

Effects of tin and sulfur chemical substitution on the structural and electrical properties of CuCr₂Se₄ selenospinel

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Supplementary Materials

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

| | <i>x</i> | <i>y</i> | <i>z</i> | <i>U</i> _{iso} [*] / <i>U</i> _{eq} | Occ. (<1) |
|----|----------|----------|----------|---|-----------|
| Cu | 1/8 | 1/8 | 1/8 | 0.0174 | |
| Sn | 1/4 | 3/4 | 1/2 | 0.0034 | 0.435 |
| Cr | 1/4 | 3/4 | 1/2 | 0.0034 | 0.565 |
| Se | 0.25484 | 0.99516 | 0.49516 | 0.0066 | 0.432 |
| S | 0.25484 | 0.99516 | 0.49516 | 0.0066 | 0.568 |

* *U*_{eq} is defined as one third of the trace of the orthogonalized *U*_{ij} tensor. Cu in 8a site; Cr/ Sn in 16d site and S/Se in 32e site.

Table S2. Frequency and proposed mode assignment of Raman peaks.

| mode | CuCrSnS ₄ ^[7] | CuCr _{1.6} Sn _{0.4} S ₂ Se ₂ ^[12] | CuCrSnS ₂ Se ₂ ^[12] | *CuCr _{1.6} Sn _{0.4} S _{2.3} Se _{1.7} | *CuCrSnS _{2.3} Se _{1.7} |
|---------------------|-------------------------------------|--|--|---|---|
| F _{2g} (1) | 130 | 133 | 124 | 128 | 119 |
| E _g | 165 | 194 | ---- | 205 | 202 |
| F _{2g} (2) | 299 | 299 | 295 | 300 | 236 |
| F _{2g} (3) | 337 | 337 | 338 | 339 | 255 |
| A _{1g} | 379 | 382 | --- | 382 | 335 |

*This work

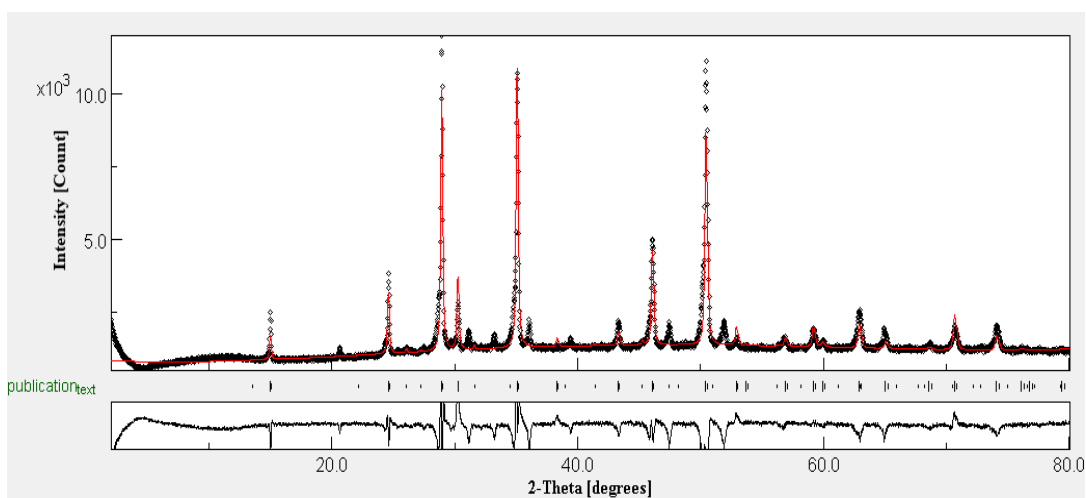
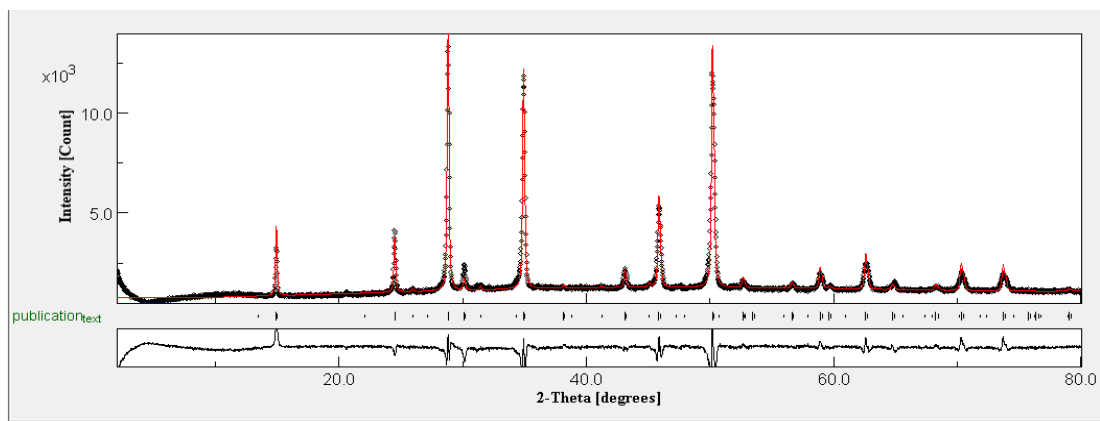


