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Electronic Supplementary Information

"Computational Identification of Promising Thermoelectric Materials Among Known Quasi-2D Binary Compounds"

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Predicted Thermoelectric Performance of Binary Quasi-2D Materials

Table S1: Material properties used to determine β_{SE} obtained from high-throughput DFT calculations. The parameters include: chemical formula, space group number (SG), Inorganic Crystal Structure Database (ICSD) identification number, β_{SE} for valence band (p-type) and conduction band (n-type) transport, lattice thermal conductivity (κ_L) in $\mathrm{Wm^{-1}K^{-1}}$, bulk modulus (B) in GPa, valence band (VB) density of states (DOS) effective mass $m^*_{DOS,VB}$ and conduction band (CB) DOS effective mass $m^*_{DOS,CB}$ in the units of m_e, and VB degeneracy $N_{b,VB}$ and CB degeneracy $N_{b,CB}$.

Compound	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
AgCl	63	056545	8.31	4.27	6.8	49	2.13	0.07	7.0	1.0
AgI	85	028230	3.18	6.14	1.6	16	1.08	0.07	2.0	1.0
AgI	186	001899	5.21	5.22	3.4	31	1.84	0.07	4.0	1.0
$AlCl_3$	12	039566	6.64	3.48	2.5	20	1.67	1.49	5.0	3.0
Al_2Te_3	14	406353	4.87	7.04	1.1	17	2.57	2.72	3.0	4.0
AsGe	12	610598	4.94	9.42	2.8	30	0.55	0.04	2.0	1.0
As_2Ge	55	023872	10.22	44.84	1.8	25	0.62	0.10	3.0	4.0
As_2O_3	14	100434	2.08	3.84	1.5	19	8.26	1.16	3.0	2.0
As_2O_4	62	010436	1.78	2.85	2.5	32	9.75	1.73	3.0	2.0
As_2S_3	14	015239	4.88	4.58	1.4	17	1.74	3.80	3.0	4.0
As_2Se_3	14	043226	3.68	8.52	1.4	19	1.37	1.70	2.0	4.0
As_2Si	55	611405	2.89	7.57	1.9	24	0.34	0.35	1.0	2.0
AuBr	138	200287	3.85	3.38	1.3	19	1.29	0.32	2.0	1.0
AuBr	141	200286	6.42	2.29	1.2	17	1.46	0.62	3.0	1.0
AuCl	141	006052	1.93	1.64	1.4	20	0.77	1.00	1.0	1.0
AuI	138	024619	4.89	13.93	1.2	17	0.86	0.76	2.0	4.0
BN	187	240999	4.70	3.31	5.3	34	6.15	1.12	8.0	3.0
BN	160	162871	1.90	4.45	6.3	34	4.28	0.53	4.0	3.0
BN	194	162870	4.68	3.35	5.4	34	6.17	1.09	8.0	3.0
BN	194	027987	5.98	5.22	4.8	30	0.81	0.52	4.0	3.0
BN	42	020946	1.71	2.30	6.2	34	1.00	0.12	2.0	1.0
BN	186	077374	5.32	4.38	5.3	33	5.01	0.27	8.0	2.0
BN	14	162883	4.21	2.21	3.9	29	1.85	1.07	4.0	2.0
BaO	129	173922	1.66	3.95	4.7	38	5.35	0.49	3.0	2.0

