Supporting Information

Optimization of the thermoelectric performance of $Cu_{22}Sn_{10}S_{32}$ through In_2O_3 alloying†

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Supplementary Figures

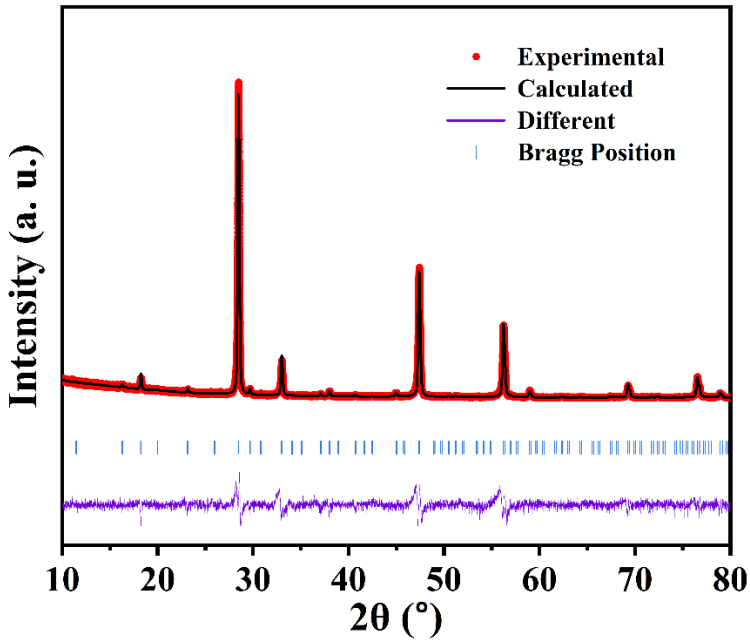

Fig. S1. Rietveld refinement of the $Cu_{22}Sn_{10}S_{32}$ sample.

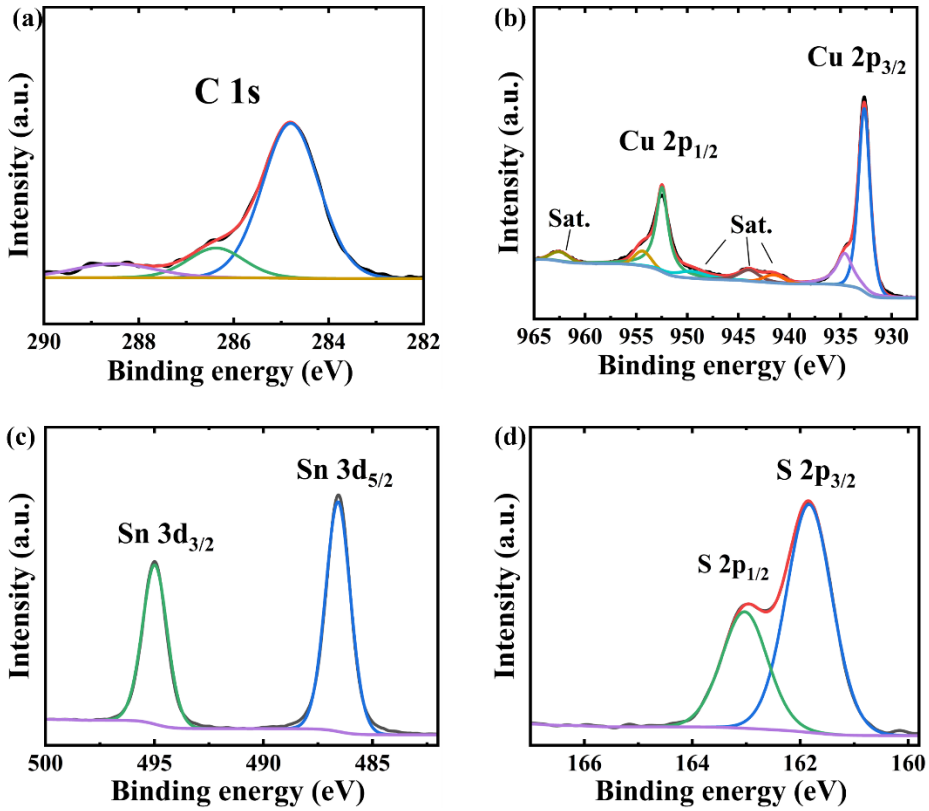

Fig. S2. XPS spectra of the CTS: (a) C 1s, (b) Cu 2p, (c) Sn 3d, (d) S 2p.

