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Supporting Information for

Giant piezoelectricity and ferroelectricity in two-dimensional ThOTe monolayer

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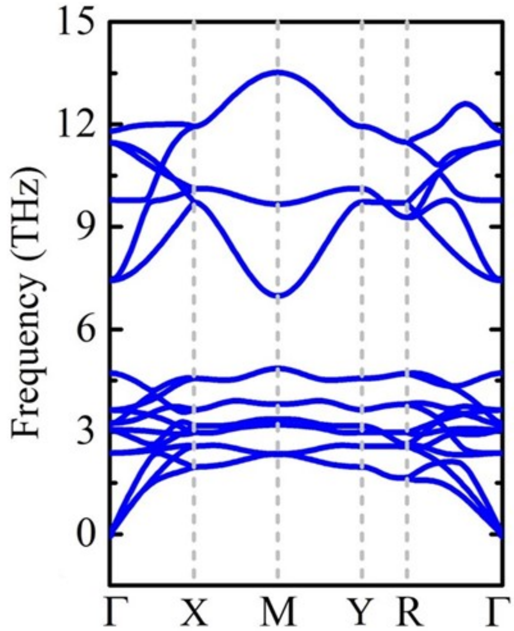

Figure S1 Phonon spectrum of ThOTe along the high symmetric points in BZ.

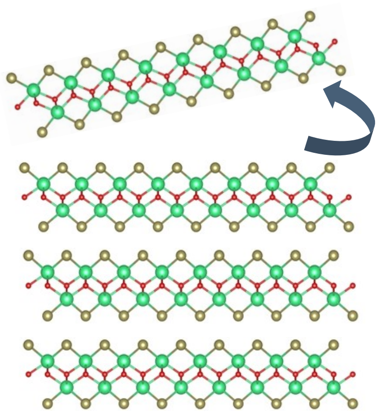

Figure S2 Schematic diagram of ThOTe monolayer exfoliation process.

We calculated the bulk modulus and shear modulus using the following formulate,

$$K^V = \frac{C_{11} + C_{22} + 2C_{12}}{4},$$

$$G^V = \frac{C_{11} + C_{22} - 2C_{12} + 4C_{66}}{8},$$

$$K^R = \frac{1}{S_{11} + S_{22} + 2S_{12}},$$

$$G^R = \frac{2}{S_{11} + S_{22} - 2S_{12} + S_{66}},$$

$$G^H = \frac{G_V + G_R}{2},$$

$$K^H = \frac{B_V + B_R}{2}$$

According to Hill, the arithmetic mean of the Voight and Reuss values can be used as an estimate of the mean shear modulus and mean bulk modulus, K and G and their ratios are shown in Table 1.

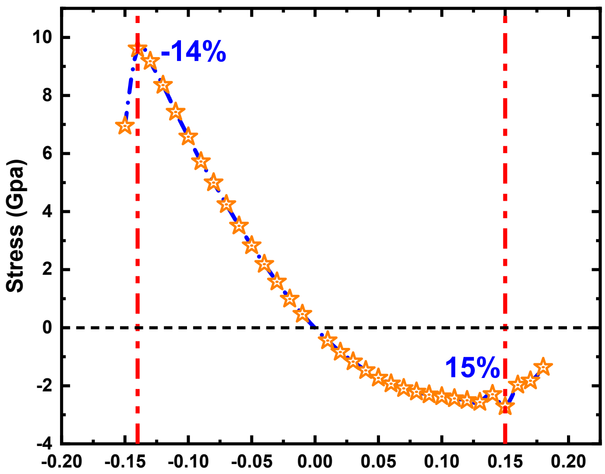

Figure S3 Stress-strain curves in the ThOTe monolayer, the black dashed line corresponds to the magnitude of the strain when the stress is zero.

