

Electronic Supplementary Information (ESI)

Promising Thermoelectric Performance in *n*-type AgBiSe₂: Effect of Aliovalent Anion Doping[†]

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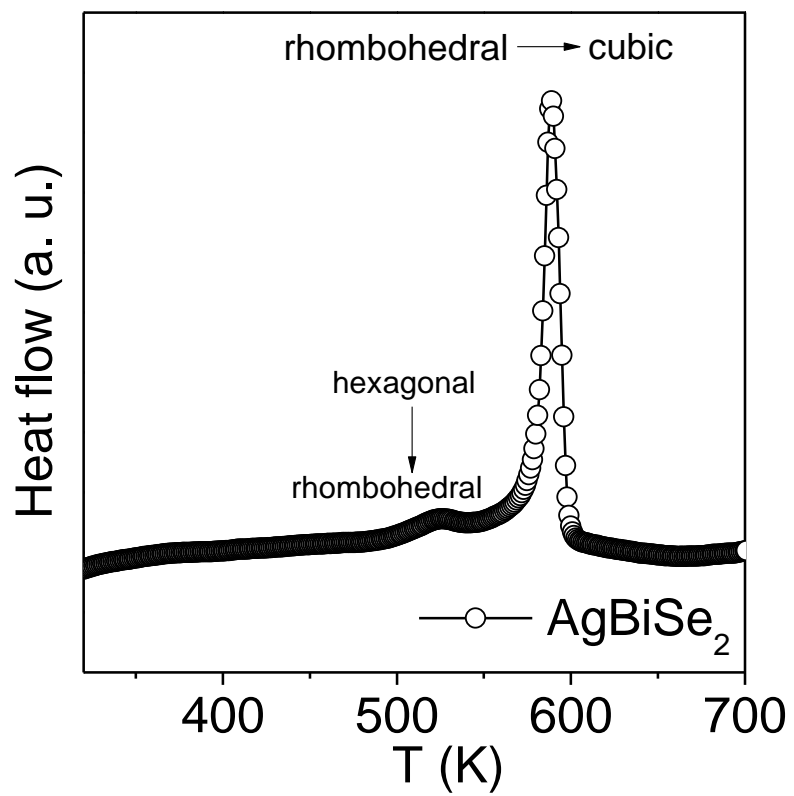


Fig.S1 DSC data for AgBiSe_2 .

