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Synergistic Effect of $CuInSe_2$ Alloying on Enhancement in Thermoelectric Performance of Cu_2SnSe_3 compounds

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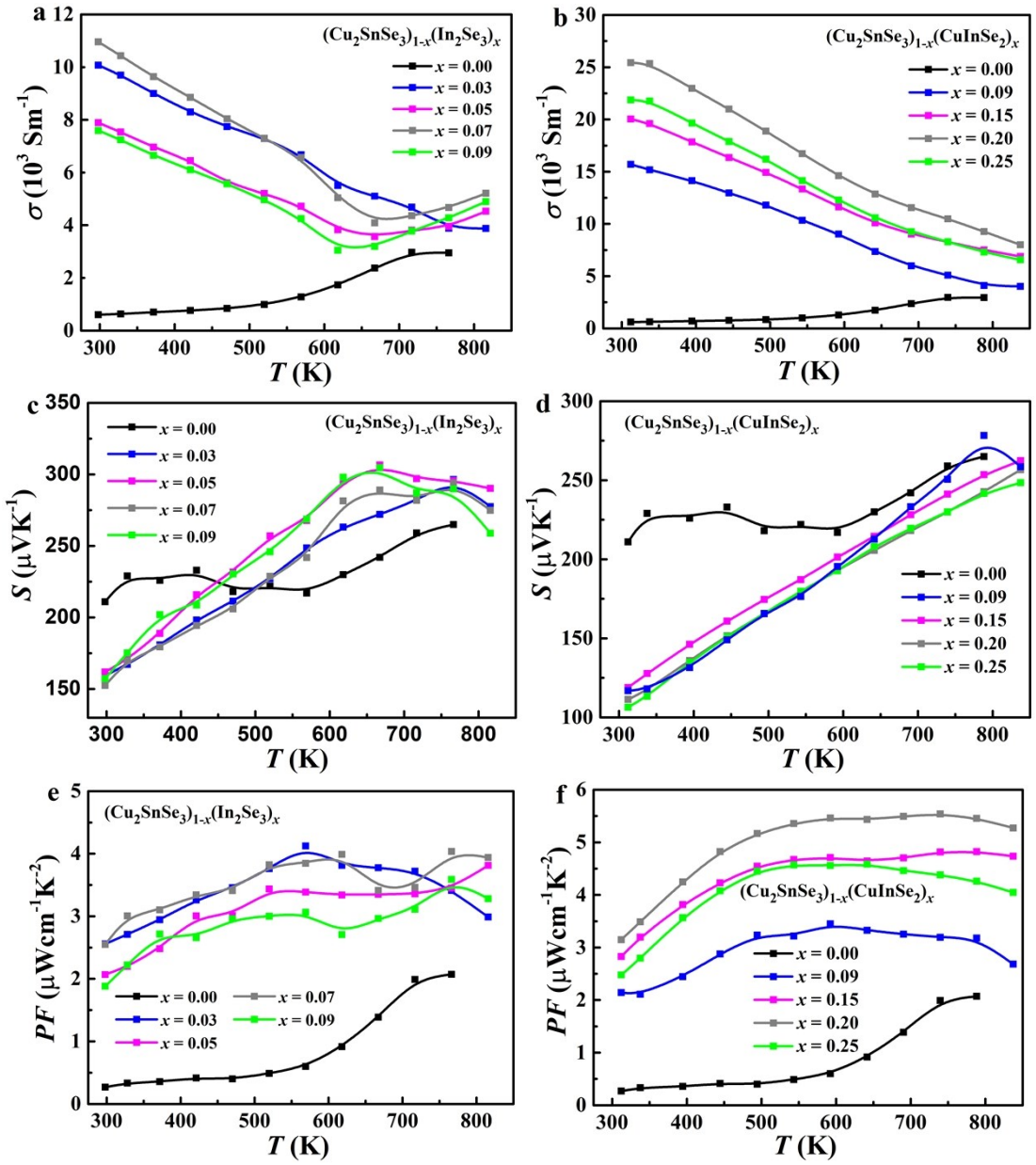

Fig. S1 Temperature dependent (a) Electrical conductivity, (c) Seebeck coefficient, and (e) Power factor for $(Cu_2SnSe_3)_{1-x}(In_2Se_3)_x$ (x = 0.00, 0.03, 0.05, 0.07, 0.09); Temperature dependent (b) Electrical conductivity, (d) Seebeck coefficient, and (f) Power factor for $(Cu_2SnSe_3)_{1-x}(CuInSe_2)_x$ (x = 0.00, 0.09, 0.15, 0.20, 0.25).

