PseudoDojo:
making and testing pseudo potentials

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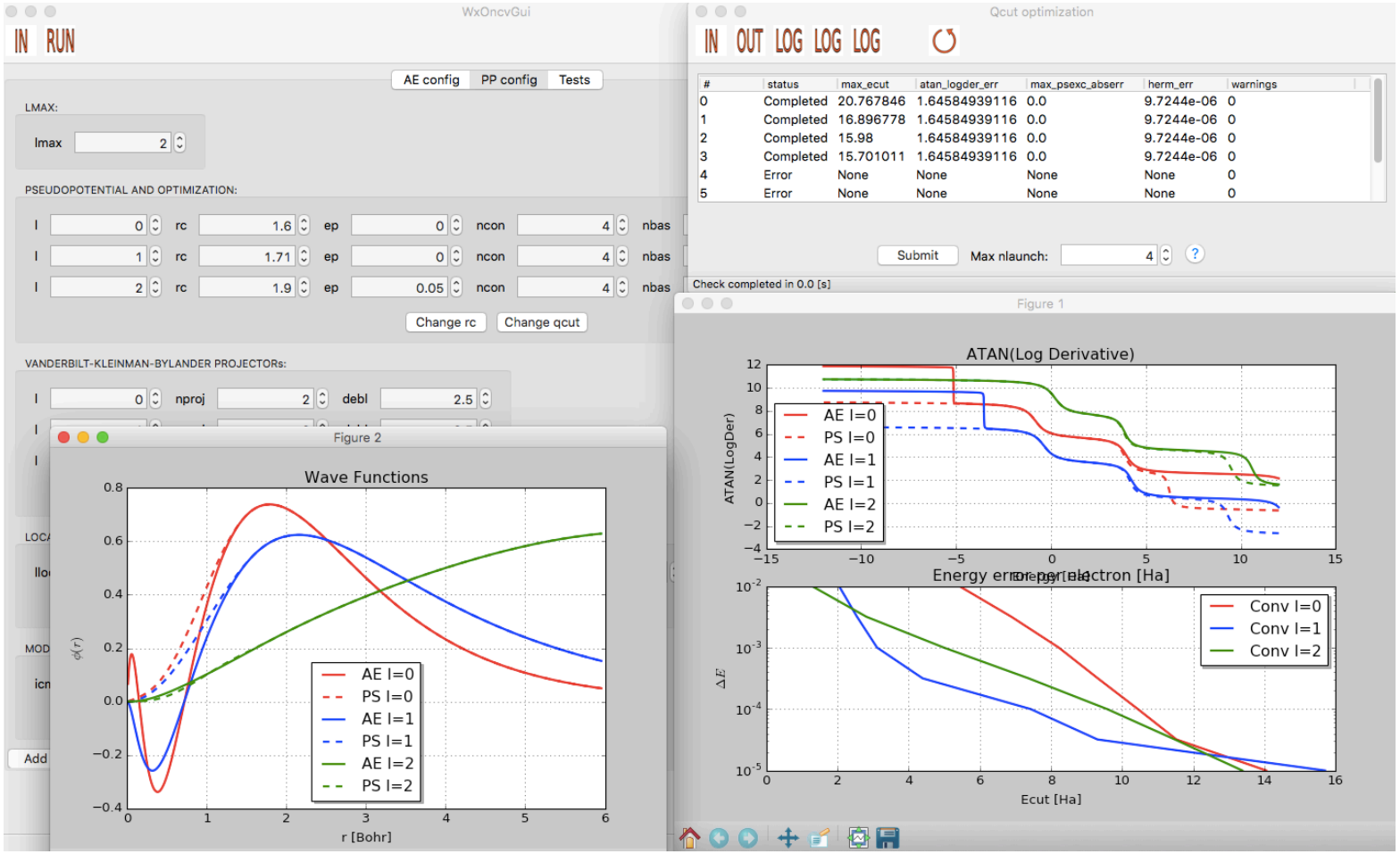
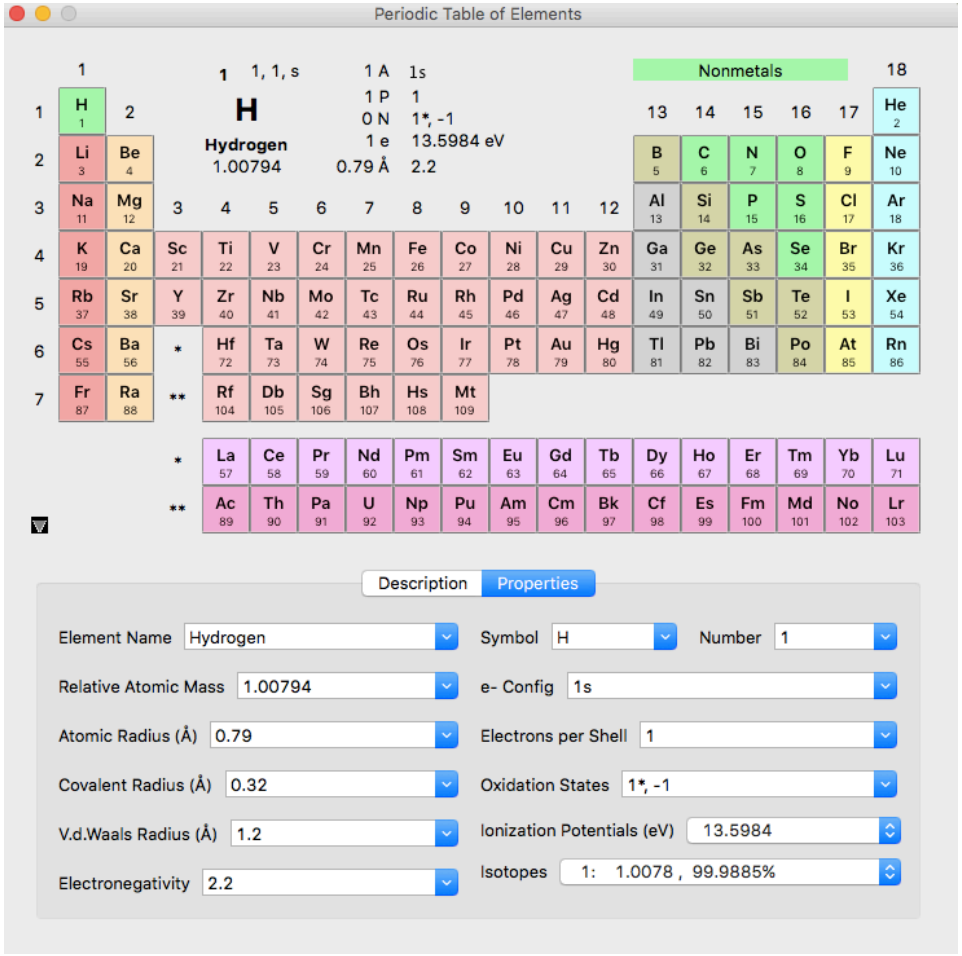
Parts of the PseudoDojo

- Tools for developing
  - GUI to ONCVPSP
- Tools for testing
  - Running test on crystals using Abipy and Abinit
  - Visualizing test results via notebooks
- Database of Pseudopotentials
  - Low, Normal, High precision hints
  - Full access via git
    - command line: git clone, git checkout …
  - Easy access via web-interface (with test results)
    - Click, click, click, …

