

# Pseudopotentials for high-throughput DFT calculations: supplementary material

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Supplementary material for “Pseudopotentials for high-throughput DFT calculations”. Note that these results are intended for pseudopotential testing and should be compared only to other calculations with identical approximations and convergence parameters (see text). They are not intended to correspond to experiment.

TABLE I: Testing data for lattice constants ( $\text{\AA}$ ) of *fcc* and *bcc* lattices. Entries marked with – were unable to be converged to sufficient accuracy for comparison.

Element	$a_{\text{AE}}$ <i>fcc</i>	$a_{\text{GBRV}}$ <i>fcc</i>	$a_{\text{VASP}}$ <i>fcc</i>	$a_{\text{PSLIB}}$ <i>fcc</i>	$a_{\text{AE}}$ <i>bcc</i>	$a_{\text{GBRV}}$ <i>bcc</i>	$a_{\text{VASP}}$ <i>bcc</i>	$a_{\text{PSLIB}}$ <i>bcc</i>
H	2.283	2.284	2.283	2.284	1.806	1.807	1.807	1.806
Li	4.335	4.332	4.336	4.359	3.427	3.425	3.429	3.454
Be	3.166	3.175	3.170	3.160	2.506	2.514	2.508	2.501
B	2.872	2.872	2.872	2.871	2.323	2.324	2.323	2.322
C	3.103	3.105	3.104	3.103	2.366	2.368	2.367	2.365
O	3.178	3.173	3.172	3.172	2.511	2.509	2.508	2.508
N	–	3.116	3.117	3.117	–	2.449	2.449	2.449
F	3.447	3.430	3.433	3.433	2.730	2.714	2.717	2.720
Na	5.294	5.294	5.292	5.294	4.199	4.196	4.205	4.195
Mg	4.526	4.527	4.530	4.521	3.581	3.582	3.582	3.577
Al	4.043	4.043	4.044	4.040	3.242	3.242	3.242	3.239
Si	3.857	3.853	3.859	3.852	3.080	3.076	3.078	3.075
P	–	3.917	3.893	3.889	–	3.060	3.043	3.041
S	3.994	3.992	3.993	3.988	3.182	3.178	3.180	3.175
Cl	4.409	4.395	4.395	4.392	3.501	3.490	3.492	3.488
K	6.684	6.668	6.670	6.667	5.294	5.279	5.285	5.281
Ca	5.532	5.523	5.529	5.514	4.400	4.392	4.396	4.386
Sc	4.622	4.621	4.624	4.623	3.680	3.679	3.683	3.681
Ti	4.114	4.114	4.110	4.105	3.259	3.258	3.255	3.249
V	3.822	3.820	3.823	3.824	3.006	3.003	3.005	3.006
Cr	3.630	3.629	3.625	3.634	2.851	2.849	2.848	2.861
Mn	3.503	3.502	3.501	3.508	2.784	2.784	2.783	2.788
Fe	3.449	3.451	3.447	3.457	2.762	2.762	2.758	2.770
