Benchmark Set for Accuracy Assessment of DFT Codes and Methods

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An obvious truth :

Any two independently written DFT codes that solve the Kohn-Sham equations in a numerically exact way, should produce identical predictions for any solid (provided the same XC-functional is used and full numerical accuracy is reached).

Goal of this work

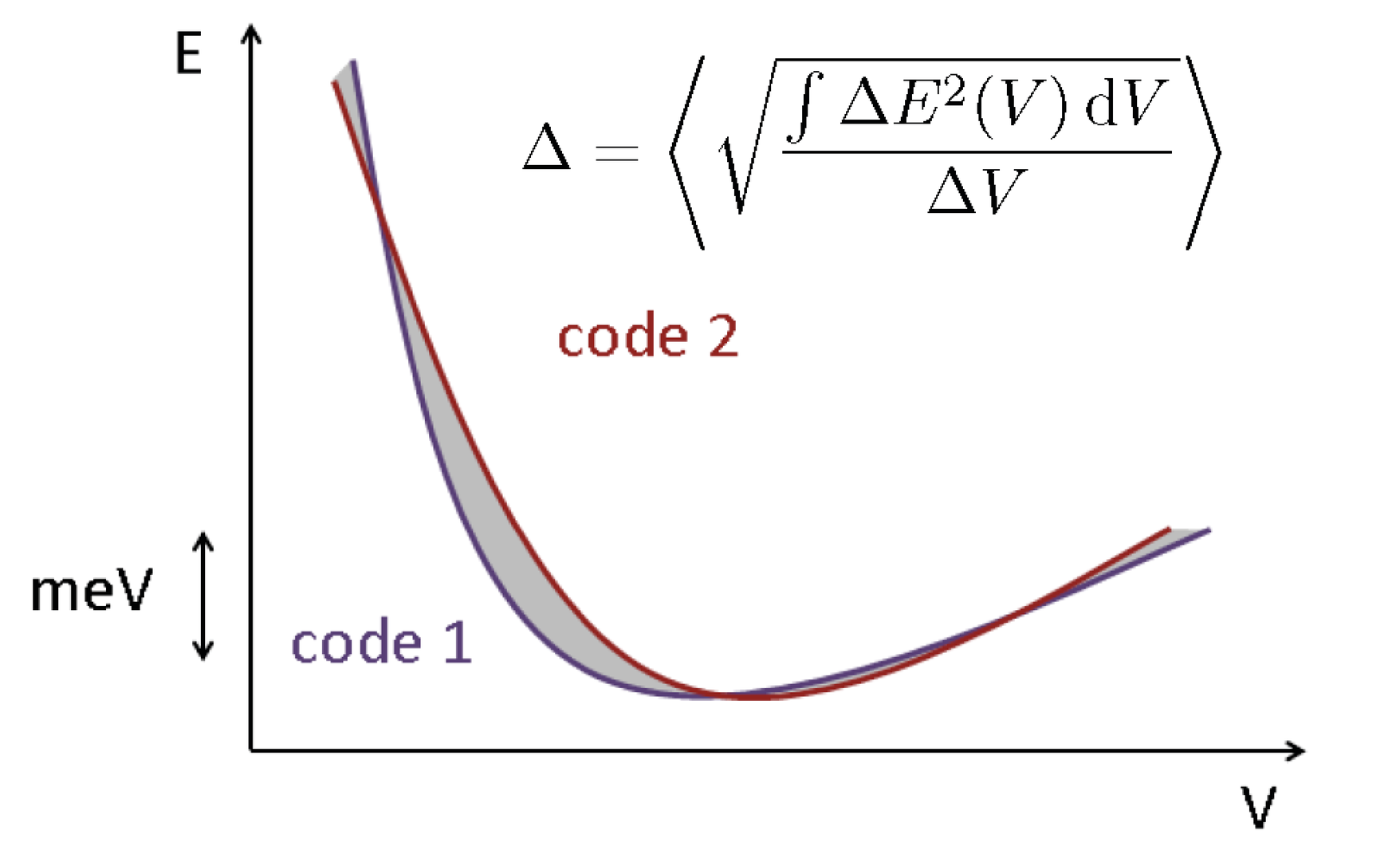
Verify this statement, by comparing predictions by different codes/methods for a standardized benchmark set of elemental solids.