Figure S1. Representative powder XRD data for $\text{CuCr}_{1.4}\text{Sn}_{0.6}\text{S}_{2.3}\text{Se}_{1.7}$ (top) and $\text{CuCr}_{1.6}\text{Sn}_{0.4}\text{S}_{2.3}\text{Se}_{1.7}$ (bottom) including profile fit, profile difference, and profile residuals from the corresponding Rietveld refinement using MAUD program. The intensities are plotted as the intensity *Q to show low-intensity reflections as well.

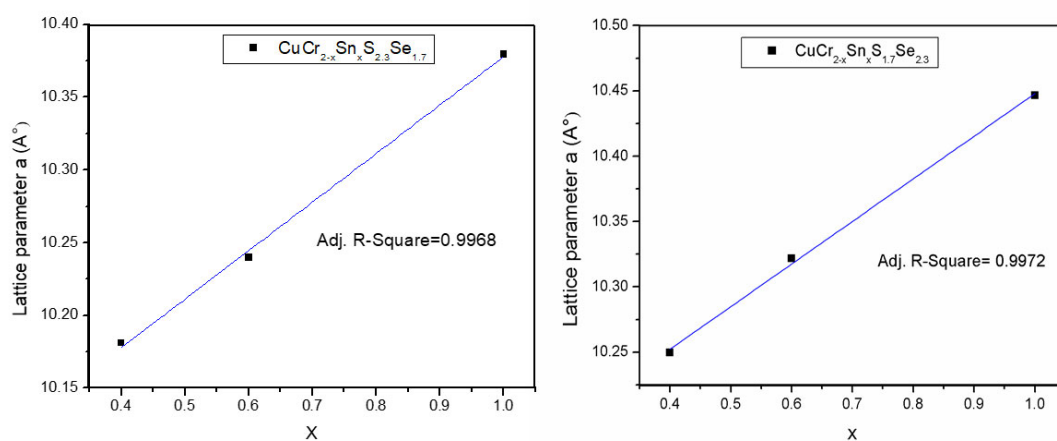


Figure S2. Vegard's Law for $\text{CuCr}_{2-x}\text{Sn}_x\text{S}_{2.3}\text{Se}_{1.7}$ and $\text{CuCr}_{2-x}\text{Sn}_x\text{S}_{1.7}\text{Se}_{2.3}$ ($x = 0.4; 0.6$ y 1.0) phases.

