Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Enhancing the solubility of Mn in $AgSbSe_2$ for high thermoelectric performance through entropy engineering

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Results and Discussion：

1. Lorenz number calculation based on the single parabolic band

In our work, the Lorenz number is obtained based on the single parabolic band:

$$\mathrm{L}=\left(\frac{\kappa_B}{e}\right)^2\left[\frac{\left(r+7/2\right)F_{r+5/2}(\eta)}{\left(r+3/2\right)F_{r+1/2}(\eta)}-\left(\frac{\left(r+5/2\right)F_{r+3/2}(\eta)}{\left(r+3/2\right)F_{r+1/2}(\eta)}\right)^2\right], \qquad (1)$$

In the equations above the integral $F_{\mathrm{n}}(\eta)$ is defined by

$$F_{\mathrm{n}}(\eta)=\int_0^{\infty}\frac{\chi^n}{1+e^{\chi-\eta}}d\chi, \qquad (2)$$

$$\eta=\frac{E_f}{k_BT}, \qquad (3)$$

Where $F_{\mathrm{n}}(\eta)$ is the Fermi integral function of order n, and η is called the reduced Fermi energy. η can be obtained by the following formula:

$$S=\pm\frac{k_B}{e}\left(\frac{\left(r+5/2\right)F_{r+3/2}(\eta)}{\left(r+3/2\right)F_{r+1/2}(\eta)}-\eta\right) \qquad (3)$$

Using the tested Seebeck coefficients, solve the above equation to get η. The scattering factor r is $-1/2$ in acoustic phonon scattering.

The average sound velocities (V_a) were calculated based on:

