Supporting Information

Improved thermoelectric performance of copper-deficient compounds $Cu_{2.5+\delta}In_{4.5}Te_8$ (δ=0-0.15) with an excess of Cu caused by formation of impurity bands and reduction in lattice thermal conductivity

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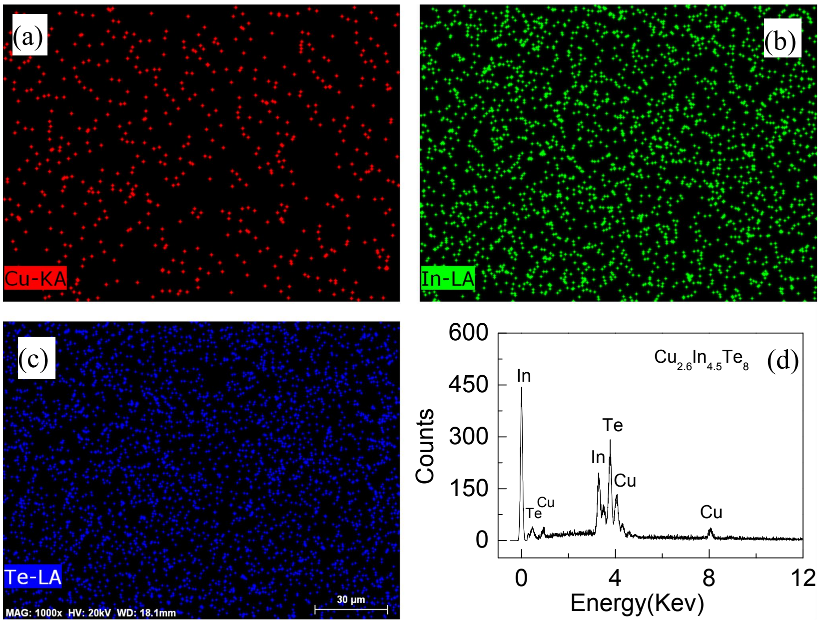

Fig. S1 EPMA mappings of three elements on polished $Cu_{2.6}In_{4.5}Te_8$ surface (a) Cu, (b) In, (c) Te, (d) an EDAX pattern.

Table S1 Average chemical compositions (relative molars) identified in $Cu_{2.5}In_{4.5}Te_8$ and $Cu_{2.6}In_{4.5}Te_8$ (taken from different mappings)

Compounds	Cu	In	Te
$Cu_{2.5}In_{4.5}Te_8$	2.53	4.51	8.0
$Cu_{2.6}In_{4.5}Te_8$	2.62	4.53	8.0

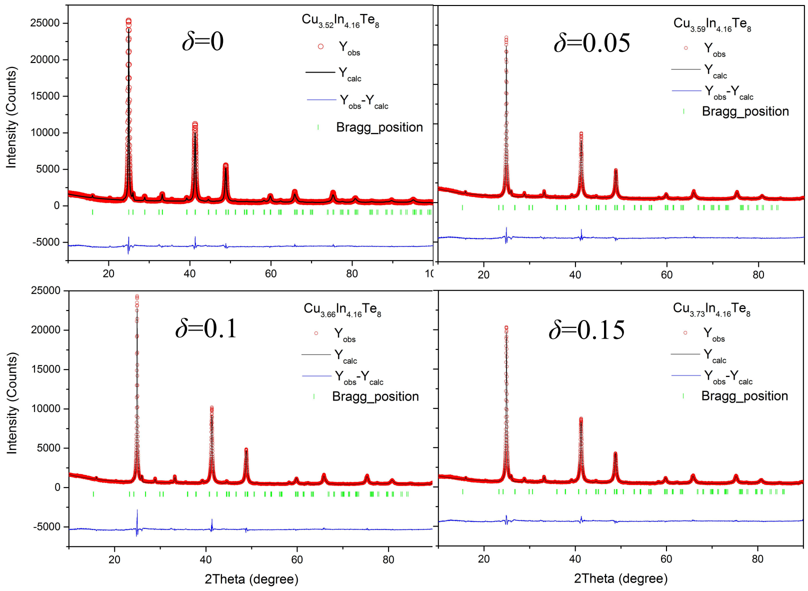

Fig. S2 Rietveld refinements using X-ray diffraction data of four compounds $Cu_{2.5+\delta}In_{4.5}Te_8$ (δ=0, 0.05, 0.1, 0.15).

