Electronic Supplementary Information

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1 Correlations.

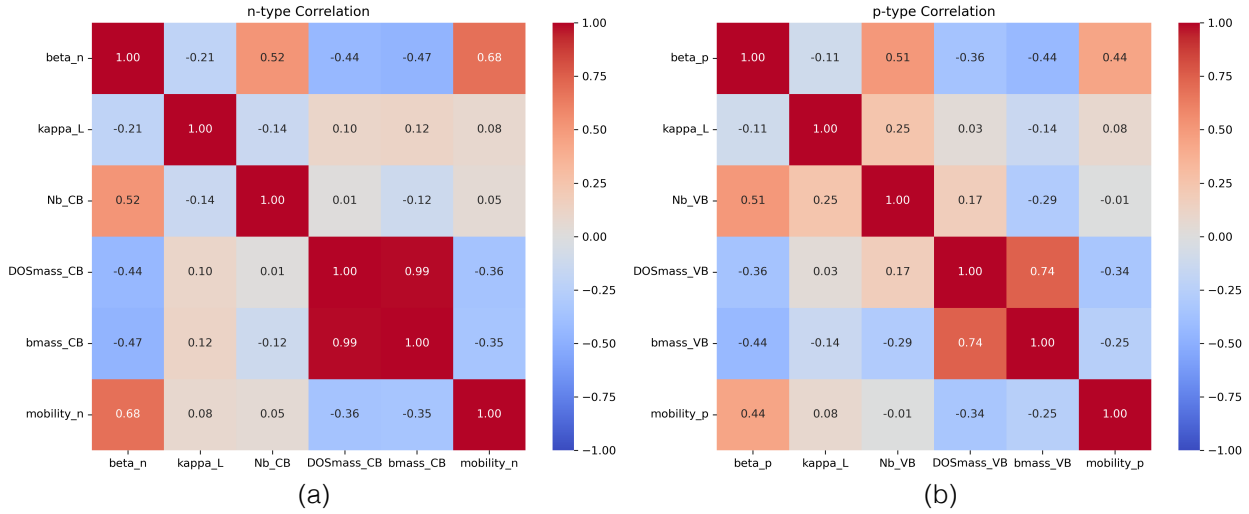

Figure S1: Pearson correlation coefficients of TE quality factor β and each of its components for n- and p-type data.

2 Band Structure Comparisons.

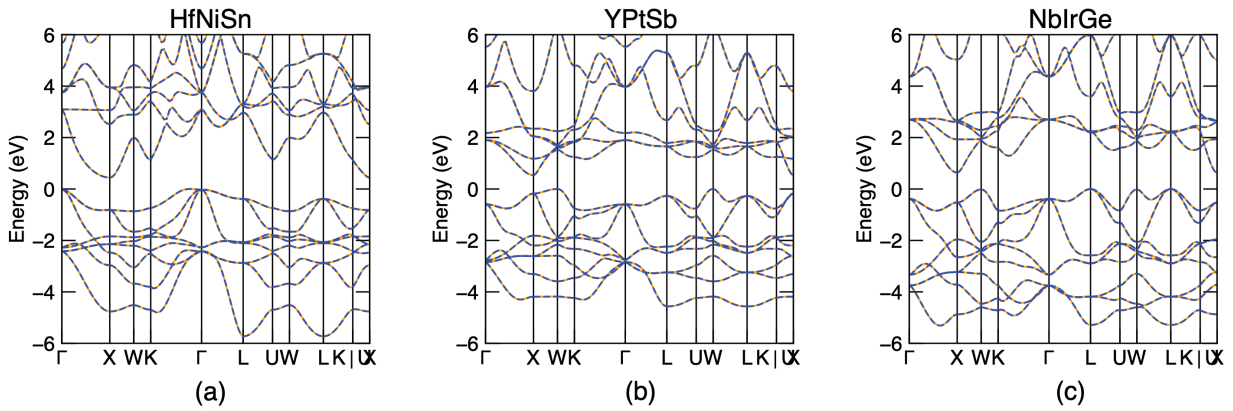

Figure S2: Calculated band structures for a) HfNiSn, a typical half-Heusler with conventional band structure features b) YPtSb, a half-Heusler predicted stable in this work with uniquely high electron moblity as anticipated by the steeper conduction band (CB) edge but still with a CB edge degeneracy of 3 at X-point and c) NbIrGe, a half-Heusler with uniquely high degeneracy at the valence band edge as seen by W, Γ, and X-points all reaching similar energy eigenvalues.

3 Effect of Mass on κ_L.

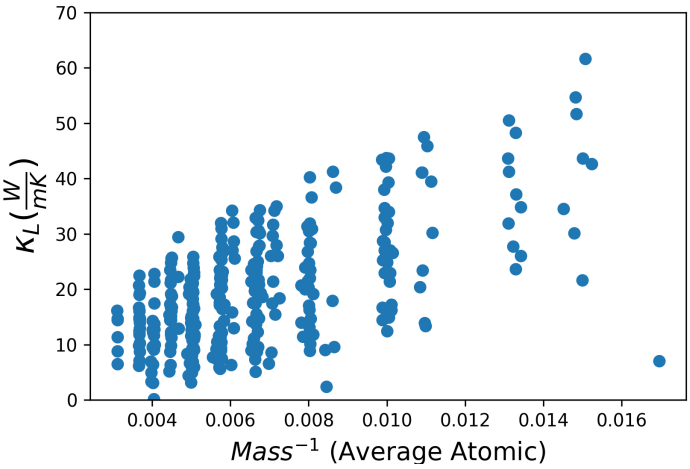

Figure S3: All half-Heuslers with a band gap are visualized here to evaluate the influence of mass and, by association, bulk modulus on the semi-empirically evaluated κ_L. The broad range of κ_L values for each mass suggests that mass alone cannot predict κ_L and that half-Heusler lattice thermal conductivity is influenced by bulk modulus as well.

4 C-element Statistical Testing.

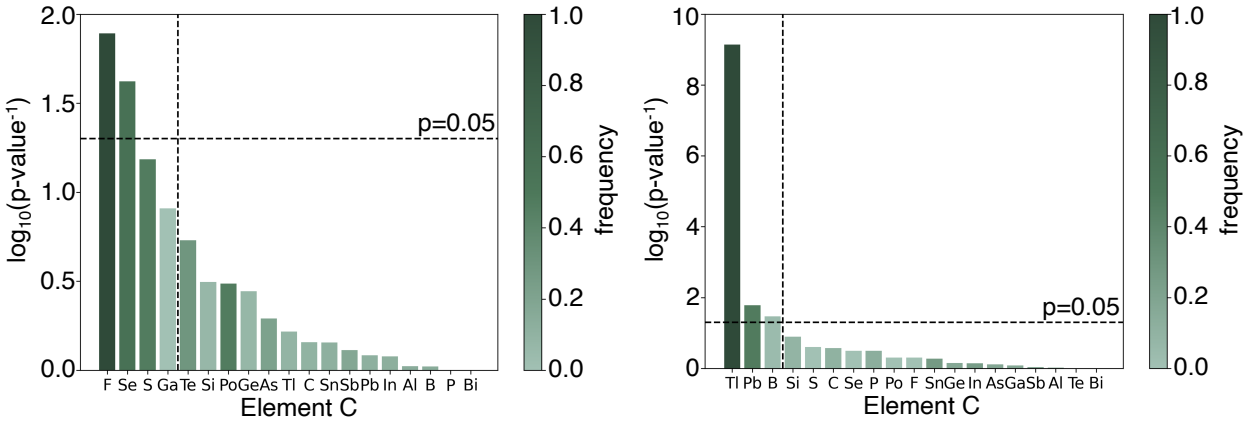

Figure S4: Additional visualization of Barnard's Exact Test used to evaluate the statistical correlation of specific C sublattice elements with high β. n-type performance is shown on the left and p-type on the right.

5 Group Number Comparisons.

As chemistry-specific trends were pursued to offer design rules in high-performing thermoelectrics, their performance alongside other descriptors were evaluated to ensure that chosen subspaces maintained high β. A common descriptor with which to analyze half-Heuslers is the group number difference between each of their ABC elements respectively. This is particularly useful in the case of our work as it is focused on 18-electron systems, so the chemistries considered fall into a rather limited range of group number differences. As seen in Figure **??**, the highest-performing half-Heuslers were spread across nearly the entirety of possible group number differences. This indicates that a selection of subspace by group number would not have captured the desirable transport trends evaluated in this work to the extent that chemistry-based subspaces did. Additionally, the highest β_n overall for each pair-wise group number comparison was often found in a compound that belonged to a high-performing subspace. The same is true for β_p as well.

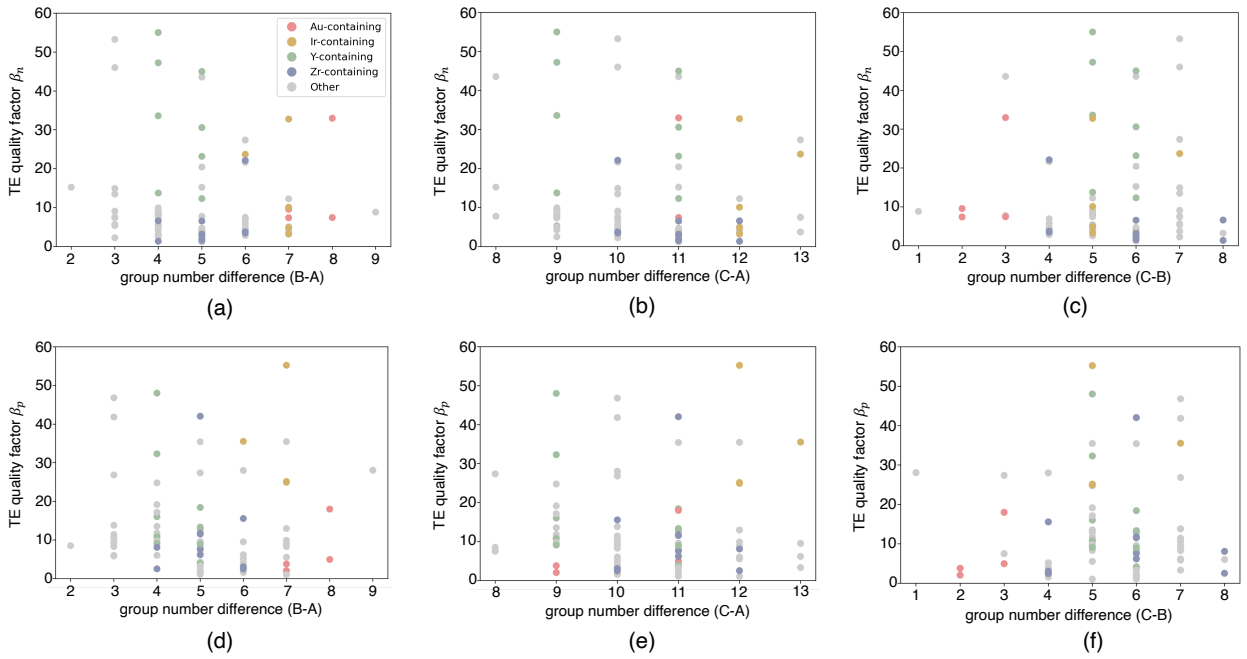

Figure S5: β values for n-type performance (a), (b), and (c) as well as for p-type performance (d), (e), and (f), visualized by difference in group numbers between ABC element pairs. Chemistries are colored accordingly if they belonged to a subspace named in this work.