Co	3.457	3.455	3.457	3.463	2.762	2.761	2.761	2.766
Ni	3.515	3.511	3.516	3.517	2.793	2.790	2.794	2.795
Cu	3.638	3.639	3.641	3.654	2.885	2.886	2.885	2.896
Zn	3.936	3.936	3.939	3.931	3.128	3.128	3.130	3.127
Ga	4.240	4.244	4.242	4.247	3.364	3.366	3.364	3.369
Ge	4.283	4.282	4.283	4.283	3.397	3.396	3.397	3.396
As	4.272	4.276	4.273	4.272	3.383	3.386	3.385	3.383
Se	4.337	4.332	4.335	4.341	3.460	3.456	3.459	3.463
Br	4.732	4.726	4.726	4.731	3.765	3.762	3.762	3.765
Rb	7.183	7.155	7.160	7.155	5.680	5.659	5.665	5.659
Sr	6.030	6.022	6.022	6.020	4.756	4.750	4.749	4.748
Y	5.062	5.057	5.055	5.060	4.044	4.040	4.040	4.042
Zr	4.522	4.520	4.521	4.527	3.569	3.566	3.568	3.572
Nb	4.217	4.214	4.215	4.217	3.309	3.306	3.307	3.308
Mo	4.007	4.002	4.008	4.005	3.166	3.160	3.164	3.162
Tc	3.875	3.872	3.876	3.874	3.082	3.080	3.085	3.082
Ru	3.809	3.806	3.808	3.809	3.058	3.054	3.056	3.057
Rh	3.836	3.839	3.834	3.842	3.071	3.072	3.069	3.075
Pd	3.951	3.951	3.951	3.956	3.137	3.136	3.135	3.141
Ag	4.158	4.161	4.165	4.167	3.299	3.299	3.303	3.304
Cd	4.511	4.512	4.515	4.491	3.628	3.629	3.632	3.612
In	4.795	4.800	4.797	4.793	3.827	3.831	3.826	3.825
Sn	4.824	4.826	4.824	4.830	3.823	3.825	3.823	3.829
Sb	4.805	4.808	4.802	4.782	3.807	3.809	3.805	3.787
Te	4.840	4.840	4.837	4.854	3.867	3.865	3.865	3.877
I	5.201	5.195	5.198	5.192	4.149	4.149	4.151	4.144
Cs	7.821	7.789	7.794	7.808	6.172	6.147	6.145	6.161
Ba	6.347	6.338	6.345	6.344	5.023	5.018	5.023	5.023
La	5.267	5.277	5.290	5.387	4.235	4.239	4.248	4.297
Hf	4.488	4.491	4.483	4.483	3.551	3.554	3.549	3.548
Ta	4.235	4.232	4.235	4.227	3.333	3.331	3.332	3.327
W	4.041	4.042	4.042	4.046	3.188	3.187	3.187	3.190
Re	3.917	3.915	3.919	3.919	3.118	3.115	3.120	3.119
Os	3.858	3.855	3.861	3.861	3.096	3.091	3.099	3.103
Ir	3.881	3.875	3.877	3.888	3.113	3.107	3.110	3.118
Pt	3.970	3.970	3.970	3.984	3.166	3.164	3.165	3.176
Au	4.168	4.163	4.166	4.180	3.306	3.302	3.304	3.316
Hg	–	–	–	–	–	–	–	–
Tl	4.996	5.004	4.997	4.962	3.977	3.980	3.975	3.974
Pb	5.045	5.039	5.044	5.044	4.008	4.003	4.007	4.007
Bi	5.038	5.035	5.035	5.041	3.984	3.981	3.982	3.979

