Electronic Supplementary Material (ESI) for Nanoscale.

Crystal structures of monoclinic bulk Al_2Te_5

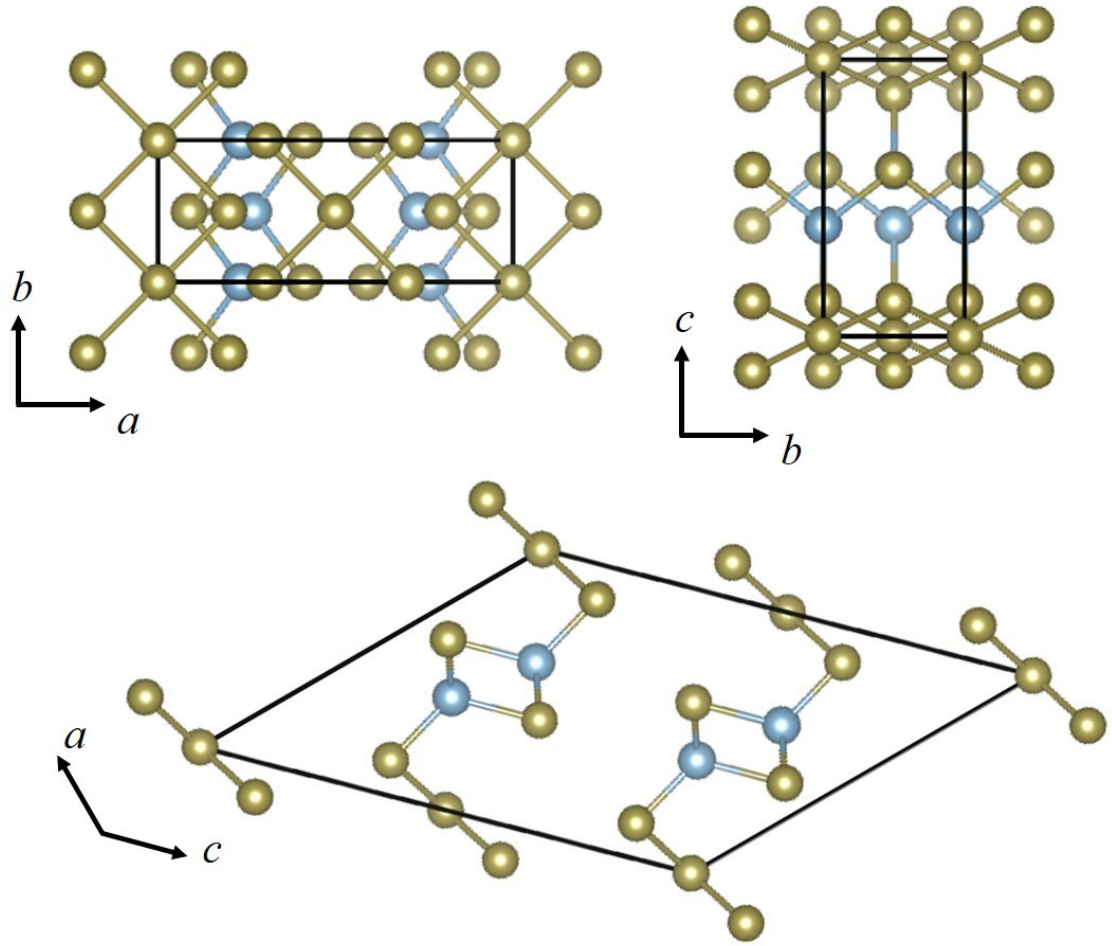


Figure S1. The geometrical structure of monoclinic bulk Al_2Te_5

The mechanical properties of single layer Al_2Te_5

The mechanical behaviors of single layer Al2Te5 is explored by calculating the in-plane Young's modulus Y(θ) and Poisson's ratio υ(θ) on the basis of the elastic constants C_{ij}. The Young's modulus Y(θ) and Poisson's ratio υ(θ) along the in-plane θ can be expressed as follows:

$$Y(\theta) = \frac{C_{11}C_{22} - C_{12}^2}{C_{11}sin^4\theta + Asin^2\theta cos^2\theta + C_{22}cos^4\theta}$$

$$\nu(\theta) = \frac{C_{12}sin^4\theta - Bsin^2\theta cos^2\theta + C_{12}sin^4\theta}{C_{11}sin^4\theta + Asin^2\theta cos^2\theta + C_{22}cos^4\theta}$$

where $A = (C_{11}C_{22} - C_{12}^2)/C_{66} - 2C_{12}$, $B = C_{11} + C_{22} - (C_{11}C_{22} - C_{12}^2)/C_{66}$. The results are plotted below.

