Testing of JTH-v1.0 PAW table for ABINIT

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A new version of the JTH table (JTHv1.0) is now available. It has been tested both against the Δ and Δ_1 factors ([1],[2]) and against the lattice parameter of fcc, bcc, rocksalt, perovskite, zinc-blende and half-heusler structures, following the GBRV testing suite [3].

I. JTH-V1.0 PAW TABLE FOR ABINIT

A new version of the JTH table (JTHv1.0) is now available. It has been generated with the code ATOMPAW (v4.0.0.12) [4]. This new version follows the XML format defined in [5].
Compared with the JTHv0.2 version, the following changes have been made:
- coefficients useful to compute the Fock operator (needed for hybrid functionals) have been added in the atomic data files for all elements of the table.
- the radius of the compensation charge has been slightly modified for the elements: As, Ar, Mg, Mo, Nb, Os, Ba, Sc, Sr, Ta, Y, Ca, Na, Li, Be, C, Ru, Ne, N, Ag, W, Ga, and Ir. (That was just to have this radius strictly lesser than the PAW radius).
- semi-core states have been added for In, Sn, Ge, Tl, Pb, Bi and Sb.
With these modifications, we obtain a table that gives good results for all the tests performed.

II. PAW ATOMIC DATA VALIDATION AGAINST THE DELTA FACTOR

We have used the delta calculation package (version 3.0 [6]) to validate our new atomic data against the Wien2k code. The electronic structure calculations have been performed thanks to the ABINIT-7.8.2 code [7]. For this, we have used the recommended values [1] for the k-point sampling (6750/N k-points in the Brillouin zone for a N-atom cell). A Fermi-Dirac broadenning of 0.002 Ha has been used. As indicated in [1], we have used the cystallographic data (CIF's files) provided with the delta calculation package. The Equation of State (EOS) of each element has been adjusted to a Birch-Murnaghan one thanks to seven calculations at seven different volumes, ranging from 0.94 to 1.06 V_S, where V_S is the equilibrium volume deduced from the CIF's file, without geometry optimisation to be exactly in the same conditions as the Wien2k calculations.

The version 3.0 of the delta calculation package gives both the Δ factor and the modified Δ_1 factor proposed by [2]. For the JTH-v1.0 table, we obtain the mean values of Δ=0.48 meV and Δ_1=1.13 meV for a 20 Ha plane-wave cutoff, which are very good results (see [6] for comparison with other PAW data).

Update: a new version of the Δ-package has been release on March 2016 (version 3.1). Some all-electron references have been updated. With these new references, the Δ mean values are:
Δ**=0.44 meV** and Δ_1**=1.04 meV** (plane-wave cutoff: 20 Ha).