Benchmark set

- Elemental materials in their ground state crystal structure (except for Mn and S).
- 7 data points in a range of ±6% around the equilibrium geometry predicted by VASP.
- Frozen geometry: only volume change, no cell shape or internal positions.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 194 hP4																	He 194 hP2
Li 166 hR9	Be 194 hP2											B 166 hR36	C 194 hP4	N 205 cP8	O 12 mS4	F 15 mS8	Ne 225 cF4
Na 166 hR9	Mg 194 hP2											Al 225 cF4	Si 227 cF8	P 64 oS8	S β-Po	Cl 64 oS8	Ar 225 cF4
K 229 cI2	Ca 225 cF4	Sc 194 hP2	Ti 194 hP2	V 229 cI2	Cr 229 cI2	Mn AF fcc	Fe 229 cI2	Co 194 hP2	Ni 225 cF4	Cu 225 cF4	Zn 194 hP2	Ga 64 oS8	Ge 227 cF8	As 166 hR6	Se 152 hP3	Br 64 oS8	Kr 225 cF4
Rb 229 cI2	Sr 225 cF4	Y 194 hP2	Zr 194 hP2	Nb 229 cI2	Mo 229 cI2	Tc 194 hP2	Ru 194 hP2	Rh 225 cF4	Pd 225 cF4	Ag 225 cF4	Cd 194 hP2	In 139 tI2	Sn 227 cF8	Sb 166 hR6	Te 152 hP3	I 64 oS8	Xe 225 cF4
Cs 229 cI2	Ba 229 cI2	Lu 194 hP2	Hf 194 hP2	Ta 229 cI2	W 229 cI2	Re 194 hP2	Os 194 hP2	Ir 225 cF4	Pt 225 cF4	Au 225 cF4	Hg 139 tI2	Tl 194 hP2	Pb 225 cF4	Bi 166 hR6	Po 221 cP1	At	Rn 225 cF4

Gauge : Δ



$$\Delta = \left\langle \sqrt{\frac{\int \Delta E^2(V)\,\mathrm{d}V}{\Delta V}} \right\rangle$$

Reference calculations

APW+lo as implemented in WIEN2k
PBE functional
R_{mt} = 2.30 a.u. or touching
basis set : very large (see bottom left table)
k-grid : corresponding to 31x31x31 for Au
l_{max} = 14
G_{max} = 3 G_{min}
FFT-mesh : factor 4

Summarized results

up-to-date table available at http://molmod.ugent.be/DeltaCodesDFT

code	*basis*	*potentials*	*Δ-factor*	*reference*
WIEN2k	APW+lo	--	0.0	by def.
ABINIT	plane waves	PAW 0.9	1.6	[3]
OpenMX	pseudo-atomic orbitals	nc MBK	1.6	[4]
GPAW	plane waves	PAW 0.9	1.7	[2]
VASP	plane waves	PAW 2012	1.9	[1]
GPAW	grid-based	PAW 0.6	3.3	[1]
DACAPO	plane waves	VdB USPP v2	8.3	[2]
ABINIT	plane waves	nc TM	21.7	[2]

Inspect Δ per element (hunt for the worst PP or PAW projector)

ABINIT / PAW 0.9

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 0.1																	He 0.0
Li 0.1	Be 2.5											B 0.7	C 1.2	N 1.4	O 1.8	F 1.4	Ne 0.0
Na 0.0	Mg 0.1											Al 0.3	Si 0.6	P 1.4	S 2.6	Cl 1.3	Ar 0.0
K 0.1	Ca 0.7	Sc 0.5	Ti 0.9	V 1.4	Cr 4.2	Mn 5.7	Fe 2.3	Co 1.4	Ni 0.3	Cu 2.3	Zn 1.7	Ga 0.7	Ge 1.7	As 1.0	Se 2.3	Br 0.3	Kr 0.1
Rb 0.0	Sr 1.7	Y 0.3	Zr 0.2	Nb 2.4	Mo 1.3	Tc N/A	Ru 5.9	Rh 1.7	Pd 2.0	Ag 0.9	Cd 2.4	In 1.2	Sn 0.2	Sb 0.5	Te 1.6	I 0.8	Xe 0.0
Cs 0.4	Ba 0.7	Lu N/A	Hf 0.1	Ta 0.5	W 5.2	Re 4.1	Os 9.2	Ir 5.9	Pt 3.8	Au 6.1	Hg 0.4	Tl 1.6	Pb 0.7	Bi 0.6	Po N/A	At N/A	Rn 0.0

