Supplementary Information

Dual doping strategy for enhancing thermoelectric performance of $Yb_{0.4}Co_4Sb_{12}$

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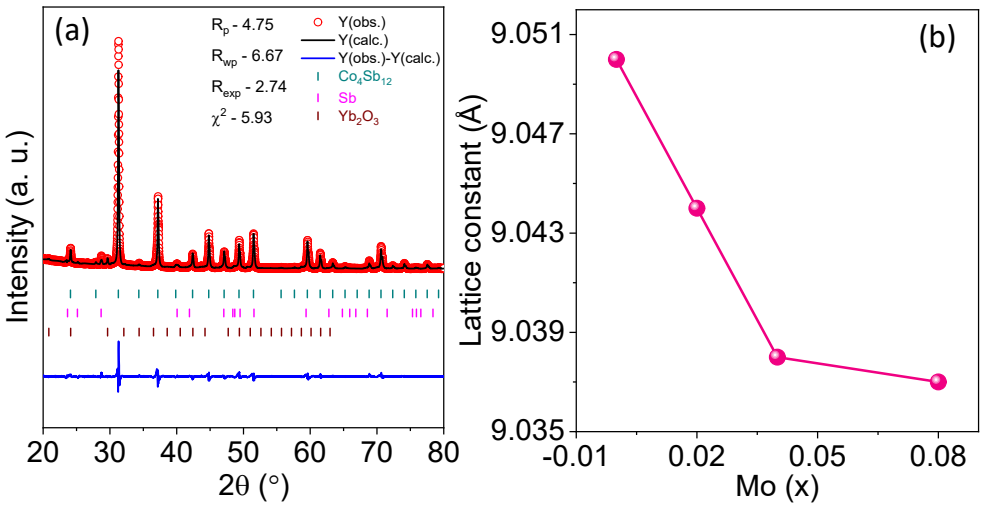


Fig. S1 (a) The Rietveld refinement of $Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$ composition (b) Variation of lattice parameter with the Mo concentration (x)

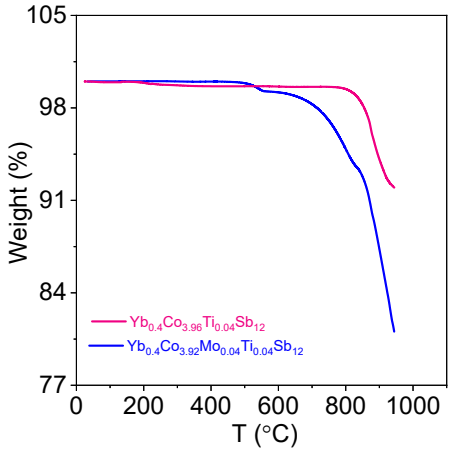


Fig. S2 Differential scanning calorimetry (DSC) measurement on $Yb_{0.4}Co_{3.96}Ti_{0.04}Sb_{12}$ and $Yb_{0.4}Co_{3.92}Mo_{0.04}Ti_{0.04}Sb_{12}$ in the temperature range 30 ºC to 950 ºC.