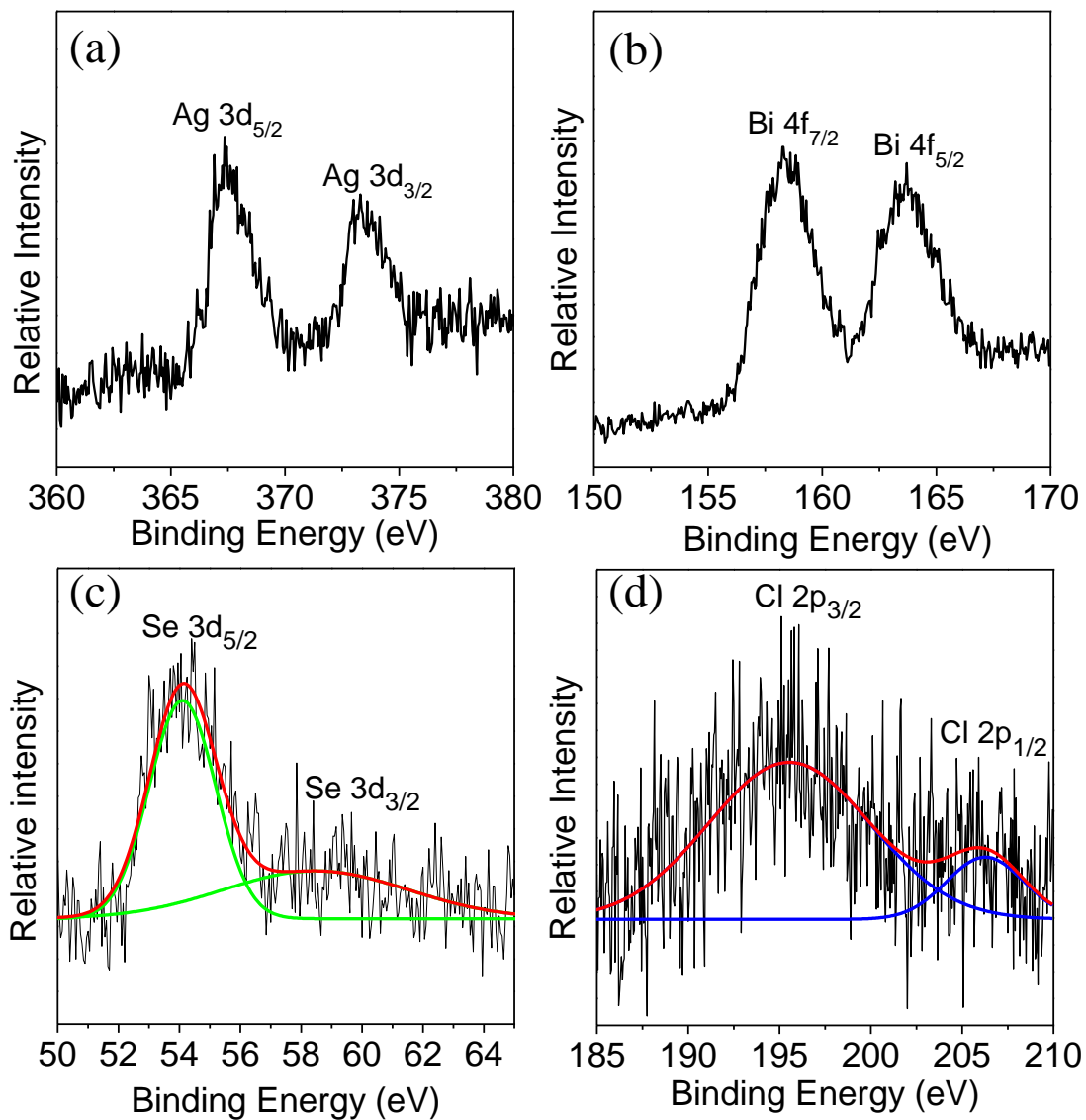


Fig. S2 XPS spectra of as prepared $\text{AgBiSe}_{1.98}\text{Cl}_{0.02}$ (a) Ag 3d, (b) Bi 4f, (c) Se 3d and (d) Cl 2p spectra.

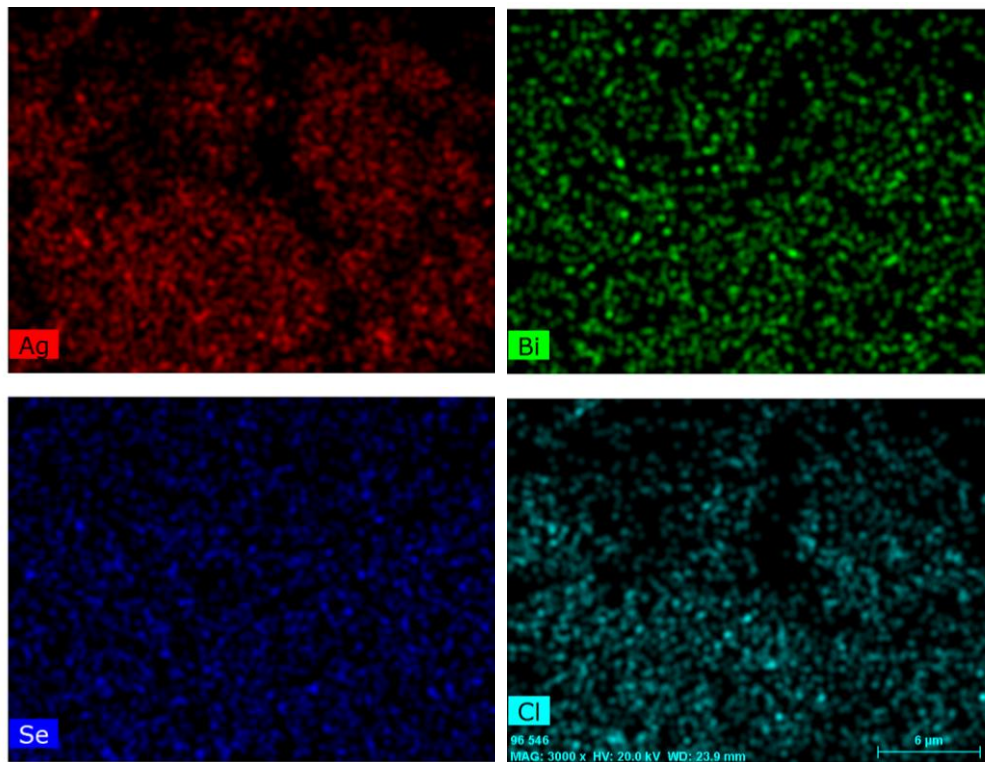


Fig. S3 EDAX elemental mapping of AgBiSe_{1.98}Cl_{0.02} sample.

