Supporting Information

"Computational Exploration of the Binary A_1B_1 Chemical Space for Thermoelectric Performance"

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Screening of A_1B_1 Chemical Space for Thermoelectric Performance

Table S1: Material properties used to determine β_{SE} obtained from high-throughput DFT calculations. The parameters include: chemical formula, space group number, Inorganic Crystal Structure Database (ICSD) identification number, β_{SE} for valence band (p) and conduction band (n) transport, bulk modulus (B) in GPa, number of atoms in the primitive cell (n), density (d) in g/cm^3, valence band density of states (DOS) effective mass $m^*_{DOS,VB}$ and conduction band DOS effective mass $m^*_{DOS,CB}$ in the units of m_e, and valence band degeneracy $N_{b,VB}$ and conduction band degeneracy $N_{b,CB}$. Hypothetical A_1B_1 rocksalts are denoted by space group number 225(h).

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
AgBr	11	056550	5.1	6.7	35	4	6.3	4.07	0.04	6.0	1.0
AgBr	225	053850	81.9	6.3	35	4	6.3	4.12	0.04	44.0	1.0
AgCl	11	056543	4.5	4.7	39	4	5.4	4.43	0.06	6.0	1.0
AgCl	63	056544	5.2	4.7	38	4	5.6	1.41	0.07	4.0	1.0
AgCl	225	056538	4.5	4.6	39	4	5.5	4.40	0.06	6.0	1.0
AgI	85	028230	2.1	4.6	26	4	5.7	1.35	0.07	2.0	1.0
AgI	11	056558	3.0	15.1	30	4	6.7	4.18	0.14	4.0	3.0
AgI	186	001899	4.1	4.9	25	8	5.5	3.20	0.09	4.0	1.0
AgI	186	015589	3.2	5.2	23	4	5.3	1.81	0.06	3.0	1.0
AgI	216	053851	2.4	3.8	22	2	5.3	2.06	0.07	3.0	1.0
AgI	225	161581	49.2	13.8	31	4	6.7	4.28	0.17	30.0	3.0
AgO	88	202055	3.8	1.8	66	16	7.7	2.44	3.49	3.0	2.0
AlAs	216	606008	1.7	3.9	67	2	3.6	1.34	0.35	3.0	3.0
AlAs	186	067771	1.5	11.7	67	4	3.6	0.97	0.57	2.0	7.0
AlCl	225(h)	–	8.7	8.1	20	2	1.8	0.24	0.27	4.0	4.0
AlF	225(h)	–	213.1	22.2	36	2	3.0	0.16	0.07	28.0	4.0
AlN	194	163950	1.1	2.4	200	4	3.4	0.21	0.06	1.0	1.0
AlN	216	082789	0.5	4.0	193	2	3.2	5.71	0.19	3.0	3.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
AlN	186	041480	0.3	2.2	193	4	3.2	1.27	0.06	1.0	1.0
AlN	63	163951	1.0	2.4	200	4	3.4	0.22	0.06	1.0	1.0
AlN	225	041358	1.0	4.2	251	2	4.0	2.22	0.20	3.0	3.0
AlP	186	067770	1.0	3.2	83	4	2.3	1.16	0.43	2.0	3.0
AlSb	216	024804	2.5	21.6	50	2	4.1	0.93	0.52	3.0	11.0
AsCd	61	000432	19.1	22.0	49	16	6.3	0.46	0.55	5.0	6.0
AsGa	186	067773	2.5	10.6	60	4	5.1	0.59	0.01	2.0	1.0
AsGa	216	610536	3.0	11.0	60	2	5.1	0.78	0.01	3.0	1.0
AsGe	12	610598	2.6	12.1	6	12	5.1	0.59	0.05	1.0	1.0
AsK	19	409653	1.1	2.5	16	16	2.9	1.23	0.31	1.0	1.0
AsLa	225	106265	2.7	5.2	63	2	5.7	0.85	0.29	3.0	3.0
AsNa	14	182159	3.3	7.6	25	16	3.4	4.72	0.23	4.0	2.0
AsNa	19	182158	3.7	3.7	23	16	3.2	0.78	0.15	2.0	1.0
AsRb	19	412594	2.8	2.9	13	16	3.6	1.66	0.30	2.0	1.0
AsSi	12	043227	3.1	11.6	2	12	3.3	1.51	0.44	2.0	3.0
AsZn	61	000431	9.6	27.1	62	16	5.8	0.38	0.34	3.0	6.0
AuBr	138	200287	2.6	2.2	39	8	7.4	1.31	0.33	2.0	1.0
AuBr	141	200286	4.6	1.7	37	8	7.3	1.31	0.53	3.0	1.0
AuCl	141	006052	2.0	2.1	7	8	7.5	1.07	1.00	1.0	1.0
AuI	138	024619	3.1	2.8	32	8	7.2	0.99	0.23	2.0	1.0
BaO	194	173921	6.2	4.8	66	4	5.9	0.73	0.57	4.0	3.0
BaO	225	616004	9.6	3.8	68	2	5.8	3.62	0.55	13.0	3.0
BaO	129	015301	2.0	4.2	20	4	5.7	5.49	0.12	3.0	1.0
BaS	225	052690	1.6	3.4	41	2	4.2	2.03	0.62	3.0	3.0
BaSe	221	052695	19.1	2.6	39	2	5.5	0.60	0.51	9.0	2.0
BaSe	225	616122	2.1	3.9	36	2	4.8	1.61	0.59	3.0	3.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
BaTe	225	616163	2.7	4.2	28	2	4.9	1.20	0.56	3.0	3.0
