Supporting Information

Surface Functionalization of Surfactant-Free Particles: A Strategy to Tailor the Properties of Nanocomposites for Enhanced Thermoelectric Performance

C. Chang, Y. Liu, S. Ho Lee, M. Chiara Spadaro, K. M. Koskela, T. Kleinhans, T. Costanzo, J. Arbiol, R. L. Brutchey, M. Ibáñez*
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1. Material processing

1.1. Chemicals

Tin (II) chloride dihydrate (SnCl₂·2H₂O, 98%), sodium hydroxide (NaOH, pellets 98%), sodium borohydride (NaBH₄, 98%), bismuth oxide (Bi₂O₃, 99.99%), and N-Methylformamide (MFA, 99%) were purchased from Fisher Scientific. Tellurium pieces (Te, 100%), ethylenediamine (en, 99%), 1, 2-ethanedithiol (EDT, ≥95.0%), anhydrous acetone (extra dry), and ethanol (95%) were purchased from Sigma-Aldrich. All chemicals were used as received without further purification. Syntheses were carried out using a standard vacuum/dry argon Schlenk line.

1.2. SnTe nanoparticle (NP) synthesis

Large scale SnTe nanoparticles (NPs) were prepared by reacting sodium stannite (Na₂SnO₂) with sodium hydrogen telluride (NaHTe) in water following a procedure previously reported by Guang Han et al with slight modifications.¹

Firstly, NaBH₄ (4.54 g, 120 mmol) was first dissolved in 200 ml deionized water, and then Te powder (5.104 g, 40 mmol) was quickly added into the solution. An Ar flow was introduced to prevent the air. The reaction rate between NaBH₄ and Te is very slow and takes ~2 h to react entirely. The suspension was stirred until the solution becomes transparent light purple, indicating the formation of NaHTe. In parallel, NaOH (16 g, 400 mmol) and SnCl₂·2H₂O (9.826 g, 40 mmol) were mixed with 200 ml of deionized water. The mixture was stirred at room temperature under Ar flow until the solution became transparent, indicating the formation of Na₂SnO₂. When NaHTe solution is ready, the Na₂SnO₂ solution was heated to its boiling point at ca. ~101 °C with a condenser to assure reflux. Then the freshly prepared NaHTe solution was rapidly injected. Since NaHTe is sensitive to the air, two 100ml syringes are prepared to inject NaHTe. Upon injection, the solution color changed from transparent to black, indicating the SnTe NP formation. The mixture was heated again to 101 °C and maintained at this temperature for 30 min. Then the mixture was cooled to room temperature with cooling water. NPs precipitated quickly when the stirring stopped. The transparent supernatant solution was carefully removed. The remaining crude was transferred into centrifuge tubes for further purification.

The SnTe NPs were washed four times with ethanol and acetone alternatively. At each step, SnTe NPs were dispersed by ethanol/acetone first and then centrifuged at 8000 rpm for 5 min. At last, the washed NPs were dried under vacuum overnight at room temperature and kept in the glovebox for further use.

1.3. Bi₂O₃/Bi₂S₃ molecular complex preparation
The Bi$_2$O$_3$/Bi$_2$S$_3$ molecular complex preparation method applied in this work was developed by R. L. Brutchey et al.\textsuperscript{2} The solubilities of Bi$_2$O$_3$ and Bi$_2$S$_3$ in en+EDT solvent (1:10) is ~15-20 % and ~10 %, respectively. Here, we dissolved 150 mg Bi$_2$O$_3$ or 90 mg Bi$_2$S$_3$ with 1.1 ml en+EDT solvent (1 ml en, 0.1 ml EDT) in N$_2$-filled vial. The mixture was sonicated for 1 min to accelerate the dissolving processing until complete dissolution. All the Bi$_2$O$_3$ and Bi$_2$S$_3$ molecular complex were prepared fresh before blending with SnTe NPs in MFA.

