A Critical Analysis of Single Band Modeling of Thermoelectric Materials

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Solving the SPB and SKB equations using MATLAB

```
%Fermi Integrand
FI=@(ene,eta,j)(ene.^j)./(1+exp(ene-eta));
%Fermi Integral
F=@(eta,j)quadgk(@(ene)FI(ene,eta,j),0,inf);
```

Define the SPB and SKB Integral

```
%Generlised Fermi integrand
FI=@(ene,eta,alpha,n,m,k)((exp(ene-eta))./((1+exp(ene-
eta)).^2).*ene.^(n+m).*((1+alpha.*ene).^m).*((1+2.*alpha.*ene)).^(k));
%Generalized Fermi Integral
F=@(eta,n,m,k)integral(@(ene)GFI(ene,eta,alpha,n,m,k),0,700);
```

```
%Seebeck Coefficient (SPB)
S=@(eta)(kb/e)*(2*F(eta,1)/F(eta,0)-eta);

%Seebeck Coefficient (SKB)
S=@(eta)(kb/e)*(F(eta,1,1,-2)/F(eta,0,1,-2)-eta);
```

Function for Seebeck coefficient

```
%Find eta from S
eta=fzero(@(eta)S(eta)-data,1);
```

Solving for η from S

Here, ene represents the reduced energy (ε), eta the reduced Fermi level (η), data is the experimental value of Seebeck coefficient

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

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

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***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	
$Mg_2Si_{0.3}Sn_{0.7}$	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
y=.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	

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***Reference no.***
y=.025	112	2536	1.9E-08	
3	76		1.9E-08	23
5	91		4.7E-08	
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	
$Mg_2Si_{0.4-x}Sn_{0.6}Sb_x$				25
x=0	647		1.0E-05	
x=.0075	156	1089	6.7E-08	
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	
0.015	136	1771	3.4E-08	
0.02	122	1854	2.9E-08	
0.03	122	2043	2.9E-08	
$Mg_{2.08}Si0_{.4-x}Sn_{0.6}Sb_x$ (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	

Composition	*S(μV/K)*	*σ(S/cm)*	*$R_H(m^{-3})$*	*Reference no.*
0.072	105	2160	1.1E-07	
$Mg_{2.08}Si_{0.4-x}Sn_{0.6}Bi_x$				29
0	456	46	1.5E-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	
$Mg_2Si_{0.4}Sn_{0.6-x}Sb_x$				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	
$YbxCo_4Sb_{12}$	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	
$CeFe_xCo_{4-x}Sb_{12}$(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,.75	166	115	1.4E-08	
$La_xCo_4Sb_{12}$(x)				34

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***Reference no.***
0.05	158	781	4.1E-08	
0.23	74	2128	3.2E-09	
$Ba_{0.3}Ni_xCo_{4-x}Sb_{12}$ (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	
$Sr_yCo_4Sb_{12}$ (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)***	***$R_H(m^{-3})$***	***Reference no.***
$Ba_xYb_yCo_4Sb_{12}$ (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	
$Tl_xCo_4Sb_{12}$ (x)				44

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	
$(Sr_{0.1}Yb_{0.1})Co_4Sb_{12}$	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	
$(Ba_{0.5}Yb_{0.5})_{0.26}Co_4Sb_{12}$	127	2890	2.0E-08	
$(Ba_{0.1}Yb_{0.1})Co_4Sb_{12}$	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	
$Sr_{0.16}Yb_{0.03}Co_4Sb_{11.82}$	116	2980	1.5E-08	46
$Sr_{0.22}Yb_{0.03}Co_4Sb_{12.12}$	109	3430	1.3E-08	
annealing temperature				47
673	213	301	3.6E-07	
773	275	228	5.8E-07	
$Yb_{0.2}Ce_{0.15}Co_4Sb_{12}$	124	2123	1.9E-08	48
$Yb_{0.2}In_{0.2}Co_4Sb_{12}$	146	1827	2.4E-08	
$Yb_{0.2}In_{0.2}Ce_{0.15}Co_4Sb_{12}$	121	1943	1.2E-08	
$Yb_{0.3}In_{0.2}Ce_{0.15}Co_4Sb_{12}$	106	2547	1.0E-08	
$Ce_yM_xCo_{4-x}Sb_{12}$				49
$Ce_{0.2}Co_4Sb_{12}$	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	
$Yb_{0.08}Ba_{0.09}Co_4Sb_{12.12}$/SQ	128	1786	2.6E-08	50
$Yb_{0.08}Ba_{0.09}Co_4Sb_{12.12}$/FQ	127	1852	2.6E-08	
$Yb_{0.13}Ba_{0.10}Co_4Sb_{12}$/SQ	122	2439	1.8E-08	
$Yb_{0.13}Ba_{0.10}Co_4Sb_{12}$/FQ	117	2174	1.9E-08	
$Yb_{0.13}Ba_{0.10}Co_4Sb_{12}$/VFQ	114	2564	1.5E-08	

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***Reference no.***
$Yb_zCo_4Sb_{12}$ (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	
$Ca_xC0_4Sb_{12}$ (x)				54
0.2	160	1285	3.2E-08	
1	103	3226	1.2E-08	
$La_xCo_4Sb_{12}$ (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_3P_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_3P_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	
$Zn_{1-x}Ag_xSb$				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	

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***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	

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***Reference no.***
LP	456	12	2.1E-05	64
MA	340	59	4.9E-06	
	250	139		65
	210	526		
	490	20	2.3E-05	
	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
I1	81	3846	3.5E-07	
I2	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 no.***
Pisa Data				
I	175		1.2E-06	
	145		1.2E-06	
	150		1.0E-06	
	130		6.9E-07	
	124		6.1E-07	
	114		5.7E-07	
	109		6.3E-07	
	104		6.1E-07	
	96		4.1E-07	
	90		4.2E-07	
	79		3.5E-07	
	74		3.1E-07	
	66		3.1E-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	
	70		2.0E-07	
	71		1.8E-07	
	55		1.5E-07	
	50		1.2E-07	
	53		1.1E-07	