BaTe	221	616162	5.7	2.8	32	2	5.7	0.38	0.48	3.0	2.0
BiLa	225	616762	4.0	6.2	45	2	7.5	0.65	0.32	3.0	3.0
BrCu	129	078277	1.1	3.6	39	4	4.9	3.19	0.08	2.0	1.0
BrCu	216	030090	1.8	3.8	39	2	5.1	2.59	0.06	3.0	1.0
BrCu	225	078280	63.9	7.0	47	4	6.1	3.88	0.03	38.0	1.0
BrIn	63	055188	4.9	8.9	12	4	4.8	0.51	0.19	2.0	2.0
BrIn	225(h)	–	10.1	11.1	16	2	4.4	0.40	0.34	4.0	4.0
BrK	221	061556	7.2	2.5	16	2	3.0	3.68	0.12	9.0	1.0
BrK	225	044282	1.1	1.8	14	2	2.6	6.14	0.21	3.0	1.0
BrNa	225	018013	1.1	2.5	19	2	3.1	6.27	0.12	3.0	1.0
BrRb	225	044286	1.1	1.9	12	2	3.2	7.55	0.23	3.0	1.0
BrRb	221	061560	12.3	2.9	14	2	3.7	4.45	0.12	13.0	1.0
CaO	227	261847	1.6	4.3	106	8	3.3	2.59	0.51	3.0	3.0
CaO	186	161831	0.5	1.6	85	4	2.8	0.88	0.13	1.0	1.0
CaO	225	052783	1.0	2.6	105	2	3.3	2.77	0.58	3.0	3.0
CaP	189	026261	2.9	1.2	53	12	2.4	0.46	0.38	2.0	1.0
CaS	225	619538	1.6	2.8	57	2	2.6	1.35	0.51	3.0	3.0
CaSe	225	052788	2.2	3.6	48	2	3.7	1.11	0.50	3.0	3.0
CaTe	62	041959	3.6	5.5	37	8	4.2	0.48	0.60	2.0	3.0
CaTe	221	052792	24.3	7.6	40	2	4.6	0.68	0.94	12.0	6.0
CaTe	225	060202	3.0	4.1	37	2	4.3	0.84	0.50	3.0	3.0
CdS	186	246892	2.2	5.7	53	4	4.6	1.86	0.03	3.0	1.0
CdS	216	081925	1.7	4.4	53	2	4.6	1.91	0.03	3.0	1.0
CdS	225	108230	1.0	9.9	72	2	5.8	5.41	0.11	3.0	3.0
CdSb	61	052831	16.2	66.3	39	16	6.4	0.20	0.10	3.0	6.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
CdSe	186	415786	2.7	9.5	44	4	5.3	1.61	0.01	3.0	1.0
CdSe	216	620439	2.1	7.5	45	2	5.3	1.71	0.01	3.0	1.0
CdTe	186	620518	3.4	10.8	35	4	5.5	1.18	0.01	3.0	1.0
CdTe	216	658983	2.5	8.1	35	2	5.5	1.36	0.01	3.0	1.0
ClCu	205	078271	2.7	7.8	38	16	4.6	3.56	0.05	3.0	1.0
ClCu	216	078270	1.4	2.6	43	2	4.1	3.51	0.09	3.0	1.0
ClCu	225	078273	0.6	3.3	53	2	4.9	5.97	0.06	2.0	1.0
ClIn	225(h)	–	9.2	11.9	18	2	3.9	0.41	0.27	4.0	4.0
ClIn	63	002430	4.7	6.2	10	4	4.1	0.53	0.33	2.0	2.0
ClK	225	044281	0.8	1.3	16	2	1.9	7.75	0.25	3.0	1.0
ClK	221	060402	8.5	1.8	19	2	2.2	4.83	0.16	13.0	1.0
ClNa	221	622368	5.6	2.1	26	2	2.3	3.71	0.12	9.0	1.0
ClNa	225	041411	0.8	1.7	24	2	2.1	7.49	0.16	3.0	1.0
ClRb	225	053829	0.8	1.6	14	2	2.7	10.82	0.26	3.0	1.0
ClRb	221	061521	12.1	2.3	16	2	3.1	6.04	0.15	16.0	1.0
CoCl	225(h)	–	0.2	4.1	58	4	4.8	32.99	0.06	2.0	1.0
CoO	216	029082	0.5	4.2	129	2	5.1	2.43	0.03	1.5	1.0
CoO	186	043458	0.7	2.4	127	4	5.1	4.22	0.10	2.0	1.0
CrCl	225(h)	–	0.3	2.9	34	4	3.6	26.66	0.11	2.0	1.0
CrN	59	053146	3.4	1.1	239	4	5.8	1.09	0.27	4.0	1.0
CrN	225	get	10.5	4.9	235	4	5.8	2.17	0.12	12.0	2.0
CrO	225(h)	–	2.5	1.9	45	4	5.0	3.81	0.32	3.5	1.0
CrS	194	626613	3.4	4.2	48	4	4.1	1.54	3.76	3.5	6.0
CrS	15	016723	2.1	3.0	48	4	3.9	2.20	3.82	3.0	5.0
CrTe	225(h)	–	4.8	6.3	26	4	5.6	0.38	1.23	2.0	4.0
CuI	156	030363	7.8	6.0	34	12	5.4	2.90	0.07	6.0	1.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
CuI	63	246690	1.0	3.0	28	4	4.7	0.81	0.12	1.0	1.0
CuI	216	163427	2.4	4.3	34	2	5.6	1.73	0.05	3.0	1.0
CuI	156	084217	1.2	4.3	34	4	5.4	2.91	0.07	2.0	1.0
CuI	129	078269	1.6	4.3	33	4	5.3	1.88	0.07	2.0	1.0
CuO	15	628618	3.6	4.8	86	4	6.4	2.18	1.39	4.0	4.0
CuO	9	069758	3.5	4.8	86	4	6.2	2.24	1.30	4.0	4.0
FK	225	053824	2.4	1.6	29	2	3.4	23.46	0.26	9.0	1.0
FK	221	061558	2.3	2.2	33	2	3.9	16.04	0.17	7.0	1.0
FNa	225	044276	0.7	1.7	45	2	3.5	13.21	0.21	3.0	1.0
FRb	225(h)	–	2.4	2.3	25	2	5.1	35.06	0.22	9.0	1.0
FRb	221	043436	2.6	3.0	28	2	5.8	18.32	0.15	7.0	1.0
FeSe	194	169290	1.2	2.3	102	4	5.9	0.32	2.85	1.0	4.0
FeSe	62	169281	1.7	1.7	130	8	5.9	0.21	2.81	1.0	3.0
FeTe	194	056142	3.2	5.2	48	4	6.5	0.58	2.20	2.0	5.0
