Electronic Supplementary Information (ESI)

Enhancing thermoelectric performance of N-type $Bi_2Te_{2.7}Se_{0.3}$ through incorporation of Ag_9AlSe_6 inclusions

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1. The measured densities for all the bulk samples

Table S1 The density(d) and the relative density(d_r) of BTS-$x$vol%Ag_9AlSe_6 (x=0, 0.15, 0.25, 0.35,0.50 and 0.70).

Table S1. The density(d) and the relative density(d_r) of $Bi_2Te_{2.7}Se_{0.3}$ -$x$vol. % Ag_9AlSe_6

$Bi_2Te_{2.7}Se_{0.3}$ -$x$vol. % Ag_9AlSe_6	d (g cm^3)	d_r (%)
x=0	7.82	98.9
x=0.15	7.78	98.4
x=0.25	7.83	99.0
x=0.35	7.76	98.1
x=0.50	7.79	98.5
x=0.70	7.69	97.3

where d_r is relative density, defined as $d_r=d/d_o$, here d is the measured density and d_o (7.91 of g cm^{-3}) is the theoretical density of $Bi_2Te_{2.7}Se_{0.3}$. For composite specimens $Bi_2Te_{2.7}Se_{0.3}$ -$x$vol. % Ag_9AlSe_6, the theoretical density is modified as: $d_o= (1-x)\, d_1 + x\, d_2$, where $d_1=d_o$ for BTS matrix and d_2 (7.14 g cm^{-3}) is the theoretical density of Ag_9AlSe_6.

2. SEM image of the BTS

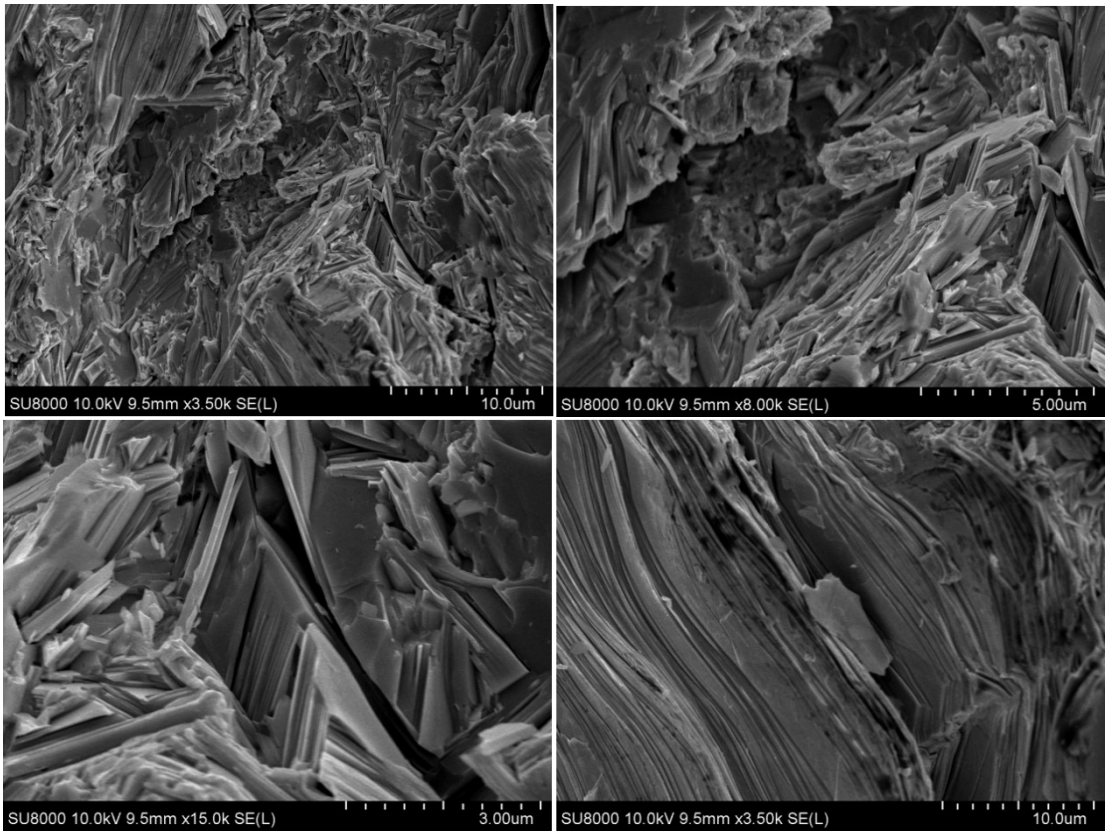

FIG.S1. SEM image of the fractured surface of the BTS.