OpenMX / nc MBK

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 0.1																	He 0.4
Li 0.9	Be 1.7											B 0.6	C 0.1	N 7.8	O 4.5	F 0.3	Ne 0.1
Na 0.3	Mg 1.4											Al 2.5	Si 0.5	P 2.6	S 2.2	Cl 0.2	Ar 2.0
K 0.2	Ca 0.1	Sc 0.1	Ti 1.9	V 2.6	Cr 1.0	Mn 3.1	Fe 1.3	Co 1.0	Ni 1.2	Cu 1.2	Zn 0.4	Ga 1.3	Ge 0.4	As 3.9	Se 5.7	Br 0.6	Kr 0.0
Rb 0.3	Sr 0.5	Y 0.6	Zr 0.5	Nb 1.1	Mo 0.3	Tc 3.7	Ru 3.3	Rh 3.3	Pd 4.0	Ag 2.8	Cd 3.5	In 0.5	Sn 0.5	Sb 2.4	Te 1.6	I 2.3	Xe 0.2
Cs 0.5	Ba 1.0	Lu 0.3	Hf 3.5	Ta 2.6	W 1.5	Re 3.5	Os 4.4	Ir 3.2	Pt 3.7	Au 2.2	Hg 0.3	Tl 0.2	Pb 0.2	Bi 1.1	Po 0.1	At N/A	Rn 0.2

GPAW / PAW 0.9

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 0.2																	He 0.1
Li 0.1	Be 2.6											B 0.3	C 0.6	N 1.2	O 0.5	F 3.9	Ne 0.2
Na N/A	Mg 0.4											Al 0.5	Si 0.6	P 1.2	S 2.9	Cl 1.0	Ar 0.1
K 0.1	Ca 0.7	Sc 0.6	Ti 0.7	V 0.9	Cr 2.7	Mn 3.9	Fe 0.7	Co 1.7	Ni 0.1	Cu 1.8	Zn 2.4	Ga 1.8	Ge 1.7	As 0.9	Se 2.2	Br 0.1	Kr 0.1
Rb 0.0	Sr 1.1	Y 0.3	Zr 1.7	Nb 3.0	Mo 3.6	Tc N/A	Ru 5.1	Rh 3.0	Pd 0.5	Ag 0.9	Cd 2.7	In 1.8	Sn 2.4	Sb 2.1	Te 2.9	I 1.0	Xe 0.0
Cs 0.2	Ba 0.8	Lu N/A	Hf 0.9	Ta 0.3	W 3.6	Re 4.8	Os 10.7	Ir 6.9	Pt 3.4	Au 6.4	Hg 1.0	Tl 1.9	Pb 1.8	Bi N/A	Po N/A	At N/A	Rn 0.1

VASP / PAW 2012

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 0.1																	He 0.0
Li 0.2	Be 0.1											B 0.3	C 0.3	N 10.6	O 8.3	F 1.5	Ne 0.1
Na 0.0	Mg 0.7											Al 0.3	Si 2.0	P 3.8	S 3.3	Cl 4.0	Ar 0.1
K 0.1	Ca 0.2	Sc 0.4	Ti 0.9	V 1.3	Cr 3.1	Mn 1.4	Fe 3.4	Co 3.4	Ni 2.0	Cu 0.4	Zn 0.3	Ga 0.2	Ge 2.4	As 1.7	Se 1.5	Br 1.5	Kr 0.1
Rb 0.1	Sr 0.1	Y 0.5	Zr 2.7	Nb 7.3	Mo 5.5	Tc 8.3	Ru 2.3	Rh 5.4	Pd 4.4	Ag 4.1	Cd 1.4	In 0.4	Sn 0.2	Sb 0.1	Te 0.5	I 0.9	Xe 0.1
Cs 0.3	Ba 0.7	Lu 4.3	Hf 1.2	Ta 1.0	W 3.5	Re 4.3	Os 3.8	Ir 1.9	Pt 2.5	Au 5.9	Hg 0.5	Tl 0.4	Pb 0.6	Bi 0.4	Po 0.4	At N/A	Rn 0.0

GPAW / PAW 0.6

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 0.2																	He 0.0
Li 0.2	Be 2.6											B 0.2	C 0.3	N 0.2	O 10.4	F 1.0	Ne 0.2
Na 0.1	Mg 0.3											Al 0.2	Si 0.6	P 1.2	S 2.2	Cl 0.9	Ar 0.1
K 0.0	Ca 1.0	Sc 0.4	Ti 3.7	V 9.3	Cr 2.3	Mn 3.7	Fe 1.0	Co 1.3	Ni 3.1	Cu 2.5	Zn 0.4	Ga 1.7	Ge 1.5	As 1.0	Se 2.3	Br 2.8	Kr 0.0
Rb 0.1	Sr 1.5	Y N/A	Zr 1.2	Nb 3.2	Mo 3.8	Tc N/A	Ru 20.9	Rh 14.5	Pd 3.3	Ag 4.4	Cd 0.1	In 0.3	Sn 0.1	Sb N/A	Te 8.4	I 3.3	Xe N/A
Cs 0.3	Ba 0.6	Lu N/A	Hf N/A	Ta 10.2	W 19.3	Re N/A	Os 18.5	Ir 13.2	Pt 6.3	Au 6.8	Hg N/A	Tl N/A	Pb 0.8	Bi 0.4	Po N/A	At N/A	Rn N/A

