

Supplementary Information Material

Strain-induced structural phase transition, electric polarization and unusual electric properties in photovoltaic materials CsMI₃ (M = Pb, Sn)

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The goal of this Supplementary Information Material is to provide more information by means of Figures.

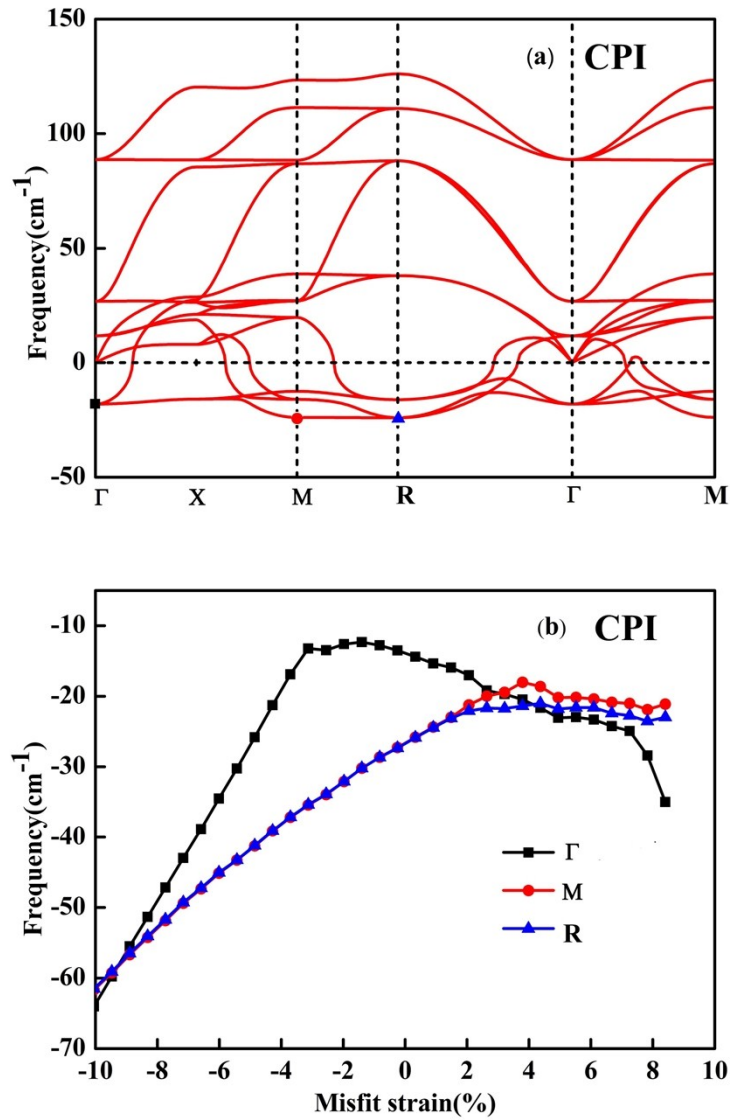


Fig. S1 (a) The Phonon dispersions curves of the ideal cubic structure CsPbI_3 within the density functional perturbation theory, where the three main unstable phonon frequencies are marked by the black, red, and blue points. (b) The unstable phonon frequencies in panel (a) vs as a function of misfit strain. Note that the symmetry in panel (b) is lowered to $P4/mmm$ by strain effect.