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***Reference no.***
	47		1.0E-07	
	40		6.7E-08	
	42		5.8E-08	
$Pb_{1-x}La_xTe$	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	
3O	69	3365	1.4E-07	72
3R	73	2952	1.5E-07	
3S	57	5213	1.3E-07	
3T	44	6748	1.1E-07	
2V	42	6962	1.1E-07	
$Pb_{(1-x)}Al_xTe$ (%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	
$Pb_{(1-x)}Cr_xTe$ (%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	

Composition	***S(μV/K)***	***σ(S/cm)***	***$R_H(m^{-3})$***	***Reference no.***
.3%NaCl	119		1.0E-06	
.1%NaCl	148		1.4E-06	
$Pb_{(1-x)}Bi_xTe$				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)
$Mg_2Si_{0.3}Sn_{0.7}$	1.1	2.19	0.0123	0.0078	0.00
$Mg_2Si_{0.4}Sn_{0.6}$	1.1	2.19	0.0123	0.0078	0.06
$CoSb_3$	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	K	$E_G(eV)$
Mg2Si0.3Sn0.7	1	0.39
Mg2Si0.4Sn0.6	1	0.44
CoSb3	5	0.22
ZnSb	1.35	0.35
PbTe	3.6	0.30

Procedure for calculating $m^*_D{}^{av}$ and $\mu_0{}^{av}$

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

1. 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)

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

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.
7. 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 $\mu_0{}^{av}$:

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. $\mu\ least\ square\ error = \sum_i (\mu_{exp} - \mu_{model})^2$ was obtained.
7. This was done for different guess values of μ_0 and the one corresponding to the minimum $\mu\ least\ square\ error$ was taken as $\mu_0{}^{av}$.

Table S4: The $m^*_D{}^{av}$ and $\mu_0{}^{av}$ values obtained from the least square fitting.

Material	SPB model		SKB model	
	$m^*_D{}^{av}$ (/m)	$\mu_0{}^{av}$ (m^2/Vs)	$m^*_D{}^{av}$ (/m)	$\mu_0{}^{av}$ (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

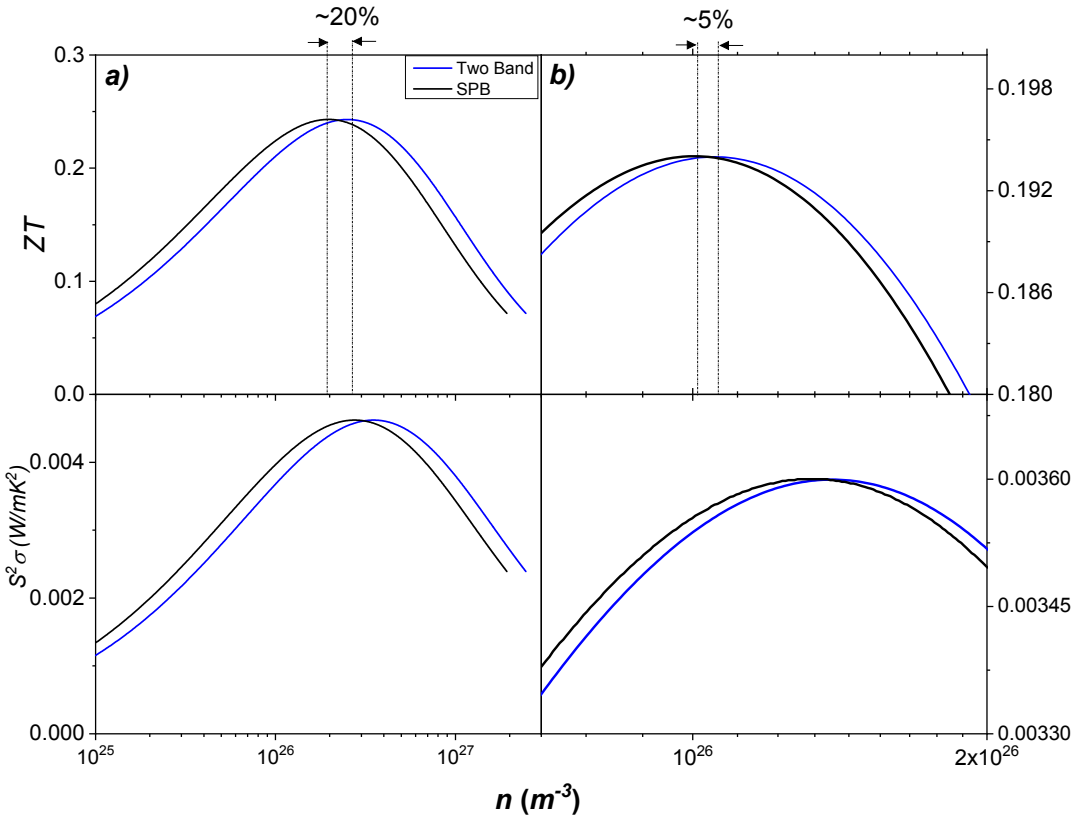

Figure S2: A comparison of errors in the actual *n* and the *n* estimated from SPB(with two band generated data as input) as obtained from the *zT* vs *n* and $S^2\sigma$ vs *n* plots. The m^*_D and μ_0 values are that of (a) $CoSb_3$ and (b) $Mg_2Si_{0.3}Sn_{0.7}$. The errors associated with the SPB *n* are shown in the figure.