Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplemental Information

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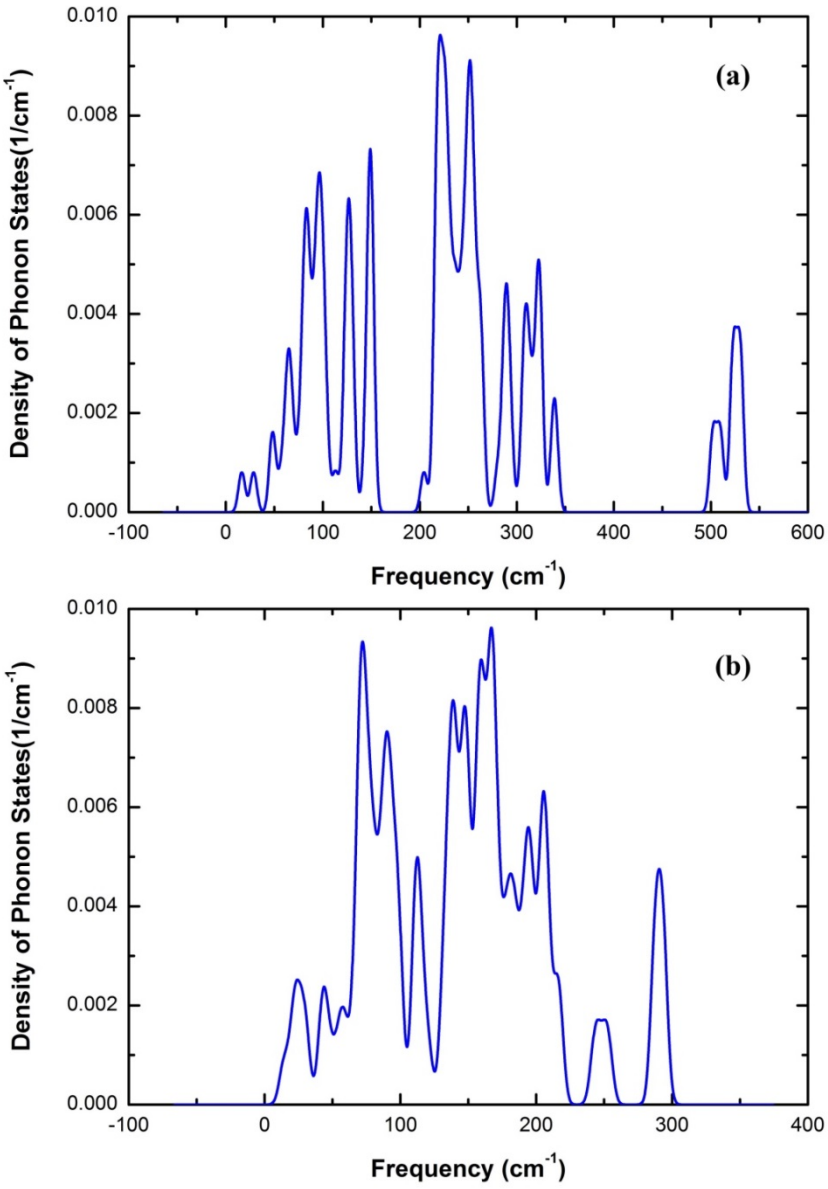

Figure S1. Computed phonon density of states (DOS) of unstrained TMTC monolayer: (a) HfS_3, (b) $HfSe_3$. The linear response method, implemented in CASTEP 7.0, was adopted to compute the phonon DOS. More specifically, the PBE functional was chosen; and the energy cut off was set to 650 eV for HfS_3 and 400 eV for $HfSe_3$, for both structural optimization and phonon DOS computation. The density of Monkhorst-Pack q-vectors 3 × 4 × 1 was selected. The vacuum space was greater than 15 Å.