Compound	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
$BiBr_3$	12	100294	6.75	1.87	0.9	11	3.61	0.72	5.0	1.0
BiI_3	148	053634	3.04	18.37	0.9	12	8.13	1.04	4.0	6.0
BiI_3	162	020676	4.14	2.93	0.8	11	8.38	0.35	5.0	1.0
BiTe	164	100654	3.84	2.17	3.0	34	0.93	0.48	2.0	1.0
Bi_2O_3	160	168810	10.29	1.08	2.4	32	4.31	1.98	7.0	1.0
Bi_2O_3	14	015752	4.88	2.31	4.9	65	2.04	0.55	3.0	1.0
Bi_2O_3	114	041764	1.87	10.17	1.9	32	5.85	0.07	2.0	1.0
Bi_2Se_3	166	042545	4.96	7.42	3.4	32	0.08	0.04	1.0	1.0
Bi_2Te_3	166	184631	6.41	6.81	3.5	32	0.05	0.05	1.0	1.0
BrIn	63	055189	5.03	9.34	2.2	19	0.38	0.13	2.0	2.0
BrTl	63	109144	13.22	20.19	1.9	19	0.48	0.24	4.0	4.0
Br_2Cd	166	052367	2.67	4.22	2.1	18	8.80	0.10	5.0	1.0
Br_2Cd	186	025782	3.32	5.32	1.8	18	12.77	0.09	6.0	1.0
Br_2Cd	166	031536	3.88	5.18	1.8	18	14.09	0.09	7.0	1.0
Br_2Fe	164	409571	0.56	0.76	13.7	72	6.11	18.61	2.0	4.0
Br_2Hg	143	151889	7.53	6.42	1.4	18	9.22	0.09	8.0	1.0
Br_2Mg	164	165972	0.68	3.73	2.5	18	1.60	0.09	1.0	1.0
Br_2Zn	166	026080	6.07	9.28	2.5	20	8.32	0.62	9.0	4.0
Br_3Fe	148	076421	0.25	0.42	8.7	61	7.70	8.37	1.0	1.5
Br_3In	12	065198	0.81	3.67	1.2	14	2.41	0.19	1.0	1.0
Br_3Rh	12	028245	15.39	5.86	1.9	21	4.56	2.15	11.0	4.0
Br_3Ti	148	039242	0.63	0.67	8.0	54	7.74	6.98	2.0	2.0
Br_3Ti	2	039784	0.63	0.66	8.0	54	7.75	7.00	2.0	2.0
CaI_2	164	052280	1.04	2.96	1.7	13	0.88	2.00	1.0	3.0
Ca_3N_2	194	162797	1.42	3.64	7.7	52	0.40	0.08	1.0	1.0
CdI_2	164	108924	8.32	17.81	1.2	17	6.24	1.22	7.0	6.0
CdI_2	164	020745	4.15	6.22	1.4	16	7.32	1.13	5.0	3.0
CdI_2	164	053983	1.78	11.11	1.9	16	5.53	1.32	3.0	6.0
ClTl	63	109143	12.06	14.89	2.0	20	0.54	0.38	4.0	4.0
Cl_2Mg	115	051245	0.36	2.22	2.3	14	16.60	0.16	2.0	1.0
Cl_2Mg	164	017063	0.47	2.34	3.3	20	2.04	0.14	1.0	1.0

Compound	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
Cl_2Mg	166	056147	0.42	2.21	3.4	20	2.45	0.15	1.0	1.0
Cl_2Mg	2	051247	2.61	1.39	2.0	13	5.24	0.35	5.0	1.0
Cl_2Pd	14	421221	4.62	2.97	1.9	19	1.38	1.12	3.0	2.0
Cl_2Zn	137	026152	0.92	3.38	2.0	17	6.04	0.14	2.0	1.0
Cl_2Zr	160	030052	4.28	1.17	4.6	31	1.55	2.68	4.0	2.0
Cl_3Mo	15	026109	1.35	1.01	13.3	87	10.37	1.70	4.0	1.5
Cl_3Mo	12	026108	1.48	0.72	16.4	87	3.15	10.44	3.0	3.0
Cl_3Sc	148	074517	0.49	1.55	1.8	15	3.28	12.28	1.0	4.0
Cl_3Y	12	015684	1.51	1.92	1.3	12	3.03	2.04	2.0	2.0
Cl_3Zr	162	043292	0.47	0.91	1.9	17	4.20	6.90	1.0	2.0
Cl_4Zr	13	026049	5.29	2.80	1.2	12	5.53	6.21	6.0	4.0
Cl_8Nb_3	164	408645	0.35	1.99	12.0	87	0.93	3.31	0.5	3.0
CrF_2	14	031827	0.24	0.48	26.4	140	5.30	1.62	1.0	1.0
Cs_2O	166	027919	7.03	3.32	1.2	12	8.29	0.17	9.0	1.0
Cs_2Te_3	36	053245	4.23	1.59	1.3	15	3.92	0.79	4.0	1.0
CuI	156	030363	6.58	7.70	1.7	22	2.25	0.07	4.0	1.0
CuI	164	080232	1.78	5.22	2.3	22	2.42	0.08	2.0	1.0
CuI	156	084217	1.78	5.26	2.3	22	2.43	0.08	2.0	1.0
CuI	129	246688	2.88	6.63	1.9	19	1.19	0.06	2.0	1.0
F_3Fe	150	029132	0.19	0.59	26.8	165	9.24	18.87	1.0	3.0
F_3Rh	150	029134	1.46	0.68	8.6	81	16.29	29.70	4.0	3.0
F_4Sn	139	016794	4.53	2.71	6.2	53	14.05	0.20	9.0	1.0
FeI_2	164	052369	0.59	1.08	10.3	60	6.68	12.22	2.0	4.0
FeSe	67	165938	3.65	0.64	24.9	121	1.20	4.36	4.0	2.0
FeSe	129	169257	3.20	0.63	24.9	121	1.50	4.42	4.0	2.0
FeSe	67	169297	3.14	0.63	24.9	121	1.54	4.47	4.0	2.0
GaP	166	635031	1.96	5.83	15.1	73	0.67	0.28	2.0	3.0
GaS	194	053587	1.61	8.96	3.2	28	0.48	0.70	1.0	4.0
GaS	166	040824	1.20	4.95	4.0	28	0.57	0.05	1.0	1.0
GaS	194	635254	1.75	17.84	3.0	27	0.44	0.86	1.0	7.0
GaTe	12	008249	2.43	9.11	1.6	20	0.42	0.24	1.0	2.0

