Trigonal Cu$_2$-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) Cu$_2$BaSnS$_4$, (b) Cu$_2$SrSnS$_4$, (c) Cu$_2$BaSnSe$_4$ and (d) Cu$_2$SrSnSe$_4$, respectively.
Figure S2. HSE calculated band structure of kesterite Cu$_2$ZnSnS$_4$.

Figure S3. HSE calculated band structures for (a) Cu$_2$BaSnSe$_4$ and (b) Cu$_2$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 Cu$_2$BaSnS$_4$. 