TABLE II: Testing data for lattice constants ( $\text{\AA}$ ) of rock salt structures. Entries marked with – were unable to be converged to sufficient accuracy for comparison.

Element	$a_{\text{AE}}$	$a_{\text{GBRV}}$	$a_{\text{VASP}}$	$a_{\text{PSLIB}}$
LiCl	5.161	5.151	5.150	5.160
NaCl	5.714	5.701	5.701	5.696
KCl	6.391	6.382	6.391	6.384
RbCl	6.710	6.698	6.705	6.701
CsCl	7.088	7.071	7.085	7.088
BeO	3.650	3.651	3.654	3.638
MgO	4.259	4.257	4.261	4.250
CaO	4.839	4.833	4.842	4.828
SrO	5.204	5.197	5.208	5.201
BaO	5.590	5.595	5.617	5.603
ScN	4.516	4.512	4.519	4.516
YN	4.911	4.907	4.906	4.915
LaN	5.314	5.313	5.328	5.349
TiO	4.288	4.284	4.288	4.283
VO	4.192	4.186	4.191	4.192
CrO	4.139	4.135	4.134	4.142
MnO	4.108	4.105	4.103	4.110
FeO	4.096	4.097	4.092	4.103
CoO	4.106	4.103	4.102	4.108
NiO	4.166	4.166	4.167	4.169
CuO	4.248	4.248	4.246	4.260
ZnO	4.332	4.336	4.340	4.330
ZrO	4.608	4.601	4.607	4.621
NbO	4.476	4.469	4.471	4.475
MoO	4.419	4.412	4.419	4.417
TcO	4.398	4.391	4.394	4.394
RuO	4.411	4.404	4.405	4.408
RhO	4.450	4.451	4.449	4.455
PdO	4.544	4.547	4.541	4.547
AgO	4.677	4.677	4.675	4.684
CdO	4.774	4.780	4.785	4.762
HfO	4.611	4.591	4.584	4.574
TaO	4.506	4.499	4.504	4.483
WO	4.466	4.465	4.467	4.466
ReO	4.455	4.454	–	4.461
OsO	4.487	4.483	4.497	4.492
IrO	4.542	4.535	4.545	4.548
PtO	4.624	4.618	4.622	4.637
AuO	4.759	4.751	4.752	4.769
HgO	4.929	4.931	4.938	4.913
BN	3.506	3.504	3.505	3.504
AlN	4.073	4.076	4.070	4.068
GaN	4.269	4.273	4.274	4.285
InN	4.708	4.710	4.711	4.714
TlN	4.957	4.961	4.963	4.968
CO	3.977	3.976	3.974	3.972
SiO	4.616	4.614	4.615	4.612
GeO	4.773	4.772	4.773	4.772
SnO	5.120	5.120	5.119	5.125
PbO	5.269	5.262	5.266	5.268
AlN	4.073	4.076	4.070	4.068
AlP	5.075	5.077	5.072	5.068
AlAs	5.303	5.307	5.298	5.301
AlSb	5.774	5.761	5.765	5.752
AlBi	5.987	5.976	5.977	5.976
SrS	6.063	6.057	6.065	6.060
SrSe	6.301	6.297	6.304	6.300
SrTe	6.724	6.720	6.726	6.728
LiF	4.076	4.074	4.067	4.081
LiBr	5.521	5.512	5.511	5.524
Lil	6.038	6.020	6.021	6.030
NaF	4.711	4.717	4.708	4.705
NaBr	6.049	6.040	6.040	6.037
NaI	6.540	6.534	6.537	6.529

TABLE III: Testing data for lattice constants ( $\text{\AA}$ ) of perovskite and anti-perovskite structures. Entries marked with – were unable to be converged to sufficient accuracy for comparison.