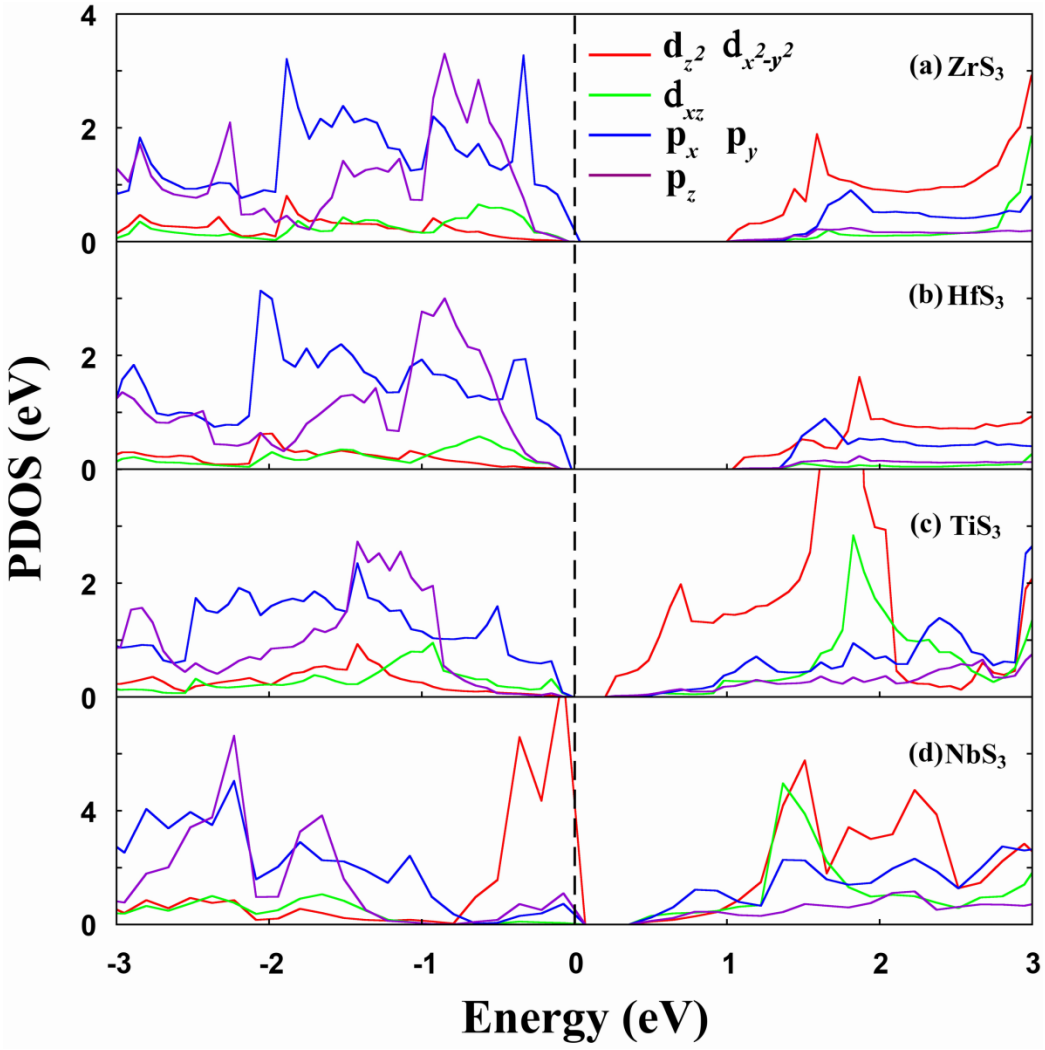

Figure S2. Computed PDOS (optB86b-vdW functional) of unstrained TMTC monolayers: (a) ZrS_3, (b) HfS_3, (c) TiS_3, and (d) NbS_3. The red lines denote the d_{z^2} and $d_{x^2-y^2}$ orbitals of M atom, the green lines denote the d_{xz} orbital of M atom. The blue lines denote the p_x and p_y orbitals of X atom, and the yellow lines denote the p_z orbital of X atom. The Vertical dashed line denotes the Fermi level.

