A Critical Analysis of Single Band Modeling of Thermoelectric Materials

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KEYWORDS: Single Parabolic Band model (SPB), Single Kane Band model (SKB), thermoelectric materials, Seebeck coefficient, Lorenz number, band mass.

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Figure S1. Representation of SPB/SKB equations using MATLAB.

Composition	S(μV/K)	σ(S/cm)	R _⊬ (m⁻³)	Reference
				no.
$Mg_{2.15}Si_{0.28}Sn_{0.71}Sb_{0.006}$	158	1740	4.1E-08	11
$Mg_2Si_{0.7}Sn_{0.3}$:Bi _{0.01}	461	7	1.3E-06	12
Mg ₂ (Si _{0.3} Sn0.7) _{1-y} Bi _y				13
y=0	447	31	2.1E-06	
0.005	211	624	9.5E-08	
0.01	150	1533	3.8E-08	
0.015	130	2004	3.1E-08	
0.02	120	2328	2.8E-08	
0.025	115	2484	2.3E-08	
0.03	114	2672	2.3E-08	
0.04	103	2692	2.0E-08	
$Mg_2(Si_{0.3}Sn_{0.7})_{0.98}Sb_{0.02}$	115	2528	3.2E-08	14
$Mg_{2.2}Si_{0.3}Sn_{0.57}Sb_{0.013}$	124	2110	1.7E-08	15
Mg ₂ (Sn _{0.3} Sn _{0.7}) _{0.98} Sb _{0.02}				16
MS-PAS	114	2947	2.5E-08	
SSR-PAS	120	2453	2.5E-08	
MS-PAS-AN	129	2294	2.8E-08	
$Mg_{2.10}Si_{0.27}Sn_{0.71}Sb_{0.017}$	128	2345	2.9E-08	17
$Mg_{2.158}(Si_{0.281}Sn_{0.719})_{0.978}Sb_{0.022}$	125	2125	2.9E-08	18
$Mg_{2.148}(Si_{0.289}Sn_{0.711})_{0.979}Sb_{0.021}$	126	2034	3.1E-08	
$Mg_{2.139}(Si_{0.306}Sn_{0.694})_{0.982}Sb_{0.018}$	128	2032	3.2E-08	
Mg _{2.082} (Si _{0.346} Sn _{0.654}) _{0.981} Sb _{0.019}	140	1868	3.7E-08	
Mg ₂ Si _{0.3} Sn _{0.7}	381	83	7.9E-07	19
Mg ₂ (Si _{0.3} Sn _{0.7}) _{0.98} Bi _{0.02}	113	2739	2.3E-08	
Mg _{1.98} Cr _{0.02} (Si _{0.3} Sn _{0.7}) _{0.98} Bi _{0.02}	129	2149	2.6E-08	
$Mg_{2}(Si_{0,3}Sn_{0,7})_{1-y}Sb_{y}$				20
v=.005	176	1032	5.3E-08	
y=.01	150	1506	3.6E-08	
y=.015	125	2370	2.0E-08	
y=.02	113	2586	1.7E-08	

Table S1: Experimental data of the various materials used for the analysis.

