Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Properties of Tin Dichalcogenide Monolayers and Effects of Hydrogenation and Tension

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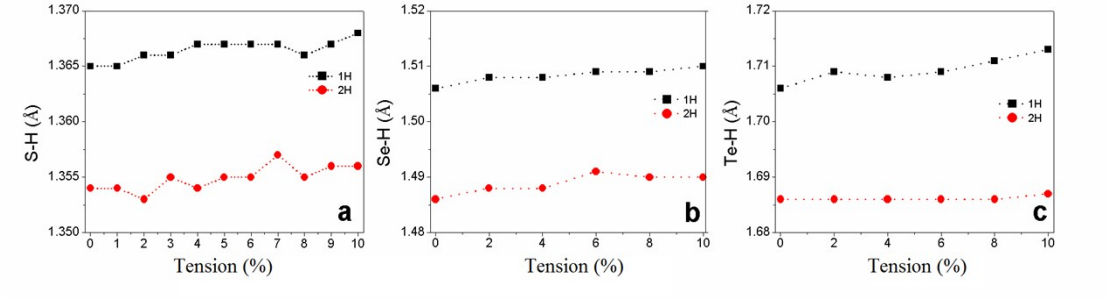
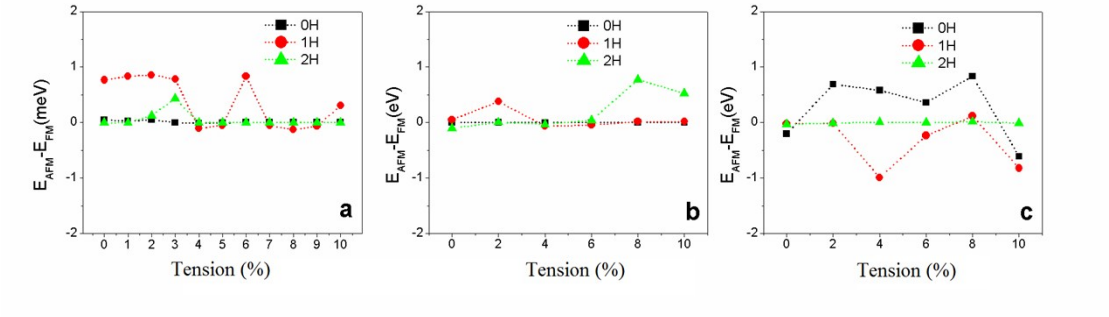
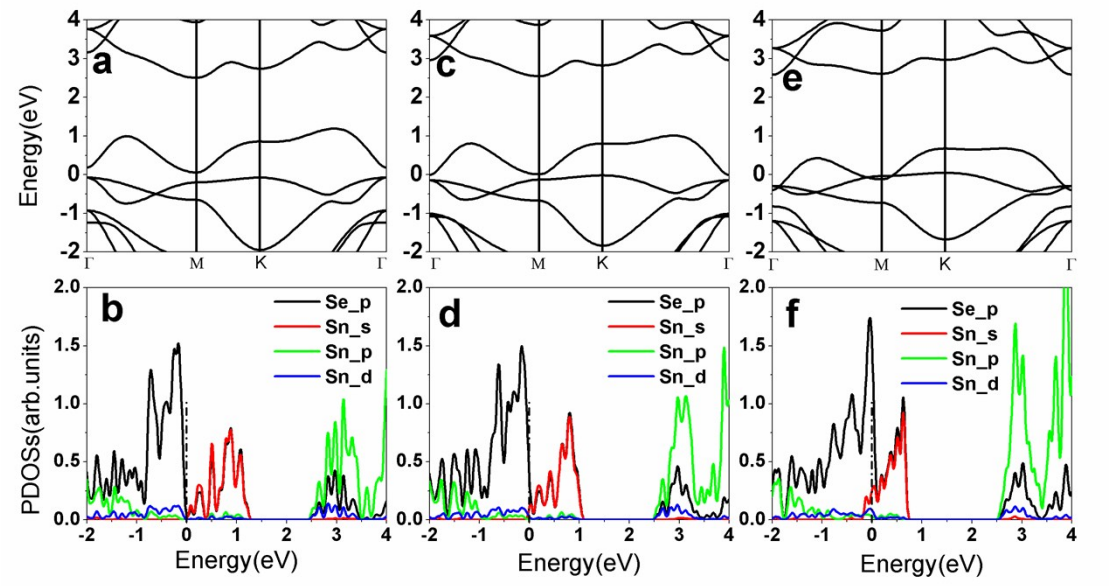
Supporting Data