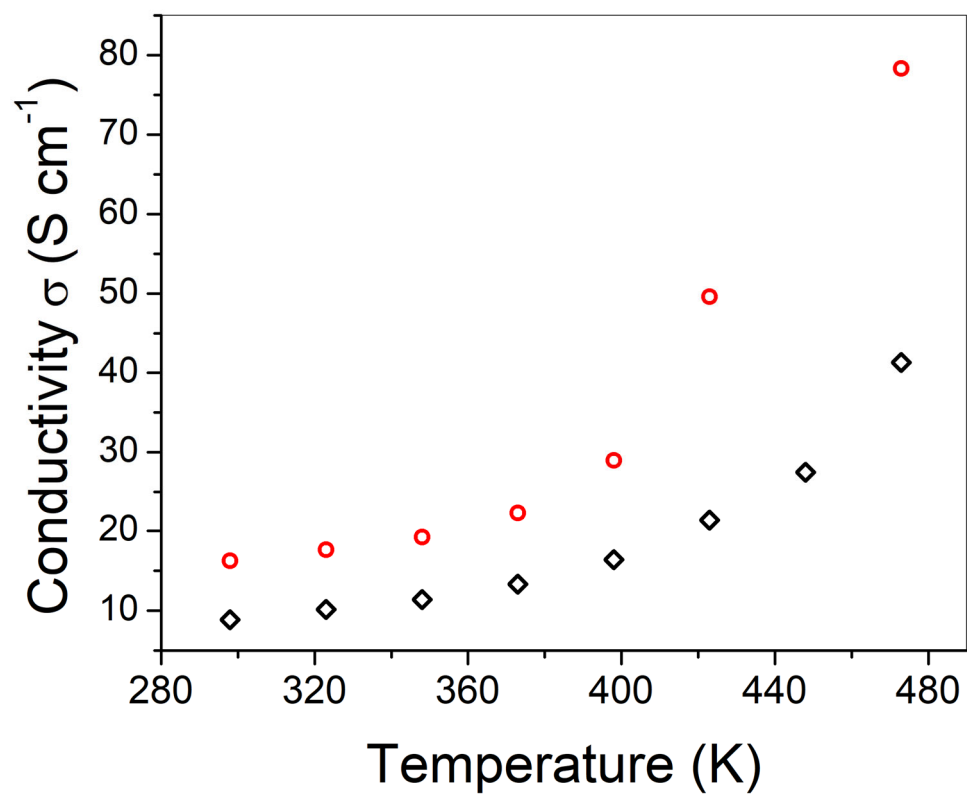


Figure S3. Electrical conductivity against Temperature of $\text{CuCr}_{2-x}\text{Sn}_x\text{S}_{2.3}\text{Se}_{1.7}$ $x = 0.4$ (red circles) and 0.6 (black diamonds) phases.