3. SEM image of the Ag_9AlSe_6 particle

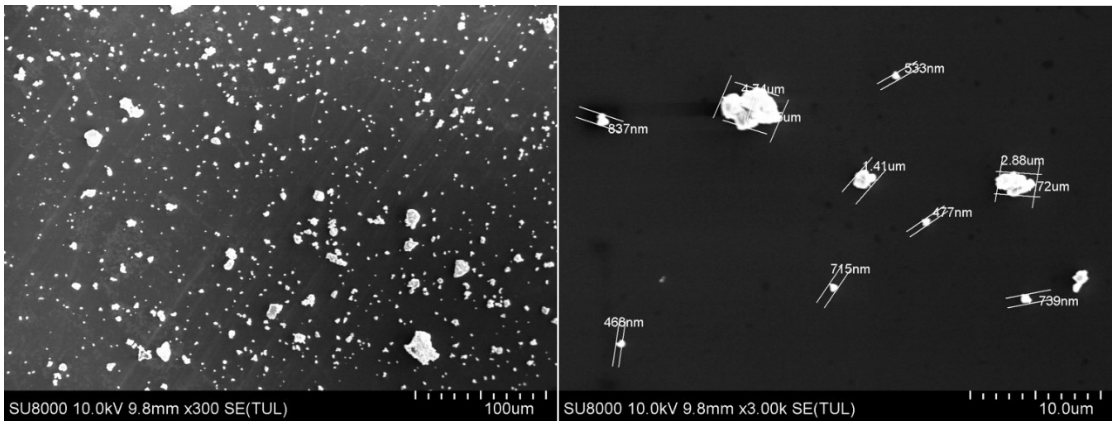

FIG.S2. SEM image of the Ag_9AlSe_6 particle.

4. SEM and EDS images of fracture surfaces of the bulk sample BTS-0.35Vol%Ag_9AlSe_6

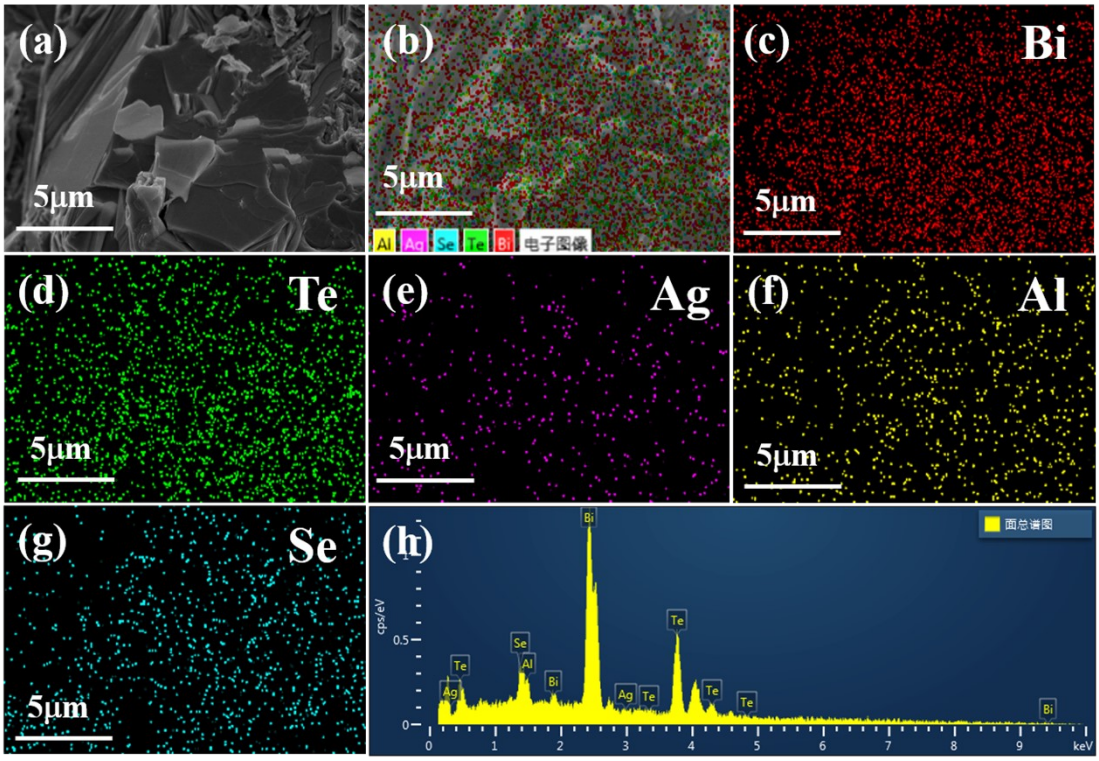

FIG. S3. SEM and EDS images of fracture surfaces of the bulk sample BTS-0.35Vol%Ag_9AlSe_6.