y=.02511225361.9E-08no.3761.9E-08235914.7E-08235914.7E-08238959.5E-08112121.2E-0724215015153.3E-08314216393.0E-08413415152.7E-08512221742.3E-08611725642.2E-08711922731.8E-08washingsba2525x=06471.0E-05x=06471.0E-05x=0.07515610896.7E-083.7E-071192253.7E-071201411301 $Mg_{216}(Sl_0,Sn_{0.6})_{1.9}Sb_{\chi}$ 26 $\gamma=.01$ 1161860 $\gamma=.02$ 1161860 $\gamma=.02$ 1161860 $\gamma=.02$ 1161845 $\gamma=.02$ 12221498 $\gamma=.02$ 1161845 $\gamma=.02$ 1221854 0.03 1222043 0.02 1222043 0.02 1222043 0.02 1221024 0.03 1232583 0.024 1521021 $3.3E-07$ 0.036 0.024 1521021 0.036 1232583 1.1120 26	Composition	S(μV/K)	σ(S/cm)	R _⊬ (m⁻³)	Reference
y=.025 112 2536 1.9E-08 3 76 1.9E-08 23 5 91 4.7E-08 23 5 91 4.7E-08 23 5 91 4.7E-08 23 5 91 4.7E-08 24 2 150 1515 3.3E-08 3 3 142 1639 3.0E-08 4 4 134 1515 2.7E-08 5 5 122 2174 2.3E-08 6 6 117 2564 2.2E-08 7 7 119 2273 1.8E-08 25 x=0075 156 1089 6.7E-08 25 x=0075 156 1089 6.7E-08 26 y=.005 190 600 1.1E-07 24 y=.015 132 1498 4.1E-08 27 y=.025 116 1845 2.9E-08 26 y=.025 120 600 1.1E-07 27 y=0					no.
3761.9f-08233761.9f-08235914.7f-088959.5f-089512121.2f-0724215015153.3f-083314216393.0f-084413415152.7f-085512221742.3f-085611725642.2f-087711922731.8f-081 $Mg_5 S_{0,4+x} Sn_0, Sb_x$ 252525x=06471.0f-05x=.0075x=007515610896.7f-08x=.0151812253.7f-07Mg_{2,16} (S_{0,4}Sn_{0,6})_{1,x} Sb_y26y=0412253.2f-06y=.0051906001.1f-07y=.0111313014.0f-08y=.02511618452.9f-08Mg_{2,16} (S_{0,4}Sn_{0,6})_{1,7} Bi_{Y}7478.3f-080.0115612794.8f-080.0212218542.9f-080.0312220432.9f-080.04456461.5f-060.02415210213.3f-070.03612325351.1f-08	y=.025	112	2536	1.9E-08	
3 76 1.9E-08 23 5 91 4.7E-08 23 8 95 9.5E-08 9.5E-08 1 212 1.2E-07 24 2 150 1515 3.3E-08 3 3 142 1639 3.0E-08 4 4 134 1515 2.7E-08 5 5 122 2174 2.3E-08 6 6 117 2564 2.2E-08 7 7 119 2273 1.8E-08 25 x=0075 155 1089 6.7E-08 25 x=.075 155 1089 6.7E-08 26 y=0 412 25 3.2E-06 9 9 y=.01 143 1301 4.0E-08 9 9 y=.025 116 1860 2.6E-08 9 9 9 y=.025 116 1845 2.9E-08 1 9 9 9 27 y=.025 116 1845 2.9E-08					
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8 95 9.5E-08 1 212 1.2E-07 24 2 150 1515 3.3E-08 3 142 1639 3.0E-08 4 134 1515 2.7E-08 5 122 2174 2.3E-08 6 117 2564 2.2E-08 7 119 2273 1.8E-08 Mg_5l_{0.4-x}Sn_{0.6}Sb_x - - 25 x=0 647 1.0E-05 x=.015 x=.075 156 1089 6.7E-08 x=.015 x=.015 181 225 3.7E-07 - Mg_{2.16}(Si_0_sSn_{0.6})_{1.9}Sb_{y} - - 26 y=0 412 25 3.2E-06 - y=.005 190 600 1.1E-07 - y=.015 132 1498 4.1E-08 - y=.02 116 1860 2.6E-08 - y=.02 116 1845 2.9E-08 - 0.01 156 1279 4.8E-08 <	5	91		4.7E-08	
12121.2E-072421501515 $3.3E-08$ 331421639 $3.0E-08$ 441341515 $2.7E-08$ 551222174 $2.3E-08$ 661172564 $2.2E-08$ 771192273 $1.8E-08$ 25x=006471.0E-05xx=.00751561089 $6.7E-08$ x=.015181225 $3.7E-07$ Mg2.16(Sl0,4Sn_0.6)1. γ Sby2626y=.0041225 $3.2E-06$ y=.011431301 $4.0E-08$ y=.021161860 $2.6E-08$ y=.021161860 $2.6E-08$ y=.021161845 $2.9E-08$ 0.011561279 $4.8E-08$ 0.011561279 $4.8E-08$ 0.011561279 $4.8E-08$ 0.021221854 $2.9E-08$ 0.031222043 $2.9E-08$ 0.031222043 $2.9E-08$ 0.0489425351.1E-08	8	95		9.5E-08	
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314216393.0E-08413415152.7E-08512221742.3E-08611725642.2E-08711922731.8E-08Mg.sl0,4.,Sn0,6Sbx25x=06471.0E-05x=.007515610896.7E-08x=.0151812253.7E-07Mg.16(sl_0,8Sn_{0,6})_1,9Sby26y=0412253.2E-06y=.0051906001.1E-07y=.01513214313014.0E-08y=.021161860y=.0211618452.9E-08y=.0211618452.9E-08y=.0211618452.9E-080.0115612794.8E-080.0212218542.9E-080.0312220432.9E-080.0415612794.8E-080.0312220432.9E-080.0415612794.8E-080.0312220432.9E-080.0415612794.8E-080.0312220432.9E-080.0415210213.8E-070.02415210213.2E-060.03612322532.7E-080.0489425351.1E-08	2	150	1515	3.3E-08	
413415152.7E-08512221742.3E-08611725642.2E-08711922731.8E-08711922731.8E-08Mg2sbi_0.4\$Sn_0.sb_k86471.0E-05x=06471.0E-05x=0.0751561089 $x=.015$ 181225 $x=0.075$ 1561089 $x=.015$ 181225 $x=0.05$ 190600 $y=0$ 41225 $y=0$ 14225 $y=0.05$ 190600 $y=.015$ 1321498 $y=.02$ 1161860 $y=.02$ 1161845 $y=.02$ 1222043 $y=.02$ 1261279 $y=.02$ 1281279 $y=.02$ 12829E-08 0.01 1561279 $4.8E-08$ 0.01 0.02 1222043 $2.9E-08$ 122 0.03 1222043 $2.9E-08$ 122 0.02 28 0 45646 $1.5E-06$ 1021 <td>3</td> <td>142</td> <td>1639</td> <td>3.0E-08</td> <td></td>	3	142	1639	3.0E-08	
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x=.00751561089 $6.7E-08$ x=.015181225 $3.7E-07$ Mg_{2.16}(Si_{0.4}Sn_{0.6})_{1.7}Sb_{y}26y=041225 $3.2E-06$ y=.005190600 $1.1E-07$ y=.011431301 $4.0E-08$ y=.021161860 $2.6E-08$ y=.021161845 $2.9E-08$ y=.0251161845 $2.9E-08$ Mg_{2.16}(Si_{0.4}Sn_{0.6})_{1-y}Bi_{y}27y=0413 $3.2E-06$ 0.005177747 $8.3E-08$ 0.011561279 $4.8E-08$ 0.0212218542.9E-080.0312220432.9E-080.04456461.5E-060.0121854131.8E-070.0241521021 $3.3E-07$ 0.03612322832.7E-080.0489425351.1E-08	x=0	647		1.0E-05	
x=.015 181 225 $3.7E-07$ Mg _{2.16} (Si _{0.4} Sn _{0.6}) _{1.y} Sb _y 26 y=0 412 25 $3.2E-06$ y=.005 190 600 $1.1E-07$ y=.01 143 1301 $4.0E-08$ y=.015 132 1498 $4.1E-08$ y=.02 116 1860 $2.6E-08$ y=.025 116 1845 $2.9E-08$ Mg _{2.16} (Si _{0.4} Sn _{0.6}) _{1-y} Bi _y 27 y=0 413 $3.2E-06$ 0.005 177 747 $8.3E-08$ 0.01 156 1279 $4.8E-08$ 0.02 122 1854 2.9E-08 Mg _{2.08} Si0 _{.4+x} Sn _{0.6} Sb _x (x) 28 2043 2.9E-08 0.02 122 1854 2.9E-08 20 0.03 122 2043 2.9E-08 20 0.04 156 1279 4.8E-08 20 20 0.02 122 1854 2.9E-08 28 28 0 122 2043 2.9E-08 28 <td>x=.0075</td> <td>156</td> <td>1089</td> <td>6.7E-08</td> <td></td>	x=.0075	156	1089	6.7E-08	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	x=.015	181	225	3.7E-07	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$					
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Mg _{2.16} (Si _{0.4} Sn _{0.6}) _{1-y} Sb _y				26
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	y=0	412	25	3.2E-06	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	y=.005	190	600	1.1E-07	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	y=.01	143	1301	4.0E-08	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	y=.015	132	1498	4.1E-08	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	y=.02	116	1860	2.6E-08	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	y=.025	116	1845	2.9E-08	
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0.005 177 747 8.3E-08 0.01 156 1279 4.8E-08 0.015 136 1771 3.4E-08 0.02 122 1854 2.9E-08 0.03 122 2043 2.9E-08 Mg _{2.08} SiO _{.4-x} Sn _{0.6} Sb _x (x) 28 28 0 456 46 1.5E-06 0.012 185 413 1.8E-07 0.024 152 1021 3.3E-07 0.036 123 2583 2.7E-08	y=0	413		3.2E-06	
0.01 156 1279 4.8E-08 0.015 136 1771 3.4E-08 0.02 122 1854 2.9E-08 0.03 122 2043 2.9E-08 Mg _{2.08} SiO _{.4-x} Sn _{0.6} Sb _x (x) 28 0 456 46 1.5E-06 0.012 185 413 1.8E-07 0.024 152 1021 3.3E-07 0.036 123 2583 2.7E-08 0.048 94 2535 1.1E-08	0.005	177	747	8.3E-08	
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0.02 122 1854 2.9E-08 0.03 122 2043 2.9E-08 Mg _{2.08} SiO _{.4-x} Sn _{0.6} Sb _x (x) 28 28 0 456 46 1.5E-06 0.012 185 413 1.8E-07 0.024 152 1021 3.3E-07 0.036 123 2583 2.7E-08 0.048 94 2535 1.1E-08	0.015	136	1771	3.4E-08	
0.03 122 2043 2.9E-08 Mg _{2.08} SiO _{.4-x} Sn _{0.6} Sb _x (x) 28 0 456 46 1.5E-06 0.012 185 413 1.8E-07 0.024 152 1021 3.3E-07 0.036 123 2583 2.7E-08 0.048 94 2535 1.1E-08	0.02	122	1854	2.9E-08	
Mg _{2.08} SiO _{.4-x} Sn _{0.6} Sb _x (x) 28 0 456 46 1.5E-06 0.012 185 413 1.8E-07 0.024 152 1021 3.3E-07 0.036 123 2583 2.7E-08 0.048 94 2535 1.1E-08	0.03	122	2043	2.9E-08	
Mg _{2.08} SiO _{.4-x} Sn _{0.6} Sb _x (x) 28 0 456 46 1.5E-06 0.012 185 413 1.8E-07 0.024 152 1021 3.3E-07 0.036 123 2583 2.7E-08 0.048 94 2535 1.1E-08					
0 456 46 1.5E-06 0.012 185 413 1.8E-07 0.024 152 1021 3.3E-07 0.036 123 2583 2.7E-08 0.048 94 2535 1.1E-08	Mg _{2.08} Si0 _{.4-x} Sn _{0.6} Sb _x (x)				28
0.0121854131.8E-070.02415210213.3E-070.03612325832.7E-080.0489425351.1E-08	0	456	46	1.5E-06	
0.02415210213.3E-070.03612325832.7E-080.0489425351.1E-08	0.012	185	413	1.8E-07	
0.036 123 2583 2.7E-08 0.048 94 2535 1.1E-08	0.024	152	1021	3.3E-07	
0.048 94 2535 1.1E-08	0.036	123	2583	2.7E-08	
	0.048	94	2535	1.1E-08	