GUI to ONCVPSP



GUI to ONCVPSP



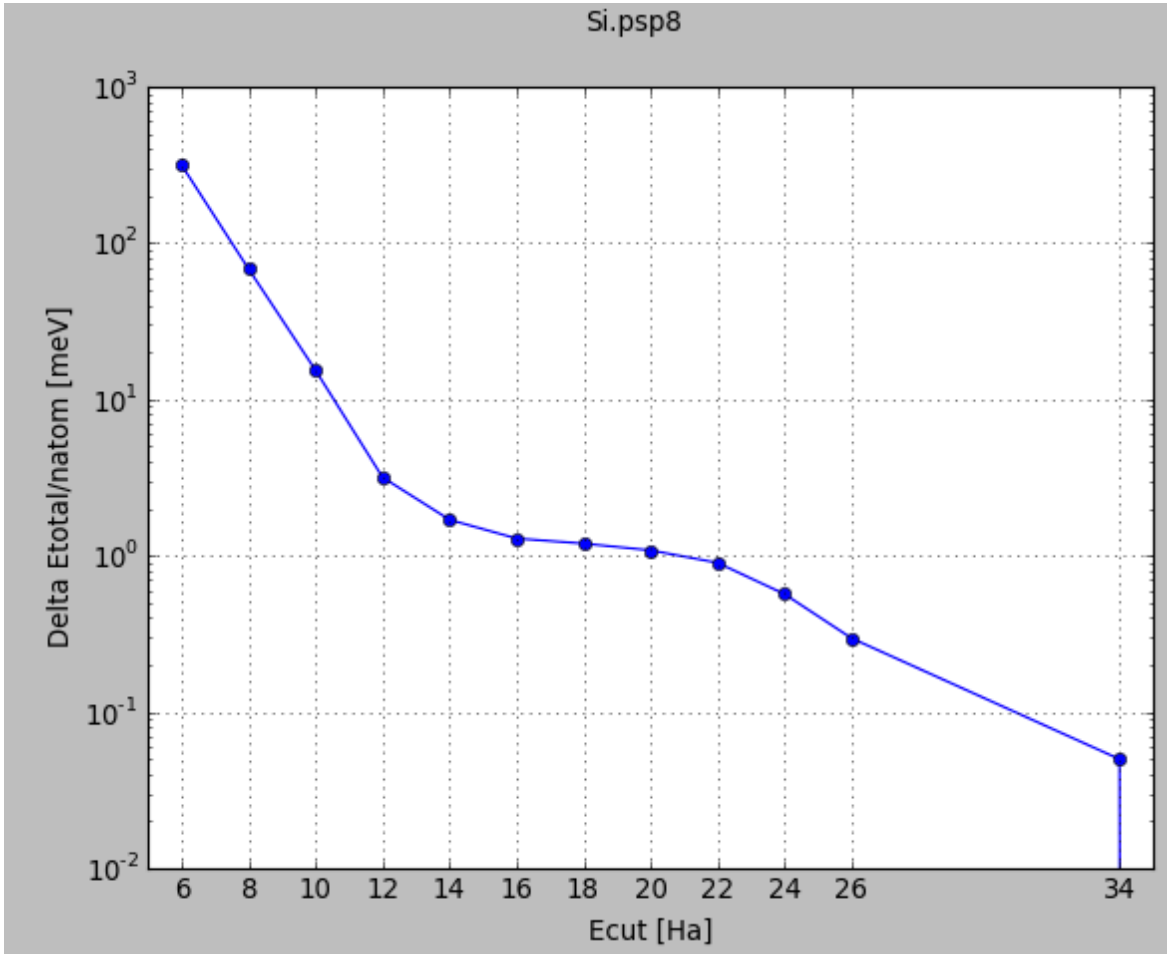
Dojorun

```
dojorun.py --help
usage: dojorun.py [-h] [-m MANAGER] [-d] [--paral-kgb PARAL_KGB] [-p]
                  [-n NEW_ECUT] [--trials TRIALS] [--loglevel LOGLEVEL]
                  path

positional arguments:
  path                  pseudopotential file.

optional arguments:
  -h, --help            show this help message and exit
  -m MANAGER, --manager MANAGER
                        Manager file
  -d, --dry-run         Dry run, build the flow without submitting it
  --paral-kgb PARAL_KGB
                        Paral_kgb input variable.
  -p, --plot            Plot convergence when the flow is done
  --trials TRIALS       List of tests e.g --trials=df,gbrv,phonon,phwoa df:
                        test delta factor against all electron refference
                        gbrv: test fcc and bcc lattice parameters agains AE
                        refference phonon: test phonon mode at gamma
                        convergence phwoa: test violation of the acoustic sum
                        rule (without enforcing it) at the min and max ecut
  --loglevel LOGLEVEL   set the loglevel. Possible values: CRITICAL, ERROR
                        (default), WARNING, INFO, DEBUG

Usage Example: dojorun.py Si.psp8 => Build pseudo_dojo flow for Si.fhi
```

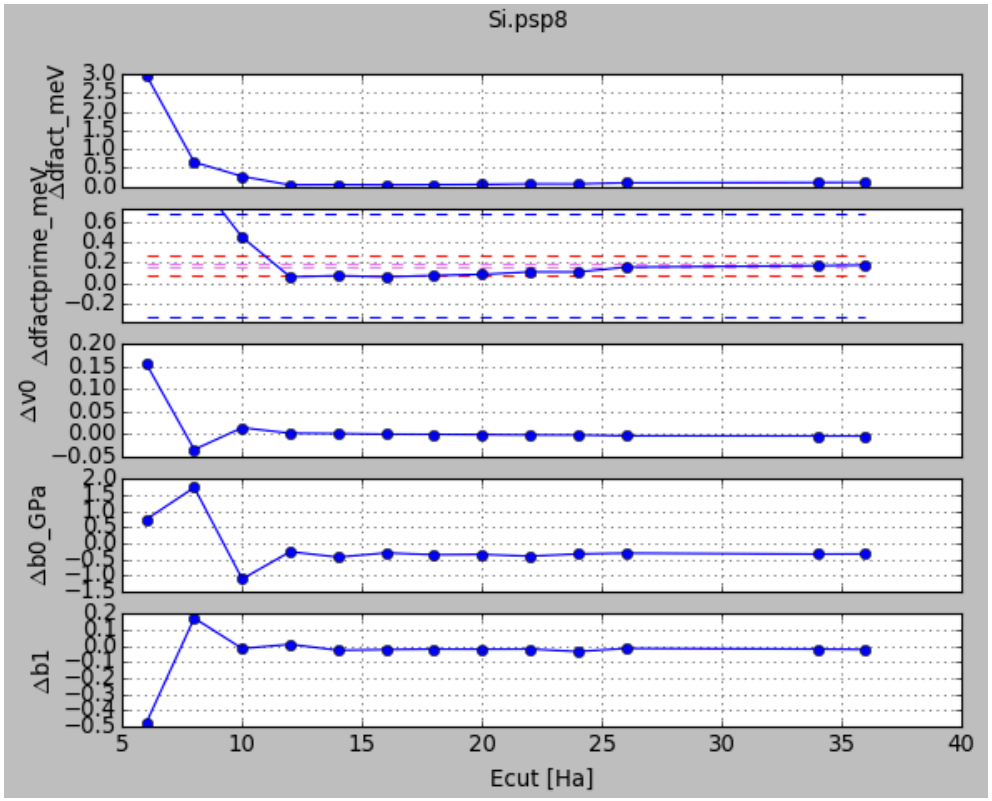
Dojodata

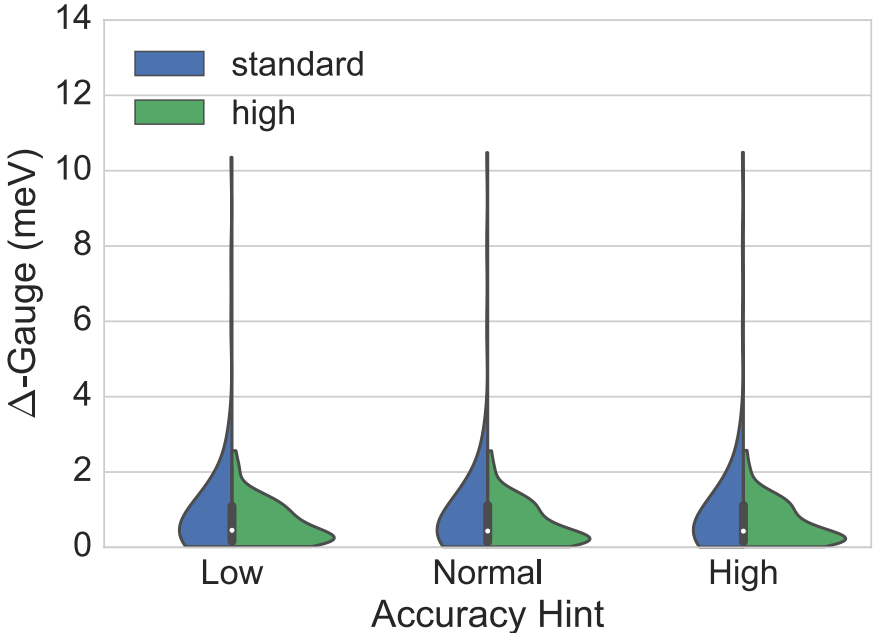
```
(dojo-new)[setten@frontal3 LDA]$ dojodata.py --help
usage: dojodata.py [-h] [--loglevel LOGLEVEL] [--seaborn]


subcommands:
  Valid subcommands

  {plot,compare,dist,make_hints,trials,figures,table,validate,check}
                        sub-command help
    plot                Plot DOJO_REPORT data.
    compare             Compare pseudos
    figures             Plot table figures
    table               Build pandas table.
    dist                Plot distribution of deltafactor and GBRV relative
                        errors.
    trials              Plot DOJO trials.
    check               Check pseudos
    validate            Validate pseudos
    make_hints          Add hints for cutoffs for pseudos

    Usage example:

    dojodata plot H.psp8                ==> Plot dojo data for pseudo H.psp8
    dojodata trials H.psp8 -r 1
    dojodata compare H.psp8 H-low.psp8  ==> Plot and compare dojo data for pseudos H.psp8 and H-low.psp8
    dojodata table .                    ==> Build table (find all psp8 files within current directory)
    dojodata figure .                   ==> Plot periodic table figures
```

