Supporting information

Efficient first-principles prediction of solid stability: Towards chemical accuracy

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Figure S1: The cumulative probability that the energy of the most stable structure predicted by PBE or SCAN lies below a threshold energy of the experimentally–reported low–temperature structure across all chemistries in our dataset.

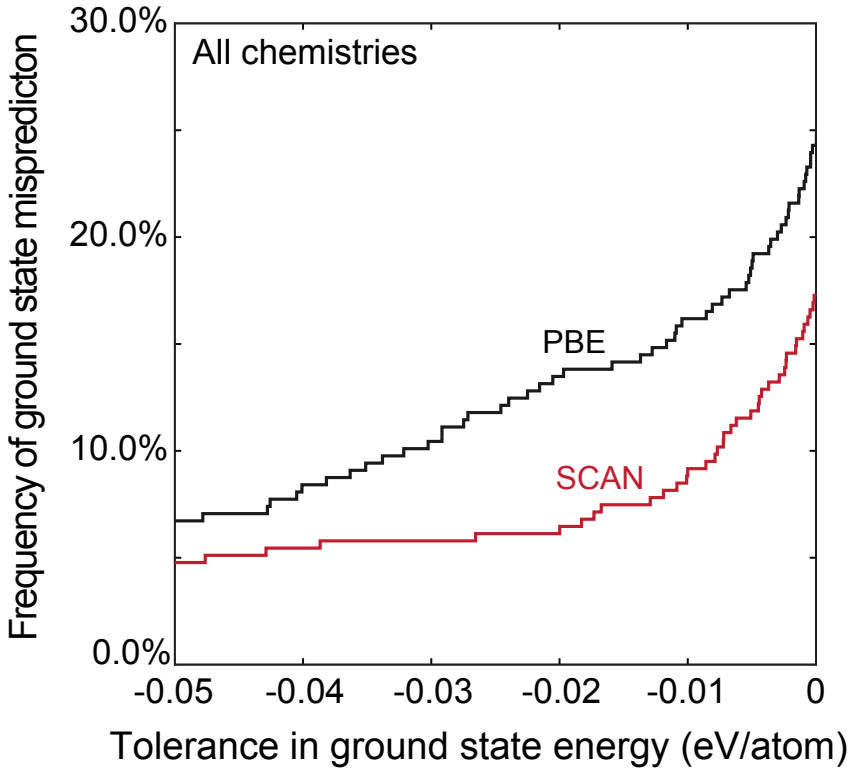

Table S1: Enthalpy of formation (eV/atom) of 101 binary compounds (including 20 oxides) without transition metal ions

System	Experiment	PBE	SCAN	PBE error	SCAN error
AlAs	-0.61	-0.487	-0.595	-0.12	-0.01
$AlCl_3$	-1.82	-1.51	-1.783	-0.31	-0.04
AlF_3	-3.90	-3.552	-4.113	-0.35	0.21
AlN	-1.61	-1.409	-1.728	-0.20	0.12
Al_2O_3	-3.47	-3.017	-3.504	-0.45	0.03
Al_2S_3	-1.50	-1.061	-1.233	-0.44	-0.27
Al_2Se_3	-1.18	-0.846	-0.981	-0.33	-0.20
Al_2Te_3	-0.68	-0.451	-0.496	-0.23	-0.18
BaO	-2.86	-2.481	-2.829	-0.38	-0.03
BaO_2	-2.19	-1.853	-2.124	-0.34	-0.07
BaS	-2.38	-2.081	-2.352	-0.30	-0.03
BeO	-3.14	-2.762	-3.215	-0.38	0.08
BeS	-1.21	-1.061	-1.338	-0.15	0.13
Be_3N_2	-1.22	-1.078	-1.399	-0.14	0.18
$CaCl_2$	-2.75	-2.403	-2.725	-0.35	-0.03
CaF_2	-4.21	-3.900	-4.456	-0.31	0.25
CaO	-3.29	-2.968	-3.353	-0.32	0.06
CaS	-2.45	-2.155	-2.432	-0.30	-0.02
GaAs	-0.37	-0.352	-0.374	-0.02	0.00
$GaCl_3$	-1.36	-1.111	-1.272	-0.25	-0.09
GaF_3	-3.01	-2.609	-3.076	-0.40	0.07
GaN	-0.81	-0.480	-0.655	-0.33	-0.16
GaS	-1.09	-0.652	-0.699	-0.44	-0.39
GaSb	-0.22	-0.165	-0.153	-0.06	-0.07
GaSe	-0.83	-0.595	-0.606	-0.24	-0.22
Ga_2O_3	-2.26	-1.858	-2.187	-0.40	-0.07
Ga_2S_3	-1.07	-0.664	-0.746	-0.41	-0.32
Ga_2Se_3	-0.85	-0.589	-0.632	-0.26	-0.22
GeS	-0.39	-0.333	-0.222	-0.06	-0.17
GeSe	-0.48	-0.249	-0.171	-0.23	-0.31
InAs	-0.31	-0.249	-0.317	-0.06	0.01
InN	-0.10	0.082	-0.109	-0.18	0.01
InS	-0.70	-0.509	-0.646	-0.19	-0.05
InSb	-0.16	-0.131	-0.174	-0.03	0.01
InTe	-0.50	-0.298	-0.308	-0.20	-0.19
In_2O_3	-1.92	-1.600	-1.952	-0.32	0.03
In_2S_3	-0.74	-0.557	-0.692	-0.18	-0.05
KC	-2.26	-1.964	-2.236	-0.30	-0.02
KF	-2.94	-2.699	-3.097	-0.24	0.16
KSb	-0.43	-0.443	-0.53	0.01	0.10