Element	$a_{\text{AE}}$	$a_{\text{GBRV}}$	$a_{\text{VASP}}$	$a_{\text{PSLIB}}$
SrLiF <sub>3</sub>	3.884	3.881	3.884	3.884
NaNbO <sub>3</sub>	3.981	3.977	3.976	3.980
KMgF <sub>3</sub>	4.059	4.058	4.062	4.052
CsMgF <sub>3</sub>	4.258	4.255	4.261	4.255
MgTiO <sub>3</sub>	3.839	3.837	3.839	3.839
CaTiO <sub>3</sub>	3.886	3.884	3.888	3.886
SrTiO <sub>3</sub>	3.941	3.939	3.943	3.942
BaTiO <sub>3</sub>	4.024	4.028	4.035	4.030
BiScO <sub>3</sub>	4.074	4.071	4.079	4.076
BiYO <sub>3</sub>	4.335	4.331	4.331	4.343
SrVO <sub>3</sub>	3.862	3.861	3.866	3.867
SrCrO <sub>3</sub>	3.820	3.820	3.819	3.826
SrMnO <sub>3</sub>	3.799	3.802	3.798	3.808
SrFeO <sub>3</sub>	3.801	3.803	3.802	3.812
SrCoO <sub>3</sub>	3.811	3.813	3.812	3.823
SrNiO <sub>3</sub>	3.843	3.846	3.849	3.853
KNiF <sub>3</sub>	4.039	4.040	4.036	4.042
KCuF <sub>3</sub>	4.085	4.086	4.084	4.095
KZnF <sub>3</sub>	4.132	4.133	4.139	4.130
SrZrO <sub>3</sub>	4.176	4.173	4.177	4.187
SrNbO <sub>3</sub>	4.067	4.063	4.064	4.066
SrMoO <sub>3</sub>	4.002	3.998	4.003	4.002
SrTcO <sub>3</sub>	3.967	3.966	3.966	3.968
SrRuO <sub>3</sub>	3.959	3.958	3.956	3.962
SrRhO <sub>3</sub>	3.982	3.985	3.981	3.991
KPdF <sub>3</sub>	4.312	4.317	4.309	4.315
SrAgF <sub>3</sub>	4.536	4.532	4.535	4.537
KCdF <sub>3</sub>	4.463	4.471	4.477	4.458
LaAlO <sub>3</sub>	3.816	3.817	3.822	3.829
SrHfO <sub>3</sub>	4.155	4.145	4.146	4.133
SrTaO <sub>3</sub>	4.066	4.064	4.067	4.050
SrWO <sub>3</sub>	4.014	4.017	4.019	4.013
SrReO <sub>3</sub>	3.986	3.987	3.997	3.994
SrOsO <sub>3</sub>	3.982	3.980	3.992	3.988
SrIrO <sub>3</sub>	3.994	4.000	4.006	4.018
SrPtO <sub>3</sub>	4.040	4.048	4.039	4.079
BiAuO <sub>3</sub>	4.151	4.149	4.147	4.171
KHgF <sub>3</sub>	4.594	4.602	4.608	4.587
TlCTi <sub>3</sub>	4.263	4.264	4.260	4.259
LaBRh <sub>3</sub>	4.288	4.285	4.287	4.306
BiAlO <sub>3</sub>	3.797	3.798	3.795	3.795
BiInO <sub>3</sub>	4.170	4.172	4.178	4.179
SrSiO <sub>3</sub>	3.695	3.693	3.698	3.694
SrGeO <sub>3</sub>	3.855	3.859	3.860	3.865
SnTiO <sub>3</sub>	3.949	3.947	3.949	3.950
PbTiO <sub>3</sub>	3.971	3.967	3.971	3.971
PNCa <sub>3</sub>	4.725	4.720	4.728	4.714
AsNCa <sub>3</sub>	4.769	4.764	4.772	4.759
SbNCa <sub>3</sub>	4.872	4.867	4.875	4.862
SrTiS <sub>3</sub>	4.786	4.781	4.785	4.781
SrTiSe <sub>3</sub>	5.030	5.031	5.033	5.034
BaZrTe <sub>3</sub>	5.681	5.677	5.684	5.691
KMgCl <sub>3</sub>	5.028	5.024	5.026	5.018
CsPbBr <sub>3</sub>	5.994	5.999	6.003	6.009
CsPbI <sub>3</sub>	6.383	6.393	6.396	6.397

TABLE IV: Testing data for lattice constants ( $\text{\AA}$ ) of half-Heusler structures. Entries marked with – were unable to be converged to sufficient accuracy for comparison. Entries are listed with the inequivalent “stuffing atom” (Wyckoff position 4c) third.