Composition	S(μV/K)	σ(S/cm)	R _н (m⁻³)	Reference
0.072	105	2160	1 1F-07	110.
	100	2100	1.12 07	
$Mg_{2.08}Si_{0.4-x}Sn_{0.6}Bi_{x}$				29
0	456	46	1.5F-06	
0.005	203	898		
0.01	150	1577	3.0E-08	
0.015	143	1820		
0.02	140	2013	2.7E-08	
0.03	132	2286	2.1E-08	
Mg ₂ Si _{0.4} Sn _{0.6-x} Sb _x				30
0.02	99	2009	3.0E-08	
0.11	273	119	8.9E-07	
0.12	90	2253	1.8E-08	
0.27	87	894	3.7E-08	
0.38	84	405	6.0E-08	
$Mg_{2.24}Si_{0.4}Sn_{0.6}$	372	8	1.4E-06	31
$Mg_{2.24}(Si_{0.4}Sn_{0.6})_{0.985}Sb_{0.015}$	317	8	2.9E-06	
Mg _{2.34} Si _{0.4} Sn _{0.6}	286	60	1.1E-06	
Mg _{2.34} (Si _{0.4} Sn _{0.6}) _{0.985} Sb _{0.015}	108	1721	2.2E-08	
YbxCo ₄ Sb ₁₂	321		1.8E-06	32
	306		1.1E-06	
	298		8.6E-07	
	241		3.0E-07	
	196		1.4E-07	
	172		8.5E-08	
	152		5.0E-08	
	119		2.2E-08	
	102		1.5E-08	
	94		1.2E-08	
CeFe _x Co _{4-x} Sb ₁₂ (y,x)				33
.05,0	185	535	1.2E-07	
.075,0	153	935	4.9E-08	
.1,0	176	1149	2.5E-08	
.15,0	152	1316	2.9E-08	
.3,./5	166	115	1.4E-08	
				24
$La_x CO_4 SD_{12}(X)$				34

