Strain Engineering of Optoelectronic and Ferroelectric Properties in R3-Phase Zn_3TeO_6: A First-Principles Study

Supporting Information

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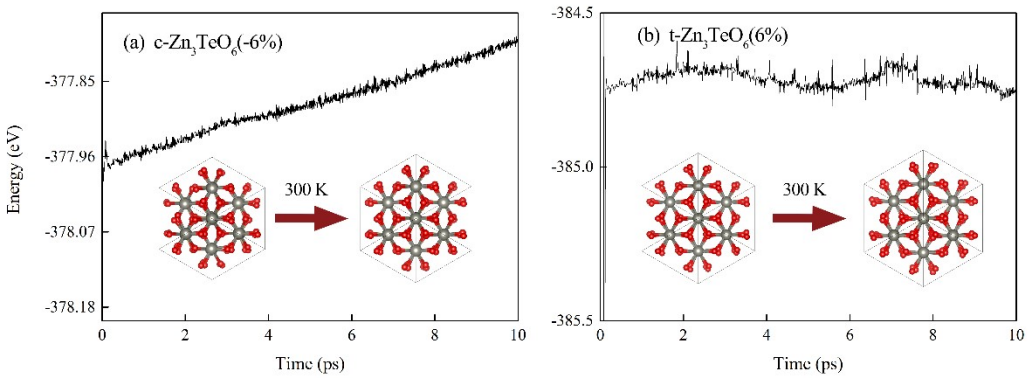

Fig.S1. AIMD energy evolution of Zn_3TeO_6 under (a) −6% compressive strain and (b) +6% tensile strain.

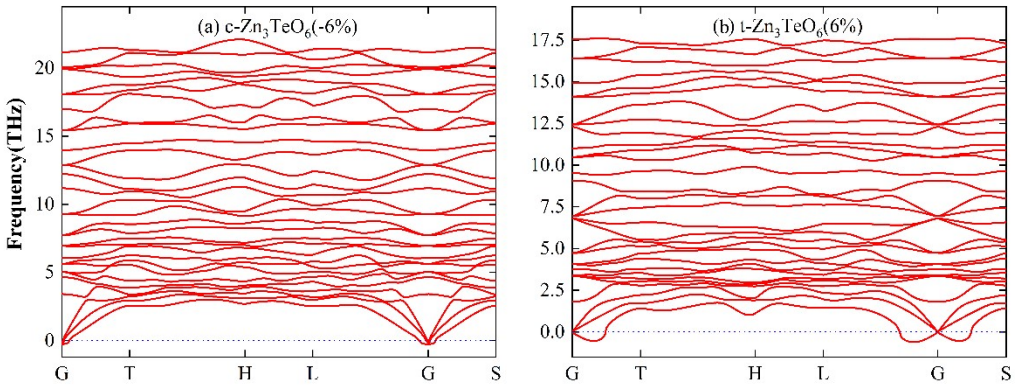

Fig.S2. The calculated phonon frequency of (a) −6% compressive strain and (b) +6% tensile strain.

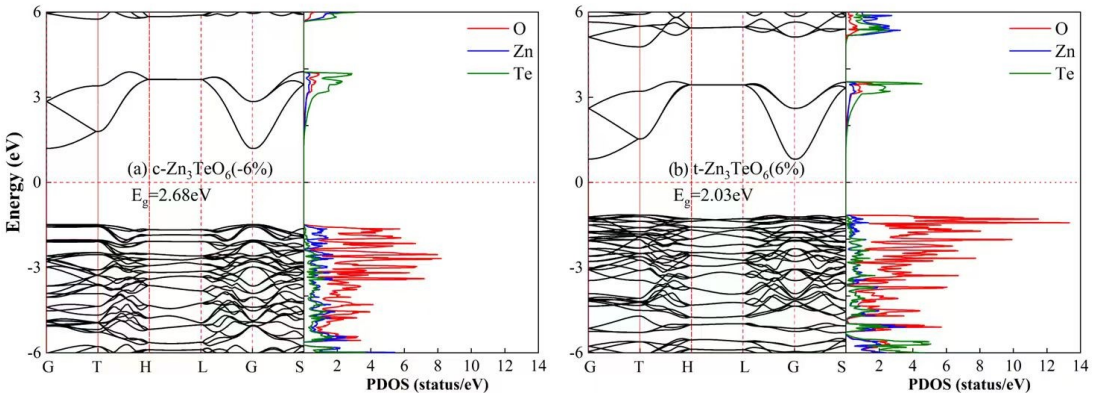

Fig.S3 The calculated band structure and density of states of (a) −6% compressive strain and (b) +6% tensile strain.

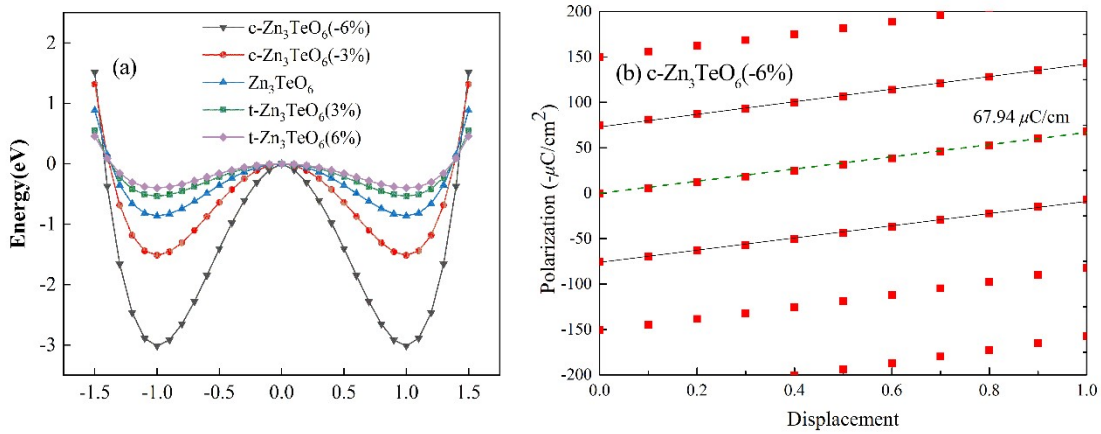

Fig.S4. (a) Potential energy curve and (b) ferroelectric polarization as a function of structural distortion under −6% compressive strain.