FROM RESEARCH TO INDUSTRY

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PAW ATOMIC DATA: THE JTH V1.0 TABLE

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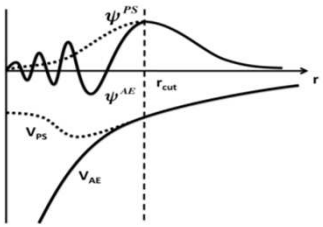


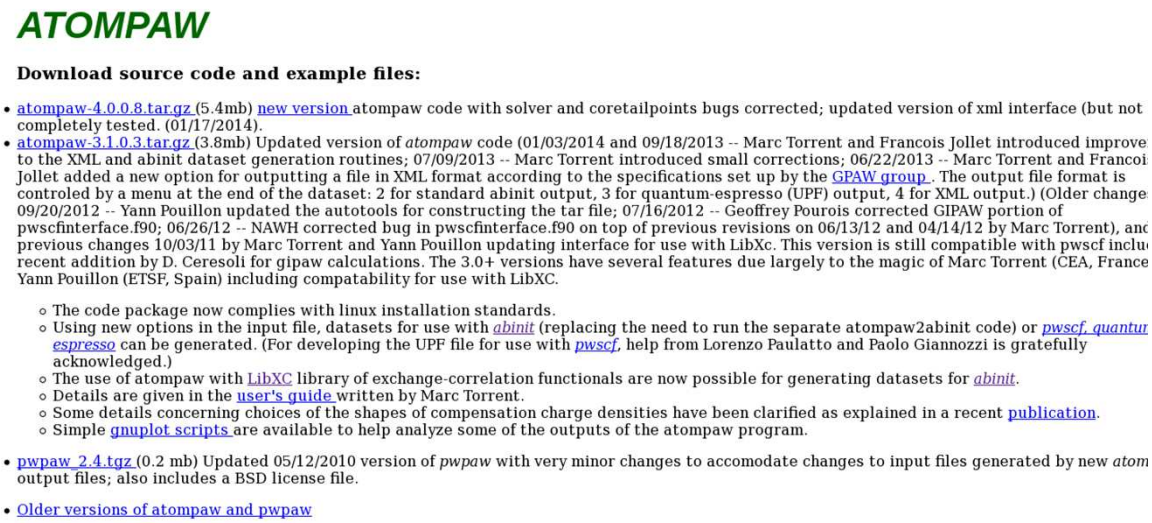
THE PAW ATOMIC DATASETS

Generation process

1- Solve "exactly" the atomic problem (for the given LDA/GGA functional)

2- Transform some quantities into smooth ones ("pseudization")

3- Build the partial wave basis and projectors



ATOMPAW

Download source code and example files:

- atompaw-4.0.0.8.tar.gz (5.4mb) new version atompaw code with solver and coretailpoints bugs corrected; updated version of xml interface (but not completely tested. (01/17/2014).
- atompaw-3.1.0.3.tar.gz (3.8mb) Updated version of *atompaw* code (01/03/2014 and 09/18/2013 -- Marc Torrent and Francois Jollet introduced improve to the XML and abinit dataset generation routines; 07/09/2013 -- Marc Torrent introduced small corrections; 06/22/2013 -- Marc Torrent and Francoi Jollet added a new option for outputting a file in XML format according to the specifications set up by the GPAW group . The output file format is controled by a menu at the end of the dataset: 2 for standard abinit output, 3 for quantum-espresso (UPF) output, 4 for XML output.) (Older change 09/20/2012 -- Yann Pouillon updated the autotools for constructing the tar file; 07/16/2012 -- Geoffrey Pourois corrected GIPAW portion of pwscfinterface.f90; 06/26/12 -- NAWH corrected bug in pwscfinterface.f90 on top of previous revisions on 06/13/12 and 04/14/12 by Marc Torrent), and previous changes 10/03/11 by Marc Torrent and Yann Pouillon updating interface for use with LibXc. This version is still compatible with pwscf inclu recent addition by D. Ceresoli for gipaw calculations. The 3.0+ versions have several features due largely to the magic of Marc Torrent (CEA, France Yann Pouillon (ETSF, Spain) including compatability for use with LibXC.
  - The code package now complies with linux installation standards.
  - Using new options in the input file, datasets for use with *abinit* (replacing the need to run the separate atompaw2abinit code) or *pwscf, quantur espresso* can be generated. (For developing the UPF file for use with *pwscf*, help from Lorenzo Paulatto and Paolo Giannozzi is gratefully acknowledged.)
  - The use of atompaw with LibXC library of exchange-correlation functionals are now possible for generating datasets for *abinit*.
  - Details are given in the user's guide written by Marc Torrent.
  - Some details concerning choices of the shapes of compensation charge densities have been clarified as explained in a recent publication.
  - Simple gnuplot scripts are available to help analyze some of the outputs of the atompaw program.
- pwpaw_2.4.tgz (0.2 mb) Updated 05/12/2010 version of *pwpaw* with very minor changes to accomodate changes to input files generated by new *atom* output files; also includes a BSD license file.
- Older versions of atompaw and pwpaw