Element	$a_{\text{AE}}$	$a_{\text{GBRV}}$	$a_{\text{VASP}}$	$a_{\text{PSLIB}}$
AgAlGe	6.224	6.220	6.223	6.221
AgAlSn	6.595	6.594	6.596	6.600
AgCaBi	7.161	7.155	7.163	7.153
AgYSi	6.501	6.496	6.499	6.502
AlBeB	4.963	4.965	4.964	4.958
AlLiGe	6.022	6.015	6.014	6.017
AlLiSi	5.931	5.933	5.936	5.938
AuLiSb	6.449	6.440	6.431	6.450
BaZnTi	6.946	6.955	6.982	6.967
BeScB	5.321	5.317	5.324	5.318
BiMgCu	6.444	6.438	6.440	6.444
BiScNi	6.271	6.261	6.265	6.267
BiYNi	6.502	6.494	6.495	6.501
BiYPd	6.736	6.731	6.734	6.738
BiZrCo	6.235	6.225	6.226	6.236
BiZrNi	6.300	6.288	6.291	6.299
CaZnSn	6.923	6.923	6.928	6.924
CaZnZr	6.834	6.823	6.834	6.829
CdPLi	5.969	5.955	5.952	5.945
CoMnSb	5.835	5.833	5.824	5.851
CoNbSn	6.186	6.176	6.175	6.186
CoSnMo	6.107	6.096	6.099	6.105
CoSnNb	6.222	6.211	6.211	6.218
CoSnTc	6.034	6.023	6.024	6.032
CoSnTi	6.121	6.115	6.115	6.118
CoZrSb	6.328	6.320	6.319	6.333
CrSbNi	5.803	5.805	5.800	5.814
CsZnBi	8.016	8.002	8.018	8.043
CuAlGe	5.920	5.912	5.910	5.916
CuAlSn	6.332	6.327	6.325	6.337
CuMgAs	6.057	6.057	6.052	6.057
CuMgSn	6.436	6.432	6.433	6.439
CuScSn	6.461	6.456	6.459	6.467
CuYSi	6.310	6.302	6.302	6.312
CuYSn	6.732	6.729	6.728	6.741
FeSnTi	6.118	6.115	6.111	6.119
InLiGe	6.398	6.397	6.394	6.397
IrMnSn	6.044	6.033	6.032	6.050
KZnBi	7.428	7.418	7.426	7.432
LiAlSn	6.459	6.454	6.453	6.459
LiAuS	6.015	5.994	5.993	6.008
LiBaP	7.139	7.148	7.164	7.158
LiCaP	6.497	6.492	6.498	6.491
LiCGa	5.088	5.091	5.091	5.100
LiCuS	5.578	5.576	5.574	5.594
LiCuSe	5.863	5.859	5.858	5.880
LiCuTe	6.273	6.273	6.261	6.294
LiLaGe	6.930	6.927	6.934	6.960
LiMgN	5.005	5.006	5.008	5.011
LiSiGa	5.881	5.882	5.881	5.887
LiSnIn	6.799	6.799	6.796	6.801
LiSrP	6.817	6.813	6.819	6.818
LiYSn	7.009	7.006	7.005	7.014
LiZnN	4.923	4.925	4.929	4.928

TABLE V: Continuation of table IV.