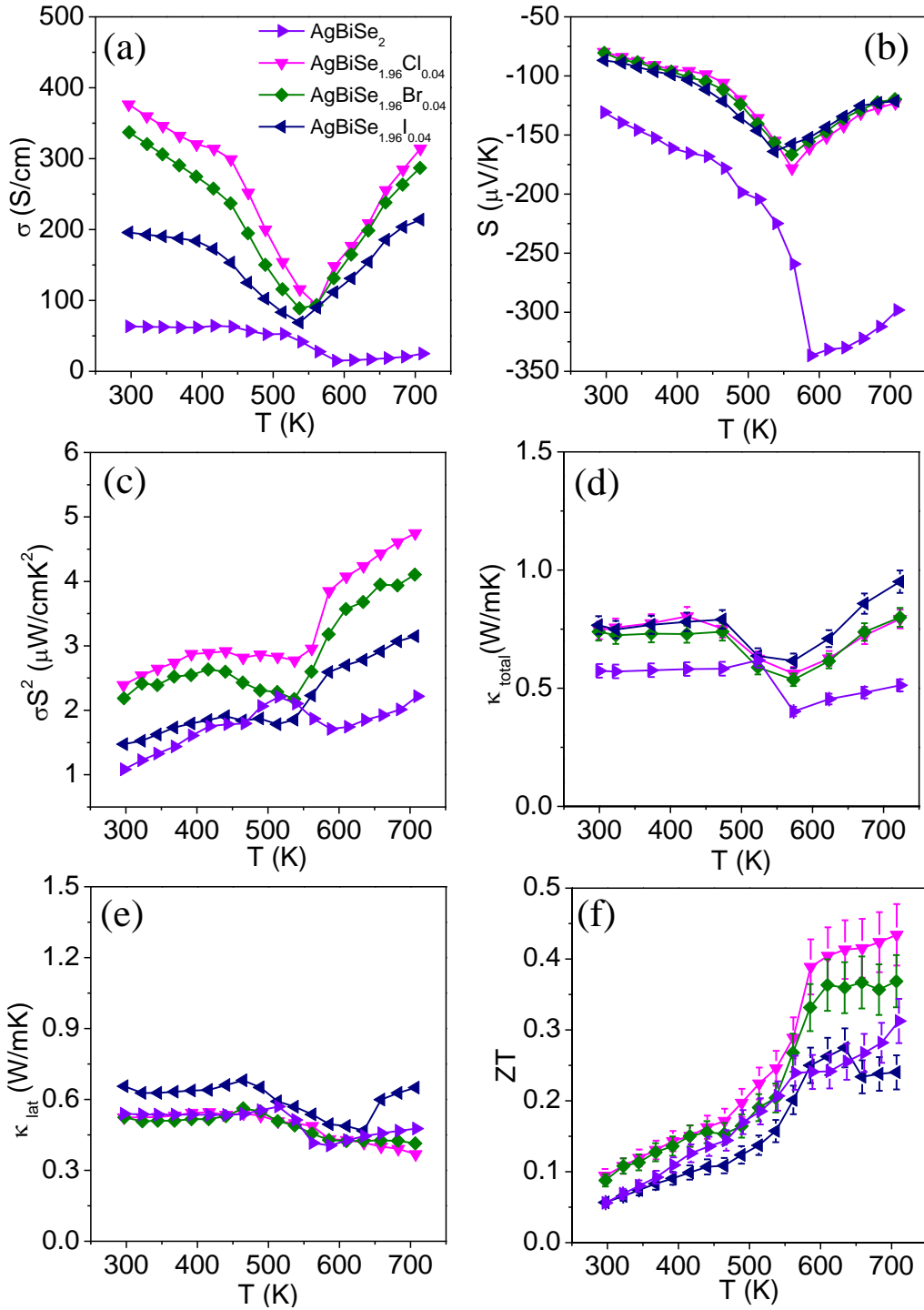


Fig. S4 Temperature-dependent (a) electrical conductivity (σ), (b) Seebeck coefficient (S), (c) power factor (σS^2), (d) total thermal conductivity (κ_{total}) with 5% error bar, (e) lattice thermal conductivity (κ_{lat}), and (f) thermoelectric figure of merit (ZT) of AgBiSe_2 and $\text{AgBiSe}_{1.96}\text{X}_{0.04}$ ($X = \text{Cl}, \text{Br}$ and I) samples with 10% error bar.

