Validation of the JTH-v2.0 PAW Dataset for ABINIT

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A new version of the JTH table (JTHv2.0) is now available. It has been thoroughly validated both against the Δ and Δ_1 factors ([1],[2]) as well as against the lattice parameter of fcc, bcc, rocksalt, perovskite, zinc-blende and half-heusler structures, following the GBRV testing protocol [3].

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I. JTH-V2.0 PAW ATOMIC DATA TABLE

A new version of the JTH table (JTHv2.0) is now available. It has been generated with the ATOMPAW code (v4.2.0.4)[4]. This new version follows the XML format defined in [5].

Relative to JTH table v1.1, the following updates have been introduced:

- All data are generated on a radial grid with 1500 or 2000 points for the elements Ag, Au, B, Bi, Br, Ce, Cl, Cu, Hf, Hg, Mo, Nb, N, Os, Pb, Pd, Po, Pt, Re, Rh, Ru, Sc, Se, S, Ta, Tc, Ti, Tl, V, W, Y, and Zr. Among these, only Cu, Rh, Re, and Os have been re-optimized due to convergence issues related to the number of radial grid points. For the other elements, only the number of points was adjusted in the ATOMPAW input file.
- In the LDA table, LDA-1/2 — half-occupation method — data are provided for C, N, O, Si, P, S, Zn, Ga, Ge, As, and In, generated according to [6] and [7] (note that for Si and Ge, LDA-1/4 is actually used).
- 3 elements (Si, Se, and Lu) have been slightly modified to avoid a non-positive definite overlap matrix.
- 14 elements (La, Cl, S, Kr, Y, Rn, Sr, Ar, B, P, Ba, Ce, Pr, Rb) have been modified to ensure a positive density when the compensation density is added to the density for the exchange-correlation term calculation (Kresse-Joubert approach). This approach is not used in ABINIT, which employs the Bloechl approach.

In addition to their 'recommended' version, all datasets are also provided in a lighter version, in which all radial functions (partial waves, projectors, etc.) are discretized on a smaller grid containing 500 points.

Once generated, the PAW data have been spline-interpolated onto a 500-point radial grid for all radial quantities (densities, potentials, and wavefunctions). These datasets were obtained from the 1500- or 2000-point sets, simply interpolated at the end of the process. These datasets can be used to slightly accelerate calculations on small systems or for applications with modest accuracy requirements, such as molecular dynamics.

II. VALIDATION OF PAW ATOMIC DATASETS USING THE Δ-FACTOR CRITERION

We have employed the *delta calculation package* (version 3.1 [8]) to validate our new atomic datasets against the WIEN2K code. Electronic structure calculations were performed using ABINIT v10.4.7 [9]. For these calculations, we applied the recommended k-point sampling values [1], specifically $(6750/N)$ k-points in the Brillouin zone for a cell containing N atoms. A Fermi-Dirac broadening of 0.002 Ha was utilized. Following [1], crystallographic data (CIF files) supplied with the delta calculation package were used. The Equation of State (EOS) for each element was fit to a Birch-Murnaghan model based on seven calculations at volumes ranging from 0.94 to 1.06 V_S, where V_S represents the equilibrium volume derived from the CIF file, without geometry optimization to match the WIEN2K calculation conditions precisely.

Version 3.1 of the *delta calculation package* provides both the Δ factor and the modified Δ_1 factor as proposed by [2].
For the JTH-v2.0 table, we obtained mean values of $\Delta = 0.43$ meV and $\Delta_1 = 1.09$ meV using a 20 Ha plane wave cutoff energy, which represent very good agreement (see [8] for comparisons with other PAW datasets).