$$V_a=\left[\frac{1}{3}\left(2/V_T^3+1/V_l^3\right)\right]^{-\frac{1}{3}}$$

2. Figures

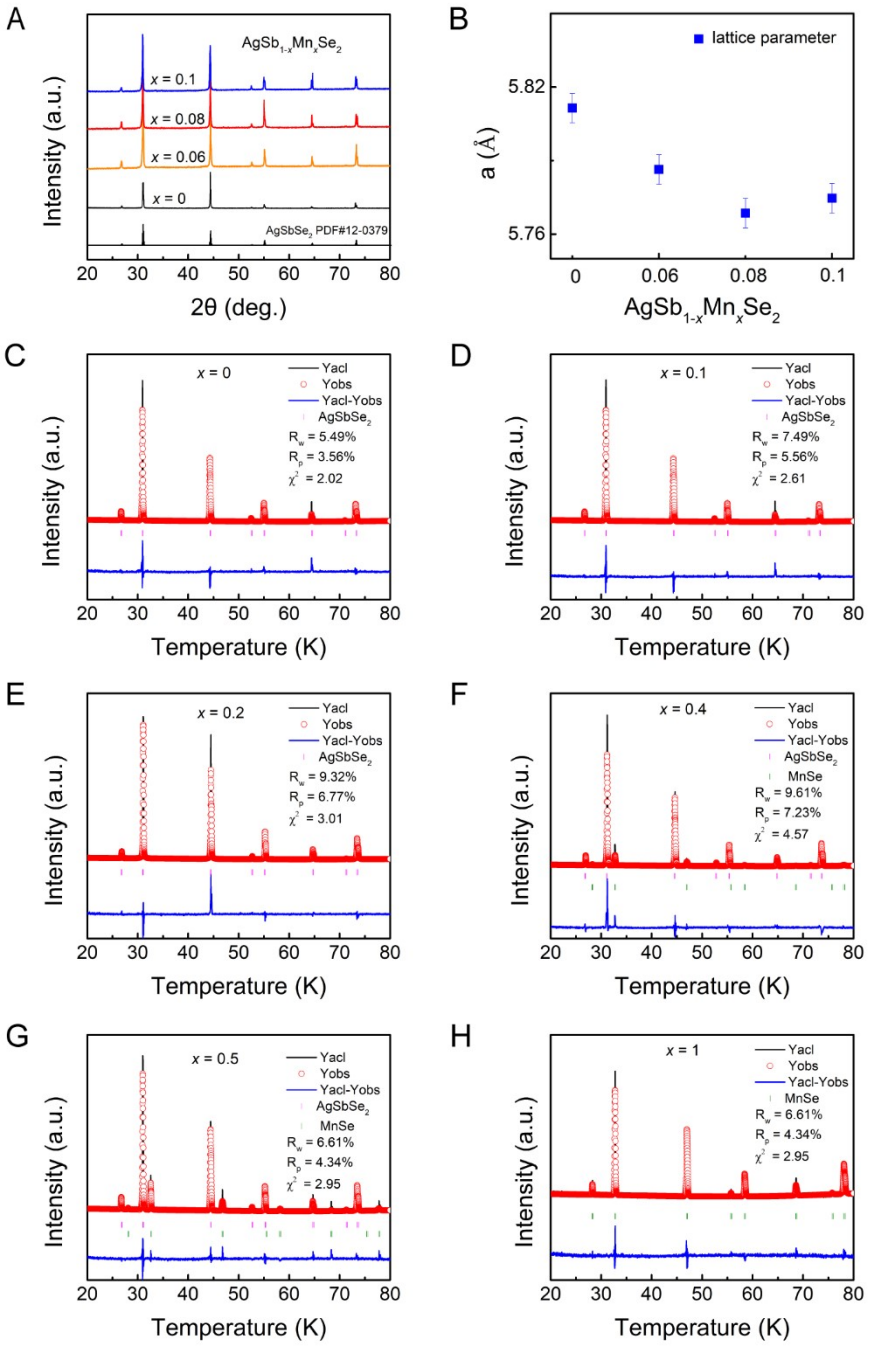

Figure S1. (A) Powder XRD patterns, (B) lattice parameters of $AgSb_{1-x}Mn_xSe_2$ (x = 0, 0.06, 0.08, 0.1) at room temperature. (C) - (H) Rietveld refinement result using X-ray diffraction data for (AgSbSe2)1-x(MnSe)x (x = 0, 0.1, 0.2, 0.4, 0.5, 1).

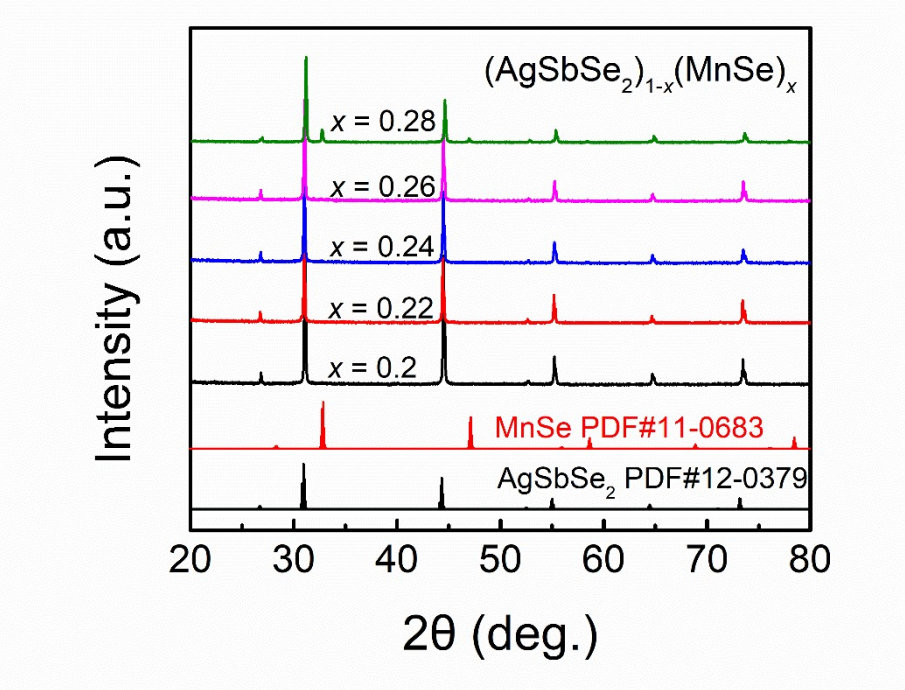

Figure S2. Powder XRD patterns for $(AgSbSe_2)_{1-x}(MnSe)_x$ (x = 0.2, 0.24, 0.26, 0.28).

