

## Supporting Information for

### Achieving higher thermoelectric performance of n-type PbTe by adjusting band structure and enhanced phonons scattering

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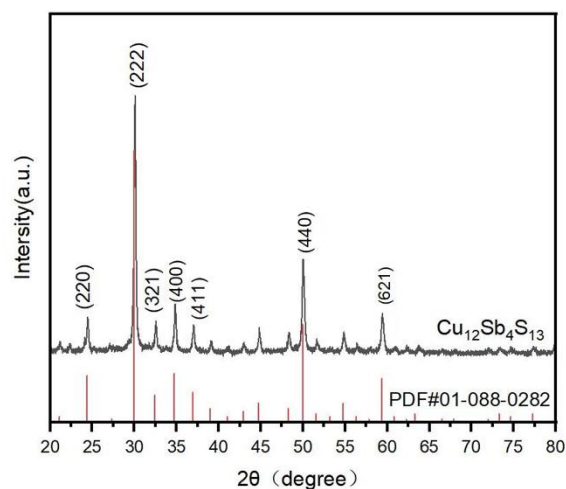
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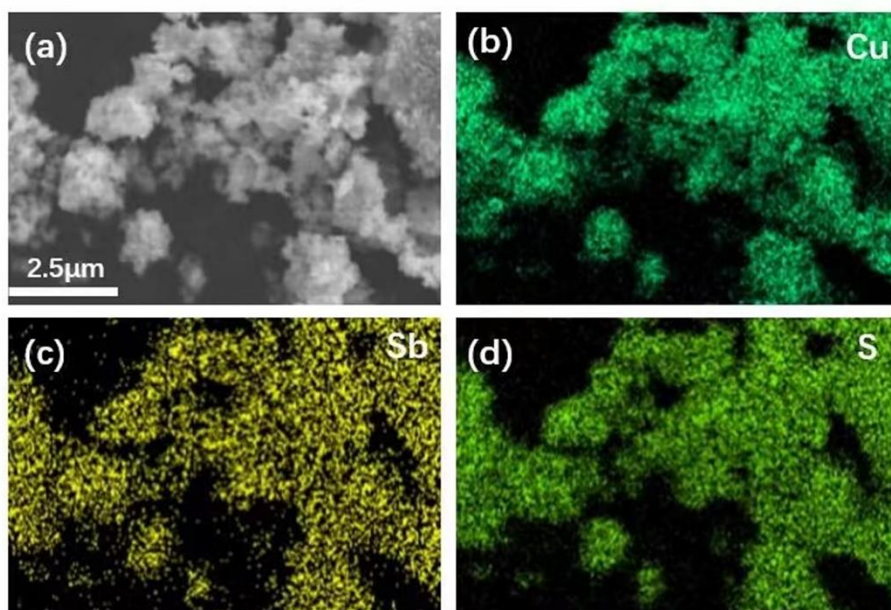
1. The raw materials, XRD pattern and FE-SEM micrographs for the  $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  nanoparticles.

Raw materials	$\text{SbCl}_3$ (99%)	$\text{CuCl}$ (97%)	S (99.5%)	ethyl alcohol (99.7%)	anhydrous ethylenediamine (99%)
Content	30mmol	90mmol	97.5mmol	-	-
Mass/Volume	6.8433g	8.9099g	3.1263g	50ml	250ml

**Table S1** Raw materials for synthesizing  $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  nanoparticles.



**Figure S1** XRD pattern for  $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  nanoparticles.



**Figure S2** FE-SEM micrographs of (a) surface of the  $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  nanoparticles, and (b)–(d) an

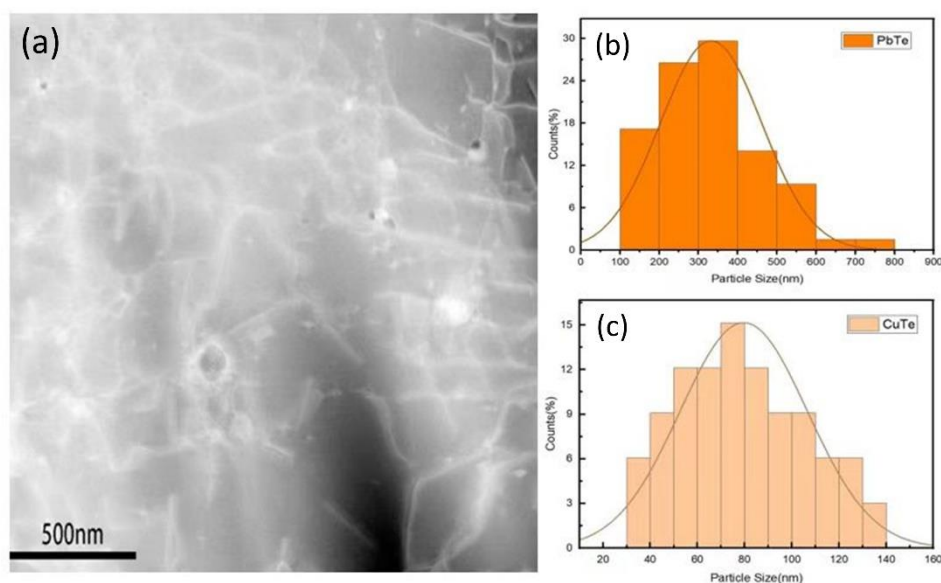
elemental (Cu, Sb and S) mapping.

**2. Theoretical densities, measured densities and relative densities for  $\text{Pb}_{0.97}\text{Sb}_{0.03}\text{Te} + y \text{ wt.}\%$   $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  ( $y = 0, 1.25, 1.5, 1.75$ ) samples.**

Composition	Theoretical density ( $\text{g cm}^{-3}$ )	Measured density ( $\text{g cm}^{-3}$ )	Relative density (%)
y=0	7.799	7.576	97.1
y=1.25	7.758	7.556	97.4
y=1.5	7.748	7.531	97.2
y=1.75	7.738	7.552	97.6

**Table S2** Theoretical densities, measured densities and relative densities for  $\text{Pb}_{0.97}\text{Sb}_{0.03}\text{Te} + y \text{ wt.}\%$   $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  ( $y = 0, 1.25, 1.5, 1.75$ ) samples.

**3. The size distribution histogram of PbTe matrix and CuTe nanoparticles.**



**Figure S3** (a) Low magnification STEM image of  $\text{Pb}_{0.97}\text{Sb}_{0.03}\text{Te} + 1.5 \text{ wt.}\%$   $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  composite sample; (b) the size distribution histogram of PbTe matrix; (c) the size distribution histogram of CuTe nanoparticles.