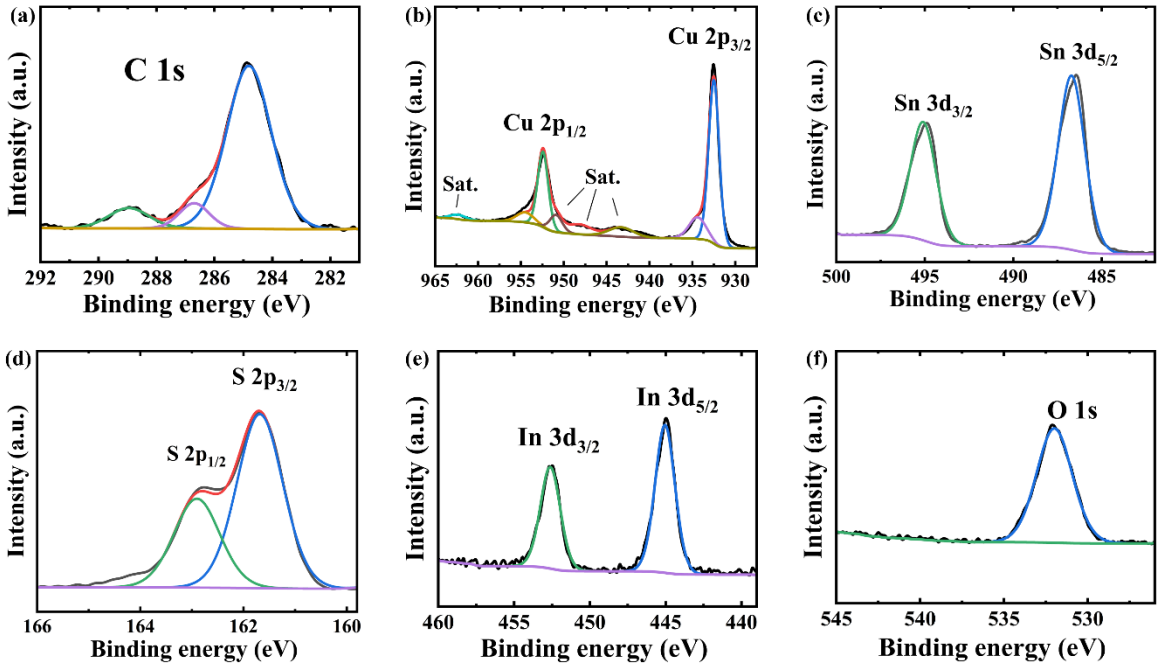

Fig. S3. XPS spectra of the CTS -5wt% In_2O_3: (a) C 1s, (b) Cu 2p, (c) Sn 3d, (d) S 2p (e) In 3d and (f) O 1s.

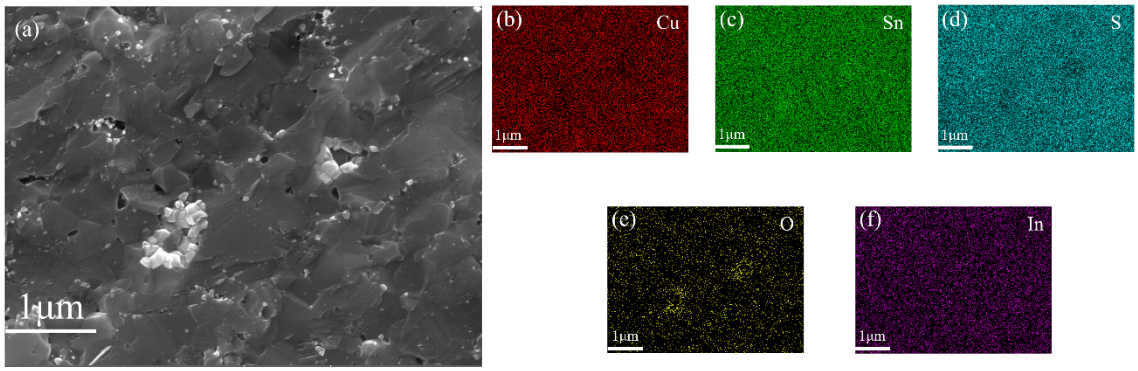

Fig. S4 (a)The enlarged view of CTS-7wt% In_2O_3 and elemental mapping analysis of (b-f) Cu; Sn; S; O; In.