The detailed results for each elements are given here:

```
--------------------
# Delta values of RUN2000_eos.txt with respect to WIEN2k.txt (in meV/atom)
# (71 elements of 71 included)
# calculated with calcDelta.py version 3.1
# from left to right: Delta [meV/atom] - relative Delta [%] - Delta1 [meV/atom]
--------------------
H  0.237  26.1 3.972
He  0.008  10.6 1.630
Li  0.011  0.8 0.121
Be  0.093  1.9 0.288
B  0.271  3.1 0.472
C  0.143  1.2 0.175
N  0.524  6.6 0.995
O  0.255  5.3 0.800
F  0.224  6.6 1.003
Ne  0.011  6.1 0.967
Na  0.500  34.0 5.209
Mg  0.251  6.0 0.916
Al  0.093  1.4 0.217
Si  0.320  3.5 0.529
P  0.358  4.8 0.734
S  0.325  4.5 0.678
Cl  0.205  5.4 0.815
Ar  0.019  9.5 1.468
K  0.071  5.3 0.806
Ca  0.115  3.1 0.473
Sc  0.274  4.1 0.615
Ti  0.915  9.3 1.410
V  2.116  17.1 2.598
Cr  0.718  6.6 1.017
Mn  0.901  13.7 2.070
Fe  0.554  5.0 0.760
Co  1.081  9.1 1.389
Ni  1.498  13.7 2.085
Cu  0.284  3.3 0.502
```

```
Zn  0.282  4.9 0.743
Ga  0.189  3.7 0.566
Ge  0.583  8.1 1.241
As  0.479  6.1 0.929
Se  0.129  1.8 0.275
Br  0.029  0.6 0.098
Kr  0.030  12.4 1.916
Rb  0.300  23.1 3.537
Sr  0.817  25.6 3.917
Y  0.308  4.5 0.683
Zr  0.144  1.3 0.197
Nb  0.307  2.0 0.299
Mo  1.506  7.2 1.103
Tc  0.402  1.8 0.279
Ru  0.177  0.8 0.124
Rh  0.335  1.8 0.277
Pd  0.131  1.0 0.153
Ag  0.367  4.4 0.680
Cd  0.121  2.4 0.362
In  0.208  4.2 0.637
Sn  0.137  2.0 0.311
Sb  0.265  3.3 0.497
Te  0.068  0.8 0.129
I  0.733  15.3 2.339
Xe  0.012  5.0 0.764
Cs  0.106  9.1 1.380
Ba  0.812  29.3 4.506
Lu  0.548  7.9 1.202
Hf  0.076  0.6 0.094
Ta  0.695  3.8 0.579
W  1.289  5.2 0.791
Re  0.217  0.8 0.120
Os  0.354  1.2 0.186
Ir  0.619  2.4 0.367
Pt  2.162  10.8 1.661
Au  1.010  7.9 1.205
Hg  0.141  10.7 1.677
Tl  0.045  1.0 0.160
Pb  0.323  5.0 0.759
Bi  0.097  1.2 0.185
Po  0.284  3.3 0.497
Rn  0.026  10.0 1.538
--------------------
np.mean  0.412  6.8 1.038
np.std   0.451  6.9 1.060
np.max   2.162  34.0 5.209   (Pt, Na, Na)
np.min   0.008  0.6 0.094   (He, Hf, Hf)
--------------------
```

We have also investigated the convergence of the delta factor with respect to the plane wave energy cutoff. We computed the delta factor for each element at energy cutoffs E_{cut} =10 Ha, 12 Ha, 15 Ha, 17.5 Ha, 20 Ha, 25 Ha and 40 Ha. The table below displays the absolute differences in the modified Δ_1 factor (measured in meV) relative to the converged value obtained at E_{cut} =40 Ha.

