Supplementary Material

Thermoelectric Properties of Al Substituted Tetrahedrite

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Table S1. Structural parameters for $Cu_{11.9}Al_{0.1}Sb_4S_{13}$ (x = 0.1) sample

Atom	Wycoff Site	*x*	*y*	*z*	U_{iso}(Å^2)	Occupancy
Cu1	12*d*	0.25000	0.50000	0	0.04140	1
Cu2	12*e*	0.21572	0	0	0.08198	1
Al	12*d*	0.25000	0.50000	0	0.04140	1
S1	24*g*	0.11395	0.11395	0.36419	0.02831	1
S2	2*a*	0	0	0	0.07771	1
Sb	8*c*	0.26828	0.26828	0.26828	0.03931	1

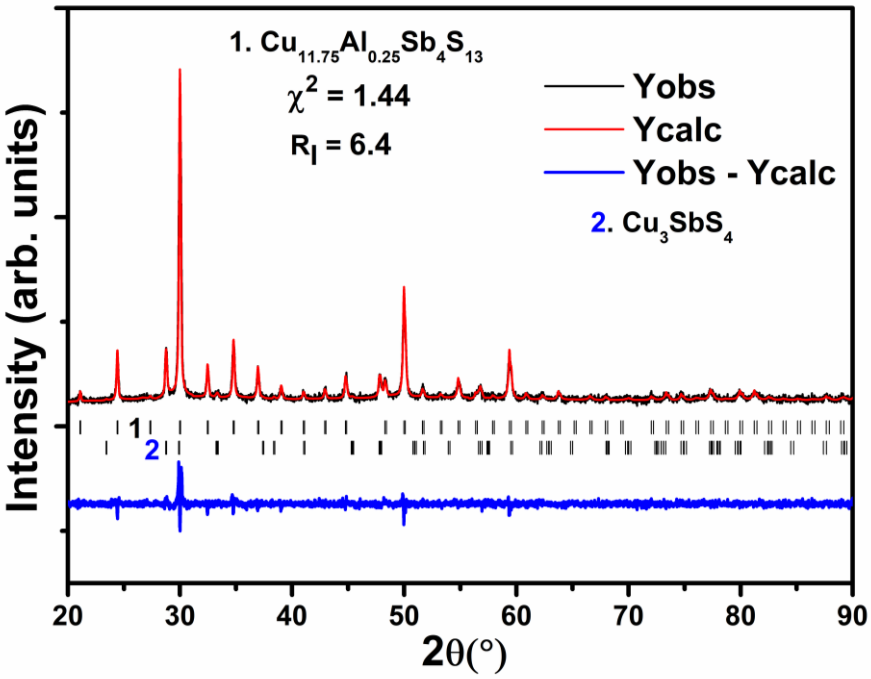

Figure S1. Refined XRD pattern for $Cu_{11.75}Al_{0.25}Sb_4S_{13}$ (x = 0.25) sample.

Table S2. Structural parameters for $Cu_{11.75}Al_{0.25}Sb_4S_{13}$ (x = 0.25) sample

Atom	Wycoff Site	x	y	z	U_{iso}(Å^2)	Occupancy
Cu1	12*d*	0.25000	0.50000	0	0.03972	1
Cu2	12*e*	0.21572	0	0	0.06692	1
Al	12*d*	0.25000	0.50000	0	0.03972	1
S1	24*g*	0.11391	0.11391	0.36417	0.03469	1
S2	2*a*	0	0	0	0.05598	1
Sb	8*c*	0.26827	0.26827	0.26827	0.04074	1