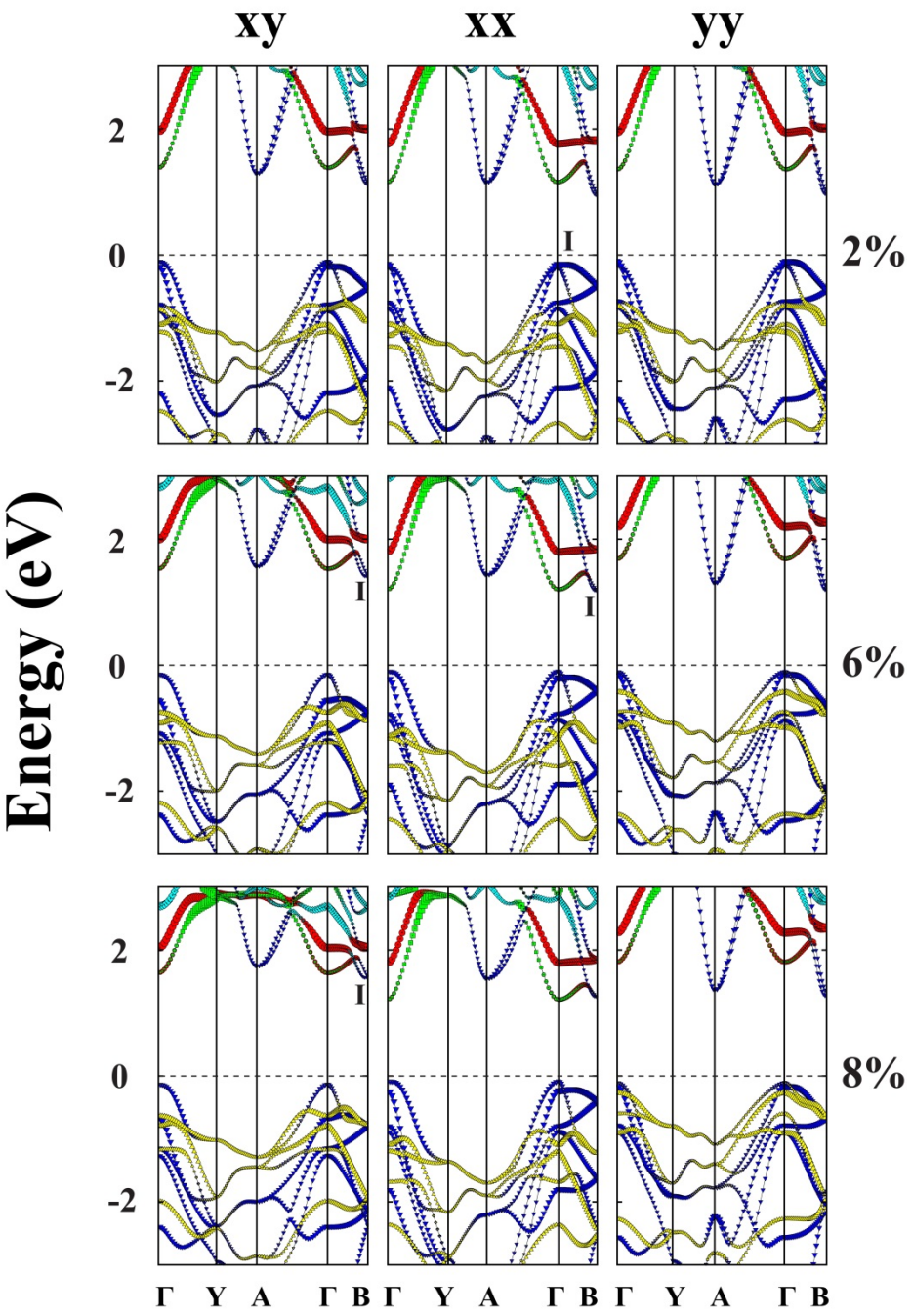

Figure S3. Computed band structures of strained monolayer $ZrSe_3$ *versus* biaxial tensile strain (xy) in both x and y directions, the uniaxial tensile strain in x direction (xx) or y direction (yy). The red lines denote the d_{z^2} orbital of the Zr atom. The green lines denote the $d_{x^2-y^2}$ orbital of Zr atom. The cyan lines denote the d_{xy}, d_{yz} and d_{xz} orbitals of Zr atom. The blue lines denote the p_x and p_y orbitals of Se atom, and the yellow lines denote the p_z orbital of Se atom. The dashed line indicates the Fermi level. I refers to either the VBM or CBM that is not located at the Γ point.