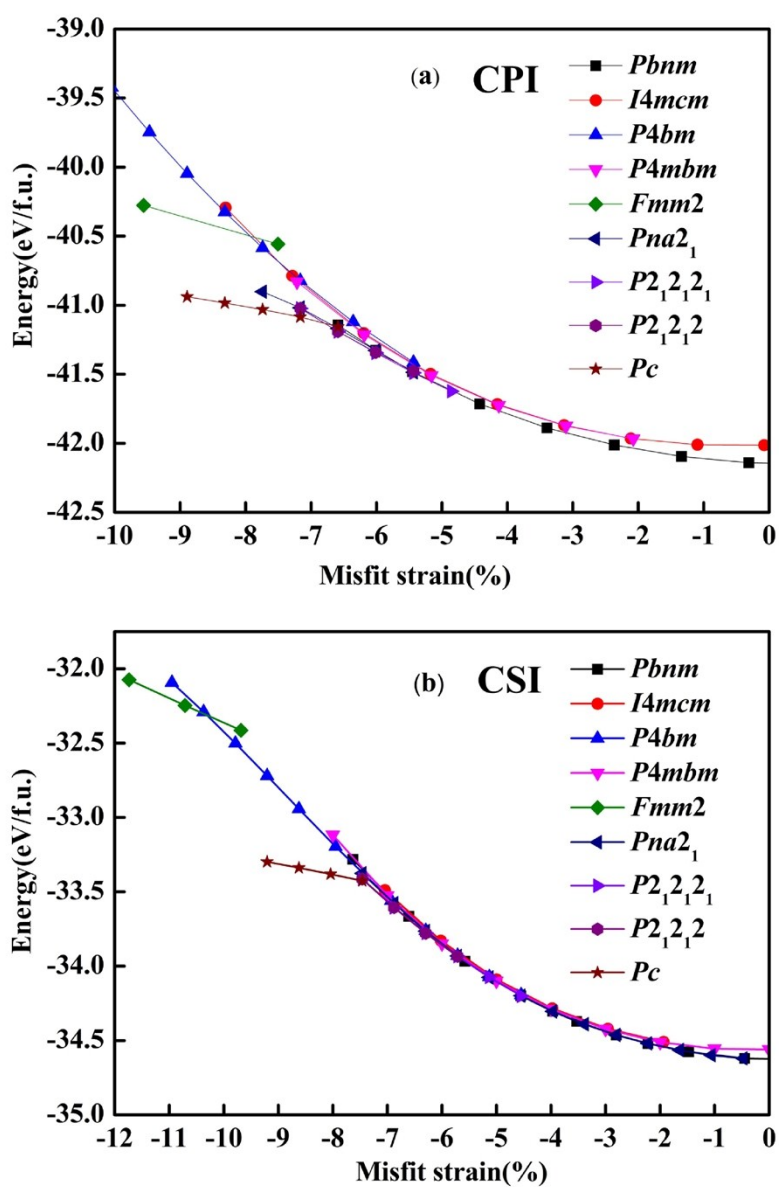


Fig. S2 The total energy of all phases contained metastable phases vs misfit strain in the (001) epitaxial CPI and CSI thin films.

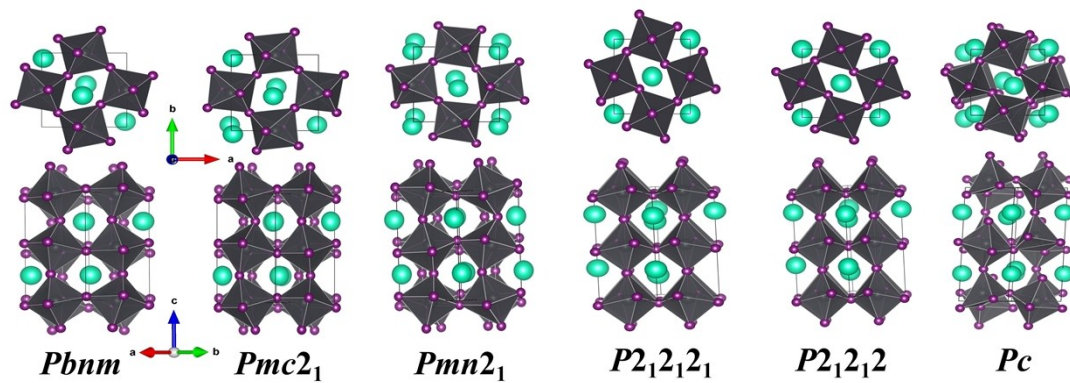


Fig. S3 Schematic description of six different phases $Pbnm$, $Pmc2_1$, $Pmn2_1$, $P2_12_12_1$, $P2_12_12$, and Pc phases for CPI films. The green and purple balls represent Cs atoms and I atoms, respectively.

