Supporting information

Supporting information for the manuscript " **Ultra-Low Thermal Conductivity in Na/Sb Chalcobismuthates: Synthesis, Crystal Structures, Optical Property and ^{23}Na NMR Spectroscopy**"

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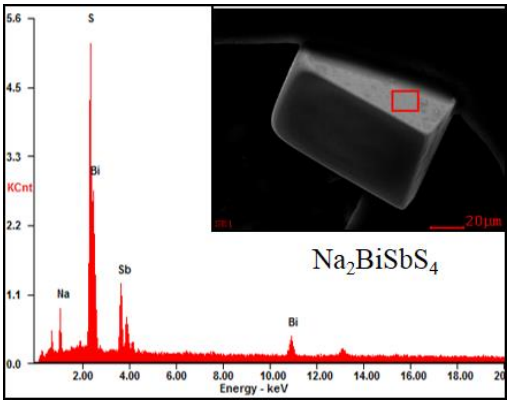
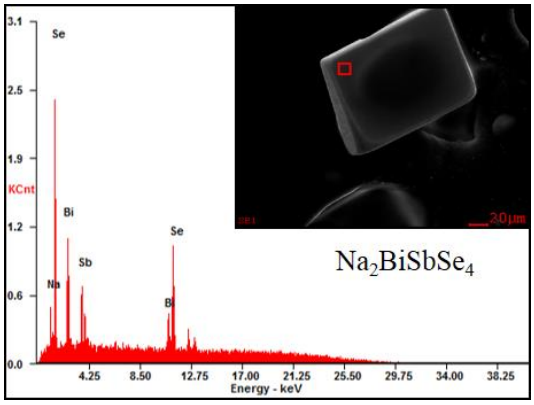
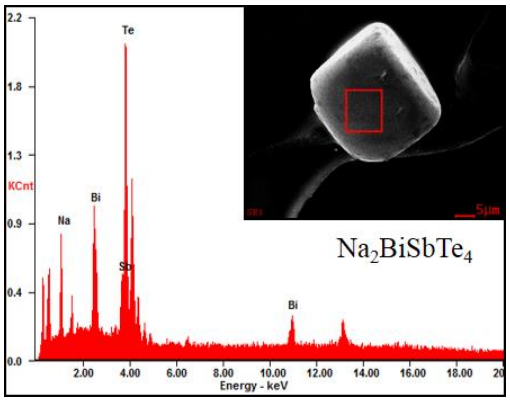


Element	Wt%	At%
NaK	09.37	25.46
SK	25.60	49.86
SbL	24.54	12.58
BiL	40.49	12.10
Matrix	Correction	ZAF



Element	Wt%	At%
NaK	07.23	24.93
SbL	16.11	12.44
BiL	31.29	12.50
SeK	45.37	50.14
Matrix	Correction	ZAF



Element	Wt%	At%
NaK	06.81	24.05
SbL	13.85	12.52
TeL	52.41	50.48
BiL	26.92	11.95
Matrix	Correction	ZAF

Figure S1. SEM/EDX analysis for Na_2BiSbS_4, $Na_2BiSbSe_4$ and $Na_2BiSbTe_4$. The estimated atomic ratio is of Na:Bi:Sb:*Q* = 2:1:1:4. The EDX analyses were carried out on different spots of the same crystal. Several crystals were measured parallel to confirm the results.

