Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental materials

First-principles investigation of in-plane anisotropies in $XYTe_4$ monolayers with X = Hf, Zr, Ti and Y = Si, Ge

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Figure S1

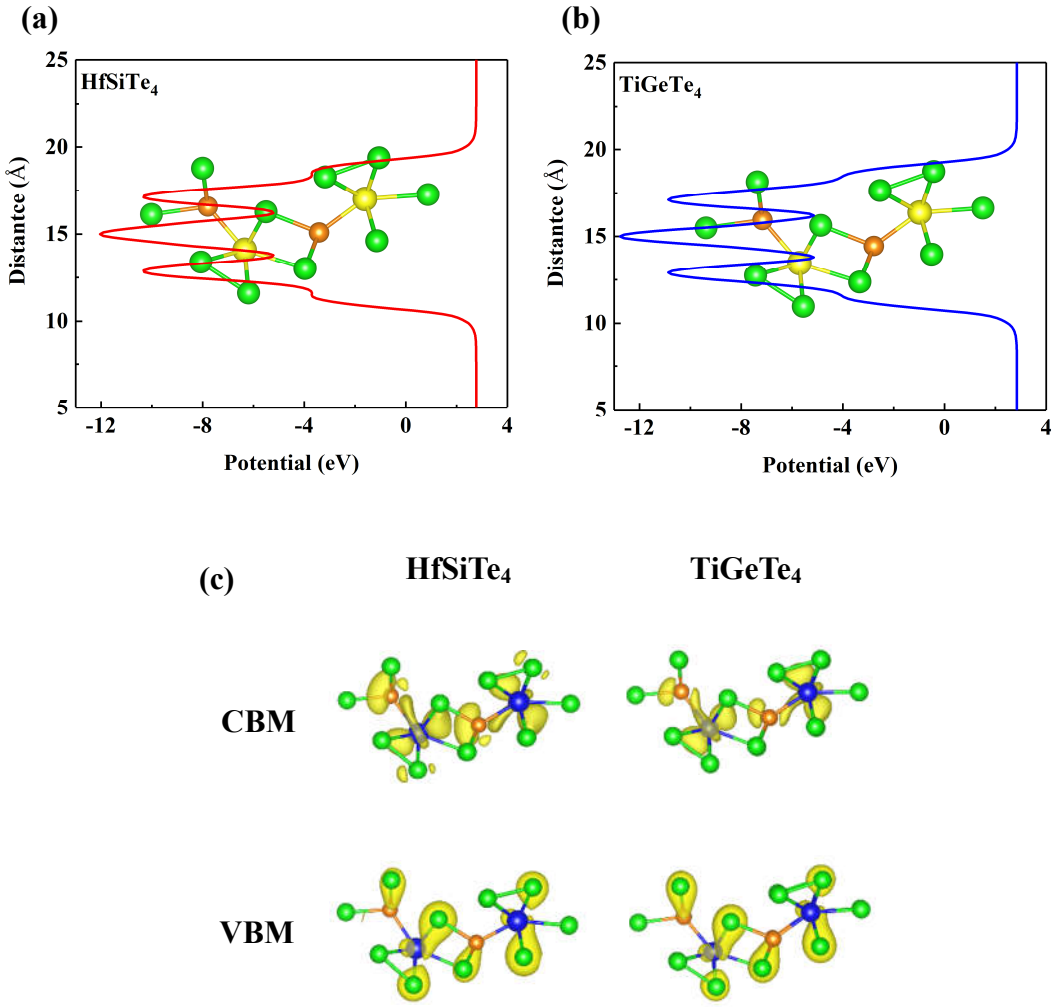

Figure S1. Potential average of (a) $HfSiTe_4$ and (b) $TiGeTe_4$ monolayer. (c) Band decomposed partial charge density of $HfSiTe_4$ and $TiGeTe_4$ at the Γ-centered of 0.002 e $Å^{-3}$ isosurface level. Transition metal atoms are turned blue for better visibility.

