

Supporting Information

Entropy-stabilized perovskite oxide $\text{Ba}_{0.1}\text{Ca}_{0.1}\text{La}_{0.05}\text{Sr}_{0.75}\text{Ti}_{0.85}\text{Nb}_{0.15}\text{O}_3$ with improved thermoelectric performance for high-temperature waste heat recovery

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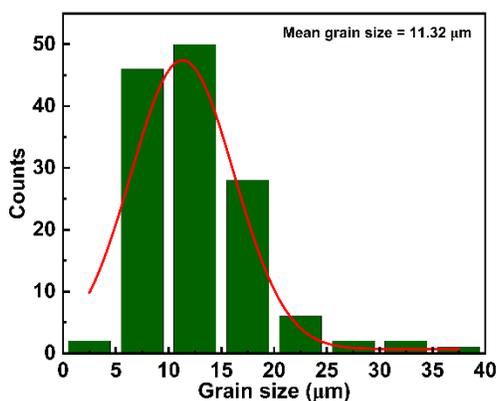


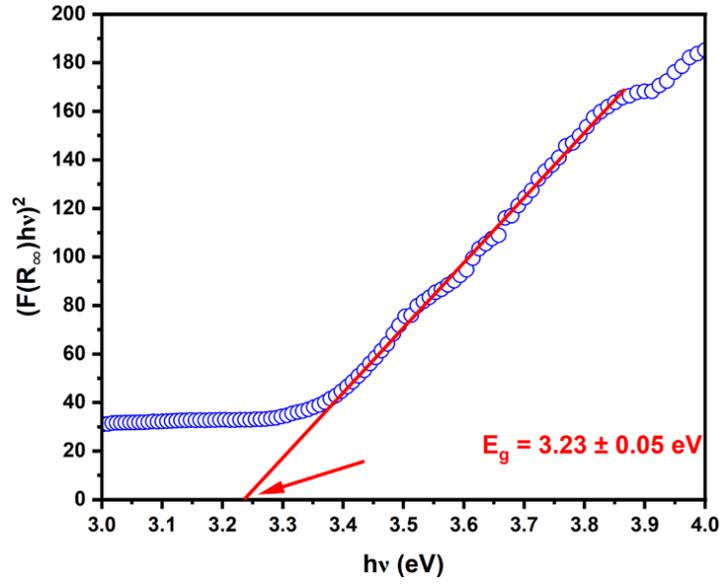
Fig. S1. Grain size distribution

Table S1. Refined structural parameters of BCLSTN ceramic after Rietveld refinement of the XRD data using $\text{Pm}\bar{3}\text{m}$ space group.

Elements	x	y	z	B_iso (Å ²)
Sr/Ca/Ba/La	0	0	0	0.59260/0.76260/0.65260/0.60260
Ti/Nb	0.5	0.5	0.5	0.16400/0.00062
O1	0.5	0	0.5	2.87452
O2	0.5	0.5	0	3.35888
a = b = c = 3.92792 Å, $\chi^2 = 1.76$				
Rp: 21.1 Rwp: 20.5 Rexp: 15.40				

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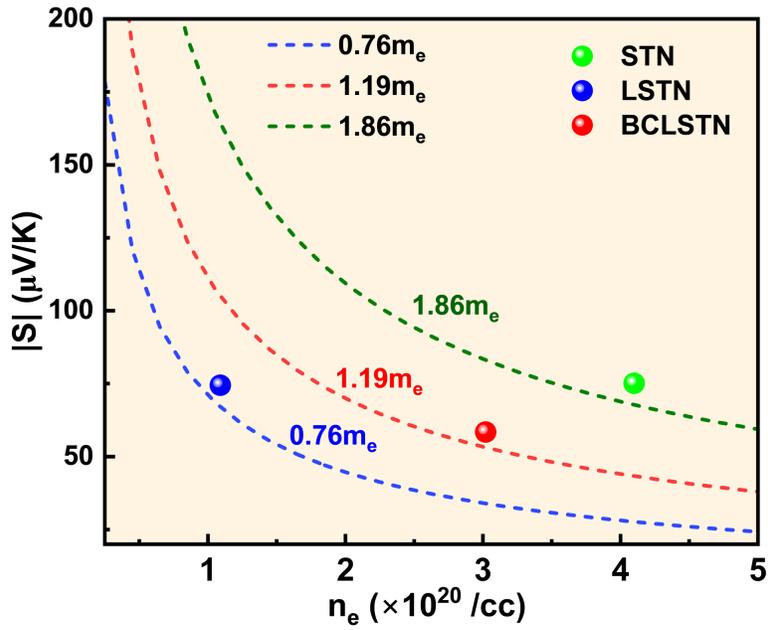
14 **S2. UV-vis analysis plot from diffusive reflectance spectroscopy (DRS):**



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Fig. S2. Bandgap calculations from the K-B plot of BCLSTN.