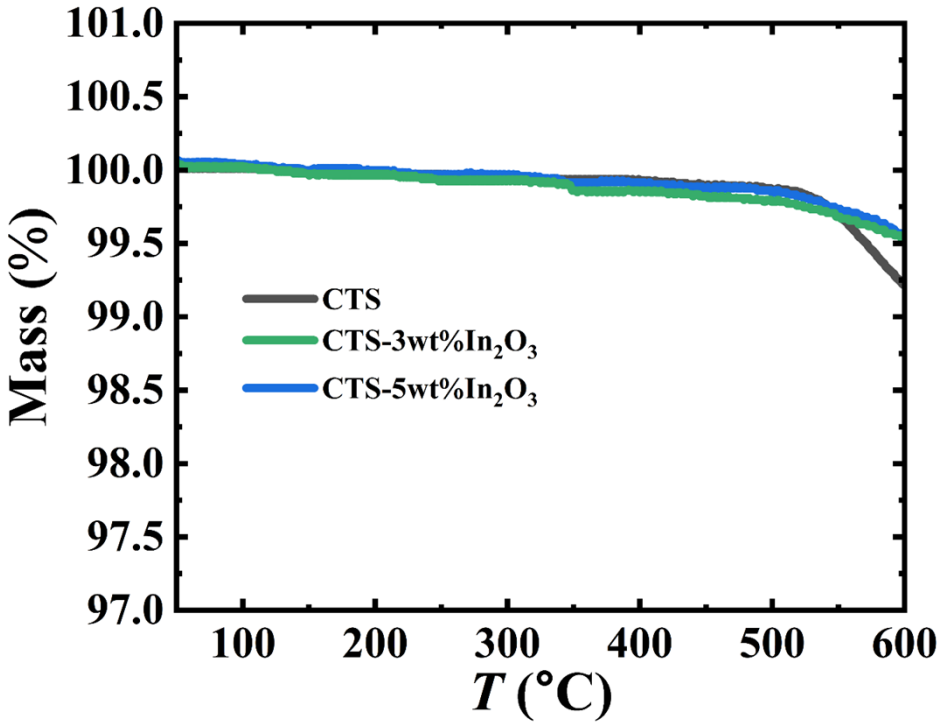

Fig. S5 The TGA curves for samples with CTS – x wt % In_2O_3(x=0, 2, and 5).

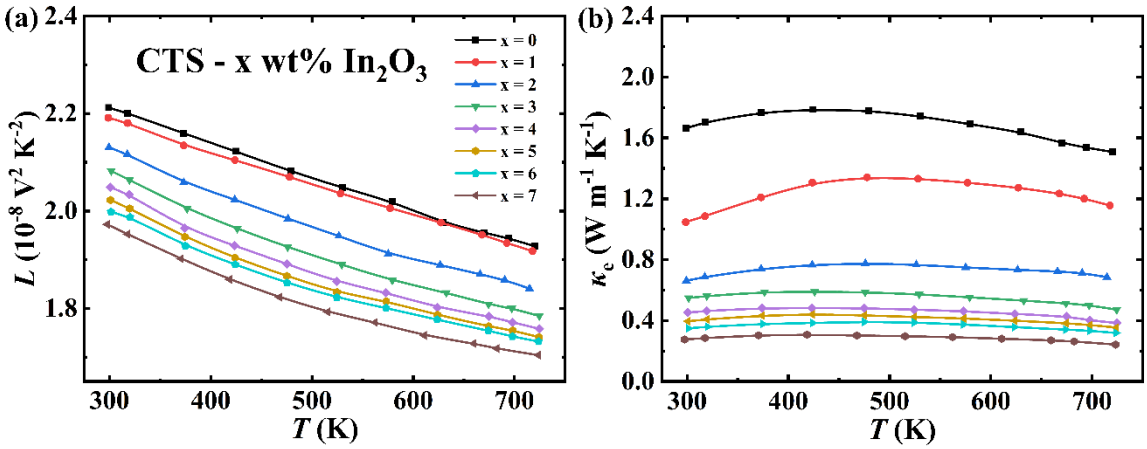

Fig. S6 Temperature dependence of (a) calculated Lorentz number L and (b) electron thermal conductivity for all sample.

Supplementary Tables

Table S1. Crystal structure parameters of $Cu_{22}Sn_{10}S_{32}$ obtained from refinement of XRD.

$Cu_{22}Sn_{10}S_{32}$ R_{wp}=9.2%, R_p=7.1%					
atom	x	y	z	Occ	U_{iso} (Å^2)
Cu1 6d	0.25	0	0	1	0.02297
Cu2 8e	0.248	x	x	1	0.01143
Cu3/Sn1 12f	0.248	0.248	0.248	0.65/0.35	0.01325
Sn2 12f	0.250	0.5	0	1	0.01601
S1 8e	0.125	0.125	0.125	1	0.01531
S2 24i	0.377	0.366	0.128	1	0.00111

Table S2. The measured density (g/cm^3) of all samples.

CTS – x wt % In_2O_3	density (g/cm^3)
x=0	4.55
x=1	4.45
x=2	4.49
x=3	4.53
x=4	4.56
x=5	4.59
x=6	4.63
x=7	4.64

Some characterization details

XRD: The working voltage was 40 kV, the current was 40 mA, the scan speed was 5°/min, and the step size was 0.02°.

SEM: Fresh cross-sections were obtained by brittle fracture using liquid nitrogen. BSE samples were obtained by polishing the samples with Al_2O_3 suspension.

TEM: The bulk material was ground into a fine powder, then subjected to ultrasonic treatment. Afterward, the sample was dropped onto a molybdenum grid and dried before testing.

XPS: A monochromatic Al target with a photon energy of 1486.6 eV was used. The resolution and sensitivity of the monochromatic source were calibrated using an Ag standard. The deconvolution analysis was performed using advantage software.