Total energy convergence

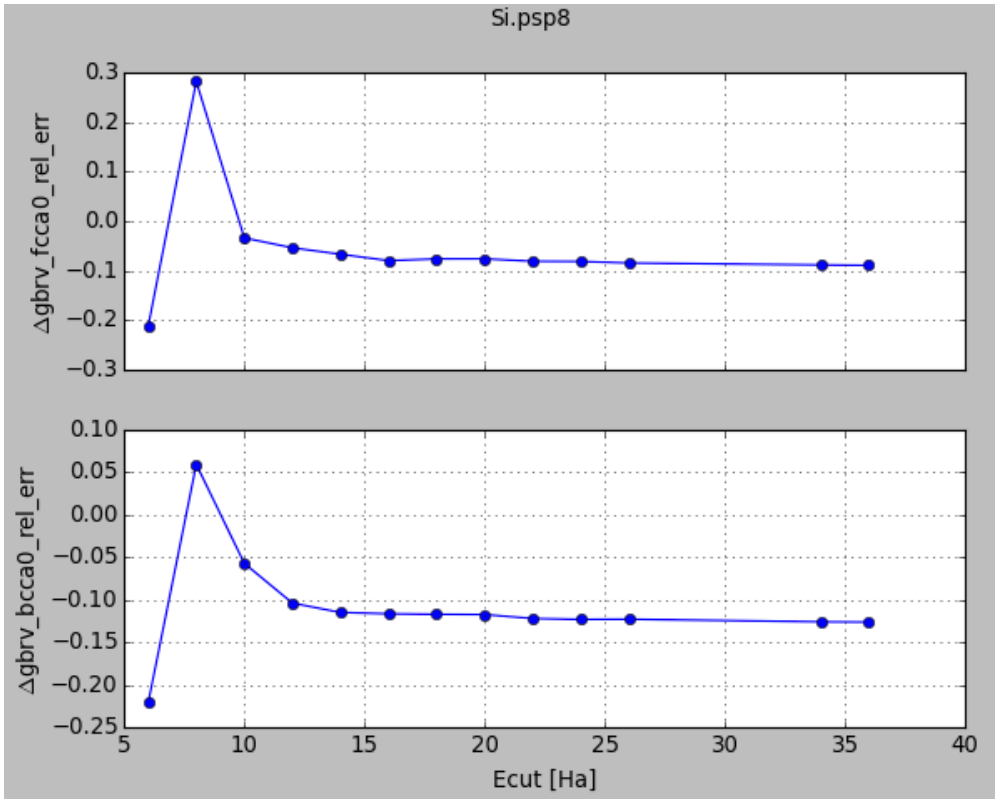


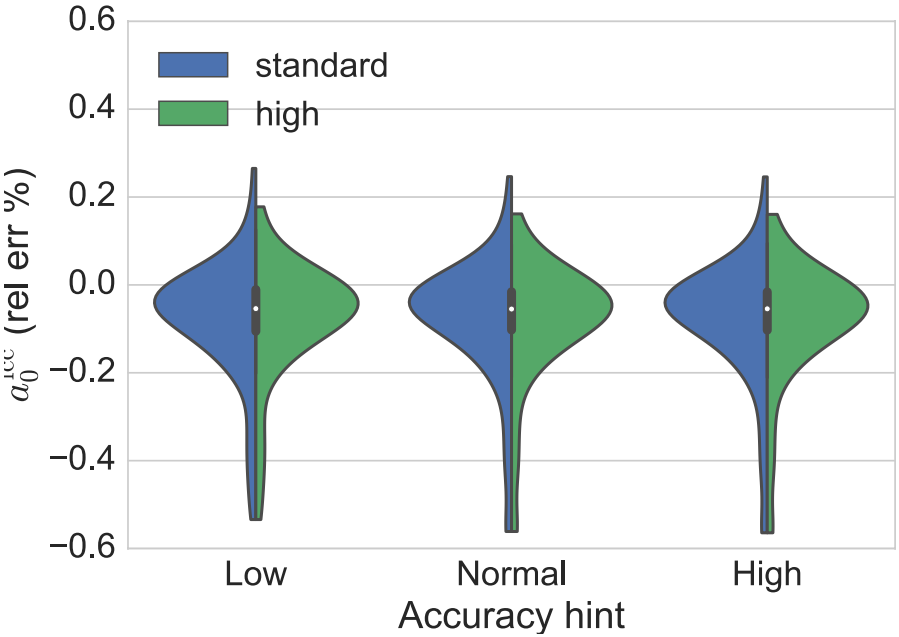
Delta Gauge (structural parameters)



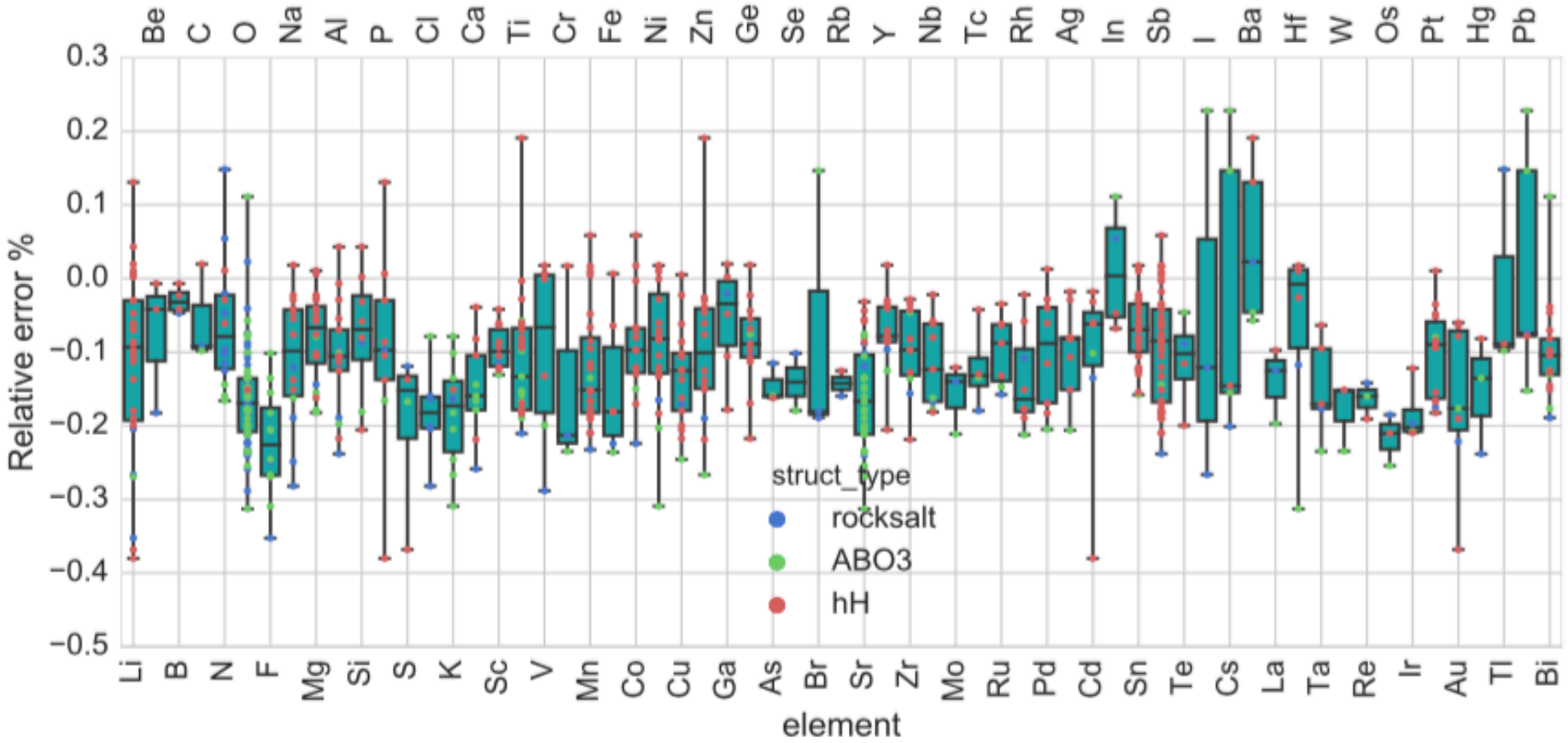


GBRV test (FCC and BCC lattice parameters)