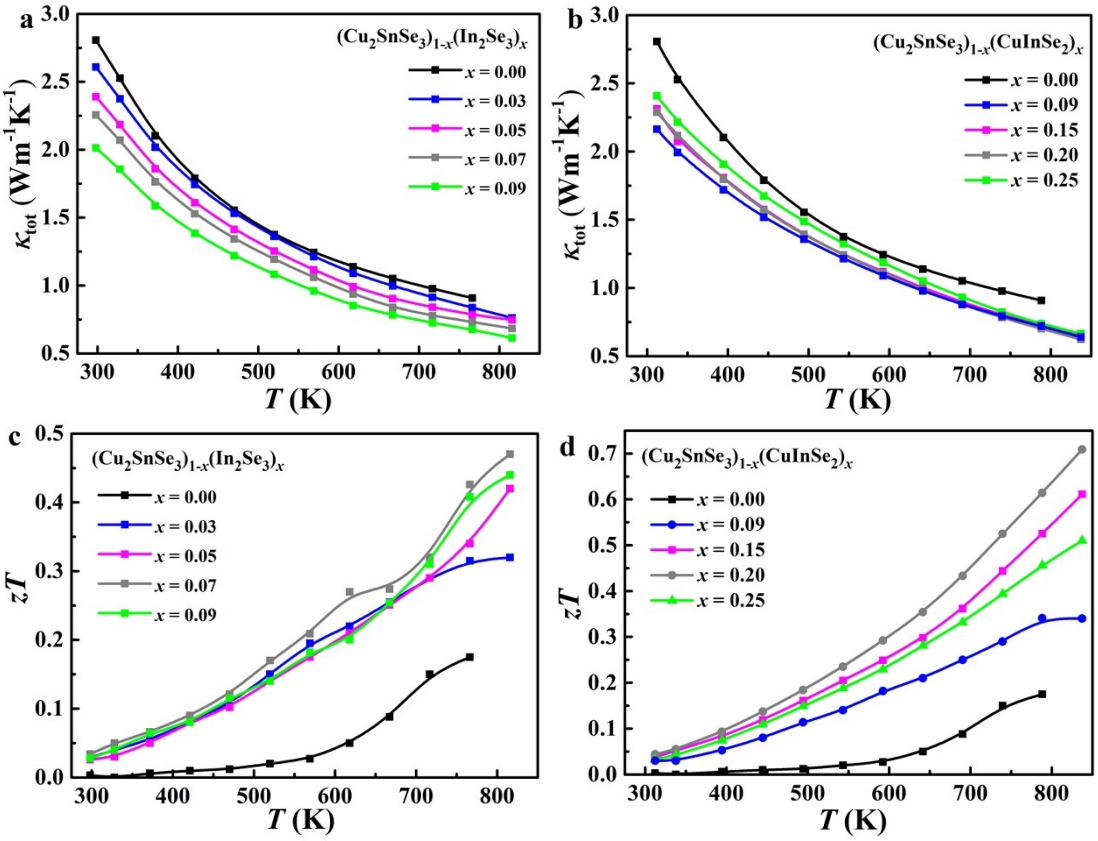

Fig. S2 Temperature dependent (a) Total thermal conductivity, and (c) zT for $(Cu_2SnSe_3)_{1-x}(In_2Se_3)_x$ (x = 0.00, 0.03, 0.05, 0.07, 0.09); Temperature dependent (b) Total thermal conductivity, and (d) zT for $(Cu_2SnSe_3)_{1-x}(CuInSe_2)_x$ (x = 0.00, 0.09, 0.15, 0.20, 0.25).