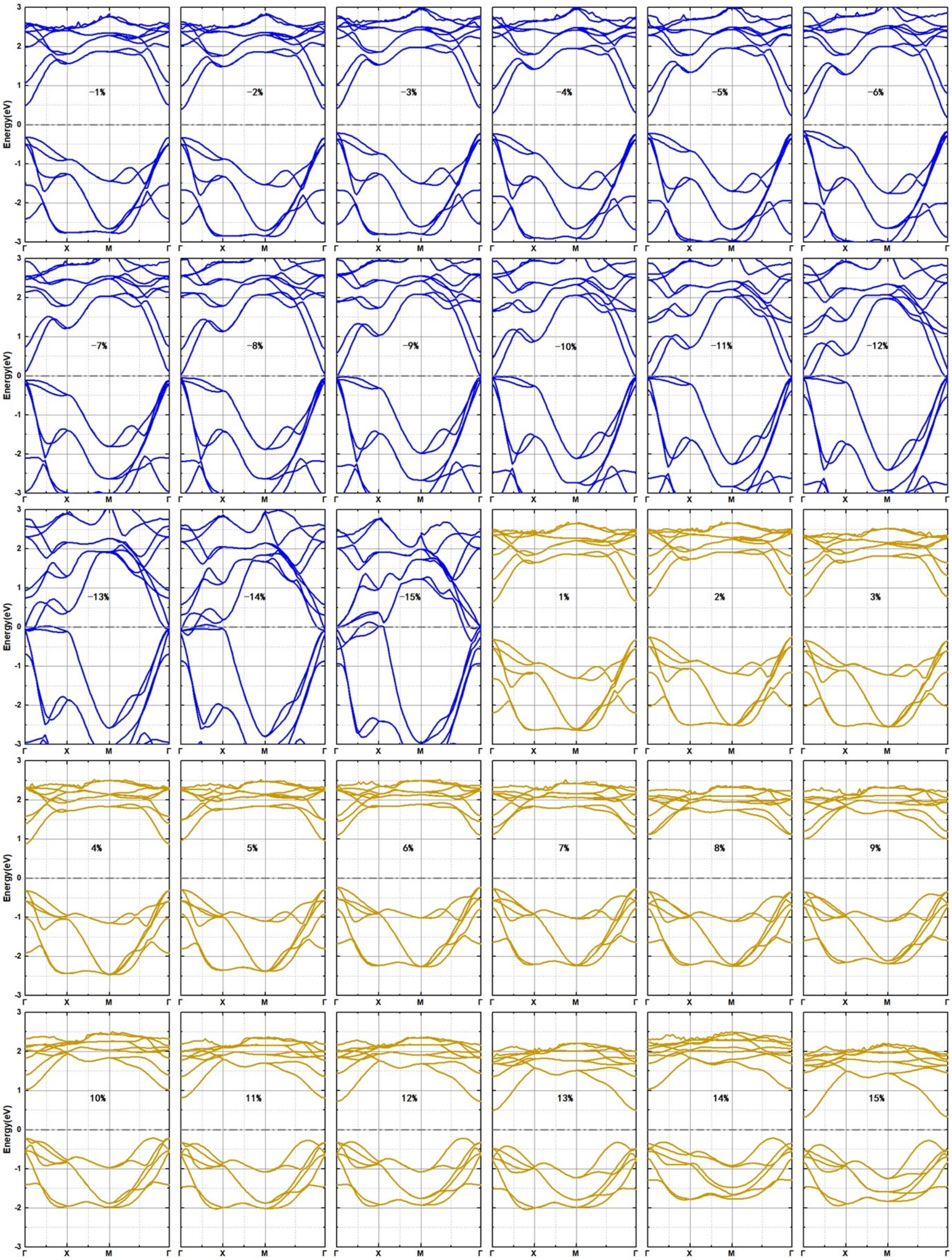

Figure S4 The band structure evolution of ThOTe monolayer under different strains. The energy at the Fermi level is set to zero.

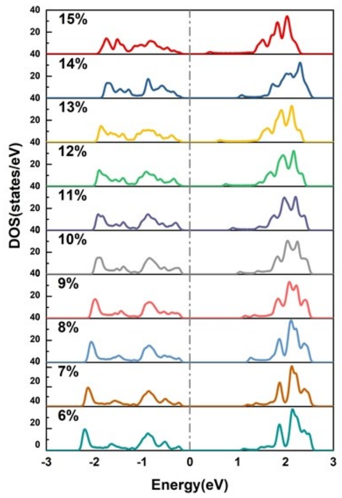

Figure S5 The evolution of Density of states in ThOTe lattice under different strains. The energy at the Fermi level is set to zero.

