Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information

Bi and Zn co-doped SnTe thermoelectrics: Interplay of resonance levels and heavy hole band dominance leading to enhanced performance and record high room temperature ZT

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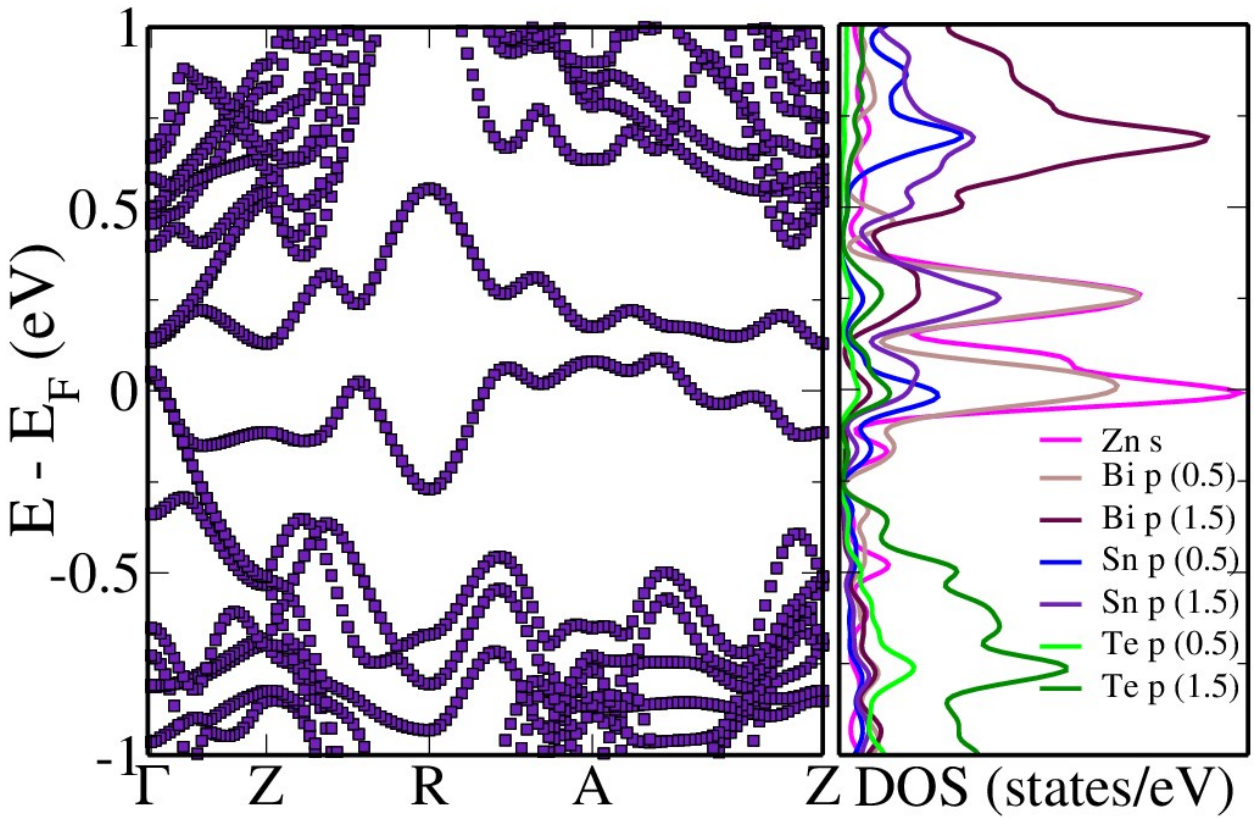

Figure S1. Electronic structure and pDOS of $Sn_{14}BiZnTe_{16}$ parallelly aligned to provide better clarity in understanding the contributions of various atomic orbitals to the electronic structure. The values within the bracket indicate the J values. The energies are shifted with respect to the Fermi level which is set at zero.