DACAPO / VdB USPP v2

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 0.7																	He N/A
Li 9.6	Be N/A											B 0.9	C 3.7	N 20.6	O 11.4	F 4.8	Ne N/A
Na 3.0	Mg 1.0											Al 0.8	Si 2.9	P 2.8	S 5.6	Cl 4.5	Ar N/A
K 0.1	Ca 0.1	Sc 0.3	Ti 0.1	V 1.9	Cr N/A	Mn 71.0	Fe 6.8	Co 1.2	Ni 1.4	Cu 9.3	Zn N/A	Ga 0.5	Ge 2.4	As 0.4	Se N/A	Br 1.5	Kr N/A
Rb N/A	Sr 0.5	Y 0.3	Zr N/A	Nb 2.2	Mo 23.7	Tc N/A	Ru 27.3	Rh 5.5	Pd 22.5	Ag 2.2	Cd 1.0	In N/A	Sn 0.8	Sb 6.9	Te 65.6	I 4.2	Xe N/A
Cs 3.1	Ba 1.5	Lu N/A	Hf N/A	Ta 3.9	W 3.6	Re 23.9	Os 12.3	Ir 18.6	Pt 17.1	Au 7.6	Hg N/A	Tl N/A	Pb N/A	Bi 1.6	Po N/A	At N/A	Rn N/A

ABINIT / nc TM

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H 1.1																	He 0.0
Li 1.5	Be 8.0											B 4.8	C 6.5	N 6.8	O 1.4	F 2.7	Ne 0.0
Na 0.3	Mg 1.0											Al 1.0	Si 2.9	P 39.8	S 4.3	Cl 2.4	Ar 0.0
K 9.4	Ca 2.3	Sc 7.2	Ti 22.6	V 59.5	Cr 20.6	Mn N/A	Fe 53.8	Co 67.3	Ni 53.7	Cu 11.1	Zn 7.1	Ga 2.2	Ge 0.6	As 7.4	Se 1.2	Br 0.3	Kr 0.1
Rb 5.9	Sr 7.5	Y 1.6	Zr 9.2	Nb 14.5	Mo 6.5	Tc 7.3	Ru 9.0	Rh 6.6	Pd 14.8	Ag 20.1	Cd 9.6	In 9.7	Sn 2.1	Sb 3.2	Te 8.0	I 1.3	Xe 0.1
Cs 9.7	Ba 2.3	Lu 3.2	Hf 8.0	Ta 25.7	W 678.9	Re 28.3	Os 34.9	Ir 21.0	Pt 15.6	Au 10.9	Hg 1.8	Tl 105.4	Pb 1.5	Bi 14.0	Po 11.5	At N/A	Rn 0.2

Raw Data

Birch-Murnaghan fits for volume per atom ($Å^3$), bulk modulus (GPa) and its pressure derivative

	highest core	lowest valence	RKmax
H		1s	5.0
He		1s	10.0
Li		1s	10.0
Be		1s	10.0
B	1s	2s	7.5
C	1s	2s	7.5
N	1s	2s	7.5
O	1s	2s	7.5
F	1s	2s	8.0
Ne	1s	2s	10.0
Na	1s	2s	10.0
Mg	1s	2s	10.0
Al	2s	2p	10.0
Si	2s	2p	10.0
P	2s	2p	9.0
S	2p	3s	10.0
Cl	2p	3s	8.0
Ar	2p	3s	10.0
K	2p	3s	10.0
Ca	2p	3s	10.0
Sc	2p	3s	10.0
Ti	2p	3s	10.0
V	2p	3s	10.0
Cr	2p	3s	10.0
Mn	2p	3s	10.0
Fe	2p	3s	10.0
Co	2p	3s	10.0
Ni	2p	3s	10.0
Cu	2p	3s	10.0
Zn	2p	3s	10.0
Ga	3p	3d	10.0
Ge	3p	3d	10.0
As	3p	3d	10.0
Se	3p	3d	10.0
Br	3p	3d	10.0
Kr	3p	3d	10.0
Rb	3d	4s	10.0
Sr	3d	4s	10.0
Y	3d	4s	10.0
Zr	3d	4s	10.0
Nb	3d	4s	10.0
Mo	3d	4s	10.0
Tc	3d	4s	10.0
Ru	3d	4s	10.0
Rh	3d	4s	10.0
Pd	3d	4s	10.0
Ag	3d	4s	10.0
Cd	3d	4s	10.0
In	4s	4p	10.0
Sn	4s	4p	10.0
Sb	4s	4p	10.0
Te	4s	4p	10.0
I	4s	4p	10.0
Xe	4s	4p	10.0
Cs	4p	4d	10.0
Ba	4p	4d	10.0
Lu	4d	5s	12.0
Hf	4d	5s	12.0
Ta	4d	5s	12.0
W	4d	5s	12.0
Re	4d	5s	12.0
Os	4d	5s	12.0
Ir	4d	5s	12.0
Pt	4d	5s	12.0
Au	4d	5s	12.0
Hg	4d	5s	12.0
Tl	4f	5p	12.0
Pb	4f	5p	12.0
Bi	4f	5p	12.0
Po	4f	5p	12.0
Rn	4f	5p	12.0