The detailed results for each elements are given here:

```
#--------------------
# Delta values of Abinit-JTHv1.0-20.txt with respect to WIEN2k.txt (in meV/atom)
# (71 elements of 71 included)
# calculated with calcDelta.py version 3.0
# from left to right: Delta [meV/atom] - relative Delta [%] - Delta1 [meV/atom]
#--------------------
 H  0.249  27.5 4.187
He  0.008  10.8 1.662
Li  0.011   0.8 0.119
Be  0.094   1.9 0.289
 B  0.244   2.8 0.426
 C  0.146   1.2 0.180
 N  0.488   6.1 0.927
 O  0.242   5.0 0.763
 F  0.220   6.5 0.984
Ne  0.010   5.6 0.891
Na  0.498  33.9 5.190
Mg  0.256   6.1 0.934
Al  0.098   1.5 0.229
Si  0.307   3.3 0.507
 P  0.488   6.6 1.003
 S  0.304   4.2 0.636
Cl  0.062   1.7 0.252
Ar  0.022  11.4 1.670
 K  0.069   5.1 0.778
Ca  0.111   3.0 0.459
Sc  0.019   0.3 0.044
Ti  1.252  12.7 1.930
 V  1.688  13.6 2.074
Cr  0.723   6.7 1.024
Mn  0.892  13.6 2.050
Fe  0.557   5.0 0.763
Co  1.235  10.4 1.584
Ni  1.604  14.6 2.230
Cu  0.821   9.5 1.444
Zn  0.092   1.6 0.242
Ga  0.137   2.7 0.410
Ge  0.555   7.7 1.181
As  0.494   6.3 0.959
Se  0.238   3.3 0.510
Br  0.109   2.4 0.369
Kr  0.021   9.3 1.441
Rb  0.288  22.4 3.415
Sr  0.755  23.7 3.616
 Y  0.332   4.8 0.735
Zr  0.245   2.2 0.336
Nb  0.193   1.2 0.188
Mo  1.631   7.8 1.195
Tc  1.031   4.7 0.715
Ru  0.344   1.6 0.241
Rh  0.944   5.1 0.781
```

```
Pd  1.161   8.9 1.360
Ag  0.215   2.6 0.397
Cd  2.015  38.0 5.886
In  0.209   4.2 0.641
Sn  0.106   1.6 0.239
Sb  0.304   3.7 0.571
Te  0.069   0.9 0.131
 I  0.727  15.2 2.319
Xe  0.010   4.2 0.645
Cs  0.115   9.9 1.500
Ba  0.739  26.6 4.080
Lu  0.211   3.1 0.464
Hf  0.192   1.6 0.239
Ta  0.434   2.4 0.362
 W  1.349   5.4 0.828
Re  0.885   3.2 0.487
Os  0.482   1.7 0.253
Ir  0.514   2.0 0.304
Pt  2.105  10.6 1.616
Au  1.108   8.6 1.323
Hg  0.206  15.4 2.420
Tl  0.056   1.3 0.201
Pb  0.293   4.5 0.690
Bi  0.110   1.4 0.209
Po  0.194   2.2 0.338
Rn  0.023   8.8 1.355
#--------------------
#np.mean  0.478  7.4 1.133
#np.std   0.503  7.7 1.179
#np.max   2.105  38.0 5.886   (Pt, Cd, Cd)
#np.min   0.008  0.3 0.044   (He, Sc, Sc)
#--------------------
```

We have also studied the convergency of the delta factor with the energy cutoff. We have calculated the delta factor for each element for Ecut=10 Ha, 12 Ha, 15 Ha, 17.5 Ha, 20 Ha, 25 Ha and 40 Ha. The following table shows the absolute difference of the Δ_1 factor in meV compared to the converged value at Ecut=40 Ha.

```
# Ecut 10 Ha    12 Ha   15 Ha   17.5 Ha   20 Ha    25 Ha    40 Ha

 H   17.325   15.781   12.047    7.064    3.670    0.291    0.000
He   26.637   75.749    2.172    3.652    1.206    3.253    0.000
Li    0.785    0.008    0.650    0.058   -0.103   -0.094    0.000
Be    0.591    0.044   -0.231   -0.219   -0.090   -0.015    0.000
 B    0.072    1.029    0.986    0.367    0.099    0.040    0.000
 C   18.620    1.786   -0.662   -0.759   -0.772   -0.194    0.000
 N    4.141   14.617   13.676    3.931    0.567   -0.204    0.000
 O   70.776   31.858    9.273    0.866    0.346    0.282    0.000
 F  111.608   13.347    7.535   -0.462    0.149   -0.224    0.000
Ne   15.490    7.554    7.878   21.914   -0.957    0.459    0.000
Na   NC       11.555   -4.554    0.189    0.025    0.305    0.000
Mg    0.418   -0.135   -0.102    0.591   -0.490    0.399    0.000
Al    3.095    1.192   -0.168   -0.210   -0.171   -0.026    0.000
```