1.4. Nanoparticle surface treatment

All surface treatments were performed in an inert atmosphere (N$_2$). We use 5 ml MFA to disperse 0.75g SnTe in a 20 ml vial. SnTe with different molar amounts of Bi$_2$O$_3$ and Bi$_2$S$_3$ molecular complex was prepared (For Bi$_2$O$_3$ molecular complex: 0.5% Bi$_2$O$_3$: 0.05ml, 1% Bi$_2$O$_3$: 0.1 ml, 1.5% Bi$_2$O$_3$: 0.16 ml, 2% Bi$_2$O$_3$: 0.2 ml, 2.5% Bi$_2$O$_3$: 0.25 ml, Bi$_2$O$_3$: 0.31 ml; For Bi$_2$S$_3$-complex: 1% Bi$_2$S$_3$: 0.1 ml, 2% Bi$_2$S$_3$: 0.2 ml, 3% Bi$_2$S$_3$: 0.31 ml. Then the mixture was vigorously stirred (800 rpm) at room temperature for 24 h. After that, the mixture was washed by acetone for 3 times. Specifically, NPs were dispersed by acetone first and then centrifuged at 7800 rpm for 5 min each time.

Samples for LC/Q-TOF were prepared from fully dissolved solutions of Bi$_2$O$_3$ (150 mg/mL, 1:10 (vol/vol) EDT/en) filtered through a 0.45 µm syringe filter and diluted with DMF to nanomolar concentrations. Fully dissolved solutions of Bi$_2$S$_3$ (90 mg/mL, 1:10 (vol/vol) EDT/en) were filtered through a 0.45 µm syringe filter and diluted with DMSO to nanomolar concentrations. Both solutions were mixed right before injection into the LC/Q-TOF instrument to avoid possible decomposition products. Samples were direct injected into an Agilent 1290 Infinity ll-6545XT AdvanceBio LC/Q-TOF. UV-vis absorption spectroscopy was performed in a 1-cm path length quartz cuvette placed within a 150 mm integrating sphere on a PerkinElmer Lambda 950 UV-vis-NIR spectrometer with roughly equimolar solutions of Bi$_2$O$_3$ (70 mg/mL) diluted in DMF and Bi$_2$S$_3$ (80 mg/mL) diluted in DMSO (2 µL ink in 3 mL of either DMF or DMSO). Spectra were collected immediately to avoid any possible absorption from decomposition products.

1.5. Bulk nanomaterial consolidation

As-prepared SnTe-xBi$_2$O$_3$/Bi$_2$S$_3$ nanocomposites (x=0.5%, 1%, 1.5%, 2%, 2.5%, and 3% Bi$_2$O$_3$ molecular complex; x=1%, 2%, and 3% Bi$_2$S$_3$ molecular complex) were firstly annealed at 650 °C for 120 min under a slow forming gas (95% N$_2$ + 5% H$_2$) flow inside a tube furnace with ca. 10 °C/min heating rate. Afterward, the annealed nano powder was ground with an agate mortar and loaded into a graphite die in the glovebox. The nano powder was then consolidated into pellet (Ø 8.6 mm × h 2 mm) under vacuum in an AGUS PECS Spark Plasma
Sintering (SPS) System-Model SPS 210Sx by applying an axial pressure of 45 MPa at 650 °C for 5 min. All consolidated pellets presented relative densities >98% of the theoretical value.

2. Structural and chemical characterization.

2.1. X-Ray Diffraction (XRD)

X-ray diffraction analyses were carried out on a Bruker AXS D8 ADVANCE powder diffractometer in a Bragg-Brentano geometry with Cu-Kα1 radiation (1.5406 Å). The height of the sample was aligned, and diffraction results were collected from 20° to 80° in 2θ at a rate of 5 °/min. The powder XRD of SnTe NPs with Bi₂O₃ and Bi₂S₃ molecular complex before and after annealing processing were carried out, as shown in Figure S3.

2.2. Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM)

The size and morphology of initial NPs, annealed NPs, and sintered pellets were examined by field-emission SEM on an Auriga Zeiss operated at 5.0 kV. STEM characterization of the Bi₂O₃ molecular complex surface coated SnTe samples has been performed using a JEOL JEM2800 microscope operated at 200 kV with a point to point resolution of 0.14 nm. Besides, STEM-EDS elemental mapping was also performed using a JEOL JEM-2800 microscope at an accelerating voltage of 200 kV with a JEOL silicon drift detector (SDD).