5. The dependence of absolute Seebeck coefficient *S* on carrier concentration (Pisarenko curve)

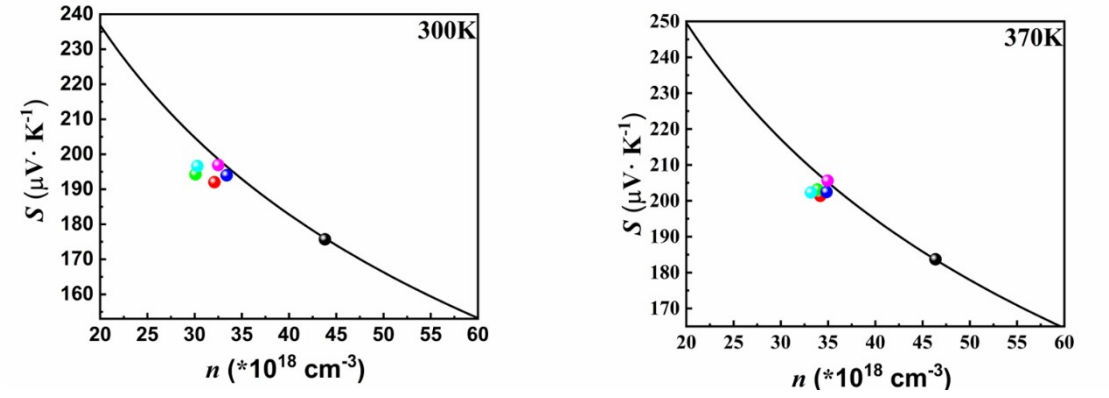

FIG.S4. The dependence of absolute Seebeck coefficient *S* on carrier concentration (Pisarenko curve) at 300 K and 370K for BTS-*x*vol%Ag_9AlSe_6 (*x*=0, 0.15, 0.25,

0.35,0.50 and 0.70).