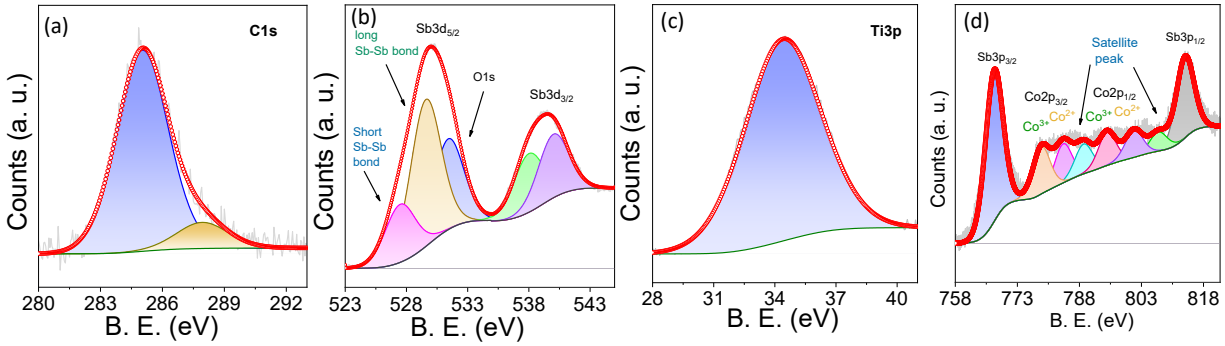
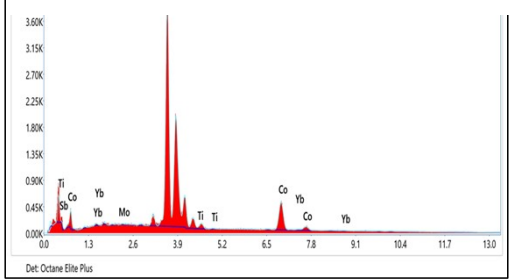
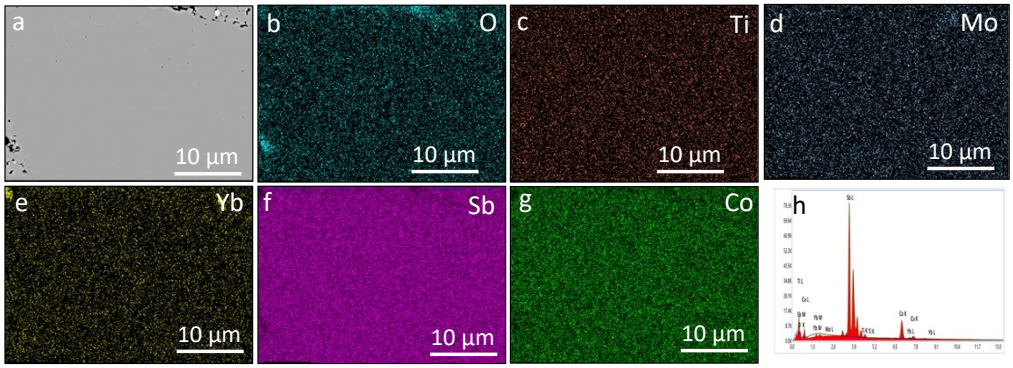


Fig. S3 XPS spectra of (a) C1s, (b) Sb3d (c) Ti3p, and (d) Co2p, Sb3p for energy levels of $Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$.

Fig. S4 EDS spectra of $Yb_{0.4}Co_{3.94}Mo_{0.02}Ti_{0.04}Sb_{12}$ composition



Ti K	0.61
Co K	23.10
Mo L	0.29
Sb L	75.65
Yb L	0.35
Total	100



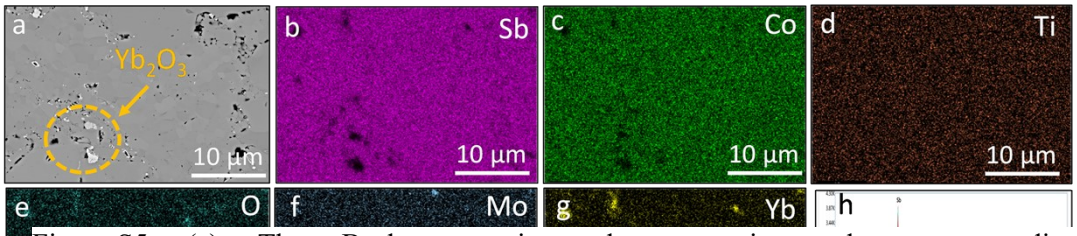


Fig. S5 (a) The Back scattering electron micrographs corresponding $Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$. (b), (c), (d), (e), (f) and (g) denotes the elemental mapping of O, Ti, Mo, Yb, Sb, and Co elements respectively. (h) EDS spectra of $Yb_{0.4}Co_{3.92}Mo_{0.04}Ti_{0.04}Sb_{12}$

Fig. S6 (a) The Back scattering electron micrographs corresponding $Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$. (b), (c), (d), (e), (f) and (g) denotes the elemental mapping of Sb, Co, Ti, O, Mo, and Yb elements respectively. (h) EDS spectra of $Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$