#Ecut	10Ha	12Ha	15Ha	175Ha	20Ha	25Ha	40Ha
H	8.087	7.749	5.744	3.245	1.504	0.037	0.000
He	26.780	58.452	0.462	0.822	0.217	1.575	0.000
Li	0.326	0.039	0.589	0.049	0.171	0.218	0.000
Be	0.748	0.062	0.278	0.156	0.006	0.021	0.000
B	0.222	1.079	1.005	0.356	0.073	0.040	0.000
C	19.211	2.544	0.276	0.325	0.321	0.185	0.000
N	7.101	15.676	12.071	3.955	0.645	0.091	0.000
O	75.261	32.130	9.297	0.886	0.588	0.391	0.000
F	113.343	13.776	7.719	0.189	0.164	0.016	0.000
Ne	14.484	10.547	6.926	10.842	1.756	0.134	0.000
Na	208.368	10.582	2.851	1.616	1.366	1.115	0.000
Mg	0.645	0.748	0.498	0.354	0.200	0.150	0.000
Al	3.109	1.207	0.155	0.212	0.174	0.024	0.000
Si	0.197	0.109	0.035	0.006	0.004	0.003	0.000
P	5.006	2.425	0.677	1.232	0.663	0.073	0.000
S	5.587	4.199	0.910	0.559	0.398	0.034	0.000
Cl	10.411	7.896	3.585	1.354	0.340	0.022	0.000
Ar	7.535	0.741	0.689	0.265	0.049	0.498	0.000
K	4.369	4.329	0.508	0.048	0.063	0.179	0.000
Ca	2.925	0.085	0.356	0.022	0.077	0.051	0.000
Sc	0.896	0.229	0.078	0.025	0.029	0.018	0.000
Ti	0.915	0.133	0.025	0.018	0.026	0.015	0.000
V	0.007	0.069	0.002	0.012	0.007	0.027	0.000
Cr	4.446	8.931	5.357	0.180	3.574	0.817	0.000
Mn	49.847	0.014	0.180	1.317	0.307	0.098	0.000
Fe	19.922	0.119	0.087	0.188	0.261	0.095	0.000
Co	28.855	1.576	0.011	1.494	0.836	0.032	0.000
Ni	2180.678	39.334	19.093	20.422	2.386	0.616	0.000
Cu	13.840	3.033	0.385	2.936	0.403	0.171	0.000
Zn	33.631	1.127	0.177	0.147	0.008	0.026	0.000
Ga	2.578	0.177	0.115	0.072	0.087	0.036	0.000
Ge	22.069	4.816	0.936	0.333	0.037	0.008	0.000
As	0.218	0.076	0.065	0.049	0.046	0.047	0.000
Se	0.002	0.005	0.005	0.003	0.002	0.002	0.000
Br	0.001	0.001	0.012	0.013	0.001	0.003	0.000
Kr	0.402	1.801	0.469	0.204	0.129	0.036	0.000
Rb	1.994	0.122	0.278	0.088	0.085	0.048	0.000
Sr	0.577	0.487	0.090	0.071	0.090	0.058	0.000
Y	0.008	0.994	0.035	0.007	0.106	0.024	0.000
Zr	3.187	0.392	0.064	0.059	0.154	0.036	0.000
Nb	0.887	0.576	0.303	0.205	0.236	0.021	0.000
Mo	0.752	0.030	0.080	0.069	0.063	0.078	0.000
Tc	1.666	0.212	0.269	0.107	0.051	0.020	0.000
Ru	0.872	0.410	0.042	0.014	0.005	0.000	0.000
Rh	1.982	2.448	0.692	0.415	0.188	0.015	0.000
Pd	19.927	13.211	4.466	0.138	0.261	0.249	0.000
Ag	3.314	0.142	0.178	0.127	0.123	0.006	0.000
Cd	3.450	0.101	0.505	0.408	0.175	0.140	0.000

In	9.265	0.731	0.116	0.104	0.025	0.009	0.000
Sn	0.590	0.070	0.165	0.074	0.005	0.001	0.000
Sb	0.101	0.143	0.011	0.015	0.005	0.006	0.000
Te	0.515	0.244	0.026	0.028	0.026	0.017	0.000
I	0.311	0.162	0.080	0.035	0.020	0.005	0.000
Xe	0.478	0.586	0.230	0.022	0.021	0.025	0.000
Cs	7.366	3.980	0.015	0.077	0.172	0.277	0.000
Ba	0.399	0.381	0.137	0.043	0.011	0.009	0.000
Lu	193.729	8.081	1.373	0.953	0.717	0.086	0.000
Hf	1.193	0.194	0.062	0.066	0.086	0.021	0.000
Ta	0.103	1.216	0.090	0.150	0.089	0.000	0.000
W	0.269	0.271	0.125	0.091	0.200	0.001	0.000
Re	5.231	0.450	0.161	0.169	0.147	0.022	0.000
Os	0.002	0.025	0.002	0.006	0.007	0.002	0.000
Ir	1.114	0.109	0.099	0.078	0.052	0.009	0.000
Pt	18.418	5.266	0.833	0.690	0.304	0.109	0.000
Au	28.700	7.642	1.326	1.008	0.279	0.133	0.000
Hg	119.053	22.394	0.307	0.114	0.046	0.075	0.000
Tl	2.189	0.031	0.178	0.287	0.274	0.175	0.000
Pb	1.227	0.364	0.211	0.373	0.102	0.067	0.000
Bi	0.883	0.289	0.234	0.137	0.033	0.024	0.000
Po	0.108	0.032	0.014	0.013	0.005	0.003	0.000
Rn	0.710	1.026	0.068	0.040	0.167	0.013	0.000