Composition	S(μV/K)	σ(S/cm)	R _н (m⁻³)	Reference
				no.
0.05	158	781	4.1E-08	
0.23	74	2128	3.2E-09	
$Ba_{0.3}Ni_{x}Co_{4-x}Sb_{12}(x)$				35
0	97	1112	1.0E-08	
0.02	88	1499	7.6E-09	
0.05	90	1942	6.0E-09	
0.08	91	2174	5.3E-09	
0.2	93	1600	3.6E-09	
$Eu_xCo_4Sb_{12-y}Ge_y(x,y)$				36
.2,0	174	1000	4.7E-08	
.43,.31	89	2941	7.2E-09	
.42,.5	119	2000	1.1E-08	
$Ca_xCo_{4-y}N_ySb12(x,y)$				37
.4,0	111	400	2.2E-08	
.4,.02	127	1010	2.0E-08	
.4,.05	127	1887	1.4E-08	
.4,.08	113	1563	1.2E-08	
$Co_4Sb_{12-x}Te_x(x)$				38
0.05	191	460	6.3E-08	
0.3	148	490	3.5E-08	
0.5	125	1000	1.1E-08	
$Sr_{y}Co_{4}Sb_{12}(y)$				39
0.25	137	904	5.3E-08	
0.3	129	1355	4.3E-08	
0.35	119	1791	2.9E-08	
0.4	110	2717	1.8E-08	
$Ca_yCo_{4-x}Ni_xSb_{12}(y,x)$				40
0.08,0	148	333	2.0E-08	
.08,.02	173	719	4.8E-08	
.1,.02	167	680	3.9E-08	
.1,.05	164	926	2.6E-08	
.2,0	128	386	2.2E-08	
.15,.02	135	1010	2.0E-08	
.18,.03	133	1587	1.4E-08	
.18,.06	127	1887	1.2E-08	

