

Supporting Information

Realization of High Thermoelectric Performance in Solution Synthesized Porous Zn and Ga codoped SnSe Nanosheets

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Lorenz number calculation in details:

In general, the total (κ) consists of the electronic thermal conductivity (κ_e) and lattice thermal conductivity (κ_L). The electronic part κ_e is directly proportional to the electrical conductivity σ through the Wiedemann-Franz relation, $\kappa_e = L\sigma T$, where L is Lorenz number and its value is calculated by SPB model. The Lorenz number can be given as:^{1,2}

$$L = \frac{k_B^2}{e^2} \left(\frac{(r+3)F_{r+2}(\eta)}{(r+1)F_r(\eta)} - \left[\frac{(r+2)F_{r+1}(\eta)}{(r+1)F_r(\eta)} \right]^2 \right) \quad (1)$$

For the Lorenz number calculation, we should get reduced Fermi energy η firstly.

The calculation of η can be derived from the measured Seebeck coefficients by using the following relationship:

$$S = \pm \frac{k_B}{e} \left(\eta - \frac{(r+2)F_{r+1}(\eta)}{(r+1)F_r(\eta)} \right) \quad (2)$$

where $F_n(\eta)$ is the n -th order Fermi integral,

$$F_n(\eta) = \int_0^{\infty} \frac{\chi^n}{1 + e^{\chi - \eta}} d\chi \quad (3)$$

where e is the electron charge, k_B is the Boltzmann constant, h is the Planck constant, r is the scattering factor. Here, r is 0 since acoustic phonon scattering has been assumed as the main carrier scattering mechanism near room temperature (RT). Lorenz number can be obtained by combining equations (1), (2) and (3).

Table S1 Lattice parameters for pure SnSe and Sn_{0.99-x}Zn_{0.01}Ga_xSe (x=0, 0.01, 0.02, 0.03)

Compositions	a (Å)	b (Å)	c (Å)	Volume (Å³)
SnSe	11.52915	4.16209	4.4541	213.73
x=0	11.52929	4.16298	4.4453	213.36
x=0.01	11.52172	4.16063	4.4441	213.04
x=0.02	11.52114	4.16419	4.43738	212.89
x=0.03	11.51765	4.16224	4.4372	212.72

Table S2 The calculated and measured densities for pure SnSe and $\text{Sn}_{0.99-x}\text{Zn}_{0.01}\text{Ga}_x\text{Se}$

(x=0, 0.01, 0.02, 0.03)

Compositions	Theoretical Density	Actual Density	Density
	(ρ, g/cm³)	(ρ, g/cm³)	%
SnSe	6.190	6.03	97.4
x=0	6.181	5.96	96.4
x=0.01	6.163	5.87	95.2
x=0.02	6.145	5.82	94.7
x=0.03	6.127	5.8	94.7

Figure S1 $\text{Sn}_{0.96}\text{Zn}_{0.01}\text{Ga}_{0.03}\text{Se}$ temperature dependent (a) total thermal conductivity(κ_T), (b) lattice thermal conductivity(κ_L), (c) electrical conductivity (σ), (d) Seebeck coefficient(S), (e) power factor (PF), (f) ZT for sample parallel to the pressing direction ($//$) and perpendicular to the pressing direction (\perp).