6 BC Element Pairs and Transport Trends.

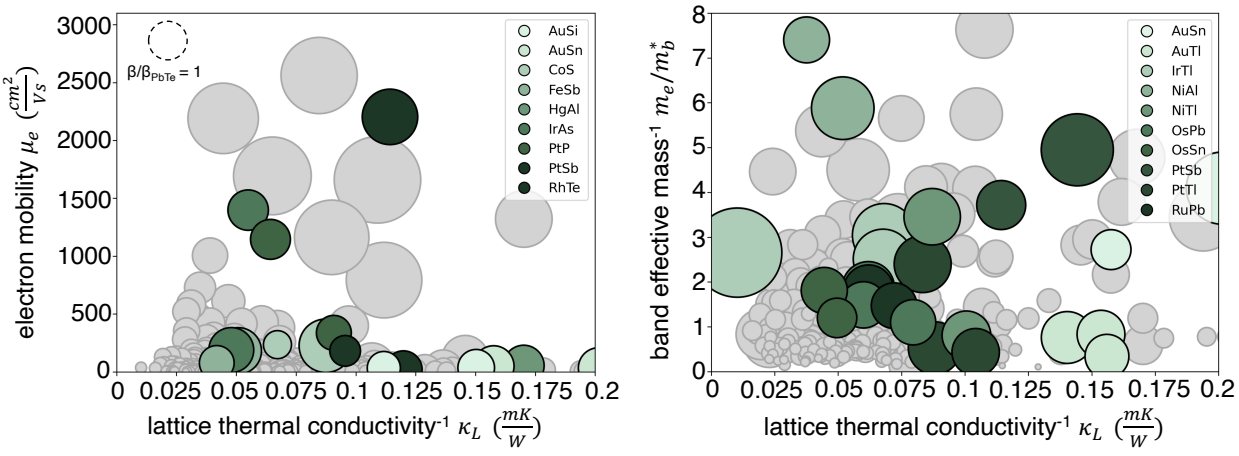

Figure S6: Additional visualization of the distribution of transport properties among all 332 half-Heusler semiconductors colored by BC element pairs. Half-heusler n-type performance is visualized by the first subfigure on the left, and p-type performance visualized on othe right. Marker size corresponds to value of TE quality factor β. Compounds with predicted values of β in the top 20% are marked in color, while lower β value compounds are marked in gray.

7 Additional Semiconductor Data - Transport.

Compounds labeled with "*" belong to one of the subspaces identified in this work.

Table S1: Electronic Transport, n-type

Compound	$m_{DOS}(m_e)$	N_b	$m_b(m_e)$	$\mu_n(\frac{cm^2}{Vs})$
AcNiAs	0.076	3	0.036	1321.419
AcNiP	2.717	3	1.306	6.633
AcNiSb	2.387	3	1.148	6.814
MoCoAl	1.961	9	0.453	55.478
CrCoAl	2.859	3	1.374	12.112
CrCoB	0.765	3	0.368	129.21
CrCoGa	1.706	3	0.82	27.171
CrCoIn	6.682	6	2.024	5.809
CrFeC	2.153	3	1.035	30.82
CrFeGe	2.168	3	1.042	21.423
CrFeSi	4.218	3	2.028	8.628
CrFeSn	1.269	3	0.61	39.375
CrIrAl	3.658	3	1.759	9.217
CrIrB	4.395	3	2.113	9.271
CrIrGa	2.505	3	1.204	16.617
CrIrIn	4.329	3	2.081	6.184
CrIrTl	2.464	3	1.185	36.501
CrOsGe	4.827	3	2.321	6.872
CrOsPb	4.195	3	2.017	6.289
CrOsSi	7.374	3	3.545	3.923
CrOsSn	4.933	3	2.372	5.726
CrReAs	4.709	3	2.264	6.973
CrReP	3.635	3	1.748	11.373
CrReSb	6.269	3	3.014	3.995
CrRhAl	5.215	3	2.507	4.821
CrRhB	1.995	3	0.959	27.765
CrRhGa	4.461	3	2.144	6.234
CrRuC	4.221	3	2.029	10.023
CrRuGe	3.751	3	1.803	9.217
CrRuPb	4.043	3	1.944	6.279
CrRuSi	5.917	3	2.845	5.017
CrRuSn	4.042	3	1.943	7.065
CrTcAs	3.799	3	1.826	9.104
CrTcP	5.317	3	2.556	6.049
CrTcSb	3.465	3	1.666	9.094
MoFeSi	6.254	3	3.007	4.057
HfAgAl	0.795	3	0.382	53.927
HfAgB	1.119	3	0.538	41.258
HfAgGa	0.906	3	0.435	44.841
HfAuAl*	1.188	3	0.571	35.27
HfAuB	1.574	3	0.757	27.838
HfAuGa	1.266	3	0.608	32.074
HfAuIn*	1.125	3	0.541	34.872
HfAuTl	1.039	3	0.499	36.495
HfCoAs	4.295	3	2.065	6.52
HfCoBi	3.523	3	1.694	6.826
HfCoP	3.888	3	1.869	8.292
HfCoSb	3.188	3	1.533	9.086
HfCuB	0.943	3	0.453	61.423
HfFeTe	0.742	3	0.357	82.067

HfIrSb*	0.282	3	0.136	381.509
HfNiC	2.696	3	1.296	14.986
HfNiGe	1.817	3	0.874	21.485
HfNiSi	1.762	3	0.847	24.24
HfNiSn	1.592	3	0.765	23.172
HfPdSn	1.464	3	0.704	25.639
HfPtGe	2.541	3	1.221	13.727
HfPtPb	1.914	3	0.92	17.359
HfPtSi	2.379	3	1.144	16.227
HfPtSn	1.902	3	0.914	19.731
HfRhAs	0.257	3	0.124	427.148
HfRhBi	0.238	3	0.114	399.445
HfRhP	0.616	3	0.296	124.674
HfRhSb	3.26	3	1.567	8.907
HfRuTe	0.207	9	0.048	1693.412
LaAuSi	1.331	6	0.403	35.932
LaAuSn	1.28	6	0.388	34.087
LaCoS	0.604	9	0.14	227.013
LaCoSe	0.248	9	0.057	792.901
LaCoTe	4.619	9	1.068	9.137
LaCuC	1.852	3	0.89	12.665
LaFeF	13.1	9	3.028	0.801
LaHgAl	1.07	9	0.247	55.481
LaHgIn	1	3	0.481	18.794
LaNiAs	2.906	9	0.672	18.786
LaNiP	3.062	9	0.708	18.906
LaNiSb	2.491	9	0.576	21.568
LaPtSb	0.056	9	0.013	6903.559
LaRhS	0.2	9	0.046	1162.399
LaRhSe	0.151	9	0.035	1659.377
LaRhTe	2.653	9	0.613	21.554
LaRuF	3.016	9	0.697	17.112
LiAlGe	1.617	3	0.777	8.989
MnNiB	19.488	3	9.369	0.81
MoIrB	1.567	3	0.753	44.496
MoIrTl	1.76	3	0.846	25.461
MoOsPb	2.861	3	1.375	12.925
MoRhB	1.143	3	0.55	66.078
NbCoC	5.046	3	2.426	7.541
NbCoGe	3.725	6	1.128	18.082
NbCoPb	3.292	3	1.582	8.505
NbCoSi	1.942	3	0.934	25.698
NbCoSn	3.463	9	0.8	26.213
NbFeAs	0.733	3	0.352	108.219
NbFeBi	1.133	3	0.544	43.533
NbFeP	0.662	3	0.318	139.896
NbFeSb	0.931	3	0.448	66.827
NbIrC	0.226	3	0.109	727.35
NbIrGe*	0.366	3	0.176	310.733
NbIrPb	0.93	3	0.447	63.195
NbIrSi	0.608	3	0.292	155.315
NbIrSn*	0.785	3	0.377	90.355
NbNiAl	0.416	3	0.2	201.235
NbNiB	2.127	3	1.023	24.087
NbNiTl	2.587	3	1.244	11.319
NbOsAs	0.733	3	0.352	112.42
NbOsBi	0.912	3	0.438	67.354

NbOsP	0.553	3	0.266	185.802
NbOsSb	0.706	3	0.34	111.517
NbPtAl	0.487	3	0.234	175.48
NbPtB	0.741	3	0.356	115.026
NbPtGa	0.453	3	0.218	198.484
NbPtIn	0.647	3	0.311	103.858
NbPtTl	4.902	3	2.357	4.722
NbRhC	2.354	3	1.131	21.15
NbRhGe	0.677	3	0.326	113.678
NbRhPb	1.246	3	0.599	36.865
NbRhSi	0.662	3	0.318	125.215
NbRhSn	0.929	3	0.446	63.614
NbRuAs	0.659	3	0.317	124.545
NbRuBi	0.967	3	0.465	57.232
NbRuP	0.634	3	0.305	143.345
NbRuSb	0.768	3	0.369	91.293
ScAgC	2.384	3	1.146	10.417
ScAuGe	1.838	3	0.884	14.266
ScAuSi	1.815	3	0.872	16.161
ScAuSn*	1.596	3	0.767	16.46
ScCdIn	2.127	3	1.023	6.778
ScCdTl	2.125	3	1.022	6.047
ScCoS	1	3	0.481	47.661
ScCoSe	0.411	3	0.197	165.818
ScCoTe	4.093	3	1.967	4.919
ScCuC	1.828	3	0.879	19.205
ScHgAl	1.155	3	0.555	22.261
ScHgB	1.625	3	0.781	16.472
ScHgGa	1.339	3	0.644	16.976
ScHgIn	1.301	3	0.626	16.335
ScHgTl	1.384	3	0.666	12.814
ScNiAs	2.667	3	1.282	9.834
ScNiBi	2.308	3	1.11	9.315
ScNiP	2.997	3	1.441	9.201
ScNiSb	2.222	3	1.068	11.478
ScPtP	0.119	3	0.057	1146.887
ScPtSb	2.984	3	1.434	8.11
ScRhTe	0.987	3	0.474	41.671
TaCoC	4.935	3	2.372	7.878
TaCoGe	3.19	3	1.533	12.12
TaCoPb	3.059	3	1.471	10.089
TaCoSi	3.444	3	1.656	11.588
TaCoSn	2.854	3	1.372	12.459
TaFeAs	0.827	3	0.397	94.991
TaFeBi	3.754	3	1.805	7.636
TaFeP	0.711	3	0.342	132.24
TaFeSb	1.036	9	0.239	182.019
TaIrGe*	0.7	3	0.337	124.639
TaIrSi	0.629	3	0.302	155.655
TaIrSn*	0.831	9	0.192	264.631
TaNiAl	1.341	3	0.645	37.487
TaNiB	1.764	3	0.848	33.493
TaNiGa	1.54	3	0.74	31.667
TaNiIn	1.574	3	0.757	26.423
TaNiTl	1.511	3	0.726	26.885
TaOsBi	2.411	3	1.159	16.368
TaOsP	0.183	3	0.088	1005.257