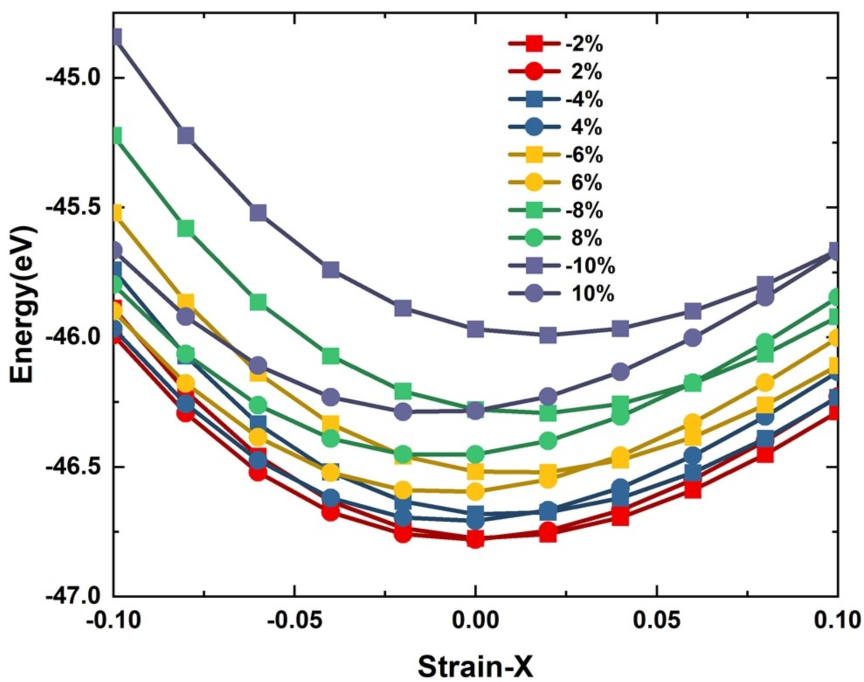

Figure S6 Energy in a monolayer ThOTe lattice at different strains in biaxial, respectively.