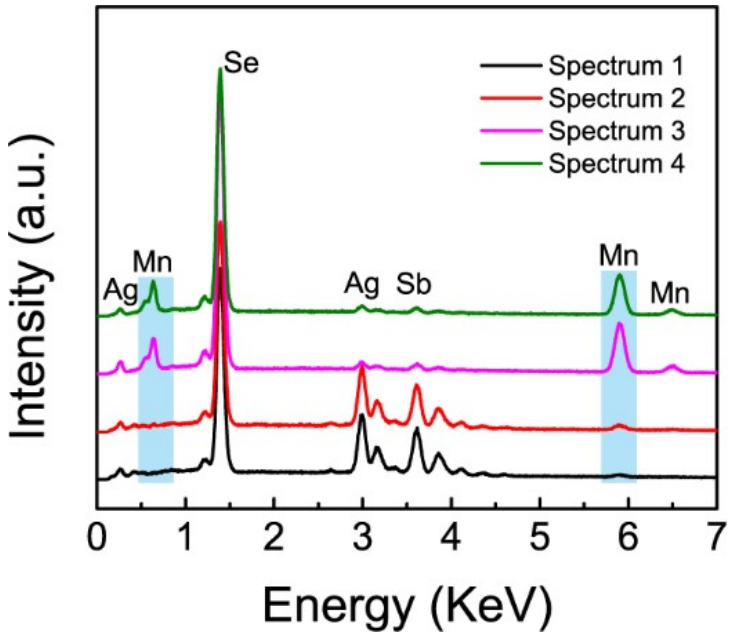

Figure S3. Wavelength dispersion spectrometer (WDS) images of elemental Ag, Mn, Sb and Se corresponding to panel C in Figure 2B.

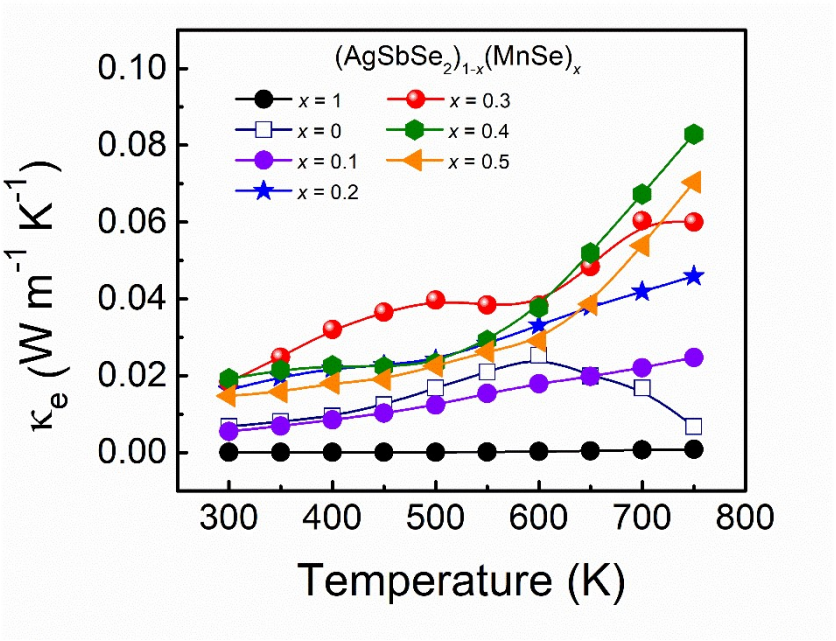

Figure S4. Electronic thermal conductivities as functions of temperature for $(AgSbSe_2)_{1-x}(MnSe)_x$ (x = 0, 0.1, 0.2, 0.3, 0.4, 0.5).