TaOsSb	0.724	3	0.348	113.447
TaPtAl	0.647	3	0.311	123.767
TaPtB	1.08	3	0.519	69.073
TaPtGa	0.895	3	0.43	77.138
TaPtIn	2.308	3	1.11	16.615
TaPtTl	3.518	3	1.691	8.342
TaRhC	0.32	3	0.154	425.167
TaRhGe	0.853	3	0.41	85.417
TaRhPb	2.86	3	1.375	11.292
TaRhSi	0.64	3	0.308	139.215
TaRhSn	1.354	3	0.651	38.52
TaRuAs	0.457	3	0.22	225.25
TaRuBi	0.365	3	0.175	260.342
TaRuP	0.647	3	0.311	144.094
TaRuSb	0.743	3	0.357	101.495
TiAgAl	1.323	3	0.636	23.199
TiAgB	2.208	3	1.062	14.625
TiAgGa	1.625	3	0.781	17.157
TiAgIn	1.929	3	0.927	11.668
TiAuAl	3.163	3	1.521	7.681
TiAuB	3.85	3	1.851	7.358
TiAuGa	3.196	3	1.537	7.535
TiAuIn	2.925	3	1.406	7.593
TiAuTl	2.888	3	1.389	7.046
TiCoAs	6.119	3	2.942	3.909
TiCoBi	5.518	3	2.653	3.439
TiCoP	5.408	3	2.6	5.305
TiCoSb	5.346	3	2.57	4.167
TiCuB	1.508	3	0.725	31.047
TiCuGa	1.098	3	0.528	35.651
TiFePo	0.952	3	0.458	48.752
TiFeS	1.777	3	0.854	26.948
TiFeSe	1.23	3	0.591	42.092
TiFeTe	1.952	3	0.939	19.394
TiIrAs*	0.984	9	0.227	189.135
TiIrBi*	2.723	3	1.309	11.076
TiIrP	1.344	3	0.646	43.503
TiIrSb*	3.139	3	1.509	10.327
TiNiC	3.714	3	1.786	10.253
TiNiGe	2.661	3	1.279	12.185
TiNiPb	2.95	3	1.418	7.873
TiNiSi	2.49	3	1.197	14.6
TiNiSn	2.688	3	1.292	10.23
TiOsTe	0.27	3	0.13	415.51
TiPtC	0.225	3	0.108	611.196
TiPtGe	4.282	3	2.058	6.274
TiPtPb	8.32	3	4	1.819
TiPtSi	1.559	3	0.75	31.021
TiPtSn	7.17	3	3.447	2.607
TiRhAs	1.86	3	0.894	22.306
TiRhBi	7.145	3	3.435	2.355
TiRhP	1.585	3	0.762	31.349
TiRhSb	4.431	3	2.13	5.536
TiRuTe	2.81	3	1.351	11.325
VCoC	1.278	3	0.615	62.521
VCoGe	1.898	3	0.913	24.372
VCoPb	5.496	3	2.642	3.659

VCoSi	1.331	3	0.64	45.403
VCoSn	3.531	3	1.697	8.095
VFeAs	1.493	3	0.718	37.493
VFeBi	4.83	3	2.322	4.697
VFeP	1.088	3	0.523	68.179
VFeSb	1.705	9	0.394	78.98
VIrC	2.387	3	1.148	22.358
VIrGe*	1.271	3	0.611	47.462
VIrPb	4.401	3	2.116	5.753
VIrSi*	0.995	3	0.478	74.254
VIrSn	1.547	3	0.744	31.143
VNiAl	6.03	3	2.899	3.489
VNiB	4.588	3	2.206	7.666
VNiGa	4.611	3	2.217	5.411
VNiIn	8.035	3	3.863	1.956
VOsAs	1.209	3	0.581	53.809
VOsBi	3.802	3	1.828	7.531
VOsP	0.984	3	0.473	80.583
VOsSb	1.788	3	0.86	26.834
VPtAl	1.141	3	0.548	46.467
VPtB	1.221	3	0.587	54.953
VPtGa	1.835	3	0.882	23.034
VPtIn	4.873	3	2.343	4.629
VPtTl	10.568	3	5.08	1.332
VReTe	1.92	3	0.923	23.038
VRhC	1.26	3	0.606	55.722
VRhGe	1.367	6	0.414	76.818
VRhPb	7.717	3	3.71	2.226
VRhSi	1.133	3	0.545	55.437
VRhSn	2.099	3	1.009	17.689
VRuAs	1.297	3	0.624	45.022
VRuBi	3.691	3	1.775	7.278
VRuP	1.034	3	0.497	69.881
VRuSb	1.482	3	0.712	32.719
VTcTe	1.23	3	0.592	41.725
WCoAl	0.584	3	0.281	157.497
WCoB	0.415	3	0.199	353.811
WCoGa	0.554	3	0.266	176.202
WCoIn	2.412	9	0.558	49.424
WFeC	0.497	3	0.239	280.748
WFeGe	0.417	3	0.201	291.356
WFeSi	0.298	3	0.143	521.644
WFeSn	0.602	3	0.289	145.838
WIrAl	1.393	3	0.67	46.587
WIrB	0.342	3	0.164	463.913
WIrGa	1.057	3	0.508	71.557
WIrIn	0.521	3	0.251	183.891
WIrTl	0.819	3	0.394	87.779
WOsGe	1.606	3	0.772	0.77
WOsPb	0.58	3	0.279	152.608
WOsSn	1.434	3	0.689	43.498
WRhAl	1.762	3	0.847	29.48
WRhB	0.28	3	0.135	582.309
WRhGa	0.644	3	0.31	136.165
WRhIn	0.763	3	0.367	93.28
WRhTl	0.929	3	0.446	65.967
WRuPb	0.578	3	0.278	142.292

YAgC	0.862	3	0.414	39.584
YAgSi	1.265	3	0.608	20.419
YAuGe	0.655	6	0.198	113.613
YAuSi	1.525	6	0.462	34.961
YAuSn*	1.082	6	0.328	51.097
YCoS	0.303	3	0.146	235.286
YCoTe	4.193	3	2.016	4.039
YCuC	1.403	3	0.674	22.965
YCuGe	1.327	3	0.638	19.454
YCuSi	1.173	3	0.564	25.146
YHgAl	0.926	6	0.28	54.494
YHgB	1.374	3	0.66	17.45
YNiAs	2.58	3	1.24	8.653
YNiBi*	2.033	3	0.977	9.807
YNiP	2.557	3	1.229	9.573
YNiSb*	2.102	3	1.01	10.664
YPtAs	0.663	3	0.319	67.794
YPtBi*	0.774	3	0.372	46.457
YPtP	0.236	3	0.114	338.009
YPtSb*	0.064	3	0.031	2203.969
YRhTe*	0.332	3	0.159	182.777
ZrAgB	1.136	6	0.344	75.632
ZrAuAl*	1.212	6	0.367	63.459
ZrAuB	1.729	6	0.524	45.178
ZrAuGa	1.362	6	0.413	53.135
ZrAuIn	1.24	3	0.596	28.123
ZrAuTl	1.425	3	0.685	21.3
ZrCoAs*	3.977	3	1.912	6.873
ZrCoBi*	3.405	3	1.637	6.802
ZrCoP	4.289	3	2.062	6.764
ZrCoSb*	3.401	3	1.635	7.75
ZrCuB	0.817	6	0.247	143.089
ZrFePo	0.335	3	0.161	221.121
ZrFeS	0.468	3	0.225	178.142
ZrFeSe	0.313	3	0.151	299.739
ZrFeTe*	7.255	3	3.488	2.518
ZrIrAs*	0.118	3	0.057	1398.387
ZrIrBi*	0.112	6	0.034	2560.732
ZrIrP	0.191	9	0.044	2190.353
ZrIrSb*	4.586	6	1.389	11.057
ZrNiC	2.625	3	1.262	15.109
ZrNiGe	1.774	3	0.853	20.922
ZrNiPb*	1.698	9	0.393	53.479
ZrNiSi	1.942	3	0.934	19.491
ZrNiSn*	1.781	3	0.856	18.318
ZrPtGe	2.535	3	1.219	12.912
ZrPtPb	2.039	3	0.98	14.95
ZrPtSi	2.737	6	0.829	24.653
ZrPtSn*	2.059	3	0.99	16.519
ZrRhAs*	3.305	3	1.589	8.892
ZrRhBi*	4.045	6	1.225	10.915
ZrRhP*	4.439	6	1.344	12.348
ZrRhSb*	3.712	3	1.785	6.933
ZrRuTe*	0.728	3	0.35	81.82