Figure S2

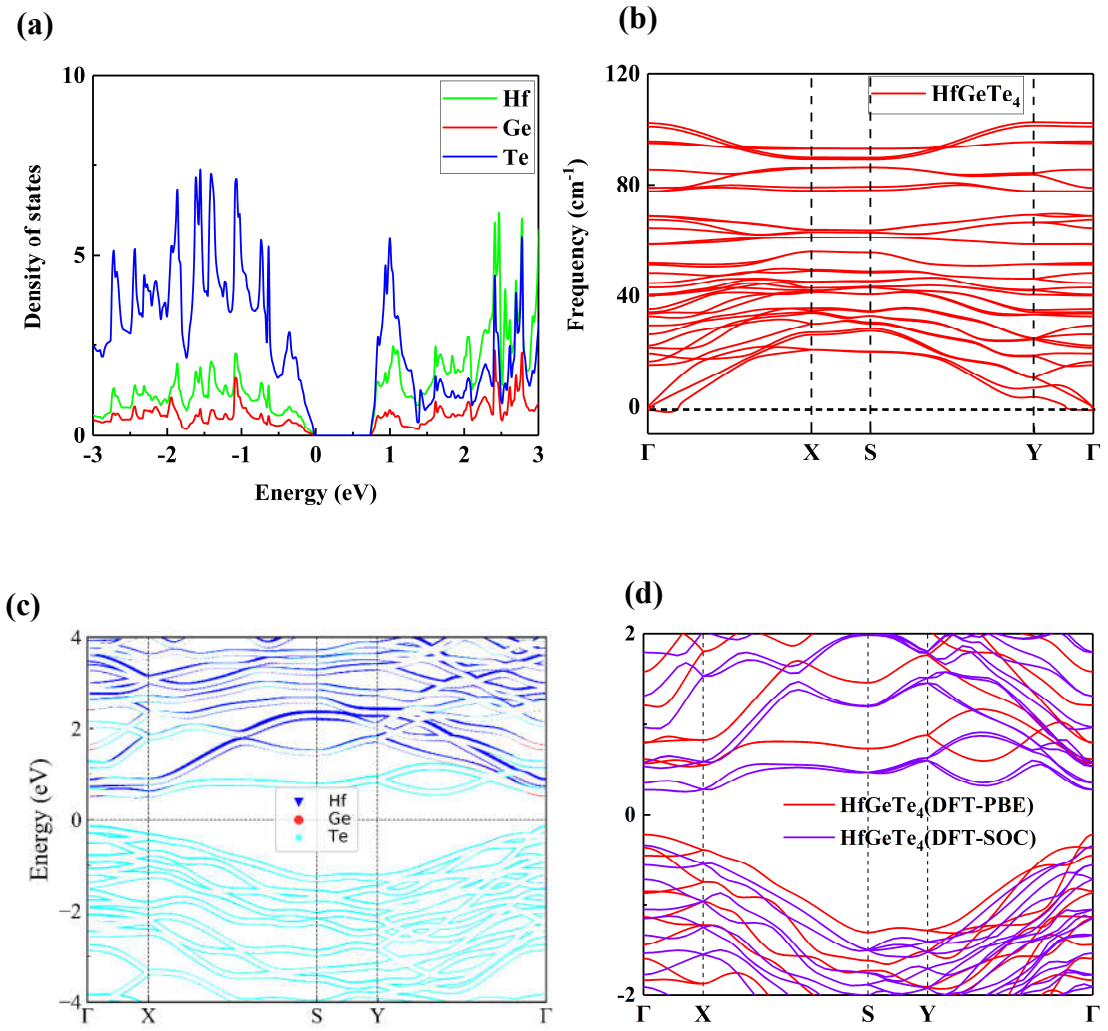

Figure S2. Projected density of states (in arb. unit) of (a) $HfGeTe_4$, showing that the dominant states at the VBM are Te *p*-states and CBM are Hf *d*-states, respectively. (b) Phonon band dispersions of $HfGeTe_4$ monolayer. (c) Atom-dependent projected electronic band structures for $HfGeTe_4$ within the scheme of DFT-PBE. (d) The electronic band structures of $HfGeTe_4$ in the frame work of DFT-PBE and SOC.