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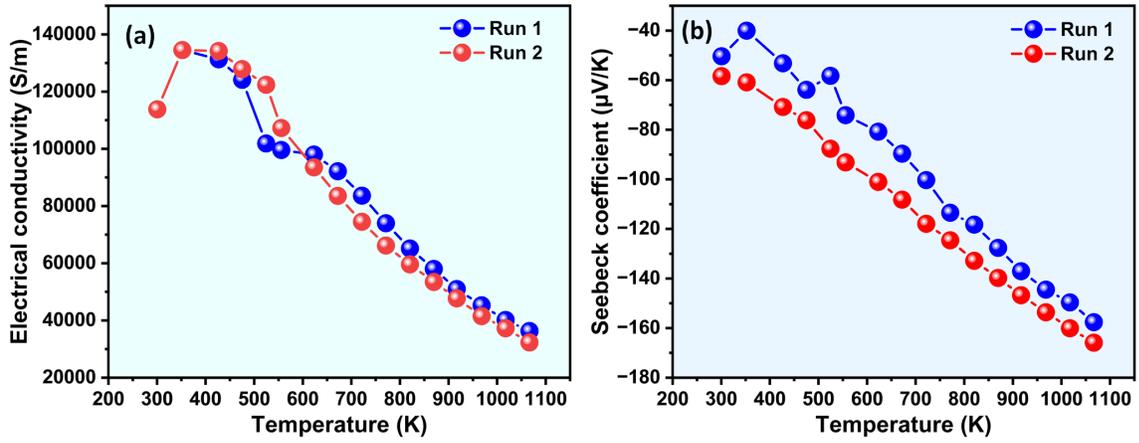
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Fig. S3. Pisarenko plot at 300 K.

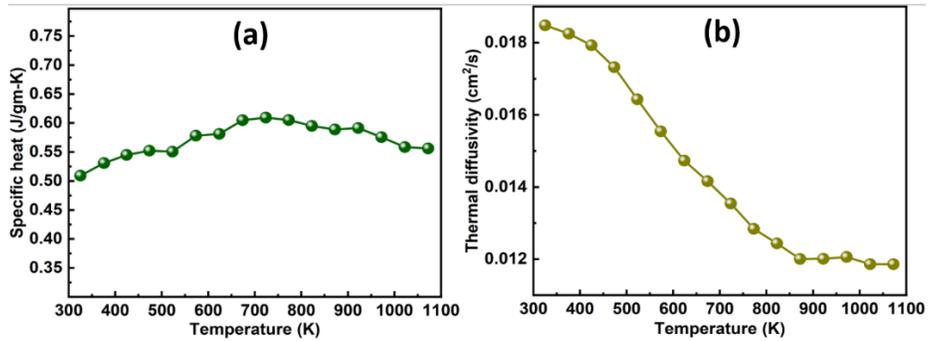
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24 Fig. S4. Reproducibility data of electrical conductivity and Seebeck coefficient of LCBSTN
25 composition.

26 **S3. Specific heat and thermal diffusivity graph of the sintered sample with a density of 5.09**
27 **g/cc:**



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29 Fig. S5. (a) Specific heat, (b) Thermal diffusivity of BCLSTN sample.