Table S2: Electronic Transport, p-type

Compound	$m_{DOS}(m_e)$	N_b	$m_b(m_e)$	$\mu_p(\frac{cm^2}{Vs})$
AcNiAs	9.703	14	1.67	4.236
AcNiP	9.032	8	2.258	2.918
AcNiSb	1.684	14	0.29	53.657
MoCoAl	1.08	14	0.186	211.221
CrCoAl	2.786	14	0.48	58.757
CrCoB	3.145	8	0.786	41.312
CrCoGa	2.492	14	0.429	71.815
CrCoIn	2.853	14	0.491	48.575
CrFeC	4.379	8	1.095	28.327
CrFeGe	9.713	8	2.428	6.026
CrFeSi	6.914	8	1.729	10.964
CrFeSn	9.504	14	1.636	8.967
CrIrAl	4.885	14	0.841	27.872
CrIrB	3.366	8	0.841	36.896
CrIrGa	4.707	14	0.81	30.109
CrIrIn	4.323	14	0.744	28.927
CrIrTl	2.488	17	0.376	203.945
CrOsGe	4.815	8	1.204	18.398
CrOsPb	5.266	14	0.907	20.864
CrOsSi	4.83	8	1.207	19.737
CrOsSn	4.83	14	0.832	27.579
CrReAs	5.28	8	1.32	15.663
CrReP	4.878	8	1.219	19.511
CrReSb	4.122	8	1.03	19.979
CrRhAl	6.964	14	1.199	14.577
CrRhB	1.911	8	0.478	78.964
CrRhGa	4.352	14	0.749	30.187
CrRuC	3.567	8	0.892	34.408
CrRuGe	4.299	14	0.74	35.058
CrRuPb	3.934	14	0.677	30.53
CrRuSi	3.889	14	0.669	43.945
CrRuSn	3.846	14	0.662	35.524
CrTcAs	3.461	8	0.865	27.919
CrTcP	5.834	8	1.458	14.037
CrTcSb	4.227	8	1.057	17.999
MoFeSi	3.714	8	0.929	23.638
HfAgAl	6.052	3	2.909	2.569
HfAgB	2.139	3	1.028	15.615
HfAgGa	3.658	3	1.759	5.523
HfAuAl*	8.699	3	4.182	1.781
HfAuB	2.319	3	1.115	15.557
HfAuGa	4.244	3	2.04	5.223
HfAuIn	3.379	3	1.624	6.701
HfAuTl	2.486	3	1.195	9.859
HfCoAs	8.412	8	2.103	6.344
HfCoBi	6.507	11	1.316	9.972
HfCoP	8.331	8	2.083	7.05
HfCoSb	9.607	8	2.402	4.632
HfCuB	2.575	3	1.238	13.613
HfFeTe	5.758	8	1.44	10.113
HfIrSb*	3.024	3	1.454	10.878
HfNiC	1.449	3	0.697	38.044
HfNiGe	2.783	3	1.338	11.334
HfNiSi	4.536	3	2.181	5.868

HfNiSn	2.761	3	1.328	10.141
HfPdSn	2.186	3	1.051	14.06
HfPtGe	2.285	3	1.098	16.099
HfPtPb	2.037	3	0.979	15.807
HfPtSi	3.227	3	1.552	10.272
HfPtSn	2.443	3	1.175	13.55
HfRhAs	1.778	3	0.855	23.533
HfRhBi	1.811	3	0.871	18.968
HfRhP	1.884	3	0.906	23.287
HfRhSb	2.129	3	1.023	16.877
HfRuTe	4.851	3	2.332	4.974
LaAuSi	1.121	6	0.339	46.514
LaAuSn	1.417	14	0.244	68.231
LaCoS	10.086	10	2.173	3.697
LaCoSe	10.47	10	2.256	3.214
LaCoTe	9.49	1	9.49	0.345
LaCuC	4.779	6	1.447	6.111
LaFeF	11.622	5	3.975	0.533
LaHgAl	4.102	17	0.62	13.964
LaHgIn	4.6	17	0.696	10.792
LaNiAs	7.573	1	7.573	0.496
LaNiP	8.187	10	1.764	4.804
LaNiSb	1.674	1	1.674	4.352
LaPtSb	1.176	14	0.202	112.472
LaRhS	4.893	5	1.673	5.334
LaRhSe	4.274	2	2.692	2.459
LaRhTe	3.247	2	2.046	3.537
LaRuF	8.297	1	8.297	0.417
LiAlGe	0.768	30	0.08	274.398
MnNiB	21.477	6	6.504	1.401
MoIrB	2.326	8	0.582	65.625
MoIrTl	1.31	6	0.397	79.26
MoOsPb	3.887	14	0.669	38.087
MoRhB	1.303	14	0.224	253.598
NbCoC	4.881	8	1.22	21.14
NbCoGe	7.198	14	1.239	15.705
NbCoPb	7.896	14	1.359	10.682
NbCoSi	7.016	6	2.125	7.486
NbCoSn	9.107	14	1.568	9.564
NbFeAs	4.522	8	1.131	18.827
NbFeBi	4.49	8	1.122	14.706
NbFeP	4.125	8	1.031	23.978
NbFeSb	4.652	10	1.002	19.955
NbIrC	2.772	8	0.693	45.077
NbIrGe*	5.902	14	1.016	22.42
NbIrPb	5.466	14	0.941	20.693
NbIrSi	4.626	14	0.796	34.512
NbIrSn*	4.541	14	0.782	30.29
NbNiAl	0.446	6	0.135	362.004
NbNiB	2.848	6	0.862	31.099
NbNiTl	1.248	9	0.289	101.285
NbOsAs	2.099	8	0.525	61.845
NbOsBi	2.562	8	0.641	38.144
NbOsP	2.14	8	0.535	65.079
NbOsSb	2.564	8	0.641	42.995
NbPtAl	2.059	6	0.624	40.375
NbPtB	2.481	6	0.751	37.532

NbPtGa	2.41	6	0.73	32.336
NbPtIn	1.538	6	0.466	56.706
NbPtTl	1.375	6	0.416	63.572
NbRhC	3.714	8	0.928	28.454
NbRhGe	2.821	6	0.854	26.74
NbRhPb	6.426	6	1.946	6.297
NbRhSi	2.086	6	0.632	44.738
NbRhSn	5.948	6	1.801	7.85
NbRuAs	2.604	8	0.651	42.265
NbRuBi	3.185	8	0.796	25.529
NbRuP	2.579	8	0.645	46.566
NbRuSb	2.952	8	0.738	32.326
ScAgC	0.956	3	0.459	41.05
ScAuGe	1.572	3	0.756	18.035
ScAuSi	1.783	3	0.857	16.592
ScAuSn	1.752	3	0.842	14.306
ScCdIn	2.674	3	1.286	4.808
ScCdTl	2.42	3	1.163	4.976
ScCoS	5.325	2	3.354	2.585
ScCoSe	4.677	3	2.249	4.312
ScCoTe	3.192	3	1.535	7.14
ScCuC	0.896	3	0.431	55.983
ScHgAl	3.62	3	1.741	4.014
ScHgB	1.802	3	0.866	14.112
ScHgGa	2.791	3	1.342	5.642
ScHgIn	2.662	3	1.28	5.583
ScHgTl	2.371	3	1.14	5.716
ScNiAs	1.418	3	0.682	25.378
ScNiBi	1.312	3	0.631	21.747
ScNiP	1.607	3	0.773	23.428
ScNiSb	1.551	3	0.746	19.676
ScPtP	1.09	2	0.687	27.739
ScPtSb	1.257	3	0.604	29.667
ScRhTe	1.18	3	0.567	31.86
TaCoC	5.02	8	1.255	20.475
TaCoGe	7.87	14	1.355	14.595
TaCoPb	9.4	17	1.422	10.612
TaCoSi	8.629	8	2.157	7.792
TaCoSn	9.229	14	1.589	9.997
TaFeAs	4.144	8	1.036	22.576
TaFeBi	4.754	8	1.188	14.288
TaFeP	4.079	8	1.02	25.664
TaFeSb	4.777	8	1.194	16.347
TaIrGe*	4.481	8	1.12	20.525
TaIrSi	6.045	8	1.511	13.927
TaIrSn*	6.442	8	1.611	10.906
TaNiAl	0.988	14	0.17	276.409
TaNiB	4.138	11	0.837	34.179
TaNiGa	1.29	14	0.222	192.613
TaNiIn	1.463	11	0.296	108.21
TaNiTl	2.564	3	1.233	12.164
TaOsBi	2.528	8	0.632	40.667
TaOsP	2.372	8	0.593	57.653
TaOsSb	2.516	8	0.629	46.648
TaPtAl	2.776	8	0.694	37.112
TaPtB	6.746	3	3.243	4.423
TaPtGa	4.401	11	0.89	25.941

TaPtIn	4.024	3	1.935	7.219
TaPtTl	3.945	3	1.896	7.025
TaRhC	5.181	11	1.047	23.982
TaRhGe	9.161	11	1.852	8.893
TaRhPb	6.398	3	3.076	3.375
TaRhSi	7.415	8	1.854	9.41
TaRhSn	8.942	11	1.808	8.321
TaRuAs	2.816	8	0.704	39.233
TaRuBi	3.106	8	0.777	27.956
TaRuP	2.795	8	0.699	42.766
TaRuSb	3.144	8	0.786	31.117
TiAgAl	8.202	3	3.943	1.503
TiAgB	3.813	3	1.833	6.445
TiAgGa	6.771	3	3.255	2.017
TiAgIn	6.134	3	2.949	2.057
TiAuAl	12.11	3	5.822	1.025
TiAuB	4.128	3	1.984	6.628
TiAuGa	8.274	3	3.978	1.809
TiAuIn	7.126	3	3.426	1.997
TiAuTl	6.068	3	2.917	2.314
TiCoAs	9.759	3	4.692	1.941
TiCoBi	7.742	3	3.722	2.07
TiCoP	10.337	11	2.09	7.361
TiCoSb	10.583	11	2.14	5.487
TiCuB	4.091	3	1.967	6.947
TiCuGa	6.622	3	3.183	2.406
TiFePo	7.996	11	1.617	7.34
TiFeS	7.086	8	1.772	9.027
TiFeSe	6.03	8	1.508	10.334
TiFeTe	6.729	8	1.682	8.081
TiIrAs	4.69	3	2.255	6.057
TiIrBi	4.564	3	2.194	5.104
TiIrP	4.86	3	2.337	6.329
TiIrSb	4.927	3	2.369	5.251
TiNiC	2.717	3	1.306	16.385
TiNiGe	5.285	3	2.541	4.354
TiNiPb	3.865	3	1.858	5.249
TiNiSi	7.874	3	3.785	2.597
TiNiSn	5.026	3	2.416	4.002
TiOsTe	6.4	3	3.077	3.598
TiPtC	2.395	2	1.509	11.756
TiPtGe	4.539	3	2.182	5.748
TiPtPb	4.069	3	1.956	5.317
TiPtSi	6.095	3	2.93	4.014
TiPtSn	5.232	3	2.515	4.183
TiRhAs	4.254	3	2.045	6.447
TiRhBi	4.25	3	2.043	5.134
TiRhP	3.384	3	1.627	10.053
TiRhSb	4.6	3	2.211	5.234
TiRuTe	5.747	3	2.763	3.872
VCoC	5.644	11	1.141	24.714
VCoGe	11.765	8	2.941	4.213
VCoPb	11.841	3	5.692	1.157
VCoSi	9.743	8	2.436	6.11
VCoSn	13.44	11	2.717	3.997
VFeAs	5.431	8	1.358	14.41
VFeBi	7.428	8	1.857	6.567