KSb_2	-0.37	-0.304	-0.354	-0.07	-0.02
K_2O	-1.25	-1.031	-1.27	-0.22	0.02
K_2O_2	-1.28	-1.066	-1.259	-0.21	-0.02
K_2S	-1.31	-1.068	-1.253	-0.24	-0.06
K_2S_2	-1.12	-0.940	-1.103	-0.18	-0.02
K_2Se	-1.36	-1.110	-1.284	-0.25	-0.08
K_3As	-0.48	-0.335	-0.439	-0.15	-0.04
K_3Bi	-0.60	-0.382	-0.460	-0.22	-0.14
K_3Sb	-0.47	-0.418	-0.507	-0.05	0.04
K_5Sb_4	-0.44	-0.444	-0.53	0.00	0.09
LiCl	-2.12	-1.816	-2.095	-0.30	-0.03
LiF	-3.19	-2.923	-3.37	-0.27	0.18
Li_2O	-2.07	-1.837	-2.113	-0.23	0.04
Li_2O_2	-1.64	-1.416	-1.636	-0.22	0.00
Li_2S	-1.52	-1.341	-1.527	-0.18	0.01
Li_2Se	-1.45	-1.267	-1.436	-0.18	-0.01
Li_3Bi	-0.60	-0.535	-0.601	-0.06	0.00
Li_3N	-0.43	-0.369	-0.510	-0.06	0.08
Li_3Sb	-0.83	-0.637	-0.699	-0.19	-0.13
$MgCl_2$	-2.21	-1.864	-2.161	-0.35	-0.05
MgF_2	-3.88	-3.550	-4.053	-0.33	0.17
MgO	-3.11	-2.715	-3.121	-0.40	0.01
MgS	-1.79	-1.433	-1.658	-0.36	-0.13
MgSe	-1.52	-1.257	-1.440	-0.26	-0.08
MgTe	-1.08	-0.879	-0.991	-0.20	-0.09
Mg_3Bi_2	-0.32	-0.208	-0.266	-0.11	-0.05
Mg_3Sb_2	-0.49	-0.370	-0.415	-0.12	-0.08
NaCl	-2.13	-1.813	-2.098	-0.32	-0.03
NaF	-2.97	-2.700	-3.137	-0.27	0.17
NaSb	-0.33	-0.333	-0.404	0.00	0.07
$NaTe_3$	-0.35	-0.388	-0.473	0.04	0.12
Na_2O	-1.43	-1.219	-1.476	-0.21	0.05
Na_2O_2	-1.32	-1.077	-1.293	-0.24	-0.03
Na_2S	-1.26	-1.074	-1.271	-0.19	0.01
Na_2S_2	-1.03	-0.833	-1.003	-0.20	-0.03
Na_2Se	-1.18	-1.074	-1.257	-0.11	0.08
Na_2Se_2	-0.97	-0.834	-0.994	-0.14	0.02
Na_3As	-0.53	-0.423	-0.528	-0.11	0.00
Na_3Bi	-0.46	-0.384	-0.452	-0.08	-0.01
Na_3Sb	-0.53	-0.441	-0.523	-0.09	-0.01
RbCl	-2.26	-1.952	-2.217	-0.31	-0.04
RbF	-2.89	-2.639	-3.036	-0.25	0.15
RbSb	-0.52	-0.433	-0.523	-0.09	0.00
$RbSb_2$	-0.35	-0.304	-0.354	-0.05	0.00
Rb_2O	-1.17	-0.919	-1.164	-0.25	-0.01

Rb_2S	-1.25	-1.009	-1.198	-0.24	-0.05
Rb_3Sb	-0.45	-0.365	-0.459	-0.09	0.01
SiO_2	-3.13	-2.980	-3.195	-0.15	0.07
SiS_2	-0.88	-0.657	-0.748	-0.22	-0.13
$SiSe_2$	-0.61	-0.376	-0.493	-0.23	-0.12
SnO	-1.48	-1.290	-1.412	-0.19	-0.07
SnO_2	-1.97b	-1.652	-1.976	-0.32	0.01
SnS	-0.57	-0.443	-0.417	-0.13	-0.15
SnS_2	-0.53	-0.379	-0.419	-0.15	-0.11
SnSe	-0.47	-0.436	-0.365	-0.03	-0.10
$SnSe_2$	-0.43	-0.348	-0.353	-0.08	-0.08
SrO	-3.07	-2.739	-3.117	-0.33	0.05
SrO	-2.19	-1.892	-2.177	-0.30	-0.01
SrS	-2.45	-2.151	-2.439	-0.30	-0.01
Sr_2Bi	-1.08	-0.761	-0.867	-0.32	-0.21
Sr_2Sb	-1.11	-0.864	-0.970	-0.25	-0.14
MAE				0.217	0.084

Table S2: Enthalpy of formation (eV/atom) of 95 binary compounds (including 27 oxides) with transition metal ions

System	Experiment	PBE	SCAN	PBE error	SCAN error
AgO	-0.06	-0.107	-0.265	0.05	0.20
Ag_2O	-0.11	-0.096	-0.189	-0.01	0.08
Ag_2S	-0.11	-0.062	-0.069	-0.05	-0.04
Ag_2Se	-0.15	-0.079	-0.079	-0.07	-0.07
$CdCl_2$	-1.35	-1.097	-1.322	-0.25	-0.03
CdF_2	-2.42	-2.159	-2.654	-0.26	0.23
CdO	-1.34	-1.031	-1.325	-0.31	-0.02
CdS	-0.78	-0.643	-0.736	-0.14	-0.04
CdSb	-0.07	-0.051	-0.062	-0.02	-0.01
CdSe	-0.75	-0.633	-0.692	-0.12	-0.06
CdTe	-0.48	-0.464	-0.477	-0.02	0.00
Cd_3As_2	-0.08	-0.103	-0.114	0.02	0.03
CoF_2	-2.39	-1.702	-2.137	-0.69	-0.25
CoF_3	-2.10	-1.712	-1.901	-0.39	-0.20
CoO	-1.23	-0.672	-0.909	-0.56	-0.32
CoS	-0.43	-0.273	-0.146	-0.16	-0.28
$CoSb_3$	-0.17	-0.192	-0.156	0.02	-0.01
CoSe	-0.32	-0.275	-0.176	-0.05	-0.14
Co_3O_4	-1.32	-0.987	-1.071	-0.33	-0.25
Co_3S_4	-0.53	-0.430	-0.350	-0.10	-0.18
CrN	-0.65	-0.343	-0.673	-0.31	0.02
CrO_2	-2.07	-1.900	-2.337	-0.17	0.27
CrS	-0.81	-0.468	-0.824	-0.34	0.01
Cr_2O_3	-2.36	-1.926	-2.392	-0.43	0.03
CuF_2	-1.88	-1.517	-1.891	-0.36	0.01
CuO	-0.82	-0.600	-0.791	-0.22	-0.03
CuS	-0.28	-0.199	-0.250	-0.08	-0.03
CuSe	-0.21	-0.137	-0.143	-0.07	-0.07
Cu_2O	-0.58	-0.414	-0.501	-0.17	-0.08
Cu_2Sb	-0.04	0.011	0.011	-0.05	-0.05
Cu_2Se	-0.21	0.013	0.030	-0.22	-0.24
Cu_2Te	0.07	0.086	0.098	-0.02	-0.03
Cu_3N	0.19	0.282	0.267	-0.09	-0.08
Cu_3Sb	-0.02	0.067	0.084	-0.09	-0.10
FeF_2	-2.46	-1.916	-2.443	-0.54	-0.02
FeO	-1.41	-0.877	-1.191	-0.53	-0.22
FeS	-0.52	-0.515	-0.365	-0.01	-0.15
FeSe	-0.39	-0.281	-0.100	-0.11	-0.29
Fe_2O_3	-1.71	-1.172	-1.155	-0.54	-0.56
Fe_3O_4	-1.66	-1.122	-1.706	-0.54	0.05

