Electronic Supplementary Material (ESI) for Materials Advances.

A synergistic approach to achieve high thermoelectric performance of La-doped SnTe using resonance state and partial band convergence

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Supplementary Information

S1: EDS spectra and corresponding quantitative analysis results for all La-doprd SnTe samples

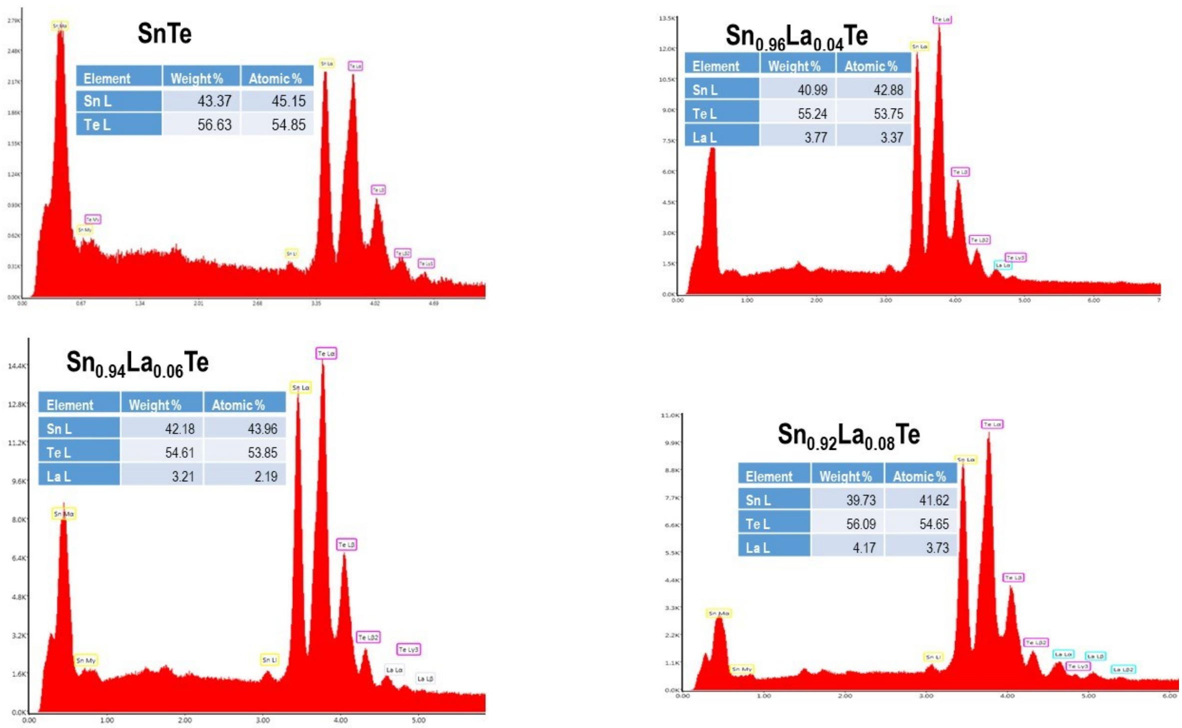


Figure S1: EDS spectra of $Sn1_{-x}La_xTe$ (x=0, 0.04, 0.06, 0.08)for quantitative analysis.

S2: Point scan of $Sn_{0.92}La_{0.08}Te$ to show the precipitation of La when the concentration (x) is 8 at%.