Figure S3

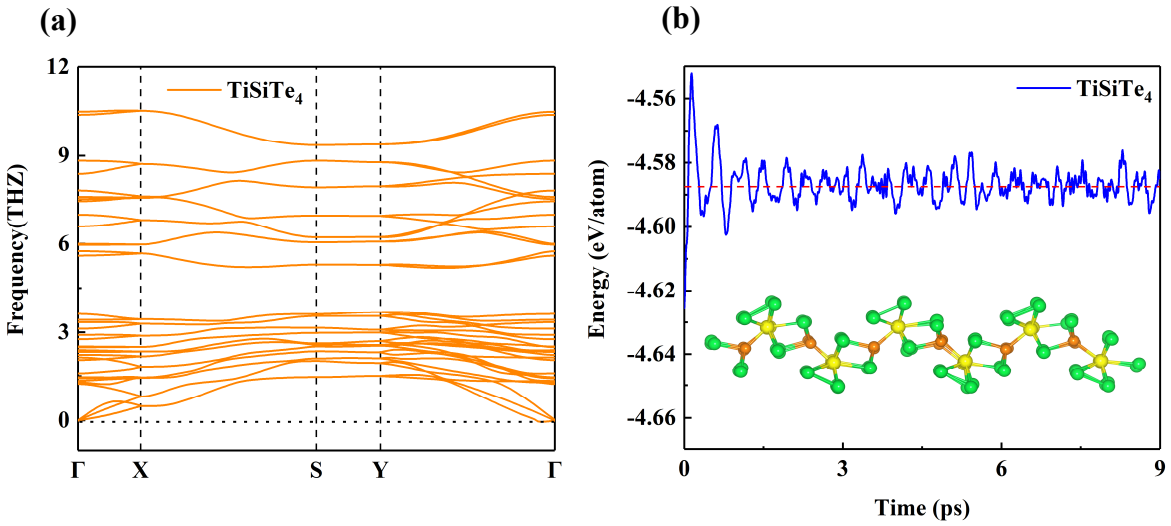

Figure S3. (a) Phonon band dispersions of $TiSiTe_4$ monolayer. (b) The variation of energy with respect to the time at 300 K for $TiSiTe_4$ monolayer, the insets show the snapshots of atomic configurations at the end of *ab initio* molecular dynamics (AIMD) simulations.