HfN	-1.91	-1.752	-1.982	-0.16	0.07
HfO_2	-3.95	-3.566	-4.026	-0.38	0.08
$HgCl_2$	-0.77	-0.605	-0.735	-0.17	-0.03
HgO	-0.47	-0.294	-0.427	-0.18	-0.04
HgS	-0.30	-0.135	-0.137	-0.17	-0.16
HgSe	-0.24	-0.215	-0.195	-0.03	-0.04
HgTe	-0.22	-0.171	-0.168	-0.05	-0.05
$LaCl_3$	-2.78	-2.414	-2.775	-0.37	0.00
LaN	-1.57	-1.33	-1.627	-0.24	0.06
LaS	-2.36	-2.17	-2.378	-0.19	0.02
La_2O_3	-3.72	-3.468	-3.876	-0.25	0.16
La_2S_3	-2.51	-2.201	-2.468	-0.31	-0.04
NbN	-1.22	-1.077	-1.249	-0.14	0.03
NbO_2	-2.75	-2.447	-2.785	-0.30	0.04
NiF_2	-2.25	-1.656	-1.98	-0.59	-0.27
NiO	-1.24	-0.472	-0.765	-0.77	-0.48
NiSb	-0.34	-0.273	-0.289	-0.07	-0.05
NiSe	-0.31	-0.287	-0.255	-0.02	-0.05
Ni_3S_2	-0.42	-0.374	-0.393	-0.05	-0.03
$PdCl_2$	-0.69	-0.482	-0.68	-0.21	-0.01
PdO	-0.44	-0.445	-0.754	0.01	0.31
PdS_2	-0.28	-0.268	-0.369	-0.01	0.09
PtO	-0.37	-0.242	-0.485	-0.13	0.12
PtO_2	-0.57	-0.465	-0.757	-0.11	0.19
PtS	-0.42	-0.411	-0.613	-0.01	0.19
PtS_2	-0.38	-0.351	-0.494	-0.03	0.11
Pt_3O_4	-0.4	-0.440	-0.690	0.04	0.29
ScAs	-1.39	-1.375	-1.521	-0.01	0.13
$ScCl_3$	-2.40	-2.125	-2.427	-0.28	0.03
ScF_3	-4.22	-3.931	-4.469	-0.29	0.25
Sc_2O_3	-3.94	-3.559	-4.002	-0.38	0.06
TiAs	-0.78	-0.926	-1.017	0.15	0.24
$TiCl_4$	-1.7	-1.597	-1.812	-0.1	0.11
TiN	-1.58	-1.723	-1.996	0.14	0.42
TiO_2	-3.26	-3.048	-3.487	-0.21	0.23
TiS	-1.41	-1.427	-1.552	0.02	0.14
TiS_2	-1.41	-1.280	-1.459	-0.13	0.05
Ti_2O_3	-3.15	-2.896	-3.307	-0.25	0.16
VN	-1.13	-0.976	-1.149	-0.15	0.02
VO_2	-2.47	-2.346	-2.742	-0.12	0.27
YAs	-1.68	-1.553	-1.753	-0.13	0.07
YCl_3	-2.59	-2.290	-2.612	-0.30	0.02
YF_3	-4.45	-4.112	-4.726	-0.34	0.28
$ZnCl_2$	-1.43	-1.149	-1.339	-0.28	-0.09
ZnF_2	-2.64	-2.318	-2.751	-0.32	0.11

ZnO	-1.81	-1.445	-1.728	-0.37	-0.08
ZnS	-1.07	-0.811	-0.921	-0.26	-0.15
ZnSb	-0.08	-0.032	-0.015	-0.05	-0.06
ZnSe	-0.85	-0.716	-0.780	-0.13	-0.07
ZnTe	-0.61	-0.470	-0.475	-0.14	-0.14
Zn_3As_2	-0.28	-0.144	-0.123	-0.14	-0.16
Zn_3N_2	-0.05	0.114	-0.034	-0.16	-0.02
ZrN	-1.89	-1.683	-2.009	-0.21	0.12
ZrO_2	-3.80	-3.360	-3.939	-0.44	0.14
ZrS_2	-1.96	-1.519	-1.760	-0.44	-0.20
MAE				0.204	0.122

Table S3: Error in unit cell volume in PBE and SCAN of the experimental ground states of binary chemistries used in ground state selection statistics

Chemistry	Exp. volume (Å^3/at.)	PBE Error (%)	SCAN Error (%)
Main group compounds			
Mean Error (%)		4.20	0.49
RMSE (%)		7.69	3.81
Al_2O_3	8.4	3.6	-0.1
Al_2S_3	21.3	5.0	1.6
Al_2Se_3	24.6	5.8	2.0
AlAs	22.2	6.2	2.8
AlF_3	10.9	5.4	-2.1
AlN	10.5	1.1	-1.6
AlP	20.0	4.3	2.0
AlSb	28.7	5.5	2.3
AsS	24.6	29.3	7.5
AsSe	26.5	19.3	6.1
$BaCl_2$	29.2	5.3	1.7
BaF_2	19.8	4.3	0.7
BaI_2	42.2	4.9	2.8
BaO	21.0	5.5	3.0
BaO_2	16.1	7.7	4.6
BaS	32.4	4.0	3.1
BaSe	35.9	3.9	3.0
$BaSe_3$	28.2	5.0	3.2
BaTe	40.0	11.3	10.9
$BaTe_2$	38.2	4.3	3.6
$BaTe_3$	34.7	4.0	4.1
$BeBr_2$	26.8	30.8	4.1
BeF_2	12.4	-5.4	-14.3
BeO	6.7	4.1	1.2
BeS	14.4	0.9	0.0
BeTe	21.5	6.0	4.5
Bi_2O_3	16.5	3.4	-1.1
Bi_2Te_3	33.7	8.1	4.8
$BiCl_3$	27.6	15.7	-2.1
BiSe	28.7	9.5	5.6
BiTe	33.9	6.1	2.6
Ca_2As_3	23.8	2.0	0.6
Ca_3N_2	18.9	-0.0	-1.7