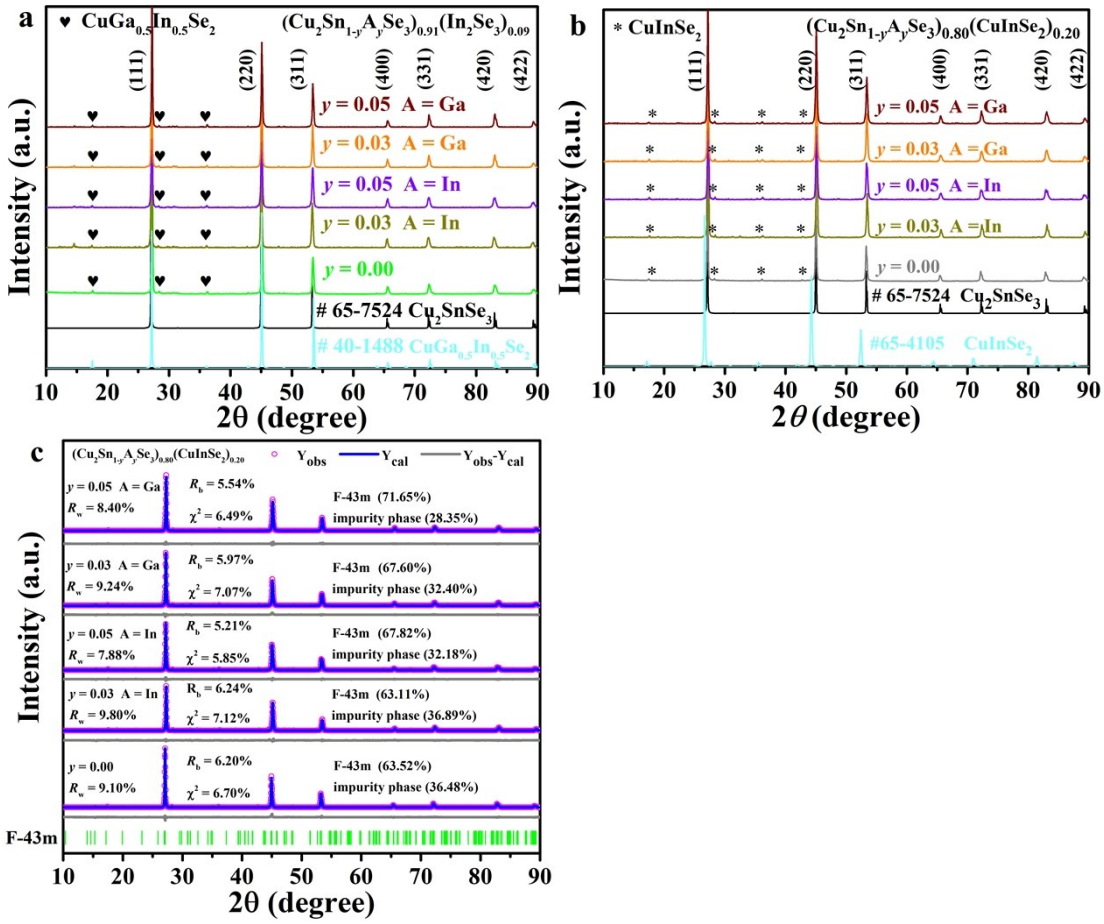

Fig. S3 Powder XRD patterns for (a) $(Cu_2Sn_{1-y}A_ySe_3)_{0.91}(In_2Se_3)_{0.09}$ (A = In, Ga; y = 0.00, 0.03, 0.05) and (b) $(Cu_2Sn_{1-y}A_ySe_3)_{0.80}(CuInSe_2)_{0.20}$ (A = In, Ga; y = 0.00, 0.03, 0.05); (c) The calculated, observed and difference Rietveld refined XRD patterns for $(Cu_2Sn_{1-y}A_ySe_3)_{0.80}(CuInSe_2)_{0.20}$ (A = In, Ga; y = 0.00, 0.03, 0.05) at room temperature.

Table S1 Density (ρ) and Dulong-Petit heat capacity (C_p) for all samples.