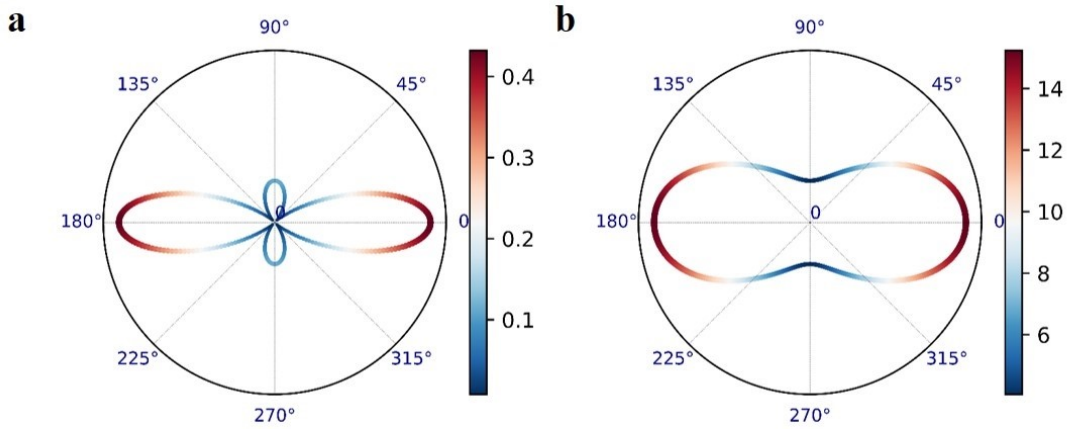


Figure S2. The mechanical properties of single layer Al_2Te_5: (a) Young's modulus Y(θ) and (b) Poisson's ratio υ(θ)

The spin-orbital coupling influences in monolayered Al_2Te_5

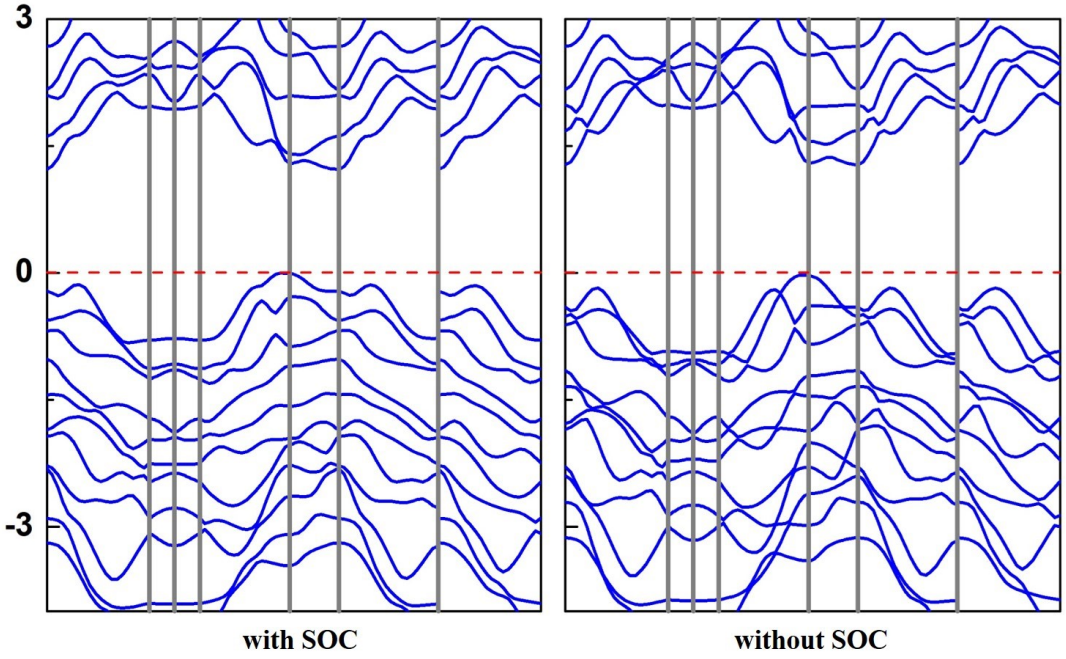


Figure S3. The band structure calculated with and without spin-orbital coupling in the monolayer.