$CaBr_2$	32.7	4.6	0.5
$CaCl_2$	28.1	2.9	0.0
CaF_2	13.6	2.9	-0.8
CaI_2	40.6	13.3	4.0
CaO	13.6	3.9	1.3
CaS	22.9	1.8	1.0
CaSe	26.0	2.1	0.7
CaTe	32.1	1.9	1.2
Cs_2O	33.1	15.0	2.5
Cs_3As	46.8	8.6	1.8
CsBr	39.2	8.3	2.1
CsCl	34.8	6.3	0.2
CsF	28.7	0.0	-6.3
CsI	47.6	7.2	1.7
Ga_2O_3	10.5	6.4	1.3
Ga_2S_3	21.3	7.9	2.6
Ga_2Se_3	24.4	7.4	2.3
GaAs	20.9	14.5	8.9
GaN	11.4	5.5	1.3
GaP	19.2	10.2	6.0
GaSb	26.2	15.2	9.4
GaSe	24.1	17.8	5.4
Ge_3N_4	12.3	6.2	2.4
GeO_2	9.2	7.2	2.1
GeSe	22.6	10.0	7.8
$GeSe_2$	29.0	19.9	6.6
GeTe	26.9	4.5	-1.2
In_2S_3	23.5	6.5	2.7
In_2Te_3	29.3	29.0	29.5
In_3Te_4	30.8	7.6	3.6
InAs	27.7	8.4	3.8
InN	15.4	7.8	4.1
InP	25.3	6.7	3.3
InSb	33.9	8.3	3.3
InTe	31.9	5.0	2.8
K_2O	22.2	2.4	-3.9
K_2O_2	19.1	3.8	-1.8
K_2S	32.9	5.8	2.2
K_2Se	37.9	2.0	-1.1
K_2Te	45.4	2.7	-0.1
K_2Te_3	37.7	2.8	-0.7
KBr	35.9	5.2	-1.1
KCl	30.9	5.0	-1.1
KF	19.1	4.4	-2.9
KI	43.8	6.2	0.5

KSe	34.6	4.3	-0.6
Li_2In	18.8	0.6	-1.8
Li_2O	8.2	1.9	-2.5
Li_2O_2	8.2	2.0	-3.1
Li_2S	15.6	-0.3	-2.0
Li_2Sb	19.8	1.1	-0.1
Li_2Se	18.2	0.0	-1.7
Li_2Te	22.7	2.0	1.2
Li_3As	16.3	-0.5	-2.3
Li_3Bi	18.9	1.5	0.0
Li_3N	11.2	-0.6	-2.6
Li_3Sb	17.6	0.0	-0.9
LiBr	20.8	23.4	18.8
LiCl	17.0	0.7	-2.9
LiF	8.2	3.4	-4.0
LiI	32.3	3.7	0.9
LiO_2	9.6	-0.6	-7.0
LiPb	21.8	4.3	0.2
LiSi	15.7	-0.5	-1.5
LiTl	20.3	5.3	-1.0
$MgBr_2$	26.4	16.6	3.1
$MgCl_2$	21.9	16.8	3.6
MgF_2	10.9	3.9	-2.1
MgI_2	34.3	15.5	4.3
MgO	9.4	1.9	-2.4
MgS	17.5	1.7	-0.3
MgSe	20.4	2.5	-0.6
MgTe	32.7	5.7	3.0
Na_2In	30.0	0.8	-4.6
Na_2O	14.2	-0.3	-7.7
Na_2O_2	12.4	-0.5	-7.9
Na_2S	23.3	0.0	-4.6
Na_2S_5	23.2	3.4	-3.5
Na_2Se	26.5	0.0	-5.0
Na_2Te	32.6	0.0	-3.9
Na_3As	25.1	0.8	-4.2
Na_3Bi	31.2	1.2	-3.7
Na_3P	23.6	-0.8	-5.2
Na_3Sb	29.7	-0.3	-3.9
NaBi	28.7	0.0	-4.9
NaBr	26.5	1.9	-5.0
NaCl	22.4	0.7	-6.6
NaF	13.7	-9.7	-18.1
NaGe	25.6	0.9	-3.9
NaI	34.0	0.9	-4.1

NaO_2	13.5	-0.6	-8.0
NaO_3	13.3	2.9	-8.0
NaP	21.6	-0.4	-4.4
NaPb	31.0	3.0	-2.3
NaS	22.3	0.2	-5.1
NaS_2	22.6	2.3	-3.5
NaSb	29.8	1.5	-2.1
NaSe	25.0	2.8	-2.4
$NaSe_2$	26.4	2.5	-2.5
NaTe	30.2	1.1	-2.8
NaTl	26.0	8.1	-3.2
P_2O_5	11.7	7.6	-1.4
P_2S_5	25.2	32.1	4.9
P_2Se_5	27.0	20.4	5.1
P_4S_7	23.9	29.0	5.1
P_4Se_5	26.5	16.5	5.7
PSe	26.2	31.0	7.0
$PbBr_2$	30.0	10.7	2.4
PbO	19.4	14.3	3.9
PbSe	28.8	3.9	1.2
Rb_2O	25.7	8.2	2.3
Rb_2S	37.5	8.1	5.6
RbBr	40.3	8.5	3.1
RbCl	35.1	8.3	3.3
RbF	22.4	7.4	2.2
RbI	49.2	7.7	2.4
Sb_2O_5	11.4	6.0	0.9
Sb_2S_3	24.4	8.1	3.7
Sb_2Te_3	31.2	8.7	5.8
SbO_2	12.8	6.1	1.2
SeCl	29.7	30.4	2.0
SeO_2	14.7	11.7	0.3
SeO_3	15.3	17.2	-1.5
SiC	10.3	2.2	0.3
SiO_2	12.6	6.7	0.5
Sn_3N_4	13.2	3.5	0.0
$SnBr_2$	31.2	14.3	3.5
$SnCl_2$	26.5	12.5	1.6
SnF_2	17.8	8.3	-4.4
SnF_3	18.0	18.0	13.9
SnI_2	38.8	8.0	2.7
SnO	17.3	9.3	1.0
SnO_2	11.9	5.8	1.6
SnS	24.1	6.5	4.7
SnSe	27.0	5.1	3.3

$SnSe_2$	25.7	16.5	7.0
SnTe	31.6	4.2	0.9
$SrBr_2$	32.1	5.2	1.0
$SrCl_2$	28.2	3.3	0.3
SrF_2	16.2	3.7	-0.4
SrI_2	41.4	5.4	2.3
SrO	17.0	3.9	1.2
SrO_2	13.8	5.3	1.3
SrS	27.1	2.9	1.5
SrSe	30.3	3.5	1.9
SrTe	36.9	2.9	2.0
Te_2O_5	13.8	8.7	1.7
Te_3As_2	28.5	8.0	3.9
TeF_6	14.6	16.9	-4.4
TeO_2	14.7	7.2	0.1
TeO_3	11.3	8.1	2.0
TePb	33.7	4.7	2.0
TlBr	31.6	3.3	-2.2
TlCl	28.3	2.3	-3.7
TlF	19.8	15.7	2.3
TlI	38.7	8.1	1.6
TlTe	32.4	4.5	0.8

Transition metal compounds

Mean Error (%)		0.96	0.28
RMSE (%)		3.95	2.62
AgBr	23.6	5.2	1.0
AgCl	21.4	3.1	-1.5
AgF	14.9	6.0	-1.0
AgI	34.2	6.1	1.7
AgO	13.3	8.0	1.7
AgSe	22.5	17.9	12.6
$CdCl_2$	24.9	16.0	2.4
CdF_2	13.0	5.5	0.1
CdO	13.0	5.4	1.1
CdS	25.1	4.2	0.4
CdSe	28.1	6.5	2.2
CdTe	32.9	10.4	5.8
CoAs	13.5	-0.7	-4.8
CoN	9.9	-3.5	-3.1
CoO	9.6	-0.6	-1.7
CoP	11.6	-1.5	-4.0
CoS	12.8	-2.8	3.8