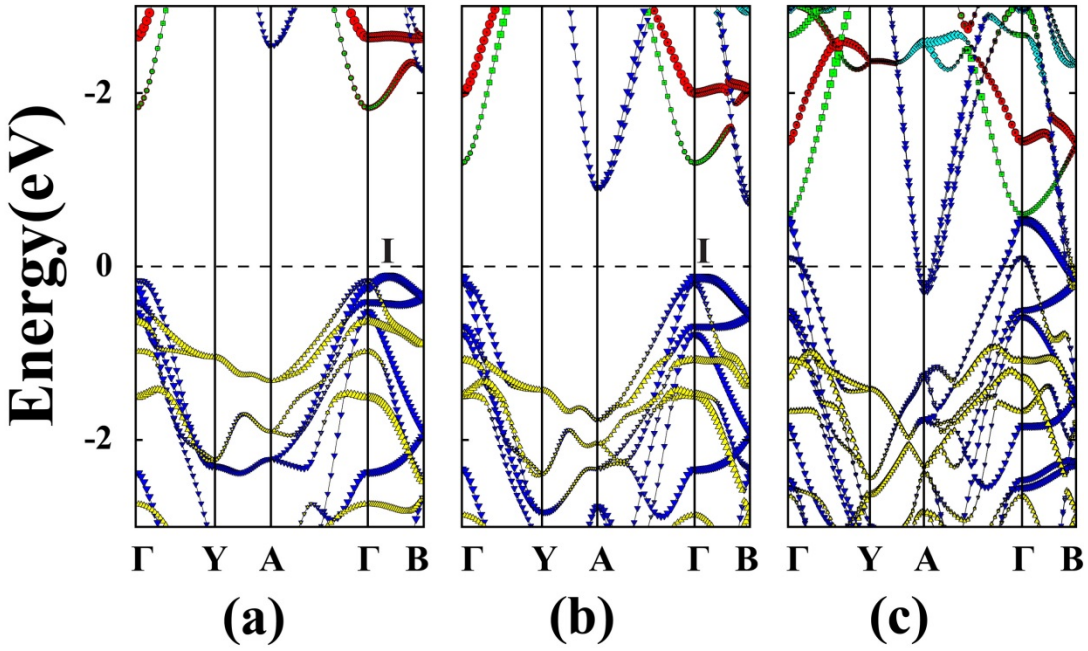

Figure S4. Band structures of unstrained monolayers: (a) HfS_3, (b) $HfSe_3$, (c) $HfTe_3$.The red lines denote the d_{z^2} orbital of Hf atom. The green lines denote the $d_{x^2-y^2}$ orbitals of Hf atom. The cyan lines denote the d_{xy}, d_{yz} and d_{xz} orbitals of Hf atom. The blue lines denote the p_x and p_y orbitals of (a) S, (b) Se, and (c) Te atom, and the yellow lines denote the p_z obital of (a) S, (b) Se, and (c) Te atom . The dashed lines indicate the Fermi level.