Figure S4

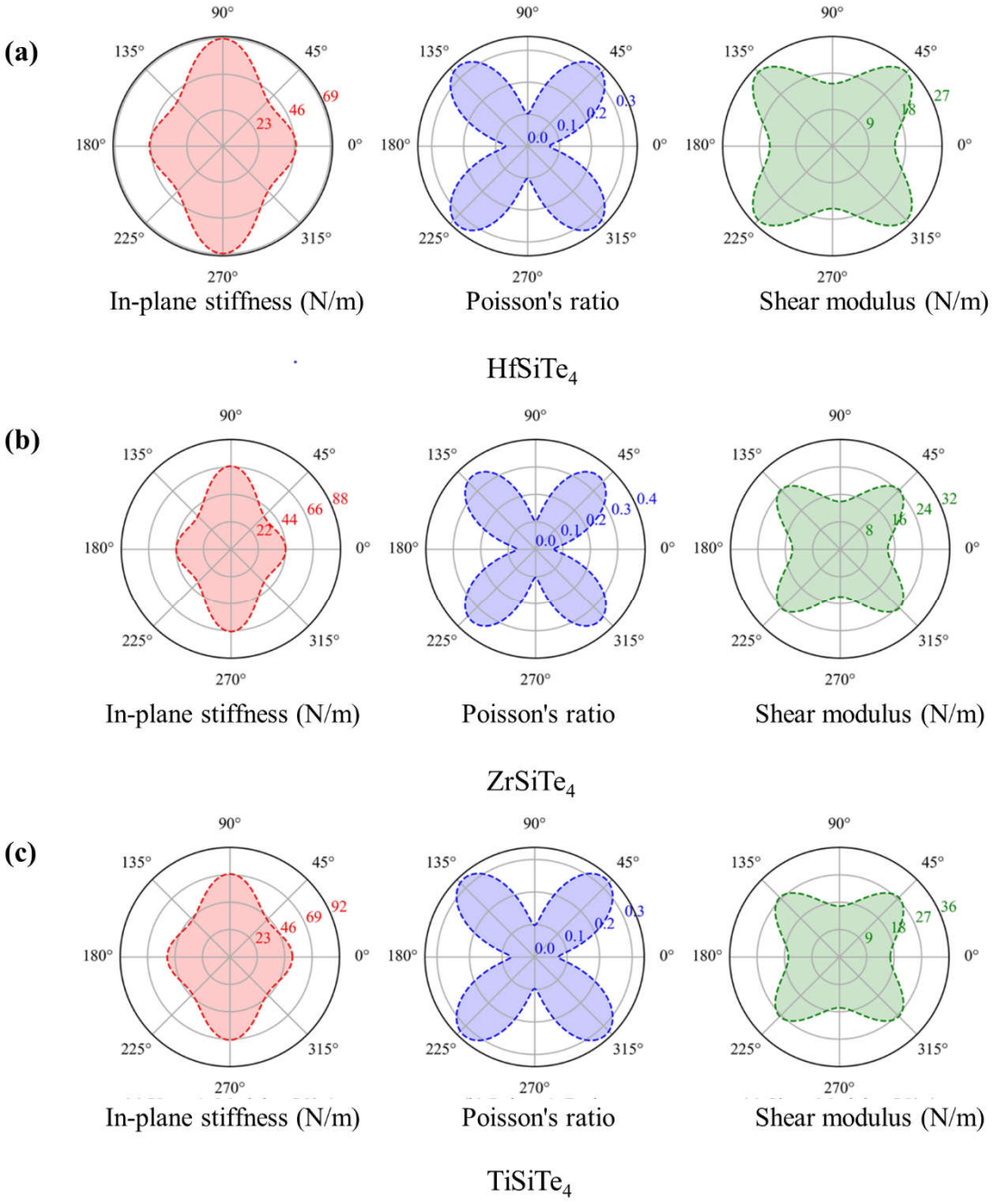

Figure S4. Orientation-dependent in-plane stiffness, Poisson's ratio and shear modulus of (a) $HfSiTe_4$, (b) $ZrSiTe_4$, and (c) $TiSiTe_4$ monolayers.