CoSb	16.9	-0.1	1.5
CoSe	15.0	-2.2	2.5
CrN	8.9	-1.2	0.0
CrO	8.6	19.9	18.5
CrP	12.5	-2.7	9.0
CrS	14.8	2.8	6.8
CrSb	20.1	0.5	0.8
Cu_2Se	16.0	4.1	-0.4
Cu_3N	13.8	1.9	-2.0
CuBr	23.0	2.1	-2.6
CuCl	20.8	-4.0	-8.2
CuI	28.4	-1.1	-5.2
CuO	10.1	11.0	5.6
CuS	16.9	1.9	-1.9
CuSe	19.8	4.4	-0.9
CuTe	22.3	6.3	1.9
FeAs	13.8	-2.1	-2.6
FeN	10.0	-5.1	8.6
FeO	10.2	-5.0	-4.9
FeP	11.7	-2.6	-4.1
FeS	14.7	-9.4	0.2
FeSb	18.3	-3.6	-2.7
FeSe	19.6	9.8	7.3
FeTe	22.9	4.9	5.5
HfN	11.5	0.9	-1.8
HgO	16.1	14.6	4.2
HgS	23.8	16.4	6.3
HgSe	28.1	9.6	3.6
HgTe	32.3	14.2	5.8
LaN	18.7	0.0	-0.8
LaS	25.1	1.1	1.1
MnAs	17.1	-7.2	-1.9
MnN	9.5	-5.6	-4.1
MnO	10.7	1.6	-0.4
MnP	12.3	-2.4	2.1
MnS	18.0	-6.2	-5.2
MnSb	21.4	-4.4	-2.0
MnSe	20.2	-2.9	-2.7
MnTe	24.8	-5.5	-4.5
MoAs	16.1	2.1	-1.0
MoP	14.5	0.1	-1.3
NbAs	17.4	2.7	0.5
NbN	10.6	3.3	2.6
NbP	15.8	2.1	1.5
NiAs	14.3	1.7	-3.8

NiO	9.1	1.5	-0.8
NiS	14.0	-0.9	-0.4
NiSb	17.1	3.0	-1.4
NiSe	15.5	0.5	4.4
NiTe	18.3	1.7	-3.3
PdO	12.2	5.5	1.4
PtO	12.3	7.5	3.3
PtS	18.4	3.6	-1.1
PtS_2	18.3	28.5	8.7
AsRh	15.3	3.8	-0.6
SbRh	18.2	3.9	0.5
AsRu	14.1	9.7	5.6
PRu	13.4	1.6	-0.4
SbRu	18.2	3.6	0.4
ScAs	20.4	1.3	0.4
ScF_3	16.3	3.8	0.5
ScN	10.9	5.3	3.9
ScP	18.7	0.1	-0.2
ScSb	25.0	2.0	0.6
TaAs	17.2	2.0	-1.4
TaN	11.3	1.5	-0.8
TaP	15.8	0.4	-1.7
TiAs	17.7	-2.0	-4.2
TiN	10.6	-9.6	-10.5
TiO	9.3	6.1	6.5
TiP	15.5	-0.1	-1.1
TiS	14.9	3.0	1.9
TiS_2	19.1	12.4	3.4
TiSb	22.6	-2.5	-5.2
TiTe	20.5	4.2	9.2
VAs	15.5	-0.8	1.5
VN	8.8	-0.4	2.3
VO	8.7	10.5	11.7
VP	13.6	-1.9	0.2
VSb	21.5	-3.2	-4.4
YAs	24.5	1.0	0.4
YN	13.7	7.8	6.8
YP	22.7	0.4	0.6
YSb	29.3	1.9	1.2
ZnO	11.8	5.0	-0.1
ZnS	19.8	2.2	-2.1
ZnSe	22.8	3.6	-1.2
ZnTe	28.0	5.7	0.7

Table S4: Binary chemistries included in the ground state structure selection statistics

Legend

- PBE and SCAN energy values, where given, indicate the energy difference, in eV per atom, between the crystal structure preferred by the functional and that of the experimentally–reported ground state. In cases where no energy is given, the crystal structure chosen by the functional agrees with the experimentally–reported ground state.
- AB denotes an incorrect ground state in PBE only
- AB denotes an incorrect ground state in SCAN only
- AB denotes an incorrect ground state in PBE and SCAN
- Source: ICSD denotes only a single known structure in the ICSD

Chemistry	PBE (eV/at.)	SCAN (eV/at.)	Spacegroup	ICSD ID	Source
Main group compounds					
Al_2O_3			$R\bar{3}c$	9770 (+80 others)	[1]
Al_2S_3	-0.002	-0.003	$P6_1$	300213	[2]
Al_2Se_3			Cc	14373	[3]
AlAs			$F\bar{4}3m$	67784 (+7 others)	[4]
AlF_3			R32	30274 (+4 others)	[5]
AlN			$P6_3mc$	31169 (+21 others)	[6]
AlP			$F\bar{4}3m$	24490 (+6 others)	[4]
AlSb			$F\bar{4}3m$	24804 (+9 others)	[4]
AsS			$P2_1/c$	15238 (+11 others)	[7]
AsSe			$P2_1/c$	2056 (+5 others)	ICSD
$BaCl_2$	-0.024		Pnma	15705 (+3 others)	[8]
BaF_2			$Fm\bar{3}m$	41649 (+5 others)	[9]
BaI_2			Pnma	15707 (+2 other)	[9]
BaO			$Fm\bar{3}m$	26961 (+7 others)	[10, 11]
BaO_2			I4/mmm	24248 (+4 others)	[12]
BaS			$Fm\bar{3}m$	30240 (+6 others)	ICSD
BaSe			$Fm\bar{3}m$	43655 (+6 others)	[13]
$BaSe_3$			$P\bar{4}2_1m$	16359	[14]
BaTe			$Fm\bar{3}m$	29152 (+4 others)	[15]
$BaTe_2$			I4/mcm	75555 (+2 other)	ICSD
$BaTe_3$			$P\bar{4}2_1m$	36366	ICSD
$BeBr_2$			Ibam	92584	ICSD

