Supporting information for

Effect of Zn substitution at Cu site on the transport behavior and thermoelectric properties in Cu_3SbSe_4

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Table S1. Refined structural parameters in *I-42m* space group of the tetragonal crystal structure of Cu_3SbSe_4 at room temperature.

Cu_3SbSe_4 *I-42m* (Tetragonal)				
Atom	**x**	**y**	**z**	**Occupancy**
Se	0.2366	0.2366	0.1310	4
Cu(1)	0	0	0	1
Sb	0	0	0.5	1
Cu(2)	0	0.5	0.25	2
$a = 5.6590$, $b = 5.6590$, $c = 11.2622$, $\alpha = 90$, $\beta = 90$, $\gamma = 90$				
$R_{Bragg} = 4.904$, $R_{RF} = 7.467$, $\chi^2 = 2.81$				

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Table S2. Refined structural parameters in $Cu_{2.5}Zn_{0.5}SbSe_4$ at room temperature.

$Cu_{2.5}Zn_{0.5}SbSe_4$ ***I-42m*** **(Tetragonal)**					**$CuSbSe_2$** ***Pnma*** **(Orthorhombic)**				
Atom	**x**	**y**	**z**	**Occupancy**	**Atom**	**x**	**y**	**z**	**Occupancy**
Se	0.23431	0.23431	0.13892	4	**Se(1)**	0.09694	0.25000	0.35828	1
Cu(1)	0	0	0	1	**Cu**	-0.11344	0.75000	0.31459	1
Sb	0	0	0.5	1	**Sb**	0.28622	0.25000	0.44470	1
Cu(2)	0	0.5	0.25	2	**Se(2)**	-0.38377	0.75000	0.37702	1
$a = 5.649473$, $b = 5.649473$, $c = 11.246007$, $\alpha = 90$, $\beta = 90$, $\gamma = 90$					$a = 6.209943$, $b = 3.983085$, $c = 14.991263$, $\alpha = 90$, $\beta = 90$, $\gamma = 90$				
$R_p = 13.0$ $R_{wp} = 10.7$ $R_{exp} = 7.03$, $\chi^2 = 2.31$									

Table S3. Refined structural parameters in $Cu_2ZnSbSe_4$ at room temperature.

$Cu_2ZnSbSe_4$ ***I-42m*** **(Tetragonal)**					**$CuSbSe_2$** ***Pnma*** **(Orthorhombic)**				
Atom	**x**	**y**	**z**	**Occupancy**	**Atom**	**x**	**y**	**z**	**Occupancy**
Se	0.24373	0.24373	0.13236	4	**Se(1)**	-0.10026	0.25000	0.39040	1
Cu(1)	0	0	0	1	**Cu**	-0.18609	0.75000	0.33349	1
Sb	0	0	0.5	1	**Sb**	0.29103	0.25000	0.43822	1
Cu(2)	0	0.5	0.25	2	**Se(2)**	-0.63791	0.75000	0.33706	1
$a = 5.651992$, $b = 5.651992$, $c = 11.229217$, $\alpha = 90$, $\beta = 90$, $\gamma = 90$					$a = 6.289621$, $b = 3.976935$, $c = 14.972906$, $\alpha = 90$, $\beta = 90$, $\gamma = 90$				
$R_p = 18.6$, $R_{wp} = 13.0$, $R_{exp} = 8.21$, $\chi^2 = 2.52$									