Sample	ρ (gcm^{-3})	C_p ($Jg^{-1}K^{-1}$)	Sample	ρ (gcm^{-3})	C_p ($Jg^{-1}K^{-1}$)
Cu_2SnSe_3	5.7753	0.3108	$(Cu_2SnSe_3)_{0.91}(CuInSe_2)_{0.09}$	5.5316	0.3099
$(Cu_2SnSe_3)_{0.97}(In_2Se_3)_{0.03}$	5.6465	0.3095	$(Cu_2SnSe_3)_{0.85}(CuInSe_2)_{0.15}$	5.5241	0.3093
$(Cu_2SnSe_3)_{0.95}(In_2Se_3)_{0.05}$	5.6803	0.3087	$(Cu_2SnSe_3)_{0.80}(CuInSe_2)_{0.20}$	5.5140	0.3088
$(Cu_2SnSe_3)_{0.93}(In_2Se_3)_{0.07}$	5.6932	0.3079	$(Cu_2SnSe_3)_{0.75}(CuInSe_2)_{0.25}$	5.5890	0.3082
$(Cu_2SnSe_3)_{0.91}(In_2Se_3)_{0.09}$	5.5080	0.3070	$(Cu_2Sn_{0.97}In_{0.03}Se_3)_{0.80}(CuInSe_2)_{0.20}$	5.5597	0.3088
$(Cu_2Sn_{0.97}In_{0.03}Se_3)_{0.91}(In_2Se_3)_{0.09}$	5.6451	0.3071	$(Cu_2Sn_{0.95}In_{0.05}Se_3)_{0.80}(CuInSe_2)_{0.20}$	5.5660	0.3089
$(Cu_2Sn_{0.95}In_{0.05}Se_3)_{0.91}(In_2Se_3)_{0.09}$	5.7350	0.3071	$(Cu_2Sn_{0.97}Ga_{0.03}Se_3)_{0.80}(CuInSe_2)_{0.20}$	5.5394	0.3096
$(Cu_2Sn_{0.97}Ga_{0.03}Se_3)_{0.91}(In_2Se_3)_{0.09}$	5.5212	0.3079	$(Cu_2Sn_{0.95}Ga_{0.05}Se_3)_{0.80}(CuInSe_2)_{0.20}$	5.5425	0.3101
$(Cu_2Sn_{0.95}Ga_{0.05}Se_3)_{0.91}(In_2Se_3)_{0.09}$	5.6861	0.3085	/	/	/

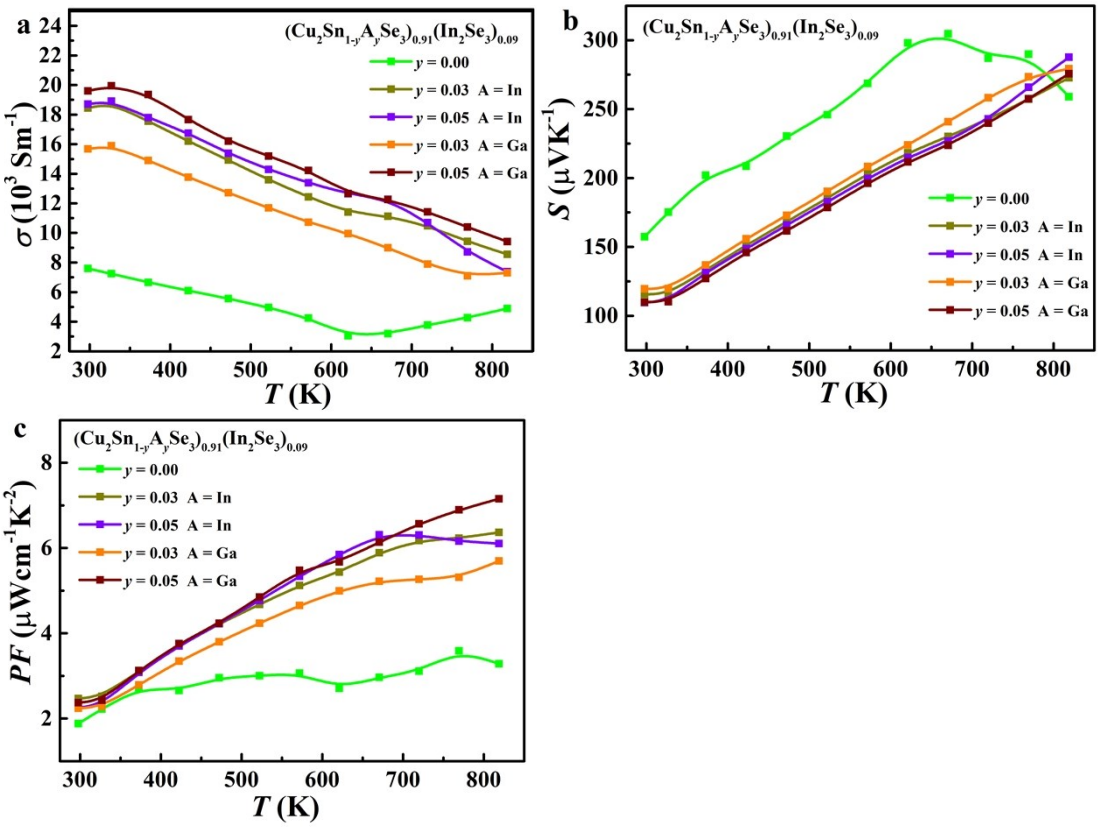

Fig. S4 Temperature dependent (a) Electrical conductivity, (b) Seebeck coefficient, and (c) Power factor for $(Cu_2Sn_{1-y}A_ySe_3)_{0.91}(In_2Se_3)_{0.09}$ (A = In, Ga; y = 0.00, 0.03, 0.05).