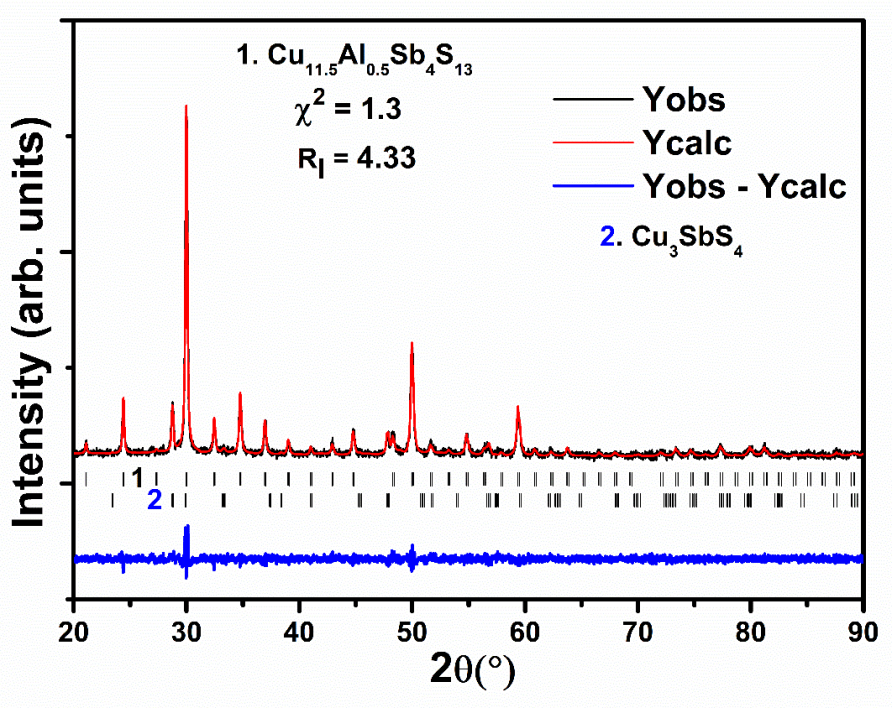

Figure S2. Refined XRD pattern for $Cu_{11.5}Al_{0.5}Sb_4S_{13}$ (x = 0.5) sample.

Table S3. Structural parameters for $Cu_{11.5}Al_{0.5}Sb_4S_{13}$ (x = 0. 5) sample

Atom	Wycoff Site	*x*	*y*	*z*	U_{iso}(Å^2)	Occupancy
Cu1	12*d*	0.25000	0.50000	0	0.03479	1
Cu2	12*e*	0.21572	0	0	0.07694	1
Al	12*d*	0.25000	0.50000	0	0.03479	1
S1	24*g*	0.11366	0.11366	0.36419	0.02914	1
S2	2*a*	0	0	0	0.05415	1
Sb	8*c*	0.26838	0.26838	0.26838	0.03575	1

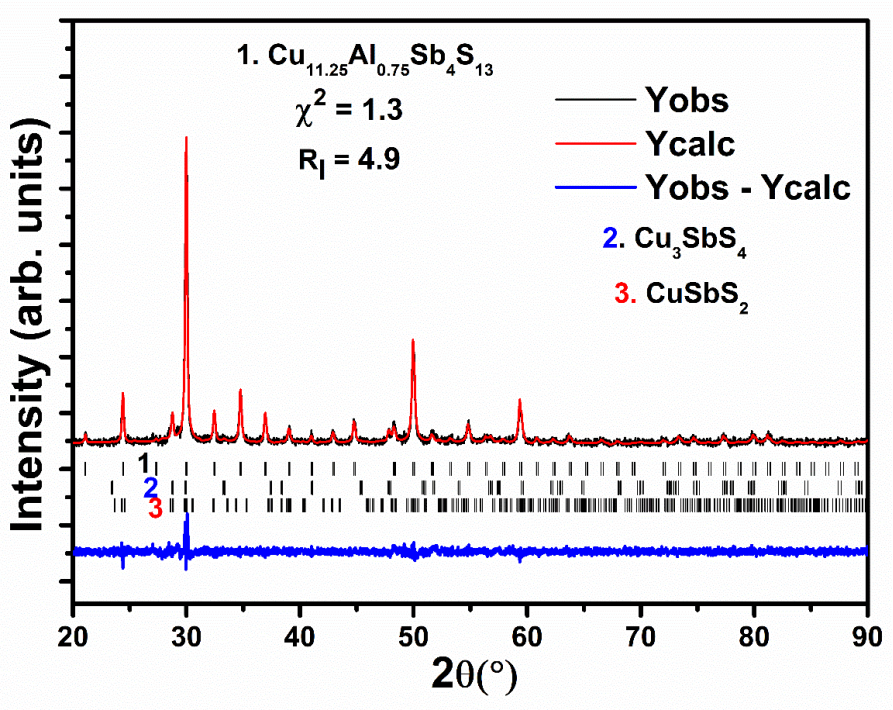

Figure S3. Refined XRD pattern for $Cu_{11.25}Al_{0.75}Sb_4S_{13}$ (x = 0.75) sample.

Table S4. Structural parameters for $Cu_{11.25}Al_{0.75}Sb_4S_{13}$ (x = 0.75) sample

Atom	Wycoff Site	*x*	*y*	*z*	U_{iso}(Å^2)	Occupancy
Cu1	12*d*	0.25000	0.50000	0	0.03351	1
Cu2	12*e*	0.21572	0	0	0.07961	1
Al	12*d*	0.25000	0.50000	0	0.03351	1
S1	24*g*	0.11274	0.11274	0.36419	0.02693	1
S2	2*a*	0	0	0	0.06224	1
Sb	8*c*	0.26827	0.26827	0.26827	0.03613	1

Table S5. Relative densities of all samples.

Sample Composition	Relative Density
$Cu_{11.9}Al_{0.1}Sb_4S_{13}$	96%
$Cu_{11.75}Al_{0.25}Sb_4S_{13}$	96%
$Cu_{11.5}Al_{0.5}Sb_4S_{13}$	95%
$Cu_{11.25}Al_{0.75}Sb_4S_{13}$	94.6%