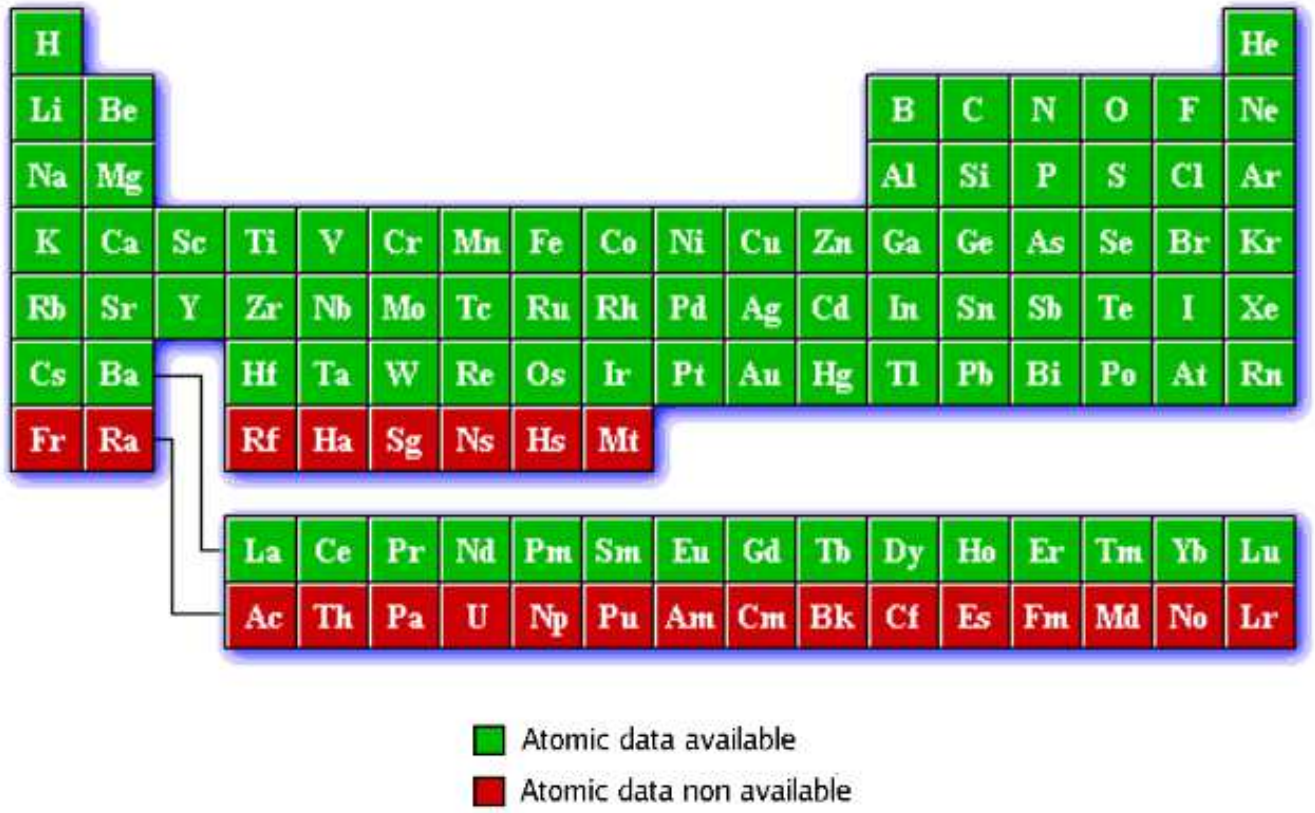
Independent of ABINIT (initiated by N. Holzwarth from Wake Forest University)