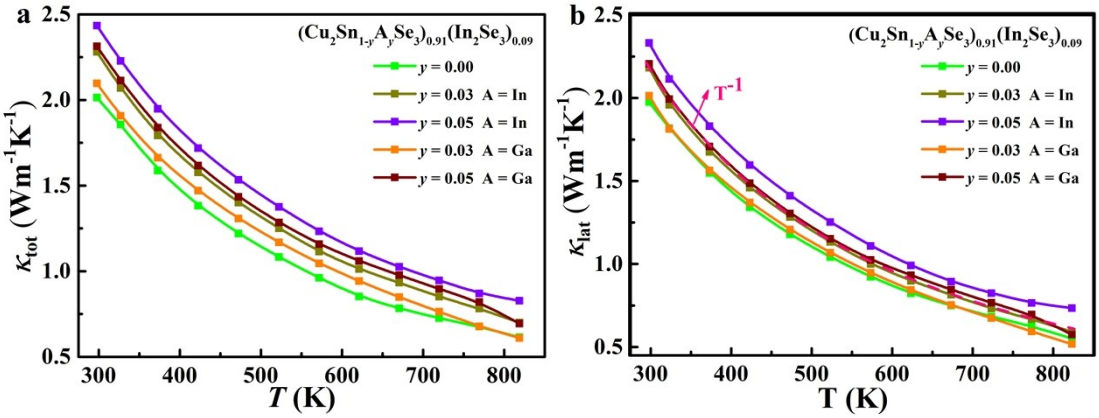

Fig. S5 Temperature dependent (a) Total thermal conductivity, and (b) Lattice thermal conductivity for $(Cu_2Sn_{1-y}A_ySe_3)_{0.91}(In_2Se_3)_{0.09}$ (A = In, Ga; y = 0.00, 0.03, 0.05).

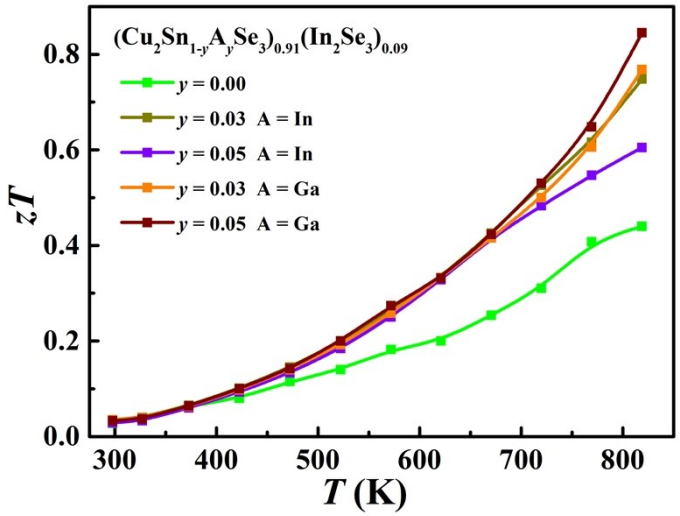

Fig. S6 Temperature dependent zT for $(Cu_2Sn_{1-y}A_ySe_3)_{0.91}(In_2Se_3)_{0.09}$ (A = In, Ga; y = 0.00, 0.03, 0.05).