The charge contribution from VBM and CBM in monolayered Al_2Te_5

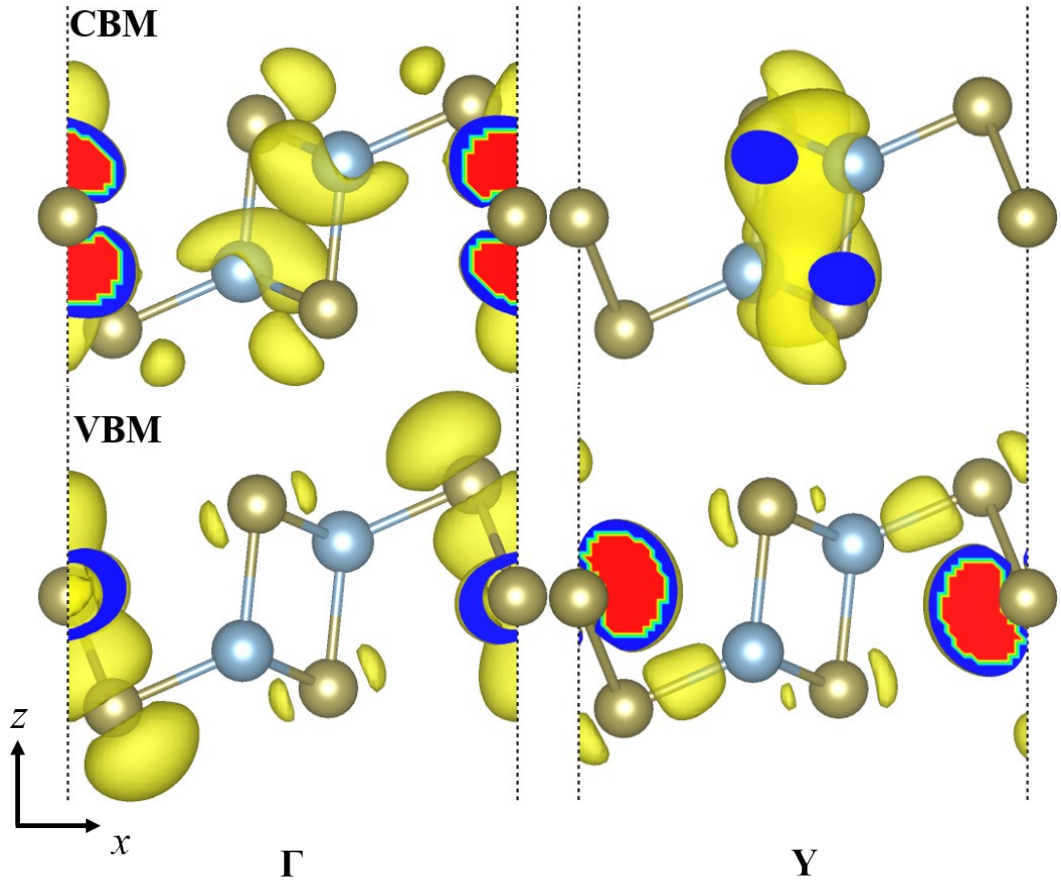
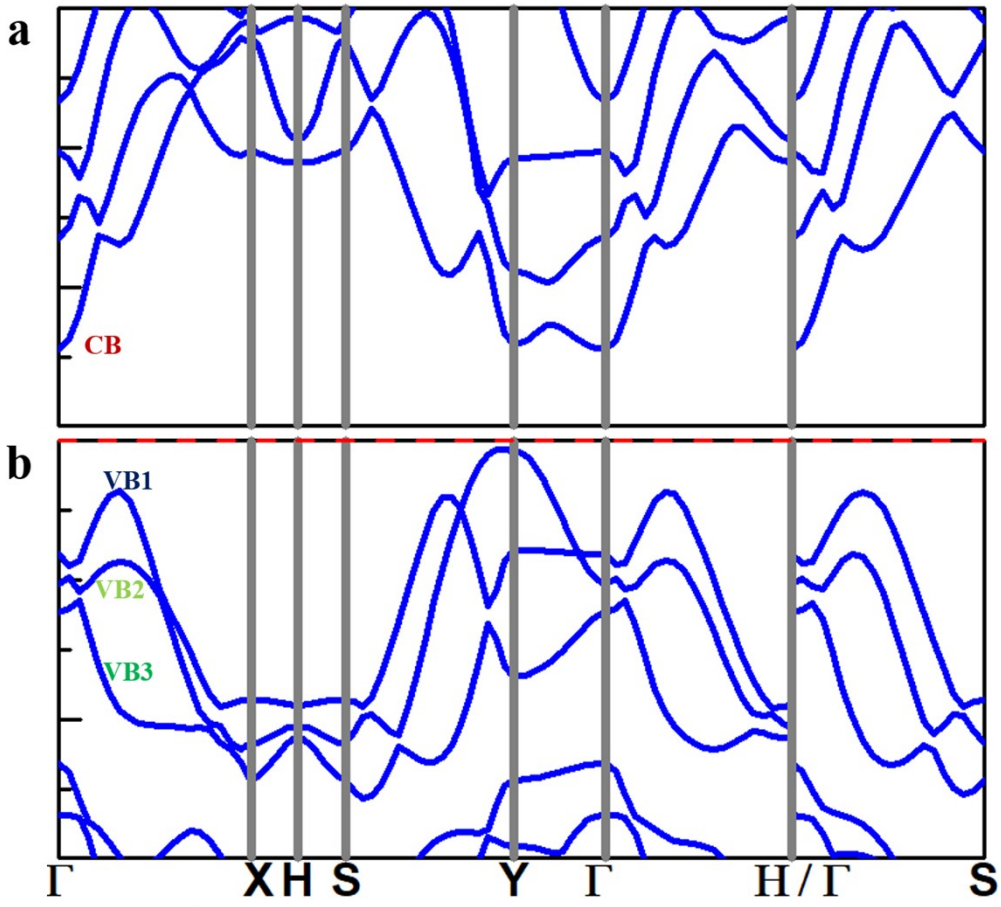