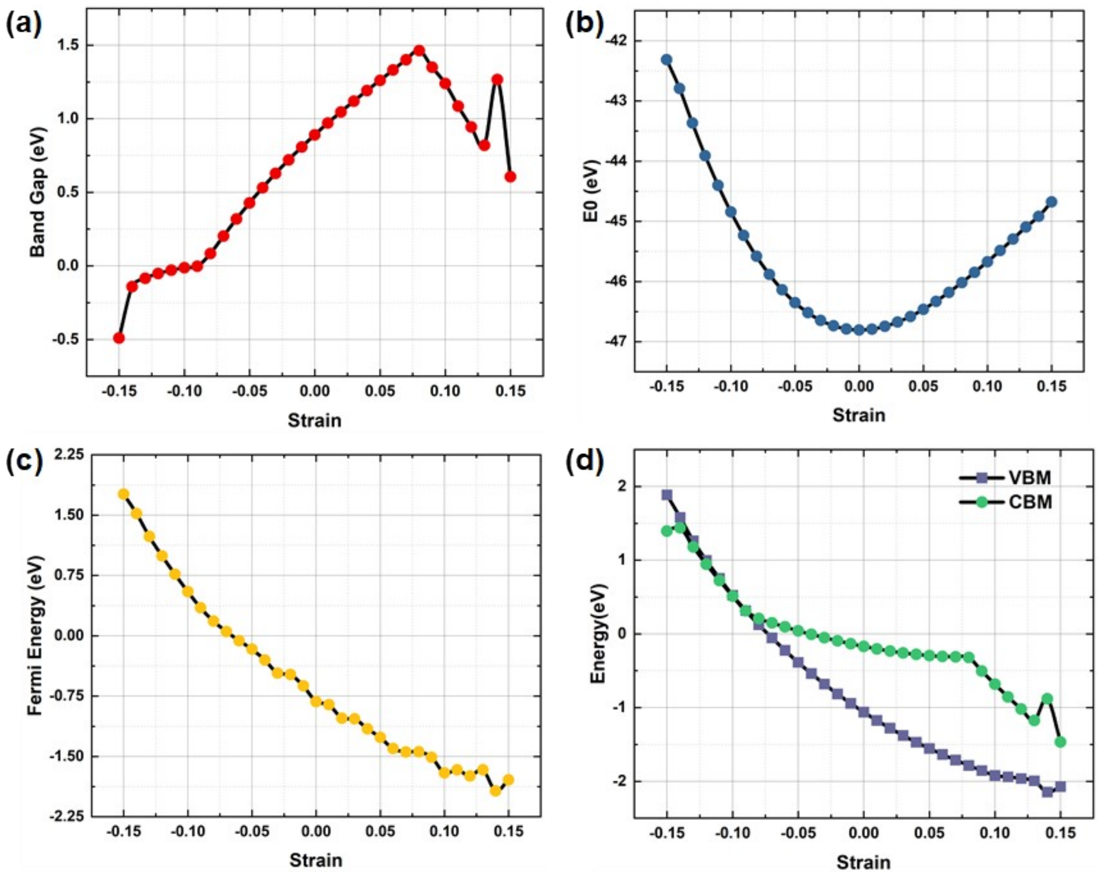

Figure S7 The evolution of (a) band gap, (b) energy, (c) Fermi level and (d) the locations of the valence band maximum (VBM) and the conduction band minimum (CBM) under different strains.

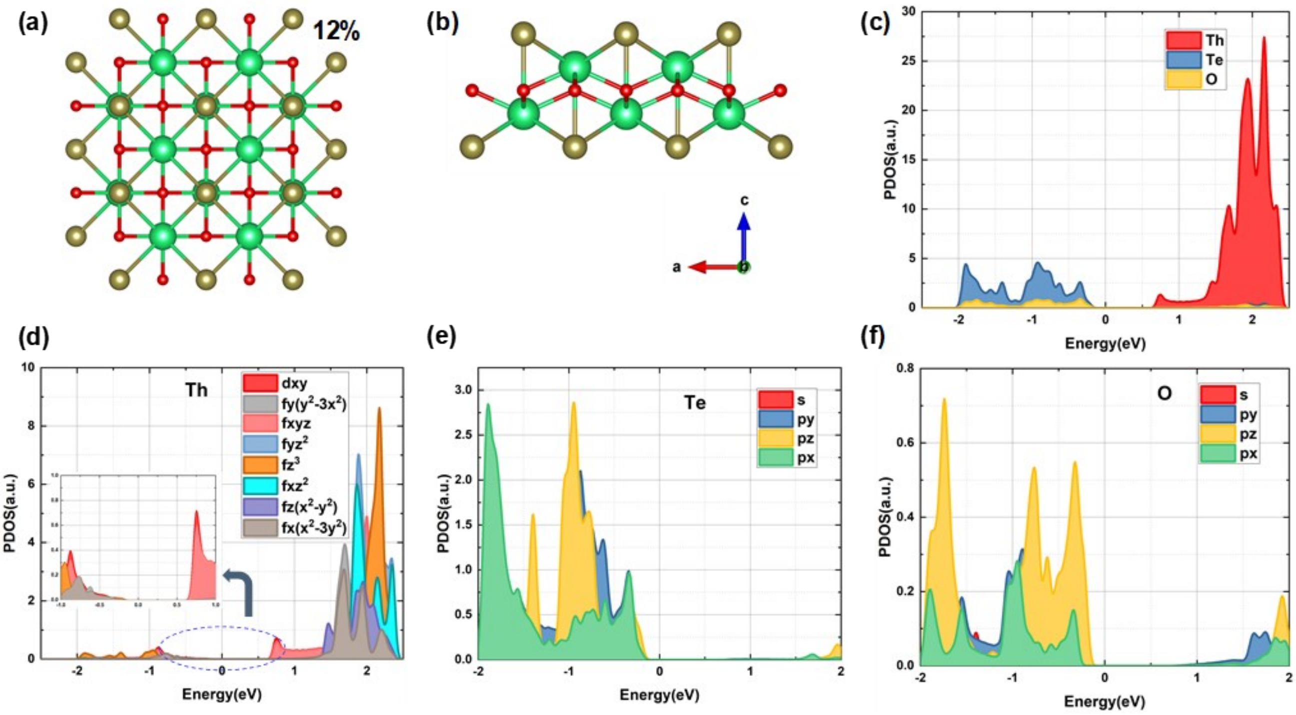

Figure S8 (a) and (b) represent the top and side views of ThOTe monolayer with 12% strain, respectively. The green, brown and red spheres represent the Th, Te and O atoms, respectively. (c) ~ (f) Electron density of states projected onto different atoms and atomic orbitals of Th, Te and O atoms.