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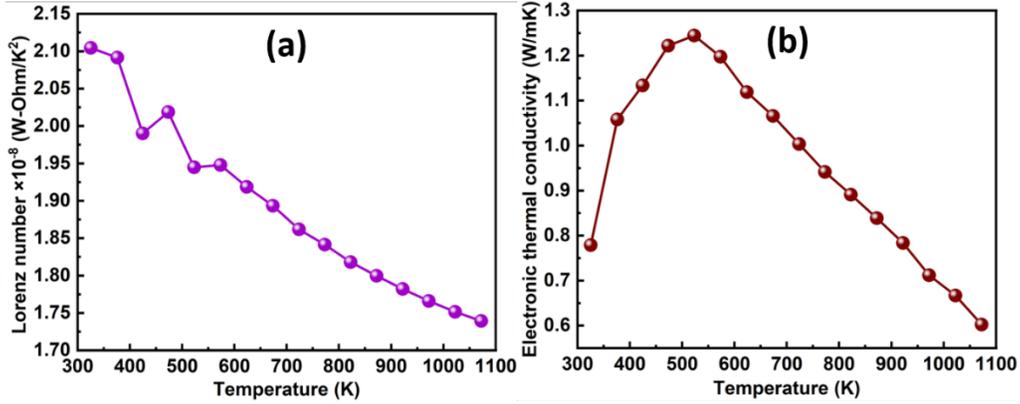
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35 **S4. Specific heat and thermal diffusivity graph:**



37 Fig. S6. (a) Lorenz number and (b) electronic thermal conductivity of BCLSTN ceramic.

38 **S5. Debye temperature determination**

39 Calculation of the Debye temperature (θ_D) of the BCLSTN system has been performed using the
40 following equation:

41
$$\theta_D = \frac{h}{k} \left[\frac{3n}{4\pi} \left(\frac{N_A \rho}{M} \right) \right]^{1/3} \vartheta_m \quad (S1)$$

42 where h stands for Planck's constant, k for Boltzmann's constant, M represents the molecular
43 weight, N_A is Avogadro's number, ρ denotes the density, n is the number of atoms per formula
44 unit, and ϑ_m is the mean sound velocity in the material. The mean sound velocity (ϑ_m), is derived
45 using the bulk modulus (B) and shear modulus (G) as follows:

46 Poisson's ratio:
$$\nu = \frac{(3B - 2G)}{(6B + 2G)} \quad (S2)$$

47
$$\vartheta_m = \left[\frac{1}{3} \left(\frac{2}{\vartheta_l^3} + \frac{1}{\vartheta_t^3} \right) \right]^{-1/3} \quad (S3)$$

48
$$\vartheta_l = \left(\frac{B + \frac{4}{3}G}{\rho} \right)^{1/2} \quad (S4)$$

49
$$\vartheta_t = (G/\rho)^{1/2} \quad (S5)$$

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51 Table S2. Table for B, G, ρ , M, ϑ_1 , ϑ_t , ϑ_l and θ_D for BCLSTN composition.

B (Pa)	G (Pa)	ρ (kg/m³)	M (gm)	ϑ_1 (m/s)	ϑ_t (m/s)	ϑ_m (m/s)	θ_D(K)
1.24×10^{11}	8.11×10^{10}	5093.3	193.02	6755.76	3990.84	4421.40	526.52

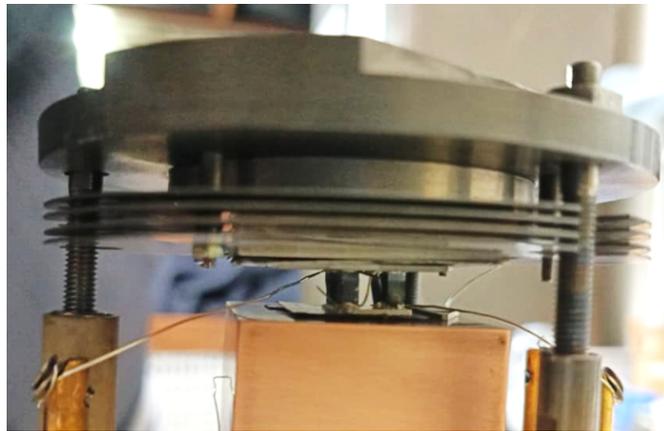
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53 Table S3. Fitting parameters of Debye-Callaway's model for Umklapp scattering pre-factor (B)
54 and electron-phonon scattering pre-factor (C).

Point defect scattering A [s³]	Phonon-phonon (Umklapp) scattering factor B [sK⁻¹]	Electron-phonon scattering factor C [s]
5.226×10^{-41}	1.257×10^{-19}	4.685×10^{-17}

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Fig. S7. Setup and fabricated TEG module.

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