Composition	S(μV/K)	σ(S/cm)	R _⊬ (m⁻³)	Reference
				no.
Ba _x Yb _y Co ₄ Sb ₁₂ (x,y)				41
0.03,0	220	399	1.4E-07	
.15,.01	125	1798	2.4E-08	
.11,.03	115	1787	1.8E-08	
0,.12	146	765	3.0E-08	
.05,.09	158	1126	2.4E-08	
.08,.09	126	2068	2.1E-08	
.11,.08	107	2114	1.5E-08	
$Co12_xM_xSb_3$ (M)				42
Pt	159		1.0E-07	
	163		6.9E-08	
	136		4.3E-08	
Ni	197		6.0E-08	
	150		2.4E-08	
	98		6.7E-09	
Pd	241		2.0E-07	
	208		1.1E-07	
	177		5.0E-08	
	157		3.3E-08	
Pd+Pt	145		4.0E-08	
	135		3.4E-08	
	126		2.5E-08	
	121		2.1E-08	
	113		2.4E-08	
	114		2.0E-08	
	107		1.8E-08	
	99		1.4E-08	
$In_xYb_yCo_4Sb_{12}(x,y)$				43
.2,0	236	532	1.2E-07	
.2,.05	189	1316	5.6E-08	
.2,.2	188	1389	5.3E-08	
.2,.2	139	1587	2.4E-08	
0,.2	168	357	3.4E-08	
.1,.1	150	1316	3.4E-08	
· · · · · · · · · · · · · · · · · · ·				
$TI_xCo_4Sb_{12}(x)$				44
· · /	I	1	1	1

Composition	S(μV/K)	σ(S/cm)	R _H (m⁻³)	Reference no.
0.1	185	741	1.1E-07	
0.22	125	1053	4.0E-08	
(Sr _{0.1} Yb _{0.1})Co ₄ Sb ₁₂	148	1062	4.3E-08	
$(Ba_{0.1}Yb_{0.1})_{0.75}(Sr_{0.1}Yb_{0.1})_{0.25}Co_4Sb_{12}$	163	2358	4.9E-08	
$(Ba_{0.1}Yb_{0.1})_{0.25}(Sr_{0.1}Yb_{0.1})_{0.75}Co_4Sb_{12}$	157	2294	4.9E-08	
$(Ba_{0.1}Yb_{0.1})_{0.5}(Sr_{0.1}Yb_{0.1})_{0.5}Co_4Sb_{12}$	157	2247	4.5E-08	
(Ba _{0.5} Yb _{0.5}) _{0.26} Co ₄ Sb ₁₂	127	2890	2.0E-08	
(Ba _{0.1} Yb _{0.1})Co ₄ Sb ₁₂	155	1558	3.1E-08	
(Ba _{0.5} Yb _{0.5}) _{0.12} Co4Sb12	189	1404	4.7E-08	
$Ba_uLa_vYb_wCo_4Sb_{12}$ (u,v,w)				45
.06,.05,.06	138	1832	2.9E-08	
.08,.05,.08	126	2398	1.9E-08	
.1,.05,.1	107	3003	1.4E-08	
.1,.05,.15	104	3058	1.2E-08	
.1,.05,.2	93	3367	8.7E-09	
Sr _{0.16} Yb _{0.03} Co ₄ Sb _{11.82}	116	2980	1.5E-08	46
Sr _{0.22} Yb _{0.03} Co ₄ Sb _{12.12}	109	3430	1.3E-08	
annealing temperature				47
673	213	301	3.6E-07	
773	275	228	5.8E-07	
Yb _{0.2} Ce _{0.15} Co ₄ Sb ₁₂	124	2123	1.9E-08	48
Yb _{0.2} In _{0.2} Co ₄ Sb ₁₂	146	1827	2.4E-08	
Yb _{0.2} In _{0.2} Ce _{0.15} Co ₄ Sb ₁₂	121	1943	1.2E-08	
Yb _{0.3} In _{0.2} Ce _{0.15} Co ₄ Sb ₁₂	106	2547	1.0E-08	
Ce _y M _x Co _{4-x} Sb ₁₂				49
Ce _{0.2} Co ₄ Sb ₁₂	145	1100	3.8E-08	
$Ce_{0.2}Co_{3.95}Fe_{0.05}Sb_{12}$	120	1800	1.8E-08	
$Ce_{0.2}Co_{3.9}Fe_{0.1}Sb_{12}$	134	1600	2.0E-08	
$Ce_{0.2}Co_{3.975}Mn_{0.025}Sb_{12}$	127	1900	2.1E-08	
Yb _{0.08} Ba _{0.09} Co ₄ Sb _{12.12} /SQ	128	1786	2.6E-08	50
Yb _{0.08} Ba _{0.09} Co ₄ Sb _{12.12} /FQ	127	1852	2.6E-08	
Yb _{0.13} Ba _{0.10} Co ₄ Sb ₁₂ /SQ	122	2439	1.8E-08	
Yb _{0.13} Ba _{0.10} Co ₄ Sb ₁₂ /FQ	117	2174	1.9E-08	
Yb _{0.13} Ba _{0.10} Co ₄ Sb ₁₂ /VFQ	114	2564	1.5E-08	