Compound	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
GaTe	194	043328	3.15	14.85	2.0	21	0.22	0.21	1.0	3.0
GeI_2	187	027674	1.69	7.89	1.6	14	2.25	0.86	2.0	4.0
GeI_2	164	023176	5.71	8.92	1.4	16	2.32	0.22	4.0	2.0
GeP	12	637492	2.04	3.47	2.4	25	0.45	0.93	1.0	2.0
GeS	63	155418	21.11	1.97	5.1	36	0.12	0.24	4.0	1.0
GeS	62	038165	9.07	2.29	3.3	30	0.72	0.28	4.0	1.0
GeSe	62	637853	5.92	2.50	2.9	29	0.35	0.30	2.0	1.0
GeTe	160	655497	16.57	8.61	6.0	37	0.37	0.22	6.0	3.0
HfO_2	137	173966	1.48	1.34	27.9	192	9.57	0.45	4.0	1.0
HfS_2	164	638847	2.10	3.44	3.6	30	1.41	1.59	2.0	3.0
$HfSe_2$	164	603743	4.90	4.55	3.2	29	1.01	1.15	3.0	3.0
HgI_2	137	281133	6.03	8.58	0.8	13	4.16	0.09	4.0	1.0
HgI_2	137	022401	2.71	6.50	1.2	14	1.67	0.08	2.0	1.0
HgI_2	137	181575	2.71	6.71	1.2	14	1.67	0.07	2.0	1.0
HgN_6	29	021029	2.23	2.26	1.1	16	3.55	8.96	2.0	3.0
Hg_2I_4	137	241172	2.70	6.55	1.2	14	1.68	0.08	2.0	1.0
IIn	63	055183	21.95	15.60	1.9	17	0.45	0.31	6.0	4.0
ITl	63	055199	19.22	17.61	1.6	17	0.69	0.31	6.0	4.0
I_2Mg	164	052279	3.41	8.34	2.0	16	1.59	1.80	3.0	6.0
I_2Pb	164	068819	1.33	2.67	1.4	14	0.78	0.24	1.0	1.0
I_2Pb	156	024264	1.87	9.47	1.1	14	0.72	0.24	1.0	2.0
I_2Pb	166	077325	1.29	2.48	1.4	13	0.82	0.28	1.0	1.0
I_2Pb	166	108914	1.59	3.09	1.2	14	0.79	0.26	1.0	1.0
I_2Pb	166	042014	1.63	3.08	1.2	14	0.76	0.26	1.0	1.0
I_2Pb	186	024263	1.62	3.08	1.2	14	0.76	0.26	1.0	1.0
I_2Sn	12	002831	18.03	3.12	1.6	18	1.22	0.24	7.0	1.0
I_2Zn	166	077058	2.13	7.83	2.1	18	3.97	0.45	3.0	3.0
I_2Zr	31	024807	9.11	10.92	1.9	23	1.17	4.36	4.0	8.0
I_2Zr	11	026418	8.21	14.46	1.9	23	1.40	1.40	4.0	6.0
I_3Y	148	170773	1.15	1.26	1.0	12	1.36	5.83	1.0	2.0
InSe	187	640503	2.08	12.06	2.4	24	0.41	0.02	1.0	1.0