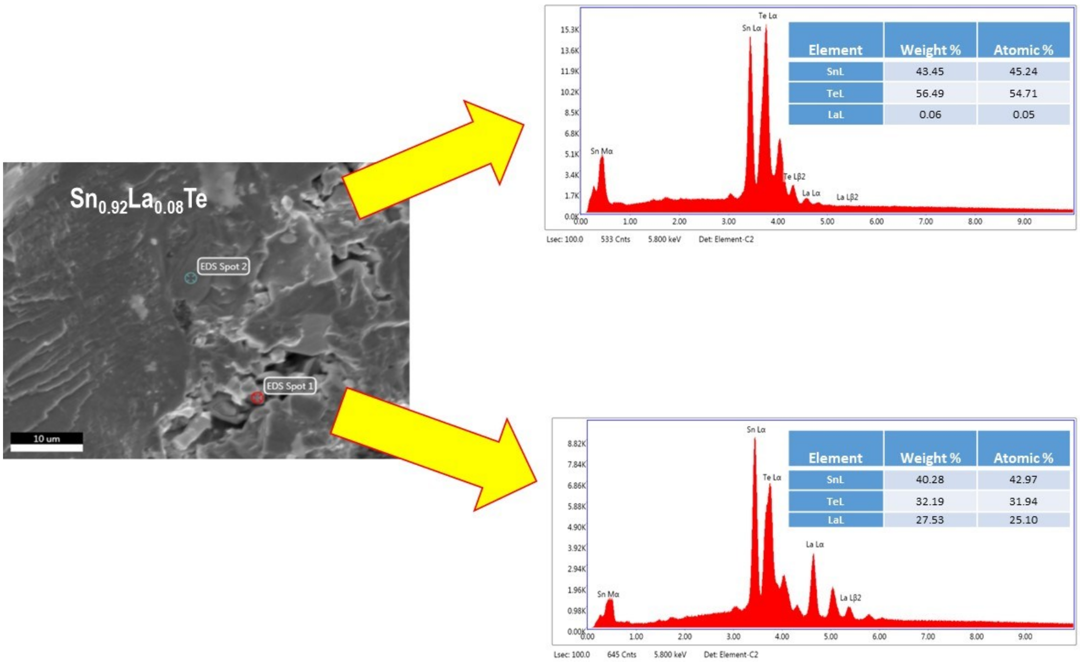


Figure S2: EDS spectra of point scan of $Sn_{0.92}La_{0.08}Te$ to show La-precipitation

S3: Band gap variation for SnTe +x% La. The behaviors for both band gap variation and change of lattice parameter indicates a ~6%La solubility in SnTe

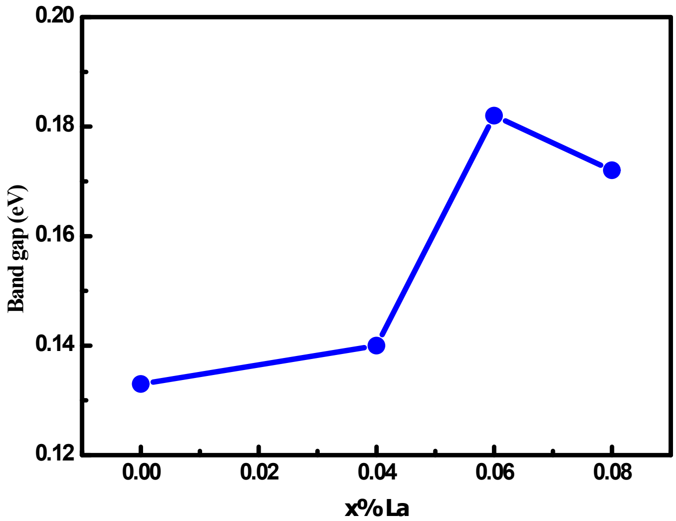
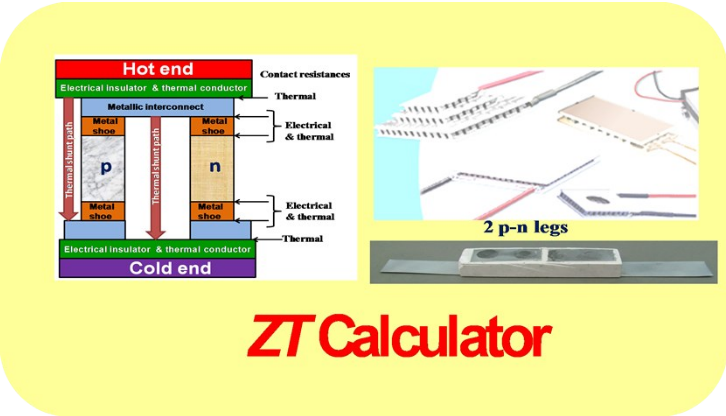


Figure S3: Band gap variation for SnTe +x% La.