GaCl	225(h)	–	7.2	8.2	21	2	3.1	0.49	0.39	4.0	4.0
GaF	225(h)	–	7.7	14.5	37	2	5.5	0.67	0.23	4.0	4.0
GaN	216	156260	1.3	4.1	170	2	5.9	2.13	0.03	3.0	1.0
GaN	225	157513	0.6	10.3	209	2	7.2	3.23	0.08	2.0	3.0
GaN	186	034476	1.7	4.9	171	4	5.9	2.04	0.03	3.0	1.0
GaP	216	635032	2.4	23.6	76	2	4.0	0.85	0.38	3.0	11.0
GaP	186	067772	1.9	2.9	76	4	4.0	0.66	0.07	2.0	1.0
GaP	166	635031	1.3	7.5	69	4	4.0	0.27	0.38	1.0	4.0
GaS	166	040824	1.0	7.1	4	4	3.6	1.94	0.07	1.0	1.0
GaS	194	635254	2.5	7.2	3	8	3.6	2.24	0.08	2.0	1.0
GaS	194	053588	2.7	7.7	3	8	3.5	1.98	0.07	2.0	1.0
GaSe	186	002002	3.7	11.6	3	16	4.6	1.56	0.05	2.0	1.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
GaSe	174	660262	4.8	13.7	3	8	4.7	0.99	0.03	2.0	1.0
GaSe	194	043540	5.0	14.0	3	8	4.7	0.93	0.03	2.0	1.0
GaSe	187	635372	5.0	14.1	3	8	4.7	0.93	0.03	2.0	1.0
GaTe	12	008249	4.2	9.5	3	12	5.0	1.49	0.38	2.0	2.0
GaTe	194	043328	2.6	29.6	3	8	4.9	0.59	0.27	1.0	4.0
GeO	225(h)	–	17.7	6.1	112	2	5.4	1.27	2.04	14.0	8.0
GeP	12	637492	1.3	7.0	2	12	4.0	1.28	0.40	1.0	2.0
GeS	225(h)	–	21.7	7.8	63	2	4.4	0.05	0.29	4.0	4.0
GeS	62	653896	5.0	2.8	16	8	4.0	1.37	0.28	3.0	1.0
GeSe	62	023953	15.9	6.8	17	8	5.2	0.45	0.36	4.0	2.0
GeSe	225	053906	26.7	14.7	57	2	5.6	0.05	0.12	4.0	4.0
GeTe	166	056042	152.0	24.7	49	2	6.1	0.07	0.29	16.0	8.0
GeTe	160	659805	14.9	9.7	30	2	5.9	0.49	0.20	6.0	3.0
GeTe	225	638007	141.1	24.2	49	2	6.1	0.08	0.30	16.0	8.0
HgO	152	024062	1.6	1.7	18	6	10.6	7.38	1.31	2.0	1.0
HgO	62	014124	15.7	4.2	20	8	10.6	4.27	1.53	8.0	2.0
HgO	154	639125	1.6	1.7	18	6	10.6	7.37	1.31	2.0	1.0
HgO	2	032561	17.9	4.8	20	16	10.6	4.39	1.53	8.0	2.0
HgS	152	081923	5.6	3.8	8	6	7.7	4.63	0.35	4.0	1.0
HgS	154	070054	5.6	3.8	8	6	7.6	4.65	0.35	4.0	1.0
HgSe	154	639202	3.0	4.1	8	6	8.5	2.65	0.32	2.0	1.0
HgTe	154	639251	2.5	4.7	12	6	8.4	0.56	0.20	1.0	1.0
HgTe	152	067861	2.6	4.9	12	6	8.4	0.53	0.18	1.0	1.0
IIn	63	055181	36.1	10.8	11	4	5.2	0.25	0.14	6.0	2.0
IIn	225(h)	–	12.0	11.5	14	2	4.7	0.34	0.36	4.0	4.0
IK	225	053827	1.4	2.1	11	2	3.0	4.74	0.19	3.0	1.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
IK	221	061555	10.1	3.0	12	2	3.4	2.51	0.11	9.0	1.0
INa	225	044279	1.4	3.1	15	2	3.6	5.05	0.10	3.0	1.0
IRb	225	053831	1.4	2.2	9	2	3.4	5.49	0.21	3.0	1.0
IRb	225	053846	1.4	2.2	9	2	3.4	5.50	0.21	3.0	1.0
IRb	221	044619	13.0	3.2	11	2	3.9	3.04	0.12	11.0	1.0
InF	225(h)	–	142.1	19.5	31	2	7.0	0.61	0.18	28.0	4.0
InP	186	180911	1.9	9.3	59	4	4.6	0.85	0.01	2.0	1.0
InP	216	600858	2.3	7.4	60	2	4.6	1.09	0.01	3.0	1.0
InS	14	409645	11.2	10.2	11	8	5.1	1.00	0.23	4.0	2.0
InS	58	081340	10.5	10.0	11	8	5.0	1.11	0.24	4.0	2.0
InSe	187	640503	0.7	7.4	4	8	5.0	4.82	0.10	1.0	1.0
InSe	12	071083	6.5	31.1	2	4	5.5	0.70	0.13	2.0	3.0
InSe	194	640490	2.7	16.2	4	8	5.2	0.58	0.03	1.0	1.0
InTe	140	169418	2.0	18.2	19	8	6.0	0.56	0.89	1.0	6.0
IrCl	225(h)	–	16.9	5.4	59	4	10.4	2.71	0.07	11.0	1.0
KP	19	014010	2.2	1.5	18	16	2.0	1.35	0.49	2.0	1.0
KSb	14	100466	3.2	15.4	13	16	3.4	3.14	0.44	3.0	4.0
KSi	142	641367	1.0	11.2	27	32	1.8	1.02	0.44	1.0	4.0
LaN	186	162195	2.0	2.2	66	4	5.6	4.30	0.15	4.0	1.0
LaN	225	162193	18.4	4.1	119	2	6.6	2.25	0.37	19.0	3.0
LaP	225	641626	2.2	4.7	70	2	4.9	1.01	0.28	3.0	3.0
LaSb	225	641893	3.5	5.5	50	2	5.9	0.65	0.30	3.0	3.0
LiCl	225(h)	–	1.0	1.4	32	2	2.1	8.55	0.19	4.0	1.0
LiF	225(h)	–	5.1	1.2	68	2	3.6	16.35	0.39	14.0	1.0
MgO	192	181463	0.7	2.7	96	24	2.4	1.03	0.12	1.0	1.0
MgO	8	181464	0.6	3.0	61	24	2.4	11.57	0.14	2.0	1.0

