Electronic Supporting Information

Improvement in the thermoelectric performance of highly reproducible *n*-type $(Bi,Sb)_2Se_3$ alloys by Cl-doping

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1. The lattice parameters of Cl-doped $BiSbSe_3$.

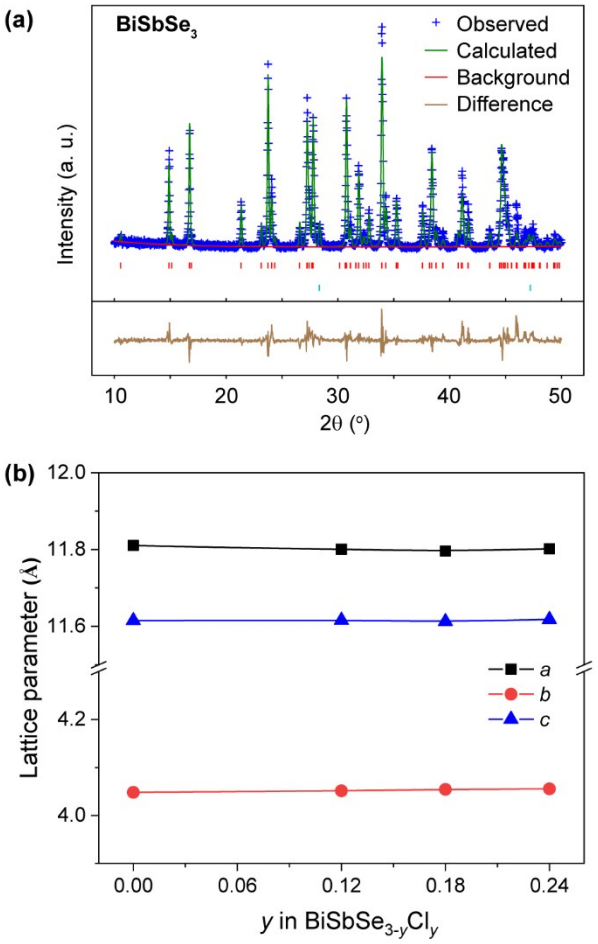

Figure S1. (a) One typical XRD refinement result of $BiSbSe_3$ sample. (b) The change in lattice parameters (*a*, *b*, and *c*) of orthorhombic $BiSbSe_3$ by Cl-doping.

2. Microstructure analysis for the SPSed $BiSbSe_{3-y}Cl_y$ (y = 0, 0.12, 0.18, 0.24) and $Bi_{1.2}Sb_{0.8}Se_{3-z}Cl_z$ (z = 0, 0.12, 0.18, 0.24) samples.