S4: Calculation of maximum efficiency



Although there is no analytic expression for Z, it can be calculated to any desired accuracy numerically with a simple procedure which can be done on a spreadsheet. To calculate the maximum efficiency Z and ZT follow these steps:

(1) Paste the temperature dependent *S(T)*, *ρ(T)*, and *κ(T)*into the *T*, *S*, *ρ*, and *κ* columns – the 4 columns in the table are shaded blue. The cold side temperature for the calculation is the first temperature, 300 K. We shall use 800 K for hot side temperature for the example in Table 1. As per the literature, 25 K temperature intervals were maintained between data points, but that can vary. Smaller temperature steps give more accurate calculations.

(2) The first entry of the relative current value u is to be optimized. The values for u at higher temperature will adjust accordingly. This is similar to setting the electrical current (or load resistance) through the device. The power and therefore efficiency will be low at low values of u because little electrical current will be flowing through the device and low at high values of u because the output voltage will drop at high currents (and even becomes negative). For good efficiency the u values should be close to the compatibility factor s in the column next to u. Calculation for u = 0 is to be avoided as some calculations become undefined, but u arbitrarily small is fine (e.g. u = 0.001).

The efficiency of this thermoelectric leg is given in the efficiency column. The calculation assumes the first row (300 K in the Table) is the cold side. For 800 K hot side we should optimize the efficiency of the last row. MS Excel has a solver add-in that makes this easy,but other methods or adjusting by hand also works.

(3) The device ZT is calculated from the maximum efficiency value found by optimizing cold side u value and the eqn. is given by $ZT = \left(\frac{T_h - T_c(1-\eta)}{T_h(1-\eta) - T_c}\right)^2 - 1$.

S.4.1 Spreadsheet for the calculation of ZT for SnTe

T (C)	Material	*T* (K)	Seebeck (μV/K)	resistivity (10-3 Ω cm)	thermal cond (W/m K)	*zT*	max red eff	*s* (1/V)	*u* (1/V)	red eff	Φ (V)	efficiency	*ZT*
27	SnTe	300	34	0.13	7.35	0.04	0.9%	1.76	1.6072	0.9%	0.632		
52	SnTe	325	35	0.14	7.16	0.04	1.0%	1.73	1.6093	1.0%	0.633	0.1%	0.04
77	SnTe	350	36	0.15	6.97	0.04	1.1%	1.70	1.6115	1.1%	0.633	0.1%	0.04
102	SnTe	375	38	0.16	6.78	0.05	1.2%	1.67	1.6139	1.2%	0.634	0.2%	0.04
127	SnTe	400	39	0.18	6.59	0.05	1.3%	1.64	1.6166	1.3%	0.634	0.3%	0.04
152	SnTe	425	41	0.19	6.41	0.06	1.4%	1.62	1.6196	1.4%	0.635	0.4%	0.05
177	SnTe	450	42	0.21	6.23	0.06	1.5%	1.60	1.6229	1.5%	0.635	0.5%	0.05
202	SnTe	475	44	0.23	6.04	0.07	1.6%	1.59	1.6266	1.6%	0.636	0.6%	0.05
227	SnTe	500	46	0.25	5.86	0.07	1.8%	1.58	1.6308	1.8%	0.636	0.6%	0.05
252	SnTe	525	49	0.26	5.68	0.08	2.0%	1.58	1.6354	2.0%	0.637	0.7%	0.06
277	SnTe	550	51	0.28	5.51	0.09	2.2%	1.59	1.6406	2.2%	0.638	0.8%	0.06
302	SnTe	575	54	0.31	5.33	0.10	2.4%	1.61	1.6465	2.4%	0.638	0.9%	0.06
327	SnTe	600	57	0.33	5.15	0.11	2.7%	1.63	1.6530	2.7%	0.639	1.0%	0.06
352	SnTe	625	60	0.35	4.98	0.13	3.0%	1.66	1.6604	3.0%	0.640	1.2%	0.07
377	SnTe	650	63	0.37	4.80	0.14	3.4%	1.70	1.6686	3.4%	0.640	1.3%	0.07
402	SnTe	675	67	0.40	4.63	0.16	3.8%	1.75	1.6779	3.8%	0.641	1.4%	0.08
427	SnTe	700	71	0.43	4.45	0.19	4.3%	1.80	1.6882	4.3%	0.642	1.6%	0.08
452	SnTe	725	76	0.45	4.28	0.22	4.9%	1.86	1.6998	4.8%	0.643	1.7%	0.09
477	SnTe	750	81	0.48	4.10	0.25	5.5%	1.93	1.7128	5.5%	0.644	1.9%	0.09
502	SnTe	775	86	0.51	3.93	0.29	6.3%	2.00	1.7274	6.2%	0.646	2.1%	0.10