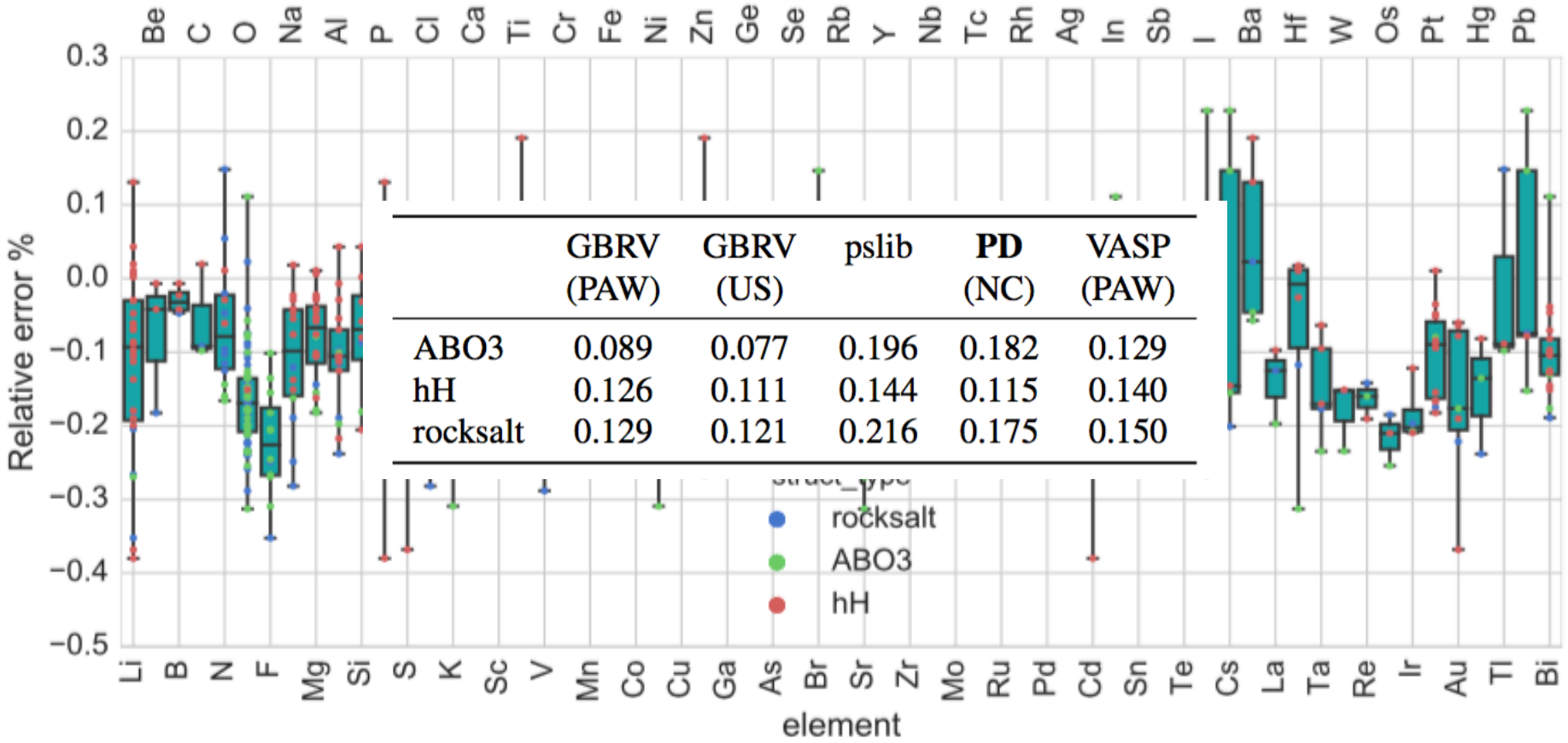




Rocksalts (63), perovskites (138) half-Heuslers (54)

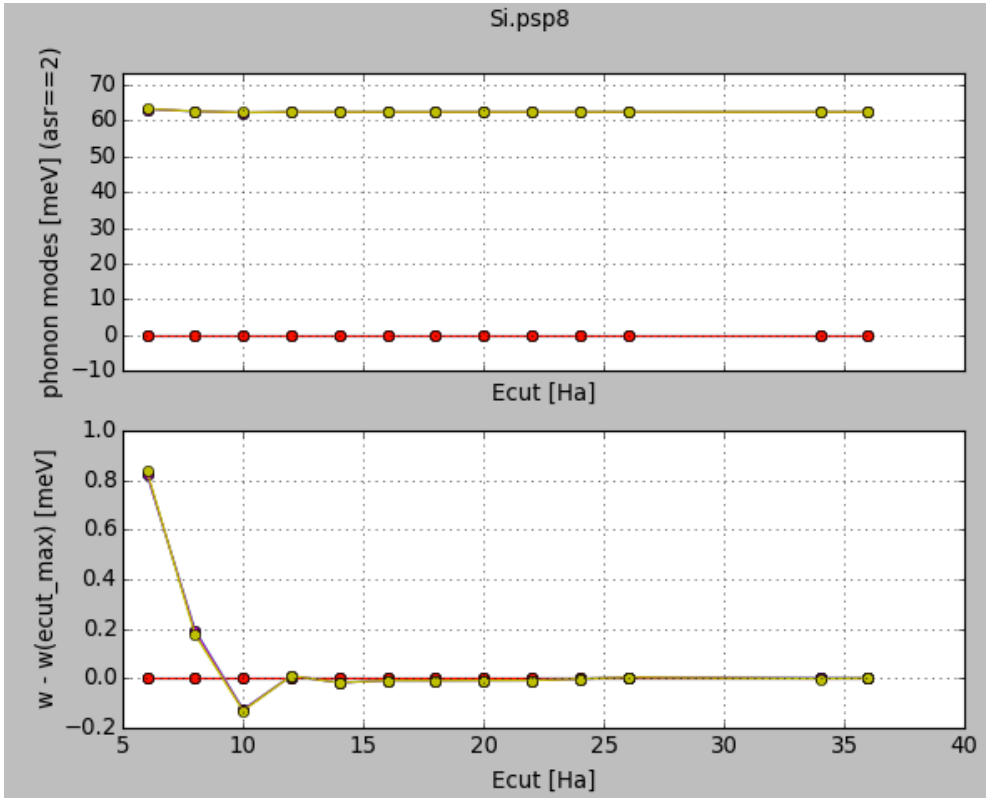


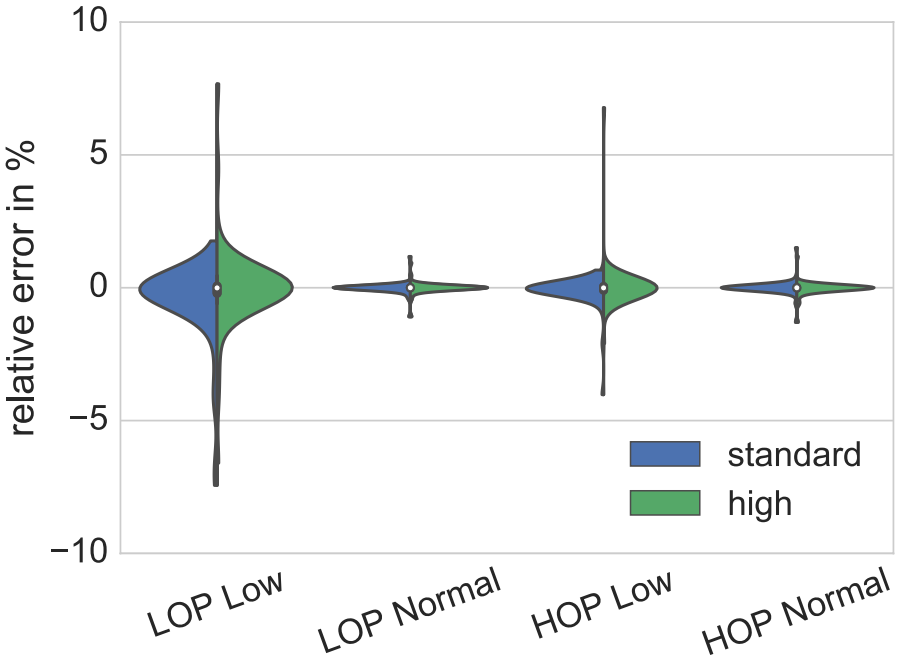
Rocksalts (63), perovskites (138) half-Heuslers (54)



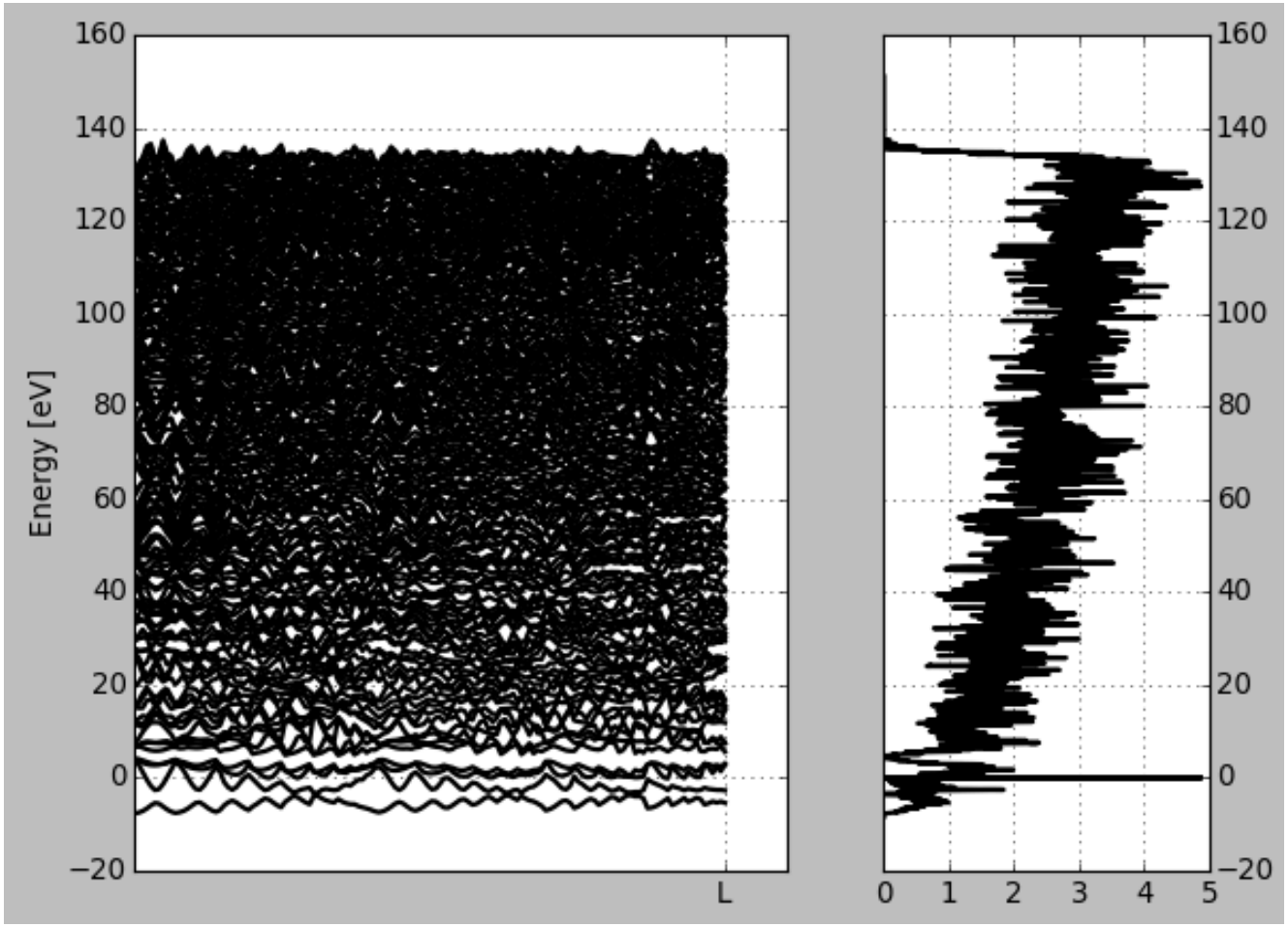
	GBRV (PAW)	GBRV (US)	pslib	**PD** (NC)	VASP (PAW)
ABO3	0.089	0.077	0.196	0.182	0.129
hH	0.126	0.111	0.144	0.115	0.140
rocksalt	0.129	0.121	0.216	0.175	0.150