Compound	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
InSe	10	032714	6.28	8.17	2.3	22	0.30	0.19	2.0	2.0
InSe	160	041477	1.94	10.41	2.7	23	0.34	0.02	1.0	1.0
InSe	194	030377	1.95	11.69	2.4	24	0.46	0.02	1.0	1.0
InSe	12	071083	6.42	7.99	2.3	22	0.28	0.20	2.0	2.0
In_2Se_3	160	017008	8.87	10.82	2.9	27	2.01	0.02	6.0	1.0
In_2Te_5	9	000501	8.01	12.21	1.5	19	1.68	0.42	4.0	3.0
MoO_3	14	644067	5.74	5.14	2.9	38	14.77	0.70	8.0	2.0
MoO_3	62	030258	8.29	8.74	2.8	33	3.42	1.22	6.0	4.0
$MoSe_2$	160	016948	1.09	10.82	4.5	36	0.81	2.27	1.0	8.0
N_4Si_3	62	156337	1.63	6.23	41.1	258	0.28	0.15	1.0	2.0
NbS_3	2	645323	0.84	1.10	18.8	117	4.11	0.52	2.0	1.0
Nb_2O_5	12	025765	3.92	0.91	32.2	153	3.77	0.46	7.0	1.0
NiO_2	12	088720	0.62	9.25	5.4	42	10.14	2.81	2.0	8.0
NiO_2	166	078698	0.59	8.89	5.5	42	10.81	2.99	2.0	8.0
OPb	29	036250	1.55	21.83	1.4	22	6.70	0.41	2.0	4.0
OPb	57	653900	1.60	20.82	1.4	22	6.28	0.44	2.0	4.0
OPb	67	062847	1.95	12.32	1.6	20	3.42	0.16	2.0	2.0
OPb	129	064778	1.95	12.55	1.6	20	3.42	0.15	2.0	2.0
OSn	129	041954	1.89	10.77	3.2	30	2.11	0.12	2.0	2.0
OSn	31	020624	1.43	21.93	1.5	17	0.92	0.25	1.0	4.0
OTl_2	166	016220	1.24	33.17	1.7	24	1.61	0.17	1.0	4.0
OTl_2	12	077699	1.22	34.83	1.7	24	1.65	0.16	1.0	4.0
OZn	186	181039	1.40	5.61	32.6	171	3.41	0.03	3.0	1.0
O_2Te	19	167816	3.44	9.72	5.0	53	4.79	0.85	4.0	4.0
O_2V	10	001503	0.28	0.39	26.4	113	14.06	7.89	2.0	2.0
O_2V	14	074705	0.75	3.82	51.2	262	18.22	0.61	4.0	3.0
O_3Sb_2	14	183102	2.24	3.83	2.0	27	3.08	1.26	2.0	2.0
O_3Y_2	62	181828	0.76	1.81	19.2	151	7.32	0.34	2.0	1.0
O_5P_2	62	079698	1.77	3.09	3.3	35	7.34	0.22	3.0	1.0
O_5Ta_2	15	280396	0.46	1.10	12.8	123	4.66	5.43	1.0	2.0
P_2Si	55	043098	1.97	17.69	2.1	21	0.45	0.76	1.0	6.0

Compound	SG	ICSD	$\beta_{\mathrm{SE}}(p)$	$\beta_{\mathrm{SE}}(n)$	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
PbS	28	183250	1.51	6.17	1.4	18	1.00	0.10	1.0	1.0
PbS	39	068701	21.58	19.90	8.3	57	0.11	0.13	4.0	4.0
PbS	36	068969	25.97	24.90	7.5	62	0.11	0.12	4.0	4.0
PbS	186	183255	10.27	12.76	4.9	39	0.49	0.18	4.0	3.0
PbS	160	183243	16.57	15.59	10.2	57	0.12	0.13	4.0	4.0
PbS	62	648451	25.99	24.67	7.4	61	0.11	0.12	4.0	4.0
PbSe	42	074334	24.20	35.61	3.9	35	0.52	0.07	7.0	4.0
PbSe	62	648514	28.97	30.52	5.6	51	0.11	0.10	4.0	4.0
PtS_2	164	659963	1.89	18.27	2.8	28	0.47	0.70	1.0	6.0
Rb_2Te_3	62	077994	3.83	7.79	1.6	20	2.66	0.32	3.0	2.0
SSn	63	100672	9.21	3.02	5.2	37	0.10	0.12	2.0	1.0
SSn	62	651025	8.74	9.81	3.7	34	0.41	0.33	3.0	3.0
S_2Sn	186	043003	5.38	8.50	2.9	25	4.33	0.40	6.0	3.0
S_2Sn	164	650993	1.18	9.37	3.4	25	3.07	1.27	2.0	6.0
S_2Ti	164	651214	3.45	3.15	5.2	32	0.38	1.13	2.0	3.0
S_2W	160	202367	1.63	14.69	4.5	38	0.47	1.52	1.0	8.0
S_2Zr	164	604434	1.79	2.84	4.6	29	1.23	1.47	2.0	3.0
Sb_2Te	164	069557	3.39	29.38	4.2	39	0.78	0.28	2.0	6.0
Sb_2Te_2	164	020459	4.35	15.41	3.7	37	0.61	0.95	2.0	6.0
Sb_2Te_3	166	002084	8.90	5.02	4.2	34	0.03	0.07	1.0	1.0
Sb_2Te_3	12	262172	49.76	25.35	2.3	26	0.53	0.19	10.0	4.0
SeSn	63	651925	16.18	2.79	4.6	36	0.22	0.16	4.0	1.0
SeSn	62	050557	5.57	13.12	3.2	32	0.38	0.23	2.0	3.0
SeZn	129	162905	2.96	7.43	2.1	20	1.06	0.23	2.0	2.0
Se_2Sn	164	651910	4.16	17.02	3.1	25	2.24	0.55	4.0	6.0
SnTe	62	652743	8.05	7.52	2.3	24	0.24	0.27	2.0	2.0
Te_5Zr	63	085506	9.36	22.86	1.8	21	0.23	1.31	2.0	8.0