BeF_2			$P6_222$	9481 (+3 others)	[16]
BeO			$P6_3mc$	15620 (+31 others)	[10, 11]
BeS			$F\bar{4}3m$	44724 (+3 others)	[11]
BeTe			$F\bar{4}3m$	53945 (+2 other)	[11]
Bi_2O_3			$P2_1/c$	2374 (+7 others)	[17]
Bi_2Te_3			$R\bar{3}m$	15753 (+6 others)	[18]
$BiCl_3$	-0.056	-0.009	$Pna2_1$	2866 (+2 other)	[19]
BiSe			$P\bar{3}m1$	20458 (+2 other)	[20]
BiTe			$P\bar{3}m1$	30525 (+4 others)	[21]
Ca_2As_3			$P2/c$	43876	ICSD
Ca_3N_2			$Ia3$	34678 (+5 others)	[22–24]
$CaBr_2$	-0.021	-0.007	$Pnnm$	14220 (+11 others)	[25]
$CaCl_2$		-0.002	$Pnnm$	26158 (+6 others)	[25]
CaF_2			$Fm\bar{3}m$	28730 (+19 others)	[26]
CaI_2			$P\bar{3}m1$	52280	ICSD
CaO			$Fm\bar{3}m$	26959 (+13 others)	[11, 27]
CaS			$Fm\bar{3}m$	28902 (+16 others)	ICSD
CaSe			$Fm\bar{3}m$	41957 (+7 others)	[4]
CaTe			$Fm\bar{3}m$	41958 (+5 others)	[4]
Cs_2O			$R\bar{3}m$	27919	ICSD
Cs_3As			$P6_3cm$	409668	ICSD
CsBr	-0.040		$Pm\bar{3}m$	22174 (+4 others)	[28]
CsCl	-0.048		$Pm\bar{3}m$	22173 (+6 others)	[28]
CsF			$Fm\bar{3}m$	44288 (+2 other)	[28]
CsI	-0.032		$Pm\bar{3}m$	44291 (+8 others)	[28]
Ga_2O_3	-0.005	-0.017	$C2/m$	34243 (+4 others)	[29]
Ga_2S_3			Cc	488 (+3 others)	[30]
Ga_2Se_3			Cc	35028 (+3 others)	ICSD
GaAs			$F\bar{4}3m$	41674 (+24 others)	[4]
GaN			$P6_3mc$	25676 (+19 others)	[4]
GaP			$F\bar{4}3m$	41676 (+17 others)	[4]
GaSb			$F\bar{4}3m$	41675 (+14 others)	[4]
GaSe			$P\bar{6}m2$	71082 (+4 others)	[31, 32]
Ge_3N_4	-0.004		$P6_3/m$	23672	[33–35]
GeO_2			$P4_2/mnm$	9162 (+22 others)	[36]
GeSe	-0.011	-0.004	$Pnma$	17006 (+9 others)	[37]
$GeSe_2$			$P2_1/c$	614	[38]
GeTe			$R3m$	43202 (+25 others)	[39]
In_2S_3			$I4_1/amd$	23844 (+3 others)	[40]
In_2Te_3			$F\bar{4}3m$	180867 (+7 others)	[41]
In_3Te_4			$R\bar{3}m$	44655	ICSD
InAs			$F\bar{4}3m$	24518 (+22 others)	[4]
InN			$P6_3mc$	25677 (+9 others)	[4]
InP			$F\bar{4}3m$	24517 (+13 others)	[4]
InSb			$F\bar{4}3m$	24519 (+25 others)	[4]

InTe	-0.013	-0.020	I4/mcm	606 (+8 others)	[42, 43]
K_2O			$Fm\bar{3}m$	44674 (+4 others)	ICSD
K_2O_2			Cmce	25527 (+3 others)	ICSD
K_2S			$Fm\bar{3}m$	26735 (+3 others)	[44]
K_2Se			$Fm\bar{3}m$	60440 (+2 other)	ICSD
K_2Te			$Fm\bar{3}m$	60441 (+4 others)	ICSD
K_2Te_3			Pnma	2453 (+2 other)	ICSD
KBr			$Fm\bar{3}m$	18015 (+6 others)	[4]
KCl			$Fm\bar{3}m$	18014 (+37 others)	[4]
KF			$Fm\bar{3}m$	52241 (+3 others)	[4]
KI			$Fm\bar{3}m$	22158 (+5 others)	[4]
KSe			$P\bar{6}2m$	73172	ICSD
Li_2In			Cmcm	51961	ICSD
Li_2O			$Fm\bar{3}m$	22402 (+11 others)	[45]
Li_2O_2			$P6_3/mmc$	25530 (+3 others)	[46]
Li_2S			$Fm\bar{3}m$	54396 (+7 others)	[47]
Li_2Sb			$P\bar{6}2c$	100020	ICSD
Li_2Se			$Fm\bar{3}m$	60433 (+5 others)	ICSD
Li_2Te			$Fm\bar{3}m$	60434 (+3 others)	ICSD
Li_3As			$P6_3/mmc$	26878 (+3 others)	[48]
Li_3Bi			$Fm\bar{3}m$	58797 (+2 other)	[49]
Li_3N	-0.008		P6/mmm	34280 (+20 others)	[50]
Li_3Sb		-0.007	$Fm\bar{3}m$	44900 (+2 other)	[49]
LiBr			$P6_3mc$		[51]
LiCl	-0.025		$Fm\bar{3}m$	26909 (+5 others)	ICSD
LiF	-0.006		$Fm\bar{3}m$	18012 (+8 others)	ICSD
LiI			$P6_3mc$	414242	[52]
LiO_2			Pnnm	180561	ICSD
LiPb			$Pm\bar{3}m$	104762 (+4 others)	ICSD
LiSi			$I4_1/a$	78364 (+4 others)	[48]
LiTl			$Pm\bar{3}m$	104789 (+4 others)	[53]
$MgBr_2$			$P\bar{3}m1$	52366 (+3 others)	ICSD
$MgCl_2$			$R\bar{3}m$	26157 (+3 others)	[54]
MgF_2			$P4_2/mnm$	394 (+22 others)	[55]
MgI_2			$P\bar{3}m1$	52279 (+2 other)	ICSD
MgO			$Fm\bar{3}m$	9863 (+51 others)	[4, 11]
MgS			$Fm\bar{3}m$	28903 (+10 others)	[11, 56]
MgSe	-0.020	-0.017	$Fm\bar{3}m$	53946	[11]
MgTe			$P6_3mc$	52363 (+4 others)	[4, 11]
Na_2In			$C222_1$	106857	ICSD
Na_2O			$Fm\bar{3}m$	60435 (+3 others)	ICSD
Na_2O_2			$P\bar{6}2m$	25526 (+4 others)	ICSD
Na_2S			$Fm\bar{3}m$	56024 (+5 others)	[57]
Na_2S_5			Pnma	38349	ICSD
Na_2Se			$Fm\bar{3}m$	54281 (+5 others)	ICSD