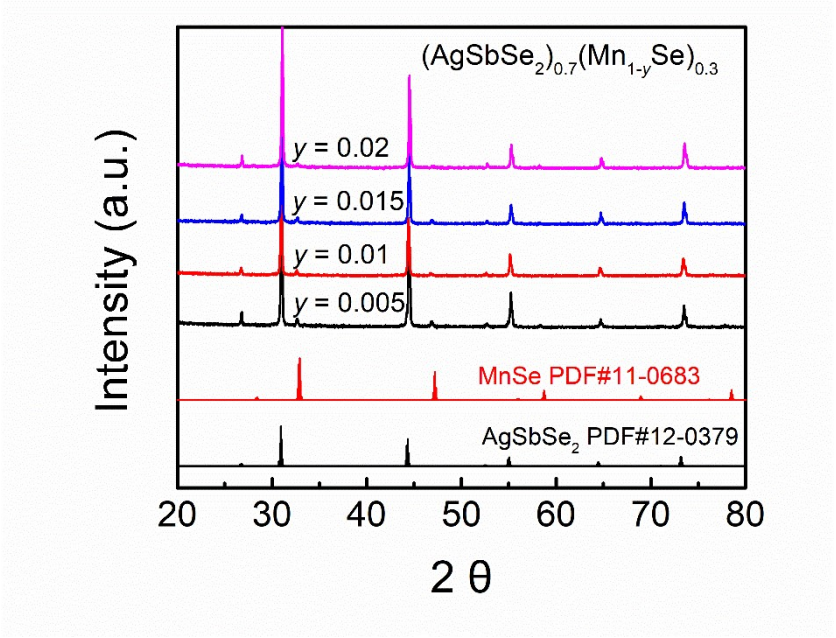

Figure S5. Powder XRD patterns for $(AgSbSe_2)_{0.7}(Mn_{1-y}Se)_{0.3}$ (y = 0.005, 0.01, 0.015, 0.02).

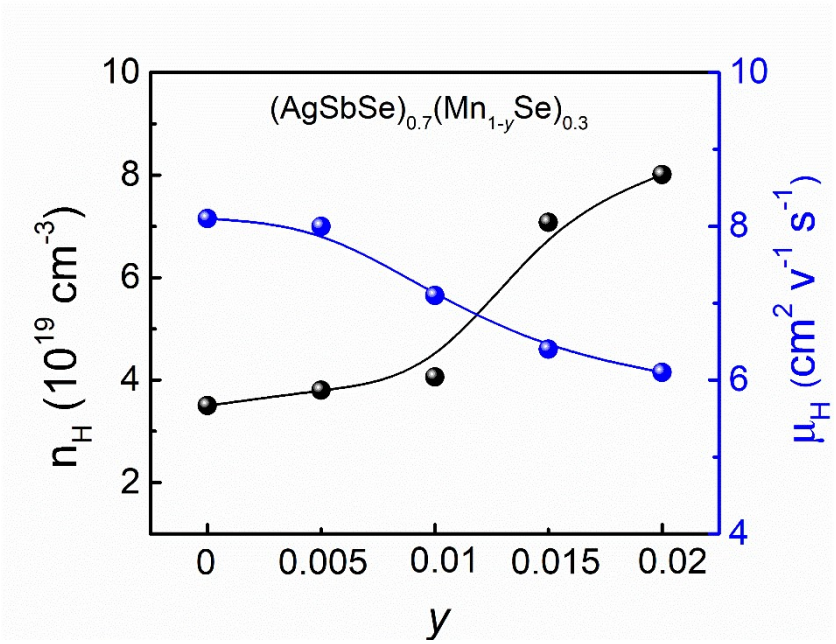

Figure S6. The Hall carrier concentration and Hall mobility of $(AgSbSe_2)_{0.7}(Mn_{1-y}Se)_{0.3}$ (y = 0.005, 0.01, 0.015, 0.02) at room temperature.