VFeP	4.795	8	1.199	19.654
VFeSb	6.419	8	1.605	9.608
VIrC	3.309	8	0.827	36.538
VIrGe*	8.13	11	1.644	10.757
VIrPb	9.422	3	4.53	1.836
VIrSi*	7.112	11	1.438	14.245
VIrSn	9.536	11	1.928	7.459
VNiAl	1.411	8	0.353	82.188
VNiB	7.435	3	3.575	3.715
VNiGa	2.466	11	0.499	50.713
VNiIn	2.816	3	1.354	9.425
VOsAs	3.18	3	1.529	12.615
VOsBi	3.644	3	1.752	8.027
VOsP	3.072	3	1.477	14.617
VOsSb	3.483	11	0.704	36.195
VPtAl	3.013	11	0.609	39.683
VPtB	6.763	3	3.252	4.216
VPtGa	4.723	3	2.271	5.58
VPtIn	7.47	3	3.591	2.439
VPtTl	4.764	3	2.29	4.403
VReTe	2.753	11	0.557	49.183
VRhC	5.386	3	2.589	6.306
VRhGe	8.75	3	4.206	2.371
VRhPb	12.27	3	5.899	1.11
VRhSi	8.628	3	4.148	2.637
VRhSn	10.81	3	5.197	1.513
VRuAs	3.868	11	0.782	32.066
VRuBi	6.888	11	1.393	10.469
VRuP	3.658	3	1.759	10.506
VRuSb	5.215	11	1.054	18.175
VTcTe	2.884	11	0.583	42.645
WCoAl	1.818	6	0.551	57.275
WCoB	2.901	8	0.725	51.013
WCoGa	2.39	6	0.724	39.291
WCoIn	2.179	6	0.66	38.372
WFeC	3.373	8	0.843	42.346
WFeGe	4.867	8	1.217	19.508
WFeSi	5.317	8	1.329	18.425
WFeSn	7.217	14	1.242	16.378
WIrAl	1.382	6	0.419	94.25
WIrB	2.766	8	0.692	53.712
WIrGa	1.073	6	0.325	139.898
WIrIn	1.28	6	0.388	95.602
WIrTl	1.083	6	0.328	115.43
WOsGe	2.414	8	0.603	1.115
WOsPb	3.1	14	0.534	57.688
WOsSn	3.207	14	0.552	60.673
WRhAl	1.729	6	0.524	60.648
WRhB	1.445	8	0.361	132.414
WRhGa	1.631	6	0.494	67.589
WRhIn	1.659	6	0.503	58.215
WRhTl	1.379	6	0.418	72.938
WRuPb	3.185	14	0.548	51.364
YAgC	0.755	9	0.174	144.993
YAgSi	1.227	6	0.372	42.74
YAuGe	1.168	6	0.354	47.681
YAuSi	1.318	6	0.399	43.52

YAuSn*	1.213	6	0.367	43.038
YCoS	10.938	4	4.341	1.445
YCoTe	8.574	8	2.143	3.684
YCuC	0.709	8	0.177	170.292
YCuGe	1.292	6	0.391	40.505
YCuSi	1.334	6	0.404	41.466
YHgAl	2.773	6	0.84	10.506
YHgB	1.524	6	0.462	29.864
YNiAs	0.974	8	0.243	99.5
YNiBi*	0.837	8	0.209	98.956
YNiP	1.161	8	0.29	83.496
YNiSb*	0.979	8	0.245	89.458
YPtAs	0.763	14	0.131	256.551
YPtBi*	0.871	6	0.264	77.731
YPtP	0.968	8	0.242	108.632
YPtSb*	0.888	6	0.269	84.551
YRhTe*	1.139	8	0.285	76.543
ZrAgB	2.825	6	0.855	19.278
ZrAuAl*	2.28	6	0.69	24.605
ZrAuB	2.752	6	0.834	22.486
ZrAuGa	6.404	6	1.939	5.212
ZrAuIn	5.693	6	1.724	5.718
ZrAuTl	4.329	6	1.311	8.045
ZrCoAs*	6.374	8	1.594	9.034
ZrCoBi*	9.252	8	2.313	4.05
ZrCoP	8.081	8	2.02	6.976
ZrCoSb*	8.241	8	2.06	5.48
ZrCuB	2.611	6	0.791	25.041
ZrFePo	4.951	4	1.965	5.187
ZrFeS	4.147	4	1.646	8.998
ZrFeSe	4.882	4	1.938	6.496
ZrFeTe*	4.843	4	1.922	6.157
ZrIrAs*	4.459	8	1.115	15.971
ZrIrBi*	2.838	8	0.71	26.811
ZrIrP	4.777	8	1.194	15.536
ZrIrSb*	4.72	8	1.18	14.12
ZrNiC	1.824	8	0.456	69.576
ZrNiGe	3.453	8	0.863	20.554
ZrNiPb*	2.766	8	0.691	22.874
ZrNiSi	11.496	8	2.874	3.61
ZrNiSn*	3.499	3	1.682	6.653
ZrPtGe	3.101	6	0.939	19.086
ZrPtPb	2.19	3	1.053	13.438
ZrPtSi	3.719	6	1.126	15.559
ZrPtSn*	3.084	3	1.483	9.011
ZrRhAs*	2.898	8	0.724	28.884
ZrRhBi*	1.911	8	0.478	44.83
ZrRhP	4.472	8	1.118	16.286
ZrRhSb*	2.587	8	0.647	31.78
ZrRuTe*	4.87	8	1.218	12.603

8 Additional Semiconductor Data - Structure.

Table S3: Half-Heusler Structure

Compound	Lattice Parameter (Å)	Mass (Average Atomic)	E_g (eV)	E_g Type	Bulk Modulus (GPa)
AcNiAs	6.583	199.605	0.145	PBE	76.206
AcNiP	6.462	175.279	0.615	PBE	82.504
AcNiSb	6.826	225.531	0.391	PBE	69.803
MoCoAl	5.772	100.67	0.306	MBJ	141.056
CrCoAl	5.461	76.335	0.545	MBJ	162.61
CrCoB	4.984	67.385	0.84	MBJ	239.975
CrCoGa	5.457	99.993	0.622	MBJ	168.191
CrCoIn	5.752	124.954	0.699	MBJ	139.333
CrFeC	4.895	66.34	0.563	MBJ	270.387
CrFeGe	5.45	99.899	0.423	MBJ	190.022
CrFeSi	5.339	75.237	0.368	MBJ	207.641
CrFeSn	5.743	125.399	0.466	MBJ	156.398
CrIrAl	5.76	150.11	0.351	MBJ	179.152
CrIrB	5.376	141.159	0.528	MBJ	237.306
CrIrGa	5.775	173.768	0.361	MBJ	182.999
CrIrIn	6.042	198.728	0.476	MBJ	154.748
CrIrTl	6.125	248.304	0.584	MBJ	392.268
CrOsGe	5.767	174.282	0.354	MBJ	202.465
CrOsPb	6.135	248.763	0.338	MBJ	150.077
CrOsSi	5.662	149.621	0.31	MBJ	218.221
CrOsSn	6.026	199.783	0.419	MBJ	174.263
CrReAs	5.794	173.319	0.152	MBJ	197.964
CrReP	5.641	148.993	0.123	MBJ	218.949
CrReSb	6.057	199.244	0.241	MBJ	174.16
CrRhAl	5.729	100.675	0.444	MBJ	159.459
CrRhB	5.315	91.724	0.63	MBJ	217.26
CrRhGa	5.733	124.333	0.44	MBJ	163.138
CrRuC	5.232	91.372	0.36	MBJ	241.483
CrRuGe	5.722	124.931	0.203	MBJ	185.993
CrRuPb	6.09	199.412	0.333	MBJ	141.803
CrRuSi	5.62	100.27	0.147	MBJ	200.581
CrRuSn	5.987	150.432	0.287	MBJ	159.508
CrTcAs	5.752	124.495	0.162	MBJ	187.237
CrTcP	5.597	100.169	0.097	MBJ	206.015
CrTcSb	6.018	150.421	0.234	MBJ	162.928
MoFeSi	5.674	99.572	0.183	MBJ	176.267
HfAgAl	6.268	173.438	0.068	PBE	106.243
HfAgB	5.862	164.487	0.147	PBE	135.707
HfAgGa	6.237	197.096	0.09	MBJ	107.349
HfAuAl*	6.263	222.755	0.641	PBE	126.918
HfAuB	5.919	213.804	0.72	PBE	152.648
HfAuGa	6.248	246.413	0.562	PBE	126.841
HfAuIn*	6.461	271.373	0.369	PBE	115.61
HfAuTl	6.526	320.949	0.254	PBE	107.31
HfCoAs	5.792	172.887	1.279	PBE	161.215
HfCoBi	6.186	247.09	0.969	PBE	125.393
HfCoP	5.649	148.561	1.368	PBE	176.58
HfCoSb	6.054	198.813	1.127	PBE	143.683
HfCuB	5.528	139.954	0.085	MBJ	156.225
HfFeTe	6.042	200.336	0.824	PBE	145.573
HfIrSb	6.32	272.587	0.881	PBE	158.922
HfNiC	5.336	137.932	0.908	PBE	184.298