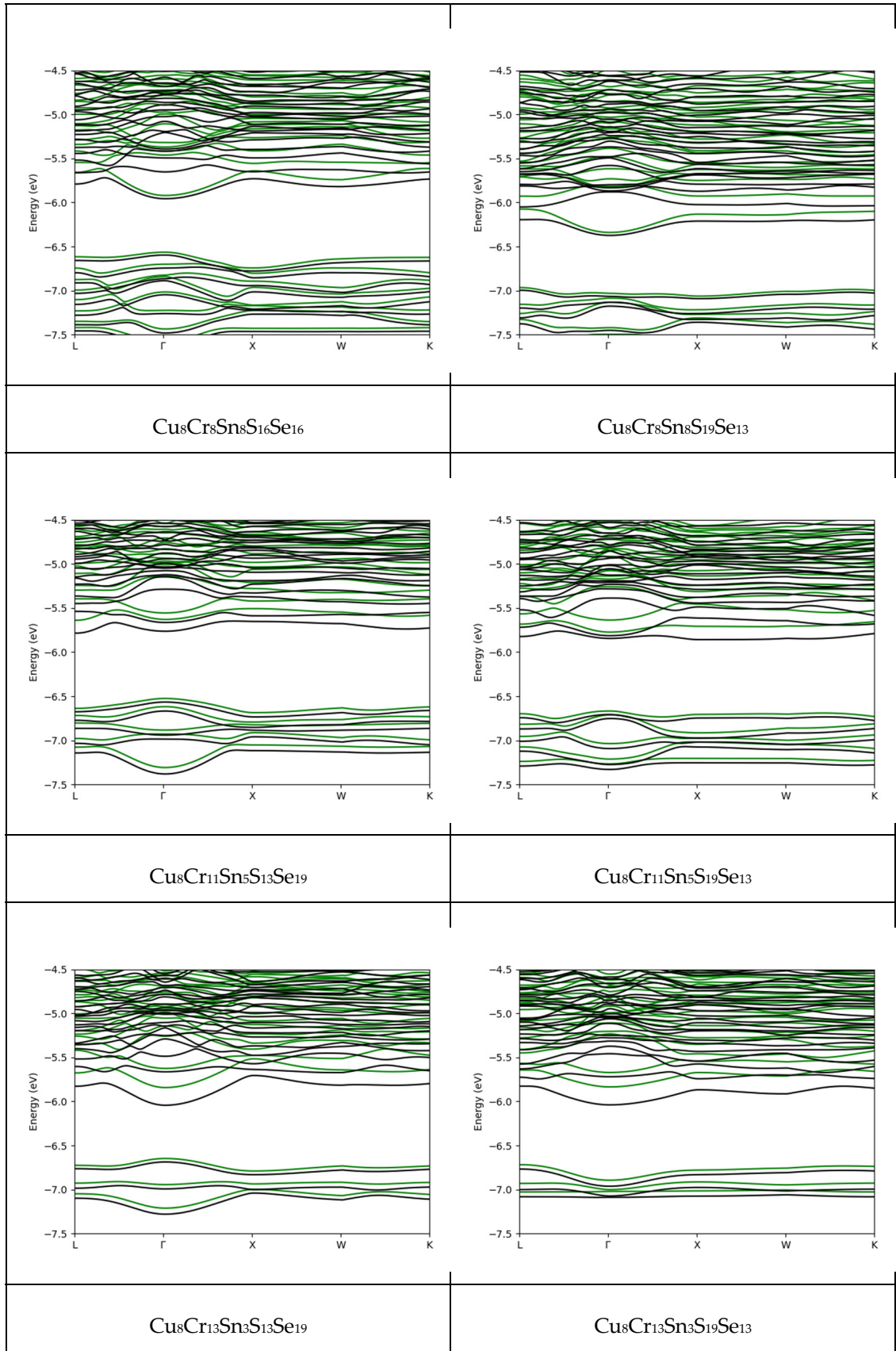
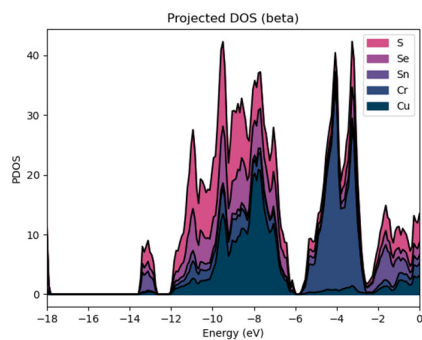
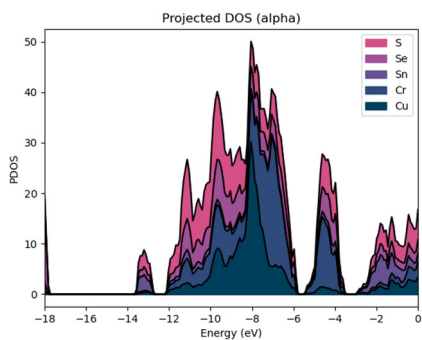
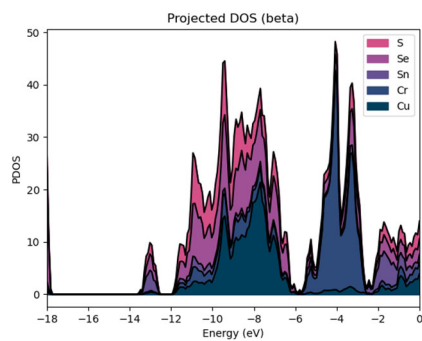
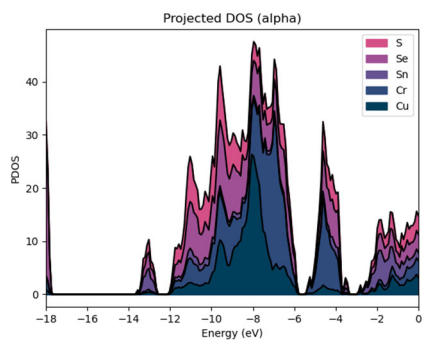