From this table we have calculated recommended values for the plane wave cutoff energy:
Low value: abs(Δ_1-$\Delta_1(40Ha)$) < 5 meV
Medium value: abs(Δ_1-$\Delta_1(40Ha)$) < 2 meV
High value: abs(Δ_1-$\Delta_1(40Ha)$) < 1 meV

These values are given below and are inserted inside each PAW data XML file.

#Sp	ecut_high	ecut_medium	ecut_low
H	25.0	20.0	17.5
He	15.0	15.0	15.0
Li	10.0	10.0	10.0
Be	10.0	10.0	10.0
B	10.0	10.0	10.0
C	15.0	15.0	12.0
N	20.0	20.0	17.5
O	17.5	17.5	17.5
F	17.5	17.5	17.5
Ne	25.0	20.0	20.0
Na	40.0	17.5	15.0
Mg	10.0	10.0	10.0
Al	15.0	12.0	10.0
Si	10.0	10.0	10.0
P	15.0	15.0	12.0
S	15.0	15.0	12.0
Cl	20.0	17.5	15.0
Ar	12.0	12.0	12.0
K	15.0	15.0	10.0
Ca	12.0	12.0	10.0
Sc	10.0	10.0	10.0

Ti	10.0	10.0	10.0
V	10.0	10.0	10.0
Cr	17.5	17.5	10.0
Mn	12.0	12.0	12.0
Fe	12.0	12.0	12.0
Co	15.0	12.0	12.0
Ni	25.0	25.0	20.0
Cu	15.0	15.0	12.0
Zn	15.0	12.0	12.0
Ga	12.0	12.0	10.0
Ge	15.0	15.0	12.0
As	10.0	10.0	10.0
Se	10.0	10.0	10.0
Br	10.0	10.0	10.0
Kr	10.0	10.0	10.0
Rb	12.0	10.0	10.0
Sr	10.0	10.0	10.0
Y	10.0	10.0	10.0
Zr	12.0	12.0	10.0
Nb	10.0	10.0	10.0
Mo	10.0	10.0	10.0
Tc	12.0	10.0	10.0
Ru	10.0	10.0	10.0
Rh	15.0	10.0	10.0
Pd	17.5	17.5	15.0
Ag	12.0	12.0	10.0
Cd	12.0	12.0	10.0
In	12.0	12.0	12.0
Sn	10.0	10.0	10.0
Sb	10.0	10.0	10.0
Te	10.0	10.0	10.0
I	10.0	10.0	10.0
Xe	10.0	10.0	10.0
Cs	15.0	15.0	12.0
Ba	10.0	10.0	10.0
Lu	17.5	15.0	15.0
Hf	12.0	10.0	10.0
Ta	10.0	10.0	10.0
W	10.0	10.0	10.0
Re	12.0	12.0	12.0
Os	10.0	10.0	10.0
Ir	12.0	10.0	10.0
Pt	15.0	15.0	15.0
Au	20.0	15.0	15.0
Hg	15.0	15.0	15.0
Tl	12.0	12.0	10.0
Pb	12.0	10.0	10.0
Bi	10.0	10.0	10.0
Po	10.0	10.0	10.0
Rn	10.0	10.0	10.0

III. VALIDATION AGAINST FCC, BCC, ROCKSALT, PEROVSKITE, HALF-HEUSLER AND ZINC-BLENDE

Following the approach described in [10], we calculated the lattice parameters for the fcc, bcc, rocksalt, perovskite, half-Heusler, and zinc-blende structures and compared the results with those obtained using WIEN2k under the same conditions.