Composition	S(μV/K)	σ(S/cm)	R _⊬ (m⁻³)	Reference
				no.
Yb _z Co ₄ Sb ₁₂ (321K)				51
0.1	192	276	4.1E-08	
0.2	155	1539	2.5E-08	
0.3	124	2053	1.4E-08	
0.4	117	2103	8.6E-09	
$Ce_yCo_{4-x}Cr_xSb_{12}$ (y,x)				52
.2,0	160	1035	3.3E-08	
.2,.025	160	1096	3.3E-08	
.2,.05	145	1346	2.1E-08	
.2,.1	170	641	3.1E-08	
.25,0	151	1413	3.0E-08	
.25,0.025	152	1437	2.7E-08	
.25,.05	149	1384	2.3E-08	
.25,.1	168	1081	2.3E-08	
CoSb _{2.9} Se _{0.1}	236	119	1.2E-07	53
CoSb _{2.825} Te _{0.15} Se _{.025}	115	1136	1.5E-08	
CoSb _{2.8} Te _{0.15} Se _{0.05}	142	1111	2.0E-08	
$CoSb_{2.75}Te_{0.15}Se_{0.1}$	126	885	1.8E-08	
$Ca_{x}CO_{4}Sb_{12}$ (x)				54
0.2	160	1285	3.2E-08	
1	103	3226	1.2E-08	
La _x Co ₄ Sb ₁₂ (x)				
0.3	164	498	7.0E-08	55
0.5	140	1163	2.9E-08	
0.7	109	2326	1.1E-08	
ZnSb				56
undoped	385	10		
.05 at% Sn	278	54	3.5E-06	
.5 at% Sn	236	97	1.6E-06	
Individual Samples	452		3.3E-05	
	437		4.6E-05	
	391		7.5E-06	
	389		1.7E-05	
	377		2.0E-05	
	372		1.7E-05	

Composition	S(μV/K)	σ(S/cm)	R _H (m⁻³)	Reference
				no.
	363		1.7E-05	
	351		1.9E-05	
	369		9.1E-06	
	359		7.8E-06	
	347		6.1E-06	
	330		8.0E-06	
	318		8.2E-06	
	303		7.3E-06	
	296		7.3E-06	
	279		6.6E-06	
	302		5.2E-06	
	318		4.0E-06	
	317		3.8E-06	
	273		1.9E-06	
	260		1.8E-06	
	247		1.6E-06	
	255		1.6E-06	
	244		1.2E-06	
	221		1.1E-06	
	226		9.6E-07	
Zn ₃ P ₂ at% (333K)				57
0	325	40	5.2E-06	
0.625	362	21	1.3E-05	
1.5	408	24	1.0E-05	
2.5	393	26	8.2E-06	
3.75	381	22	1.4E-05	
Zn ₃ P ₂ at %,Cu at % (313K)				
2.5,0.05	175	204	1.2E-06	
2.5,0.1	148	500	3.8E-07	
2.5,0.2	137	714	3.4E-07	
Zn _{1-x} Ag _x Sb				58
x=0	284		5.2E-06	
x=.002	181		2.4E-07	
x=.02	171		1.6E-07	
Cu at %				59
0.6	134	640	2.5E-07	
0.3	140	570	2.3E-07	
0.15	142	935	2.6E-07	
				1