HfNiGe	5.849	171.491	0.563	PBE	146.182
HfNiSi	5.771	146.83	0.685	PBE	157.476
HfNiSn	6.105	196.992	0.376	PBE	129.269
HfPdSn	6.343	223.409	0.394	PBE	126.208
HfPtGe	6.161	246.985	1.138	PBE	154.42
HfPtPb	6.462	321.466	0.753	PBE	127.647
HfPtSi	6.082	222.324	1.293	PBE	165.434
HfPtSn	6.366	272.486	0.906	PBE	143.738
HfRhAs	6.061	197.226	0.295	PBE	154.922
HfRhBi	6.404	271.429	0.145	PBE	128.435
HfRhP	5.936	172.9	0.855	PBE	167.249
HfRhSb	6.282	223.152	1.126	PBE	145.615
HfRuTe	6.277	225.368	0.066	PBE	147.603
LaAuSi	6.751	201.455	0.241	PBE	76.672
LaAuSn	6.995	251.617	0.143	PBE	68.537
LaCoS	6.13	127.255	0.32	PBE	98.687
LaCoSe	6.295	153.212	0.066	PBE	90.744
LaCoTe	6.545	180.135	0.632	PBE	83.991
LaCuC	6.009	118.708	0.333	PBE	88.674
LaFeF	6.494	118.313	0.056	MBJ	35.166
LaHgAl	7.012	202.85	0.066	PBE	56.874
LaHgIn	7.165	251.468	0.121	PBE	52.197
LaNiAs	6.37	150.844	0.626	PBE	86.178
LaNiP	6.247	126.518	0.698	PBE	93.785
LaNiSb	6.619	176.769	0.453	PBE	78.517
LaPtSb	6.859	252.263	0.05	PBE	85.383
LaRhS	6.404	151.594	0.366	PBE	96.228
LaRhSe	6.545	177.551	0.128	PBE	90.539
LaRhTe	6.76	204.474	0.749	PBE	86.242
LaRuF	6.037	143.345	0.056	MBJ	82.975
LiAlGe	6.061	58.984	0.371	PBE	51.337
MnNiB	5.057	68.881	0.06	PBE	193.676
MoIrB	5.599	165.494	0.325	MBJ	242.51
MoIrTl	6.217	272.638	0.169	MBJ	165.141
MoOsPb	6.237	273.098	0.116	MBJ	173.706
MoRhB	5.529	116.059	0.497	MBJ	224.441
NbCoC	5.224	90.693	1.446	PBE	237.448
NbCoGe	5.706	124.252	1.071	PBE	180.535
NbCoPb	6.051	198.733	0.942	PBE	141.093
NbCoSi	5.623	99.591	0.862	PBE	193.214
NbCoSn	5.962	149.753	0.982	PBE	156.446
NbFeAs	5.694	123.806	0.581	PBE	188.598
NbFeBi	6.081	198.009	0.596	PBE	145.74
NbFeP	5.552	99.48	0.507	PBE	209.284
NbFeSb	5.951	149.732	0.507	PBE	166.863
NbIrC	5.656	164.468	0.283	PBE	216.764
NbIrGe*	6.019	198.027	0.634	PBE	191.362
NbIrPb	6.321	272.507	0.715	PBE	157.385
NbIrSi	5.941	173.365	0.485	PBE	204.37
NbIrSn*	6.23	223.527	0.631	PBE	174.466
NbNiAl	5.771	98.847	0	PBE	149.911
NbNiB	5.349	89.896	0.58	PBE	207.562
NbNiTl	6.045	197.041	0.091	PBE	130.811
NbOsAs	6.015	198.19	0.242	PBE	195.936
NbOsBi	6.346	272.393	0.318	PBE	162.956
NbOsP	5.893	173.864	0.16	PBE	212.157
NbOsSb	6.226	224.115	0.264	PBE	183.893

NbPtAl	6.065	174.341	0.143	PBE	165.732
NbPtB	5.741	165.39	0.808	PBE	203.722
NbPtGa	6.058	197.999	0.457	PBE	168.077
NbPtIn	6.274	222.96	0.449	PBE	150.271
NbPtTl	6.337	272.535	0.592	PBE	142.36
NbRhC	5.567	115.032	1.048	PBE	212.12
NbRhGe	5.972	148.592	0.649	PBE	176.01
NbRhPb	6.279	223.072	0.763	PBE	142.467
NbRhSi	5.896	123.93	0.473	PBE	187.189
NbRhSn	6.193	174.092	0.659	PBE	158.157
NbRuAs	5.962	148.839	0.332	PBE	185.055
NbRuBi	6.303	223.042	0.421	PBE	151.15
NbRuP	5.839	124.513	0.245	PBE	200.906
NbRuSb	6.184	174.764	0.356	PBE	170.766
ScAgC	5.736	91.238	0.228	PBE	106.52
ScAuGe	6.268	174.114	0.297	PBE	98.743
ScAuSi	6.174	149.453	0.386	PBE	109.741
ScAuSn*	6.493	199.615	0.146	PBE	92.178
ScCdIn	6.676	150.658	0.068	MBJ	58.41
ScCdTl	6.748	200.233	0.113	MBJ	52.036
ScCoS	5.585	75.252	0.672	PBE	132.323
ScCoSe	5.776	101.209	0.292	PBE	121.174
ScCoTe	6.043	128.132	0.889	PBE	113.128
ScCuC	5.352	66.705	0.118	PBE	131.888
ScHgAl	6.441	150.847	0.103	PBE	76.804
ScHgB	6.029	141.897	0.17	PBE	94.817
ScHgGa	6.431	174.505	0.077	PBE	73.059
ScHgIn	6.665	199.466	0.378	MBJ	67.349
ScHgTl	6.76	249.042	0.153	MBJ	57.973
ScNiAs	5.822	98.841	0.467	PBE	119.007
ScNiBi	6.247	173.045	0.179	PBE	90.751
ScNiP	5.669	74.516	0.58	PBE	132.603
ScNiSb	6.103	124.767	0.263	PBE	105.623
ScPtP	6.019	150.01	0.085	PBE	131.587
ScPtSb	6.375	200.261	0.659	PBE	116.107
ScRhTe	6.294	152.471	0.463	PBE	113.466
TaCoC	5.216	139.425	1.536	PBE	239.881
TaCoGe	5.698	172.984	1.206	PBE	191.789
TaCoPb	6.041	247.465	0.973	PBE	149.931
TaCoSi	5.614	148.323	1.238	PBE	205.737
TaCoSn	5.952	198.485	1.039	PBE	166.828
TaFeAs	5.688	172.538	0.9205	PBE	198.364
TaFeBi	6.072	246.741	0.92	PBE	154.273
TaFeP	5.545	148.212	0.837	PBE	220.237
TaFeSb	5.943	198.464	0.856	PBE	177.775
TaIrGe	6.013	246.759	0.932	PBE	202.793
TaIrSi	5.935	222.097	0.795	PBE	215.602
TaIrSn	6.219	272.259	0.942	PBE	185.752
TaNiAl	5.76	147.579	0.585	MBJ	161.643
TaNiB	5.338	138.629	0.778	PBE	217.954
TaNiGa	5.737	171.237	0.243	PBE	168.074
TaNiIn	5.989	196.198	0.181	PBE	145.008
TaNiTl	6.032	245.773	0.427	MBJ	138.713
TaOsBi	6.338	321.125	0.132	MBJ	170.245
TaOsP	5.89	222.596	0.049	PBE	219.375
TaOsSb	6.217	272.847	0.551	PBE	193.959
TaPtAl	6.052	223.073	0.572	PBE	178.819

TaPtB	5.733	214.123	1.327	PBE	215.282
TaPtGa	6.045	246.731	0.94	PBE	181.458
TaPtIn	6.259	271.692	0.923	PBE	161.87
TaPtTl	6.322	321.267	0.952	PBE	152.878
TaRhC	5.557	163.765	0.645	PBE	214.239
TaRhGe	5.961	197.324	1.07	PBE	186.818
TaRhPb	6.266	271.804	1.049	PBE	151.718
TaRhSi	5.885	172.662	0.868	PBE	197.92
TaRhSn	6.18	222.824	1.047	PBE	168.556
TaRuAs	5.955	197.571	0.452	PBE	193.138
TaRuBi	6.293	271.774	0.455	PBE	159.409
TaRuP	5.831	173.245	0.533	PBE	208.181
TaRuSb	6.175	223.496	0.631	PBE	180.683
TiAgAl	6.112	101.136	0.151	PBE	98.093
TiAgB	5.66	92.185	0.337	PBE	133.312
TiAgGa	6.088	124.794	0.177	PBE	98.73
TiAgIn	6.342	149.755	0.072	PBE	86.833
TiAuAl	6.094	150.453	0.695	PBE	120.029
TiAuB	5.7	141.503	0.864	PBE	154.407
TiAuGa	6.09	174.111	0.622	PBE	119.601
TiAuIn	6.337	199.072	0.424	PBE	105.515
TiAuTl	6.419	248.647	0.326	PBE	96.077
TiCoAs	5.601	100.585	1.3	PBE	164.368
TiCoBi	6.026	174.789	0.896	PBE	123.841
TiCoP	5.44	76.26	1.375	PBE	185.328
TiCoSb	5.881	126.511	1.053	PBE	143.102
TiCuB	5.3	67.653	0.216	PBE	159.657
TiCuGa	5.773	100.261	0.065	PBE	113.889
TiFePo	6.035	173.09	0.69	PBE	125.729
TiFeS	5.412	75.154	1.101	PBE	177.363
TiFeSe	5.604	101.111	0.901	PBE	159.409
TiFeTe	5.874	128.034	0.957	PBE	146.945
TiIrAs*	5.931	174.36	0.758	PBE	170.904
TiIrBi*	6.302	248.563	0.617	PBE	138.221
TiIrP	5.791	150.034	0.896	PBE	188.372
TiIrSb*	6.165	200.285	0.807	PBE	159.534
TiNiC	5.099	65.631	0.97	PBE	203.885
TiNiGe	5.661	99.19	0.625	PBE	146.947
TiNiPb	6.042	173.67	0.339	PBE	110.792
TiNiSi	5.568	74.528	0.743	PBE	159.361
TiNiSn	5.942	124.69	0.442	PBE	125.264
TiOsTe	6.163	202.418	0.478	PBE	161.82
TiPtC	5.553	141.125	0.418	PBE	181.595
TiPtGe	5.983	174.684	0.845	PBE	154.395
TiPtPb	6.33	249.164	0.712	PBE	121.255
TiPtSi	5.889	150.022	0.863	PBE	167.809
TiPtSn	6.218	200.184	0.764	PBE	139.058
TiRhAs	5.882	124.925	0.795	PBE	157.132
TiRhBi	6.264	199.128	0.69	PBE	124.931
TiRhP	5.74	100.599	0.799	PBE	173.82
TiRhSb	6.13	150.85	0.719	PBE	143.445
TiRuTe	6.126	153.067	0.745	PBE	148.165
VCoC	4.948	67.465	0.936	PBE	251.033
VCoGe	5.507	101.024	0.66	PBE	177.083
VCoPb	5.899	175.505	0.638	PBE	130.946
VCoSi	5.404	76.363	0.526	PBE	193.569
VCoSn	5.795	126.525	0.614	PBE	149.172

