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Enhancing the thermoelectric performance of SnTe-$CuSbSe_2$ with an ultra-low lattice thermal conductivity†

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Calculation of the Lorenz number (*L*) and effective mass (*m)**

For a degenerate semiconductor like SnTe, *L* and *m** can be approximatively calculated by the single parabolic band (SPB) model.[1–4]

The value of *L* is generally related to the scattering factors (*r*) as well as the reduced Fermi energy (*η*), and *m** can be obtained by a relation with Hall carrier concentration (*n*). Here, acoustic phonon scattering is considered to be the prime scattering mechanism (*r*=−1/2), and η can be deduced by (1), (2) and (3) below:

$$S(\eta) = \frac{\kappa_B}{e}\left[\frac{\left(r+\frac{5}{2}\right)\cdot F_{r+\frac{3}{2}}(\eta)}{\left(r+\frac{3}{2}\right)\cdot F_{r+\frac{1}{2}}(\eta)} - \eta\right] \tag{1}$$

$$F_x(\eta) = \int_0^\infty \frac{\epsilon^x}{1+e^{(\epsilon-\eta)}}d\epsilon \tag{2}$$

$$\eta = \frac{E_f}{k_B T} \tag{3}$$

Therefore, *L* and *m**can be computed as follows:

$$L = \frac{\kappa_B}{e}\left\{\frac{\left(r+\frac{7}{2}\right)\cdot F_{r+\frac{5}{2}}(\eta)}{\left(r+\frac{3}{2}\right)\cdot F_{r+\frac{1}{2}}(\eta)} - \left[\frac{\left(r+\frac{5}{2}\right)\cdot F_{r+\frac{3}{2}}(\eta)}{\left(r+\frac{3}{2}\right)\cdot F_{r+\frac{1}{2}}(\eta)}\right]^2\right\} \tag{4}$$

$$n = \frac{1}{e\cdot R_H} = \frac{(2m^*\cdot\kappa_B T)^{3/2}}{3\pi^2 h^3}\cdot\frac{\left(r+\frac{3}{2}\right)^2\cdot F^2_{r+\frac{1}{2}}(\eta)}{\left(2r+\frac{3}{2}\right)\cdot F_{2r+\frac{1}{2}}(\eta)} \tag{5}$$

Where the k_B, *e*, E_f, *T*, $F_x(\eta)$, R_H and *h* is the Boltzmann constant, the electron charge, the Fermi energy, the absolute temperature, the Fermi integrals, the Hall coefficient and the Plank's constant, respectively.

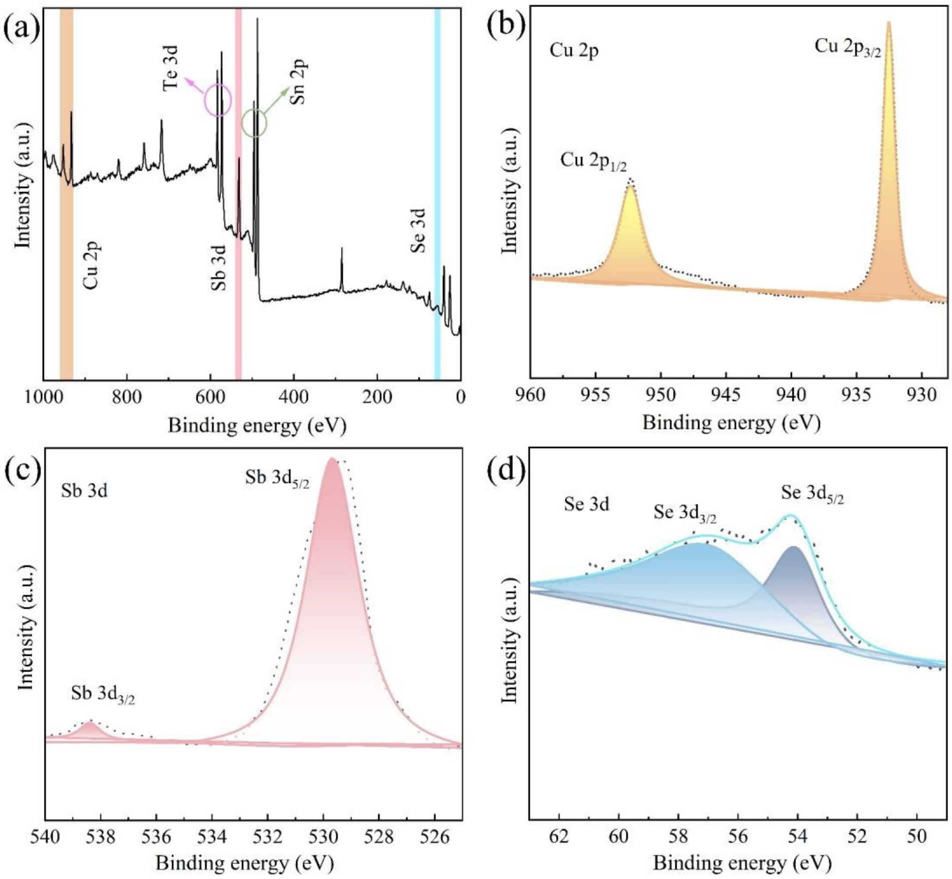

Fig. S1 XPS spectra of the SnTe-5% $CuSbSe_2$ sample: (a) the total survey XPS spectrum; (b) high-resolution Cu 2p XPS spectrum; (c) high-resolution Sb 3d XPS spectrum; (d) high-resolution Se 3d XPS spectrum.