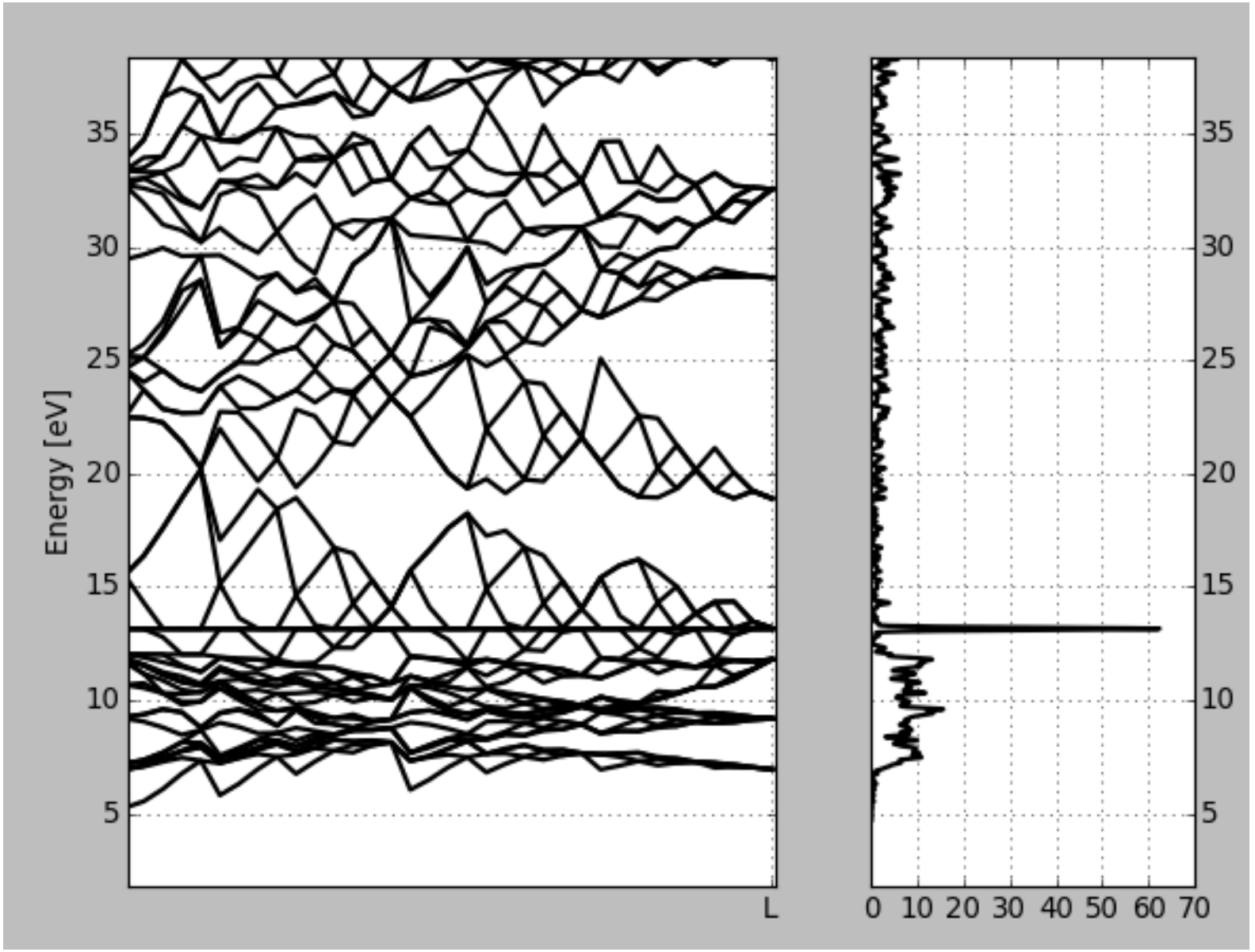
Phonon convergence





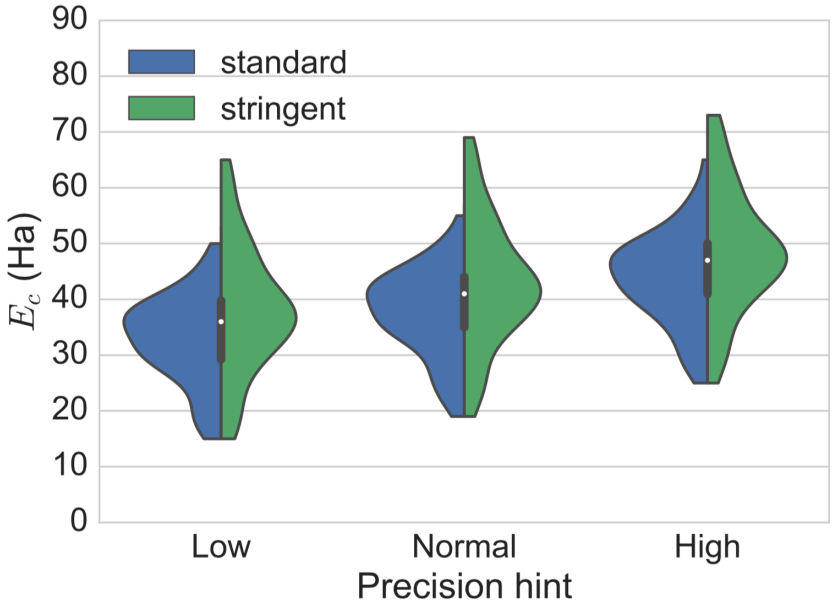
Ebands test (ghost states)




Energy [eV]
35
30
25
20
15
10
5
L
0 10 20 30 40 50 60 70

Hints

Observable	unit	low	normal	high
$\epsilon - \epsilon_{AE}$	(mHa/electron)	–	< 1	< 1
$\Delta_1 - \Delta_1^c$	(meV)	< 2	< 1	< 0.5
TE - TE^c	(meV/atom)	< 10	< 5	< 2