S.4.2 Spreadsheet for the calculation of ZT for $Sn_{0.96}La_{0.04}Te$

T (C)	Material	*T* (K)	Seebeck (μV/K)	resistivity (10-3 Ω cm)	thermal cond (W/m K)	*zT*	max red eff	*s* (1/V)	*u* (1/V)	red eff	Φ (V)	efficiency	*ZT*
27	Sn0.96La0.04Te	300	41	0.17	5.53	0.05	1.3%	2.15	2.1237	1.3%	0.483		
52	Sn0.96La0.04Te	325	42	0.18	5.39	0.06	1.5%	2.16	2.1281	1.5%	0.484	0.1%	0.06
77	Sn0.96La0.04Te	350	44	0.19	5.26	0.07	1.6%	2.15	2.1328	1.6%	0.484	0.2%	0.06
102	Sn0.96La0.04Te	375	46	0.20	5.13	0.07	1.8%	2.16	2.1380	1.8%	0.485	0.3%	0.06
127	Sn0.96La0.04Te	400	47	0.21	5.01	0.08	2.0%	2.16	2.1438	2.0%	0.485	0.5%	0.07
152	Sn0.96La0.04Te	425	49	0.23	4.88	0.09	2.2%	2.16	2.1501	2.2%	0.486	0.6%	0.07
177	Sn0.96La0.04Te	450	51	0.24	4.75	0.10	2.4%	2.16	2.1571	2.4%	0.487	0.7%	0.08
202	Sn0.96La0.04Te	475	53	0.26	4.62	0.11	2.7%	2.17	2.1648	2.7%	0.487	0.9%	0.08
227	Sn0.96La0.04Te	500	56	0.28	4.50	0.12	2.9%	2.17	2.1732	2.9%	0.488	1.0%	0.08
252	Sn0.96La0.04Te	525	58	0.30	4.38	0.14	3.2%	2.17	2.1824	3.2%	0.489	1.2%	0.09
277	Sn0.96La0.04Te	550	61	0.32	4.26	0.15	3.5%	2.17	2.1925	3.5%	0.490	1.3%	0.09
302	Sn0.96La0.04Te	575	63	0.34	4.15	0.16	3.8%	2.16	2.2035	3.8%	0.490	1.5%	0.10
327	Sn0.96La0.04Te	600	66	0.37	4.02	0.18	4.1%	2.16	2.2155	4.1%	0.491	1.6%	0.10
352	Sn0.96La0.04Te	625	69	0.39	3.90	0.20	4.5%	2.16	2.2286	4.5%	0.492	1.8%	0.11
377	Sn0.96La0.04Te	650	72	0.42	3.79	0.21	4.8%	2.15	2.2428	4.8%	0.493	2.0%	0.11
402	Sn0.96La0.04Te	675	76	0.45	3.68	0.23	5.2%	2.15	2.2582	5.2%	0.494	2.2%	0.12
427	Sn0.96La0.04Te	700	79	0.49	3.57	0.25	5.6%	2.14	2.2750	5.6%	0.495	2.4%	0.13
452	Sn0.96La0.04Te	725	82	0.52	3.46	0.27	6.0%	2.13	2.2932	6.0%	0.496	2.6%	0.13
477	Sn0.96La0.04Te	750	86	0.56	3.36	0.29	6.4%	2.13	2.3130	6.4%	0.497	2.8%	0.14
502	Sn0.96La0.04Te	775	90	0.61	3.25	0.31	6.8%	2.11	2.3345	6.8%	0.498	3.0%	0.15