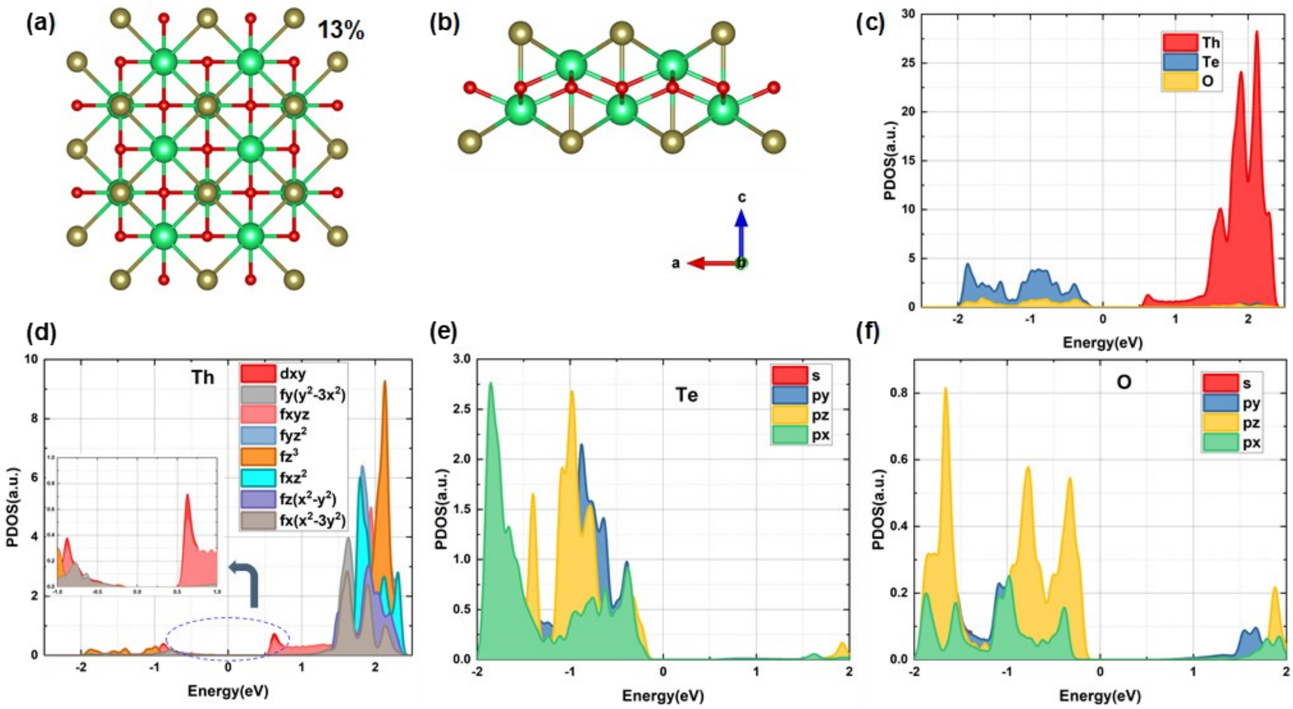

Figure S9 (a) and (b) represent the top and side views of ThOTe monolayer with 13% strain, respectively. The green, brown and red spheres represent the Th, Te and O atoms, respectively. (c) ~ (f) Electron density of states projected onto different atoms and atomic orbitals of Th, Te and O atoms.