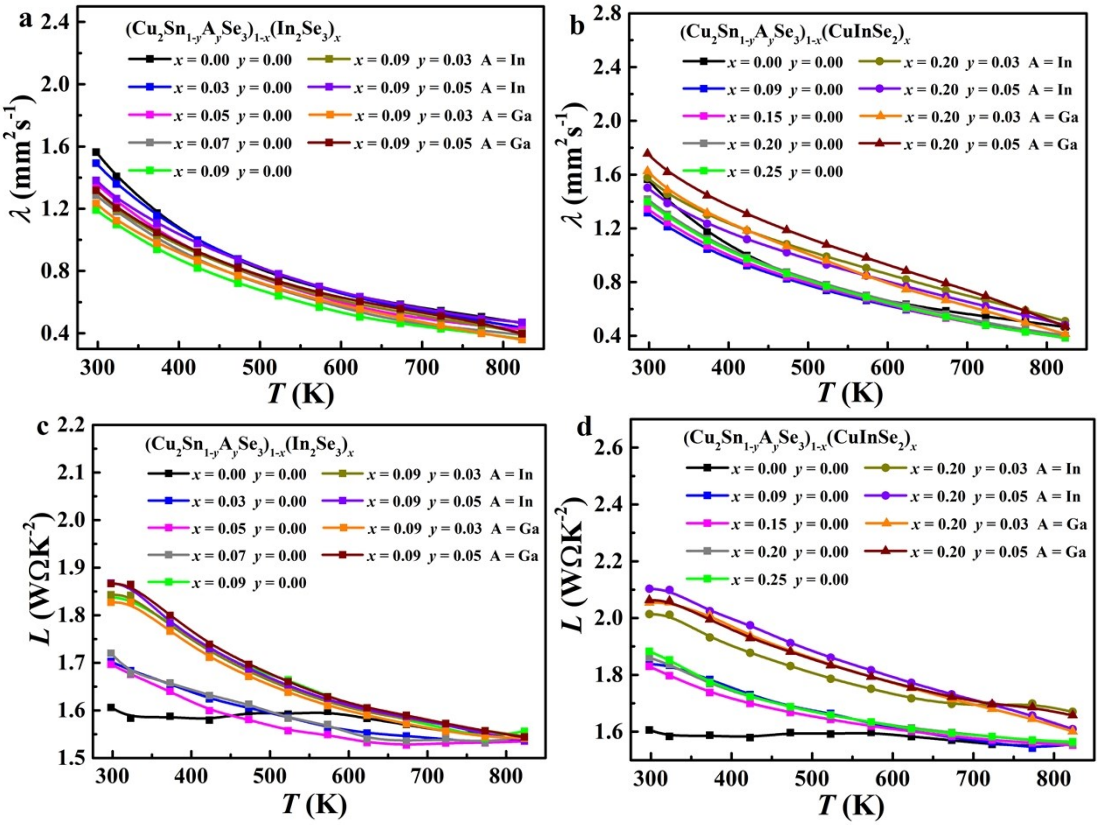

Fig. S7 Temperature dependent (a) Thermal diffusivity, and (c) Calculated Lorenz number for $(Cu_2Sn_{1-y}A_ySe_3)_{1-x}(In_2Se_3)_x$ (x = 0.00, 0.03, 0.05, 0.07, 0.09; y = 0.00, 0.03, 0.05; A = In, Ga); Temperature dependent (b) Thermal diffusivity, and (d) Calculated Lorenz number for $(Cu_2Sn_{1-y}A_ySe_3)_{1-x}(CuInSe_2)_x$ (x = 0.00, 0.09, 0.15, 0.20, 0.25; y = 0.00, 0.03, 0.05; A = In, Ga).

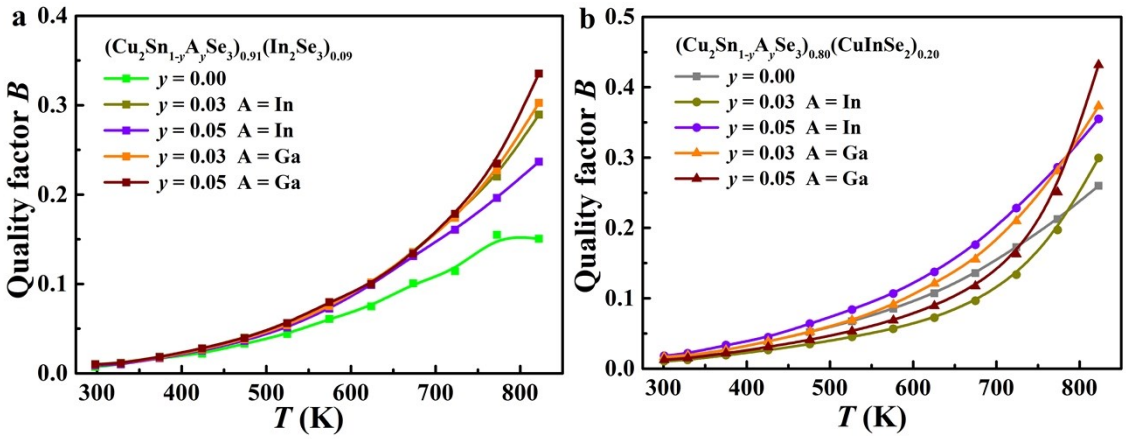

Fig. S8 Temperature dependent Quality factor for (a) $(Cu_2Sn_{1-y}A_ySe_3)_{0.91}(In_2Se_3)_{0.09}$ (y = 0.00, 0.03, 0.05; A = In, Ga) and (b) $(Cu_2Sn_{1-y}A_ySe_3)_{0.80}(CuInSe_2)_{0.20}$ (y = 0.00, 0.03, 0.05; A = In, Ga).