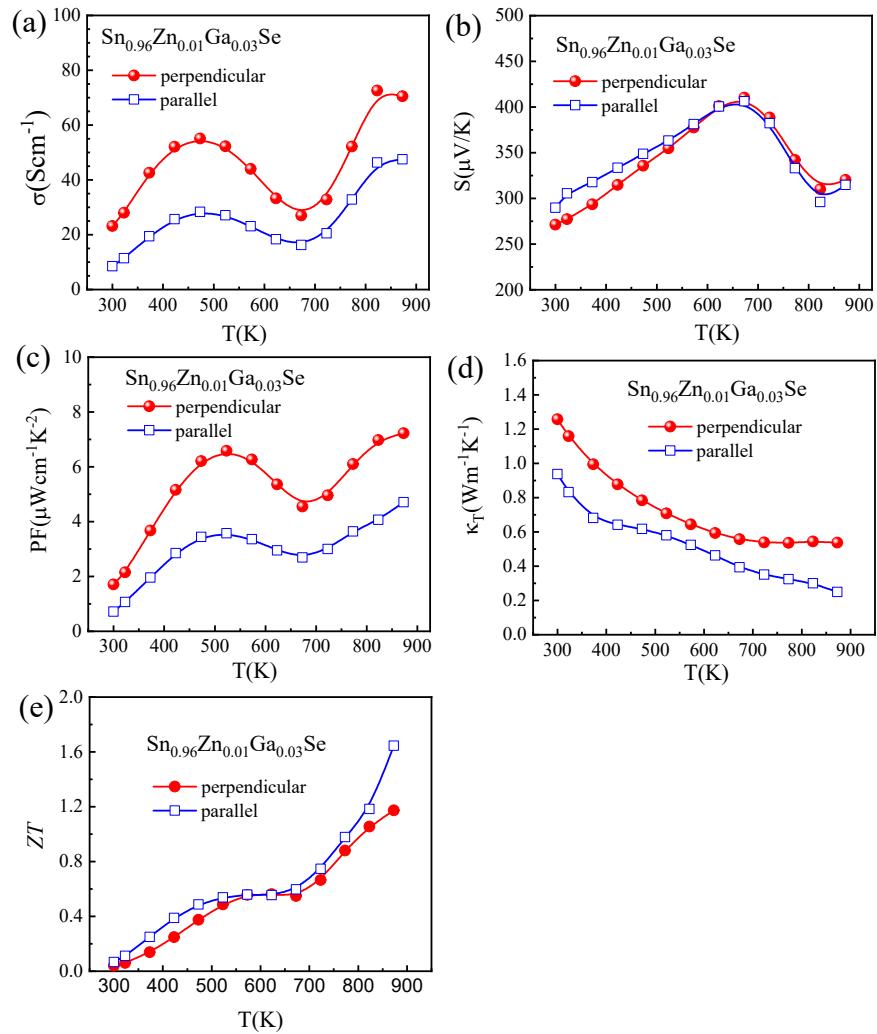


Figure S2 The thermal diffusivity (D) for pure SnSe and $\text{Sn}_{0.99-x}\text{Zn}_{0.01}\text{Ga}_x\text{Se}$ ($x=0, 0.01, 0.02, 0.03$)

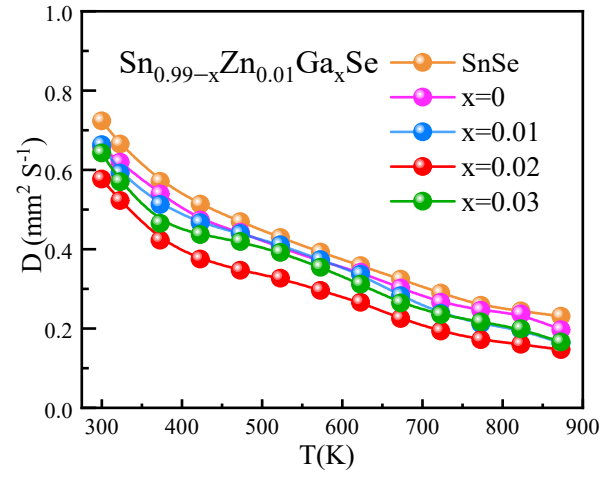


Figure S3 Comparison of the temperature dependent (a) total thermal conductivity(κ_T) (b)

lattice thermal conductivity(κ_L)

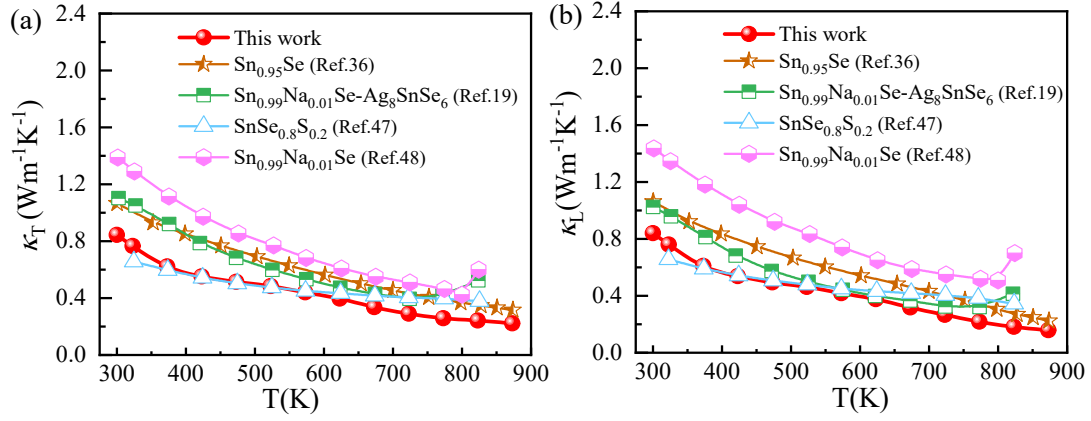


Figure S4 (a) Lorenz number (L) (b) electronic thermal conductivity (κ_e) as a function of temperature for pure SnSe and $\text{Sn}_{0.99-x}\text{Zn}_{0.01}\text{Ga}_x\text{Se}$ ($x=0, 0.01, 0.02, 0.03$)