Si	-0.375	-0.277	-0.070	-0.090	-0.026	-0.018	0.000
P	4.953	2.296	-1.333	-1.013	-0.591	-0.044	0.000
S	5.416	4.192	0.911	-0.659	-0.573	-0.047	0.000
Cl	40.114	8.118	2.845	0.196	-0.813	-0.112	0.000
Ar	21.102	NC	0.716	6.629	0.244	0.539	0.000
K	4.136	4.020	0.680	-0.046	-0.012	-0.224	0.000
Ca	3.294	0.415	0.672	0.448	0.146	-0.002	0.000
Sc	0.788	0.495	0.101	0.001	-0.034	-0.021	0.000
Ti	-0.620	0.333	0.003	-0.007	0.014	-0.021	0.000
V	0.335	-0.034	0.008	-0.035	-0.003	-0.027	0.000
Cr	4.227	8.864	5.156	0.205	-3.626	-0.780	0.000
Mn	49.221	1.189	0.293	1.564	-0.026	0.306	0.000
Fe	19.818	-0.151	0.010	-0.193	-0.056	0.209	0.000
Co	30.284	1.326	0.097	1.766	0.939	0.328	0.000
Ni	NC	NC	18.881	21.212	-1.858	-0.565	0.000
Cu	12.597	13.509	1.787	2.840	1.095	-0.027	0.000
Zn	43.927	1.891	0.572	0.737	0.214	0.141	0.000
Ga	2.920	0.292	-0.105	-0.110	-0.050	0.002	0.000
Ge	22.142	4.919	1.008	0.328	0.038	-0.021	0.000
As	-0.595	-0.161	0.143	0.056	-0.012	-0.049	0.000
Se	0.103	1.198	0.129	0.377	0.043	0.007	0.000
Br	-0.335	0.499	-0.234	-0.293	-0.046	0.011	0.000
Kr	0.783	2.318	0.215	0.565	0.242	-0.127	0.000
Rb	1.886	0.008	-0.711	-0.157	-0.178	0.067	0.000
Sr	0.761	0.443	0.298	-0.203	0.022	0.012	0.000
Y	0.372	1.031	0.074	0.049	-0.079	-0.020	0.000
Zr	3.456	0.270	0.035	0.054	0.164	0.038	0.000
Nb	1.211	0.882	-0.125	-0.158	-0.220	0.019	0.000
Mo	1.091	0.129	0.109	-0.070	-0.026	-0.082	0.000
Tc	1.047	-0.534	-0.229	-0.116	-0.062	-0.011	0.000
Ru	0.298	0.454	-0.056	-0.140	-0.070	0.061	0.000
Rh	1.606	1.432	-0.814	0.293	-0.296	-0.337	0.000
Pd	21.532	14.000	5.090	0.018	0.351	0.295	0.000
Ag	2.043	-0.099	-0.109	-0.124	-0.100	0.001	0.000
Cd	29.805	-1.707	-0.676	-0.291	0.179	0.029	0.000
In	8.225	-0.735	0.273	-0.073	-0.252	-0.260	0.000
Sn	3.254	1.046	1.291	0.439	-0.329	0.429	0.000
Sb	-0.350	-0.219	0.021	0.031	0.038	-0.010	0.000
Te	0.505	0.151	-0.108	-0.033	-0.021	-0.010	0.000
I	0.296	0.046	0.075	0.066	-0.011	0.007	0.000
Xe	3.969	8.409	7.455	4.665	-1.216	1.554	0.000
Cs	5.666	4.324	7.542	-0.026	0.861	0.182	0.000
Ba	1.170	-0.097	-1.551	-0.206	-0.335	0.133	0.000
Lu	8.428	1.500	0.670	0.133	0.051	0.061	0.000
Hf	1.692	0.080	0.053	0.011	0.062	0.019	0.000
Ta	0.416	1.417	0.015	0.375	0.250	0.034	0.000
W	0.712	0.233	0.077	0.097	0.222	0.005	0.000
Re	1.769	0.692	0.108	0.078	0.245	0.015	0.000
Os	20.674	10.299	0.390	0.055	0.082	0.046	0.000
Ir	1.378	-0.080	-0.169	0.063	-0.063	0.054	0.000
Pt	18.814	5.866	0.787	0.724	0.343	0.101	0.000
Au	29.222	7.812	1.280	0.992	0.318	0.122	0.000
Hg	122.942	23.485	1.260	0.955	0.292	0.080	0.000
Tl	2.111	0.488	0.205	0.605	-0.085	-0.094	0.000

```
Pb    1.363   -0.325   -0.254   -0.281   -0.117   -0.014    0.000
Bi    0.808    0.297    0.242    0.156    0.032    0.019    0.000
Po    0.035    0.056    0.164   -0.054    0.004    0.028    0.000
Rn    2.910    3.614    0.041    0.374   -0.031    0.928    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 here and are inserted inside each PAW data XML file for each element.