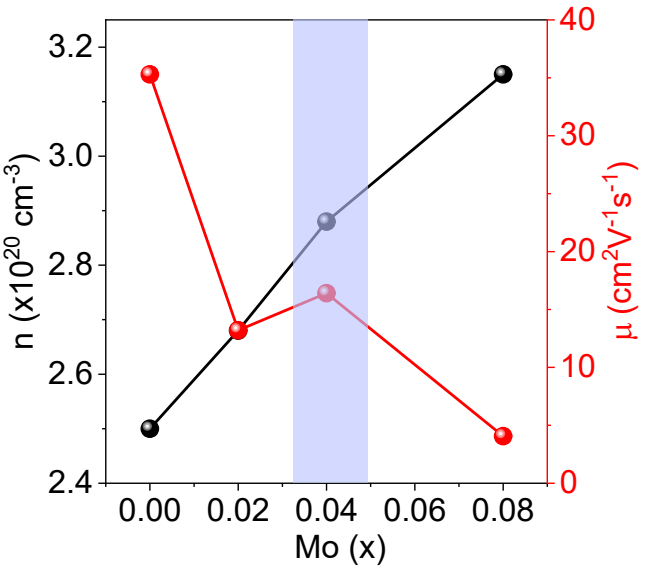


Fig. S7 Variation of carrier concentration and mobility with respect to Mo concentration in all the compositions

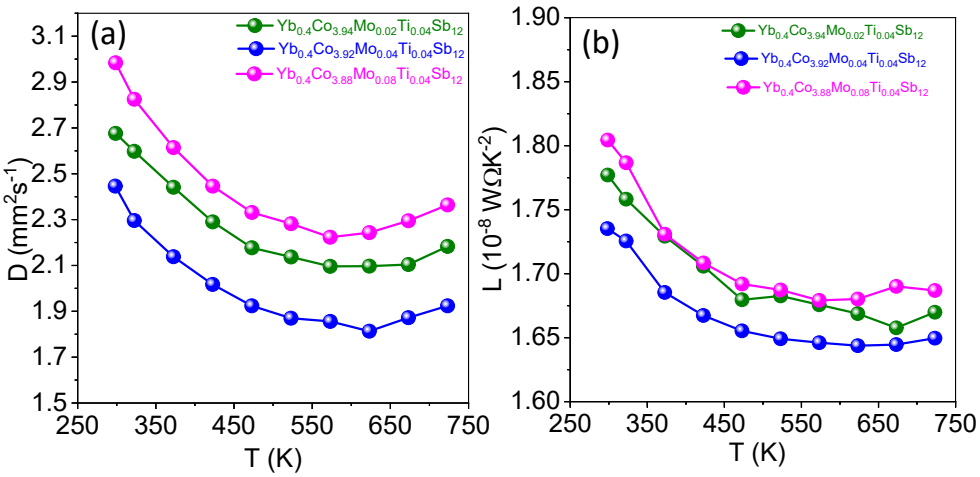


Fig. S8 (a) Thermal diffusivity as a function of temperature (b) Variation of Lorenz number with temperature