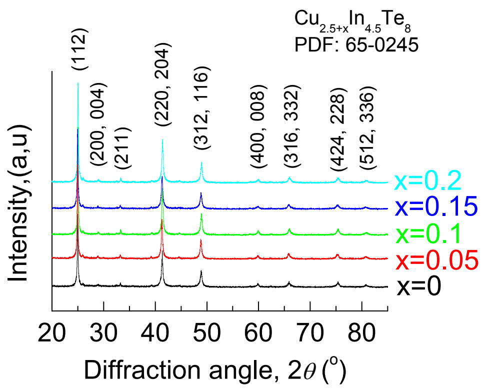

Fig. S3 XRD patterns of the powders of $Cu_{2.5+\delta}In_{4.5}Te_8$ (δ=0, 0.05, 0.1, 0.15, 0.2).

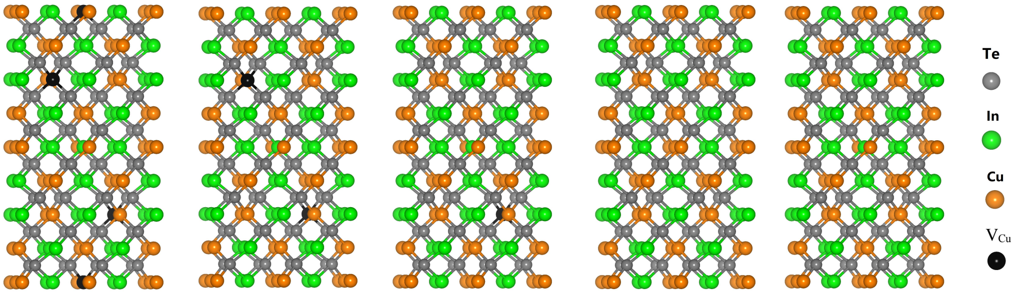

Fig. S4 Crystal structures of $Cu_{28+y}In_{33}Te_{64}$ (y=0-4) assuming that added Cu atoms reside in the Cu vacancy.

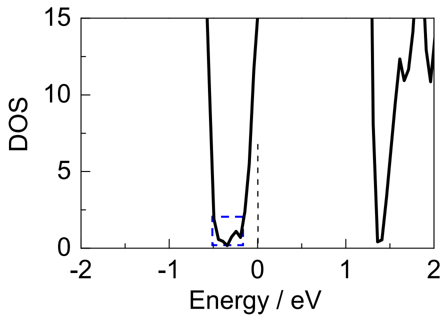

Fig. S5 Close-up view of the impurity band (IB) in the density of the states (DOS) of $Cu_{28+y}In_{33}Te_{64}$ (y=0-4) system.

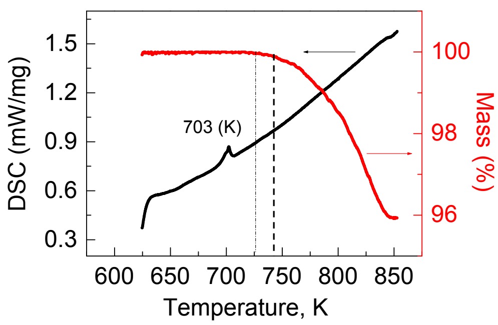

Fig. S6 Differential scanning calorimetry (DSC) and weight loss (TG) signals as a function of temperature for $Cu_{2.5}In_{4.5}Te_8$.