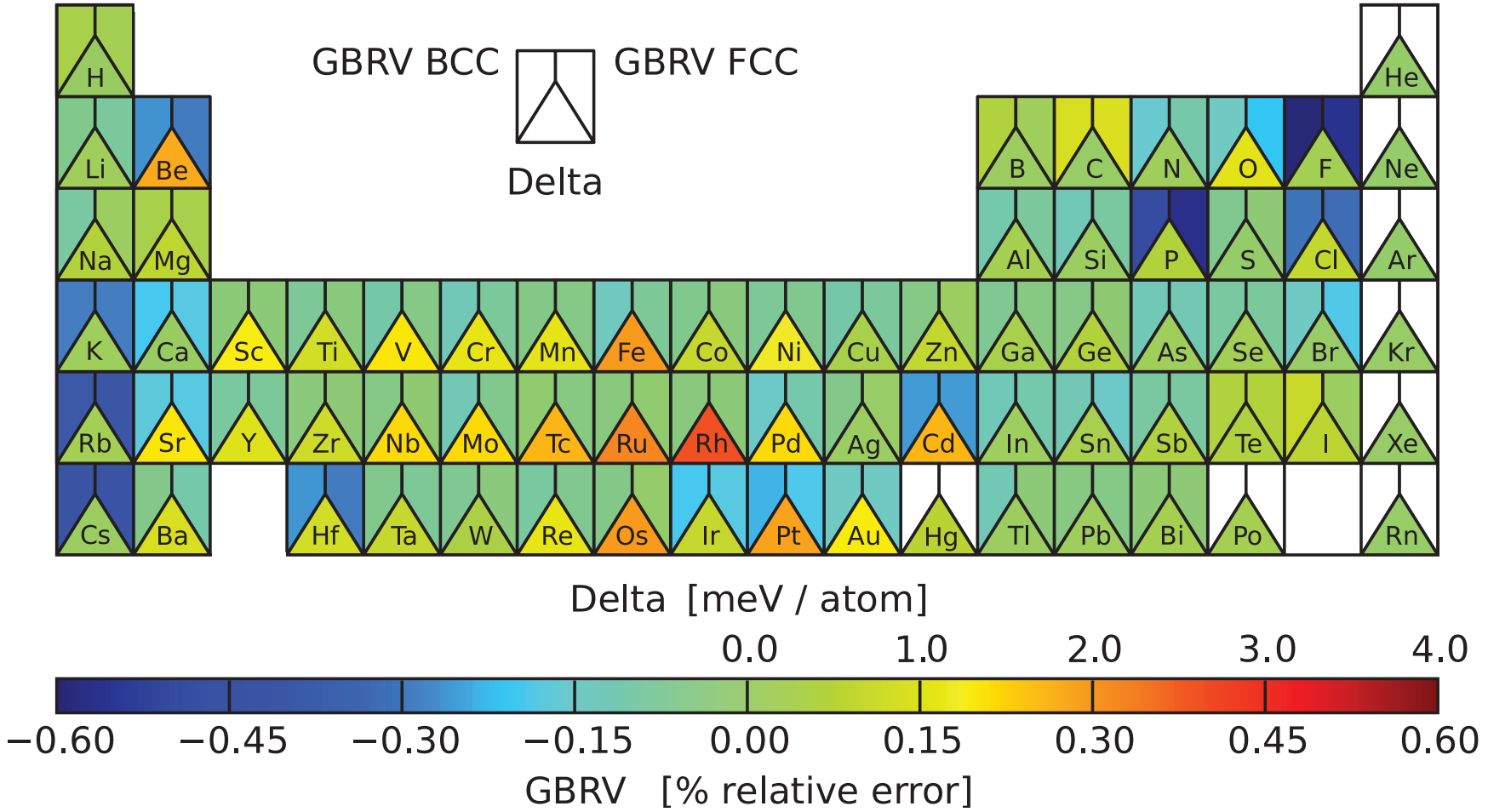
	E_c^l	E_c^n	E_c^h
count	72.00	72.00	72.00
mean	32.86	37.60	43.72
std	7.80	7.70	8.04
min	15.00	19.00	25.00
25%	29.00	34.00	39.75
50%	34.00	38.00	44.00
75%	38.00	42.25	48.25
max	50.00	55.00	65.00

Database

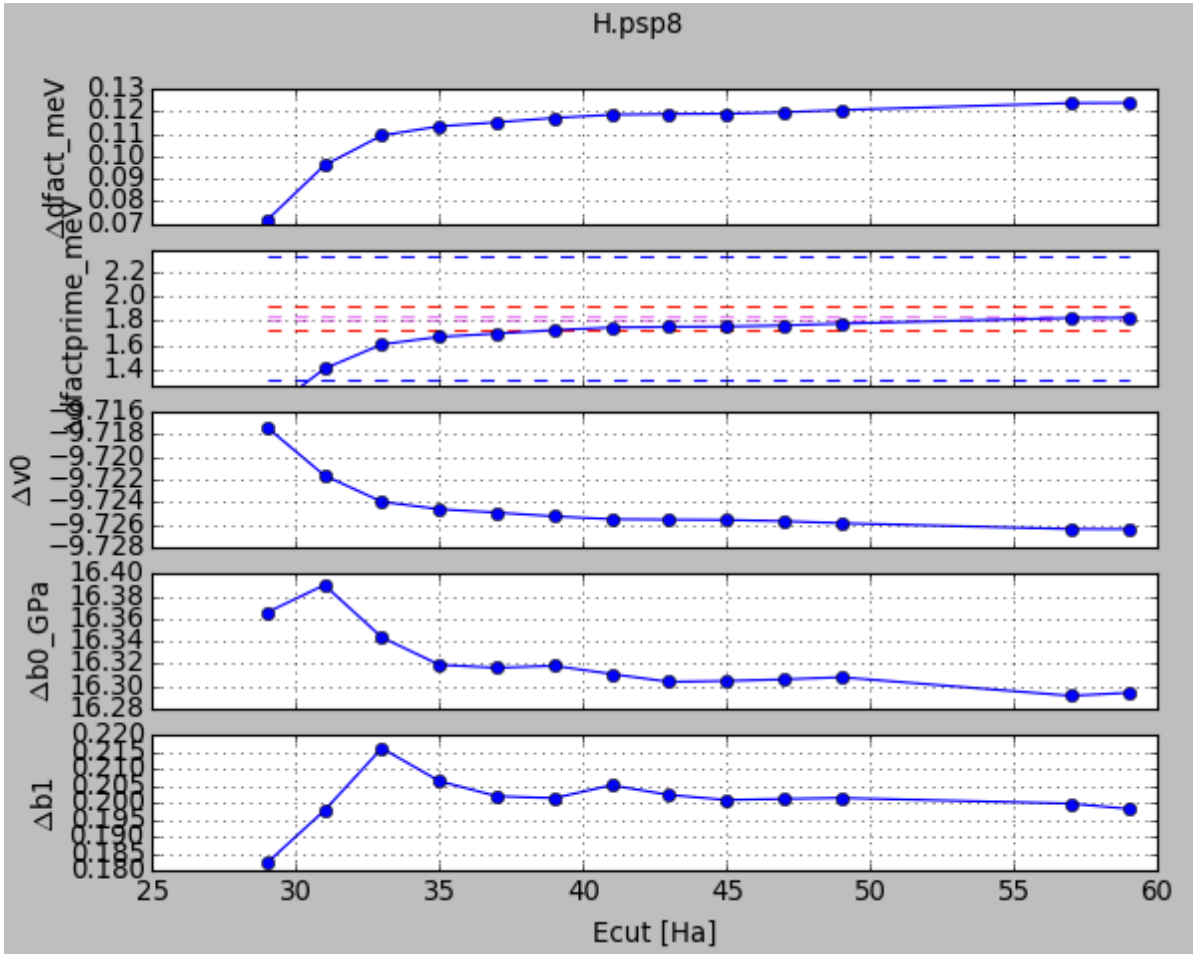
- PBE, PBEsol, LDA
  - 126 potentials in total per functional
  - Divided in a standard and stringent accuracy table
  - High, Normal, Low precision hints
- Scalar relativistic, Fully relativistic
- PSP8, UPF, PSML
- Other GGAs

Via web interface and git
Only via git (still in a testing phase)
Machinery in place, developmental phase
Machinery in place, generation on demand