The calculations were performed with the ABINIT code, using the following input files:

Common part of the general input file for all structures

```
ndtset 7
nsym 0
occopt 3
pawovlp -1
prteig 0
prtden 0
prtcif 1
tsmear 0.001
ecutsm 0.5
ecut 20
pawecutdg 40
chkprim 0
usexcnhat -1
ngkpt 8 8 8
chksymbreak 0
paral_kgb 0
nstep 99
toldfe 1.0d-8

getwfk2 -1
getwfk3 -1
getwfk4 -1
getwfk5 -1
getwfk6 -1
getwfk7 -1

scalecart3 3*0.9932883883792687
scalecart2 3*0.986484829732188
scalecart1 3*0.9795861087155615
scalecart5 3*1.006622709560113
scalecart6 3*1.0131594038201772
scalecart7 3*1.0196128224222163
```

For fcc structures (example for Al)

```
shiftk 0.0 0.0 0.0
acell  4.040210000000    4.040210000000    4.040210000000  angstrom
xred 0 0 0
rprim 0.0 0.5 0.5
      0.5 0.0 0.5
      0.5 0.5 0.0
```

```
natom 1 typat 1
ntypat 1
znucl  13
nband 8
```

For bcc structures(example for Al)

```
shiftk 0.5 0.5 0.5
acell  3.240000000000    3.240000000000    3.240000000000  angstrom
xred 0 0 0
rprim -0.5 0.5 0.5
      0.5 -0.5 0.5
      0.5 0.5 -0.5
natom 1 typat 1
ntypat 1
znucl  13
nband 8
```

For rocksalt structures(example for NaCl)

```
shiftk 0.0 0.0 0.0
acell  5.714000000000    5.714000000000    5.714000000000  angstrom
xred 0 0 0
 0.5 0.5 0.5
rprim 0.0 0.5 0.5
      0.5 0.0 0.5
      0.5 0.5 0.0
natom 2 typat 1 2
ntypat 2
znucl  11   17
nband 21
```

For perovskite structures(example for BaTiO3)

```
shiftk 0.0 0.0 0.0
acell  4.024000000000    4.024000000000    4.024000000000  angstrom
xred 0.5 0.5 0.5
 0 0 0
 0.5 0 0
 0 0.5 0
 0 0 0.5
rprim 1.0 0.0 0.0
      0.0 1.0 0.0
      0.0 0.0 1.0
natom 5 typat 1 2 3 3 3
ntypat 3
znucl  56   22    8
nband 55
```

For half-heusler structures(example for AgAlGe)

```
shiftk 0.0 0.0 0.0
acell  6.224000000000    6.224000000000    6.224000000000  angstrom
xred 0.25 0.25 0.25
 0.5 0.5 0.5
 0 0 0
rprim 0.0 0.5 0.5
      0.5 0.0 0.5
      0.5 0.5 0.0
natom 3 typat 3 2 1
ntypat 3
znucl  47   13   32
nband 33
```

For zinc-blende structures(example for ZnS)

```
shiftk 0.0 0.0 0.0
acell  5.442518477764    5.442518477764    5.442518477764  angstrom
xred 0 0 0
 0.25 0.25 0.25
rprim 0.0 0.5 0.5
      0.5 0.0 0.5
      0.5 0.5 0.0
natom 2 typat 1 2
ntypat 2
znucl  30   16
nband 23
```

A summary of the results is presented in **Table I**. The GBRV values in ABINIT and the AE reference values are taken from [10].

Test	GBRV-Abinit	JTHv1.2-Abinit
fcc latt. const. (%)	0.13	0.13
bcc latt. const. (%)	0.15	0.14
rocksalt latt. const. (%)	0.13	0.16
perovskite latt. const. (%)	0.09	0.14
half-heusler latt. const. (%)	0.13	0.14
zinc-blend Δ (meV/atom)	1.2	0.95
zinc-blend $\Delta 1$ (meV/atom)	2.1	1.73

Table I: Summary of PAW data files testing (RMS errors reltative to AE calculations and Δ factor for zinc-blende structures

Detailed results for each crystal structure are shown in **Fig. 1** (fcc), **Fig. 2** (bcc), **Fig. 3** (rocksalt), **Fig. 4** (perovskite), **Fig. 5** (half-Heusler), and **Fig. 6** (zinc-blende).