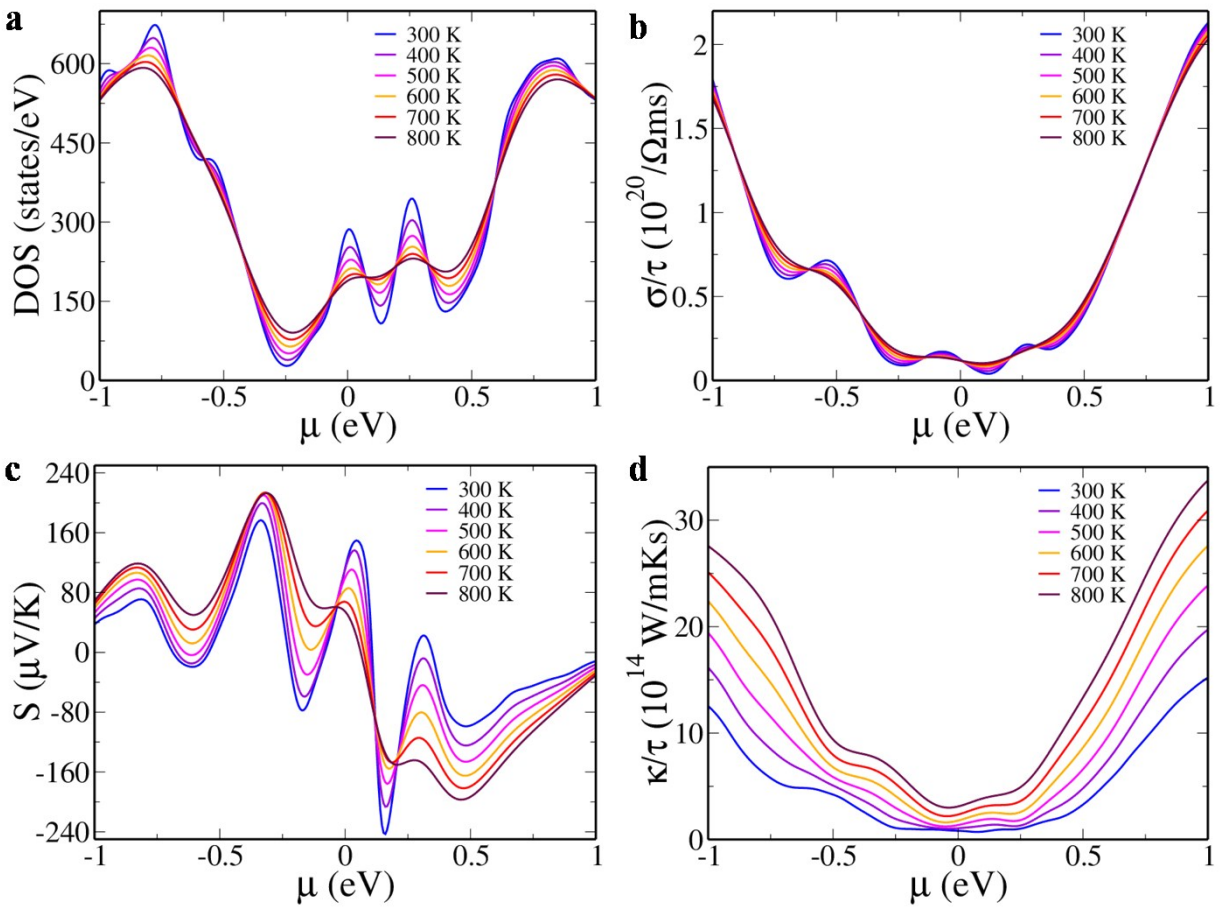

Figure S2. a) Density of states; b) electrical conductivity; c) Seebeck co-efficient and d) thermal conductivity of $Sn_{14}BiZnTe_{16}$ as a function of chemical potential (μ) at various temperatures. The Fermi level is set at zero. The negative 'μ' corresponds to p-type hole doping while the positive 'μ' corresponds to n-type electron doping. The Seebeck peaks found around the Fermi level shows a decreasing trend with increasing temperature representing a classic case of resonant dopant contribution.