```
# Ecut low medium high

 H  20.00  25.00  25.00
He  15.00  25.00  25.00
Li  10.00  10.00  10.00
Be  10.00  10.00  10.00
 B  10.00  10.00  15.00
 C  12.00  12.00  15.00
 N  17.50  20.00  20.00
 O  17.50  17.50  17.50
 F  17.50  17.50  17.50
Ne  20.00  20.00  20.00
Na  15.00  17.50  17.50
Mg  10.00  10.00  10.00
Al  10.00  12.00  15.00
Si  10.00  10.00  10.00
 P  10.00  15.00  20.00
 S  12.00  15.00  15.00
Cl  15.00  17.50  17.50
Ar  20.00  20.00  20.00
 K  10.00  15.00  15.00
Ca  10.00  12.00  12.00
Sc  10.00  10.00  10.00
Ti  10.00  10.00  10.00
 V  10.00  10.00  10.00
Cr  17.50  25.00  25.00
Mn  12.00  12.00  20.00
Fe  12.00  12.00  12.00
Co  12.00  12.00  20.00
Ni  20.00  20.00  25.00
Cu  15.00  20.00  25.00
Zn  12.00  12.00  15.00
Ga  10.00  12.00  12.00
Ge  12.00  15.00  17.50
As  10.00  10.00  10.00
Se  10.00  10.00  15.00
Br  10.00  10.00  10.00
Kr  10.00  15.00  15.00
Rb  10.00  10.00  12.00
```