$\mathbf{A}_1\mathbf{B}_1$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
MgO	72	181462	0.8	3.5	105	16	2.9	0.87	0.07	1.0	1.0
MgO	15	181466	1.6	2.3	85	24	2.2	17.49	0.15	6.0	1.0
MgO	225	159373	0.8	1.9	152	2	3.5	4.39	0.07	3.0	1.0
MgO	223	181465	0.6	2.2	95	12	2.3	11.24	0.12	3.0	1.0
MgO	143	166273	1.1	2.3	139	2	3.4	5.01	0.06	4.0	1.0
MgO	194	181458	0.6	2.3	127	4	3.0	0.75	0.07	1.0	1.0
MgS	216	159401	0.6	1.8	56	2	2.0	5.17	0.07	3.0	1.0
MgS	225	028903	1.0	4.4	74	2	2.6	2.89	0.24	3.0	3.0
MgSe	186	658986	1.8	3.7	45	4	3.2	2.09	0.05	3.0	1.0
MgSe	216	159398	1.0	2.9	45	2	3.2	4.03	0.05	3.0	1.0
MgSe	225	053946	1.3	6.6	61	2	4.1	2.83	0.19	3.0	3.0
MgTe	225	168346	2.2	9.1	46	2	4.7	2.78	0.14	4.0	3.0
MgTe	216	159402	1.4	3.5	34	2	3.7	2.87	0.05	3.0	1.0
MgTe	194	168349	0.9	3.4	46	4	4.7	0.69	0.38	1.0	2.0
MgTe	186	052363	1.8	4.3	34	4	3.7	2.62	0.05	3.0	1.0
MnO	186	262928	0.6	2.9	109	4	4.3	4.73	0.07	2.0	1.0
MnO	225	–	1.2	3.6	144	4	5.3	1.54	0.05	2.0	1.0
MnS	186	044765	0.8	1.8	56	4	3.2	2.79	6.24	2.0	5.0
MnS	225	158650	0.3	1.5	80	2	3.9	1.81	0.38	1.0	1.5
MnS	216	076205	0.8	0.7	58	2	3.1	1.06	2.50	1.5	2.0
MnSe	194	076218	2.9	4.7	64	4	5.4	0.49	2.88	2.0	6.0
MnSe	216	041526	1.0	12.1	48	2	4.1	0.92	0.01	1.5	1.5
MnSe	129	162900	19.5	3.5	2	4	4.4	2.28	1.54	8.0	2.0
MnSe	186	643594	1.1	3.5	47	4	4.2	2.38	0.06	2.0	1.0
MnSe	225	104970	0.3	4.2	68	2	5.3	2.19	0.09	1.0	1.5
MnTe	62	643799	17.8	8.0	50	8	6.0	0.34	0.15	5.0	2.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
MnTe	194	643804	8.2	3.3	50	4	6.0	0.52	0.48	4.0	2.0
MnTe	225(h)	–	4.1	12.8	50	4	5.9	0.32	0.12	2.0	3.0
MnTe	216	181324	1.2	0.9	37	2	4.5	0.74	2.40	1.5	2.0
MoCl	225(h)	–	1.9	1.6	29	4	4.9	1.56	0.41	2.0	1.0
MoN	225(h)	–	6.6	6.4	218	4	8.1	1.19	0.10	6.0	2.0
NSc	225	157501	2.8	4.1	189	2	4.1	0.42	0.22	3.0	3.0
NV	225(h)	–	2.8	1.1	232	4	5.6	7.17	0.26	8.0	1.0
NY	225	037413	2.4	5.2	148	2	5.5	0.72	0.20	3.0	3.0
NY	186	161078	1.2	3.4	121	4	4.7	0.25	0.22	1.0	2.0
NY	216	161077	1.0	1.9	106	2	4.4	9.40	0.08	5.0	1.0
NaP	19	014009	2.4	2.2	27	16	2.1	1.00	0.23	2.0	1.0
NaS	194	644958	0.9	1.9	24	8	2.0	3.92	0.24	2.0	1.0
NaSb	14	026473	16.3	7.7	20	16	3.9	1.01	0.27	6.0	2.0
NaSi	15	174082	9.5	2.7	36	16	1.8	2.48	0.12	9.0	1.0
NbCl	225(h)	–	3.2	4.3	145	4	4.6	0.91	0.55	4.0	4.0
NbO	225(h)	–	0.9	0.6	158	4	7.3	7.05	1.08	3.0	1.0
NbS	225(h)	–	4.1	3.6	81	4	5.5	6.14	0.30	8.0	2.0
NbSe	225(h)	–	7.4	4.1	66	4	6.5	4.89	0.30	10.0	2.0
NbTe	225(h)	–	12.8	5.0	52	4	6.8	0.97	0.25	7.0	2.0
NiO	225	–	0.9	4.6	188	4	6.7	2.60	2.27	2.0	6.0
NiO	166	043740	3.3	0.2	186	2	6.6	2.75	0.81	6.0	0.5
NiO	12	246910	3.3	0.2	186	2	6.6	2.74	0.81	6.0	0.5
NiS	186	042493	1.8	10.6	98	4	5.3	0.91	3.17	2.0	12.0
NiS	194	646338	1.8	10.7	98	4	5.3	0.91	3.12	2.0	12.0
OPb	225(h)	–	19.8	4.7	87	2	10.2	2.58	1.13	16.0	4.0
OPb	67	062848	3.0	13.5	7	4	8.6	2.79	0.22	2.0	2.0