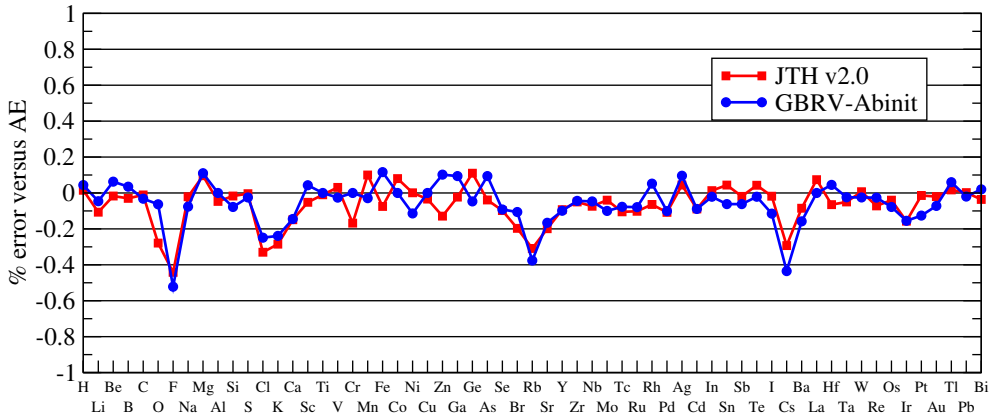

Figure 1: Percent difference between AE and PAW lattice constants for FCC structures

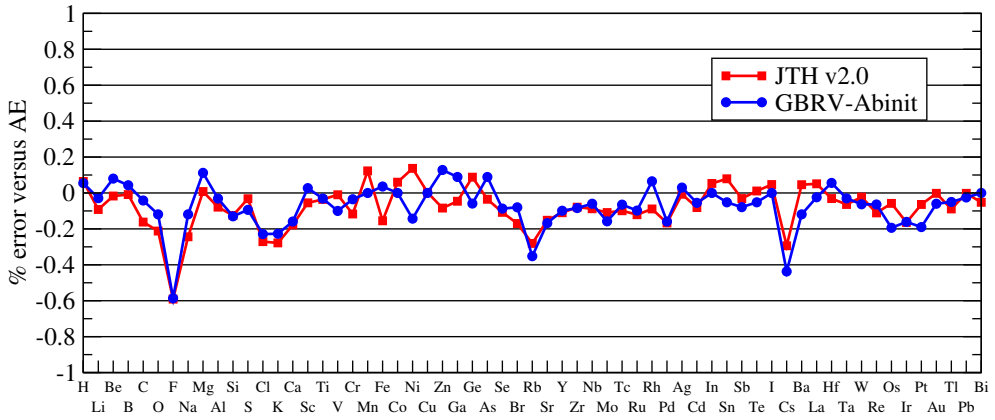

Figure 2: Percent difference between AE and PAW lattice constants for BCC structures