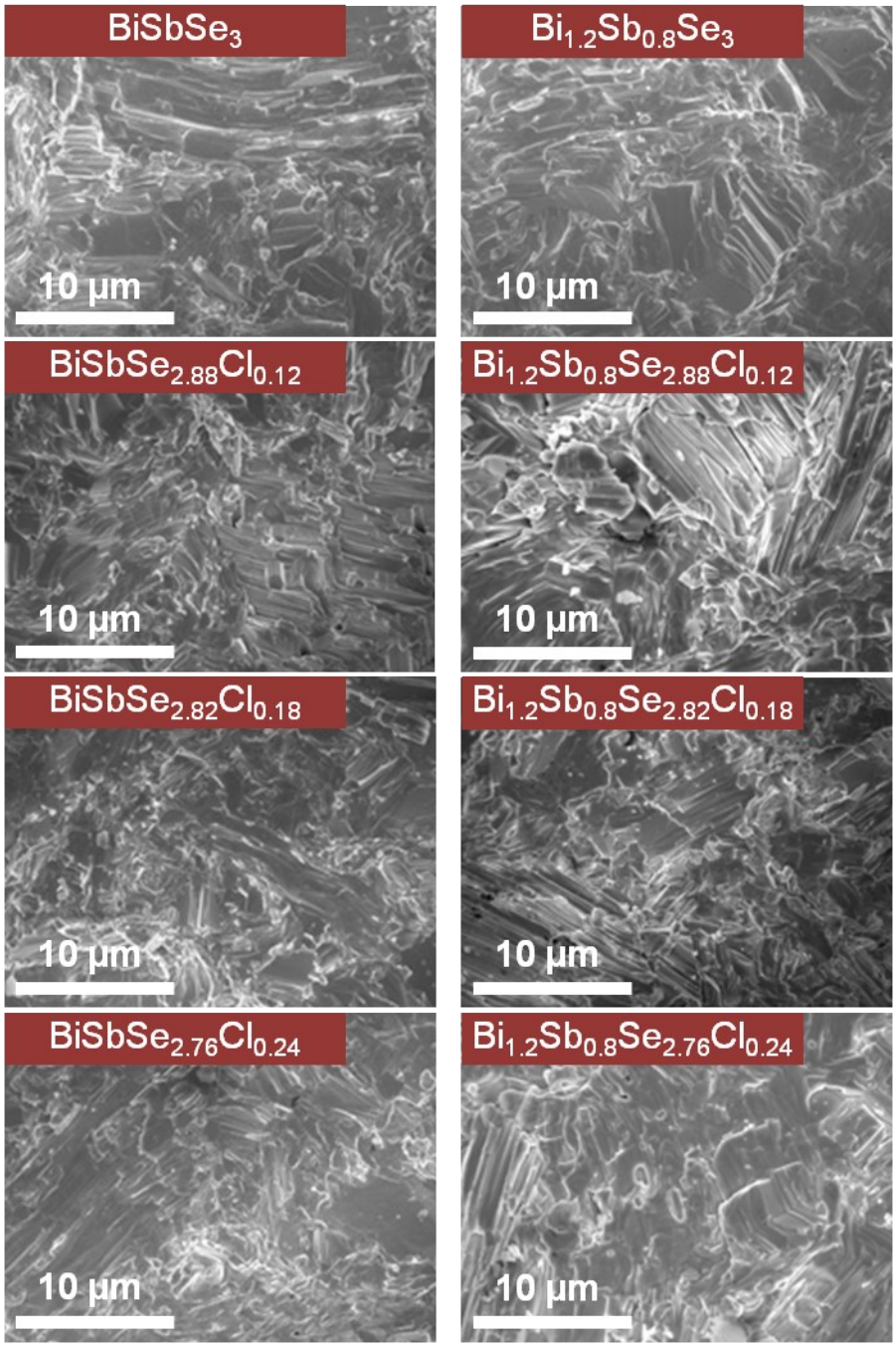

Figure S2. SEM images of fractured surfaces for the SPSed $BiSbSe_{3-y}Cl_y$ (y = 0, 0.12, 0.18, 0.24) and $Bi_{1.2}Sb_{0.8}Se_{3-z}Cl_z$ (z = 0, 0.12, 0.18, 0.24).

3. The mole fraction of rhombohedral phase in $Bi_{1.2}Sb_{0.8}Se_{3-z}Cl_z$ (z = 0, 0.12, 0.18, 0.24).

Table S1. The mole fraction of rhombohedral phase in $Bi_{1.2}Sb_{0.8}Se_{3-z}Cl_z$ (z = 0, 0.12, 0.18, 0.24), which is calculated by Rietveld refinement. The relative densities of the samples measured by the Archimedes principle (AlfaMiracle, MD-300S) are also shown.

Compositions (nominal)	Mole fraction		Relative density (%)
	Rhombohedral	Orthorhombic	
$Bi_{1.2}Sb_{0.8}Se_3$	0.743	0.257	97.4%
$Bi_{1.2}Sb_{0.8}Se_{2.88}Cl_{0.12}$	0.744	0.256	97.4%
$Bi_{1.2}Sb_{0.8}Se_{2.82}Cl_{0.18}$	0.745	0.255	95.5%
$Bi_{1.2}Sb_{0.8}Se_{2.76}Cl_{0.24}$	0.747	0.253	97.1%