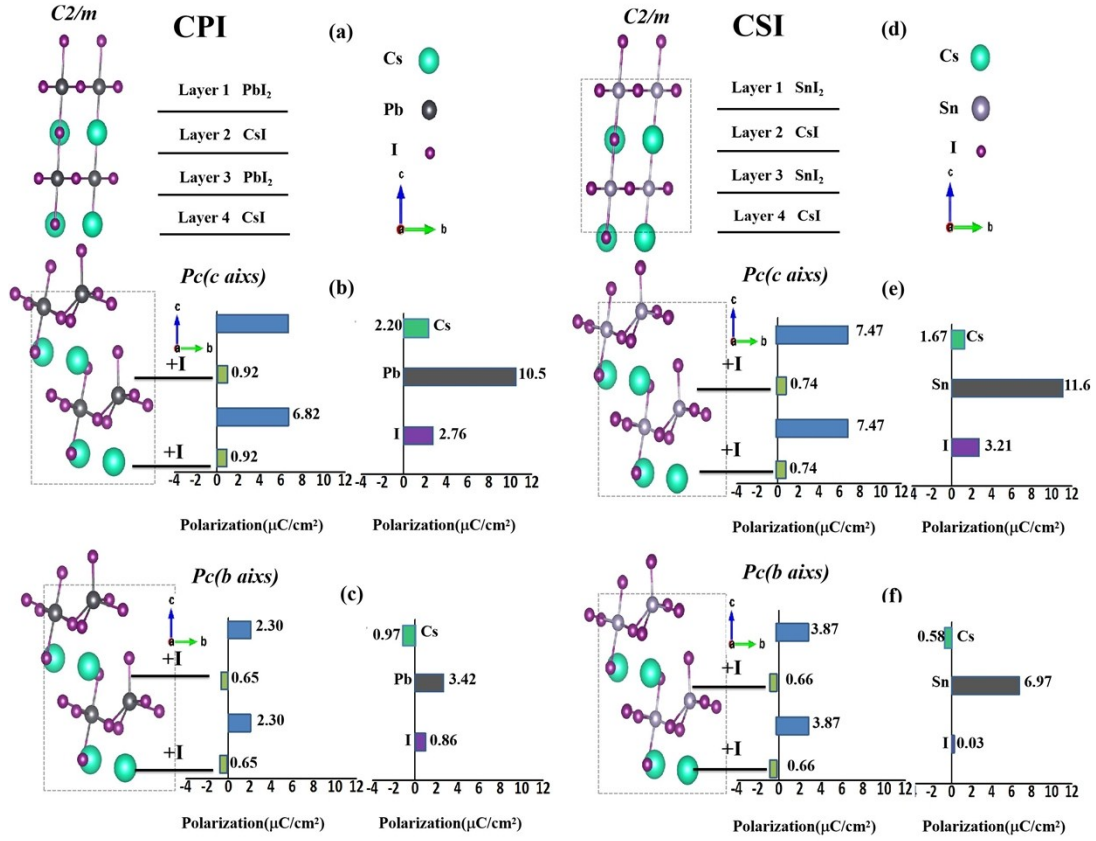


Fig. S4 The layer-decomposed polarization in corresponding strained phases for CPI and CSI. Panel (a) and (d) display the schematic configuration of the centrosymmetric $C2/m$ structure for CPI and CSI, respectively. Panel (b), (c), (e) and (f) represent the layer-decomposed polarization in Pc phase along c , b axis, respectively.

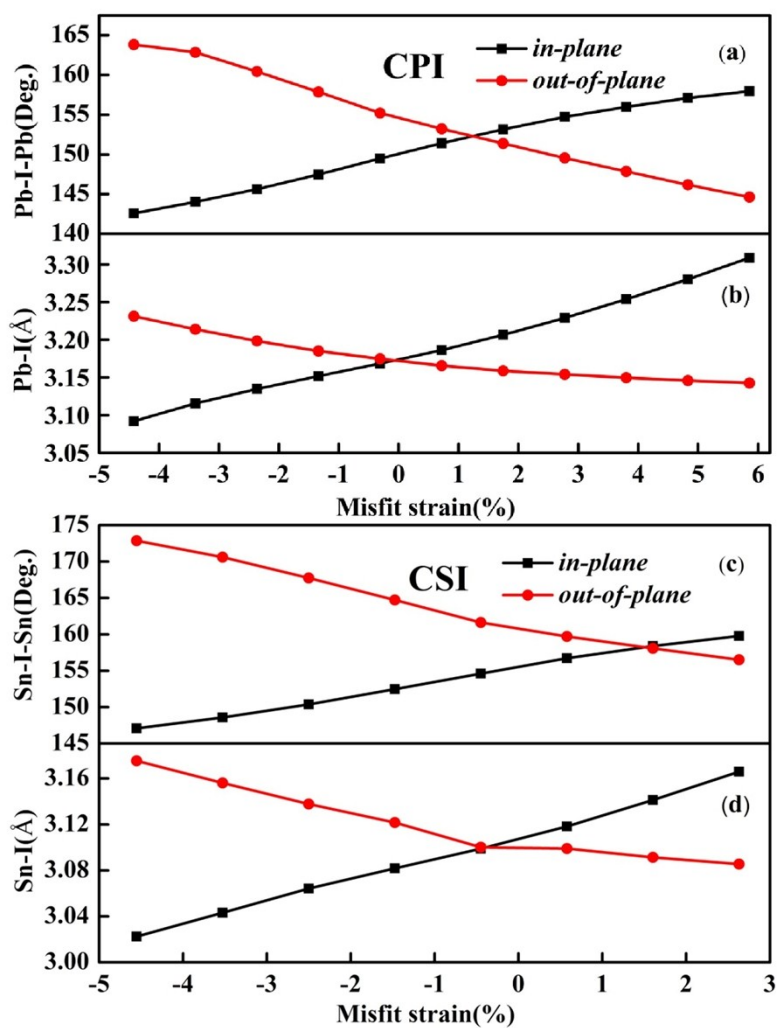


Fig. S5 Bond angles and bond lengths of *Pbnm* state of CsPbI_3 and CsSnI_3 thin films under misfit strain. (Bond angles represent Pb-I-Pb , Sn-I-Sn , respectively. Bond lengths represent Pb-I , Sn-I , respectively).