Na_2Te			$Fm\bar{3}m$	60437 (+4 others)	ICSD
Na_3As			$P6_3cm$	79586 (+6 others)	[58]
Na_3Bi	-0.002	-0.002	$P6_3/mmc$	26881	[59]
Na_3P			$P6_3/mmc$	26884 (+3 others)	[60]
Na_3Sb			$P6_3/mmc$	26882	[59]
NaBi			P4/mmm	58816 (+2 other)	ICSD
NaBr			$Fm\bar{3}m$	18013 (+7 others)	[4]
NaCl			$Fm\bar{3}m$	18189 (+25 others)	[4]
NaF			$Fm\bar{3}m$	29128 (+8 others)	ICSD
NaGe			$P2_1/c$	43275	ICSD
NaI			$Fm\bar{3}m$	44279 (+6 others)	[4]
NaO_2	-0.001	-0.001	Pnnm	26583 (+5 others)	[61]
NaO_3			Imm2	85587 (+3 others)	ICSD
NaP		-0.005	$P2_12_12_1$	14009	[62]
NaPb			$I4_1/acd$	105156	ICSD
NaS			$P6_3/mmc$	43407 (+3 others)	[63]
NaS_2			$I\bar{4}2d$	2586	ICSD
NaSb			$P2_1/c$	26473	ICSD
NaSe			$P6_3/mmc$	43408	ICSD
$NaSe_2$			$I\bar{4}2d$	402584	ICSD
NaTe			Pbcn	61382	ICSD
NaTl			$Fd\bar{3}m$	105169 (+12 others)	[64]
P_2O_5	-0.005		Pnma	16611 (+4 others)	[65]
P_2S_5			$P\bar{1}$	23843 (+3 others)	ICSD
P_2Se_5			$P2_1/c$	74546	ICSD
P_4S_7			$P2_1/c$	23842 (+3 others)	ICSD
P_4Se_5			$Pna2_1$	16140	ICSD
PSe			$P2_1/c$	74878	ICSD
$PbBr_2$	-0.029		Pnma	36170	ICSD
PbO			P4/nmm	15466 (+20 others)	[66]
PbSe			$Fm\bar{3}m$	38294 (+24 others)	[67]
Rb_2O	-0.003		$Fm\bar{3}m$	77676 (+3 others)	ICSD
Rb_2S			$Fm\bar{3}m$	29208	[68]
RbBr			$Fm\bar{3}m$	18017 (+5 others)	[4]
RbCl			$Fm\bar{3}m$	18016 (+8 others)	[67]
RbF			$Fm\bar{3}m$	53828	[4]
RbI			$Fm\bar{3}m$	22168 (+5 others)	[4]
Sb_2O_5			C2/c	1422 (+2 other)	[69]
Sb_2S_3			Pnma	22176 (+25 others)	[70]
Sb_2Te_3			$R\bar{3}m$	2084 (+3 others)	[71]
SbO_2		-0.002	Pnna	919 (+6 others)	[72, 73]
SeCl			$P2_1/c$	37018	ICSD
SeO_2			$P4_2/mbc$	24022 (+7 others)	[74]
SeO_3			$P\bar{4}2_1c$	18180	[75]
SiC			$F\bar{4}3m$	24217 (+9 others)	[76, 77]

SiO_2	-0.011		$P3_221$	174 (+138 others)	[78]
Sn_3N_4			$Fd\bar{3}m$	89525	ICSD
$SnBr_2$	-0.003		Pnma	411177	ICSD
$SnCl_2$			Pnma	15452 (+2 other)	[79]
SnF_2	-0.002		C2/c	308 (+3 others)	[80]
SnF_3			$Fm\bar{3}m$	33786	ICSD
SnI_2	-0.034	-0.013	C2/m	2831	ICSD
SnO			P4/nmm	15516 (+5 others)	[66]
SnO_2			$P4_2/mnm$	9163 (+29 others)	[81]
SnS			Pnma	24376 (+18 others)	[82]
SnSe			Pnma	16997 (+32 others)	[82]
$SnSe_2$			$P\bar{3}m1$	43594 (+6 others)	[83]
SnTe			$Fm\bar{3}m$	52489 (+23 others)	[84]
$SrBr_2$	-0.014		P4/n	26092 (+2 other)	[85, 86]
$SrCl_2$			$Fm\bar{3}m$	18011 (+3 others)	ICSD
SrF_2			$Fm\bar{3}m$	40414 (+5 others)	[87]
SrI_2	-0.027	-0.008	Pbca	15101 (+4 others)	[86]
SrO			$Fm\bar{3}m$	26960 (+10 others)	[4, 11]
SrO_2	-0.029	-0.011	I4/mmm	24249 (+2 other)	[88]
SrS			$Fm\bar{3}m$	28900 (+16 others)	[4]
SrSe			$Fm\bar{3}m$	28901 (+4 others)	[4]
SrTe			$Fm\bar{3}m$	53950 (+3 others)	[4]
Te_2O_5			$P2_1$	2523	ICSD
Te_3As_2			C2/m	18208 (+3 others)	[89]
TeF_6			Pnma	67609 (+2 other)	ICSD
TeO_2	-0.011		$P4_12_12$	25706 (+10 others)	[90]
TeO_3	-0.022		$R\bar{3}c$	27019 (+4 others)	[91]
TePb			$Fm\bar{3}m$	38295 (+44 others)	[92]
TlBr	-0.043	-0.004	$Pm\bar{3}m$	44936 (+4 others)	[93]
TlCl	-0.043		$Pm\bar{3}m$	29107 (+5 others)	[93]
TlF	-0.007		Pbcm	16112 (+9 others)	[94]
TlI	-0.023		Cmcm	26761 (+8 others)	[93]
TlTe			I4/mcm	69027 (+7 others)	[95]

Compounds containing transition metals

AgBr	-0.041		$Fm\bar{3}m$	52246 (+8 others)	[4, 96]
AgCl	-0.028		$Fm\bar{3}m$	56538 (+5 others)	[4, 96]
AgF	-0.009	-0.012	$Fm\bar{3}m$	18008	[4]
AgI		-0.005	$F\bar{4}3m$	52361 (+11 others)	[96]
AgO	-0.036		$P2_1/c$	69095	[97]
AgSe	-0.092	-0.164	$F\bar{4}3m$	52601 (+2 other)	ICSD
AsRh			Pnma	42572 (+3 others)	ICSD
AsRu			Pnma	42577 (+2 other)	ICSD
$CdCl_2$			$R\bar{3}m$	30255 (+3 others)	ICSD