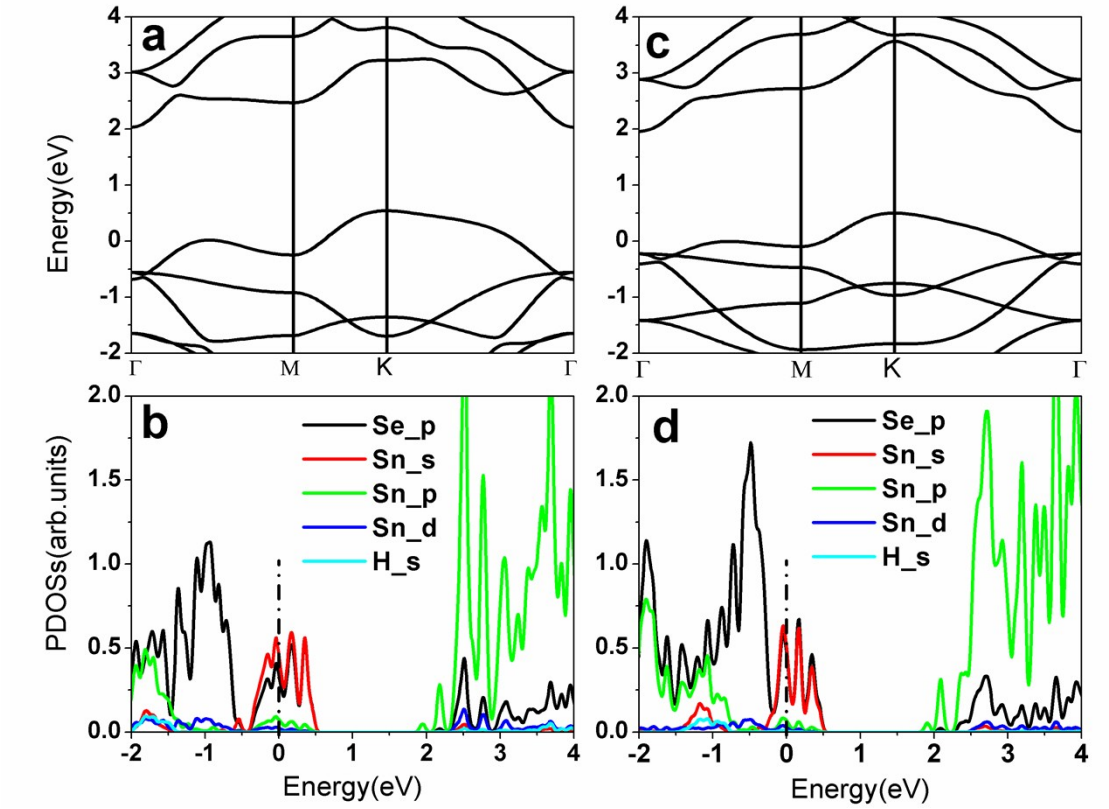
S-1, The bond length of (a) S-H, (b) Se-H, and (c) Te-H on SnX_2-nH monolayers (X = S, Se, and Te; n = 1 and 2).