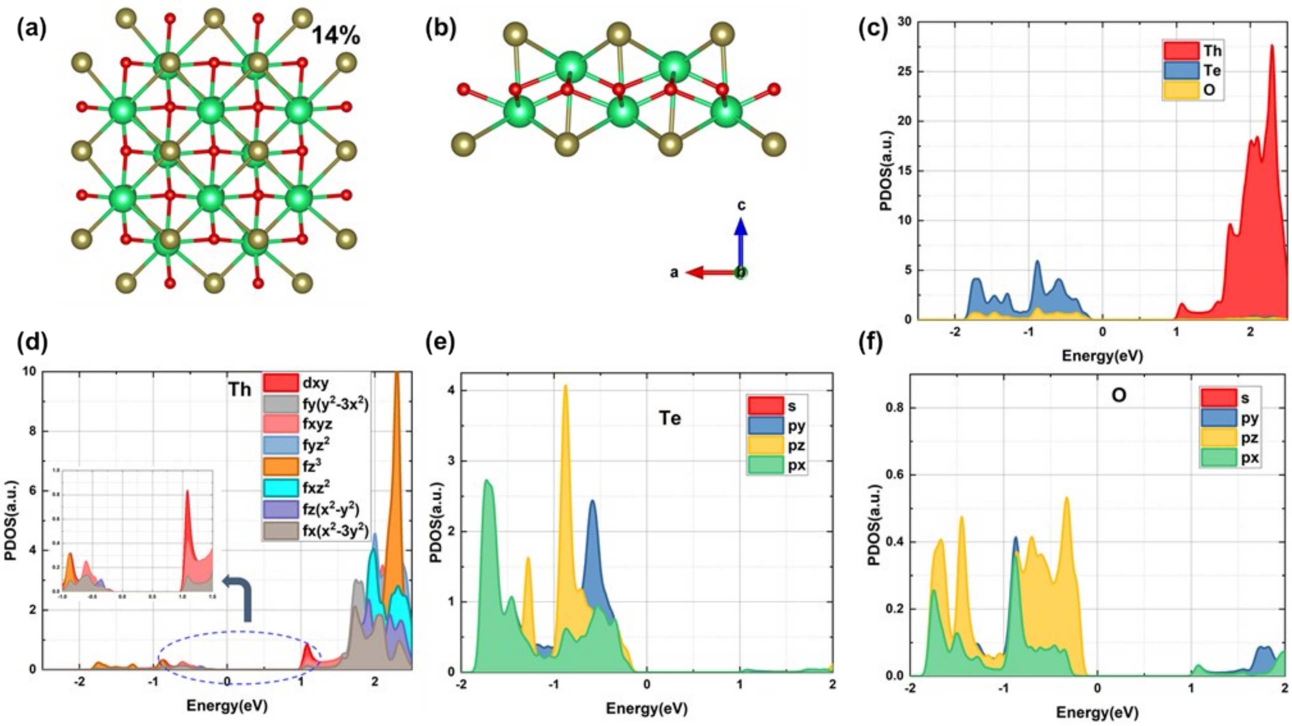

Figure S10 (a) and (b) represent the top and side views of ThOTe monolayer with 14% strain, respectively. The green, brown and red spheres represent the Th, Te and O atoms, respectively. (c) ~ (f) Electron density of states projected onto different atoms and atomic orbitals of Th, Te and O atoms.