$\mathbf{A}_1\mathbf{B}_1$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
OPb	57	015402	0.8	24.0	6	8	8.9	6.05	0.54	1.0	4.0
OPb	129	600296	3.0	13.5	7	4	8.6	2.77	0.22	2.0	2.0
OPd	225(h)	–	4.6	8.5	158	4	8.6	1.10	1.02	4.0	6.0
OPt	131	026599	7.9	0.7	180	4	13.3	1.43	1.23	6.0	1.0
OSn	225(h)	–	28.2	13.0	94	2	6.6	0.97	0.70	16.0	8.0
OSn	36	060619	3.0	15.5	19	8	6.0	1.67	0.11	2.0	2.0
OSn	129	015516	2.4	12.7	19	4	6.2	1.98	0.12	2.0	2.0
OSr	221	181275	13.6	1.9	88	2	5.5	1.58	0.64	12.0	2.0
OSr	225	163625	1.1	3.5	84	2	4.9	3.41	0.53	3.0	3.0
OV	225	647611	0.2	4.5	161	2	5.0	25.42	0.05	2.5	1.5
OV	225(h)	–	0.2	2.3	157	4	5.3	30.44	0.10	2.0	1.0
OZn	186	076641	1.6	5.1	129	4	5.5	2.72	0.03	3.0	1.0
OZn	216	162753	1.1	4.2	129	2	5.5	3.27	0.03	3.0	1.0
OZn	225	057156	0.4	4.6	166	2	6.6	6.47	0.03	2.0	1.0
PSi	36	023724	3.7	13.9	2	24	2.2	3.75	1.07	4.0	6.0
PSr	189	026262	2.8	2.1	45	12	3.4	0.69	0.22	2.0	1.0
PbS	63	183240	24.3	23.5	17	4	7.3	0.78	0.37	7.0	5.0
PbS	38	183252	4.4	8.7	18	8	6.0	0.75	1.23	2.0	4.0
PbS	39	068701	23.5	24.5	49	4	7.4	0.11	0.10	4.0	4.0
PbS	186	183255	9.1	15.1	28	4	7.1	0.75	0.16	4.0	3.0
PbS	160	183243	18.1	12.3	48	2	7.3	0.12	0.11	4.0	3.0
PbS	62	648451	27.5	28.2	48	8	7.4	0.12	0.11	4.0	4.0
PbS	11	183248	5.8	4.6	18	8	6.7	0.55	0.16	2.0	1.0
PbS	225	648436	16.9	16.3	53	2	7.4	0.12	0.13	4.0	4.0
PbSe	62	648514	31.5	36.6	43	8	7.9	0.10	0.08	4.0	4.0
PbSe	225	600730	18.2	19.8	47	2	8.0	0.12	0.10	4.0	4.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
PbTe	225	600843	14.7	16.7	38	2	7.9	0.18	0.15	4.0	4.0
PdS	84	648749	2.4	3.6	107	16	6.5	3.02	0.12	3.0	1.0
PdSe	135	409568	2.1	31.8	89	48	7.5	3.14	0.43	2.0	6.0
PtS	131	031131	5.3	0.9	118	4	9.9	2.51	0.71	6.0	1.0
RbSb	19	014030	3.4	3.2	11	16	3.8	1.30	0.28	2.0	1.0
RbSi	142	650058	1.1	13.4	24	32	2.8	1.26	0.47	1.0	4.0
RhCl	225(h)	–	0.5	4.4	48	4	5.9	33.68	0.07	3.0	1.0
RhO	225(h)	–	0.2	2.4	140	4	9.1	8.76	0.79	1.0	2.0
SSi	225(h)	–	2.0	7.2	66	2	2.9	0.39	3.13	2.0	12.0
SSn	216	043409	12.3	3.0	35	2	3.6	1.81	0.76	12.0	3.0
SSn	225	052107	17.2	12.2	54	2	5.1	1.15	0.79	12.0	8.0
SSn	62	052109	5.7	13.3	22	8	4.9	1.03	0.10	3.0	2.0
SSn	39	067442	9.3	0.5	29	4	2.8	1.70	1.35	9.0	1.0
SSn	63	651004	9.8	3.4	23	4	5.06	0.13	0.14	2.0	1.0
SSr	225	651061	1.7	3.3	48	2	3.6	1.70	0.53	3.0	3.0
SSr	221	052111	14.2	2.1	52	2	4.0	0.69	0.52	9.0	2.0
SV	62	651366	5.6	1.0	85	8	4.1	2.11	0.59	6.0	1.0
SV	225(h)	–	3.2	2.0	82	4	4.0	7.47	0.62	8.0	2.0
SV	194	651358	0.9	1.5	87	4	4.0	5.67	1.02	3.0	2.0
SZn	186	031076	2.3	4.6	69	4	4.0	1.43	0.03	3.0	1.0
SZn	216	181741	1.6	3.5	69	2	4.0	1.70	0.04	3.0	1.0
SbZn	61	076937	11.5	83.1	47	16	6.2	0.12	0.06	2.0	6.0
SeSn	63	050562	23.9	3.0	23	4	6.0	0.06	0.19	4.0	1.0
SeSn	62	050549	6.1	22.9	22	8	5.9	0.25	0.06	2.0	3.0
SeSr	225	053949	2.2	3.9	41	2	4.4	1.39	0.53	3.0	3.0
SeV	194	652157	0.7	1.6	73	4	5.4	4.83	1.16	2.0	2.0