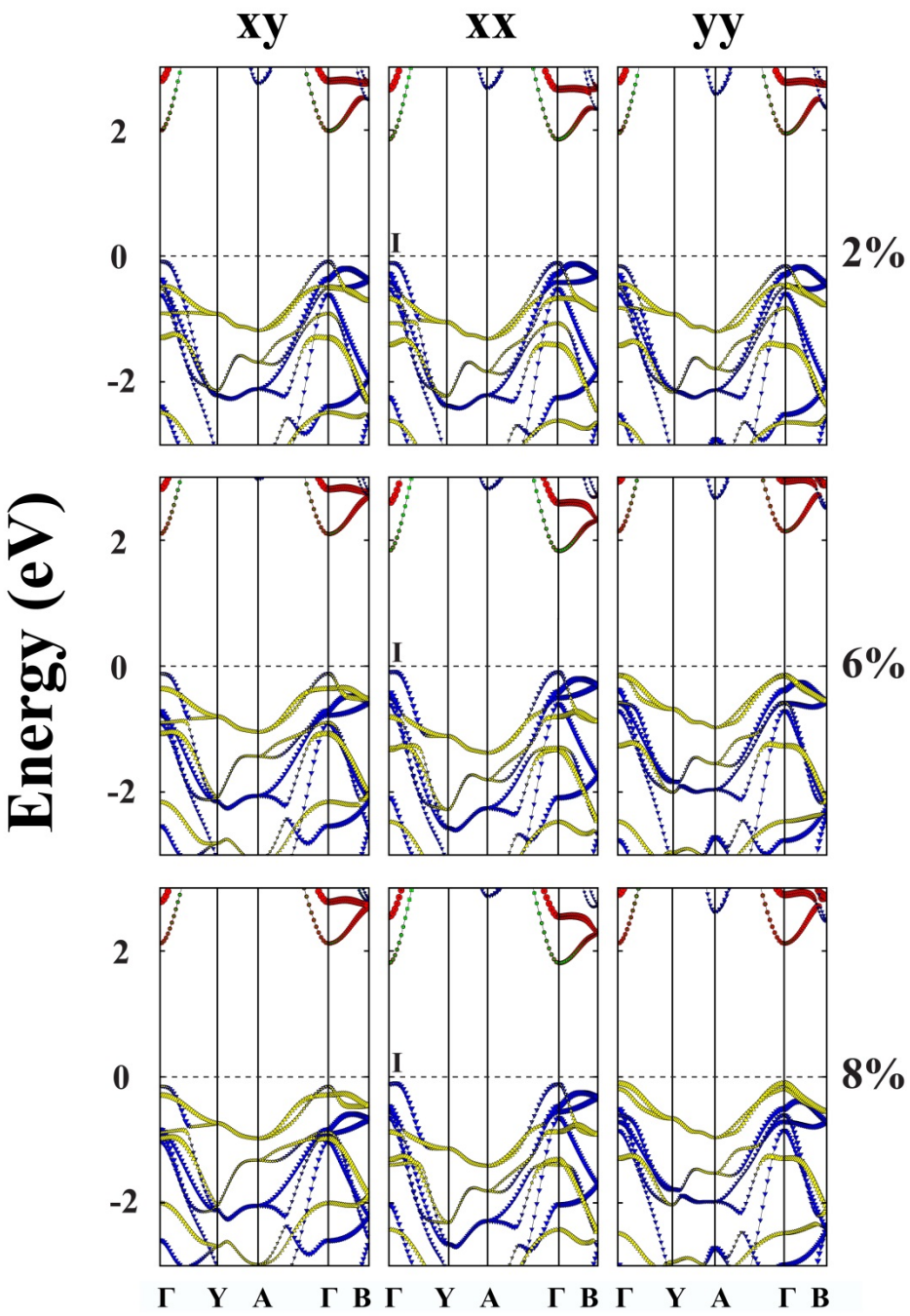

Figure S5. Computed band structures of strained monolayer HfS_3 *versus* biaxial tensile strain in both x and y directions (xy), the uniaxial tensile strain in x direction (xx) or y direction (yy). The red and green lines illustrate the d_{z^2} orbital and the $d_{x^2-y^2}$ orbital of Hf atom, respectively. The cyan lines denote the d_{xy}, d_{yz} and d_{xz} orbitals of Hf atom. The blue lines denote the p_x and p_y orbitals of S atom, and the yellow lines denote the p_z obital of S atom. The dashed lines indicate the Fermi level.