S.4.3 Spreadsheet for the calculation of ZT for $Sn_{0.96}La_{0.04}Te$

T	Material	*T*	Seebeck	resistivity	thermal cond	*zT*	max red eff	*s*	*u*	red eff	Φ	efficiency	*ZT*
(C)		(K)	(μV/K)	(10-3 Ω cm)	(W/m K)			(1/V)	(1/V)		(V)		
27	Sn0.94La0.06Te	300	43	0.16	6.16	0.06	1.4%	2.13	2.0457	1.3%	0.502		
52	Sn0.94La0.06Te	325	44	0.17	5.95	0.06	1.5%	2.12	2.0492	1.5%	0.502	0.1%	0.06
77	Sn0.94La0.06Te	350	45	0.18	5.75	0.07	1.6%	2.09	2.0531	1.6%	0.503	0.2%	0.06
102	Sn0.94La0.06Te	375	46	0.20	5.55	0.07	1.8%	2.07	2.0575	1.8%	0.503	0.3%	0.06
127	Sn0.94La0.06Te	400	48	0.21	5.36	0.08	1.9%	2.06	2.0625	1.9%	0.504	0.5%	0.07
152	Sn0.94La0.06Te	425	50	0.23	5.17	0.09	2.1%	2.05	2.0682	2.1%	0.505	0.6%	0.07
177	Sn0.94La0.06Te	450	52	0.25	4.98	0.10	2.3%	2.05	2.0747	2.3%	0.505	0.7%	0.07
202	Sn0.94La0.06Te	475	54	0.27	4.79	0.11	2.6%	2.06	2.0820	2.6%	0.506	0.8%	0.08
227	Sn0.94La0.06Te	500	56	0.29	4.62	0.12	2.8%	2.06	2.0902	2.8%	0.507	1.0%	0.08
252	Sn0.94La0.06Te	525	59	0.31	4.45	0.13	3.1%	2.07	2.0993	3.1%	0.507	1.1%	0.09
277	Sn0.94La0.06Te	550	62	0.34	4.28	0.15	3.4%	2.08	2.1096	3.4%	0.508	1.3%	0.09
302	Sn0.94La0.06Te	575	65	0.36	4.12	0.16	3.8%	2.10	2.1210	3.8%	0.509	1.4%	0.10
327	Sn0.94La0.06Te	600	69	0.39	3.96	0.18	4.2%	2.13	2.1336	4.2%	0.510	1.6%	0.10
352	Sn0.94La0.06Te	625	72	0.42	3.80	0.20	4.6%	2.16	2.1476	4.6%	0.511	1.8%	0.11
377	Sn0.94La0.06Te	650	76	0.45	3.66	0.23	5.2%	2.20	2.1630	5.2%	0.512	2.0%	0.11
402	Sn0.94La0.06Te	675	80	0.48	3.52	0.26	5.7%	2.25	2.1799	5.7%	0.513	2.2%	0.12
427	Sn0.94La0.06Te	700	84	0.51	3.39	0.29	6.4%	2.31	2.1985	6.4%	0.514	2.4%	0.13
452	Sn0.94La0.06Te	725	89	0.53	3.26	0.33	7.1%	2.38	2.2188	7.1%	0.515	2.6%	0.14
477	Sn0.94La0.06Te	750	94	0.56	3.13	0.38	8.0%	2.47	2.2410	7.9%	0.516	2.9%	0.15
502	Sn0.94La0.06Te	775	99	0.59	3.01	0.43	8.9%	2.55	2.2652	8.8%	0.518	3.1%	0.15
527	Sn0.94La0.06Te	800	105	0.62	2.90	0.49	9.9%	2.64	2.2946	9.8%	0.519	**3.4%**	0.17
552	Sn0.94La0.06Te	825	110	0.65	2.79	0.55	10.98%	2.71	2.3249	10.79%	0.52108	3.72%	0.18