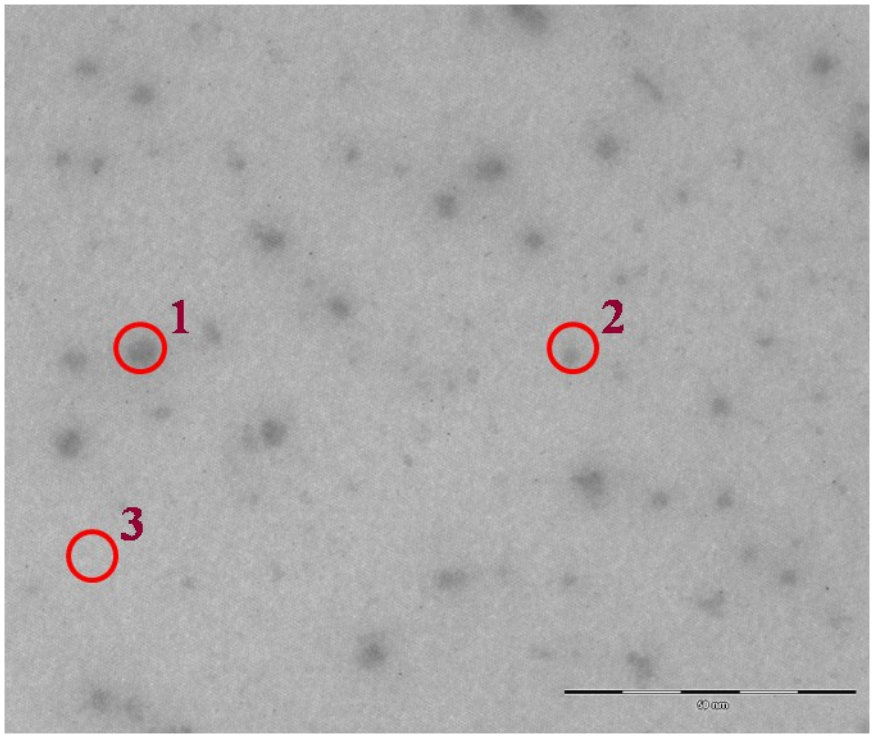

Figure S3. TEM image of $Sn_{0.92}Bi_{0.04}Zn_{0.04}Te$ revealing *Zn* nanoprecipitates. The scale bar represents 50 nm. The percentage elemental compositions of the area marked in red circles are given in Table S2.

Table S1. Elemental percentage composition of $Sn_{0.92}Bi_{0.04}Zn_{0.04}Te$ using EDS analysis at various area marked in TEM image (Figure S3).

Element	Percentage composition (%)		
	Spot 1	Spot 2	Spot 3
Sn	45.21	45.58	46.10
Te	49.86	50.01	49.96
Bi	1.82	1.91	1.98
Zn	3.11	2.5	1.96

Table S2. Carrier concentration (n) and mobility (μ) of SnTe and doped samples.

Sample	n (10^{20} cm^{-3})	μ ($cm^2V^{-1}S^{-1}$)
SnTe	3.5	144.5
$Sn_{0.96}Bi_{0.04}Te$	1.67	138.3
$Sn_{0.96}Zn_{0.04}Te$	1.98	148.2
$Sn_{0.92}Bi_{0.04}Zn_{0.04}Te$	0.947	141.7

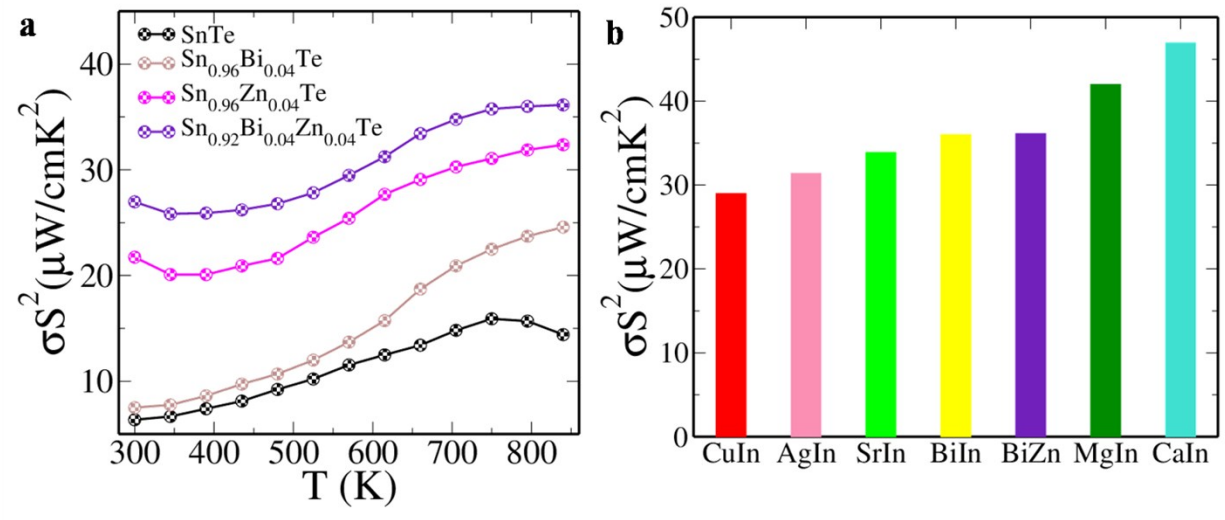

Figure S4. a) Power factor as a function of temperature for pristine SnTe and doped samples; b) Comparison of power factor of $Sn_{0.92}Bi_{0.04}Zn_{0.04}Te$ with state of the art SnTe based materials with high power factor.[1-6]

References

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