Figure S4. The charge contributed from CBM and VBM of Γ and Y points in the Brillouin zone

The symmetry analysis of VBs and CB in Al_2Te_5



	Γ	X	H	S	Y
CB	+	+	+	+	+
VB1	-	-	-	-	-
VB2	-	-	+	-	+
VB3	+	+	+	+	+

Figure S5. (a) and (b) different parts of the CB and VB band structure on the path of BZ, where the bands are labeled according to the energy. (c) the parity of the bands on high symmetry point in BZ.

The work function of Al_2Te_5

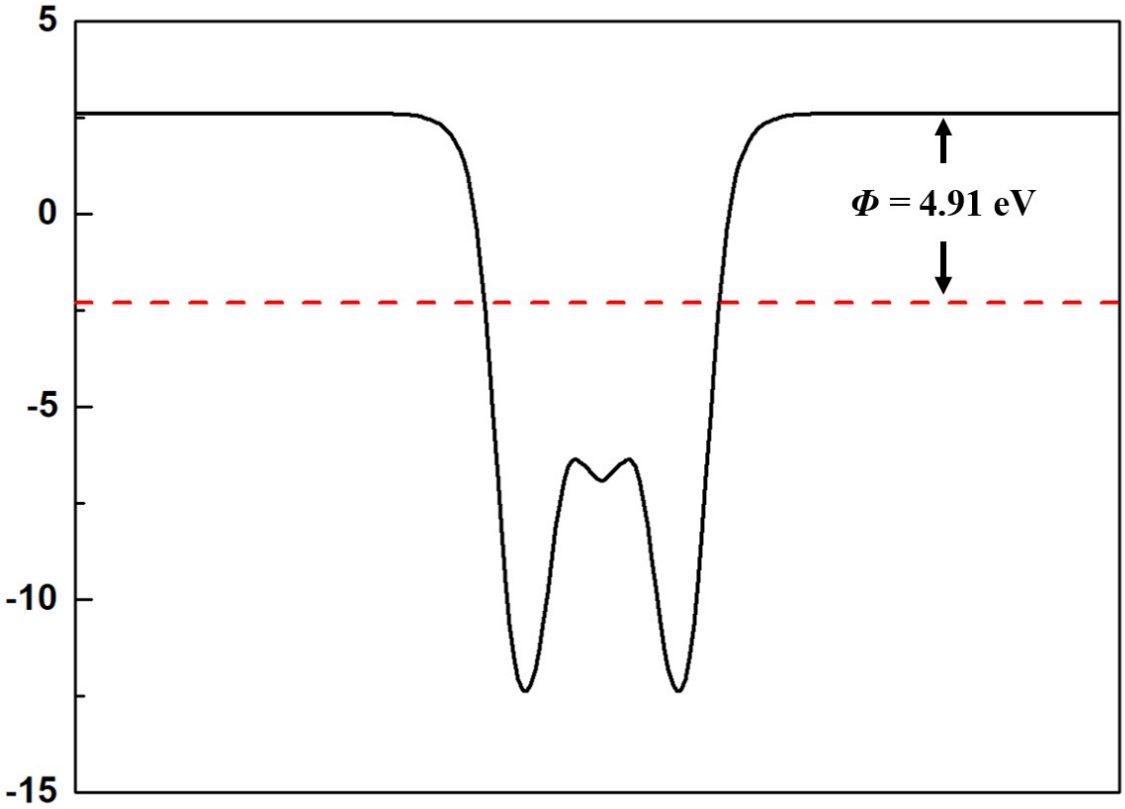


Figure S6. The calculated work function for layer Al_2Te_5 crystal.

Absorbance calculations

The interband optical transition is relevant with the imaginary part of the dielectric tensor $\varepsilon_2(\omega)$ as a function of photon frequency ω, at energies relevant for interband optical ransitions. Starting from $\varepsilon_2(\omega)$, the monolayer absorbance $A(\omega)$ of monolayer defined as the fraction of photons of energy $E = \hbar\omega$ absorbed by the monolayer, is obtained using an approximation analogous to what used by Yang et al. for graphene

$$A(\omega) = \frac{\omega}{c}\varepsilon_2 \Delta z$$