	WIEN2k			ABINIT PAW 0.9			OpenMX			GPAW PAW 0.9		
	V/at	B	B'	V/at	B	B'	V/at	B	B'	V/at	B	B'
H	17.387	10.315	3.025	17.454	10.309	2.770	17.334	10.251	2.227	17.459	10.340	2.705
He	17.778	0.847	6.534	17.778	0.874	6.317	16.437	1.215	6.762	17.264	1.047	6.060
Li	20.216	13.879	3.754	20.260	14.038	3.371	19.943	14.719	3.900	20.259	14.058	3.365
Be	7.915	123.039	3.154	8.005	123.602	3.348	7.852	126.156	3.273	8.008	123.494	3.348
B	7.245	237.599	3.476	7.231	237.908	3.469	7.234	236.297	3.405	7.241	237.967	3.464
C	11.654	209.648	3.565	11.627	209.526	3.566	11.656	210.013	3.585	11.645	209.686	3.566
N	28.896	54.288	3.753	28.780	54.363	3.772	29.499	54.725	3.559	28.797	54.159	3.694
O	18.564	51.231	3.927	18.403	52.101	3.876	18.947	50.146	3.860	18.525	51.715	3.895
F	19.347	35.015	4.246	19.164	34.603	4.141	19.323	32.960	3.648	19.049	37.197	3.735
Ne	24.349	1.242	8.664	24.342	1.219	8.348	24.118	1.287	6.759	23.938	1.430	6.456
Na	37.089	7.728	3.736	37.078	7.688	3.745	37.232	8.238	2.672	37.321	7.609	-1.136
Mg	22.934	35.748	4.263	22.917	36.110	3.964	23.104	36.052	3.981	22.892	36.231	4.033
Al	16.503	77.512	4.667	16.519	77.528	4.612	16.356	76.493	4.150	16.517	77.660	4.609
Si	20.553	88.673	4.227	20.523	88.388	4.310	20.524	89.302	4.380	20.520	88.516	4.326
P	21.614	68.863	4.416	21.519	68.108	4.352	21.441	68.790	4.206	21.532	68.002	4.348
S	17.346	85.495	4.440	17.207	83.940	4.210	17.231	86.014	4.063	17.187	84.008	4.207
Cl	39.175	19.324	4.489	38.862	19.091	4.257	39.211	18.857	4.349	38.949	19.016	4.378
Ar	52.209	0.704	7.838	52.295	0.661	4.758	48.559	2.464	11.119	52.201	0.788	7.033
K	73.710	3.586	3.734	73.649	3.521	3.645	73.486	3.550	4.456	73.563	3.608	3.772
Ca	42.208	17.300	3.167	42.383	17.424	3.332	42.190	17.130	3.331	42.395	17.422	3.273
Sc	24.621	54.559	3.402	24.662	54.274	3.446	24.633	54.814	3.279	24.573	54.613	3.393
Ti	17.407	112.712	3.591	17.444	112.007	3.564	17.329	115.575	3.969	17.437	112.194	3.594
V	13.517	185.231	3.731	13.553	180.517	3.935	13.454	193.477	3.947	13.543	182.429	3.802
Cr	11.910	183.841	7.374	11.803	160.850	7.061	11.915	167.075	7.939	11.852	161.406	7.241
Mn	11.611	131.159	0.852	11.370	111.339	2.648	11.733	126.605	-1.022	11.471	121.430	0.493
Fe	11.451	196.127	6.137	11.511	189.140	4.951	11.420	186.257	8.095	11.472	193.380	5.620
Co	10.948	216.191	5.076	10.917	212.332	5.378	10.929	214.191	4.807	10.910	215.828	5.115
Ni	10.986	204.685	4.852	10.993	204.230	4.744	10.960	201.770	4.822	10.982	203.940	4.947
Cu	12.017	143.702	5.198	12.095	137.663	4.902	12.058	138.499	4.779	12.081	137.188	5.078
Zn	15.270	75.617	5.377	15.169	75.320	5.289	15.293	74.375	5.440	15.122	76.379	5.407
Ga	20.377	49.087	5.330	20.443	49.810	5.290	20.506	47.242	4.917	20.538	49.728	5.378
Ge	24.094	59.486	5.084	23.963	59.882	4.920	24.080	56.656	6.167	23.967	60.210	4.906
As	22.571	69.732	4.294	22.635	68.831	4.281	22.818	68.087	4.896	22.637	68.795	4.294
Se	29.973	47.637	4.548	29.748	47.392	4.481	29.412	47.320	4.575	29.761	47.304	4.481
