Supplementary Information

Co-alloying of Sn and Te Enables High Thermoelectric Performance in Ag_9GaSe_6

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Calculation of the minimum lattice thermal conductivity

Based on the simplified Cahill's model, the minimum lattice thermal conductivity κ_{min} for a normal solid can be expressed as[1, 2]

$$\kappa_{min} = \frac{1}{2}\left(\frac{\pi}{6}\right)^{1/3} k n^{2/3} (2v_t + v_l)$$

where v_t is the transverse speed of sound, v_l is the longitudinal speed of sound, and n is the number density of atoms. Besides, an assessment of the high temperature diffusion limit of the lattice thermal conductivity is made possible by the obtained sound velocities based on the following equation[3, 4]:

$$\kappa_{diff} = 0.76 k n^{2/3} \frac{1}{3}(2v_t + v_l).$$

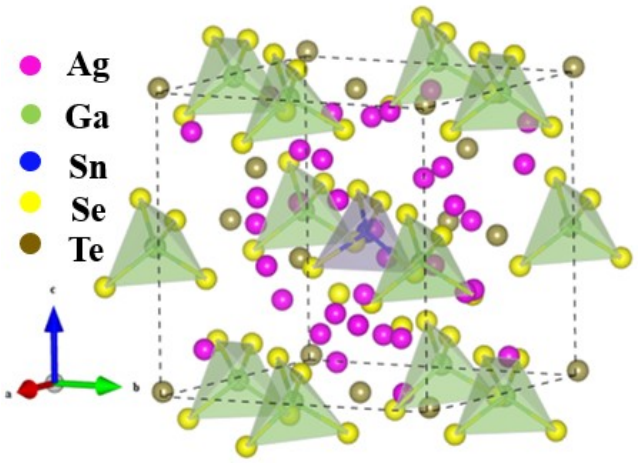

Figure S1. The crystal structure of $Ag_{8.75}Ga_{0.75}Sn_{0.25}Se_{4.5}Te_{1.5}$ used for theoretical calculations.

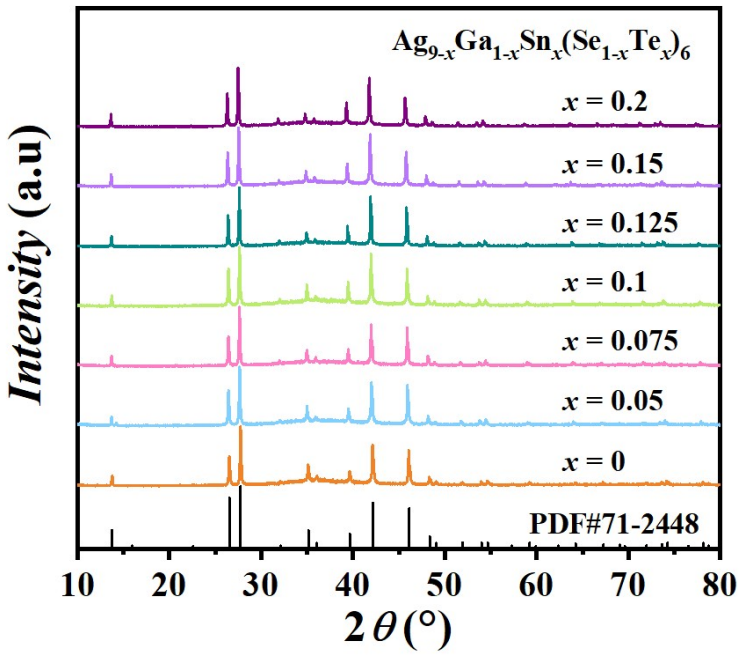

Figure S2. The room temperature PXRD patterns for $Ag_{9-x}Ga_{1-x}Sn_x(Se_{1-x}Te_x)_6$ (x = 0, 0.05, 0.075, 0.1, 0.125, 0.15, and 0.2).