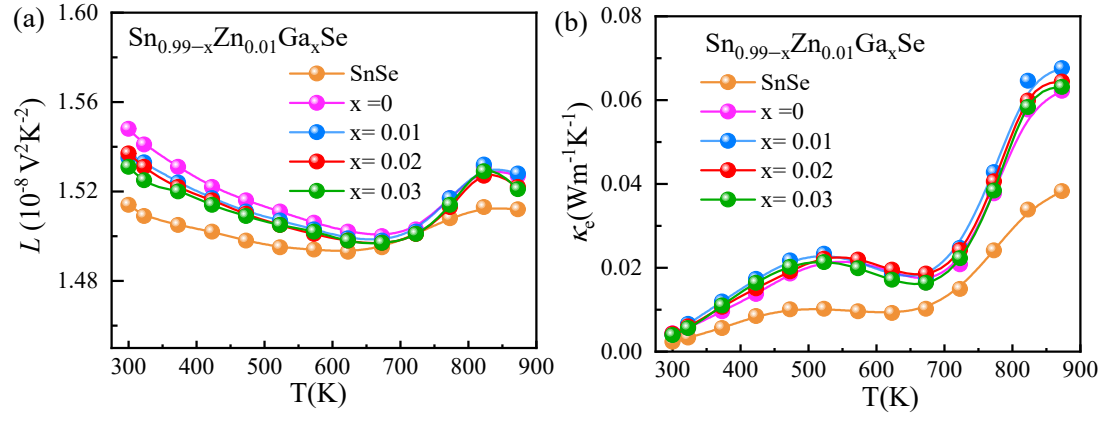


Figure S5 SEM image of as-synthesized $\text{Sn}_{0.99}\text{Zn}_{0.01}\text{Se}$ powder sample.

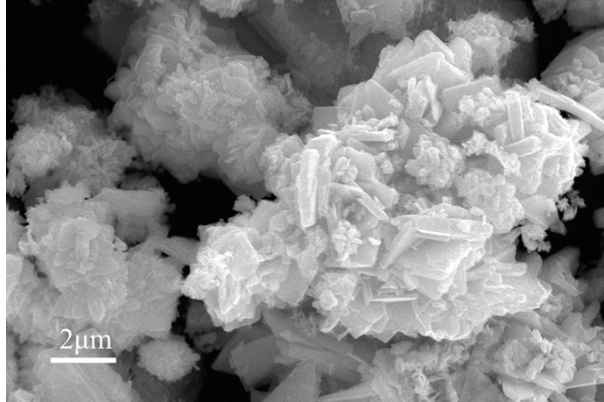
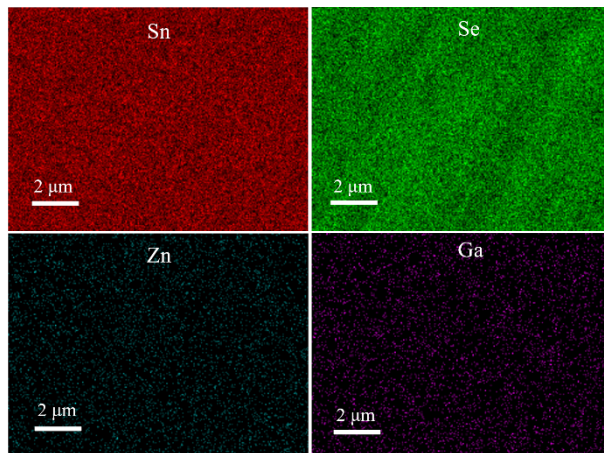
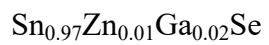


Figure S6 Energy Dispersive Spectrometer (EDS) elemental mapping image for



Reference

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- [2] A. F. May; E. S. Toberer; A. Saramat; G. J. Snyder, *Phys. Rev. B* **2009**, *80*, 125205.