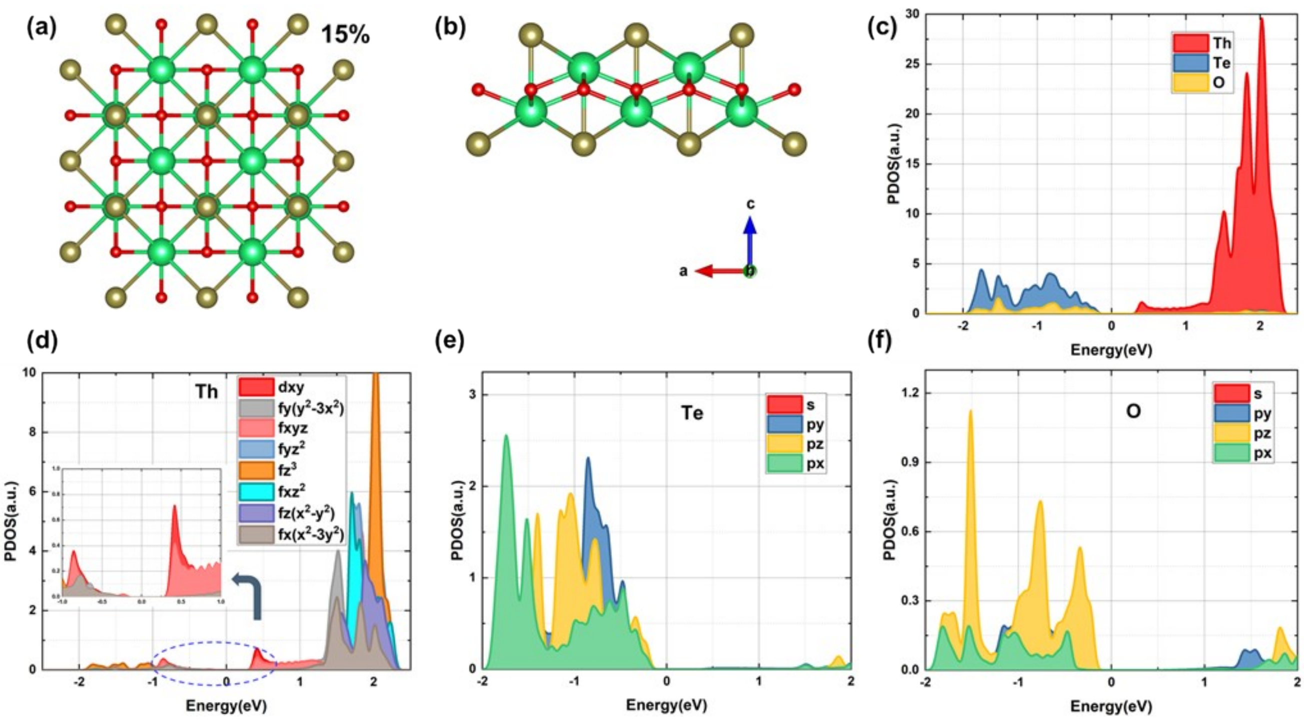

Figure S11 (a) and (b) represent the top and side views of ThOTe monolayer with 15% strain, respectively. The green, brown and red spheres represent the Th, Te and O atoms, respectively. (c) ~ (f) Electron density of states projected onto different atoms and atomic orbitals of Th, Te and O atoms.

