

Trigonal $\text{Cu}_2\text{-II-Sn-VI}_4$ (II=Ba, Sr and VI=S, Se) Quaternary Compounds for Earth-Abundant Photovoltaics

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Supporting Information

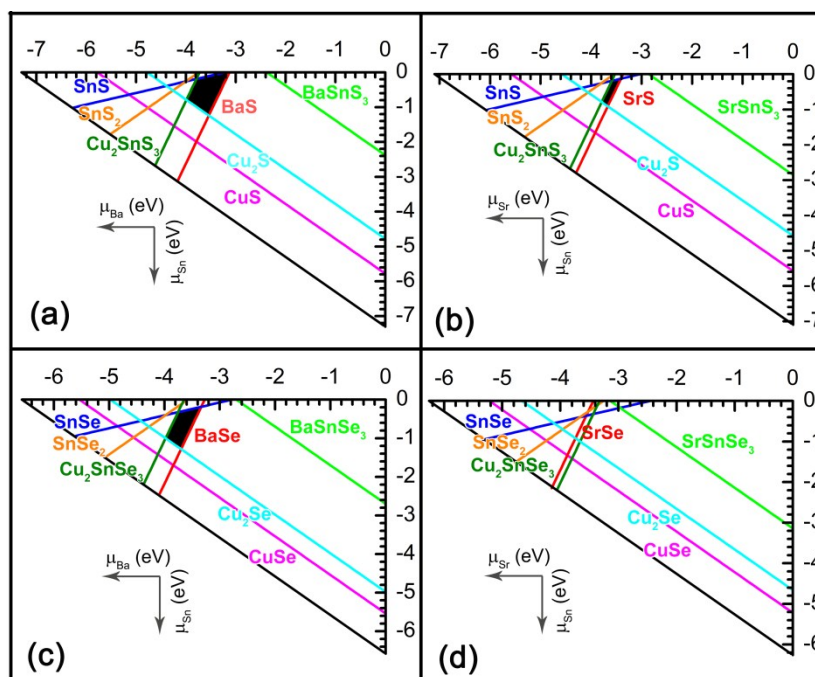


Figure S1. Thermodynamically stable range at $\mu_{\text{Cu}} = -0.2$ eV plane for (a) $\text{Cu}_2\text{BaSnS}_4$, (b) $\text{Cu}_2\text{SrSnS}_4$, (c) $\text{Cu}_2\text{BaSnSe}_4$ and (d) $\text{Cu}_2\text{SrSnSe}_4$, respectively.

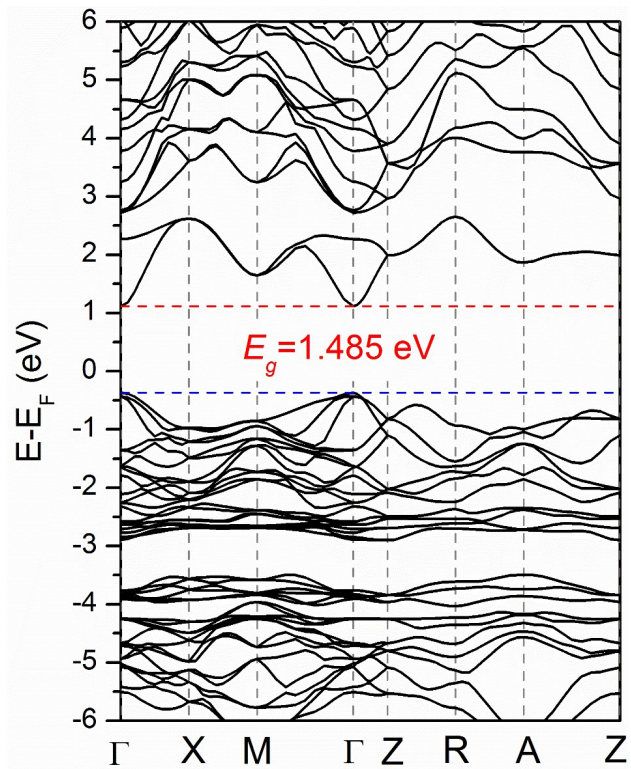


Figure S2. HSE calculated band structure of kesterite $\text{Cu}_2\text{ZnSnS}_4$.