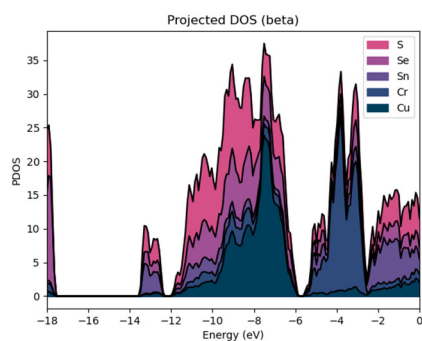
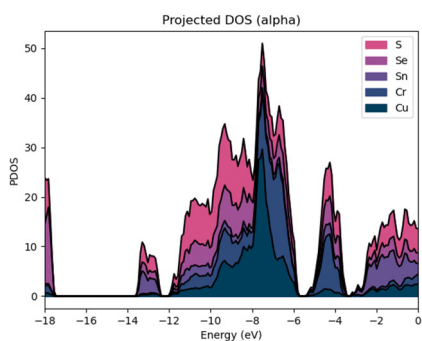
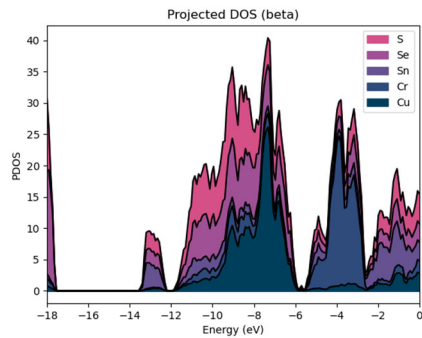
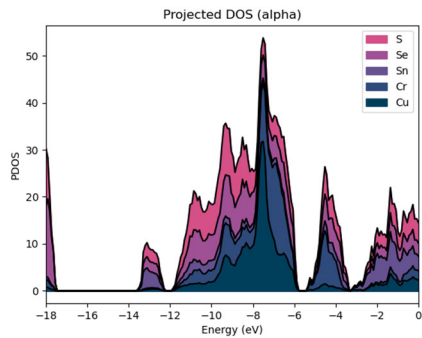