where c is the speed of light, and Δz is the size of the simulation cell in the layer-normal direction, it is set to be 1nm in the calculation in the manuscript for comparing with other materials. This formula can be seen as a Taylor expansion for small thickness $\Delta z \rightarrow 0$ of the absorbance $A = 1 - e^{-\alpha\Delta z}$ for a flat layer of a bulk material with thickness Δz and absorption coefficient. $\alpha(\omega) = \frac{\varepsilon_2 \omega}{cn}$ with refractive index $n = 1$ due to the presence of vacuum in the vast majority of the simulation cell. Equivalently, it can be seen as deriving from the polarizability per unit area or from the optical conductivity of the monolayer. The absorbance defined with this approach is independent of the simulation cell size, since $\varepsilon_2 \propto \Delta z^{-1}$ when a large vacuum is introduced.

The feasibility for applying biaxial strain

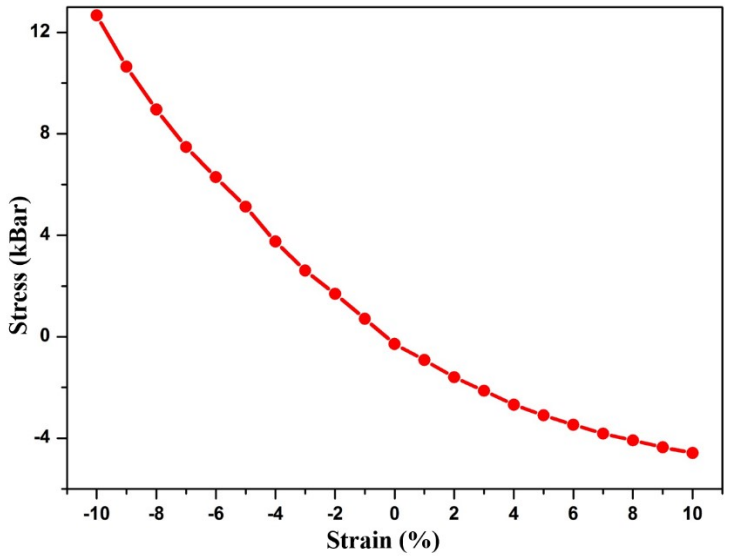


Figure S7. The calculated stress of Al_2Te_5 monolayer under the biaxial strain (from -10% to 10%).