```
Sr  10.00  10.00  10.00
 Y  10.00  10.00  15.00
Zr  10.00  12.00  12.00
Nb  10.00  10.00  12.00
Mo  10.00  10.00  12.00
Tc  10.00  10.00  12.00
Ru  10.00  10.00  10.00
Rh  10.00  10.00  15.00
Pd  17.50  17.50  17.50
Ag  10.00  12.00  12.00
Cd  12.00  12.00  15.00
In  12.00  12.00  12.00
Sn  10.00  12.00  17.50
Sb  10.00  10.00  10.00
Te  10.00  10.00  10.00
 I  10.00  10.00  10.00
Xe  17.50  20.00  25.00
Cs  17.50  17.50  17.50
Ba  10.00  10.00  17.50
Lu  12.00  12.00  15.00
Hf  10.00  10.00  12.00
Ta  10.00  10.00  15.00
 W  10.00  10.00  10.00
Re  10.00  10.00  12.00
Os  15.00  15.00  15.00
Ir  10.00  10.00  12.00
Pt  15.00  15.00  15.00
Au  15.00  15.00  17.50
Hg  15.00  15.00  17.50
Tl  10.00  12.00  12.00
Pb  10.00  10.00  12.00
Bi  10.00  10.00  10.00
Po  10.00  10.00  10.00
Rn  10.00  15.00  15.00
#n_low(10)= 42 n_low(12)= 10 n_low(15)=  8 n_low(17.5)=  7 n_low(20)=  4 n_low(25)=  0
#n_med(10)= 31 n_med(12)= 15 n_med(15)= 10 n_med(17.5)=  6 n_med(20)=  6 n_med(25)=  3
#n_high(10)= 17 n_high(12)= 15 n_high(15)= 16 n_high(17.5)= 11 n_high(20)=  6 n_high(25)=  6
```

III. PAW ATOMIC DATA VALIDATION AGAINST FCC, BCC, ROCKSALT, PEROVSKITE, HALF-HEUSLER AND ZINC-BLENDE STRUCTURES

Following [8], we have calculated the lattice parameters for fcc, bcc, rocksalt, perovskite, half-heusler and zinc-blende structures and compare the results to a WIEN2k calculation in the same conditions. The calculations were performed with the ABINIT code with the following input files:
Common part of general input file for all the 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 . The values for GBRV in ABINIT and the values used for AE reference calculations come from [8].

Test	GBRV-Abinit	JTHv1.0-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	0.15
zinc-blend Δ (meV/atom)	1.2	0.95
zinc-blend $\Delta 1$ (meV/atom)	2.1	1.7

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

The detailed results for each element is given on Fig. 1 for fcc structures, Fig. 2 for bcc structures, Fig. 3 for rocksalt structures, Fig. 4 for perovskite structures, Fig. 5 for half-heusler structures and Fig. 6 for zinc-blende structures.

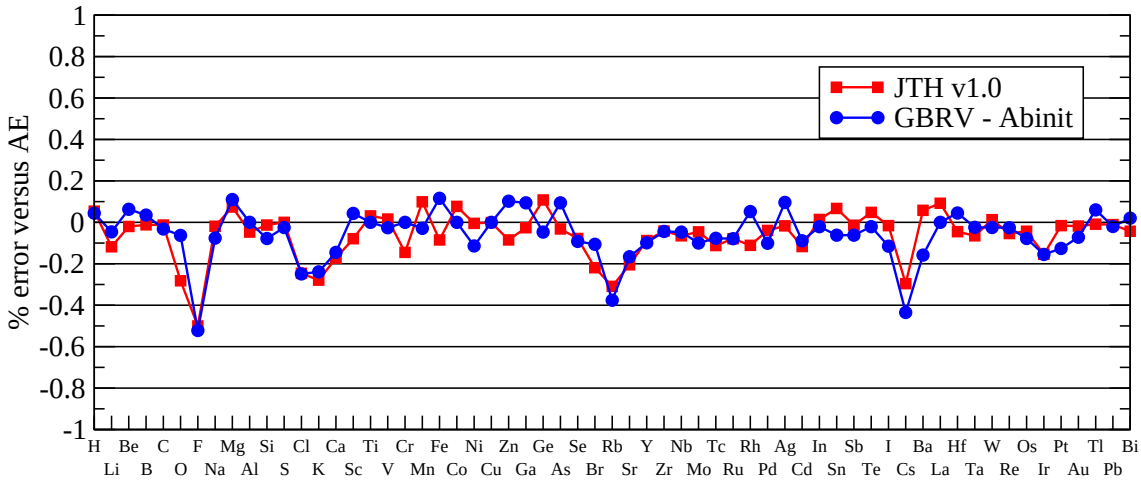

Figure 1: Percent difference in AE versus PAW data calculations for fcc lattice constant

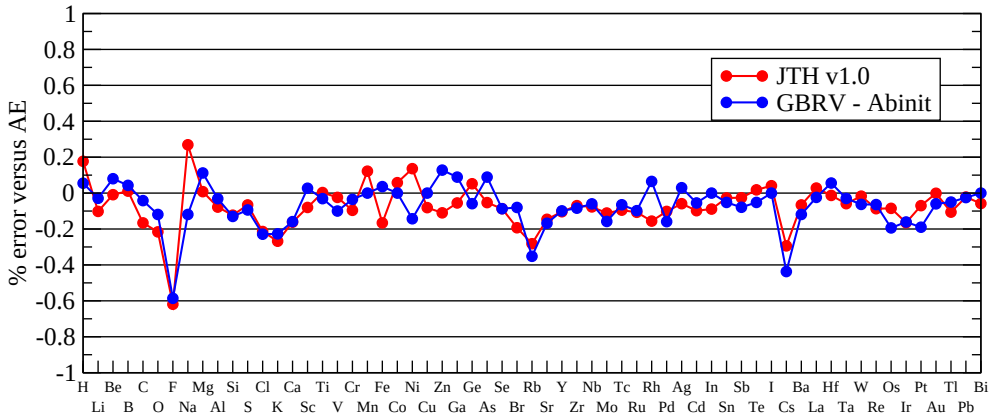

Figure 2: Percent difference in AE versus PAW data calculations for bcc lattice constant

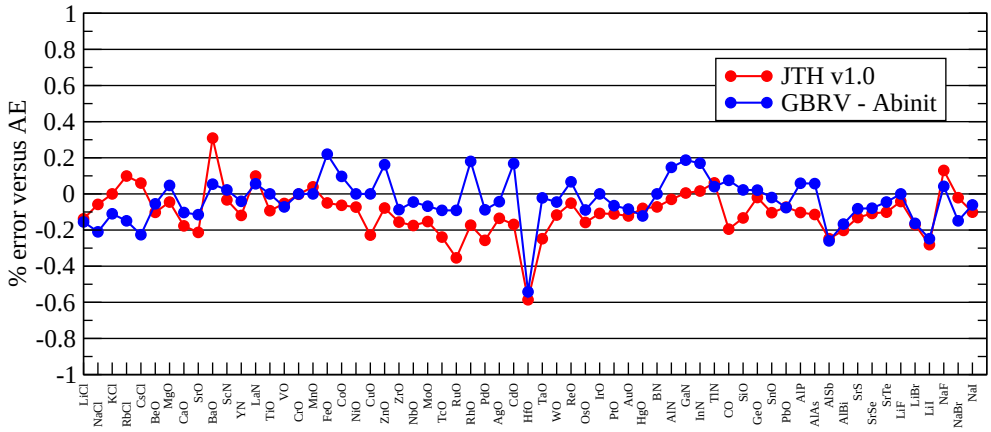

Figure 3: Percent difference in AE versus PAW data calculations for rocksalt lattice constant

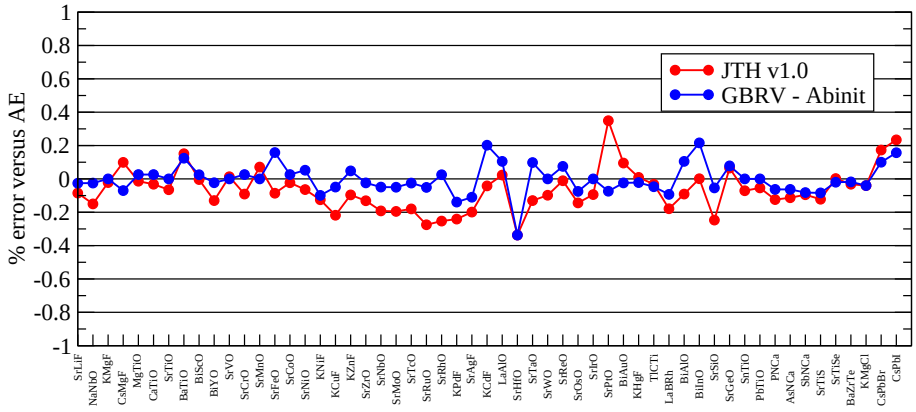

Figure 4: Percent difference in AE versus PAW data calculations for perovskite lattice constant

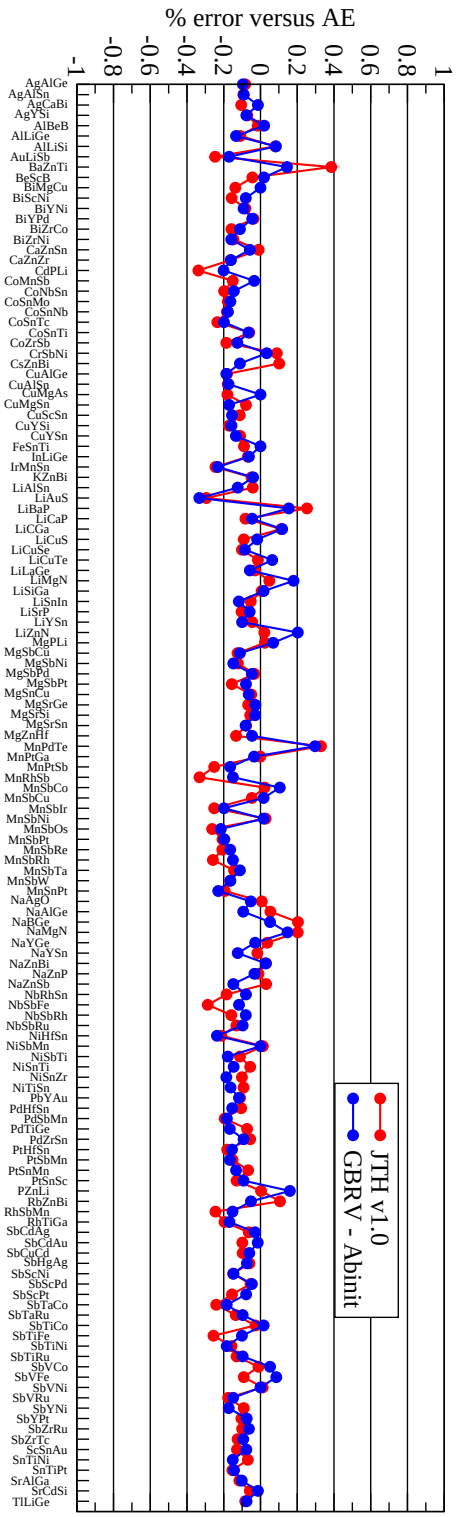

Figure 5: Percent difference in AE versus PAW data calculations for half-heusler lattice constant

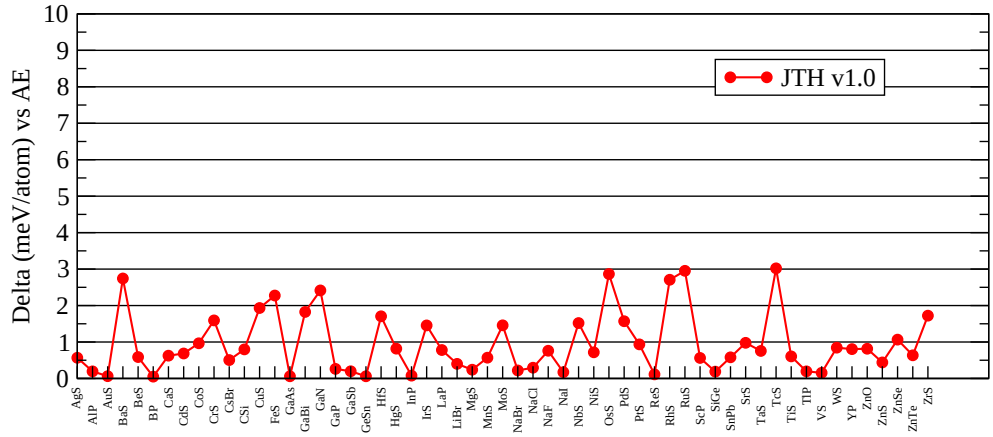