Figure S4. Band structures for calculated models. Alpha bands are depicted in black and beta bands are presented in green.



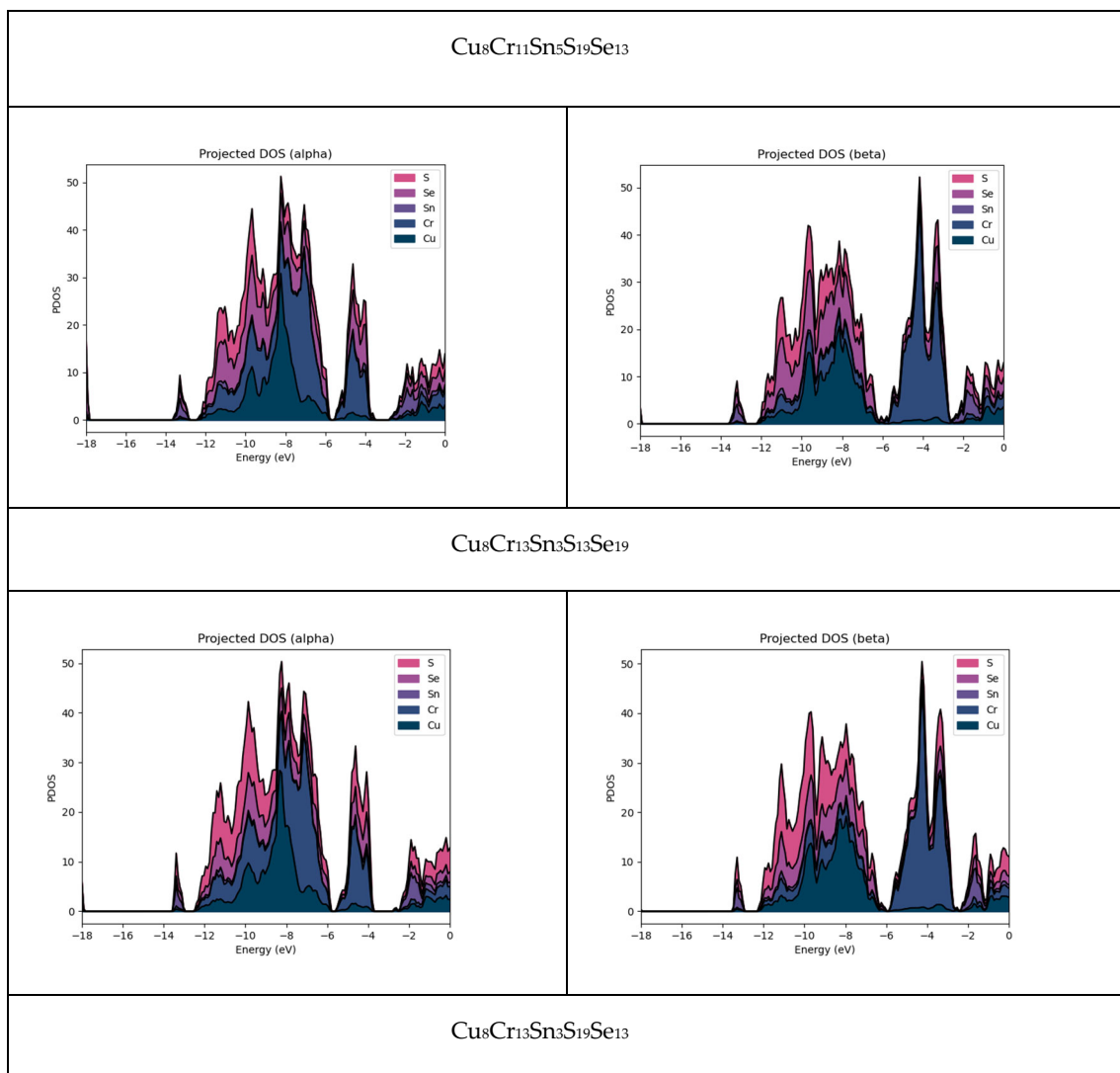


Figure S5 Element and spin resolved Density of states for all calculated systems.

Supplementary Materials: The following materials are available online at www.mdpi.com/xxx/s1. Table S1: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ; Figure S1: Representative powder XRD data for $\text{CuCr}_{1.0}\text{Sn}_{1.0}\text{S}_{2.3}\text{Se}_{1.7}$; Figure S2. Vegard's Law; Figure S3: Electrical conductivity against Temperature of $\text{CuCr}_{2-x}\text{Sn}_x\text{S}_{2.3}\text{Se}_{1.7}$; Figure S4. Band structures for calculated models. Alpha bands are depicted in black and beta bands are presented in green; Figure S5: Element and spin resolved Density of states for all calculated systems.

Author Contributions: conceptualization, A.G. and S.M.; methodology and experiments, P.V.G., P.B., A.G., and S.M.; writing—original draft preparation, S.M., P.V-G., D.A., and A.G.; electrical measurements, A.G. and P.V-G; DFT calculations, D.A. All authors have read and agreed to the final version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.



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