Br	39.780	22.629	5.154	39.716	22.388	4.873	39.675	22.296	4.613	39.768	22.302	4.866
Kr	65.226	0.851	22.009	66.050	0.653	6.838	65.732	0.801	9.878	66.260	0.636	7.271
Rb	91.130	2.842	2.321	91.092	2.781	3.752	90.508	2.674	4.958	91.121	2.786	3.770
Sr	54.561	11.333	4.172	55.197	11.640	3.349	54.791	11.440	2.212	54.662	12.391	4.328
Y	32.864	41.320	2.952	32.892	40.801	3.064	32.801	42.920	3.225	32.858	41.220	3.014
Zr	23.402	94.061	3.247	23.393	93.373	3.292	23.420	95.861	3.253	23.323	93.990	3.322
Nb	18.155	168.691	3.504	18.089	168.216	3.727	18.146	179.901	4.798	18.034	170.426	3.920
Mo	15.825	260.410	4.264	15.806	255.693	4.083	15.820	263.805	4.363	15.765	259.394	4.367
Tc	14.472	301.391	4.555				14.530	302.326	4.004			
Ru	13.810	315.359	4.955	13.722	309.294	4.991	13.857	315.034	4.938	13.735	309.531	4.858
Rh	14.082	260.576	5.440	14.113	252.579	5.234	14.141	262.221	4.686	14.137	253.502	5.260
Pd	15.326	170.442	5.854	15.273	169.252	5.548	15.435	168.458	5.274	15.304	169.253	5.614
Ag	17.855	91.328	5.799	17.811	92.116	5.737	17.983	91.874	6.581	17.807	92.333	5.751
Cd	22.866	44.247	7.089	22.617	45.826	6.822	22.547	53.581	7.952	22.575	46.346	6.714
In	27.497	34.759	4.870	27.337	36.230	5.214	27.574	36.728	2.350	27.244	36.050	5.299
Sn	36.883	36.020	5.038	36.864	35.700	4.897	36.831	36.910	4.603	36.581	36.313	4.912
Sb	31.786	50.718	4.495	31.745	50.159	4.494	32.007	49.043	4.604	31.593	50.484	4.485
Te	35.009	44.806	4.703	34.843	45.093	4.713	35.179	44.421	4.506	34.708	45.262	4.716
I	50.339	18.699	5.222	50.547	18.600	5.084	50.890	18.253	4.910	50.594	18.551	5.083
Xe	87.318	0.569	-0.724	86.767	0.542	7.214	88.907	0.497	7.823	87.204	0.529	7.235
Cs	117.748	1.964	3.592	116.834	1.958	3.329	118.844	1.928	4.786	117.310	1.961	3.492
Ba	63.200	8.431	3.299	63.569	8.880	2.719	63.672	9.099	3.373	63.575	8.813	2.853
Lu	29.060	47.725	4.048				29.070	49.294	4.041			
Hf	22.551	108.082	3.225	22.544	108.682	3.462	22.400	109.783	3.855	22.586	108.630	3.452
Ta	18.296	193.730	4.774	18.291	195.569	3.747	18.238	199.819	4.233	18.302	193.805	3.813
W	16.175	302.590	4.300	16.096	304.221	4.151	16.150	305.293	4.670	16.115	304.826	4.245
Re	14.987	364.610	4.466	14.935	363.901	4.507	14.942	369.686	4.579	14.926	365.244	4.435
Os	14.320	402.199	4.352	14.211	398.861	4.800	14.368	398.124	4.787	14.194	400.169	4.813
Ir	14.533	341.743	6.958	14.464	347.474	4.959	14.578	356.806	4.829	14.452	348.912	5.111
Pt	15.678	251.750	5.342	15.610	245.082	5.309	15.742	256.315	5.190	15.613	246.217	5.496
Au	17.993	139.863	5.985	18.184	138.750	6.077	18.045	147.161	6.982	18.208	138.897	5.823
Hg	29.716	8.155	8.077	29.548	9.542	8.300	29.365	10.588	25.163	28.515	10.958	11.346
Tl	31.456	26.683	4.565	31.173	27.036	5.379	31.472	26.618	6.254	31.107	27.488	5.364
Pb	32.000	39.551	5.954	31.931	40.319	5.019	32.018	39.992	6.211	31.872	37.943	4.848
Bi	36.939	42.556	4.626	37.001	42.405	4.625	37.053	42.867	4.673	36.831	42.751	4.640
Po	37.570	45.523	5.018				37.566	44.965	5.680			
Rn	92.765	0.544	13.133	92.762	0.544	7.377	91.382	0.556	7.446	93.543	0.523	7.228

