

Supporting Information

Title: Significant improvement in thermoelectric performance of Sb-incorporated chalcopyrite compounds $\text{Cu}_{18}\text{Ga}_{25}\text{Sb}_x\text{Te}_{50-x}$ ($x=0-3.125$) through the coordination of energy band and crystal structures

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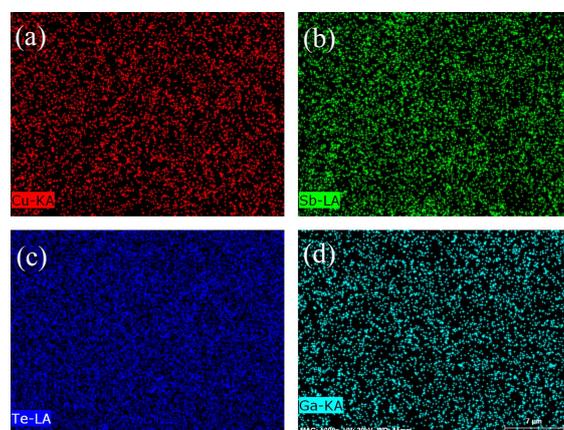


Fig.S1 EPMA mapping of four elements on polished $\text{Cu}_{18}\text{Ga}_{25}\text{Sb}_{2.5}\text{Te}_{47.5}$ surface (a) Cu, (b) Sb, (c) Te and (d) Ga.

Table S1 Chemical compositions (relative molars)
identified for $x=0, 2.5$ (taken from mappings)

Compounds	Cu	Ga	Sb	Te
$\text{Cu}_{18}\text{Ga}_{25}\text{Te}_{50}$	18.05	24.93	---	50.0
$\text{Cu}_{18}\text{Ga}_{25}\text{Sb}_{2.5}\text{Te}_{47.5}$	17.92	24.88	2.48	47.5

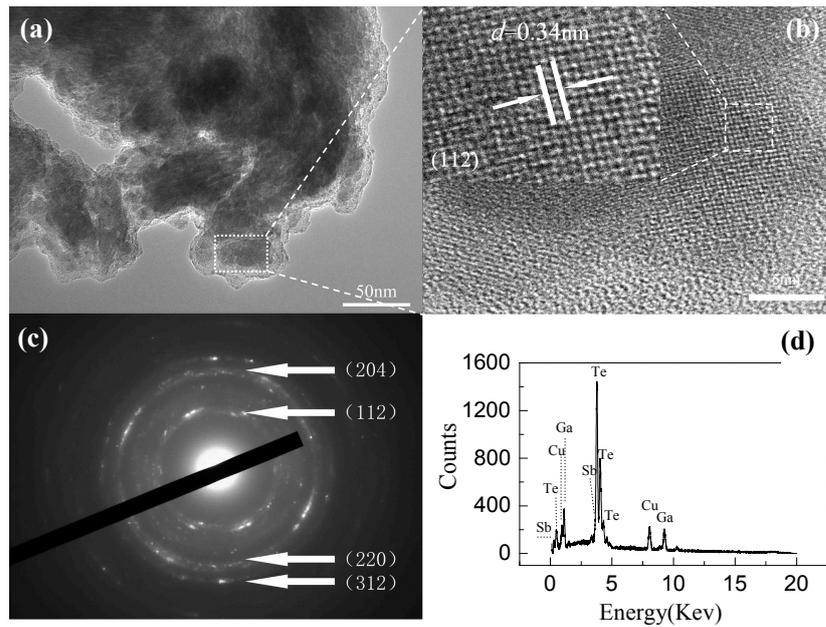


Fig.S2 High resolution transmission electron microscopy (HRTEM) image observed in $\text{Cu}_{18}\text{Ga}_{25}\text{Sb}_{2.5}\text{Te}_{47.5}$. (a) TEM image; (b) The corresponding high resolution TEM image, the inset is the magnified high resolution TEM image, which shows that the spacing between (112) crystal planes is about 0.34 nm. (c) The selected area electron diffraction (SAED) pattern; (d) Chemical compositions analyses.

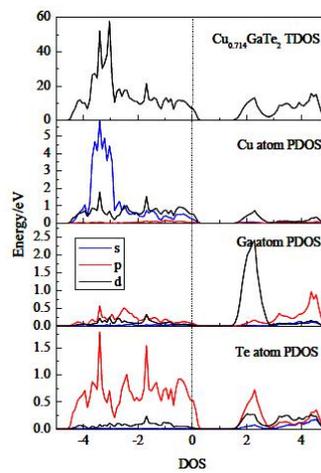


Fig. S3 The state of the densities (DOS) of the pristine ternary semiconductor $\text{Cu}_{18}\text{Ga}_{25}\text{Te}_{50}$.