

Supplementary information

Different Structural Evolutions of inorganic perovskite CsGeI₃

Tian Luo,^{‡a} Yufan Xia,^{‡a} Jiawei Huang,^a Xi Huang,^a Zhenyuan Wu,^a Yuxuan Chen,^b
Xin Xu,^a Weiguang Xie,^a Pengyi Liu,^a Cuiying Hu,^a Xing Lu,^{*a} and Tingting Shi^{*a}

^a Siyuan Laboratory, Guangzhou Key Laboratory of Vacuum Coating Technologies and New Energy Materials, Guangdong Provincial Engineering Technology Research Center of Vacuum Coating Technologies and New Energy Materials, Department of Physics, Jinan University, Guangzhou 510632, China

^b School of Physics, Sun Yat-sen University, Guangzhou 510275, China

[†] Electronic supplementary information (ESI) available.

[‡] These authors contribute equally to this work.

Corresponding Author

*E-mail: tjnuxlu@jnu.edu.cn

*E-mail: ttshi@jnu.edu.cn

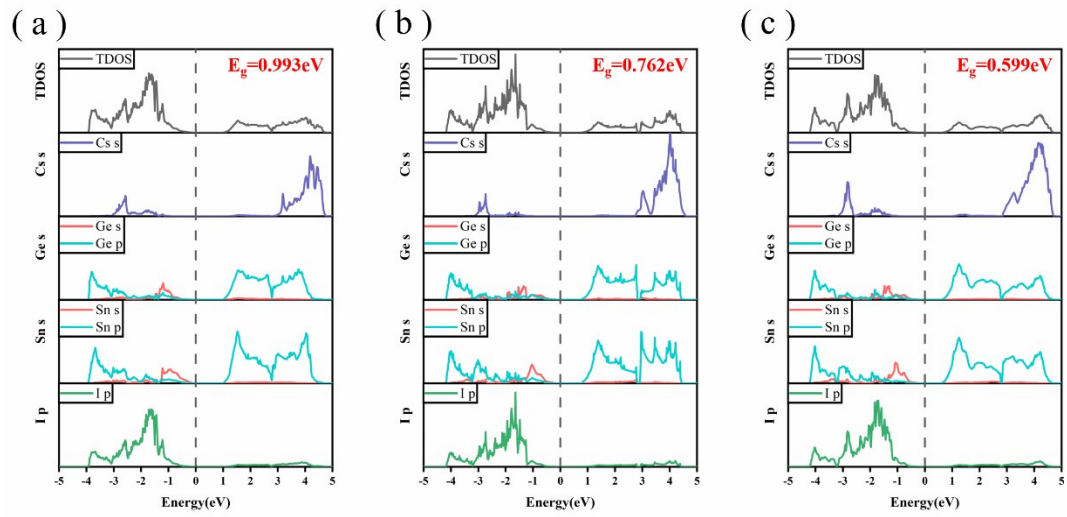


Figure S1. TDOS and PDOS of CsSn_{0.5}Ge_{0.5}I₃ using GGA method: (a) stable structure, (b) R3m, (c) P4/mbm.