Automatically download and installed by ABINIT build system

http://users.wfu.edu/natalie/papers/pwpaw/man.html

THE PAW DATASETS

JTH table : from ABINIT website – http://www.abinit.org/downloads/PAW2



F. Jollet, M. Torrent and N. Holzwarth, Computer Physics Communications, **185** (2014) 1246-1254

CHANGES COMPARED TO JTH_V0.2

Generator: code ATOMPAW (v4.0.0.12) with XML format

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

Error estimation: the delta factor

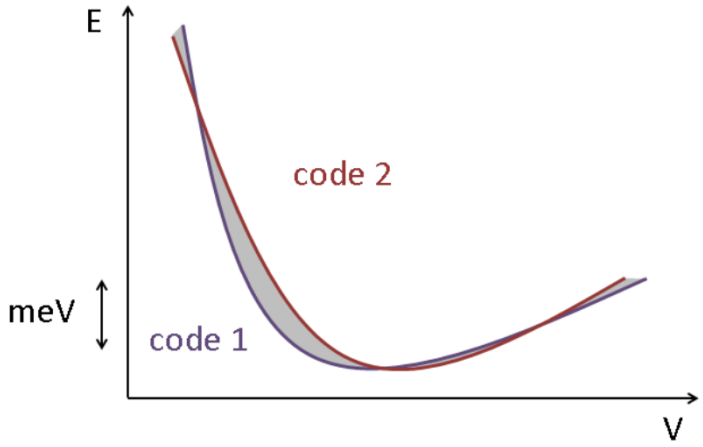
« Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals »,

by K. Lejaeghere, V. Van Speybroeck, G. Van Oost and S. Cottenier

submitted to Critical Reviews in Solid State and Materials Sciences, 39 (1), (2014) 1-24

The Delta parameter:

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



With the delta calculation package, CIF files for 71 elements are available.

- 71 input files are generated (python script)
- 6750/N kpoints for a N atoms unit cell
- 7 calculations with volumes from 0.94 V_0^{ref} to 1.06 V_0^{ref}
- V_0, B_0, B'_0 are deduced from the E(V) curve
- The delta factor is calculated comparing the two codes

Error estimation: the delta factor

Reference point: WIEN2k 13.1 with basis LAPW/APW+lo and potential all-electron

Code: ABINIT 7.8.2 with basis plane waves and potential PAW JTH v1.0

Maximum at Pt. Minimum at He

All values are in meV.

Δ=0.44 meV
Δ1=1.04 meV
Ecut=20 Ha

H 0.25																	He 0.01
Li 0.01	Be 0.09											B 0.24	C 0.15	N 0.49	O 0.24	F 0.22	Ne 0.01
Na 0.50	Mg 0.26											Al 0.10	Si 0.31	P 0.49	S 0.30	Cl 0.06	Ar 0.02
K 0.07	Ca 0.11	Sc 0.02	Ti 1.25	V 1.69	Cr 0.72	Mn 0.89	Fe 0.56	Co 1.07	Ni 1.46	Cu 0.65	Zn 0.28	Ga 0.14	Ge 0.56	As 0.49	Se 0.24	Br 0.11	Kr 0.02
Rb 0.29	Sr 0.76	Y 0.33	Zr 0.25	Nb 0.19	Mo 1.63	Tc 1.03	Ru 0.34	Rh 0.94	Pd 1.16	Ag 0.21	Cd 0.02	In 0.21	Sn 0.11	Sb 0.30	Te 0.07	I 0.73	Xe 0.01
Cs 0.12	Ba 0.74		Hf 0.19	Ta 0.43	W 1.35	Re 0.89	Os 0.48	Ir 0.51	Pt 2.10	Au 1.11	Hg 0.14	Tl 0.06	Pb 0.29	Bi 0.11	Po 0.19	At	Rn 0.02
Fr	Ra																
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu 0.21	
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Error estimation: the delta factor

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https://molmod.ugent.be/deltacodesdft