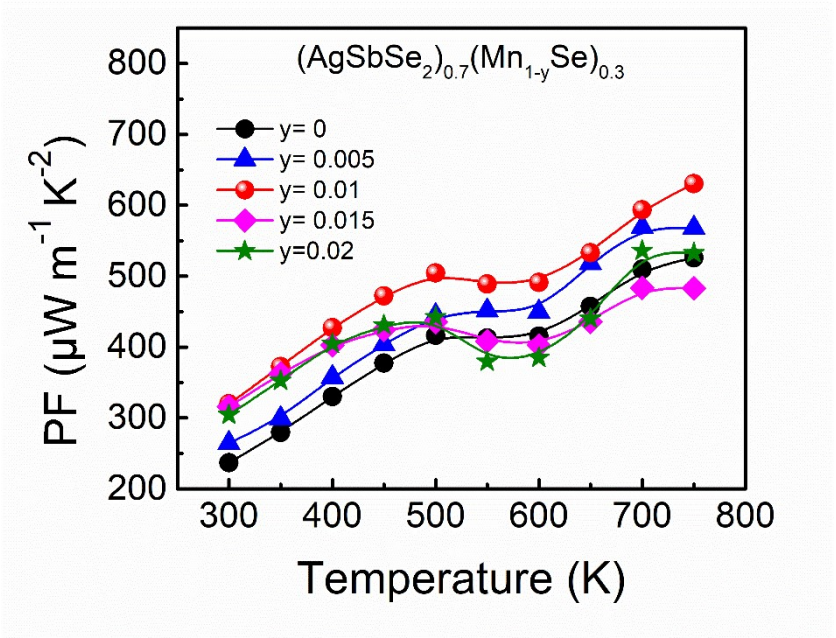

Figure S7. Power factors as a function of temperature for $(AgSbSe_2)_{0.7}(Mn_{1-y}Se)_{0.3}$ (y = 0.005, 0.01, 0.015, 0.02).

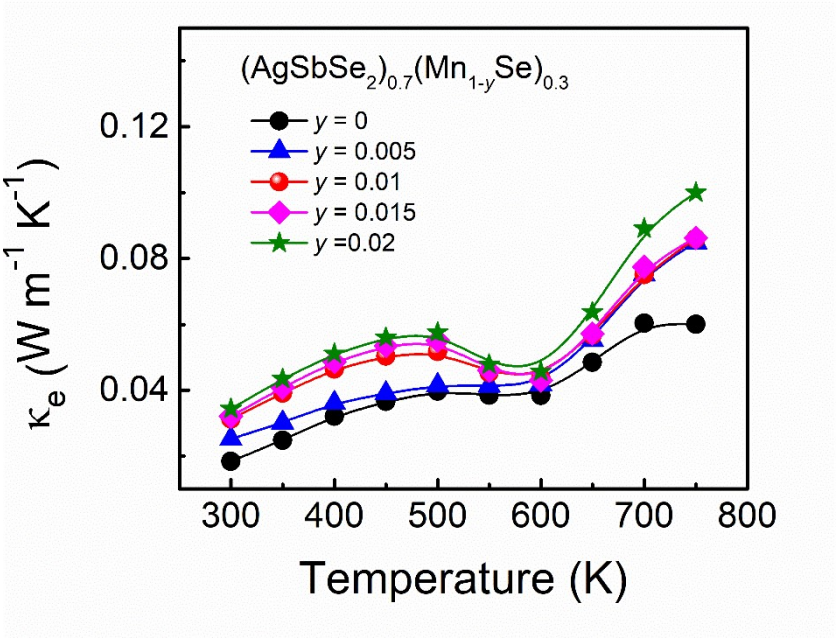

Figure S8. Electronic thermal conductivities as functions of temperature for $(AgSbSe_2)_{0.7}(Mn_{1-y}Se)_{0.3}$ (y = 0.005, 0.01, 0.015, 0.02).

3. Table

Table S1. Density ρ of $(AgSbSe_2)_{1-x}(MnSe)_x$ (x = 0, 0.1, 0.2, 0.3, 0.4, 0.5) and $(AgSbSe_2)_{0.7}(Mn_{1-y}Se)_{0.3}$ (y = 0.005, 0.01, 0.015, 0.02) at room temperature

Sample	ρ (g cm^{-3})
$AgSbSe_2$	6.35
MnSe	5.51
x = 0.1	6.26
x = 0.2	6.17
x = 0.3	6.10
x = 0.4	6.02
x = 0.5	6.00
y = 0.005	6.01
y = 0. 01	6.05
y = 0.015	6.04

y = 0.02	6.03