Supplementary Materials

Tuning the band gap and polarization in $BaSnO_3/SrSnO_3$ superlattices for photovoltaic applications

Yajun Zhang[1], MPK Sahoo[1,2,3], Jie Wang[1,2*]

[1]*Department of Engineering Mechanics, School of Aeronautics and Astronautics, Zhejiang University, 38 Zheda Road, Hangzhou 310007, China*

[2]*Key Laboratory of Soft Machines and Smart Devices of Zhejiang Province, Zhejiang University, 38 Zheda Road, Hangzhou 310007, China*

[3]*Department of Physics, RGUKT IIIT, Nuzvid Campus, Andhra Pradesh, India*

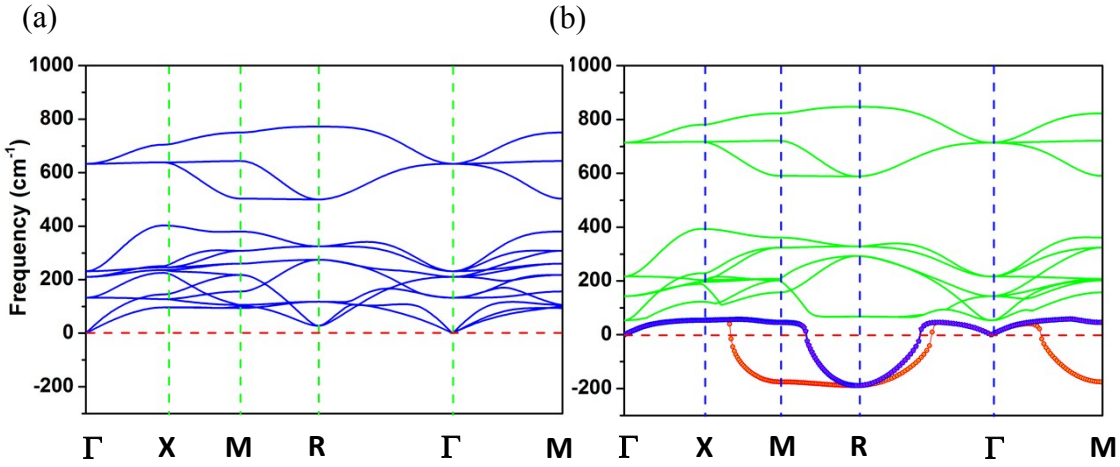

Fig. S1 Phonon dispersion curves of cubic phase for (a) $BaSnO_3$ and (b) $SrSnO_3$. The imaginary frequencies (unstable modes) are depicted as negative values.

* E-mail:jw@zju.edu.cn

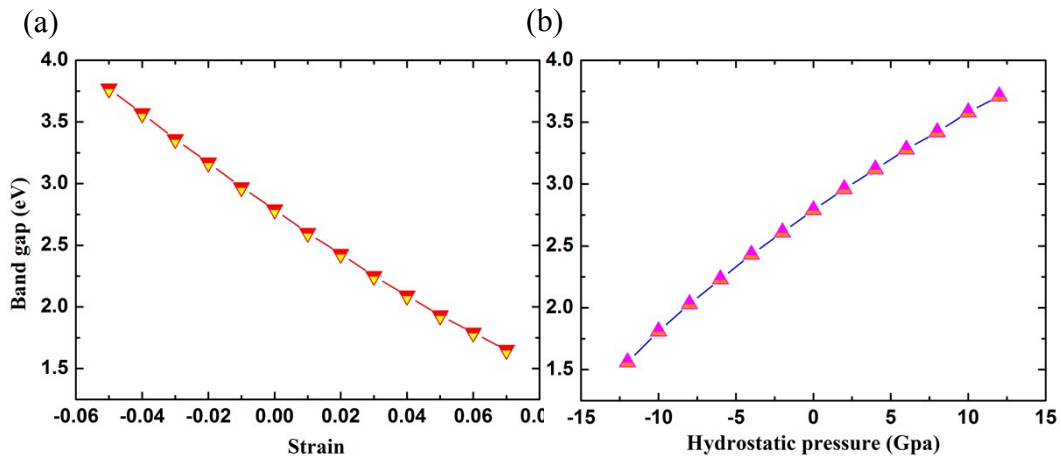

Fig. S2 The calculated band gap for cubic $BaSnO_3$ as a function of (a) biaxial strain and (b) hydrostatic pressure.

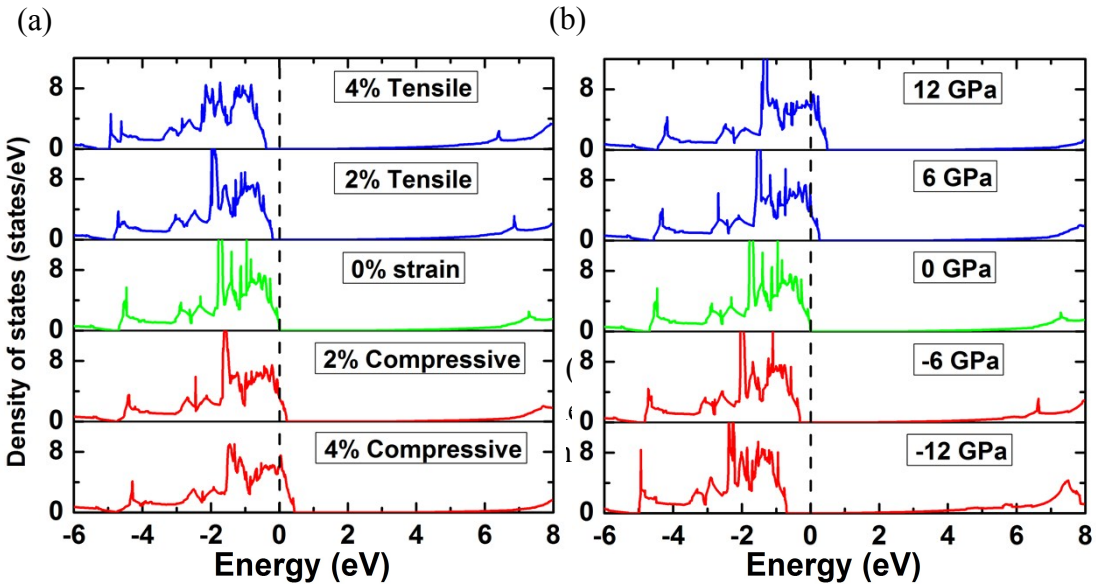

Fig. S3 Total density of states of cubic $BaSnO_3$, (a) under different biaxial strains and (b) under different hydrostatic pressure. The Fermi level is set to zero.