Composition	S(μV/K)	σ(S/cm)	R _⊬ (m⁻³)	Reference
				no.
0.1	158	770	3.7E-07	
CuSb at %				
0.3	129	830	2.6E-07	
0.6	130	885	2.7E-07	
Cu at%				60
0.05	203	403	5.7E-07	
0	305	110	4.8E-06	
at% Cu (322K)				61
0	333	53	5.2E-06	
0.025	255	175	1.2E-06	
0.05	246	304	9.0E-07	
0.075	213	382	5.6E-07	
0.1	198	522	4.3E-07	
0.2	190	587	4.0E-07	
0.3	190	484	3.8E-07	
Cu at %and 0.2% P (323K)				
0	283	56	3.4E-06	
0.05	221	117	1.6E-06	
0.1	239	205	7.4E-07	
0.2	188	282	5.3E-07	
0.3	170	336	4.1E-07	
0.4	145	561	3.8E-07	
Zn _{1-x} Sb (%x)				62
0	399	5	1.8E-05	
1	345	6	1.4E-05	
2	281	7	1.1E-05	
3	266	8	9.5E-06	
4	263	8	9.4E-06	
%Sn				63
0.1	169	470	4.6E-07	
0.2	194	314	5.7E-07	
0.5	295	107	3.0E-06	
%ZnSn				
0.1	238	192	1.2E-06	
0.2	222	243	8.7E-07	
0.5	194	252	7.6E-07	
L	I	1	1	1

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490 20 2.3E-05 375 20 5.6E-06
375 20 5.6E-06
375 20 5.6E-06
404 25 1.7E-05
288 33 9.4E-06
400 50 8.8E-06
181 625 2.7E-07
250 1.5E-06
134 2.7E-07
142 2.9E-07
Ag0.04PbTe+x% 67
1 299 119 6.1E-06
2 315 97 7.3E-06
3 323 74 8.4E-06
4 314 91 7.1E-06
0.04 316 82 7.7E-06
PbTe _(1-x) I _x 68
0.0004 149 1613 1.1E-06
0.0007 117 2564 6.3E-07
0.0012 83 4255 3.7E-07
0.002 65 7813 2.2E-07
0.0028 50 8333 1.5E-07
0.004 31 11001 1.1E-07
0.0055 25 11001 7.9E-08
0.01 25 11001 4.3E-08
69
11 81 3846 3.5E-07
12 60 4950 2.2E-07
La1 90 2564 3.5E-07
La2 70 3268 2.0E-07

Composition	S(μV/K)	σ(S/cm)	R _H (m⁻³)	Reference
Pisa Data				110.
	175		1.2F-06	
· 	145		1.2F-06	
	150		1.0E-06	
	130		6.9F-07	
	124		6.1F-07	
	114		5.7E-07	
	109		6.3F-07	
	104		6.1F-07	
	96		4.1E-07	
	90		4.2F-07	
	79		3.5E-07	
	74		3.1E-07	
	66		3.1F-07	
	71		2.7E-07	
	75		2.7E-07	
	66		2.2E-07	
	60		2.2E-07	
	58		2.0E-07	
	55		1.8E-07	
	50		1.5E-07	
	40		1.4E-07	
	42		1.2E-07	
	38		1.1E-07	
	30		1.2E-07	
	31		1.1E-07	
	34		9.9E-08	
	28		7.7E-08	
	21		5.6E-08	
	21		5.2E-08	
	24		4.3E-08	
La	170		1.5E-06	
	124		6.5E-07	
	90		3.3E-07	
	73		2.3E-07	1
	70		2.0E-07	1
	71		1.8E-07	
	55		1.5E-07	
	50		1.2E-07	
	53		1.1E-07	

Composition	S(μV/K)	σ(S/cm)	R _⊬ (m⁻³)	Reference
				no.
	47		1.0E-07	
	40		6.7E-08	
	42		5.8E-08	
Pb _{1-x} La _x Te	171		1.5E-06	70
	126		6.4E-07	
	93		3.3E-07	
	76		2.7E-07	
	72		2.0E-07	
	72		1.7E-07	
	54		1.1E-07	
	41		6.6E-08	
at. %				71
0.3	320	151	4.9E-06	
0.4	240	473	2.2E-06	
0.6	151	1420	8.6E-07	
0.8	74	3160	3.0E-07	
30	69	3365	1.4E-07	72
3R	73	2952	1.5E-07	
35	57	5213	1.3E-07	
ЗТ	44	6748	1.1E-07	
2V	42	6962	1.1E-07	
$Pb_{(1-x)}AI_{x}Te$ (%x)				73
0.125	117		5.2E-07	
0.25	82		2.7E-07	
0.5	51		1.6E-07	
1	57		1.6E-07	
Pb _(1-x) Cr _x Te (%x)				74
0.25	185		1.3E-06	
0.5	175		1.2E-06	
1	159		9.9E-07	
2	152		8.5E-07	
				75
0.5%Cl	59		1.7E-07	
.3%Cl	89		3.0E-07	
L		1	1	1