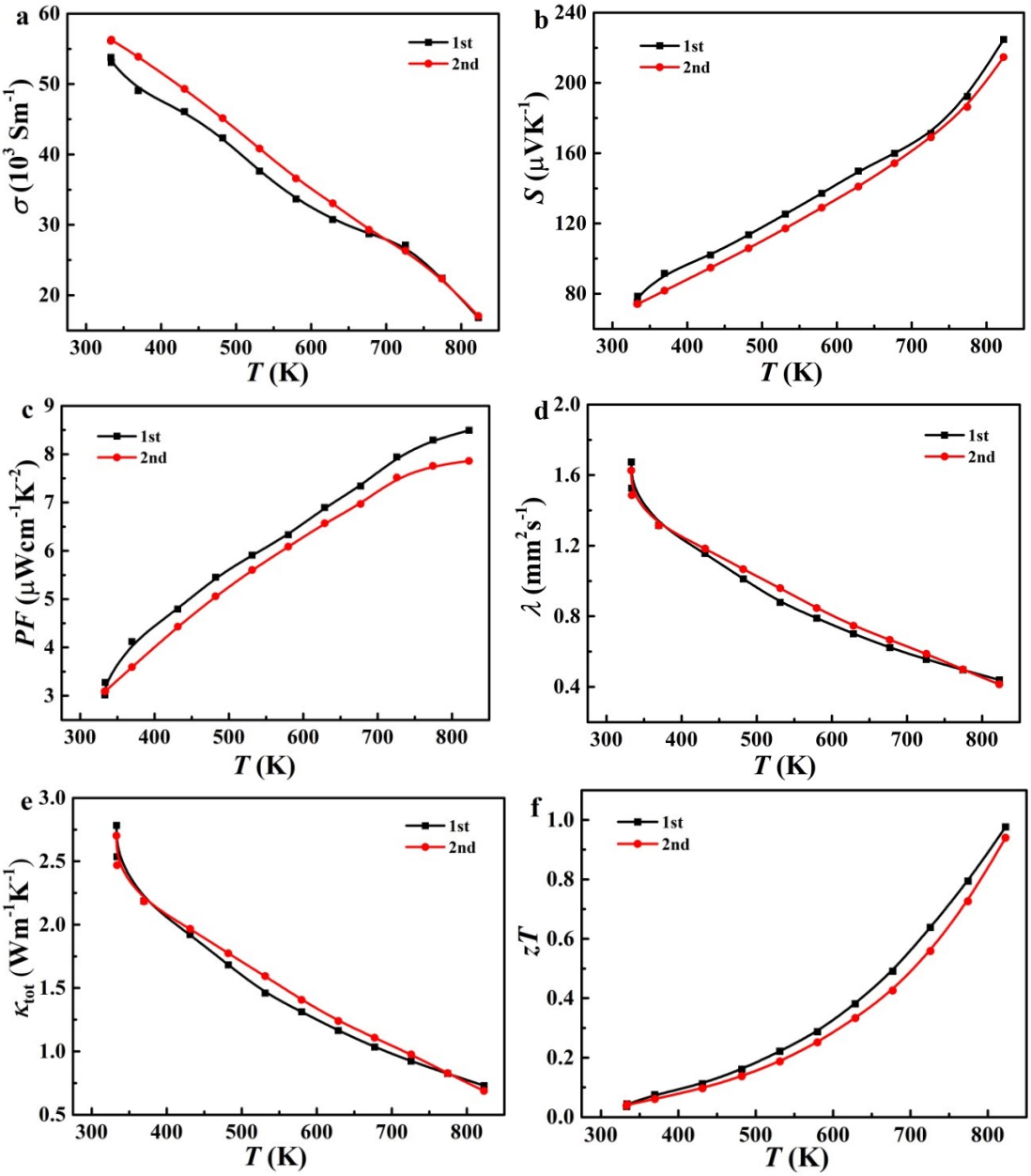

Fig. S9 Thermoelectric properties for $(Cu_2Sn_{0.97}Ga_{0.03}Se_3)_{0.80}(CuInSe_2)_{0.20}$ sample after thermal cycling.