$\mathbf{A_1B_1}$	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	B	n	d	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
SeV	225(h)	–	4.9	2.2	70	4	5.4	4.91	0.75	8.0	2.0
SeZn	216	167830	2.1	6.2	57	2	5.1	1.51	0.02	3.0	1.0
SeZn	186	043595	2.9	8.2	56	4	5.1	1.24	0.02	3.0	1.0
SiO	225(h)	–	19.1	7.4	125	2	3.0	0.89	0.85	16.0	8.0
SiSe	225(h)	–	2.8	16.5	62	2	4.3	0.31	1.07	2.0	12.0
SnTe	225	652742	32.2	19.1	40	2	6.2	0.04	0.10	4.0	4.0
SnTe	216	053956	18.0	3.0	24	2	4.4	1.28	0.99	12.0	3.0
SrTe	225	652879	2.8	4.3	32	2	4.7	1.04	0.52	3.0	3.0
SrTe	221	052491	5.7	6.0	36	2	5.2	0.34	0.32	3.0	3.0
TeV	194	052509	3.8	2.1	56	4	6.1	0.07	0.97	1.0	2.0
TeV	225(h)	–	3.0	13.8	54	4	6.0	0.10	1.05	1.0	8.0
TeZn	216	184481	2.7	6.9	43	2	5.4	1.17	0.02	3.0	1.0
TeZn	186	067779	3.7	8.5	43	4	5.4	0.96	0.02	3.0	1.0
TeZn	144	080076	4.3	10.3	43	6	5.4	0.92	0.02	3.0	1.0
TeZn	152	184487	1.3	13.7	47	6	6.0	0.59	0.01	1.0	1.0
VCl	225(h)	–	1.1	4.4	28	4	3.6	3.44	0.32	2.0	2.0