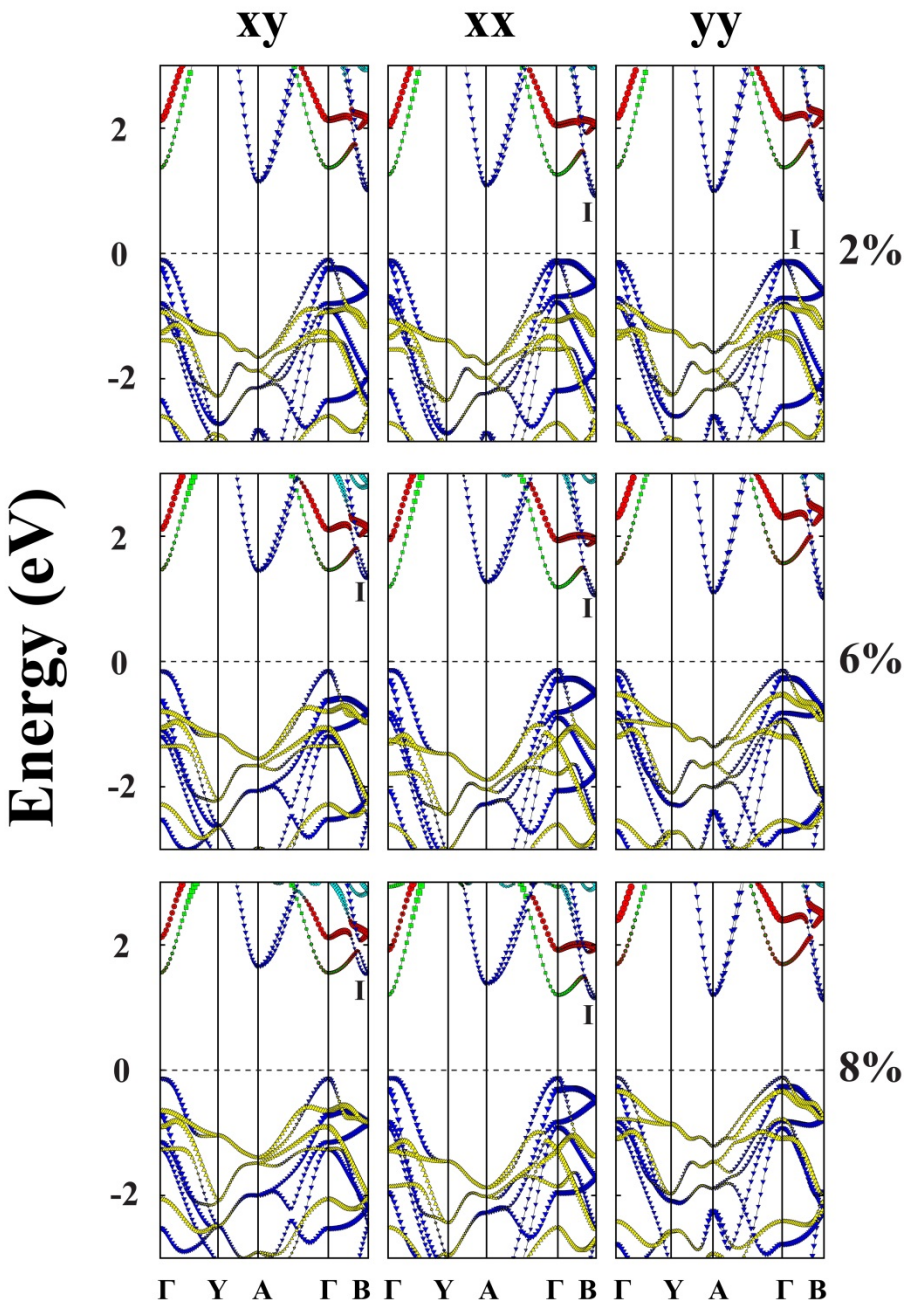

Figure S6. Computed band structures of stained monolayer $HfSe_3$ *versus* biaxial tensile strain (xy) in both x and y directions, the uniaxial tensile strain in x direction (xx) or y direction (yy). The red lines denote the d_{z^2}orbital of Hf atom. The green lines denote the $d_{x^2-y^2}$ orbital of Hf atom. The cyan lines denote the d_{xy}, d_{yz} and d_{xz} orbitals of Hf atom. The blue lines denote the p_x and p_y orbitals of Se atom, and the yellow lines denote the p_z obital of Se atom. The dashed lines indicate the Fermi level.