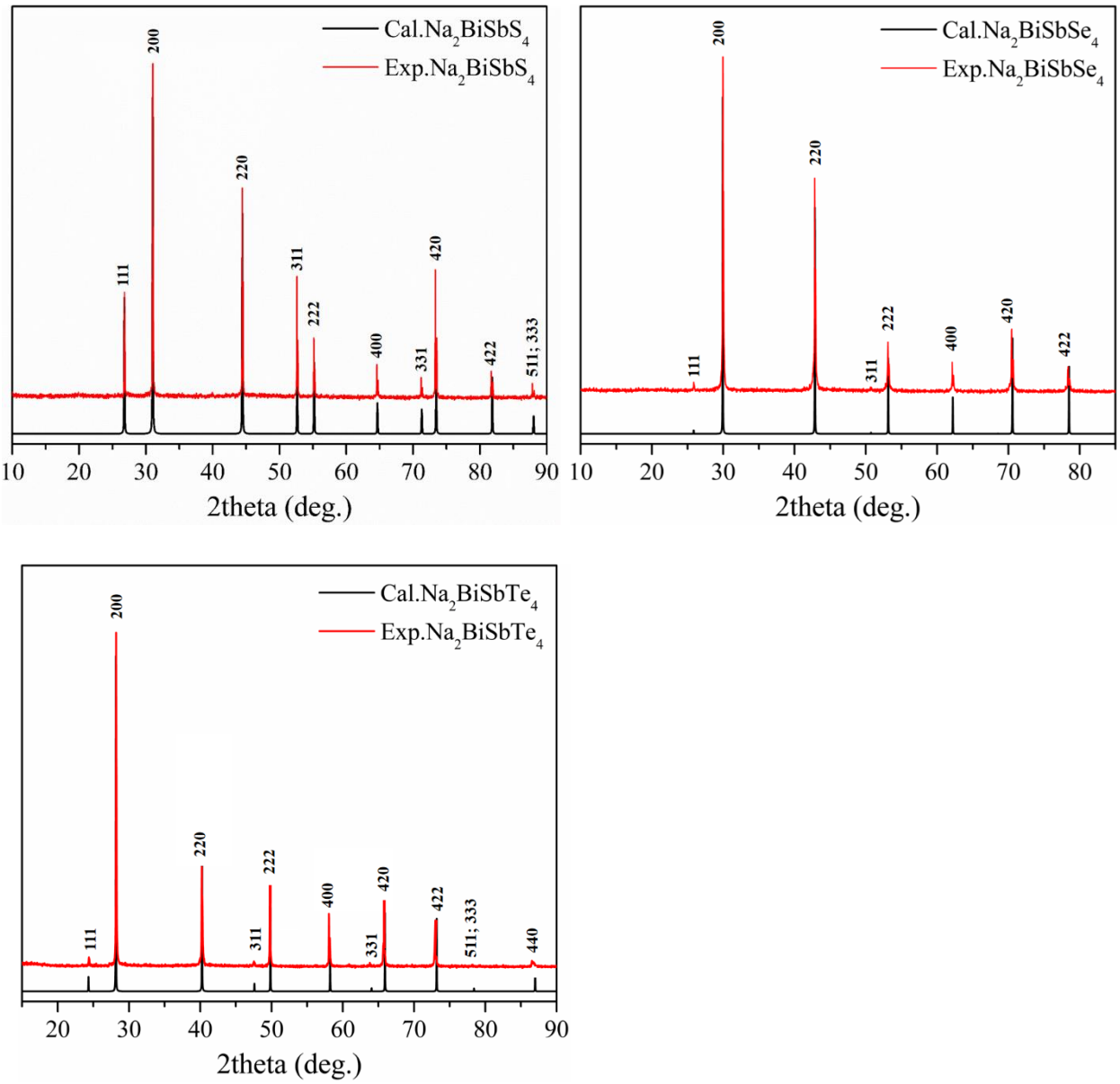


Figure S2. PXRD analysis for Na_2BiSbS_4, $Na_2BiSbSe_4$ and $Na_2BiSbTe_4$.