Table S2: Energy above known A_1B_1 ground state (ΔE_{GS}) and calculated enthalpy of formation (ΔH_f) for hypothetical A_1B_1 rocksalt structures, which are predicted to be better thermoelectric materials than PbTe. Values of β_{SE} can be found in Table S1. ΔE_{GS} cannot be determined where there are no known polymorphs of the A_1B_1 stoichiometry. ΔH_f is calculated using fitted elemental-phase reference energies (FERE)*.

$\mathbf{A_1B_1}$	ΔE_{GS} (eV/atom)	ΔH_f (eV/atom)
AlF	–	-1.51
InF	–	-1.84
SnO	0.45	-1.07
GeS	0.06	-0.50
PbO	0.20	-1.00
SiO	–	-0.68
GeO	–	-1.02
IrCl	–	+0.77

* Stevanović, V.; Lany, S.; Zhang, X.; Zunger, A. *Phys. Rev. B* **2012**, *85*, 115104.

Orthorhombic Crystals Exhibit Lower κ_L than Cubic Crystals

For a given composition in the A_1B_1 chemical space, the orthorhombic structures exhibit lower lattice thermal conductivities (κ_L) than cubic structures. This decrease is primarily driven by the decrease in bulk modulus (B) in orthorhombic structures that are predominantly layered and anisotropic. This observation is confirmed in Figure S1, where the ratio of average κ_L of orthorhombic to cubic structures is shown for a given A_1B_1 composition (compounds that have at least one cubic and orthorhombic polymorph). This ratio is less than or roughly equal to one suggesting average κ_L of orthorhombic structures is lower. The corresponding ratio of average bulk modulus (B) closely follows a trend similar to κ_L ratio (Figure S1) indicating that B is the "stronger" driver of κ_L. Variations in the number of atoms in the primitive cell (n), density (d) and average mass ($\bar{M}$) account for the observed κ_L ratios to a lesser extent.

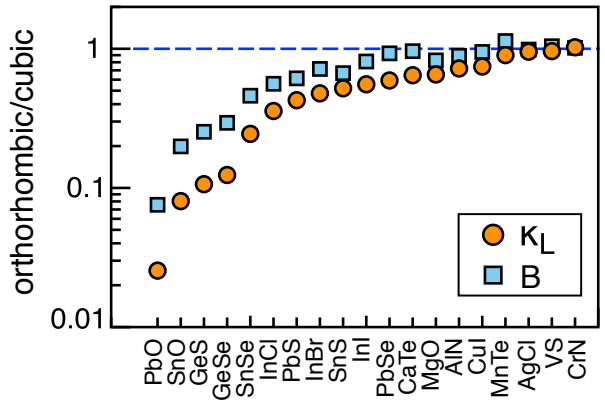

Figure S1: Ratio of average lattice thermal conductivity κ_L (circle) and bulk modulus B (square) of orthorhombic to cubic crystals for a given A_1B_1 composition.