4. The lattice parameters of Cl-doped $Bi_{1.2}Sb_{0.8}Se_3$.

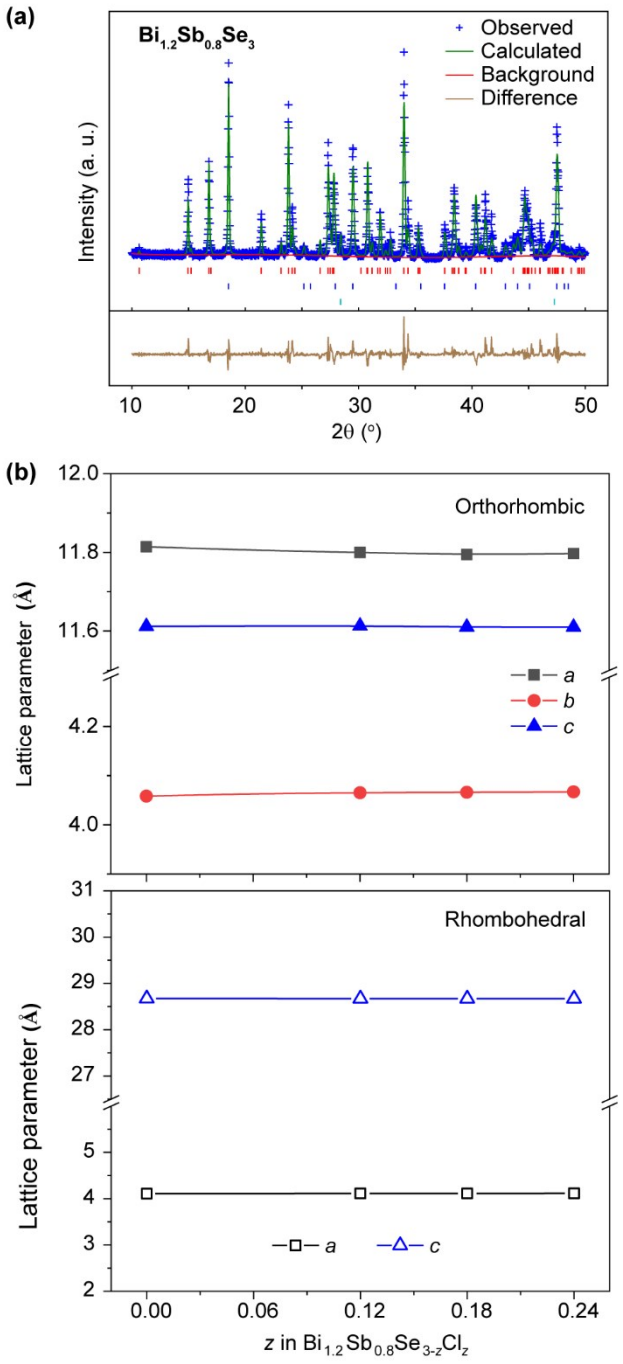

Figure S3. (a) One typical XRD refinement result of $Bi_{1.2}Sb_{0.8}Se_3$ sample. (b) The change in lattice parameters of rhombohedral (*a* and *c*) and orthorhombic (*a*, *b*, and *c*) phases of $Bi_{1.2}Sb_{0.8}Se_3$ by Cl-doping.

