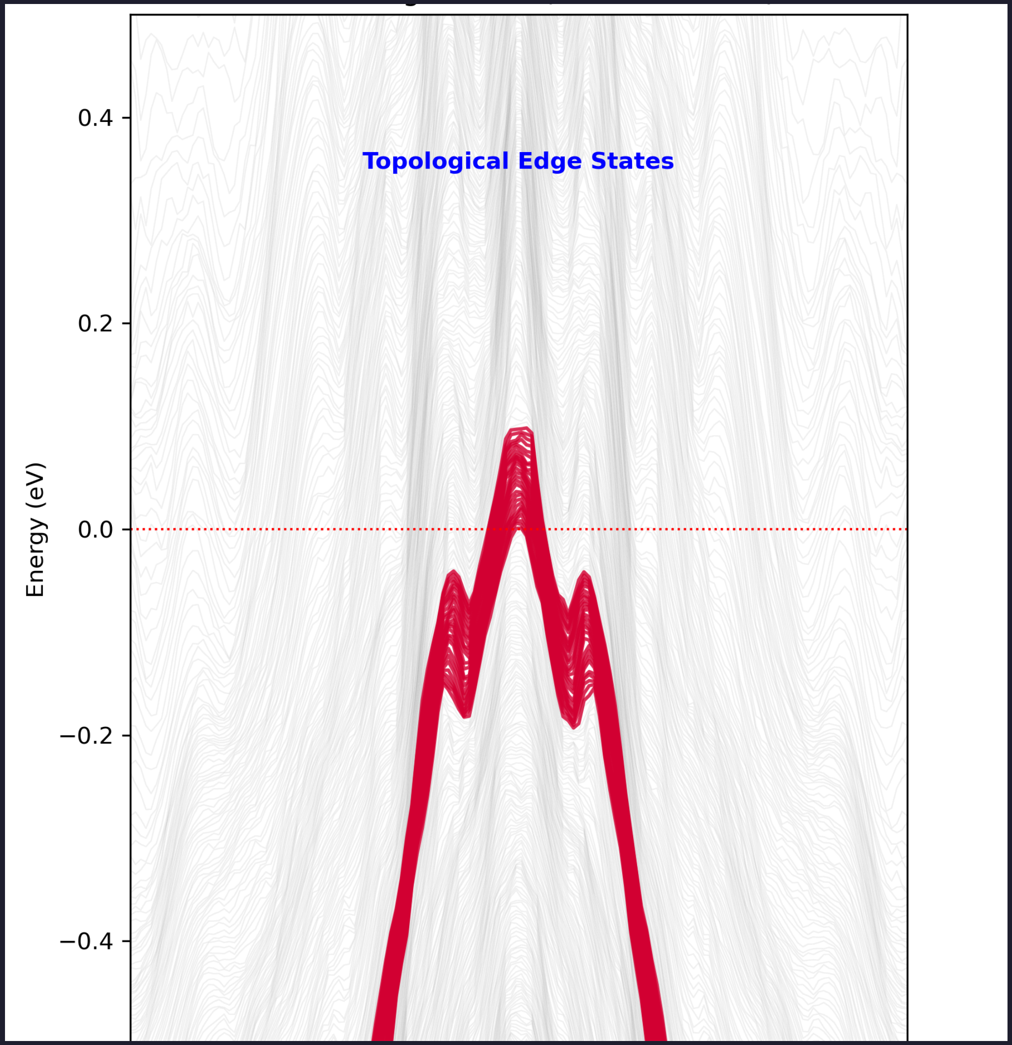
Bulk-Boundary Correspondence: If the bulk is topological, the boundary must be metallic.

Simulation:

- 30-Unit Cell Ribbon.
- Constructed from Maximally Localized Wannier Functions.

Observation:

- **Red States:** Gapless modes crossing the Fermi level.
- These are the topologically protected edge channels.



Summary

- **Conclusion:**
  - We have robustly characterized monolayer 1T'-WTe_2 as a QSH insulator.
  - Verified via orbital inversion, quantized SHC, and edge states.
  - Established a reproducible workflow for topological materials.
- **Future Work:**
  - Investigation of strain tuning and electric field effects.