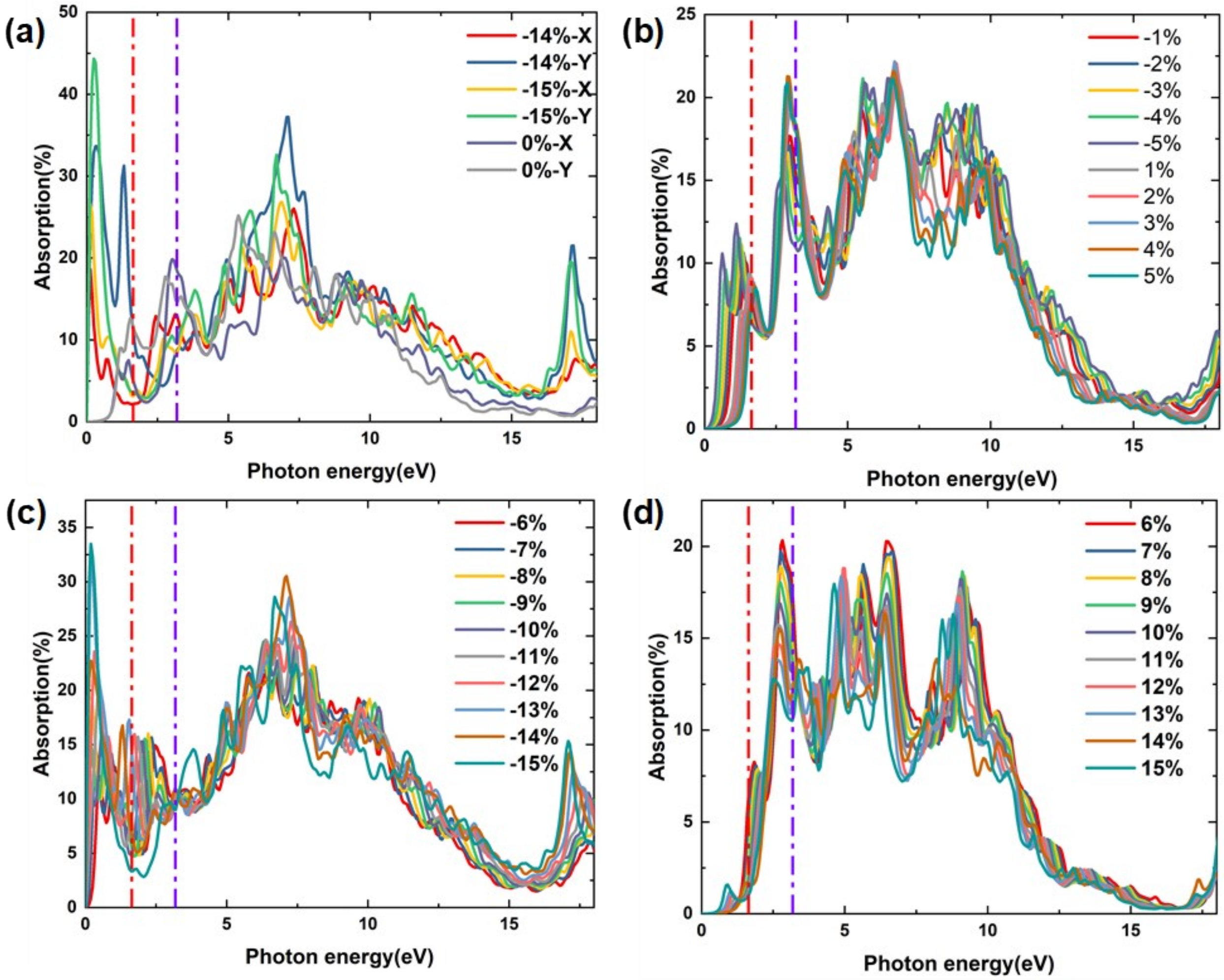

Figure S12 The photon energy absorption coefficients of ThOTe under different strains. (a) The x and y directions photon energy absorption coefficients of ThOTe under no strain, 14%, and 15% compressive strains. (b) The average photon energy absorption coefficients of ThOTe under 1%-5% tensile and compressive strains. (c) The average photon energy absorption coefficients of ThOTe under 6%-15% compressive strains. (d) The average photon energy absorption coefficients of ThOTe under 6%-15% tensile strains.

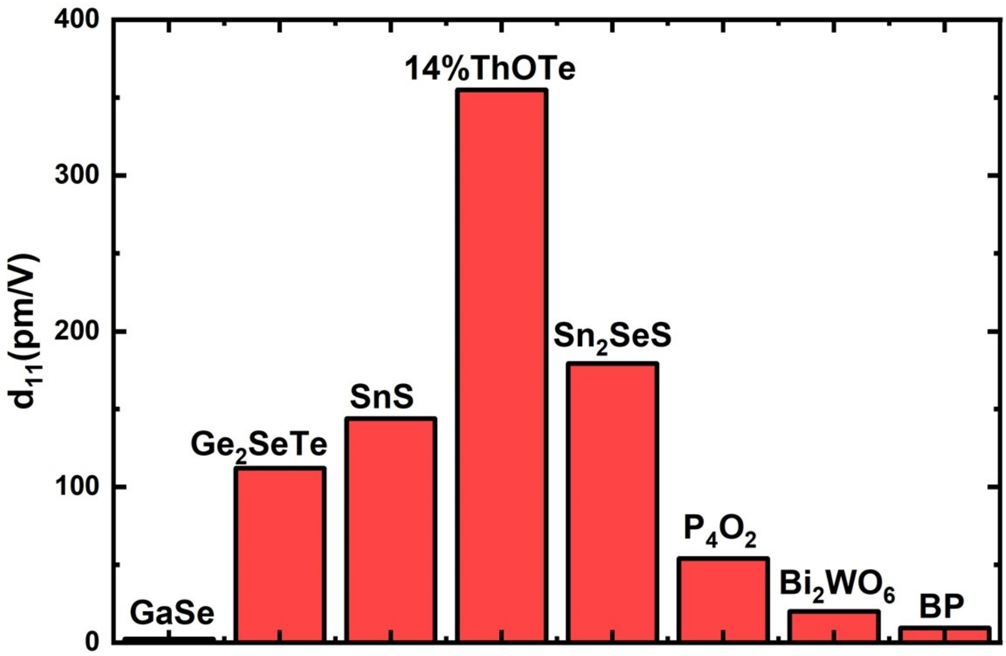

Figure S13 d_{11} of ThOTe at 14% strain and some other 2D materials by DFT calculation. [1-5]

References

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