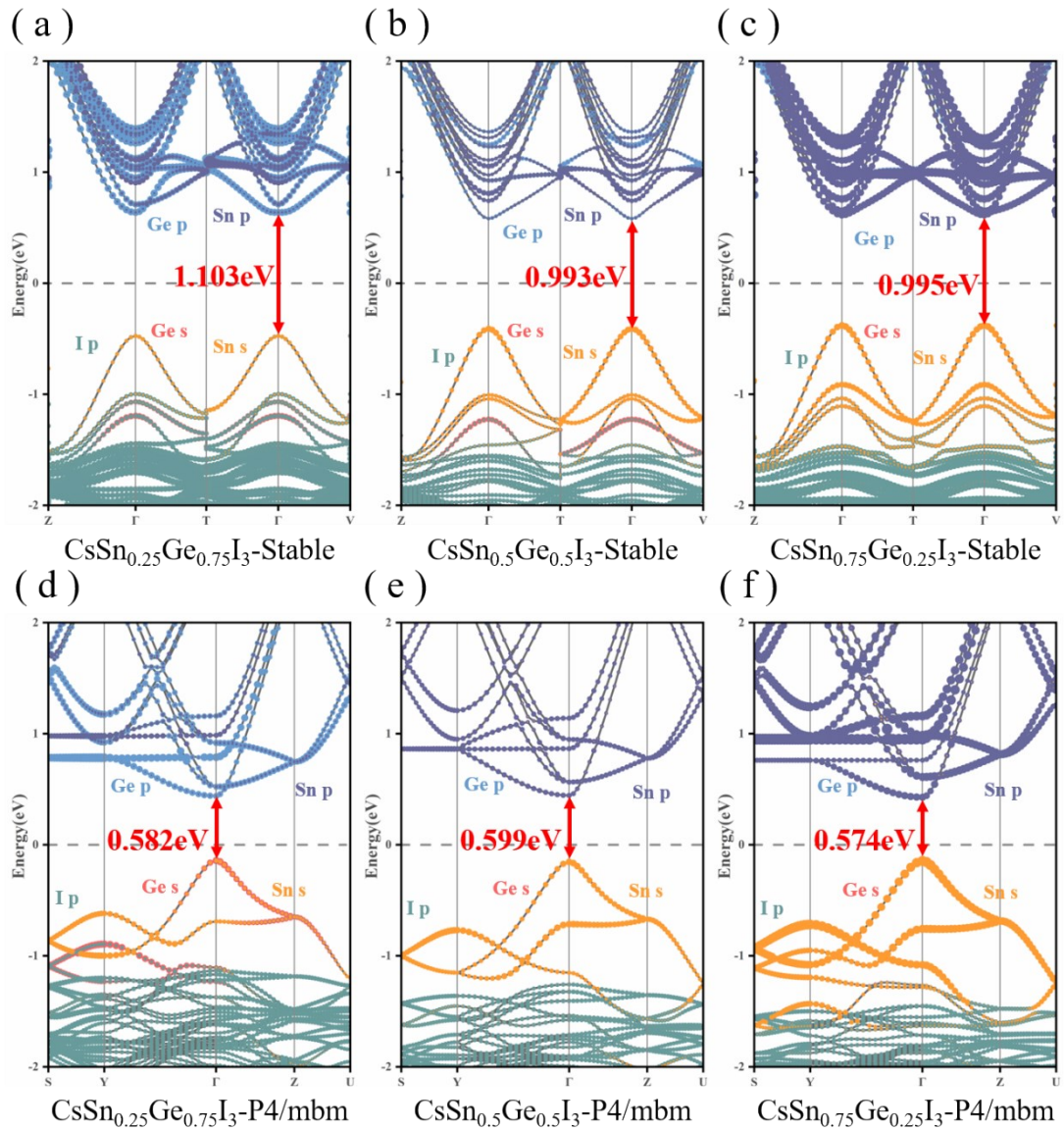


Figure S2. Projected band structures of $\text{CsSn}_x\text{Ge}_{1-x}\text{I}_3$ using GGA method.

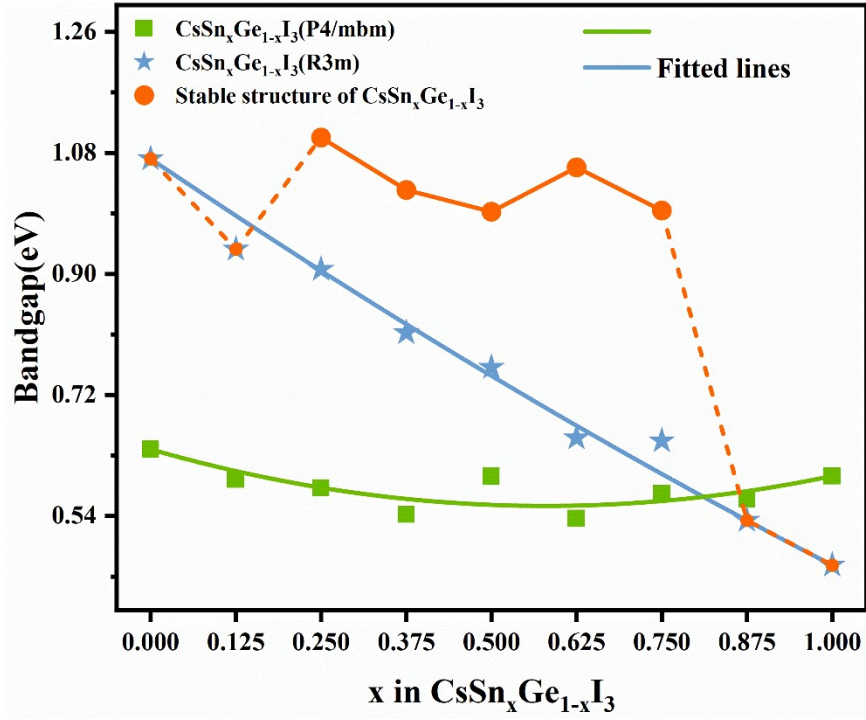


Figure S3. Calculated band gap evolutions of CsSn_xGe_{1-x}I₃ as a function of composition x using GGA method.

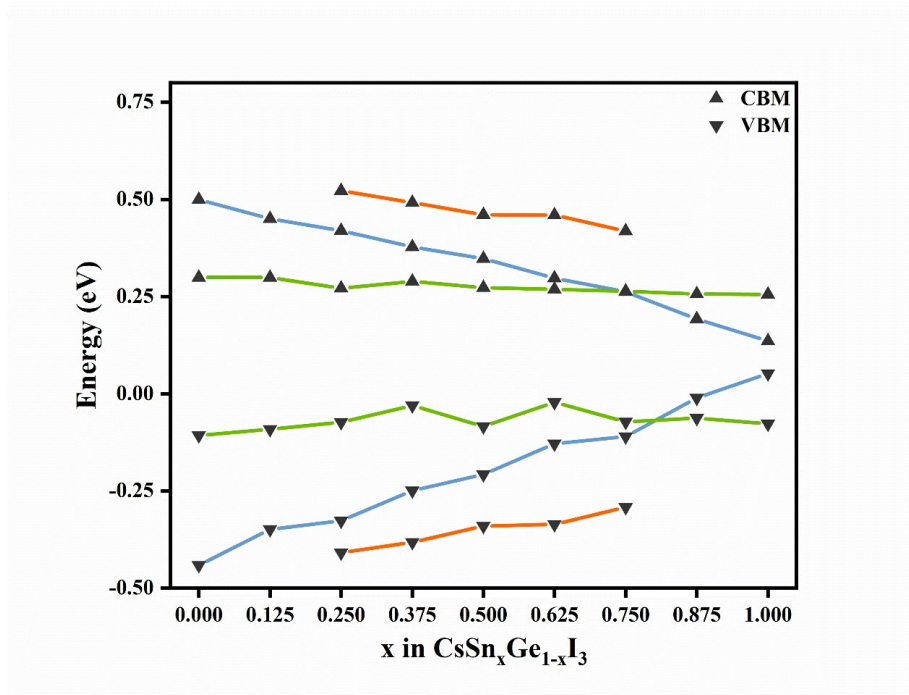


Figure S4. The band edge variation of CsSn_xGe_{1-x}I₃ as a function of composition x using GGA+SOC method.