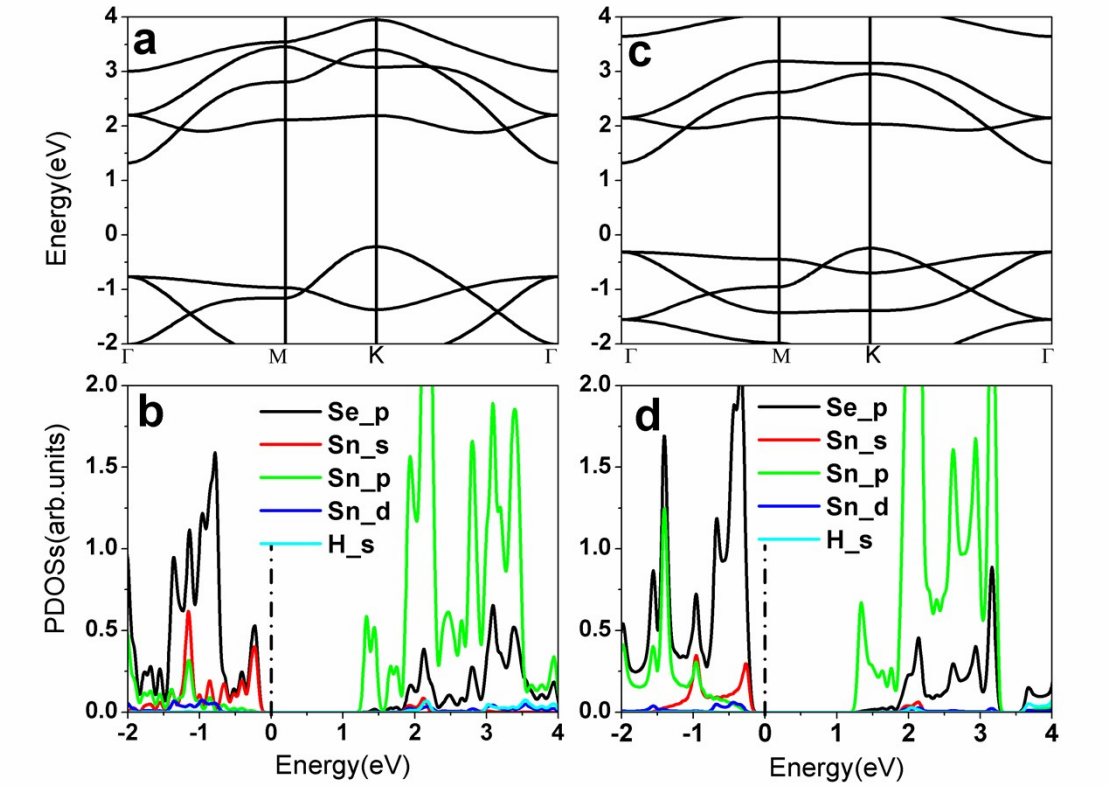
S-2, Total energy difference between ferromagnetic (FM) and anti-ferromagnetic (AFM) states for (a) SnS_2, (b) $SnSe_2$, and (c) $SnTe_2$ monolayers with and without hydrogenation under tension.



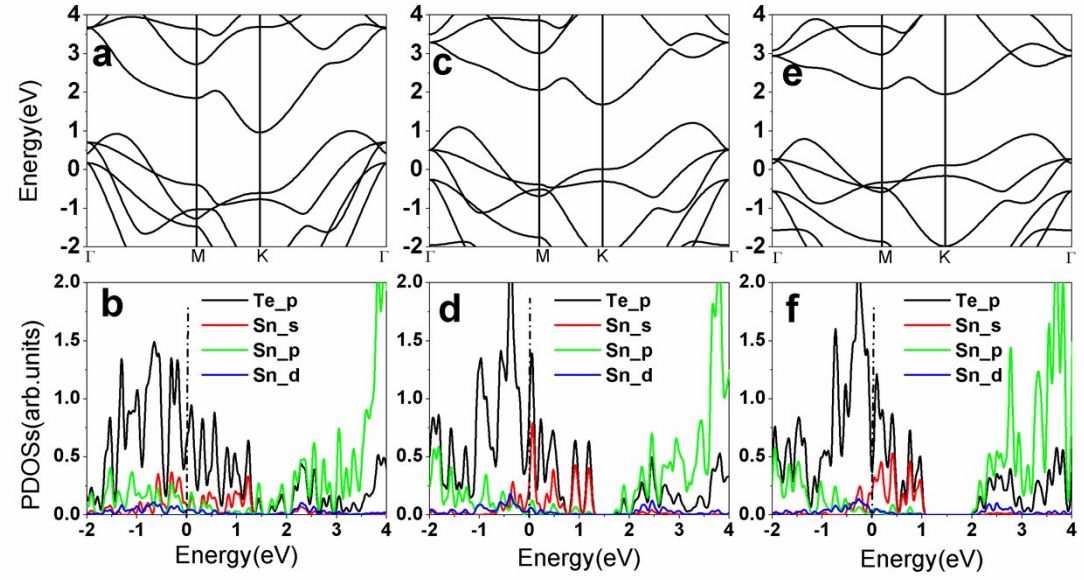
S-3, Calculated band structures of $SnSe_2$-0H-ML at a tension of (a) 4 %, (c) 6 % and (e) 10% and partial density of states at a tension of (b) 4%, (d) 6 % and (f) 10 %. Fermi level is at 0 eV.