2.3. Elemental analysis

The overall material composition was investigated by using an Oxford energy dispersive X-ray spectrometer (EDX) attached to the Zeiss Auriga SEM at 15.0 kV.

3. Thermoelectric property measurement

3.1. Electrical Properties

Seebeck coefficients were measured by using a static DC method. Electrical resistivity data was obtained by a standard four-probe method. Both the Seebeck coefficient and the electrical resistivity were simultaneously measured in an LSR-3 LINSEIS system from room temperature to 873 K, under a helium atmosphere. The temperature was increased at a rate of 10 K min⁻¹. Data approximately was taken every 30 degrees.
Room-temperature hall charge carrier concentrations \((n)\) and mobilities \((\mu)\) were measured with the Van der Pauw method using a magnetic field of 0.6 T (ezHEMS, NanoMagnetics). Each sample is measured five times to get the average value. Temperature-dependent Hall charge carrier concentrations \((n)\) and mobilities \((\mu)\) from 300 K to 873 K were measured utilizing Hall Effect Analyzer by Linseis Company.

3.2. Thermal properties

An XFA 500 Xenon Flash Apparatus and an LFA 1000 Laser Flash were used to determine the thermal diffusivities \((\alpha)\) of the samples with an estimated error of ca. 5%. The total thermal conductivity was calculated by \(\kappa = \alpha C_p \rho\), where \(\alpha\) is the thermal diffusivity, \(C_p\) is the heat capacity, and \(\rho\) is the mass density of the specimen. The temperature-dependent \(C_p\) values were derived from reference 3. Notably, we applied the \(C_p\) of bare SnTe to estimate \(C_p\) in this work because the real Bi content in all samples are below 3.5%. In Figure S15, we compared \(C_p\) values measured by different groups.

We estimated the lattice thermal conductivity \((\kappa_L)\) simply by subtracting the electronic thermal conductivity \((\kappa_e)\) from the measured total thermal conductivity \((\kappa_{tot})\):

\[
\kappa_L = \kappa_{tot} - \kappa_{el}
\]  

(S1)

The electronic part \(\kappa_e\) is directly proportional to the electrical conductivity \(\sigma\) by the Wiedemann-Franz law:

\[
\kappa_{ele} = L \sigma T
\]  

(S2)

An estimation of \(L\) can be made using a single parabolic band (SPB) model with acoustic phonon scattering. The calculations based on SPB model results in an \(L\) with a deviation of less than 10% as compared with a more rigorous single non-parabolic band and multiple band model calculations. It is well known that the \(L\) value is used to estimate the lattice thermal conductivity, which will not change the total thermal conductivity and final \(zT\) values. The Lorenz number is given by the formula:

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

(S3)

where \(k_B\) is the Boltzmann constant and \(\eta\) represents the reduced Fermi energy, which can be derived from the measured Seebeck coefficients via the following equations:

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

(S4)
where $F_n(\eta)$ is the $n$th order Fermi integral:

$$F_n(\eta) = \int_0^{\infty} \frac{x^n}{1 + e^{x-\eta}} \, dx$$  \hspace{2cm} (S5)

$$\eta = \frac{E_i}{k_B T}$$  \hspace{2cm} (S6)

### 3.3. Error estimation

Taking the system accuracy and the measurement precision (including the measurement of sizes/distances) into account, we estimate an error of ca. 4% in the measurement of both electrical conductivity and Seebeck coefficient. Combining the uncertainties of electrical conductivity and Seebeck coefficient, so the uncertainty of the power factor is ca. 12%. An LFA 1000 Laser Flash were used to determine the thermal diffusivities ($\alpha$) of the samples with an estimated error of ca. 5%. The density ($\rho$) error is ~2%. To avoid cluttering the plots, error bars were not included in the figures except $zT$. Therefore, the combined uncertainty for all measurements involved in $zT$ determination shown in the plot is estimated to be ca. 17%.