VFeAs	5.491	100.578	0.342	PBE	189.975
VFeBi	5.927	174.781	0.332	PBE	138.494
VFeP	5.325	76.252	0.302	PBE	214.973
VFeSb	5.782	126.503	0.321	PBE	162.745
VIrC	5.386	141.239	0.305	PBE	229.091
VIrGe*	5.831	174.799	0.295	PBE	188.927
VIrPb	6.188	249.279	1.132	MBJ	147.514
VIrSi*	5.732	150.137	0.184	PBE	204.679
VIrSn	6.08	200.299	0.293	PBE	166.402
VNiAl	5.578	75.619	0.12	PBE	143.521
VNiB	5.088	66.668	0.904	PBE	209.252
VNiGa	5.56	99.277	0.319	PBE	148.818
VNiIn	5.847	124.238	0.223	PBE	123.72
VOsAs	5.822	174.962	0.079	PBE	198.697
VOsBi	6.208	249.165	0.119	PBE	155.111
VOsP	5.674	150.636	1.099	MBJ	218.599
VOsSb	6.07	200.887	0.109	PBE	178.244
VPtAl	5.876	151.113	1.015	MBJ	157.257
VPtB	5.488	142.162	0.369	PBE	205.983
VPtGa	5.881	174.771	0.167	PBE	159.105
VPtIn	6.141	199.732	0.699	MBJ	138.323
VPtTl	6.222	249.307	0.29	PBE	127.158
VReTe	6.107	201.893	0.244	MBJ	170.237
VRhC	5.301	91.804	0.452	PBE	218.964
VRhGe	5.787	125.363	0.319	PBE	170.445
VRhPb	6.147	199.844	0.405	PBE	132.571
VRhSi	5.69	100.702	0.187	PBE	185.625
VRhSn	6.042	150.864	0.346	PBE	149.417
VRuAs	5.773	125.61	0.14	PBE	184.823
VRuBi	6.166	199.814	0.199	PBE	143.372
VRuP	5.625	101.285	0.074	PBE	204.176
VRuSb	6.029	151.536	0.176	PBE	163.953
VTcTe	6.074	153.069	0.727	MBJ	158.193
WCoAl	5.63	149.313	0.455	MBJ	195.013
WCoB	5.232	140.362	0.753	PBE	262.595
WCoGa	5.622	172.971	0.346	PBE	201.667
WCoIn	5.874	197.931	0.377	PBE	171.453
WFeC	5.164	139.317	0.518	PBE	273.211
WFeGe	5.623	172.876	0.201	PBE	218.169
WFeSi	5.532	148.214	0.048	PBE	235.323
WFeSn	5.875	198.376	0.235	PBE	188.992
WIrAl	5.929	223.087	0.143	MBJ	212.737
WIrB	5.627	214.136	0.591	MBJ	257.422
WIrGa	5.933	246.745	0.233	MBJ	215.895
WIrIn	6.149	271.706	0.363	MBJ	192.332
WIrTl	6.214	321.281	0.577	MBJ	180.593
WOsGe	5.937	247.26	0.104	MBJ	4.356
WOsPb	6.238	321.74	0.347	MBJ	187.378
WOsSn	6.147	272.76	0.244	MBJ	207.395
WRhAl	5.889	173.652	0.206	MBJ	191.566
WRhB	5.553	164.701	0.764	MBJ	239.525
WRhGa	5.884	197.31	0.266	MBJ	195.501
WRhIn	6.107	222.271	0.23	MBJ	172.84
WRhTl	6.163	271.846	0.078	PBE	163.997
WRuPb	6.192	272.389	0.159	MBJ	173.822
YAgC	6.061	115.565	0.851	MBJ	88.025
YAgSi	6.45	124.463	0.113	MBJ	80.654

YAuGe	6.539	198.441	0.324	MBJ	83.594
YAuSi	6.458	173.78	0.239	PBE	91.42
YAuSn*	6.736	223.942	0.077	MBJ	79.89
YCoS	5.874	99.579	0.061	PBE	108.87
YCoTe	6.296	152.459	0.872	PBE	96.335
YCuC	5.698	91.032	0.085	PBE	105.963
YCuGe	6.233	124.591	0.299	MBJ	82.585
YCuSi	6.158	99.93	0.559	MBJ	88.692
YHgAl	6.715	175.174	0.084	PBE	67.389
YHgB	6.355	166.224	0.096	PBE	78.041
YNiAs	6.101	123.168	0.492	PBE	99.593
YNiBi*	6.493	197.371	0.193	PBE	78.934
YNiP	5.964	98.842	0.594	PBE	108.756
YNiSb*	6.359	149.094	0.285	PBE	90.264
YPtAs	6.423	198.662	0.826	MBJ	101.692
YPtBi*	6.746	272.865	0.424	MBJ	87.827
YPtP	6.305	174.336	0.917	MBJ	107.722
YPtSb*	6.615	224.588	0.094	PBE	98.29
YRhTe*	6.53	176.798	0.158	PBE	96.961
ZrAgB	5.925	116.184	0.24	PBE	127.111
ZrAuAl*	6.316	174.452	0.472	PBE	117.633
ZrAuB	5.976	165.501	0.79	PBE	142.609
ZrAuGa	6.3	198.11	0.594	PBE	117.321
ZrAuIn	6.509	223.07	0.455	PBE	107.861
ZrAuTl	6.572	272.646	0.344	PBE	100.641
ZrCoAs*	5.836	124.584	1.208	PBE	151.444
ZrCoBi*	6.223	198.787	0.985	PBE	118.732
ZrCoP	5.699	100.258	1.284	PBE	166.917
ZrCoSb*	6.094	150.51	1.057	PBE	135.048
ZrCuB	5.587	91.651	0.084	PBE	146.73
ZrFePo	6.232	197.089	0.096	PBE	119.041
ZrFeS	5.669	99.153	0.326	PBE	158.293
ZrFeSe	5.838	125.11	0.112	PBE	145.997
ZrFeTe*	6.084	152.033	1.156	PBE	136.714
ZrIrAs*	6.157	198.358	0.265	PBE	156.638
ZrIrBi*	6.48	272.562	0.204	PBE	133.524
ZrIrP	6.038	174.033	0.782	PBE	168.954
ZrIrSb*	6.358	224.284	1.407	PBE	150.824
ZrNiC	5.397	89.629	0.953	PBE	178.536
ZrNiGe	5.895	123.188	0.665	PBE	137.365
ZrNiPb*	6.239	197.669	0.365	PBE	109.603
ZrNiSi	5.818	98.527	0.786	PBE	146.561
ZrNiSn*	6.148	148.689	0.486	PBE	120.938
ZrPtGe	6.205	198.682	1.192	PBE	144.778
ZrPtPb	6.502	273.163	0.826	PBE	120.947
ZrPtSi	6.129	174.021	1.337	PBE	155.002
ZrPtSn*	6.407	224.183	0.974	PBE	135.589
ZrRhAs*	6.104	148.923	1.204	PBE	148.399
ZrRhBi*	6.443	223.127	1.023	PBE	123.348
ZrRhP	5.984	124.598	1.427	PBE	160.409
ZrRhSb*	6.324	174.849	1.18	PBE	137.754
ZrRuTe*	6.318	177.065	0.888	PBE	141.107

9 Additional Semiconductor Data - TE Quality Factor (β) and Lattice Thermal Conductivity (κ_L).

Table S4: β and κ_L Predictions

Compound	β_n	β_p	κ_L
AcNiAs	34.134	16.016	5.876
AcNiP	3.49	6.702	7.25
AcNiSb	4.487	47.799	5.157
MoCoAl	10.671	28.335	22.953
CrCoAl	1.517	13.314	31.889
CrCoB	3.046	5.148	51.699
CrCoGa	2.742	18.875	24.873
CrCoIn	3.845	20.981	17.093
CrFeC	1.546	3.986	61.675
CrFeGe	2.086	3.349	31.988
CrFeSi	1.012	2.971	48.319
CrFeSn	3.528	9.109	21.467
CrIrAl	1.955	14.202	23.511
CrIrB	1.72	7.971	31.7
CrIrGa	2.805	16.603	21.008
CrIrIn	2.237	19.349	16.043
CrIrTl	1.305	82.541	97.764
CrOsGe	1.71	6.763	25.716
CrOsPb	2.82	21.259	12.579
CrOsSi	1.123	5.717	32.723
CrOsSn	1.852	16.21	20.175
CrReAs	1.724	6.355	25.314
CrReP	1.738	5.752	32.444
CrReSb	1.557	7.904	20.774
CrRhAl	1.158	8.416	28.548
CrRhB	1.953	7.91	41.078
CrRhGa	1.582	13.879	23.483
CrRuC	1.196	5.224	47.53
CrRuGe	1.542	12.278	30.488
CrRuPb	2.466	21.667	13.891
CrRuSi	0.915	10.169	42.159
CrRuSn	1.709	15.217	22.551
CrTcAs	1.47	30.813	31.938
CrTcP	0.966	29.387	43.702
CrTcSb	1.781	30.895	24.251
MoFeSi	0.965	5.206	33.98
HfAgAl	6.512	1.927	10.457
HfAgB	5.447	3.693	13.008
HfAgGa	7.068	3.059	9.005
HfAuAl*	5.684	1.722	11.248
HfAuB	5.046	3.998	12.876
HfAuGa	6.223	3.011	9.886
HfAuIn*	6.915	3.575	8.702
HfAuTl	8.999	23.766	6.512
HfCoAs	2.282	6.018	16.463
HfCoBi	3.597	15.348	9.148
HfCoP	2.097	5.241	20.825
HfCoSb	2.883	5.871	13.888
HfCuB	5.855	3.205	15.441
HfFeTe	6.95	8.022	14

HfIrSb*	12.742	3.071	14.884
HfNiC	3.085	4.478	18.405
HfNiGe	3.997	3.095	14.278
HfNiSi	3.368	1.91	18.593
HfNiSn	4.631	3.328	11.798
HfPdSn	4.739	3.727	11.835
HfPtGe	3.586	3.823	13.747
HfPtPb	5.503	5.3	8.779
HfPtSi	3.276	2.728	16.772
HfPtSn	4.351	3.744	12.551
HfRhAs	11.844	3.715	16.498
HfRhBi	16.492	4.874	10.308
HfRhP	6.18	3.159	20.229
HfRhSb	2.641	3.411	15.157
HfRuTe	64.32	2.082	15.359
LaAuSi	14.3	15.856	6.657
LaAuSn	17.556	54.069	4.964
LaCoS	30.347	6.495	11.445
LaCoSe	60.886	7.472	8.946
LaCoTe	11.238	0.337	7.761
LaCuC	3.789	5.661	9.033
LaFeF	8.288	3.911	2.357
LaHgAl	32.005	34.815	4.438
LaHgIn	8.808	28.036	3.311
LaNiAs	13.558	0.352	8.716
LaNiP	10.904	7.004	11.431
LaNiSb	16.116	0.944	7.328
LaPtSb	179.94	53.926	6.935
LaRhS	59.1	3.811	11.125
LaRhSe	79.688	1.308	9.172
LaRhTe	14.972	1.615	8.343
LaRuF	16.932	0.426	6.573
LiAlGe	3.056	119.951	7.035
MnNiB	0.527	1.312	34.551
MoIrB	3.022	9.412	34.243
MoIrTl	4.446	36.728	14.783
MoOsPb	3.096	22.26	16.684
MoRhB	2.804	22.408	41.263
NbCoC	1.095	4.41	45.876
NbCoGe	4.262	9.4	28.371
NbCoPb	2.888	14.765	13.353
NbCoSi	1.843	2.251	39.32
NbCoSn	9.071	9.427	21.288
NbFeAs	4.106	5.439	30.924
NbFeBi	5.137	8.875	14.71
NbFeP	3.433	4.521	43.627
NbFeSb	4.027	8.278	24.157
NbIrC	10.311	9.04	28.682
NbIrGe*	7.908	48.052	24.695
NbIrPb	6.29	18.779	14.604
NbIrSi	4.971	12.71	30.969
NbIrSn*	5.326	16.052	21.168
NbNiAl	5.327	21.862	26.615
NbNiB	1.866	4.135	39.501
NbNiTl	3.598	33.139	11.483
NbOsAs	5.101	10.711	25.856
NbOsBi	5.996	12.736	16.047