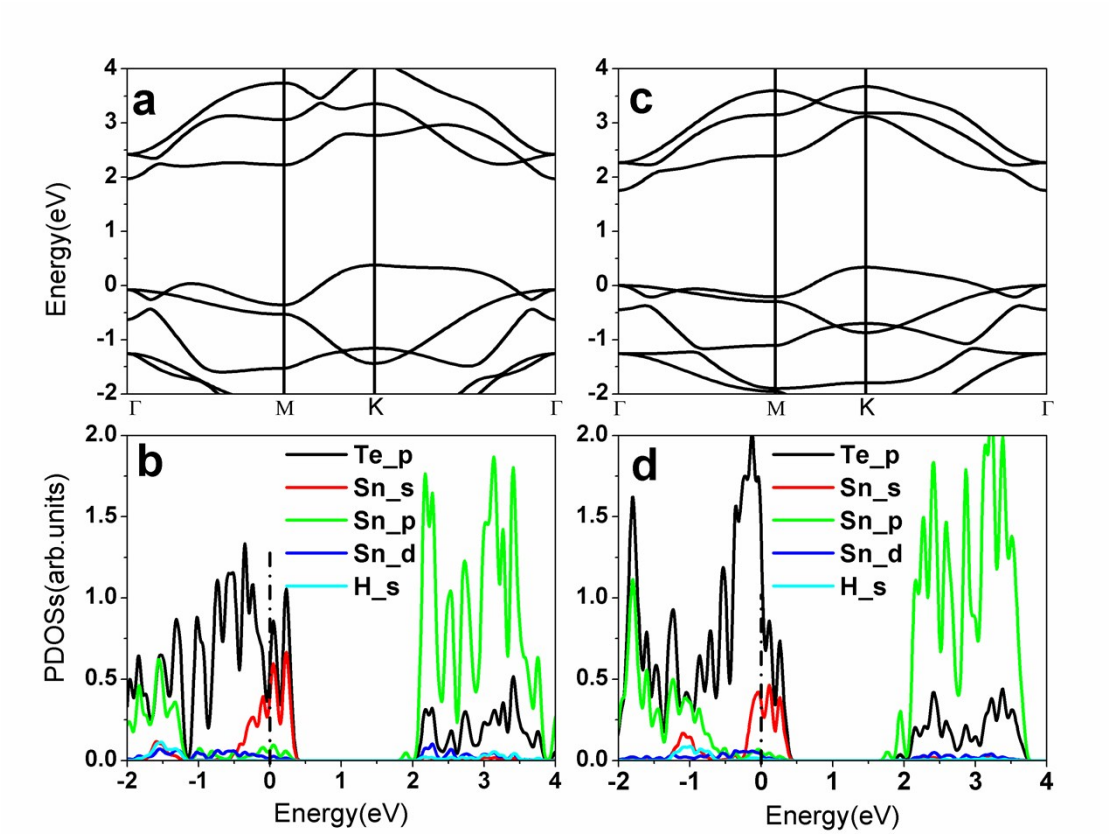
S-4, Calculated band structures of $SnSe_2$-1H-ML at a tension of (a) 2 % and (c) 10 % and partial density of states at a tension of (b) 2 % and (d) 10 %. Fermi level is at 0 eV.