### 3.4. Klemens model

At a temperature above the Debye temperature $\Theta_D$, the ratio of the lattice thermal conductivities including point defects and that of parent material can be expressed as the following equation:\(^3\)

$$\frac{\kappa_{\text{lat}}}{\kappa_{\text{lat,p}}} = \tan^{-1} \frac{U}{U}$$  \hspace{2cm} (S7)

where $\kappa_{\text{lat}}$ and $\kappa_{\text{lat,p}}$ are the lattice thermal conductivities of the defected and parent materials, respectively. In this work, $\kappa_{\text{lat,p}} = 2.43 \, \text{W m}^{-1} \text{K}^{-1}$. $U$ is defined as:

$$U = \left( \frac{\pi^2 \Theta \Omega}{h \nu_a^2} \kappa_{\text{lat,p}} \Gamma \right)^\frac{1}{2}$$  \hspace{2cm} (S8)

where $\Theta_D$, $\Omega$, $h$ and $\nu_a$ represent the Debye temperature, average atom volume, Planck constant and average sound velocity, respectively. $\Gamma$, the imperfection scaling parameter is a weighted sum of the mass fluctuation $\Gamma_M$ and strain field fluctuation $\Gamma_S$ and can be written as:

$$\Gamma = \Gamma_M + \epsilon \Gamma_S$$

where $\epsilon$ is a phenomenological adjustable parameter related to the Poisson ratio ($\nu_p$) and Grüneisen parameter ($\gamma$). $\nu_p$ and $\gamma$ can be written as:
\[ v_p = \frac{1 - 2 \left( \frac{v_l}{v_s} \right)^2}{2 - 2 \left( \frac{v_l}{v_s} \right)^2} \]  
\[ \gamma = \frac{3}{2} \left( \frac{1 + \frac{v_p}{2v_s}}{2 - 3v_p} \right) \]

where \( v_l \) and \( v_s \) denote longitudinal and shear sound velocities, respectively. Then, we can obtain \( v_a \) as

\[ v_a = \left[ \frac{1}{3} \left( \frac{1}{v_l^3 \gamma} + \frac{1}{v_s^3 \gamma} \right) \right]^{\frac{1}{3}} \]

Setting Bi alloying as an example. \( \Gamma \) is defined as:

\[ \Gamma_{\text{Sn}, \text{Bi}, \text{Te}} = \frac{1}{2} \left( \frac{M_{\text{(Sn,Bi)}}}{M} \right)^2 \Gamma_{\text{(Sn,Bi)}} \]  
\[ \overline{M} = \frac{1}{2} \left( M_{\text{Sn}} + M_{\text{Bi}} \right) \]

\[ \Gamma_{\text{(Sn,Bi)}} = \Gamma_{M(\text{Sn,Bi})} + \Delta \Gamma_{S(\text{Sn,Bi})} \]

\[ \Gamma_{M(\text{Sn,Bi})} = x(1 - x) \left( \frac{\Delta M}{M_{\text{(Sn,Bi)}}} \right)^2 \]

\[ \Gamma_{S(\text{Sn,Bi})} = x(1 - x) \left( \frac{\Delta r}{r_{\text{(Sn,Bi)}}} \right)^2 \]

where \( M_{\text{(Sn,Bi)}} = (1 - x)M_{\text{Sn}} + xM_{\text{Bi}} \), \( \Delta M = M_{\text{Bi}} - M_{\text{Sn}} \) and \( r_{\text{(Sn,Bi)}} = (1 - x)r_{\text{Sn}} + xr_{\text{Bi}} \),

\[ \Delta r = r_{\text{Bi}} - r_{\text{Sn}} \]

Then we get:

\[ \Gamma_{\text{Sn}, \text{Bi}, \text{Te}} = \frac{1}{2} x(1 - x) \left( \frac{M_{\text{(Sn,Bi)}}}{M} \right)^2 \left[ \left( \frac{\Delta M}{M_{\text{(Sn,Bi)}}} \right)^2 + \varepsilon \left( \frac{\Delta r}{r_{\text{(Sn,Bi)}}} \right)^2 \right] \]

The mass fluctuation \( \Gamma_M \) and strain field fluctuation \( \Gamma_S \) of S alloying can be obtained using the same method.
Back to the equation S7, we can obtain the theoretical predication $\kappa_{\text{lat}}$ with Klemens model.
4. Figures

**Figure S1.** Annular dark-field scanning transmission electron microscope (ADF-STEM) images of SnTe-1.5%Bi$_2$O$_3$ molecular complex NPs.