S.4.4 Spreadsheet for the calculation of ZT for $Sn_{0.92}La_{0.08}Te$

T (C)	Material	*T* (K)	Seebeck (µV/K)	resistivity (10-3 Ω cm)	thermal cond (W/m K)	*zT*	max red eff	*s* (1/V)	*u* (1/V)	red eff	Φ (V)	efficiency	*ZT*
27	Sn0.92La0.08Te	300	41	0.16	5.67	0.06	1.4%	2.27	2.2220	1.4%	0.462		
52	Sn0.92La0.08Te	325	43	0.17	5.50	0.06	1.6%	2.27	2.2266	1.6%	0.463	0.1%	0.06
77	Sn0.92La0.08Te	350	44	0.18	5.35	0.07	1.7%	2.25	2.2316	1.7%	0.464	0.2%	0.06
102	Sn0.92La0.08Te	375	46	0.19	5.19	0.08	1.9%	2.25	2.2371	1.9%	0.464	0.4%	0.07
127	Sn0.92La0.08Te	400	47	0.21	5.04	0.09	2.1%	2.24	2.2434	2.1%	0.465	0.5%	0.07
152	Sn0.92La0.08Te	425	49	0.22	4.90	0.10	2.3%	2.24	2.2503	2.3%	0.465	0.6%	0.08
177	Sn0.92La0.08Te	450	51	0.24	4.74	0.11	2.5%	2.25	2.2581	2.5%	0.466	0.8%	0.08
202	Sn0.92La0.08Te	475	54	0.25	4.59	0.12	2.8%	2.26	2.2668	2.8%	0.467	0.9%	0.08
227	Sn0.92La0.08Te	500	56	0.27	4.45	0.13	3.1%	2.26	2.2764	3.1%	0.467	1.1%	0.09
252	Sn0.92La0.08Te	525	59	0.29	4.31	0.15	3.4%	2.27	2.2870	3.4%	0.468	1.2%	0.09
277	Sn0.92La0.08Te	550	62	0.31	4.17	0.16	3.7%	2.28	2.2988	3.7%	0.469	1.4%	0.10
302	Sn0.92La0.08Te	575	65	0.34	4.04	0.18	4.1%	2.29	2.3117	4.1%	0.470	1.5%	0.10
327	Sn0.92La0.08Te	600	68	0.36	3.90	0.20	4.5%	2.31	2.3260	4.5%	0.471	1.7%	0.11
352	Sn0.92La0.08Te	625	71	0.39	3.76	0.22	4.9%	2.33	2.3417	4.9%	0.471	1.9%	0.12
377	Sn0.92La0.08Te	650	75	0.41	3.63	0.24	5.4%	2.35	2.3588	5.4%	0.472	2.1%	0.12
402	Sn0.92La0.08Te	675	78	0.44	3.51	0.27	5.9%	2.38	2.3776	5.9%	0.473	2.3%	0.13
427	Sn0.92La0.08Te	700	82	0.47	3.39	0.30	6.5%	2.41	2.3981	6.5%	0.475	2.5%	0.14
452	Sn0.92La0.08Te	725	86	0.50	3.27	0.33	7.1%	2.45	2.4205	7.1%	0.476	2.8%	0.15
477	Sn0.92La0.08Te	750	90	0.53	3.15	0.37	7.8%	2.51	2.4448	7.8%	0.477	3.0%	0.15
502	Sn0.92La0.08Te	775	95	0.55	3.03	0.41	8.6%	2.58	2.4713	8.6%	0.478	3.3%	0.16
527	Sn0.92La0.08Te	800	99	0.58	2.92	0.47	9.6%	2.66	2.5000	9.5%	0.480	**3.6%**	0.17
552	Sn0.92La0.08Te	825	104	0.60	2.81	0.53	10.63%	2.77	2.5312	10.57%	0.48103	3.86%	0.18