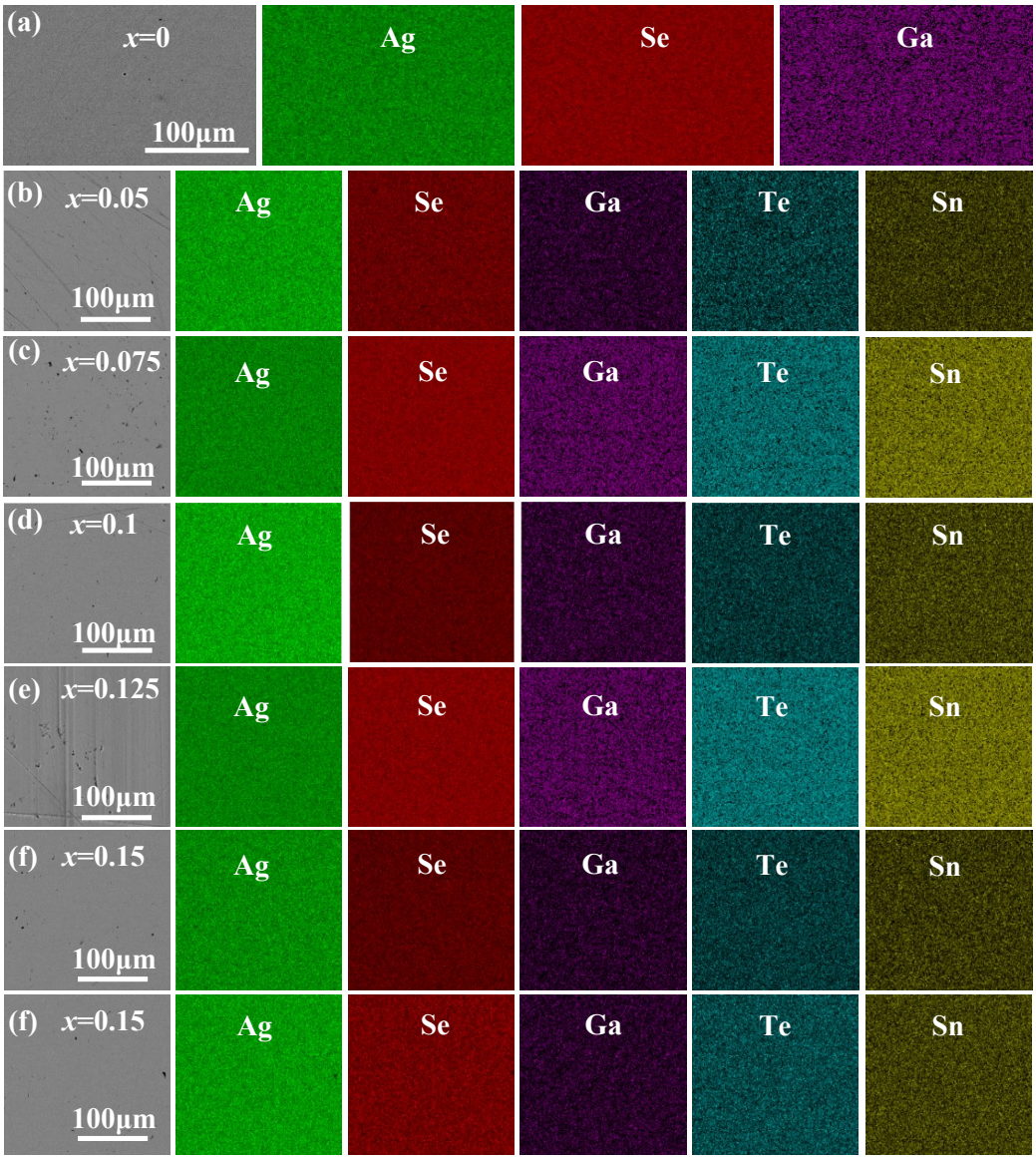

Figure S3. (a) SEM images (BSE model) and corresponding EDS mappings observed in $Ag_{9-x}Ga_{1-x}Sn_x(Se_{1-x}Te_x)_6$ (x = 0, 0.05, 0.075, 0.1, 0.125, 0.15, and 0.2).