6. The temperature dependence of thermal conductivity of electric component κ_E

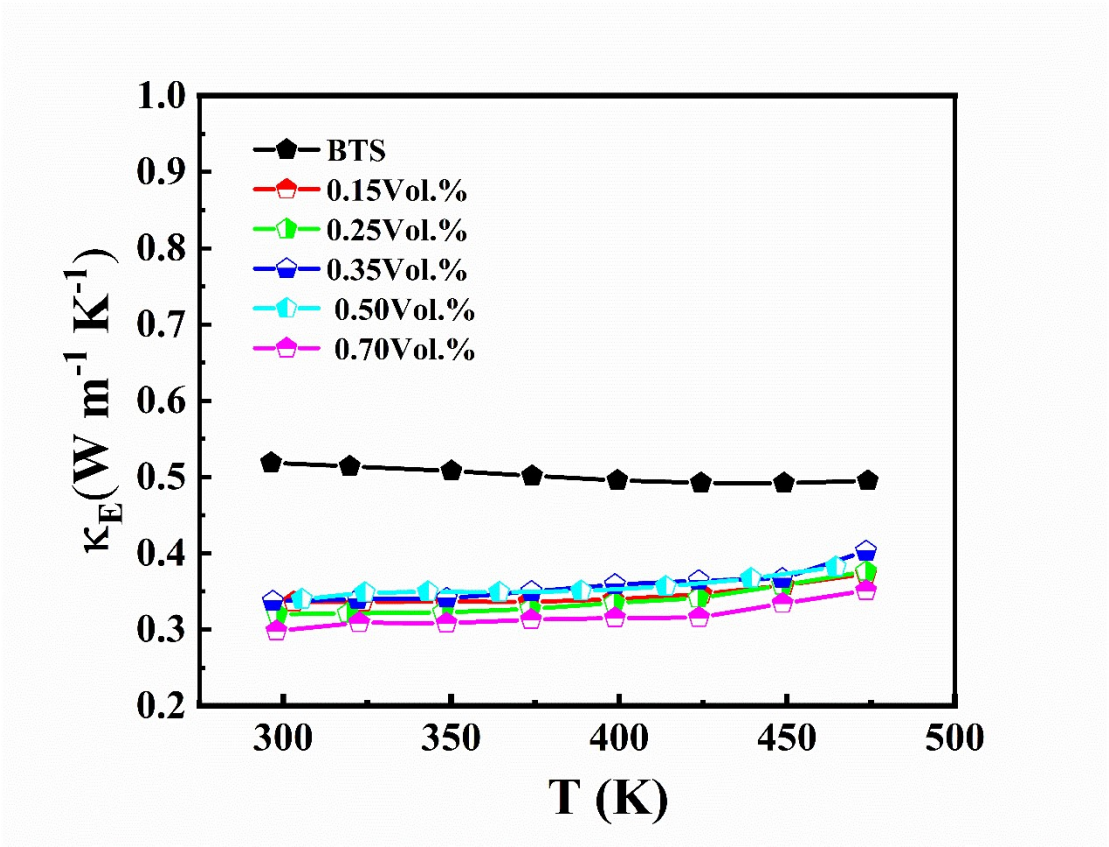

FIG.S5. The temperature dependence of thermal conductivity of electric component κ_E for BTS-*x*vol%Ag_9AlSe_6 (*x*=0, 0.15, 0.25, 0.35,0.50 and 0.70).

7. The thermal stability for BTS-0.35vol%Ag_9AlSe_6 sample

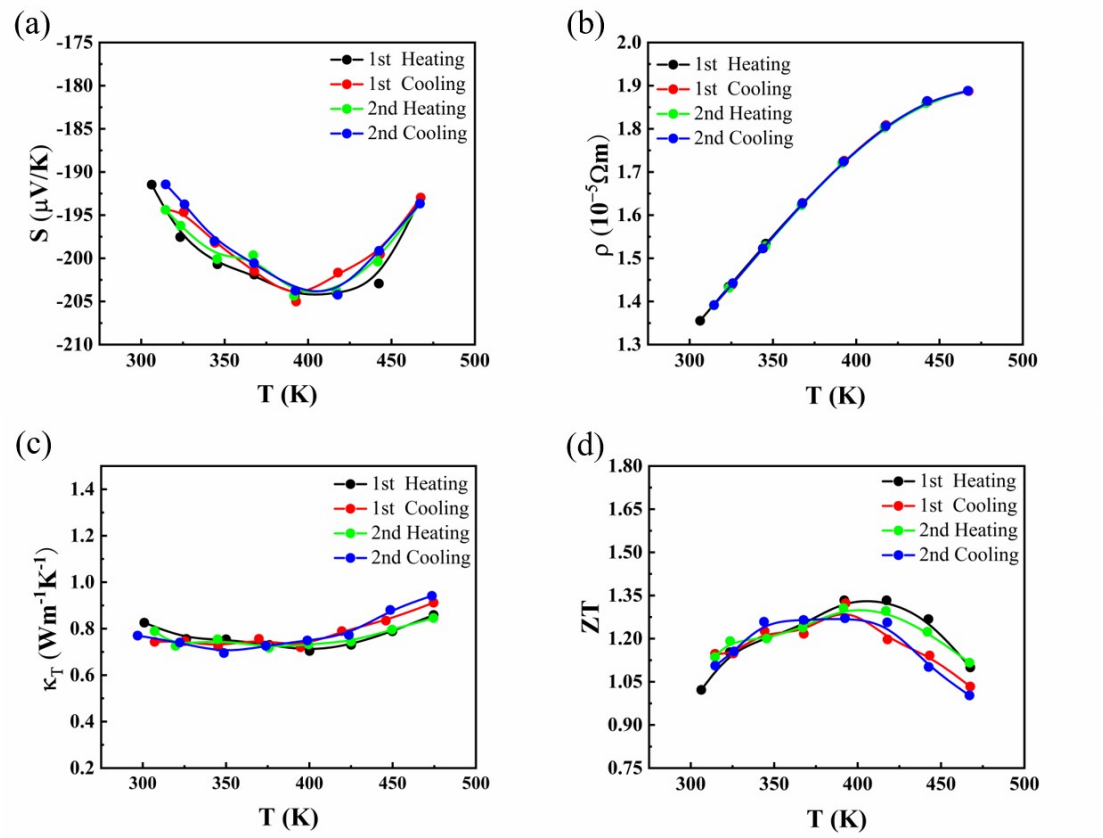

FIG.S6. The cyclic measurements for the BTS-0.35vol%Ag_9AlSe_6 sample. Temperature-dependent (a) Seebeck coefficient, (b) electrical resistivity, (c) total thermal conductivity and (d) ZT, wherein the symbol 1st Heating and Cooling, 2nd Heating and Cooling stand for the first heating and cooling, second heating and cooling measurements.