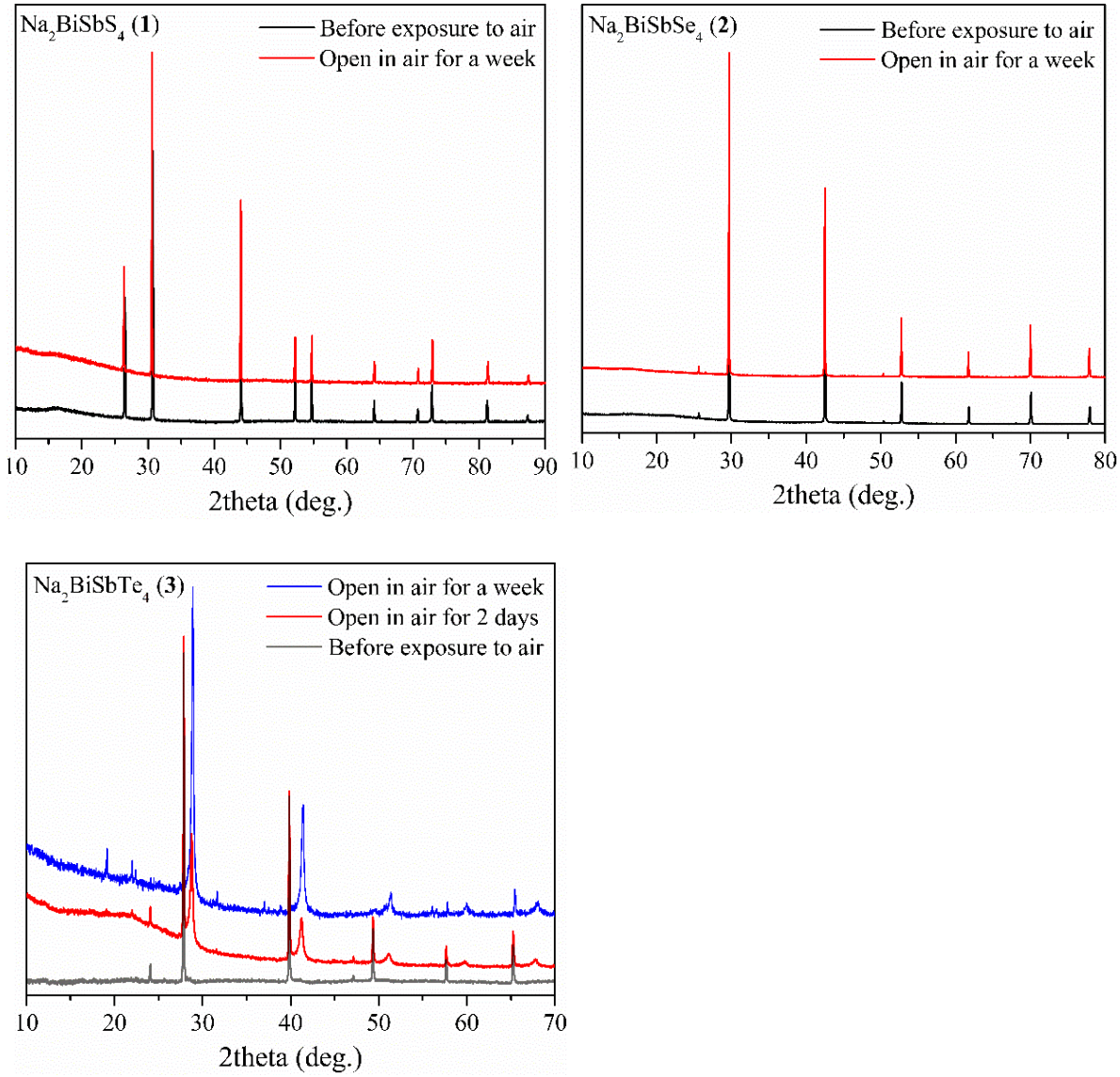
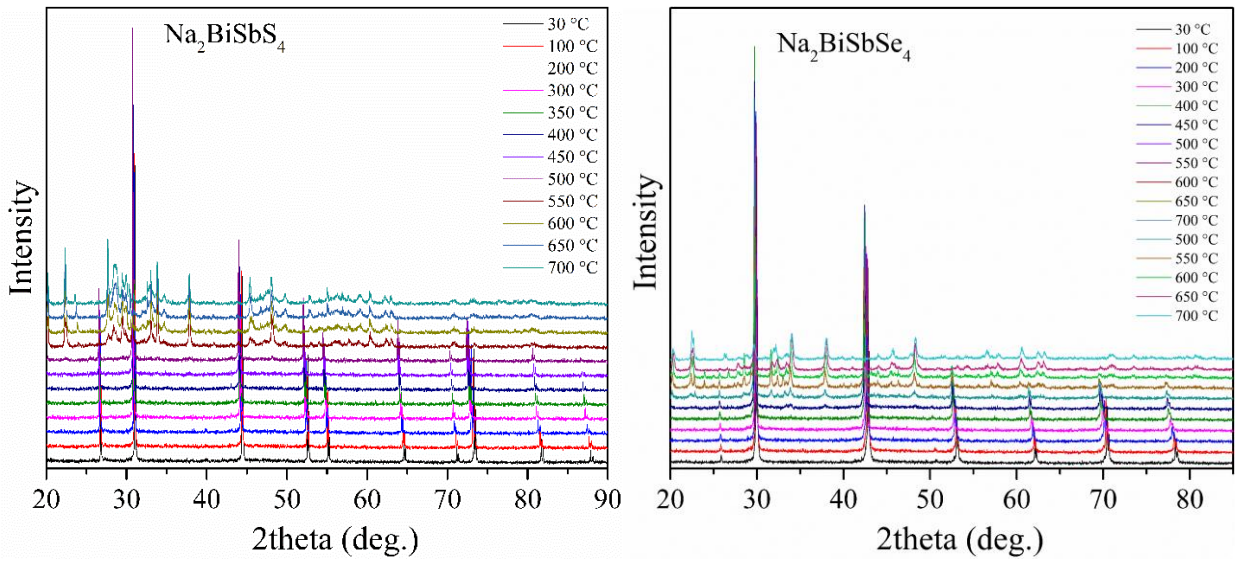