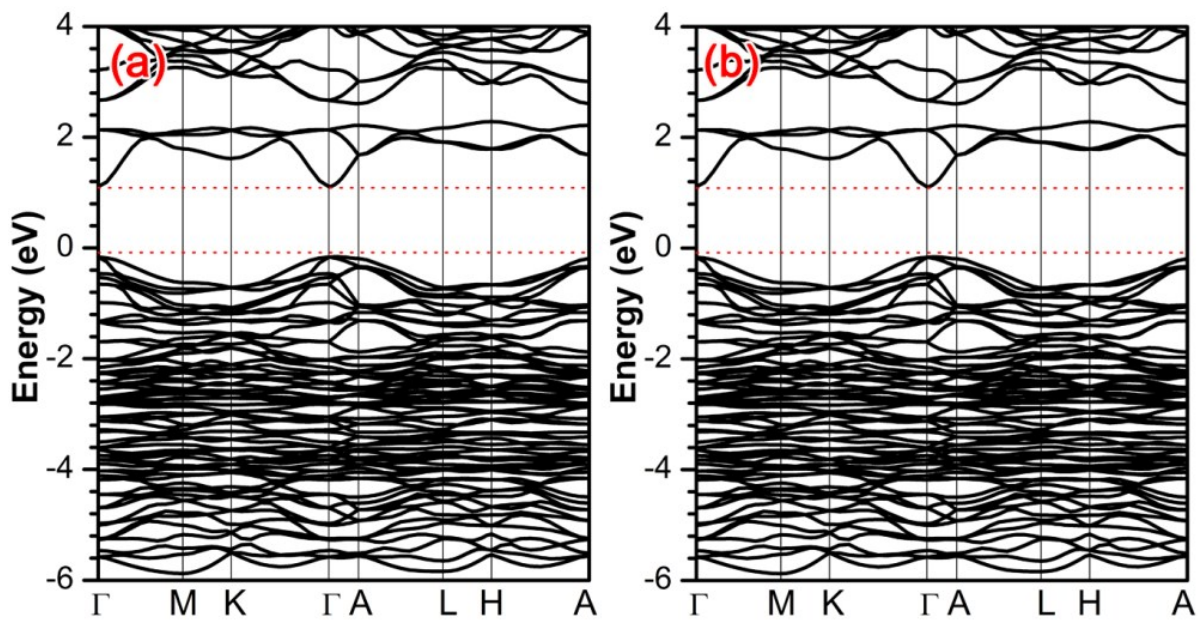


Figure S3. HSE calculated band structures for (a) $\text{Cu}_2\text{BaSnSe}_4$ and (b) $\text{Cu}_2\text{SrSnSe}_4$ with $P3_1$ structures, respectively.

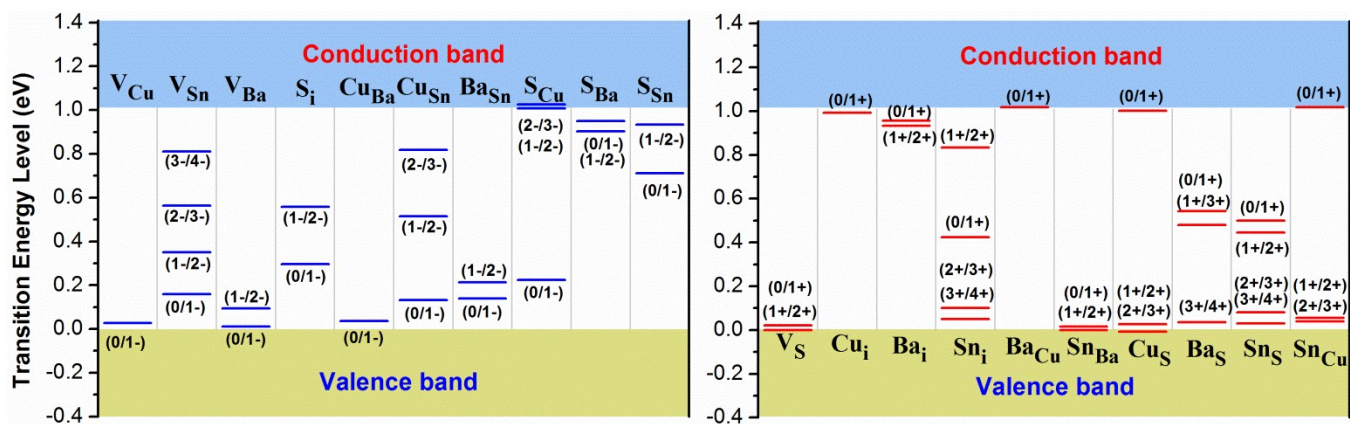


Figure S4. GGA+U calculated ($U=6$ eV for Cu $3d$ orbital) transition energy levels of (a) acceptor-like and (b) donor-like intrinsic defects in $\text{Cu}_2\text{BaSnS}_4$.