Figure 6: Δ factor for zinc- blende structure

Following [8], we have also calculated magnetic moments of transition metal oxides with non-zero magnetic moments at the AE non-spin polarized lattice constant. The magnetic moments are given in μ_B per primitive cell. The AE results come from [8]. The calculations have been done with a 12x12x12 k-point mesh .

Compound	μ_{AE}	$\mu_{GBRV-Abinit}$	$\mu_{JTHv1.0-Abinit}$
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	3.86
CoO	2.42	2.53	2.56
NiO	1.68	1.47	1.36
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	1.50
IrO	0.62	0.62	0.75

Table II: Magnetic moments of transition metal oxides

In addition, we have generated atomic data for rare-earth elements. The lattice parameters found for the fcc struture are the following :

Element	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
fcc lattice parameter (Å)	5.272	4.769	4.608	4.531	4.499	4.516	4.630	4.723	4.835	4.918	5.012	5.073	5.120	5.163	5.589

Table III: fcc lattice parameters obtained with JTHv1.0 atomic data in Abinit for the rare-earth elements

IV. CONCLUSIONS

The JTHv1.0 table has good accuracy and efficiency compared to other similar datasets. It makes it a good candidate for high-throughput calculations. This new table is provided as XML files, that makes it easily readable by all PAW codes (ABINIT, GPAW, PWPAW, SOCORRO, ...). It is distributed on the ABINIT web site [9].

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