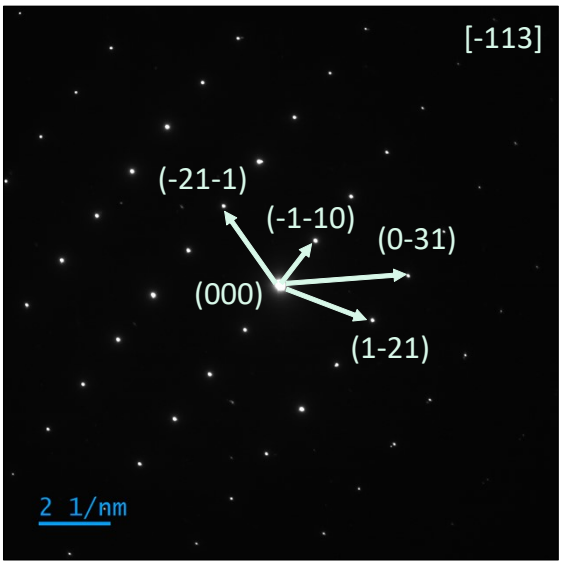


Fig. S9 BCC SAED single orientation pattern captured from single grain

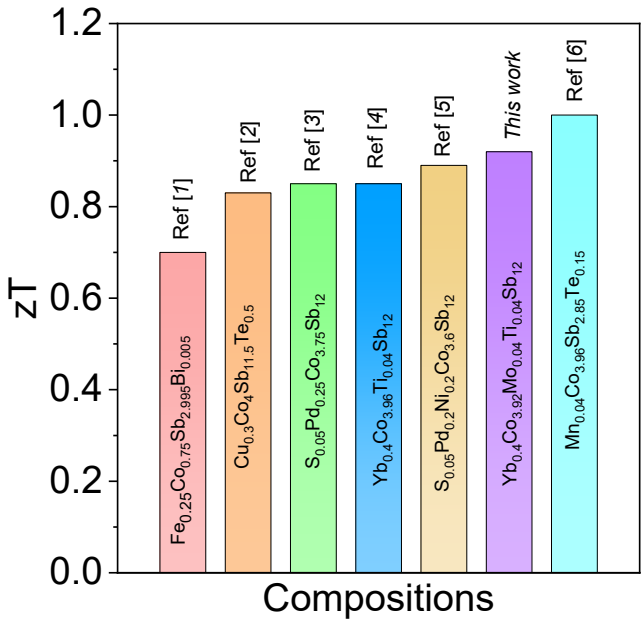


Figure S10 Bar diagram showing the comparison of figure of merit with the previous reports such as; $Fe_{0.25}Co_{0.75}Sb_{2.995}Bi_{0.005}$,[1] $Cu_{0.3}Co_4Sb_{11.5}Te_{0.5}$,[2] $S_{0.05}Pd_{0.25}Co_{3.75}Sb_{12}$,[3] $Yb_{0.4}Co_{3.96}Ti_{0.04}Sb_{12}$,[4] $S_{0.05}Pd_{0.2}Ni_{0.2}Co_{3.6}Sb_{12}$,[5] and $Mn_{0.04}Co_{3.96}Sb_{2.85}Te_{0.15}$,[6]

Table S1

Composition	d (gcm^{-3})	Lattice parameter (Å)	Volume (cm^{-3})
$Yb_{0.4}Co_{3.96}Ti_{0.04}Sb_{12}$	7.34 (> 98%)	9.050(0)	741.22
$Yb_{0.4}Co_{3.94}Mo_{0.02}Ti_{0.04}Sb_{12}$	7.32 (> 98%)	9.044(7)	739.92
$Yb_{0.4}Co_{3.92}Mo_{0.04}Ti_{0.04}Sb_{12}$	7.30 (> 98%)	9.038(8)	738.54
$Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$	7.31 (> 98%)	9.037(4)	738.18

Sample	Sb3d - energy level (eV)				Sb3p - energy level (eV)		Ti3p - energy level
	$Sb3d_{5/2}$		$Sb3d_{3/2}$		$Sb3p_{3/2}$	$Sb3p_{1/2}$	
Co_4Sb_{12}	527.66	529.83	537.13	539.02	811.95	765.95	-
$Yb_{0.4}Co_{3.94}Mo_{0.02}Ti_{0.04}Sb_{12}$	527.97	530.14	537.68	539.34	813.26	767.14	34.22
$Yb_{0.4}Co_{3.92}Mo_{0.04}Ti_{0.04}Sb_{12}$	527.62	529.54	537.56	539.61	813.72	767.46	34.50
$Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$	527.50	529.57	538.00	539.99	813.54	767.39	34.38

Table S2: Quantitative analysis of Sb3d, Sb3p and Ti3p energy levels

Sample	Co2p - energy level						O1s Energy level
	$Co2p_{3/2}$		$Co2p_{1/2}$		Satellite peak		
	Co^{3+}	Co^{2+}	Co^{3+}	Co^{2+}	Co^{3+}	Co^{2+}	
Co_4Sb_{12}	777.66	782.88	792.31	797.40	786.61	802.52	-
$Yb_{0.4}Co_{3.94}Mo_{0.02}Ti_{0.04}Sb_{12}$	778.62	783.73	794.74	800.92	788.79	806.33	-
$Yb_{0.4}Co_{3.92}Mo_{0.04}Ti_{0.04}Sb_{12}$	779.13	784.69	795.74	802.20	790.23	808.14	530.96

Table S3: Quantitative analysis of Co2p energy levels

$Yb_{0.4}Co_{3.88}Mo_{0.08}Ti_{0.04}Sb_{12}$	778.78	784.08	794.69	801.18	789.01	807.09	531.40

References:

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