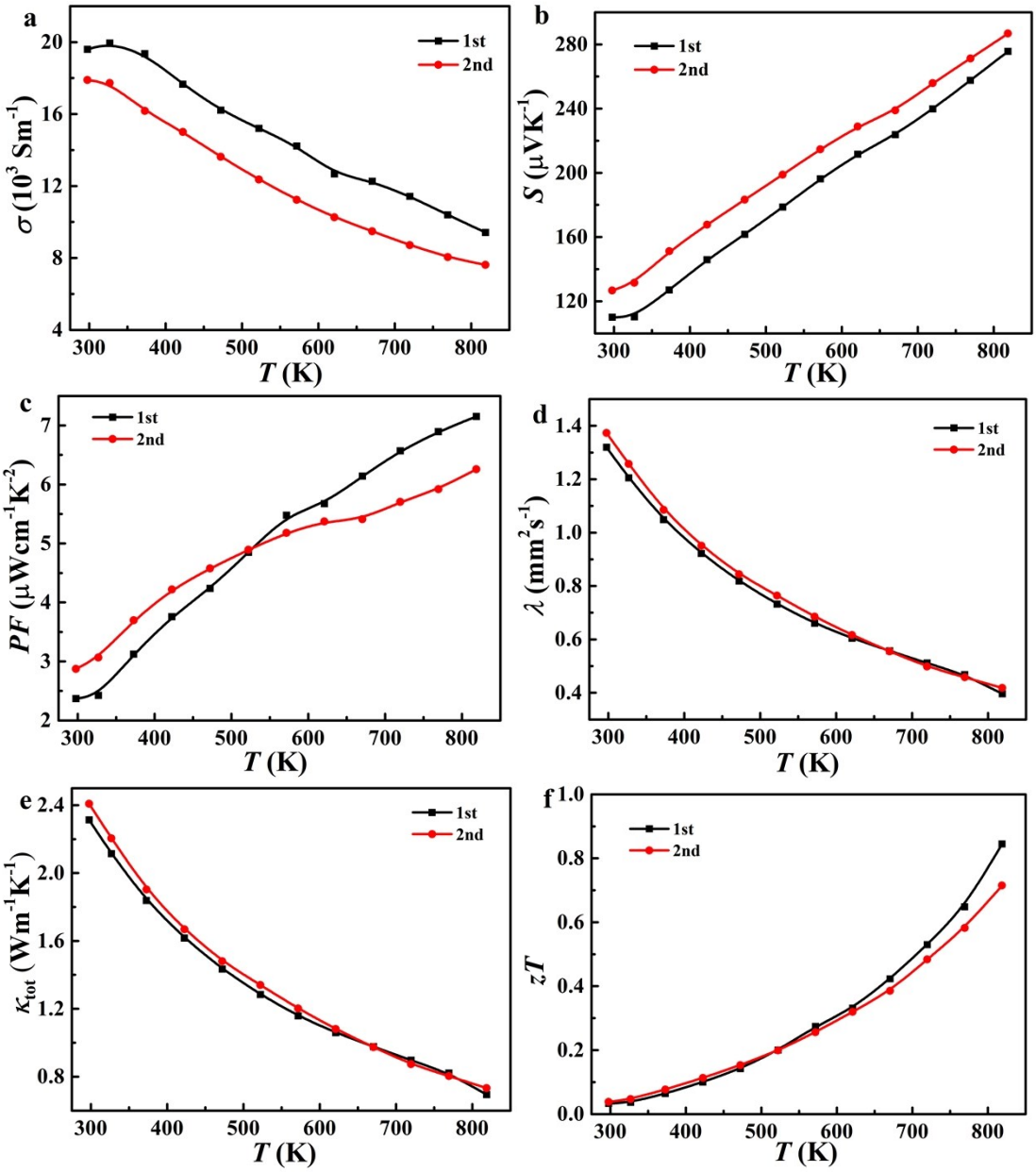

Fig. S10 Thermoelectric properties for $(Cu_2Sn_{0.95}Ga_{0.05}Se_3)_{0.91}(In_2Se_3)_{0.09}$ sample after thermal cycling.