

Supporting Information:

Strain Tuning of the Anisotropy in the Optoelectronic Properties of TiS_3

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- In Fig. S1 we show the evolution of the band structure with strain, ranging from +7.5% (tensile) to -1.5% (compressive).
- In Table S1 we show the fit ($y = a \cdot x + b$) of the effective masses for the three bands of interest of the TiS_3 single-layer (see Fig. 4 of the main text).

- In Fig. S2 we show a polar plot the optical conductivity depending on the polarization angle of the incident light for energies coinciding at the peak in the optical conductivity of each case (that is 1.47 eV for the case of -1.5% strain, 1.6 eV for the case of 0.0% strain and 1.74 eV for the case of +1.5% strain).

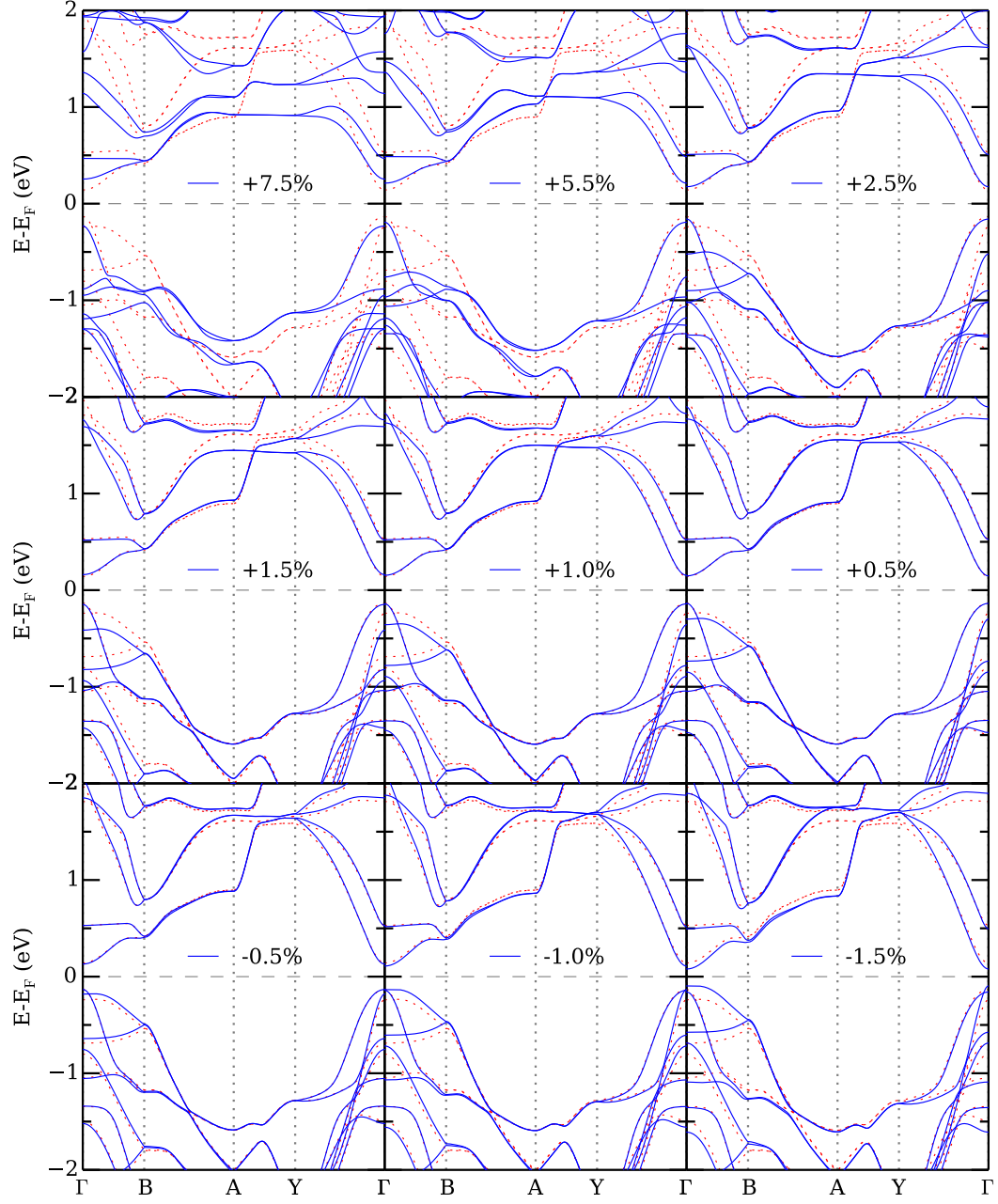


Figure S1: Band structure of TiS_3 single-layer under tensile and compressive strain (solid line). We also plot the band structure for the case with no strain for clarity (dashed line). $\Gamma = (0, 0, 0)$, $B = (1/2, 0, 0)$, $A = (1/2, 1/2, 0)$ and $Y = (0, 1/2, 0)$ in units of the reciprocal lattice vectors.

Table S1: Fit ($y = a \cdot x + b$) of the effective masses for the three bands of interest of the TiS_3 single-layer (see Fig. 4).

| | $b(m_{e-}/\text{strain})$ | $a(m_{e-})$ |
|-------------------------|---------------------------|-------------|
| $\text{CB}_{\Gamma-B}$ | 0.11104436 | 1.61517364 |
| $\text{CB}_{Y-\Gamma}$ | 0.02077982 | 0.39255455 |
| $\text{VB1}_{\Gamma-B}$ | -2.18016636 | 7.50028 |
| $\text{VB1}_{Y-\Gamma}$ | 0.014358 | 0.15574545 |
| $\text{VB2}_{\Gamma-B}$ | -0.01392509 | 0.31911182 |
| $\text{VB2}_{Y-\Gamma}$ | -0.03831873 | 0.93913 |

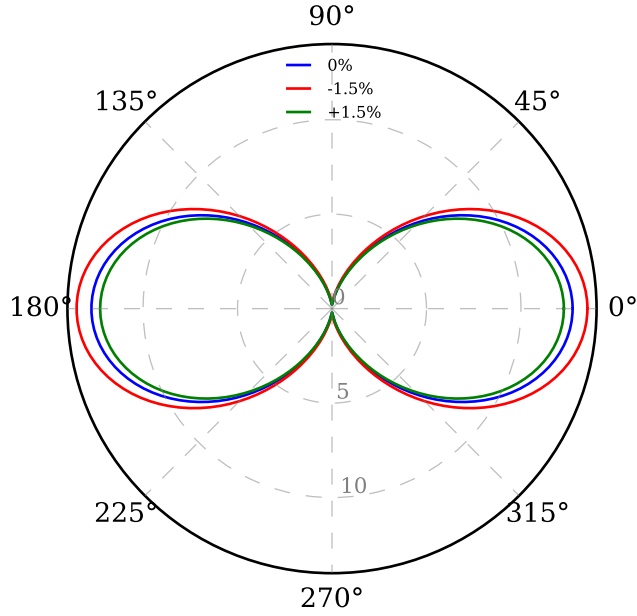


Figure S2: Optical conductivity depending on the polarization angle of the incident light for energies coinciding at the peak in the optical conductivity in units of $10^5 (\Omega \cdot m)^{-1}$ of each case (that is 1.47 eV for the case of -1.5% strain, 1.6 eV for the case of 0.0% strain and 1.74 eV for the case of +1.5% strain).