Projected Density of States (DOS): ZnSb

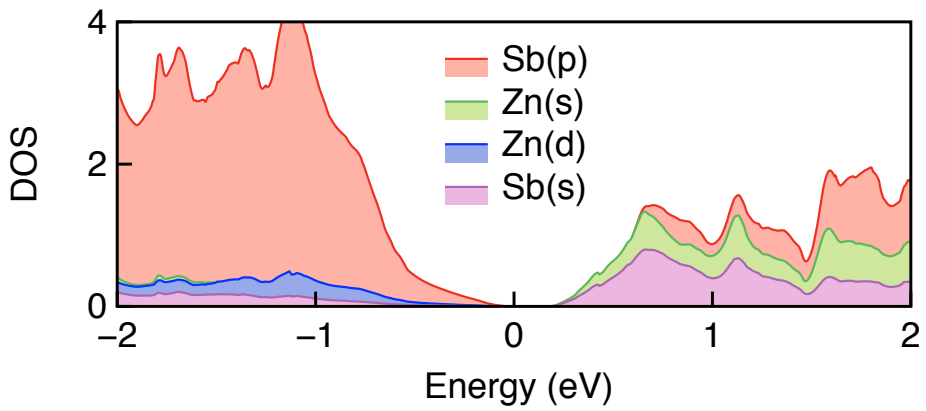

Figure S2: Orbital-projected density of states of ZnSb (*Pbca*).

Dependence of β_{SE} on μ_0 and κ_L

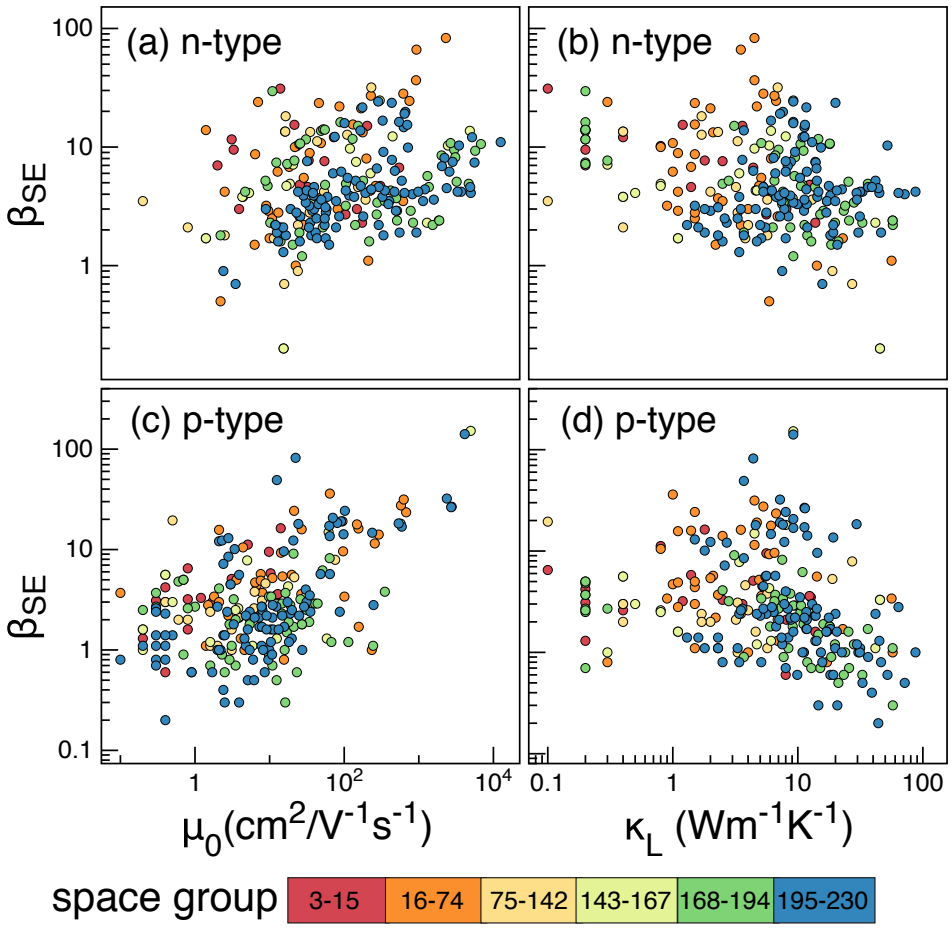

Figure S3: Variation of β_{SE} with μ_0 and κ_L. The marker color corresponds to the crystal system. For example, space group numbers 195-230 belong to the cubic crystal system.