CdF_2			$Fm\bar{3}m$	28731 (+4 others)	ICSD
CdO			$Fm\bar{3}m$	24802 (+14 others)	[4, 11]
CdS			$P6_3mc$	31074 (+22 others)	[4, 11, 98, 99]
CdSe			$F\bar{4}3m$	41528 (+6 others)	[4, 11, 99, 100]
CdTe			$F\bar{4}3m$	31844 (+39 others)	[4, 11, 99]
CoAs			$Pna2_1$	15065 (+9 others)	[101]
CoN			$F\bar{4}3m$	79936 (+2 other)	ICSD
CoO	-0.206	-0.056	$Fm\bar{3}m$	9865 (+22 others)	[102]
CoP			Pnma	43249 (+4 others)	ICSD
CoS	-0.142	-0.073	$P6_3/mmc$	29305 (+6 others)	[103]
CoSb			$P6_3/mmc$	76118 (+11 others)	ICSD
CoSe	-0.129		$P6_3/mmc$	42541 (+8 others)	[104]
CrAs			$P6_3/mmc$	1261	[105]
CrN	-0.030		$Fm\bar{3}m$	37412 (+9 others)	[106]
CrO	-0.279	-0.328	$Fm\bar{3}m$	61633 (+2 other)	ICSD
CrP			Pnma	42079 (+12 others)	ICSD
CrS		-0.027	P1	16718	[107]
CrSb			$P6_3/mmc$	53210 (+9 others)	ICSD
Cu_2Se	-0.093	-0.097	$Fm\bar{3}m$	56025	[108]
Cu_3N			$Pm\bar{3}m$	25675 (+14 others)	[109]
CuBr	-0.004		$F\bar{4}3m$	23989 (+5 others)	[96, 110]
CuCl	-0.016		$F\bar{4}3m$	23988 (+4 others)	[96]
CuI		-0.002	$F\bar{4}3m$	9098 (+12 others)	[96, 110, 111]
CuO			C2/c	69095	[97]
CuS			$P6_3/mmc$	26968 (+13 others)	[112]
CuSe	-0.005	-0.008	Cmcm	240 (+20 others)	[113]
CuTe			Pmmn	42591 (+5 others)	[114]
FeAs			Pnma	15009 (+16 others)	ICSD
FeN			$F\bar{4}3m$	41258	ICSD
FeO	-0.093	-0.077	$Fm\bar{3}m$	27856 (+14 others)	ICSD
FeP			$Pna2_1$	15057 (+7 others)	ICSD
FeS	-0.274	-0.077	$P6_3/mmc$	29302 (+5 others)	[103]
FeSb			$P6_3/mmc$	53535 (+3 others)	ICSD
FeSe			P4/nmm	26889 (+47 others)	[115]
FeTe			P4/nmm	44753 (+4 others)	[116]
HfN			$Fm\bar{3}m$	53025 (+16 others)	[117]
HgO			Pnma	14124 (+3 others)	[118]
HgS			$P3_121$	31129 (+8 others)	[119]
HgSe			$F\bar{4}3m$	24175 (+11 others)	[11, 99]
HgTe			$F\bar{4}3m$	31845 (+28 others)	[11, 99]
LaN	-0.012	-0.003	$Fm\bar{3}m$	44684 (+16 others)	[120, 121]
LaS			$Fm\bar{3}m$	29394 (+10 others)	[122]
MnAs	-0.035		$P6_3/mmc$	9497 (+9 others)	[123]
MnN	-0.052		I4/mmm	106932	[124]
MnO	-0.122	-0.039	$Fm\bar{3}m$	9864 (+14 others)	ICSD

MnP			Pnma	30412 (+12 others)	ICSD
MnS	-0.122	-0.052	$Fm\bar{3}m$	18007 (+24 others)	[125]
MnSb			$P6_3/mmc$	53970 (+22 others)	ICSD
MnSe	-0.144	-0.048	$Fm\bar{3}m$	24251 (+16 others)	[126]
MnTe	-0.107	-0.078	$P6_3/mmc$	43541 (+17 others)	[127]
MoAs	-0.001	-0.006	Pnma	43188 (+2 other)	ICSD
MoP			$P\bar{6}m2$	76367 (+4 others)	ICSD
NbAs			$I4_1md$	16585 (+3 others)	ICSD
NbN	-0.038	-0.043	$P6_3/mmc$	76384 (+3 others)	[128–131]
NbP			$I4_1md$	76027 (+2 other)	ICSD
NiAs			$P6_3/mmc$	29303 (+6 others)	[132]
NiO			$Fm\bar{3}m$	9866 (+29 others)	ICSD
NiS		-0.085	R3m	29312 (+11 others)	[103]
NiSb			$P6_3/mmc$	29304 (+11 others)	ICSD
NiSe			$P6_3/mmc$	29310 (+10 others)	[133]
NiTe			$P6_3/mmc$	42557 (+8 others)	[134]
PRu			Pnma	109139 (+2 other)	ICSD
PdO			$P4_2/mmc$	24692 (+3 others)	[66]
PtO	-0.093	-0.188	$P4_2/mmc$	26599 (+2 other)	[66]
PtS			$P4_2/mmc$	31131 (+4 others)	ICSD
PtS_2			$P\bar{3}m1$	41375 (+6 others)	ICSD
SbRh			Pnma	991 (+4 others)	ICSD
SbRu			Pnma	990	ICSD
ScAs			$Fm\bar{3}m$	1331 (+4 others)	[135]
ScF_3			R32	36011 (+31 others)	[136]
ScN			$Fm\bar{3}m$	26948 (+7 others)	[137]
ScP			$Fm\bar{3}m$	77798 (+4 others)	[138]
ScSb			$Fm\bar{3}m$	1335 (+5 others)	[135, 139]
TaAs			$I4_1md$	44068 (+3 others)	[140]
TaN		-0.005	$P\bar{6}2m$	1396 (+5 others)	[141, 142]
TaP			$I4_1/amd$	108656	ICSD
TiAs			$P6_3/mmc$	16773 (+2 other)	[135]
TiN			$Fm\bar{3}m$	26947 (+26 others)	ICSD
TiO	-0.181	-0.202	$Fm\bar{3}m$	40125 (+10 others)	[143, 144]
TiP			$P6_3/mmc$	24337 (+2 other)	ICSD
TiS	-0.137	-0.155	$R\bar{3}m$	25561	[145, 146]
TiS_2			$P\bar{3}m1$	26861 (+16 others)	[147]
TiSb			$P6_3/mmc$	76406 (+2 other)	[148]
TiTe	-0.058	-0.018	$P6_3/mmc$	653080	[148]
VAs		-0.007	$Pna2_1$	42445 (+5 others)	[149]
VN	-0.191	-0.126	$Fm\bar{3}m$	22321 (+22 others)	[150]
VO	-0.075	-0.010	$Fm\bar{3}m$	28681 (+10 others)	[143, 151]
VP	-0.007		$P6_3/mmc$	42444 (+2 other)	[149]
VSb	-0.005		$P6_3/mmc$	23910	[152]
YAs			$Fm\bar{3}m$	44087 (+6 others)	[153]

YN			$Fm\bar{3}m$	37413 (+5 others)	[137]
YP			$Fm\bar{3}m$	77857 (+4 others)	[138]
YSb			$Fm\bar{3}m$	43632 (+6 others)	[139]
ZnO			$P6_3mc$	26170 (+56 others)	[4, 11]
ZnS			$F\bar{4}3m$	41985 (+19 others)	[4, 11]
ZnSe			$F\bar{4}3m$	41527 (+26 others)	[4, 11]
ZnTe			$F\bar{4}3m$	31843 (+19 others)	[4, 11]

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