NbOsP	5.283	9.259	32.018
NbOsSb	5.383	9.805	23.51
NbPtAl	6.471	7.191	22.028
NbPtB	5.039	6.439	27.043
NbPtGa	7.769	7.52	19.438
NbPtIn	6.768	10.626	16.101
NbPtTl	2.551	33.771	12.012
NbRhC	1.848	5.55	38.361
NbRhGe	4.469	5.01	27.798
NbRhPb	4.825	4.759	14.454
NbRhSi	3.655	4.843	36.656
NbRhSn	4.132	3.578	22.356
NbRuAs	4.342	7.514	30.583
NbRuBi	5.163	9.968	16.689
NbRuP	3.667	6.237	40.237
NbRuSb	4.301	7.572	25.982
ScAgC	2.539	4.394	13.918
ScAuGe	4.262	4.681	8.983
ScAuSi	3.498	3.535	12.259
ScAuSn*	4.864	4.599	7.998
ScCdIn	4.052	3.532	5.12
ScCdTl	5.783	12.857	3.198
ScCoS	3.123	0.649	23.676
ScCoSe	6.92	1.608	16.688
ScCoTe	1.946	2.258	13.946
ScCuC	2.369	3.634	21.654
ScHgAl	5.372	2.707	7.324
ScHgB	4.608	4.331	8.589
ScHgGa	6.111	3.933	5.606
ScHgIn	6.541	4.258	4.911
ScHgTl	8.541	15.121	3.12
ScNiAs	2.143	3.132	17.218
ScNiBi	4.086	5.735	7.512
ScNiP	1.473	2.141	26.032
ScNiSb	2.781	3.45	13.143
ScPtP	16.906	2.543	15.557
ScPtSb	2.902	4.875	11.6
ScRhTe	4.505	4.046	14.184
TaCoC	1.837	7.18	27.988
TaCoGe	2.462	12.374	21.702
TaCoPb	3.673	21.24	11.659
TaCoSi	1.965	4.47	27.858
TaCoSn	2.86	12.222	17.37
TaFeAs	5.364	8.05	23.159
TaFeBi	3.059	10.481	12.74
TaFeP	5.009	6.933	30.139
TaFeSb	22.982	7.791	19.694
TaIrGe*	6.547	8.485	21.433
TaIrSi	6.176	6.271	25.763
TaIrSn*	28.408	7.052	18.999
TaNiAl	3.92	40.677	19.322
TaNiB	3.329	12.304	26.023
TaNiGa	4.198	40.332	17.265
TaNiIn	4.54	29.256	13.59
TaNiTl	6.084	24.585	9.943
TaOsBi	3.89	14.93	14.417
TaOsP	13.24	11.253	25.608

TaOsSb	6.346	11.861	20.732
TaPtAl	6.776	11.162	19.148
TaPtB	5.153	1.716	22.289
TaPtGa	6.208	14.719	17.454
TaPtIn	3.712	2.659	14.747
TaPtTl	3.532	28.83	11.369
TaRhC	9.259	10.749	25.588
TaRhGe	5.133	7.614	22.374
TaRhPb	3.482	2.148	12.957
TaRhSi	5.234	4.751	27.616
TaRhSn	4.147	8.237	18.934
TaRuAs	7.243	9.601	23.838
TaRuBi	11.097	12.121	14.695
TaRuP	5.183	8.502	29.147
TaRuSb	5.546	9.217	21.745
TiAgAl	3.2	1.071	14.475
TiAgB	2.272	1.637	20.379
TiAgGa	3.646	1.549	11.304
TiAgIn	3.749	1.873	8.723
TiAuAl	2.457	1.098	13.674
TiAuB	2.2	2.11	17.467
TiAuGa	2.908	1.643	11.444
TiAuIn	3.323	1.947	9.318
TiAuTl	4.428	19.956	6.414
TiCoAs	1.147	0.867	27.012
TiCoBi	2.143	1.749	11.586
TiCoP	0.911	3.807	41.292
TiCoSb	1.461	5.982	20.007
TiCuB	2.313	1.271	30.147
TiCuGa	4.062	1.382	14.812
TiFePo	5.941	10.215	12.179
TiFeS	1.886	3.248	37.198
TiFeSe	3.116	4.737	25.25
TiFeTe	2.652	4.983	20.72
TiIrAs*	21.5	1.809	20.877
TiIrBi*	3.467	2.543	12.211
TiIrP	3.274	1.514	26.911
TiIrSb*	2.381	1.816	18.847
TiNiC	1.216	1.467	42.616
TiNiGe	1.989	1.318	22.947
TiNiPb	3.427	2.914	9.439
TiNiSi	1.477	0.74	34.866
TiNiSn	2.376	1.632	16.271
TiOsTe	10.355	1.549	19.158
TiPtC	11.588	1.591	21.407
TiPtGe	2.045	1.975	17.623
TiPtPb	1.997	3.067	9.516
TiPtSi	3.115	1.375	23.056
TiPtSn	1.608	1.943	14.813
TiRhAs	2.447	1.489	24.728
TiRhBi	1.73	2.362	12.402
TiRhP	2.125	1.348	34.664
TiRhSb	1.609	1.573	20.385
TiRuTe	2.084	1.356	21.373
VCoC	2.214	5.6	54.667
VCoGe	2.342	3.095	28.749
VCoPb	2.271	1.433	11.589

VCoSi	2.089	2.497	43.617
VCoSn	1.936	5.354	20.19
VFeAs	2.529	4.6	33.002
VFeBi	2.246	6.85	13.387
VFeP	2.261	26.847	50.492
VFeSb	12.835	4.912	23.948
VIrC	2.558	8.303	29.679
VIrGe*	3.892	7.882	23.481
VIrPb	2.676	1.694	12.661
VIrSi*	3.778	7.156	30.364
VIrSn	3.739	7.74	19.14
VNiAl	0.984	9.285	27.727
VNiB	1.073	0.803	43.682
VNiGa	1.552	13.924	21.417
VNiIn	1.351	2.534	14.656
VOsAs	3.827	2.142	25.884
VOsBi	2.719	2.789	14.302
VOsP	3.742	1.89	32.945
VOsSb	3.214	13.283	21.861
VPtAl	4.116	14.168	19.725
VPtB	3.925	1.405	26.006
VPtGa	3.603	2.043	17.137
VPtIn	2.173	1.682	13.752
VPtTl	1.798	23.346	9.599
VReTe	3.157	15.68	20.366
VRhC	2.589	1.083	41.134
VRhGe	7.775	0.967	26.799
VRhPb	1.718	21.472	12.653
VRhSi	2.532	0.749	38.003
VRhSn	2.601	0.973	20.572
VRuAs	2.817	9.017	31.356
VRuBi	2.418	10.255	15.129
VRuP	2.572	1.206	43.453
VRuSb	2.94	8.521	24.605
VTcTe	3.328	34.722	23.452
WCoAl	6.005	8.013	25.067
WCoB	7.271	8.936	34.205
WCoGa	7.152	7.848	22.46
WCoIn	15.265	9.197	17.223
WFeC	6.635	8.302	34.998
WFeGe	7.75	7.008	26.57
WFeSi	7.933	5.555	34.286
WFeSn	6.794	13.223	21.081
WIrAl	3.93	10.419	24.788
WIrB	9.303	10.472	29.443
WIrGa	5.121	13.393	22.785
WIrIn	8.232	12.674	19.291
WIrTl	7.743	41.701	14.692
WOsGe	9.744	30.129	0.188
WOsPb	8.976	28.385	16.166
WOsSn	4.15	22.122	22.495
WRhAl	2.964	7.91	25.705
WRhB	8.955	13.206	32.079
WRhGa	6.186	9.35	22.988
WRhIn	6.044	10.01	18.786
WRhTl	6.856	36.704	13.97
WRuPb	8.362	25.959	16.132

YAgC	5.616	28.319	9.571
YAgSi	3.879	10.425	10.09
YAuGe	23.151	16.358	6.864
YAuSi	11.682	12.752	8.958
YAuSn*	17.698	16.524	6.347
YCoS	8.372	1.456	14.88
YCoTe	2.242	5.763	10.156
YCuC	3.62	21.515	13.348
YCuGe	4.372	11.725	8.906
YCuSi	3.626	16.372	12.422
YHgAl	17.707	9.166	5.878
YHgB	5.676	14.075	6.348
YNiAs	2.668	18.898	11.81
YNiBi*	4.834	32.497	5.961
YNiP	2.136	13.548	16.19
YNiSb*	3.36	20.98	9.611
YPtAs	7.829	33.973	9.285
YPtBi*	9.258	22.748	6.182
YPtP	12.982	21.985	11.022
YPtSb*	32.755	24.938	8.753
YRhTe*	10.029	18.882	10.473
ZrAgB	9.681	5.603	17.937
ZrAuAl*	11.602	7.943	13.318
ZrAuB	9.576	7.244	15.809
ZrAuGa	12.723	5.027	11.294
ZrAuIn	5.399	5.709	9.81
ZrAuTl	6.378	27.894	7.128
ZrCoAs*	1.678	4.991	22.023
ZrCoBi*	2.938	6.367	10.823
ZrCoP	1.267	3.422	30.713
ZrCoSb*	2.073	4.813	17.458
ZrCuB	10.434	5.196	23.408
ZrFePo	11.588	3.444	11.063
ZrFeS	5.156	2.082	27.06
ZrFeSe	8.054	2.319	20.319
ZrFeTe*	1.326	2.528	17.543
ZrIrAs*	17.353	7.734	18.216
ZrIrBi*	61.934	13.331	11.814
ZrIrP	52.883	6.494	22.455
ZrIrSb*	5.158	7.585	17.285
ZrNiC	1.85	9.088	30.211
ZrNiGe	2.836	7.509	19.182
ZrNiPb*	22.131	14.006	9.374
ZrNiSi	2.066	2.807	26.606
ZrNiSn*	3.24	2.161	14.748
ZrPtGe	2.881	6.736	16.067
ZrPtPb	4.507	4.319	9.775
ZrPtSi	6.161	5.125	20.274
ZrPtSn*	3.407	2.674	14.412
ZrRhAs*	1.863	7.957	21.726
ZrRhBi*	6.412	15.044	12.261
ZrRhP	3.404	5.071	28.405
ZrRhSb*	1.886	9.247	18.575
ZrRuTe*	4.98	6.284	19.157