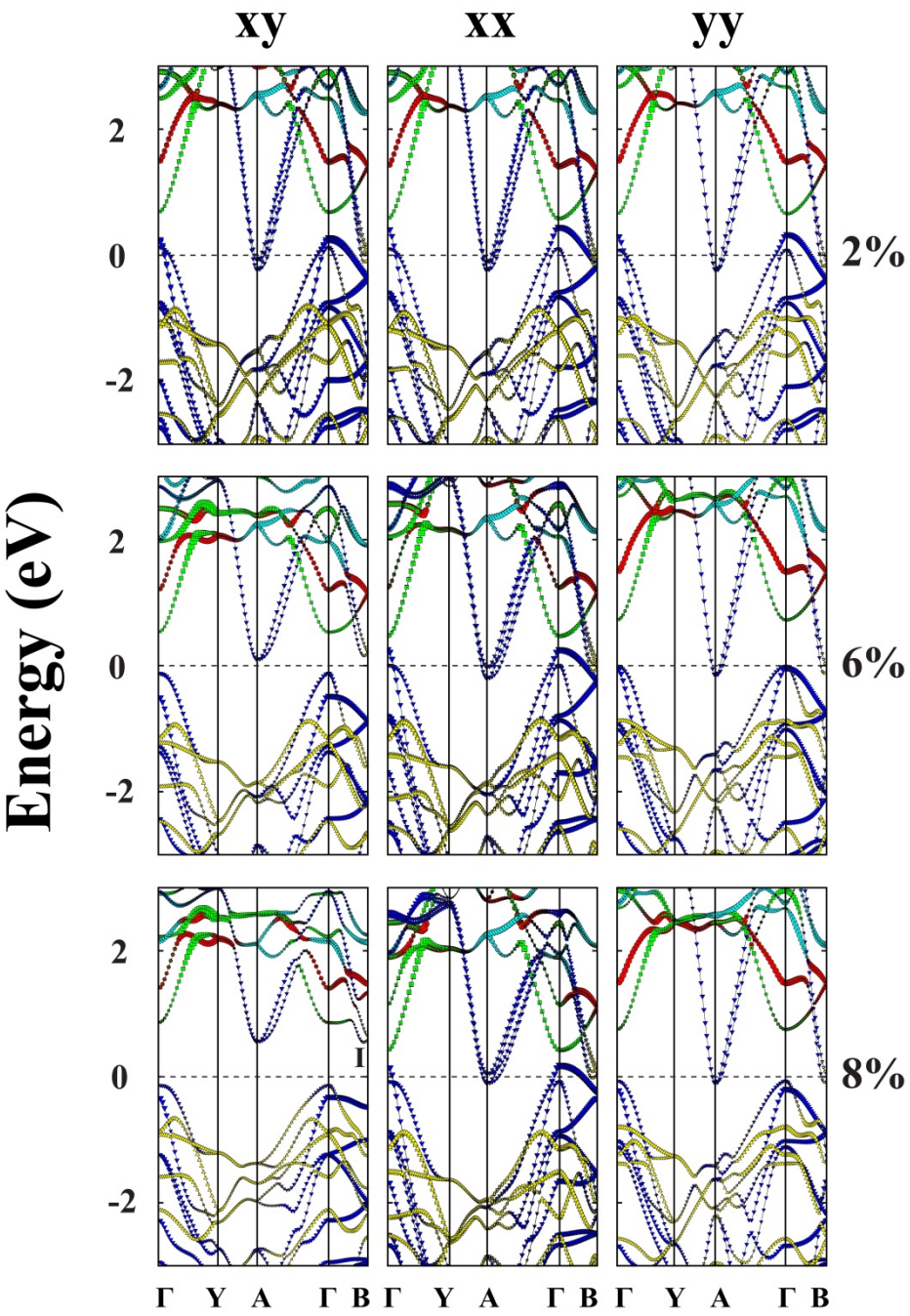

Figure S7. Computed band structures of strained monolayer $HfTe_3$ *versus* biaxial tensile strain in both x and y directions (xy), the uniaxial tensile strain in x direction (xx) or y direction (yy). The red and green lines illustrate the d_{z^2} orbital and the $d_{x^2-y^2}$ orbital of Hf atom, respectively. The cyan lines denote the d_{xy}, d_{yz} and d_{xz} orbitals of Hf atom. The blue lines denote the p_x and p_y orbitals of Te atom, and the yellow lines denote the p_z obital of Te atom. The dashed lines indicate the Fermi level.