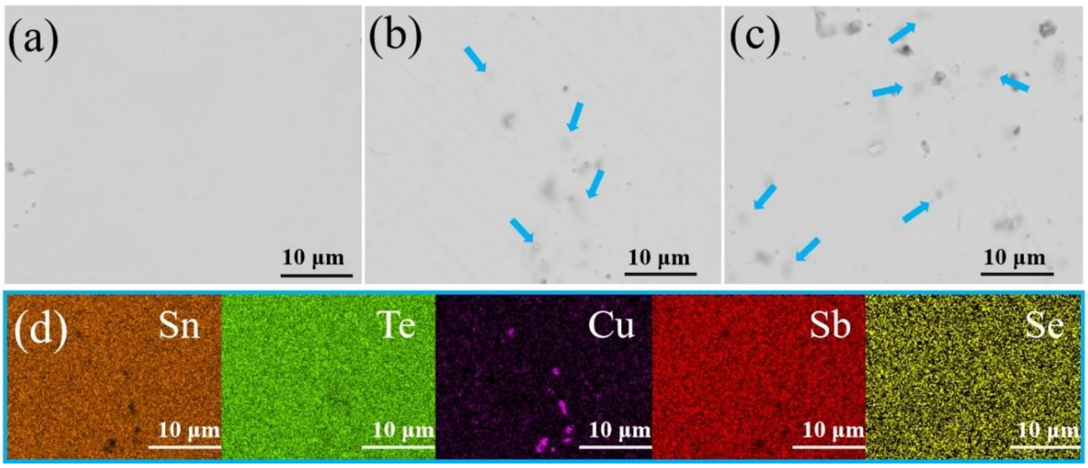

Fig. S2 SEM micromorphology of SnTe-*x*% $CuSbSe_2$ (*x*=0, 5, 8): (a-c) BSE images of the SnTe (a), SnTe-5% $CuSbSe_2$ (b), and SnTe-8% $CuSbSe_2$ (c) samples. The blue arrows indicate the positions of Cu-based nanoprecipitates; (d-h) element mapping images of Sn, Te, Cu, Sb and Se for the SnTe-5% $CuSbSe_2$ sample.

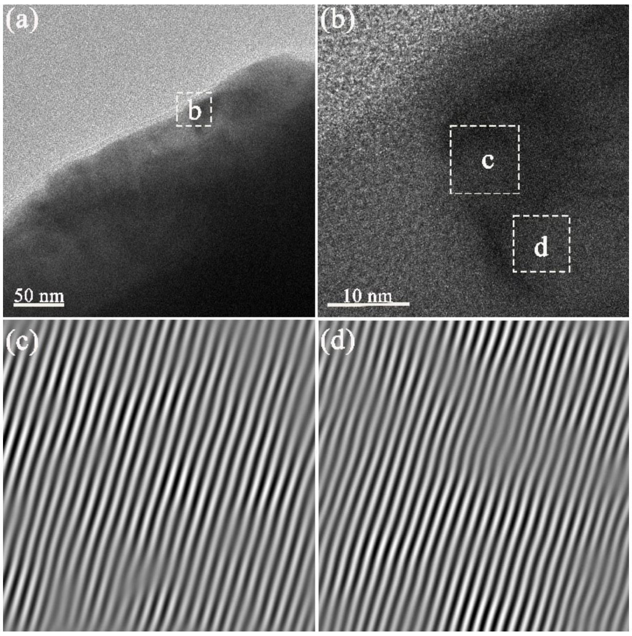

Fig. S3 (a) Low resolution TEM images for the pristine SnTe. (b) High resolution TEM (HR-TEM) image of the marked square in (a). (c-d) IFFT of the selected region in (b).

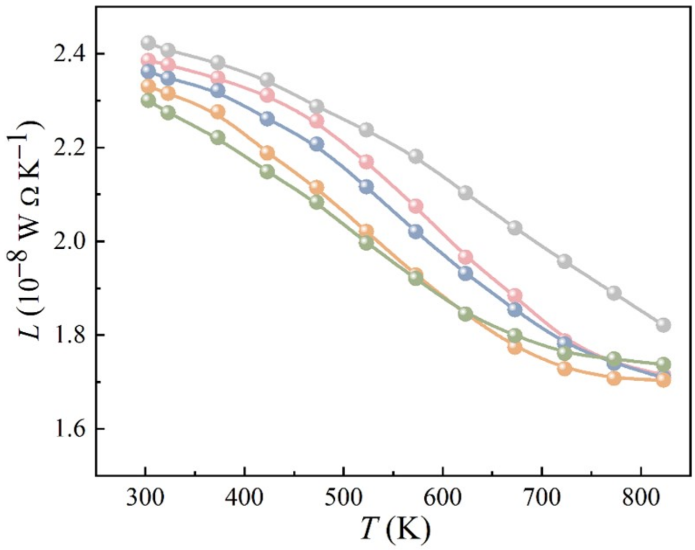

Fig. S4 The calculated Lorenz number (L) as a function of temperature for SnTe-x% $CuSbSe_2$ (x=0, 3, 5, 8, 11).

Reference

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