**Figure S2.** XRD patterns of SnTe-Bi$_2$O$_3$ molecular complex NPs (a) before and (b) after annealing processing, and (c) the corresponding SnTe-Bi$_2$S$_3$ nanocomposites; XRD patterns of SnTe-Bi$_2$S$_3$ molecular complex NPs (d) before and (e) after annealing processing, and (f) the corresponding SnTe-*Bi$_2$S$_3$* nanocomposites.
Figure S3. Negative ion mode LC/Q-TOF spectra of direct injected (a) Bi₂O₃ (150 mg/mL, 1:10 (vol/vol) EDT/en) molecular complex diluted in DMF and (b) Bi₂S₃ (90 mg/mL, 1:10 (vol/vol) EDT/en) molecular complex diluted in DMSO.

Figure S4. UV-vis absorption spectra of (a) a Bi₂O₃ molecular complex (70 mg/mL, 1:10 (vol/vol) EDT/en) diluted in DMF (2 mL complex in 3 mL DMF). Solvent blank ran with DMF; (b) a Bi₂S₃ molecular complex (80 mg/mL, 1:10 (vol/vol) EDT/en) dissolved in DMF (2 mL complex in 3 mL DMSO). Solvent blank ran with DMSO.
Figure S5. SEM images of SnTe (a) NPs before annealing; (b) NPs after annealing; (c) pellet.

Figure S6. SEM images of the NPs before annealing obtained from (a) SnTe-0.5% Bi$_2$O$_3$ molecular complex; (b) SnTe-1% Bi$_2$O$_3$ molecular complex; (c) SnTe-1.5% Bi$_2$O$_3$ molecular complex; (d) SnTe-2% Bi$_2$O$_3$ molecular complex; (e) SnTe-2.5% Bi$_2$O$_3$ molecular complex and (f) SnTe-3% Bi$_2$O$_3$ molecular complex.
**Figure S7.** SEM images of the NPs after annealing obtained from (a) SnTe-0.5% Bi$_2$O$_3$ molecular complex; (b) SnTe-1% Bi$_2$O$_3$ molecular complex; (c) SnTe-1.5% Bi$_2$O$_3$ molecular complex; (d) SnTe-2% Bi$_2$O$_3$ molecular complex; (e) SnTe-2.5% Bi$_2$O$_3$ molecular complex and (f) SnTe-3% Bi$_2$O$_3$ molecular complex.

**Figure S8.** SEM images of the pellets obtained from (a) SnTe-0.5% Bi$_2$S$_3$; (b) SnTe-1% Bi$_2$S$_3$; (c) SnTe-1.5% Bi$_2$S$_3$; (d) SnTe-2% Bi$_2$S$_3$; (e) SnTe-2.5% Bi$_2$S$_3$ and (f) SnTe-3% Bi$_2$S$_3$ nanocomposites produced with Bi$_2$O$_3$ molecular complexes as precursor.

**Figure S9.** SEM images of SnTe-1% Bi$_2$S$_3$ molecular complex (a) NPs before annealing; (b) NPs after annealing; (c) the corresponding pellet.
Figure S10. STEM overview in SnTe-Bi$_2$S$_3$ nanocomposites produced with 1.5% Bi$_2$O$_3$ molecular complexes as precursor.

Figure S11. HRTEM of grain boundaries in SnTe-Bi$_2$S$_3$ nanocomposites produced with 1.5% Bi$_2$O$_3$ molecular complexes as precursor.
**Figure S12.** HRTEM of nanoprecipitate in SnTe-Bi$_2$S$_3$ nanocomposites produced with 1.5% Bi$_2$O$_3$ molecular complexes as precursor.

