Supporting Information

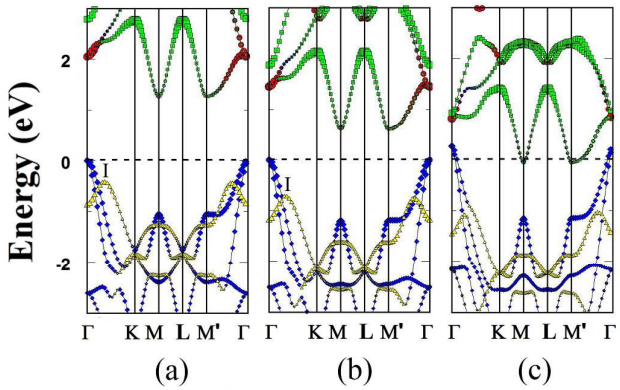

Figure S1. Computed electronic band structures of unstrained monolayer (a) HfS_2, (b) $HfSe_2$, and (c) $HfTe_2$. The red line denotes d_{xy}, d_{yz}, and d_{xz} orbitals of Hf atom, the green line denotes d_z^2 and $d_{x^2-y^2}$ orbitals of Hf atom, the blue line denotes p_x and p_y orbitals of S atom, and the yellow line denotes p_z orbital of S atom. The dashed line represents the Fermi level.

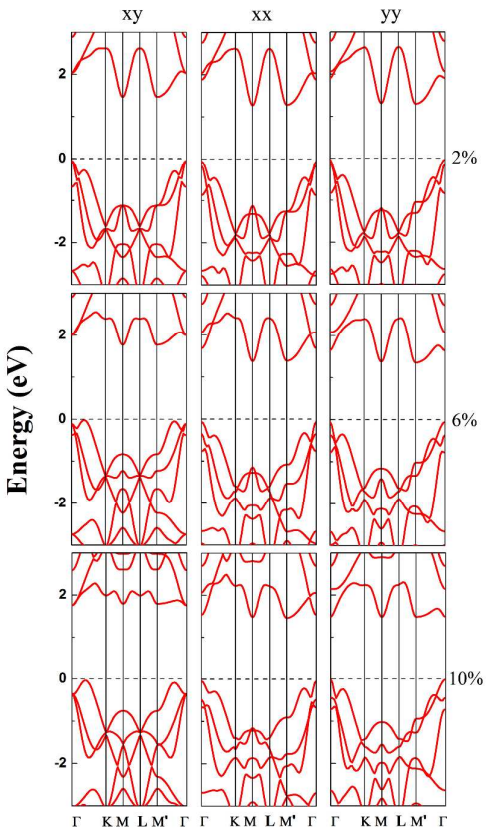

Figure S2. Computed band structures of HfS_2 monolayer with respect to the biaxial tensile strain (*xy*), or uniaxial tensile strain in *x*-direction (*xx*) or *y*-direction (*yy*). The applied strain □ = 2% (upper panel), 6% (middle panel) and 10% (lower panel).