	VASP			GPAW PAW 0.6			DACAPO			ABINIT FHI-PP		
	V/at	B	B'	V/at	B	B'	V/at	B	B'	V/at	B	B'
H	17.445	10.101	3.032	17.465	10.332	2.932	17.683	10.617	2.728	16.894	10.145	2.618
He	17.721	0.923	7.416	17.693	0.841	6.728				17.685	0.845	7.426
Li	20.286	13.801	3.159	20.278	14.000	3.412	22.156	12.196	3.532	19.715	13.526	3.199
Be	7.920	123.305	3.293	8.009	123.300	3.371				7.633	122.773	3.201
B	7.251	237.006	3.467	7.242	237.100	3.527	7.228	236.231	3.450	7.152	238.116	3.613
C	11.661	208.405	3.558	11.648	208.700	3.623	11.573	211.609	3.598	11.509	208.886	3.541
N	29.648	56.413	3.859	28.910	54.000	3.666	30.218	55.628	3.389	28.320	53.958	3.638
O	19.186	51.428	4.058	19.280	53.600	3.964	19.338	53.354	3.722	18.434	50.633	3.735
F	19.541	34.185	4.203	19.207	33.700	4.501	19.872	35.781	4.621	18.873	26.594	6.434
Ne	24.606	1.071	14.475	23.751	2.100	20.674				24.242	1.281	7.040
Na	37.074	7.688	3.044	37.045	7.800	3.913	35.524	8.072	3.724	36.882	7.559	3.608
Mg	22.847	36.471	3.919	22.971	36.255	4.182	23.058	35.951	4.052	22.801	35.795	4.025
Al	16.487	77.287	4.651	16.515	78.209	4.610	16.455	77.260	5.027	16.565	76.010	4.504
Si	20.446	88.790	4.296	20.521	88.830	4.361	20.403	88.872	4.307	20.399	87.921	4.280
P	21.359	68.513	4.338	21.531	68.072	4.436	21.427	67.695	4.196	23.861	40.815	4.611
S	17.167	83.524	4.136	17.224	83.735	4.316	17.037	83.932	4.452	17.108	84.292	4.204
Cl	38.207	19.154	4.334	38.953	19.016	4.590	38.077	19.690	6.753	38.591	19.134	4.362
Ar	52.652	0.788	7.351	52.661	0.838	3.274				52.248	0.777	8.446
K	73.844	3.592	3.818	73.782	3.600	2.491	73.872	3.893	1.431	66.621	3.979	3.689
Ca	42.169	17.518	3.017	42.456	17.400	3.193	42.217	17.175	1.979	42.760	17.826	3.480
Sc	24.659	54.370	3.406	24.659	54.200	3.097	24.643	54.266	3.418	25.173	54.732	3.320
Ti	17.371	112.521	3.599	17.257	114.400	3.714	17.404	111.643	3.831	18.148	111.345	3.654
V	13.484	181.621	4.020	13.729	185.500	4.379	13.470	180.486	3.601	14.510	172.570	3.832
Cr	11.834	176.751	7.166	11.870	161.800	6.665				12.246	228.158	4.972
Mn	11.569	115.449	0.354	11.746	126.600	1.116	10.748	277.287	4.329			
Fe	11.375	185.742	4.910	11.478	196.700	5.034	11.626	162.557	8.238	12.309	178.916	3.975
Co	10.875	210.783	4.994	10.921	212.400	4.997	10.973	214.957	5.157	10.839	1613.396	53.914
Ni	10.942	193.681	4.919	10.917	203.600	4.602	10.954	203.148	4.772	10.975	769.967	60.404
Cu	12.026	136.757	5.097	12.100	139.400	4.594	12.306	133.614	5.029	12.342	136.174	5.198
Zn	15.288	74.193	5.624	15.250	75.100	4.797				15.662	74.030	4.416
Ga	20.356	48.928	5.087	20.524	50.300	5.242	20.345	49.928	3.377	20.171	49.675	5.053
Ge	23.911	58.826	4.777	23.979	60.100	4.840	23.907	59.757	4.804	24.053	57.745	4.754
As	22.686	68.726	4.294	22.636	68.900	4.434	22.548	69.623	4.089	23.040	66.841	4.242
Se	29.829	47.229	4.480	29.749	47.200	4.607				30.092	46.475	4.443
Br	39.467	22.463	4.850	40.382	20.800	4.658	39.468	22.404	4.667	39.729	22.254	4.842
Kr	66.559	0.683	4.824	65.583	0.800	13.160				66.033	0.641	6.957
Rb	91.238	2.790	3.729	91.172	2.700	3.056				84.304	2.986	3.731
Sr	54.541	11.132	4.594	55.154	11.200	3.684	54.752	11.506	3.321	52.296	13.500	3.205
Y	32.921	41.378	3.203				32.899	40.972	3.065	32.687	42.037	3.300