Composition	S(μV/K)	σ(S/cm)	R _н (m⁻³)	Reference
				no.
.3%NaCl	119		1.0E-06	
.1%NaCl	148		1.4E-06	
Pb _(1-x) Bi _x Te				76
0.005	101	661	6.9E-07	
0.01	91	1410	4.5E-07	
0.02	86	2006	2.6E-07	
0.05	72	2528	1.1E-07	

Table S2: Parameters used for the two band model

Material	m_{d1}^{*} (/m _e)	m_{d2}^{*} (/m _e)	$\mu_{01}(m^2/Vs)$	$\mu_{02}(m^2/Vs)$	Interband
					Separation (eV)
Mg ₂ Si _{0.3} Sn _{0.7}	1.1	2.19	0.0123	0.0078	0.00
Mg ₂ Si _{0.4} Sn _{0.6}	1.1	2.19	0.0123	0.0078	0.06
CoSb₃	0.7	4.8	0.0147	0.0040	0.08
ZnSb	0.2	0.8	0.0276	0.0281	0.08

Table S3: Parameters used for SKB model

Material	К	E _G (eV)
Mg2Si0.3Sn0.7	1	0.39
Mg2Si0.4Sn0.6	1	0.44
CoSb3	5	0.22
ZnSb	1.35	0.35
РЬТе	3.6	0.30

Procedure for calculating $m^{*}{}_{\mathsf{D}}{}^{\mathsf{av}}$ and $\mu_{0}{}^{\mathsf{av}}$

Following procedure has been used to calculate m^{*}_D^{av}:

- Experimental values of Seebeck coefficient (S_{exp}) and corresponding charge carrier concentration (n) values (obtained using single band model equations) were taken as input.
- 2. For a guess value of m_{D}^* , Reduced Fermi level (η) value was calculated for *i*th n using (here *i* represents a set of S,n data)

$$n = \frac{\left(2m_D^* k_B T\right)^{3/2}}{3\pi^2 \hbar^3} F_{1/2}(\eta)$$

3. Using that η , theoretical S (S_{model}) value was obtained.

$$S_{model} = \frac{k_B}{e} \left(\frac{2F_1(\eta)}{F_0(\eta)} - \eta \right)$$

- 4. $(S_{exp} S_{model})^2$ was obtained.
- 5. Steps 2-4 were repeated for all input S and n (all *i* values).
- 6. *S* least square error = $\sum_{i} (S_{exp} S_{model})^2$ was obtained.
- This was done for different guess values of m^{*}_D and the one corresponding to the minimum S least square error was taken as m^{*}_D^{av}.

8.
$$S^{rms}_{error}$$
 value is given by $\sqrt{\frac{\sum_{i=1}^{N} (S_{exp} - S_{model})^2}{N}}$, with S_{model} calculated using $m^*_{D}^{av}$ value.

These steps were repeated with SKB equations for obtaining the corresponding $m^*_{\ D}{}^{av}$.

For μ_0^{av} :

- 1. n and μ_{exp} (mobility) obtained from single band models along with m_{D}^{*av} were taken as input.
- 2. Reduced Fermi level (η) was calculated for *i*th n.
- 3. Hall prefactor was calculated using η .
- 4. For a guess value of μ_0 , μ_{model} was calculated.
- 5. Steps 2-4 were repeated for all input n and μ .
- 6. μ least square error = $\sum_{i} (\mu_{exp} \mu_{model})^2$ was obtained.
- 7. This was done for different guess values of μ_0 and the one corresponding to the minimum μ least square error was taken as μ_0^{av} .

Material	SPB model		SKB model	
	$m_{D}^{*av}(/m)$	μ_0^{av} (m ² /Vs)	$m_{D}^{*}(m)$	μ_0^{av} (m ² /Vs)
Mg2Si0.3Sn0.7	2.689	0.0090	3.397	0.0118
Mg2Si0.4Sn0.6	1.755	0.0091	2.208	0.0125
CoSb3	2.787	0.0063	3.645	-
ZnSb	0.463	0.0295	0.589	0.0412
PbTe	0.318	0.150	0.403	0.245

Table S4: The m_{D}^{*av} and μ_{0}^{av} values obtained from the least square fitting.



Figure S2: A comparison of errors in the actual *n* and the *n* estimated from SPB(with two band generated data as input) as obtained from the *zT* vs *n* and $S^2 \sigma$ vs *n* plots. The m_p^* and μ_0 values are that of (a) CoSb₃ and (b) Mg₂Si_{0.3}Sn_{0.7}. The errors associated with the SPB *n* are shown in the figure.