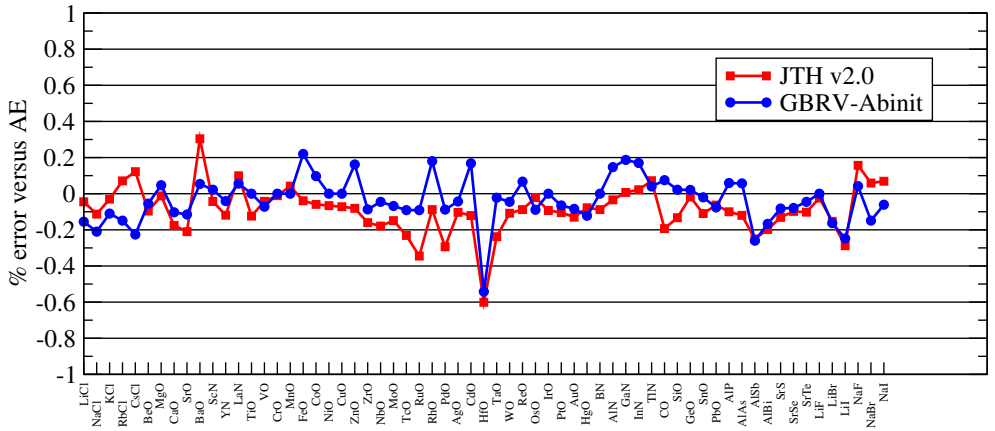

Figure 3: Percent difference between AE and PAW lattice constants for rocksalt structures

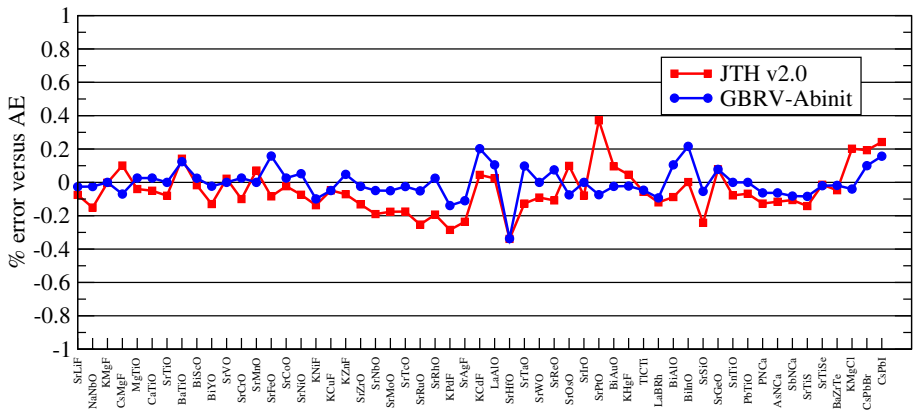

Figure 4: Percent difference between AE and PAW lattice constants for perovskite structures

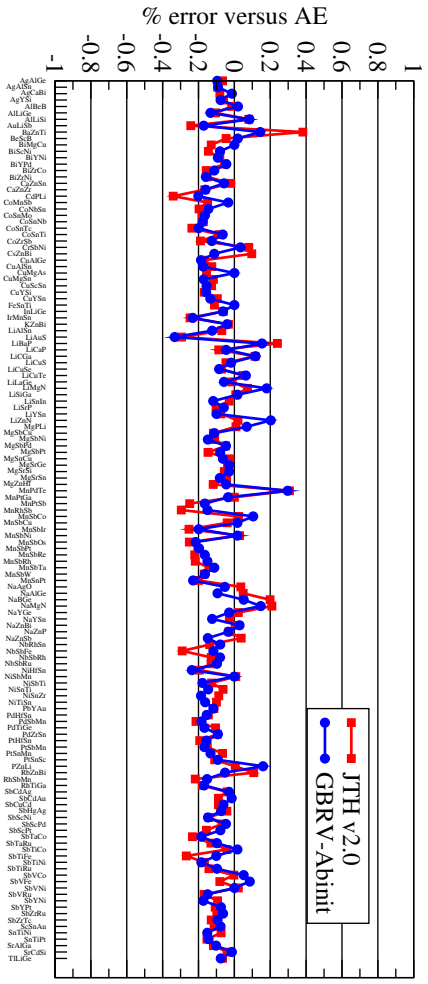

Figure 5: Percent difference between AE and PAW lattice constants for half-Heusler structures