5. Phase formation in $Bi_{1.2}Sb_{0.8}Se_{2.7}Cl_{0.3}$.

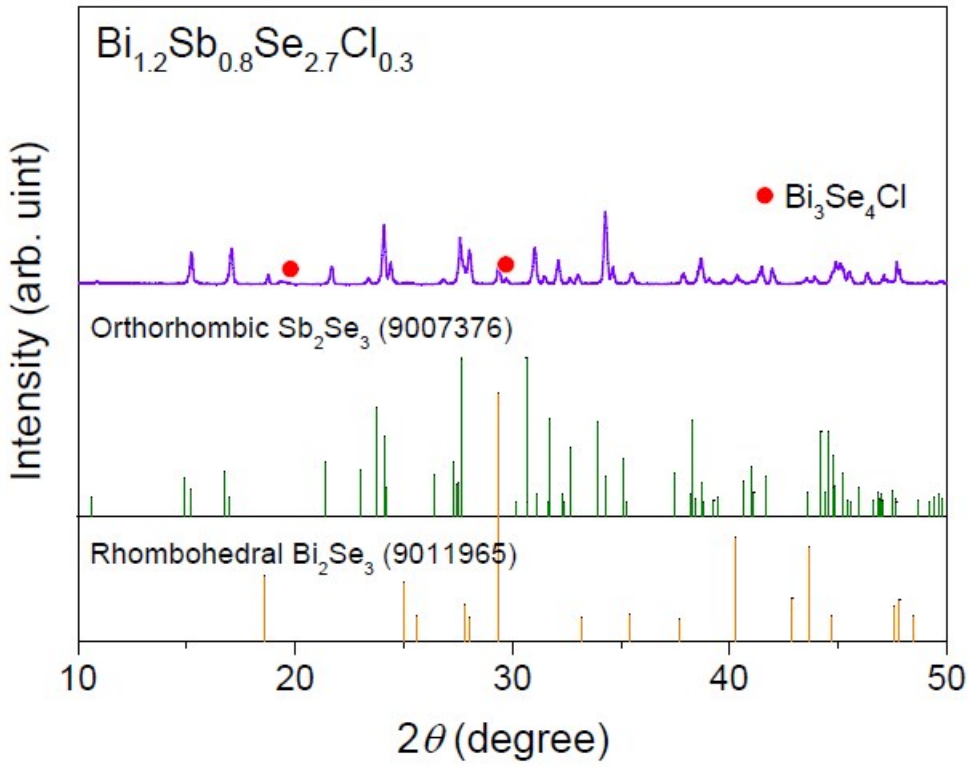

Figure S4. XRD pattern of SPSed $Bi_{1.2}Sb_{0.8}Se_{2.7}Cl_{0.3}$.

6. Calculation of electronic thermal condutivity

The electronic thermal conductivity (κ_{ele}) is estimated by the Wiedemann-Franz law ($\kappa_{ele} = L\sigma T$, where L, σ, and T are the Lorenz number, electrical conductivity, and the absolute temperature). Temperature dependent L is obtained by using Eq. S1 assuming a single parabolic band model [1].

$$L = 1.5 + \exp\left(-\frac{|S|}{116}\right) \quad \text{(S1)}$$

Figure S5 shows the temperature dependences of L for Cl-doped $BiSbSe_3$ and $Bi_{1.2}Sb_{0.8}Se_3$.

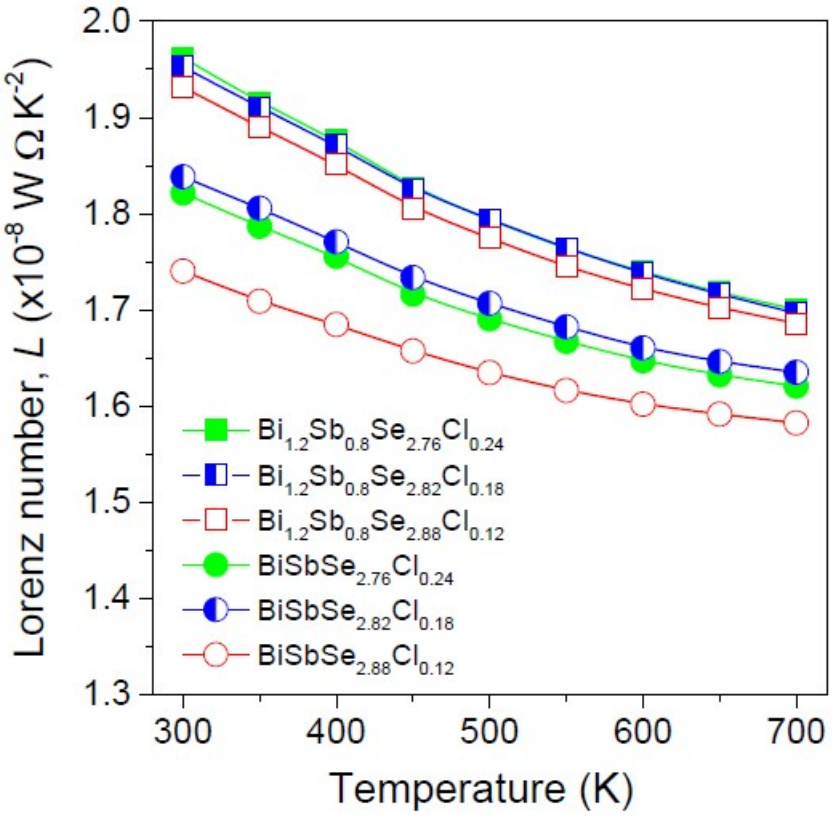

Figure S5. Temperature dependences of L for Cl-doped $BiSbSe_3$ and $Bi_{1.2}Sb_{0.8}Se_3$.

References

[1] H. S. Kim, Z. M. Gibbs, Y. Tang, H. Wang, and G. J. Snyder, APL Mater. 3 (2015) 041506.