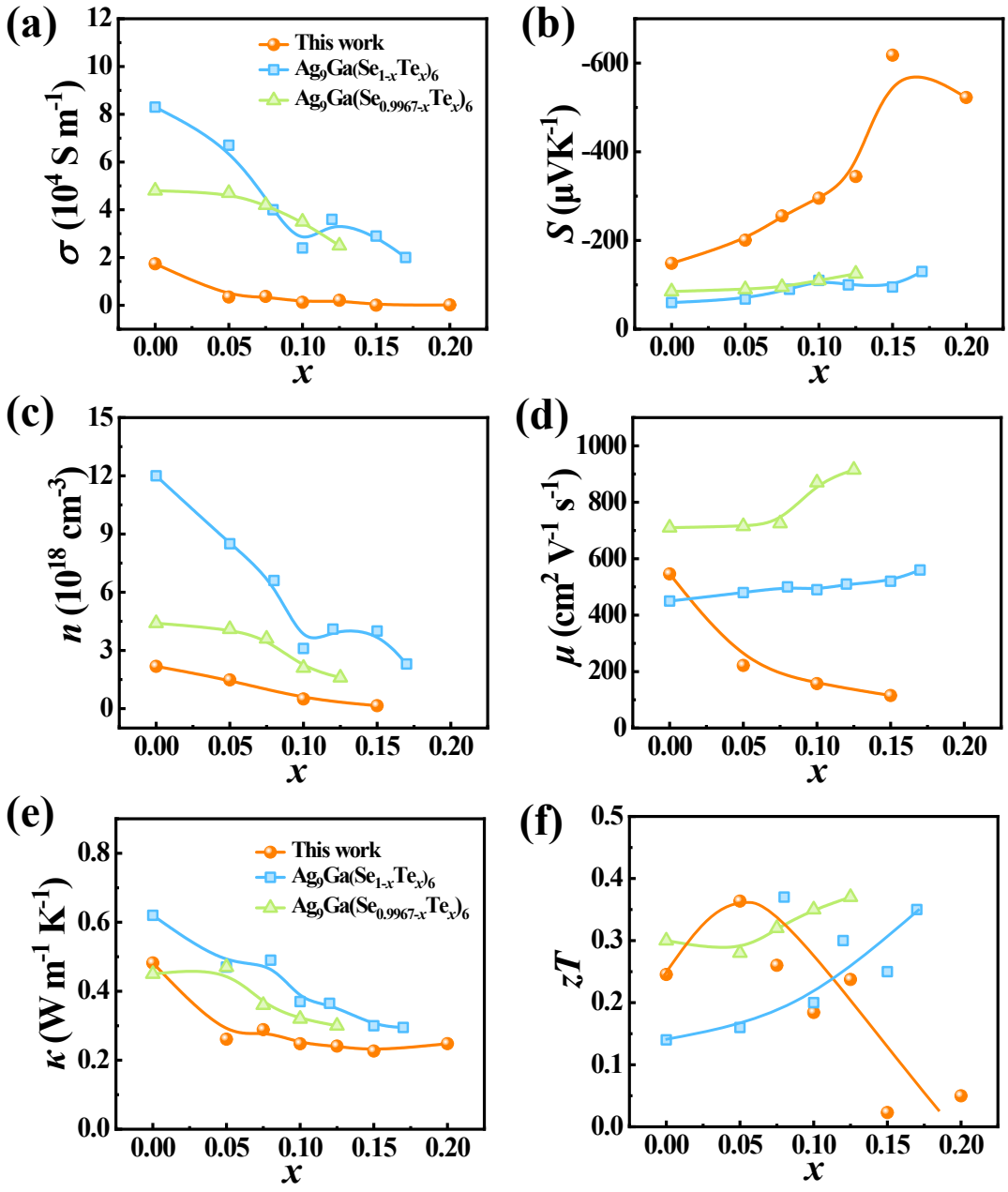

Figure S4. Room temperature (a) electrical conductivity (σ), (b) Seebeck coefficient (S), (c) carrier concentration (n), (d) carrier mobility (μ), (e) thermal conductivity (κ), and (f) TE figure of merit zT as a function of alloying content x for $Ag_{9-x}(Ga_{1-x}Sn_x)(Se_{1-x}Te_x)_6$. The data of $Ag_9Ga(Se_{0.9967-x}Te_x)_6$ from Ref [5] and $Ag_9Ga(Se_{1-x}Te_x)_6$ from Ref [6] are included for comparison.

Table S1. Element composition obtained from the EDS results for $Ag_{9-x}Ga_{1-x}Sn_x(Se_{1-x}Te_x)_6$ (x = 0, 0.05, 0.075, 0.1, 0.125, 0.15, and 0.2).

Samples	Ag	Ga	Sn	Se	Te
x = 0	56.4	6.1		37.5	
x = 0.05	56.0	5.8	0.1	36.0	2.1
x = 0.075	56.2	5.7	0.2	35.3	2.9
x = 0.1	55.9	5.7	0.3	34.2	3.9
x = 0.125	55.9	5.4	0.4	33.5	4.8
x = 0.15	55.8	5.3	0.6	32.6	5.7
x = 0.2	55.6	5.0	1.0	30.8	7.6

References

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