Figure S5

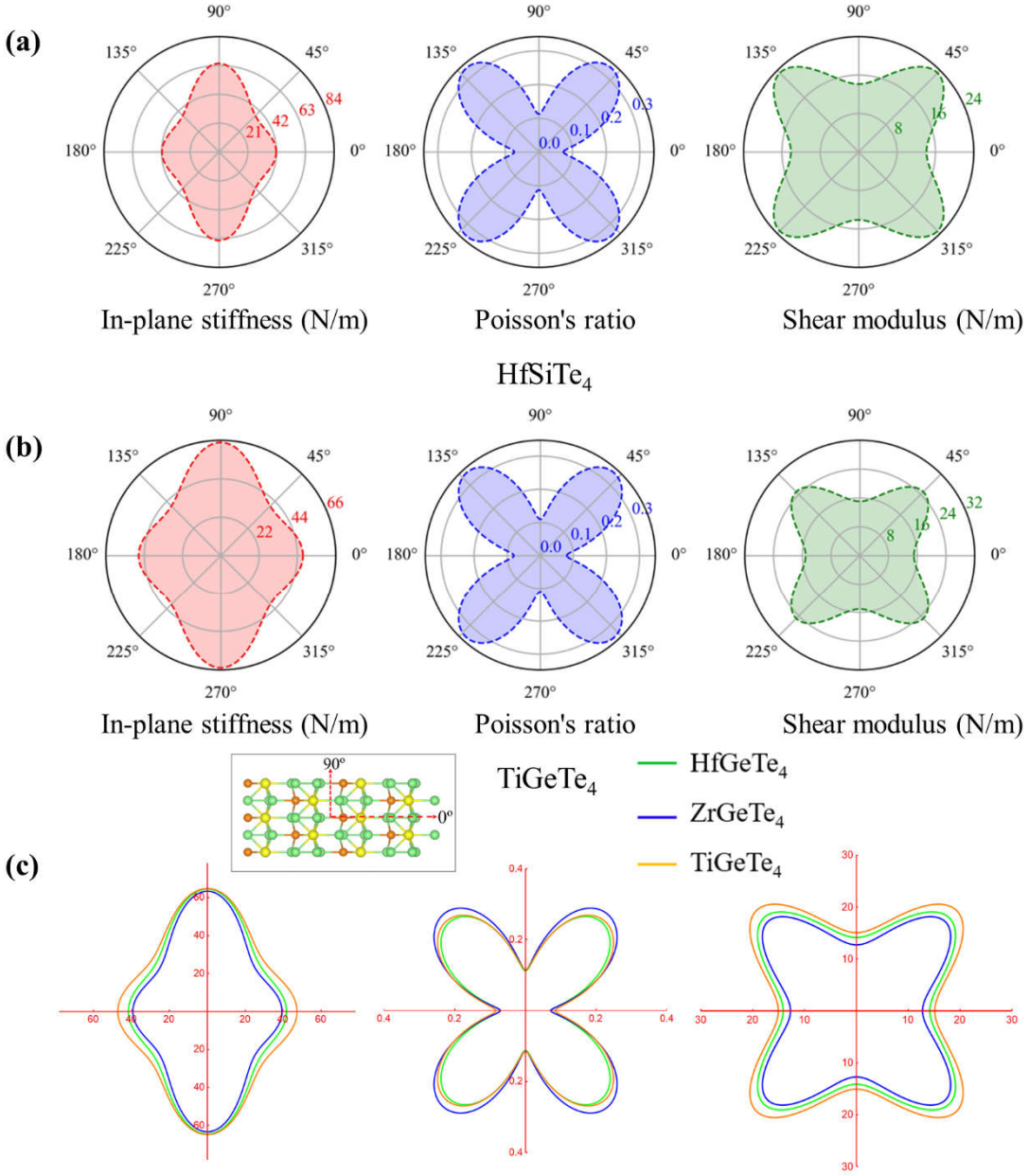

Figure S5. Orientation-dependent in-plane stiffness, Poisson's ratio and shear modulus of (a) $HfGeTe_4$ and (b) $TiGeTe_4$ monolayers. (c) Orientation-dependent linear-elastic constants of $XGeTe_4$ (X = Hf, Zr or Ti).

Figure S6

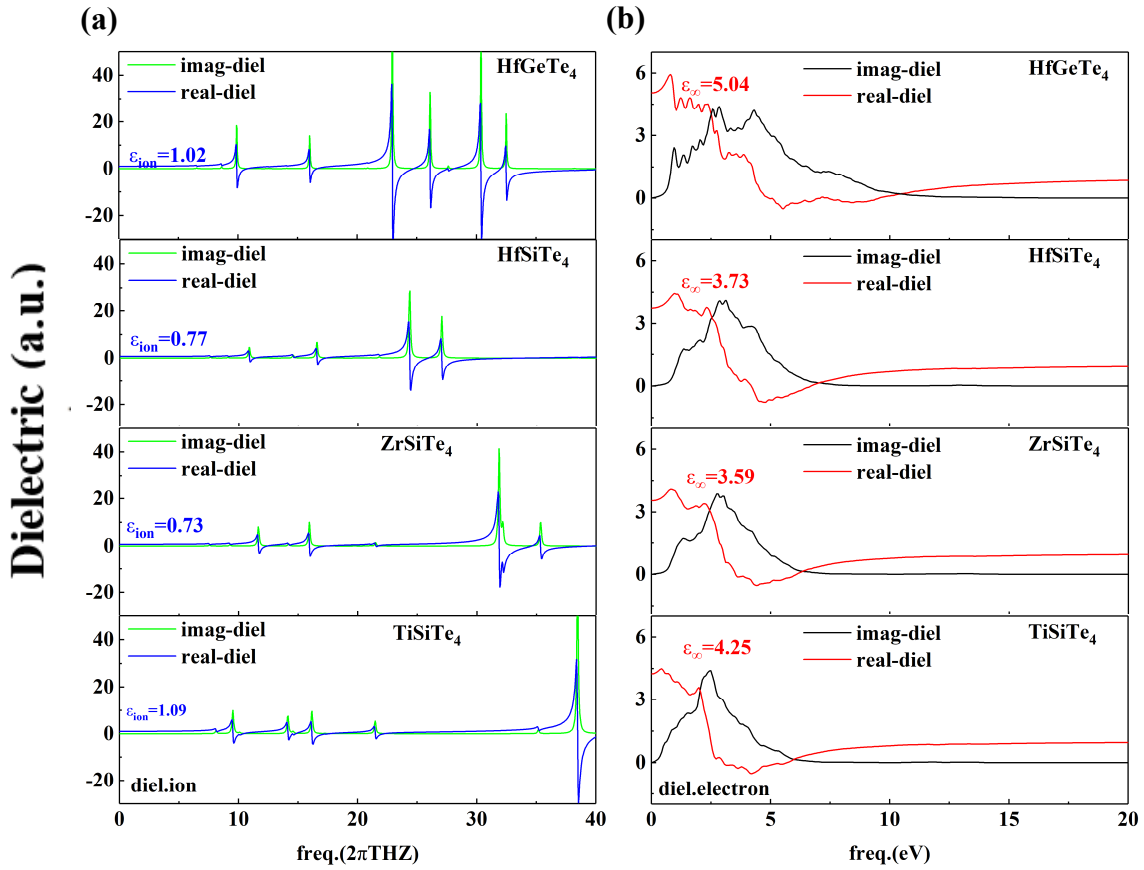

Figure S6. Imaginary and real parts of dielectric function of $XYTe_4$ as a function of photon frequencies, ionic contribution on the left (a) and electron contribution on the right (b).