Zr	23.530	93.781	3.584	23.458	94.900	3.384				23.800	97.628	3.502
Nb	18.337	171.753	3.970	18.232	174.200	3.783	18.093	170.578	3.971	18.503	175.175	3.559
Mo	15.917	262.885	4.342	15.888	263.700	4.375	16.182	267.884	4.531	15.933	266.090	4.191
Tc	14.596	298.498	4.545							14.572	313.646	4.519
Ru	13.844	311.518	4.951	14.090	310.900	4.874	14.120	344.792	5.059	13.930	322.632	4.948
Rh	14.179	254.234	5.250	14.321	255.200	5.424	13.985	259.049	5.120	14.189	267.957	5.269
Pd	15.444	168.191	5.636	15.415	167.300	5.975	15.820	170.298	5.644	15.677	169.784	5.655
Ag	18.054	89.106	5.778	18.067	90.700	5.520	17.744	92.462	5.863	18.639	87.613	5.813
Cd	23.008	43.780	7.225	22.875	43.300	6.282	22.766	44.499	6.813	23.715	40.166	7.044
In	27.538	35.433	5.335	27.533	35.100	5.603				26.377	37.905	5.059
Sn	36.859	35.843	4.852	36.899	36.000	4.899	36.792	35.194	4.237	36.611	35.403	4.733
Sb	31.794	50.899	4.544				31.192	54.089	4.649	31.497	50.988	4.474
Te	34.961	44.964	4.721	34.171	46.100	4.812	38.558	41.165	4.833	34.201	45.968	4.680
I	50.123	18.720	5.090	51.154	17.600	4.878	49.319	19.099	5.063	50.024	18.775	5.032
Xe	87.770	0.525	7.764							86.650	0.544	7.208
Cs	116.957	1.974	3.483	117.011	2.100	3.588	123.835	1.793	3.432	105.515	2.261	3.677
Ba	63.554	8.863	3.107	63.514	8.900	2.947	62.410	8.497	2.585	64.298	9.013	2.870
Lu	29.469	47.159	3.438							29.339	50.015	3.922
Hf	22.496	107.831	3.478							22.870	108.981	3.362
Ta	18.325	194.286	3.972	18.523	198.400	3.991	18.210	194.071	3.724	18.830	194.065	3.715
W	16.226	304.396	4.298	16.440	307.500	4.351	16.120	306.074	4.283	18.899	530.281	-0.516
Re	14.933	372.481	4.548				14.689	371.713	4.440	15.305	367.036	4.452
Os	14.360	400.928	4.948	14.517	397.900	4.975	14.177	408.197	4.723	14.676	393.568	4.814
Ir	14.566	345.973	5.173	14.699	351.600	5.385	14.296	352.890	5.150	14.787	351.566	5.173
Pt	15.723	248.060	5.534	15.790	247.600	5.666	15.971	243.678	5.562	15.937	250.890	5.566
Au	18.182	136.424	5.914	18.207	137.800	5.772	18.227	138.628	5.811	18.315	139.871	5.739
Hg	29.944	7.623	12.941							32.928	-0.428	4.667
Tl	31.521	26.464	5.429							25.455	36.408	5.303
Pb	32.079	39.787	4.403	32.103	39.100	5.556				32.226	37.430	2.694
Bi	36.985	42.539	4.550	36.973	42.900	4.761	36.777	43.893	4.081	35.540	44.094	4.603
Po	37.534	45.385	4.633							36.460	47.203	4.809
Rn	93.106	0.553	7.240							91.520	0.730	14.805

Conclusions and Outlook

- Convenient test set for code accuracy verification
- Convenient test set for pseudopotential and PAW projector generation
- Disagreement between codes/methods is one order of magnitude smaller than disagreement between DFT and experiment (good !)
- General call: run this test for your favourite code (all input and scripts available)
- Interesting question: would other APW+lo implementations yield Δ-values well below 1.6 meV/atom ?

References

[1] K. Lejaeghere, V. Van Speybroeck, G. Van Oost, S. Cottenier, Critical Reviews in Solid State Physics and Materials Sciences 39 (2014) p. 1 (http://arxiv.org/abs/1204.2733)
[2] by M. Dulak
[3] by F. Jollet and M. Torrent
[4] by T. Ozaki

Input files to run your own tests as well as scripts for analysis are available at http://molmod.ugent.be/DeltaCodesDFT