Comparing Solid State DFT Codes, Basis Sets and Potentials

Code	Version	Basis	Electron treatment	Δ-value	Authors
WIEN2k	13.1	LAPW/APW+lo	all-electron	0 meV/atom	S. Cottenier [16]
FHI-aims	081213	tier2 numerical orbitals	all-electron (relativistic atomic_zora scalar)	0.2 meV/atom	ASE [2,16]
Exciting	development version	LAPW+xlo	all-electron	0.2 meV/atom	Exciting [10,16]
VASP	5.2.12	plane waves	PAW 2015 GW-ready (5.4)	0.3 meV/atom	K. Lejaeghere [16]
FHI-aims	081213	tier2 numerical orbitals	all-electron (relativistic zora scalar 1e-12)	0.3 meV/atom	ASE [2]
Quantum ESPRESSO	5.1	plane waves	SSSP Accuracy (mixed NC/US/PAW potential library)	0.3 meV/atom	QuantumESPRESSO [12,16]
Elk	3.1.5	APW+lo	all-electron	0.3 meV/atom	Elk [14,16]
ABINIT	7.8.2	plane waves	PAW JTH v1.0	0.4 meV/atom	F. Jollet and M. Torrent
FLEUR	0.26	LAPW (+lo)	all-electron	0.4 meV/atom	FLEUR [9,16]
Quantum ESPRESSO	5.1	plane waves	SSSP Efficiency (mixed NC/US/PAW potential library)	0.4 meV/atom	QuantumESPRESSO [12]
CASTEP	9.0	plane waves	OTFG CASTEP 9.0	0.5 meV/atom	CASTEP [7,16]
ABINIT	7.7.3	plane waves	PAW JTH v0.2	0.5 meV/atom	F. Jollet and M. Torrent [16]
FHI-aims	081213	tight numerical orbitals	all-electron (relativistic atomic_zora scalar)	0.5 meV/atom	ASE [2,16]

The GBRV suite

K. F. Garrity, J. W. Bennett, K.M. Rabe and D. Vanderbilt, *Comput. Mater. Sci.* **81**, 446 (2014)

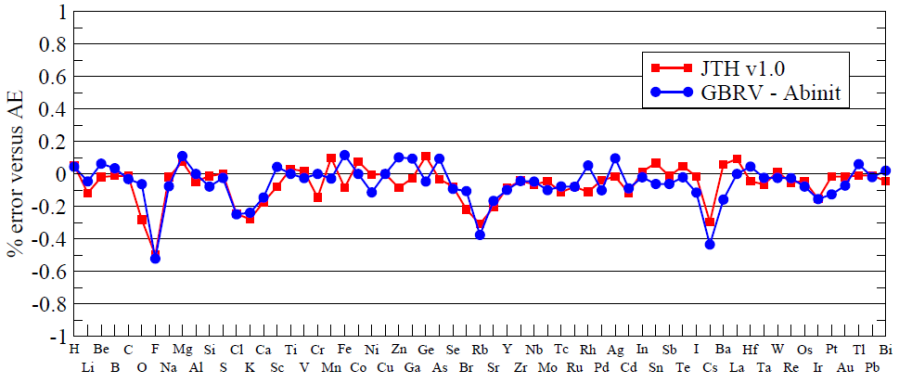

Figure 1: Percent difference in AE versus PAW data calculations for fcc lattice constant

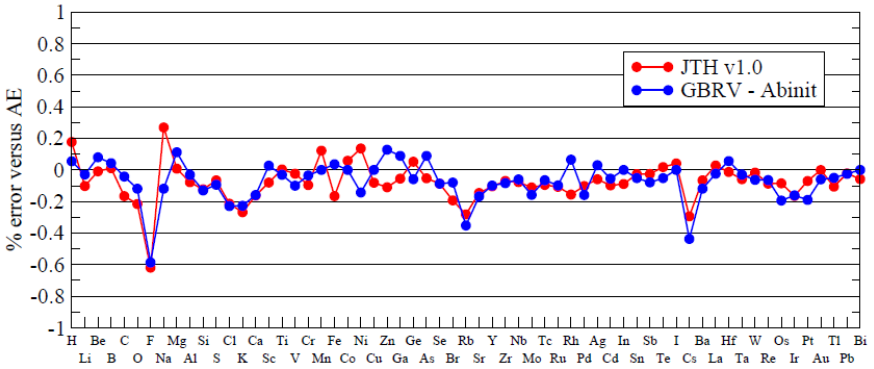

Figure 2: Percent difference in AE versus PAW data calculations for bcc lattice constant