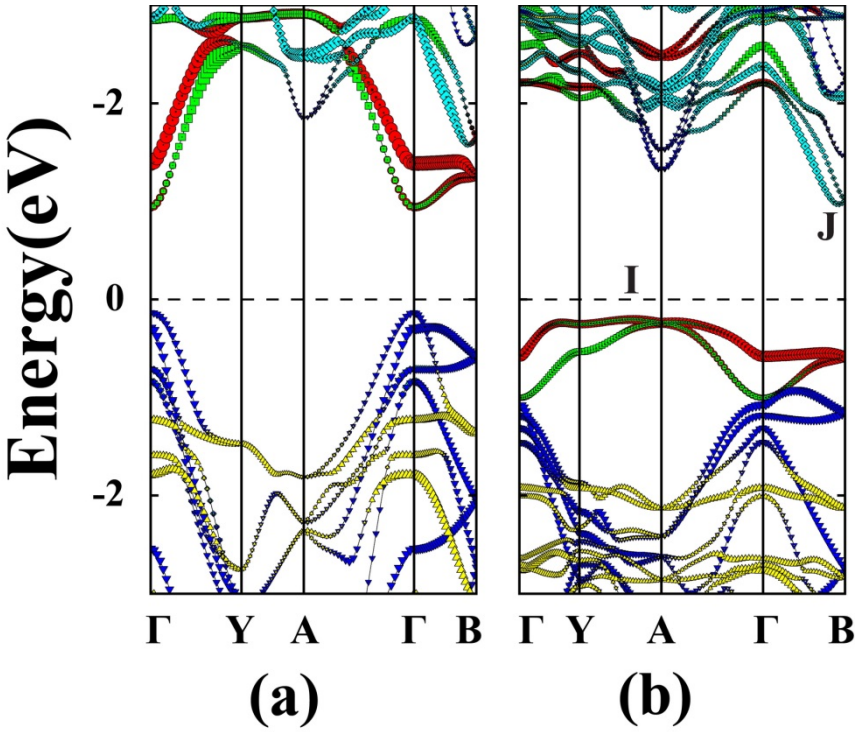

Figure S8. Band structures of unstrained monolayers: (a) TiS_3 and (b) $NbSe_3$. The red lines denote the d_{z^2} orbital of (a) Ti atom and (b) Nb atom. The green lines denote the $d_{x^2-y^2}$ orbitals of (a) Ti atom and (b) Nb atom. The cyan lines denote the d_{xy}, d_{yz} and d_{xz} orbitals of (a) Ti atom and (b) Nb atom. The blue lines denote the p_x and p_y orbitals of S atom, and the yellow lines denote the p_z obital of the S atom. The dashed lines indicate the Fermi level.