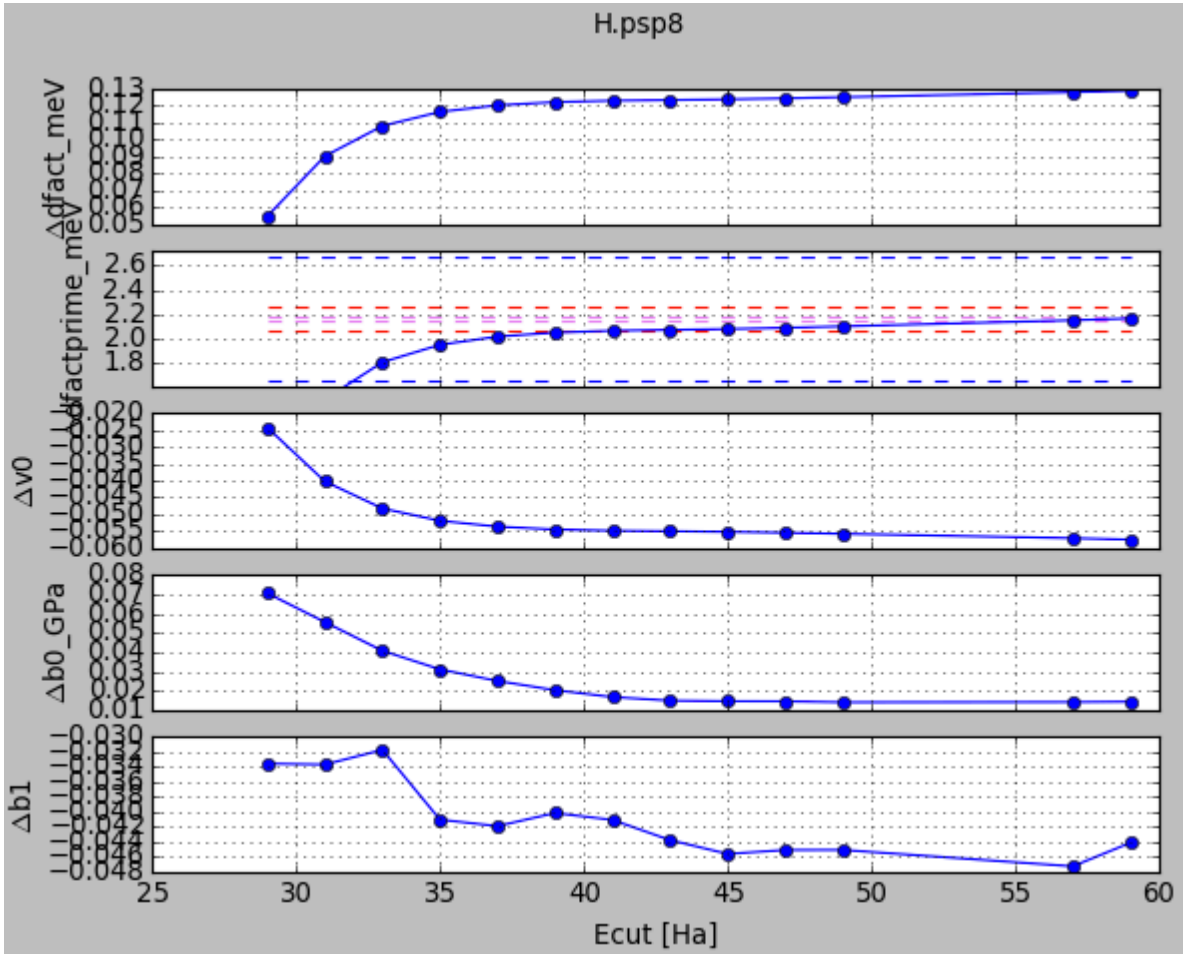
ONCVPSP PBE table



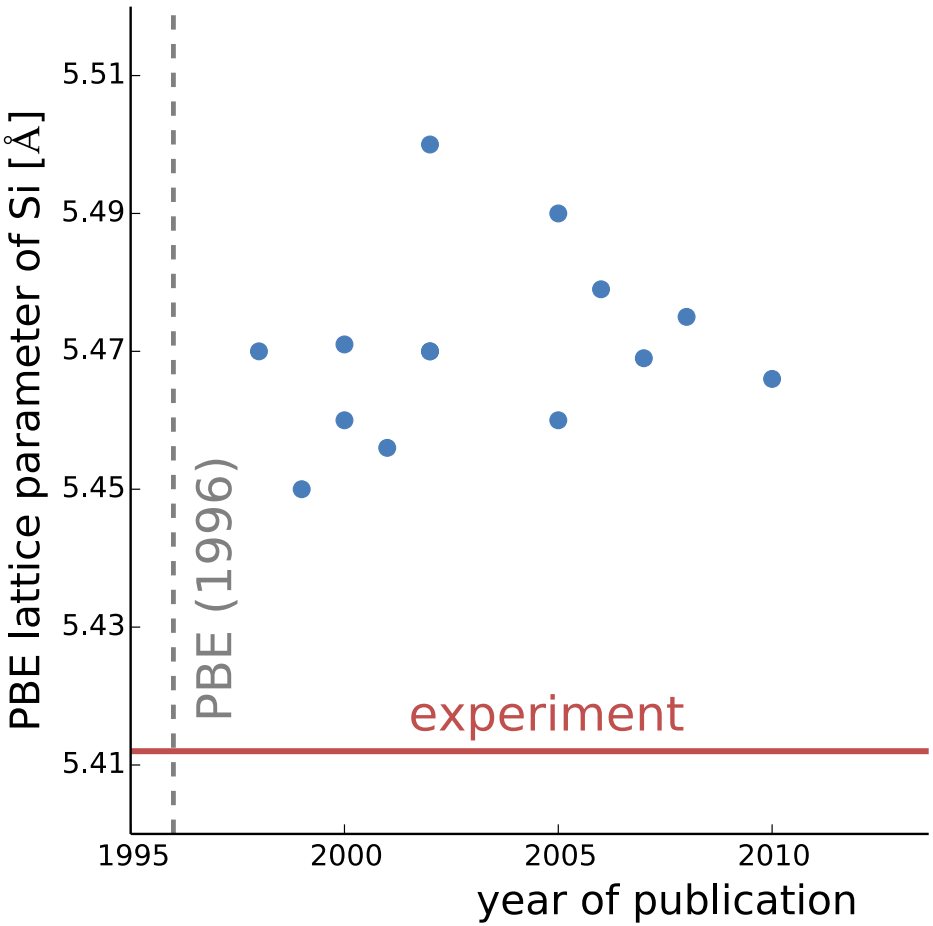
H (LDA)


H.psp8
Δdfact_meV
0.13
0.12
0.11
0.10
0.09
0.08
0.07
Δdfactprime_meV
2.2
2.0
1.8
1.6
1.4
Δv0
−9.716
−9.718
−9.720
−9.722
−9.724
−9.726
−9.728
Δb0_GPa
16.40
16.38
16.36
16.34
16.32
16.30
16.28
Δb1
0.220
0.215
0.210
0.205
0.200
0.195
0.190
0.185
0.180
25
30
35
40
45
50
55
60
Ecut [Ha]

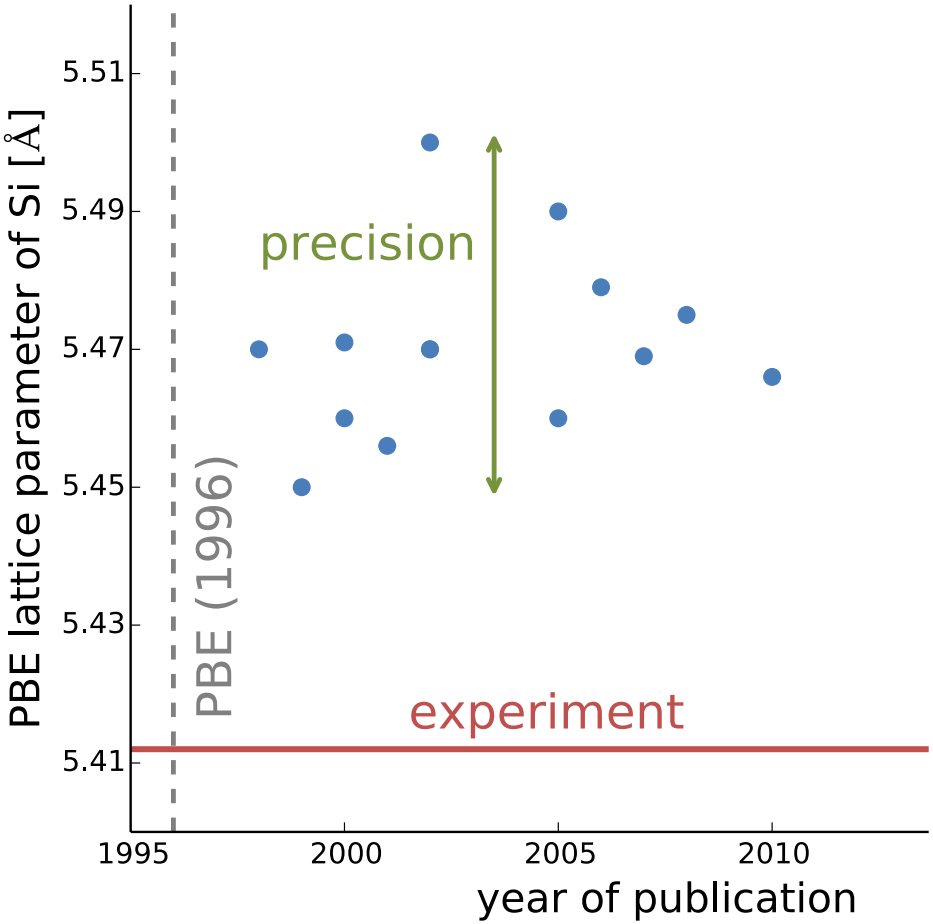
H (PBE)



The problem


PBE lattice parameter of Si [Å]
5.51
5.49
5.47
5.45
5.43
5.41
PBE (1996)
experiment
1995
2000
2005
2010
year of publication