8. Calculation of Lattice Thermal Conductivity

The lattice thermal conductivity κ_L can be calculated by using the Debye-Callaway model[1]:

$$\kappa_L = \frac{4\pi k_B^4 T^3}{vh^3} \int_0^{\theta_D/T} \tau_T \frac{z^4 exp(z)}{[\exp(z) - 1]^2} dz \quad \text{(S1)}$$

$$\tau_T^{-1} = \tau_U^{-1} + \tau_N^{-1} + \tau_{PD}^{-1} + \tau_E^{-1} + \tau_B^{-1} + \tau_{NP}^{-1} \quad \text{(S2)}$$

where τ_U, τ_N, τ_{PD}, τ_E, τ_B and τ_{NP} are relaxation time corresponding to the scattering from phonon-phonon U- and N-process (U+N), point defects (PD), electron-phonon (E), phase boundaries (B), and nanoparticles (NP), respectively. Here, this model is used to analysis the lattice thermal conductivity. To analyze the κ_L the expression of the

different scattering mechanisms can be rewritten as below:

$$\tau_U^{-1} = \frac{\hbar\gamma^2\omega^2 T}{M v^2 \theta_D} e^{-\theta_D/3T} \quad \text{(S3)}$$

$$\tau_N^{-1} = \beta\tau_U^{-1} = \beta\frac{\hbar\gamma^2\omega^2 T}{M v^2 \theta_D} e^{-\theta_D/3T} \quad \text{(S4)}$$

$$\tau_{PD}^{-1} = \frac{V\omega^4}{4\pi v^3}\Gamma \quad \text{(S5)}$$

$$\tau_E^{-1} = \frac{E_{def}^2 m^* \omega^2}{2\pi\hbar^3 \rho v} \quad \text{(S6)}$$

$$\tau_B^{-1} = v/l \quad \text{(S7)}$$

$$\tau_{NP}^{-1} = v\left[(2\pi R)^2 + \left(\frac{4\pi R^2}{9}\left(\frac{\Delta_D}{D}\right)^2\left(\frac{\omega R}{v}\right)^4\right)^{-1}\right]^{-1} N_P \quad \text{(S8)}$$

$$A = \frac{V}{4\pi v^3}\Gamma \quad \text{(S9)}$$

$$B = (1+\beta)\frac{\hbar\gamma^2}{M v^2 \theta_D} \quad \text{(S10)}$$

$$C = \frac{E_{def}^2 m^*}{2\pi\hbar^3 \rho v} \quad \text{(S11)}$$

Thus

$$\tau_T^{-1} = A\omega^4 + B\omega^2 T exp\left(-\frac{\theta_D}{3T}\right) + C\omega^2 + {}^{v}/_{l} + v\sigma N_P \quad \text{(S12)}$$

To quantitatively calculate κ_L, the literature values [2]of Debye temperature θ_D=164K and sound velocity ν=1778m s^{-1} are used for BTS - *x*vol% Ag_9AlSe_6 (*x*=0, 0.15, 0.25, 0.35,0.50 and 0.70). *l* is the average spatial distance between the Ag_9AlSe_6 nanoparticles in the BTS, $\Delta D/D$ = 0.022 and the average radius of Ag_9AlSe_6 R = 628 nm; the pre-factors of point defect A, U- and N- process B, electron-phonon scattering C and the number density of nanoparticles N_P were provided in Table S2.

Table S2 Parameters for the calculation of lattice thermal conductivity by using the Debye-Callaway model

Sample	A($10^{-42}s^3$)	B($10^{-17}sK^{-1}$)	C($10^{-16}S$)	*l*(nm)	N_p($10^{13}m^{-3}$)
0	**4.6**	**3.9**	**1.8**	**--**	**--**
0.15	**4.6**	**3.9**	**1.8**	**533**	**4.54**
0.25	**4.6**	**3.9**	**1.8**	**477**	**4.81**
0.35	**4.6**	**3.9**	**1.8**	**404**	**6.34**

0.50	**4.6**	**3.9**	**1.8**	**352**	**6.83**
0.70	**4.6**	**3.9**	**1.8**	**430**	**5.37**

Reference

[1] J. Callaway, H.C. von Baeyer, Physical Review, 120 (1960) 1149-1154.

[2] B. Jabar, X. Qin, D. Li, J. Zhang, A. Mansoor, H. Xin, C. Song, L. Huang, Journal of Materials Chemistry A, 7 (2019) 19120-19129.