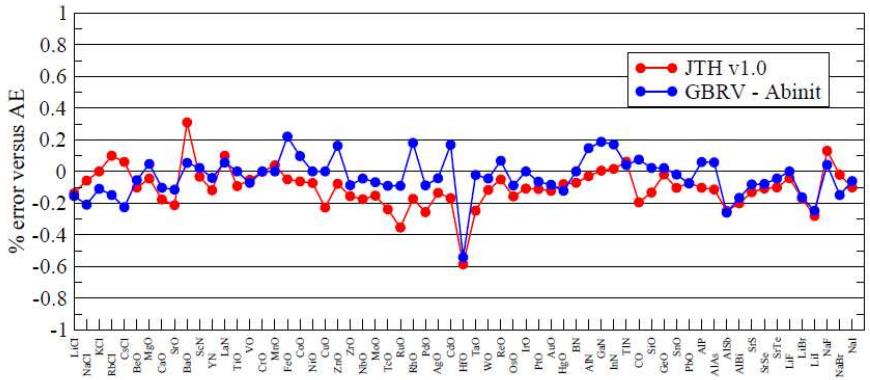

Figure 3: Percent difference in AE versus PAW data calculations for rocksalt lattice constant

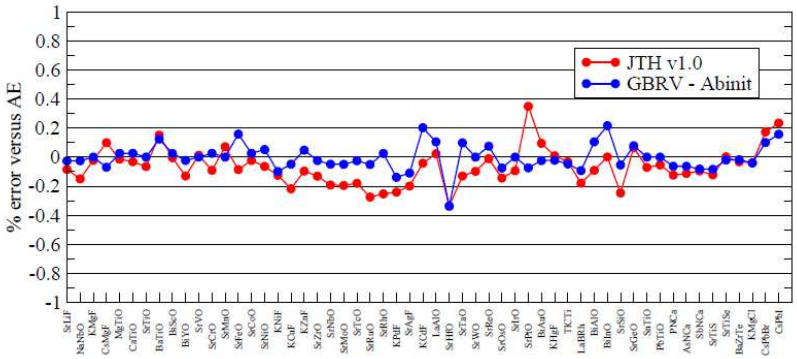

Figure 4: Percent difference in AE versus PAW data calculations for perovskite lattice constant

The GBRV suite

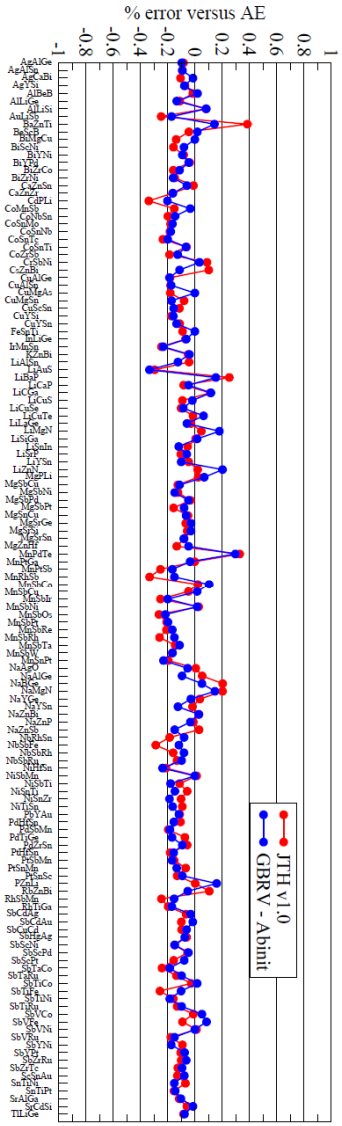

Figure 5: Percent difference in AE versus PAW data calculations for half-heusler lattice constant

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

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

TO DO …

- Numerical problems may happen with H and Li
- The table has been generated for PBE calculations
- The LDA atomic data have not been tested
    - Pb with Fe?

Commissariat à l’énergie atomique et aux énergies alternatives

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