Element	$a_{\text{AE}}$	$a_{\text{GBRV}}$	$a_{\text{VASP}}$	$a_{\text{PSLIB}}$
MgPLi	5.775	5.776	5.776	5.776
MgSbCu	6.259	6.257	6.257	6.256
MgSbNi	6.099	6.094	6.094	6.093
MgSbPd	6.354	6.351	6.349	6.351
MgSbPt	6.364	6.359	6.357	6.362
MgSnCu	6.247	6.248	6.248	6.257
MgSrGe	7.069	7.067	7.072	7.064
MgSrSi	7.012	7.009	7.016	7.008
MgSrSn	7.427	7.424	7.428	7.422
MgZnHf	6.579	6.576	6.573	6.572
MnPdTe	6.059	6.075	6.036	6.068
MnPtGa	5.744	5.743	5.744	5.756
MnPtSb	6.064	6.053	6.048	6.076
MnRhSb	6.001	5.991	5.982	6.010
MnSbCo	5.720	5.724	5.718	5.737
MnSbCu	5.853	5.857	5.850	5.868
MnSbIr	6.033	6.022	6.017	6.035
MnSbNi	5.758	5.760	5.755	5.771
MnSbOs	6.017	6.004	6.003	6.015
MnSbPt	6.106	6.096	6.090	6.112
MnSbRe	6.045	6.036	6.033	6.040
MnSbRh	5.996	5.988	5.980	5.998
MnSbTa	6.246	6.239	6.237	6.233
MnSbW	6.116	6.107	6.104	6.110
MnSnPt	6.093	6.081	6.082	6.098
NaAgO	5.708	5.708	5.709	5.706
NaAlGe	6.387	6.384	6.386	6.380
NaBGe	5.750	5.753	5.754	5.748
NaMgN	5.446	5.449	5.450	5.439
NaYGe	6.897	6.897	6.899	6.899
NaYSn	7.286	7.282	7.284	—
NaZnBi	6.951	6.948	6.954	6.995
NaZnP	6.150	6.148	6.149	6.143
NaZnSb	6.765	6.765	6.764	6.764
NbRhSn	6.295	6.289	6.289	6.301
NbSbFe	5.972	5.963	5.956	5.970
NbSbRh	6.220	6.215	6.213	6.220
NbSbRu	6.197	6.191	6.189	—
NiHfSn	6.341	6.334	6.329	6.332
NiSbMn	5.817	5.818	5.813	5.824
NiSbTi	6.177	6.169	6.167	6.160
NiSnTi	6.167	6.162	6.162	6.162
NiSnZr	6.467	6.459	6.462	6.467
NiTiSn	6.146	6.141	6.142	6.145
PbYAu	6.856	6.845	6.849	6.857
PdHfSn	6.483	6.477	6.474	6.481
PdSbMn	6.002	5.994	5.987	5.999
PdTiGe	5.980	5.971	5.973	5.972
PdZrSn	6.507	6.503	6.506	6.514
PtHfSn	6.449	6.442	6.439	6.448
PtSbMn	5.998	5.989	5.985	6.001
PtSnMn	5.996	5.990	5.990	6.007
PtSnSc	6.494	6.487	6.493	6.496
PZnLi	5.637	5.642	5.639	5.645
RbZnBi	7.694	7.683	7.689	7.697
RhSbMn	5.922	5.912	5.906	5.919
RhTiGa	5.917	5.907	5.910	5.910

TABLE VI: Continuation of tables IV and V.

Element	$a_{\text{AE}}$	$a_{\text{GBRV}}$	$a_{\text{VASP}}$	$a_{\text{PSLIB}}$
SbCdAg	6.688	6.693	6.693	6.679
SbCdAu	6.684	6.685	6.682	6.676
SbCuCd	6.566	6.570	6.567	6.554
SbHgAg	6.735	6.738	6.738	6.725
SbScNi	6.127	6.119	6.122	6.123
SbScPd	6.385	6.381	6.383	6.384
SbScPt	6.399	6.393	6.396	6.398
SbTaCo	5.983	5.971	5.970	5.970
SbTaRu	6.196	6.189	6.188	—
SbTiCo	5.896	5.897	5.894	5.902
SbTiFe	5.943	5.936	5.929	5.942
SbTiNi	5.965	5.956	5.953	5.957
SbTiRu	6.165	6.159	6.157	—
SbVCo	5.810	5.811	5.809	5.821
SbVFe	5.795	5.798	5.792	5.809
SbVNi	5.867	5.868	5.866	5.874
SbVRu	6.053	6.044	6.042	—
SbYNi	6.371	6.365	6.364	6.368
SbYPt	6.623	6.620	6.620	6.626
SbZrRu	6.347	6.343	6.342	—
SbZrTc	6.402	6.398	6.399	6.403
ScSnAu	6.518	6.512	6.515	6.521
SnTiNi	5.959	5.953	5.953	5.958
SnTiPt	6.239	6.231	6.236	6.239
SrAlGa	6.875	6.870	6.876	6.872
SrCdSi	6.966	6.966	6.974	6.961
TlLiGe	6.564	6.563	6.559	6.561