Figure S3. PXRD analysis for Na_2BiSbS_4, $Na_2BiSbSe_4$ and $Na_2BiSbTe_4$ before and after exposure to air for a week.



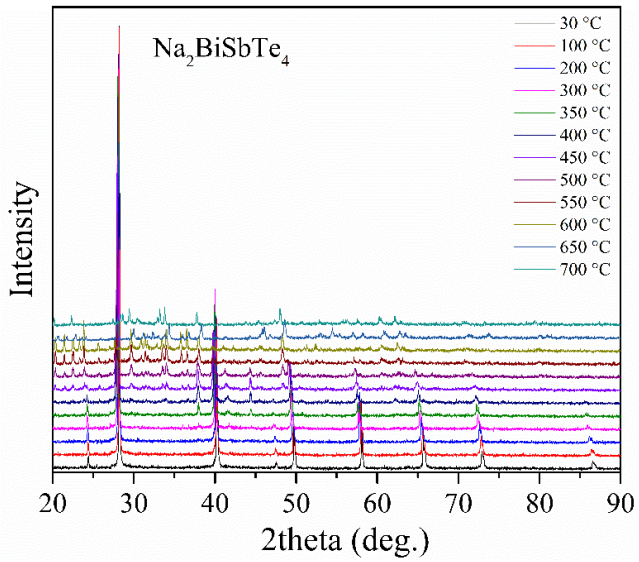


Figure S4.Varible temperature PXRD analysis for Na_2BiSbS_4, $Na_2BiSbSe_4$ and $Na_2BiSbTe_4$ up to 700 °C.

Table S1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for Na_2BiSbS_4 at 170 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Na(1)	0	5000	5000	0.5	27(1)
Bi(1)	0	5000	5000	0.25	27(1)
Sb(1)	0	5000	5000	0.25	27(1)
S(1)	5000	5000	5000	1	38(1)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Anisotropic displacement parameters ($Å^2x10^3$) for Na_2BiSbS_4 at 170 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	27(1)	27(1)	27(1)	0	0	0
Bi(1)	27(1)	27(1)	27(1)	0	0	0
Sb(1)	27(1)	27(1)	27(1)	0	0	0
S(1)	38(1)	38(1)	38(1)	0	0	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S3. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for $Na_2BiSbSe_4$ at 200 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Na(1)	0	5000	5000	0.5	28(1)
Sb(1)	0	5000	5000	0.2501	28(1)
Bi(1)	0	5000	5000	0.2501	28(1)
Se(1)	5000	5000	5000	1	14(1)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S4. Anisotropic displacement parameters ($Å^2x10^3$) for $Na_2BiSbSe_4$ at 200 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	28(1)	28(1)	28(1)	0	0	0
Sb(1)	28(1)	28(1)	28(1)	0	0	0
Bi(1)	28(1)	28(1)	28(1)	0	0	0
Se(1)	14(1)	14(1)	14(1)	0	0	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Table S5. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for $Na_2BiSbTe_4$ at 150 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Na(1)	0	5000	5000	0.5	21(1)
Sb(1)	0	5000	5000	0.2501	21(1)
Bi(1)	0	5000	5000	0.2501	21(1)
Te(1)	5000	5000	5000	1	17(1)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S6. Anisotropic displacement parameters ($Å^2x10^3$) for $Na_2BiSbTe_4$ at 150 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	21(1)	21(1)	21(1)	0	0	0
Sb(1)	21(1)	21(1)	21(1)	0	0	0
Bi(1)	21(1)	21(1)	21(1)	0	0	0
Te(1)	17(1)	17(1)	17(1)	0	0	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$