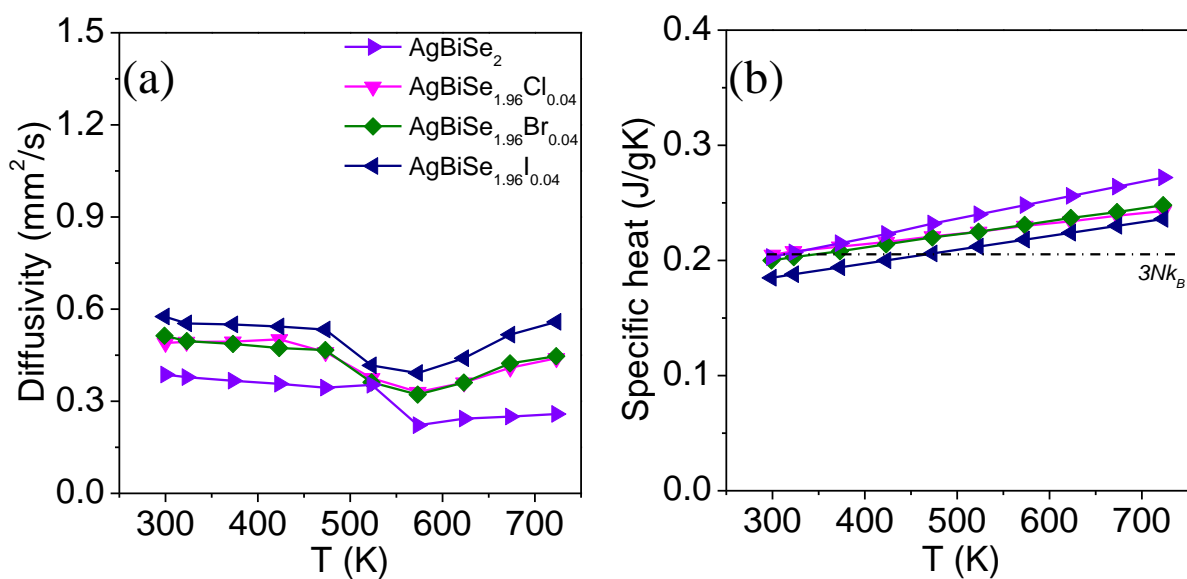


Fig. S5 Temperature dependent (a) thermal diffusivity (D) and (b) specific heat (C_p) of AgBiSe_2 and $\text{AgBiSe}_{1.96}\text{X}_{0.04}$ ($X = \text{Cl}, \text{Br}$ and I) samples.