**Figure S13.** (a) HRTEM of nanoprecipitate in SnTe-Bi$_2$S$_3$ nanocomposites produced with 1.5% Bi$_2$O$_3$ molecular complexes as precursor. (b) power spectrum of the marked yellow square region. Both SnTe (FM3-M) and Bi$_2$S$_3$ (PMCN) are characterized. (c-e) phase-filtered composition maps showing the SnTe phase marked as green and blue and Bi$_2$S$_3$ phase marked as red.

**Figure S14.** EDS mapping of (a) SnTe-2.5% Bi$_2$S$_3$ and (b) SnTe-3.0% Bi$_2$S$_3$ nanocomposites produced with Bi$_2$O$_3$ molecular complexes as precursor. The EXD resolution is too low to detect the element distribution at the grain boundary.
Figure S15. EDS mapping of SnTe-1% Bi$_2$S$_3$ nanocomposite produced with Bi$_2$S$_3$ molecular complexes as precursor.
**Figure S16.** The temperature dependent TE properties of SnTe-xBi$_2$S$_3$ nanocomposites produced with Bi$_2$S$_3$ molecular complexes as precursor (x=0, 1%, 2%, 3%). (a) electrical conductivity; (b) Seebeck coefficient; (c) power factor; (d) Lorenz number; (e) thermal diffusivity; (f) total thermal conductivity; (g) electronic thermal conductivity; (h) lattice thermal conductivity; (f) $zT$.

![Graph showing temperature dependent TE properties of SnTe-xBi$_2$S$_3$ nanocomposites](image)

**Figure S17.** The relative band structure energy of SnTe and Bi$_2$S$_3$ to vacuum. The work function of SnTe and Bi$_2$S$_3$ are taken from reference 4-5.

![Graph showing relative band structure energy of SnTe and Bi$_2$S$_3$](image)

**Figure S18.** The hall mobility, weighted mobility and effective mass as a function of nominal Bi$_2$S$_3$ amount in percentage.

![Graph showing hall mobility, weighted mobility and effective mass](image)
Figure S19. (a) The heat capacity \( C_p \) of SnTe as a function of temperature. This figure of \( C_p \) values is taken from previous work by Zhao et al.\textsuperscript{36} \( C_p \) in some other references are listed for comparison.\textsuperscript{7-10} The temperature dependent TE properties of SnTe-xBi\textsubscript{2}S\textsubscript{3} nanocomposites produced with Bi\textsubscript{2}O\textsubscript{3} molecular complexes as precursor (x=0, 0.5%, 1%, 1.5%, 2%, 2.5%, 3%). (b) thermal diffusivity; (c) Lorenz number; (d) electronic thermal conductivity.
Figure S20. The reproduced TE properties measurement of SnTe-xBi$_2$S$_3$ nanocomposites (x=1.5, 3%) produced with Bi$_2$O$_3$ molecular complexes as precursor. 1$^{st}$ and 2$^{nd}$ indicates the first and second heating measurement processing (a) electrical conductivity; (b) Seebeck coefficient; (c) power factor; (d) thermal diffusivity; (e) total thermal conductivity; (f) $zT$.

Figure S21. The reproduced TE properties measurement of SnTe-1.5% Bi$_2$S$_3$ nanocomposites produced with Bi$_2$O$_3$ molecular complexes as precursor. R1 and R2 indicates the SnTe-1.5% Bi$_2$S$_3$ nanocomposite synthesized in another two separate batches. (a) electrical conductivity; (b) Seebeck coefficient; (c) power factor; (d) thermal diffusivity; (e) total thermal conductivity; (f) $zT$.