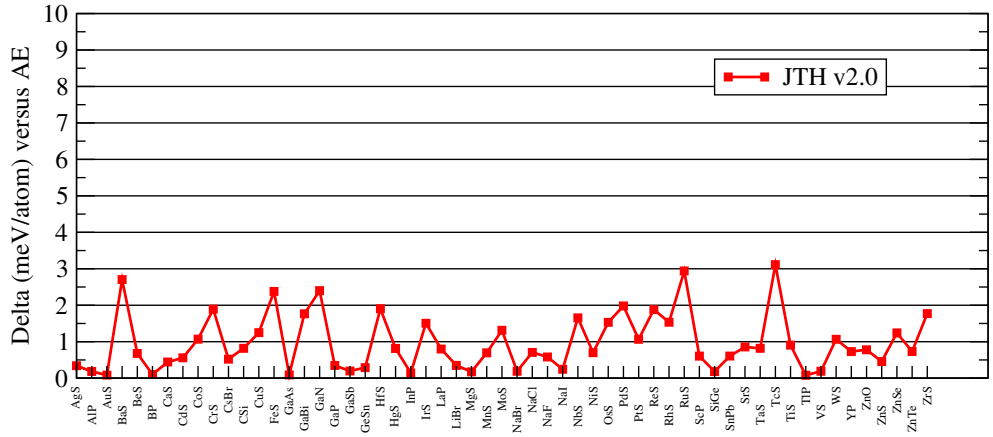

Figure 6: Δ factor for zinc-blende structures

Following [10], we also calculated the magnetic moments of transition metal oxides with non-zero magnetic moments at the AE non-spin-polarized lattice constant. The magnetic moments, expressed in μ_B per primitive cell, are provided in **Table II**. The AE reference values are taken from [10]. All calculations were performed using a 12×12×12 k-point mesh.

Compound	μ_{AE}	$\mu_{GBRV-Abinit}$	$\mu_{JTHv1.1-Abinit}$
VO	1.32	1.27	1.24
CrO	2.99	3.04	3.05
MnO	3.85	3.84	3.86
FeO	3.83	3.84	3.85
CoO	2.42	2.53	2.56
NiO	1.68	1.47	1.35
MoO	0.54	0.53	0.49
TcO	1.92	1.90	1.95
RuO	1.64	1.63	1.67
OsO	1.56	1.50	1.69
IrO	0.62	0.62	0.74

Table II: Magnetic moments of transition metal oxides

Additionally, we generated atomic data for rare-earth elements. The calculated lattice parameters for their fcc structures are presented in **Table III** (for some elements, these values differ slightly from the JTH-v1.1 table due to insufficient convergence criteria in the previous calculations.).

Element	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
fcc lattice parameter (Å)	5.293	4.779	4.616	4.544	4.527	4.573	4.693	4.780	4.889	4.973	5.066	5.087	5.140	5.163	4.875

Table III: FCC lattice parameters obtained with JTHv1.2 atomic data in ABINIT for the rare-earth elements

IV. CONCLUSIONS

The JTH-v2.0 table offers improved accuracy and efficiency compared to similar datasets, making it suitable for high-throughput calculations. It is provided as XML files, ensuring compatibility with major PAW codes (ABINIT, GPAW, etc.). This table is distributed via the ABINIT website [11].

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[1] K. Lejaeghere, V. Van Speybroeck, G. Van Oost, and S. Cottenier, Crit. Rev. Solid State Mater. Sci. **39**, 1 (2014).
[2] F. Jollet, M. Torrent, and N. Holzwarth, Computer Physics Communications **185**, 1246 (2014).
[3] K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, Comp. Mat. Sci. **81**, 446 (2014).
[4] https://users.wfu.edu/natalie/papers/pwpaw/man.html (2014).
[5] https://http://esl.cecam.org/mediawiki/index.php/Paw-xml (2016).
[6] L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B **78**, 125116 (2008), URL `https://link.aps.org/doi/10.1103/PhysRevB.78.125116`.
[7] K.-H. Xue, L. R. Fonseca, and X.-S. Miao, arXiv:1603.01300 (2016).
[8] https://molmod.ugent.be/DeltaCodesDFT (2014).
[9] M. J. Verstraete, J. Abreu, G. E. Allemand, B. Amadon, G. Antonius, M. Azizi, L. Baguet, C. Barat, L. Bastogne, R. Béjaud, et al., The Journal of Chemical Physics **163**, 164126 (2025), URL `https://doi.org/10.1063/5.0288278`.
[10] https://www.physics.rutgers.edu/gbrv/ (2014).
[11] https://abinit.org (2014).