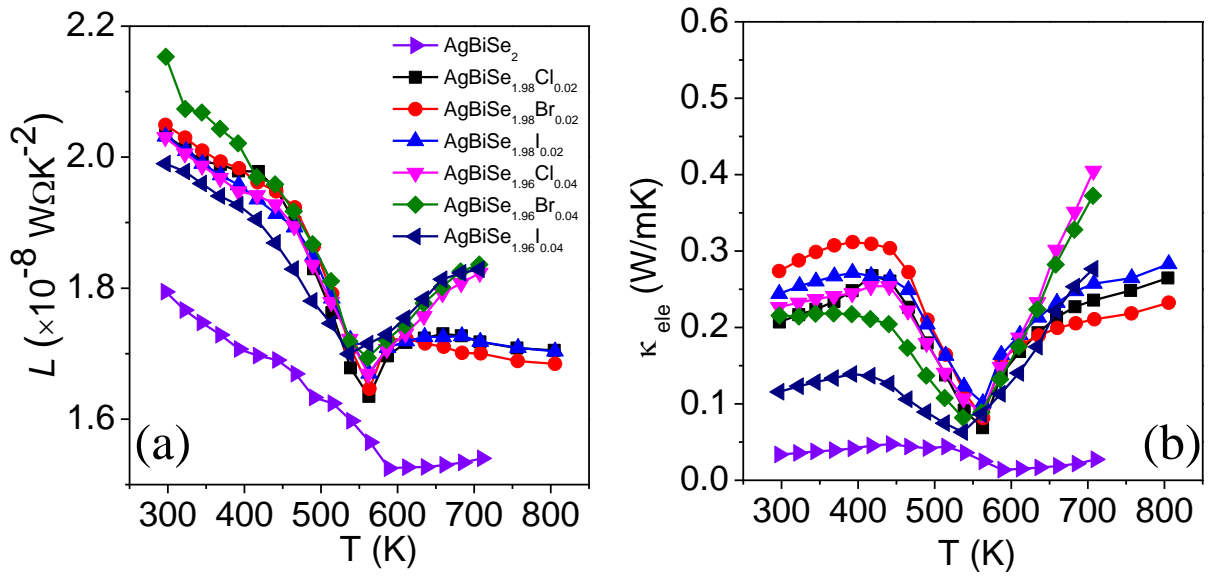


Fig. S6 Temperature dependent (a) calculated Lorenz numbers and (b) electronic thermal conductivity (κ_{lat}) for pristine and halogen doped AgBiSe₂ samples.

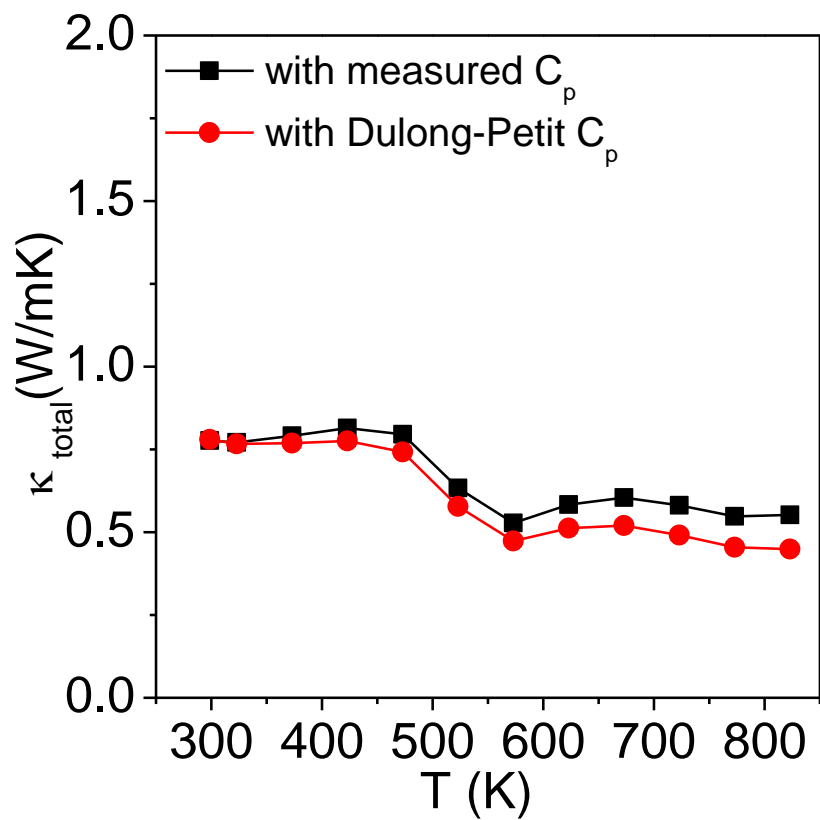


Fig. S7 Temperature-dependent total thermal conductivity (κ_{total}) of $\text{AgBiSe}_{1.98}\text{Cl}_{0.02}$ estimated using measured and Dulong- Petit C_p value.

Table S1 Measured room temperature κ_{total} and κ_{lat} value of present samples in comparison with the previously reported samples of AgBiSe₂

Sample	κ_{total} (W/mK) at 300 K	κ_{lat} (W/mK) at 300 K
AgBiSe ₂ (Present work)	~0.58	~0.54
AgBiSe ₂ (<i>J. Am. Chem. Soc.</i> , 2013, 135 , 4914)	~0.63	~0.58
AgBiSe ₂ (<i>Energy Environ. Sci.</i> 2013, 6 , 570)	~0.6	–
AgBiSe _{1.98} Cl _{0.02} (Present work)	~0.77	~0.57
Ag _{0.98} Nb _{0.02} BiSe ₂ (<i>J. Am. Chem. Soc.</i> , 2013, 135 , 4914)	~0.70	~0.58