5. Tables

Table S1. Composition of SnTe-xBi$_2$S$_3$/Bi$_2$S$_3^*$ nanocomposites produced with 2O$_3$/Bi$_2$S$_3$ molecular complexes as precursor obtained from SEM-EDS analysis.

| Sample       | Sn (atomic %) | Te (atomic %) | Bi (atomic %) | S (atomic %) |
|--------------|---------------|---------------|---------------|--------------|
| SnTe         | 46.14         | 53.86         | -             | -            |
| SnTe-0.5% Bi$_2$S$_3$ | 44.98        | 53.44         | 0.67          | 0.91         |
| SnTe-1.0% Bi$_2$S$_3$ | 44.83        | 53.05         | 0.87          | 1.26         |
| SnTe-1.5% Bi$_2$S$_3$ | 44.98        | 53.85         | 0.73          | 0.43         |
| SnTe-2.0% Bi$_2$S$_3$ | 44.60        | 53.57         | 0.94          | 0.89         |
| SnTe-2.5% Bi$_2$S$_3$ | 43.83        | 53.78         | 1.68          | 0.71         |
| SnTe-3.0% Bi$_2$S$_3$ | 43.42        | 53.90         | 1.86          | 0.81         |
| SnTe-1.0% *Bi$_2$S$_3^*$* | 45.59        | 53.90         | 0.40          | 0.11         |
| SnTe-2.0% *Bi$_2$S$_3^*$* | 44.48        | 54.26         | 1.11          | 0.15         |
| SnTe-3.0% *Bi$_2$S$_3^*$* | 44.10        | 54.32         | 1.49          | 0.09         |
Table S2. Room temperature Hall carrier concentration and mobility of SnTe-Bi$_2$S$_3$/Bi$_2$S$_3*$ nanocomposites produced with Bi$_2$O$_3$/Bi$_2$S$_3$ molecular complexes as precursor.

| Sample            | $n_{H_{\text{ave}}}$ (cm$^{-3}$) | $\mu_{H_{\text{ave}}}$ (cm$^2$ V s$^{-1}$) |
|-------------------|---------------------------------|------------------------------------------|
| SnTe              | 1.40×10$^{21}$                  | 33.63                                    |
| SnTe-0.5% Bi$_2$S$_3$ | 9.37×10$^{19}$                  | 251.11                                   |
| SnTe-1.0% Bi$_2$S$_3$ | 6.82×10$^{19}$                  | 208.90                                   |
| SnTe-1.5% Bi$_2$S$_3$ | 1.56×10$^{20}$                  | 155.42                                   |
| SnTe-2.0% Bi$_2$S$_3$ | 4.47×10$^{19}$                  | 355.11                                   |
| SnTe-2.5% Bi$_2$S$_3$ | 2.98×10$^{19}$                  | 381.435                                  |
| SnTe-3.0% Bi$_2$S$_3$ | 2.53×10$^{19}$                  | 376.695                                  |
| SnTe-1.0% *Bi$_2$S$_3*$ | 4.21×10$^{20}$                  | 98.21                                    |
| SnTe-2.0% *Bi$_2$S$_3*$ | 9.70×10$^{19}$                  | 194.00                                   |
| SnTe-3.0% *Bi$_2$S$_3*$ | 3.79×10$^{19}$                  | 256.24                                   |

Table S3. Densities of SnTe-xBi$_2$S$_3$/Bi$_2$S$_3*$ pellets produced with Bi$_2$O$_3$/Bi$_2$S$_3$ molecular complexes as precursor measured with the Mass-and-volume method.

| Sample            | Density (g/cm$^3$) |
|-------------------|--------------------|
| SnTe              | 6.38               |
| SnTe-0.5% Bi$_2$S$_3$ | 6.37               |
| SnTe-1.0% Bi$_2$S$_3$ | 6.35               |
| SnTe-1.5% Bi$_2$S$_3$ | 6.39               |
| SnTe-2.0% Bi$_2$S$_3$ | 6.38               |
| SnTe-2.5% Bi$_2$S$_3$ | 6.37               |
| SnTe-3.0% Bi$_2$S$_3$ | 6.40               |
| SnTe-1.0% *Bi$_2$S$_3*$ | 6.40               |
| SnTe-2.0% *Bi$_2$S$_3*$ | 6.40               |
| SnTe-3.0% *Bi$_2$S$_3*$ | 6.38               |

6. References
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