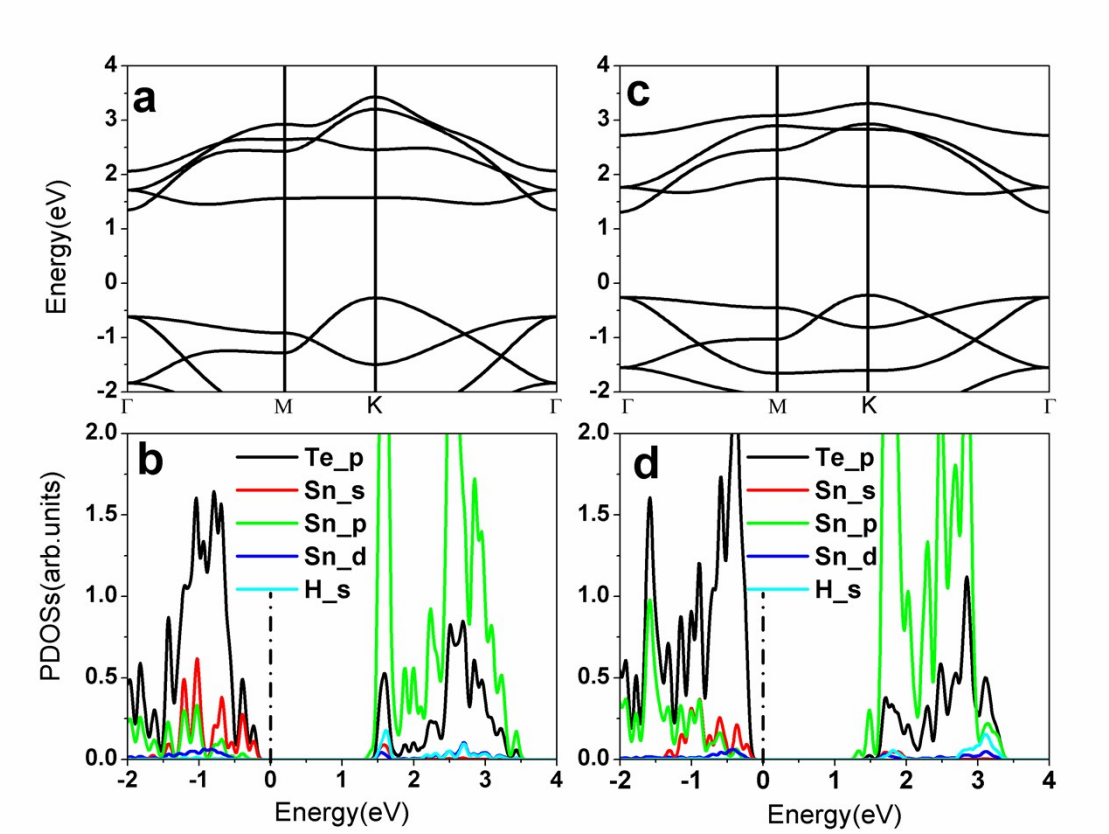
S-5, Calculated band structures of $SnSe_2$-2H-ML at a tension of (a) 2 % and (c) 10 % and partial density of states at a tension of (b) 2 % and (d) 10 %. Fermi level is at 0 eV.



S-6, Calculated bond structures of $SnTe_2$-0H-ML at a tension of (a) 2 %, (c) 6 % and (e) 10 %, and partial density of states at a tension of (b) 2 %, (d) 6 % and (f) 10 %. Fermi level is at 0 eV.



S-7, Calculated band structures of $SnTe_2$-1H-ML at a tension of (a) 2 % and (c) 10 % and partial density of states at a tension of (b) 2 % and (d) 10 %. Fermi level is at 0 eV.



S-8, Calculated bond structures of $SnTe_2$-2H-ML at a tension of (a) 2 % and (c) 10 % and partial density of states at a tension of (b) 2 % and (d) 10 %. Fermi level is at 0 eV.