The problem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precision
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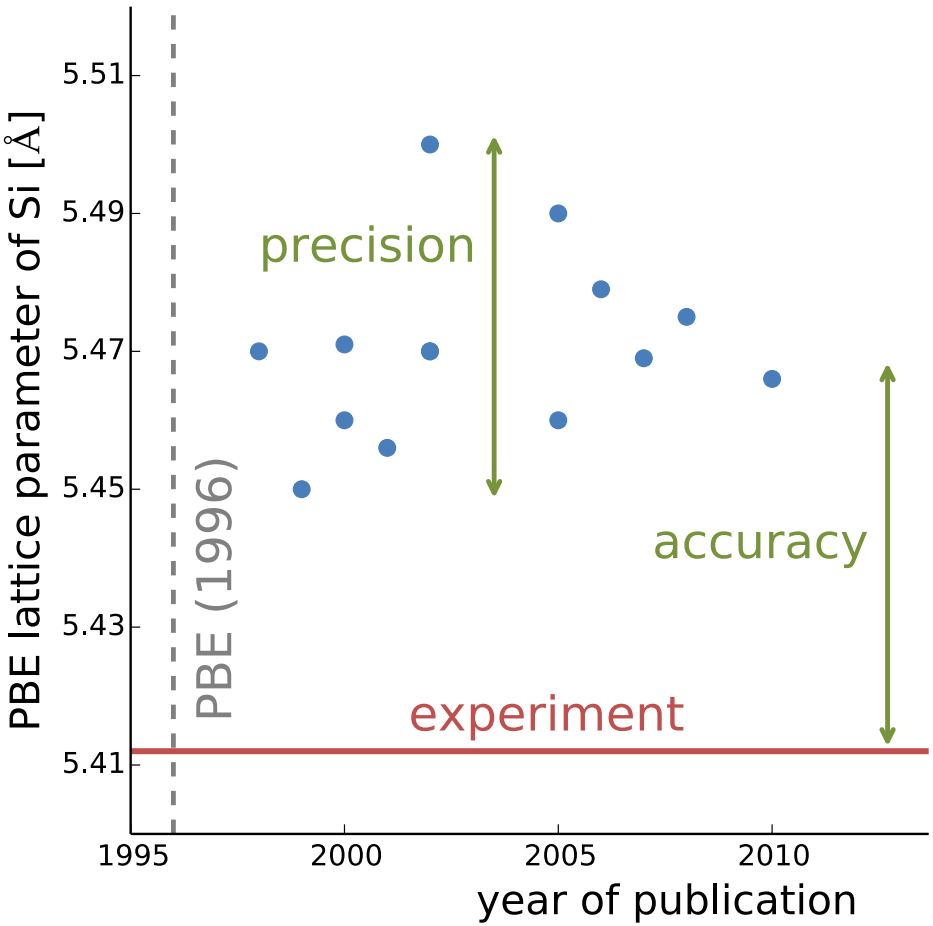
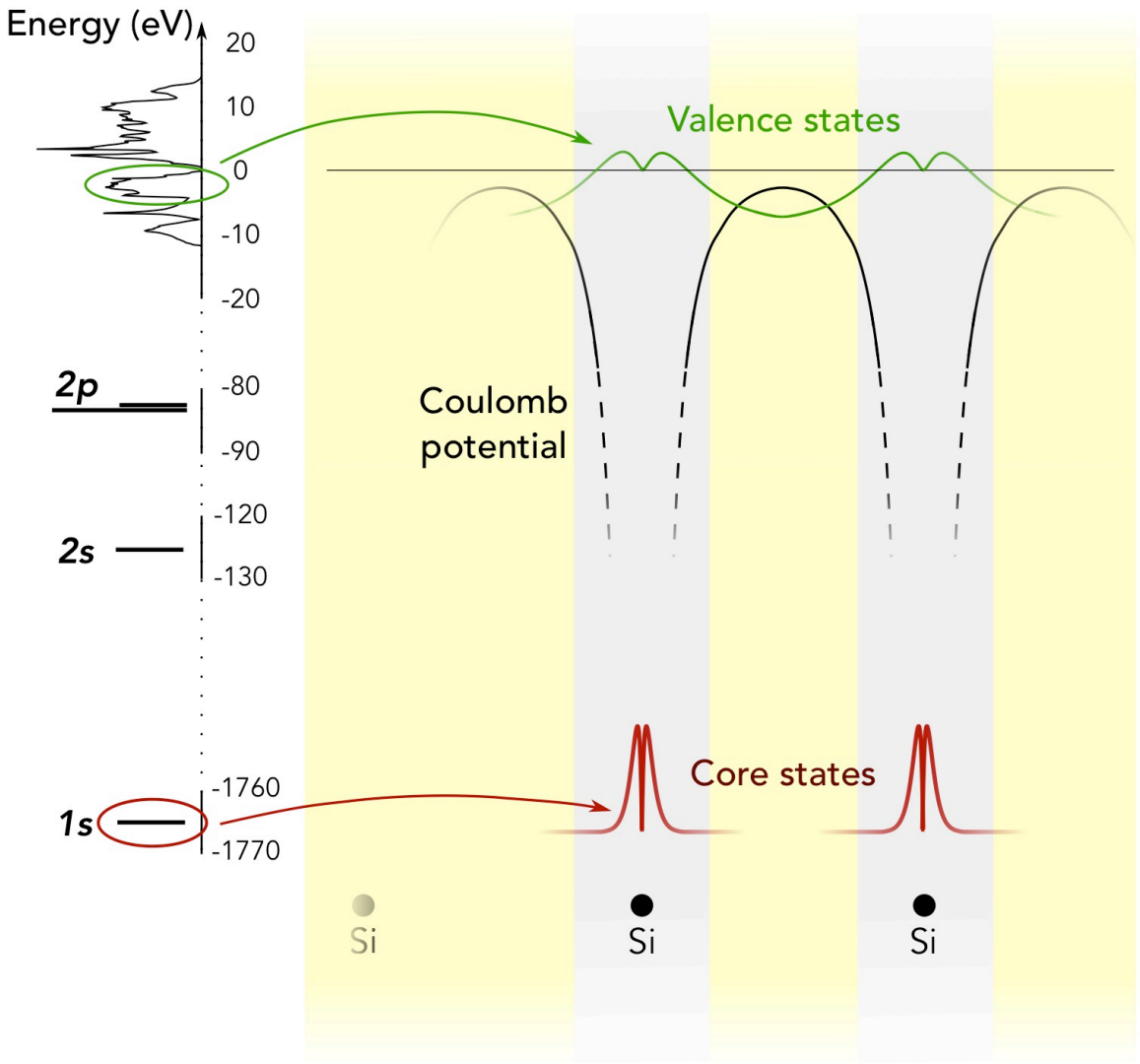
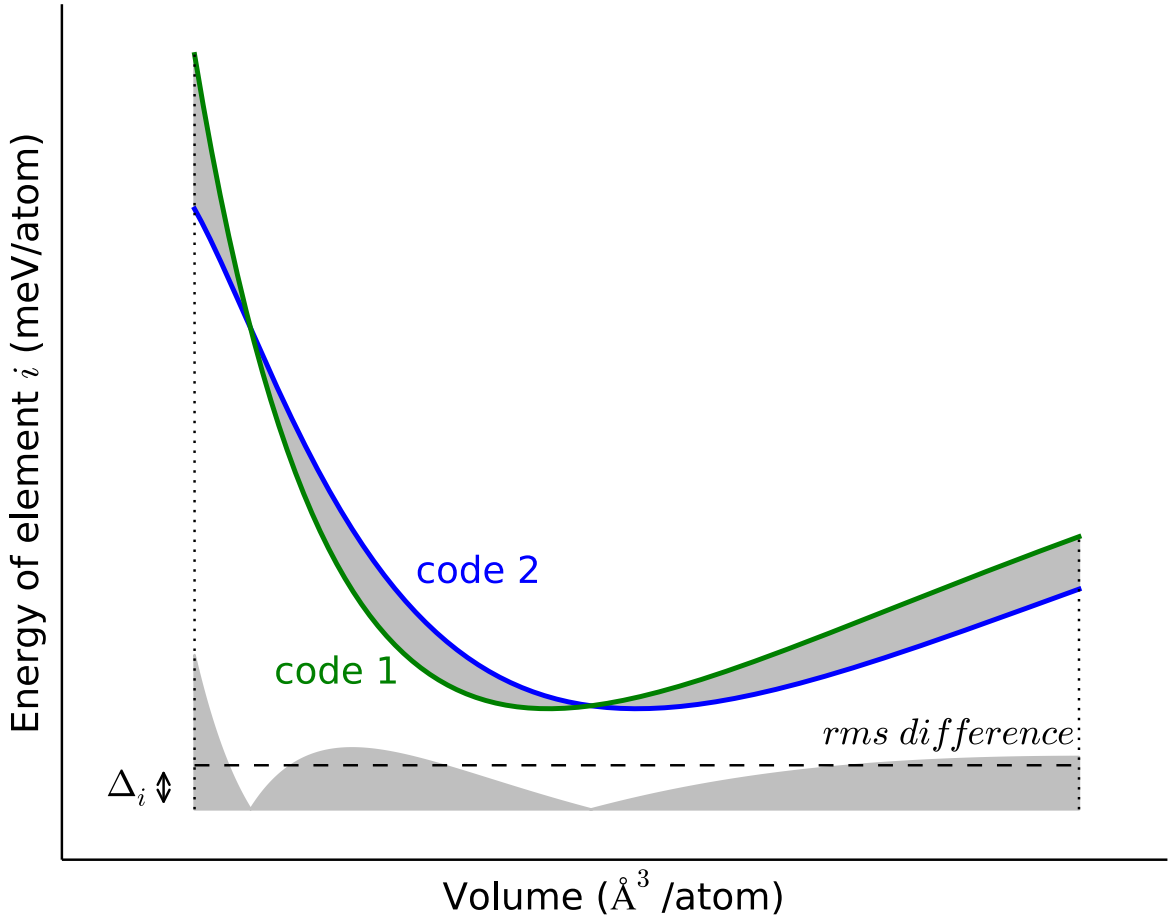
The problem

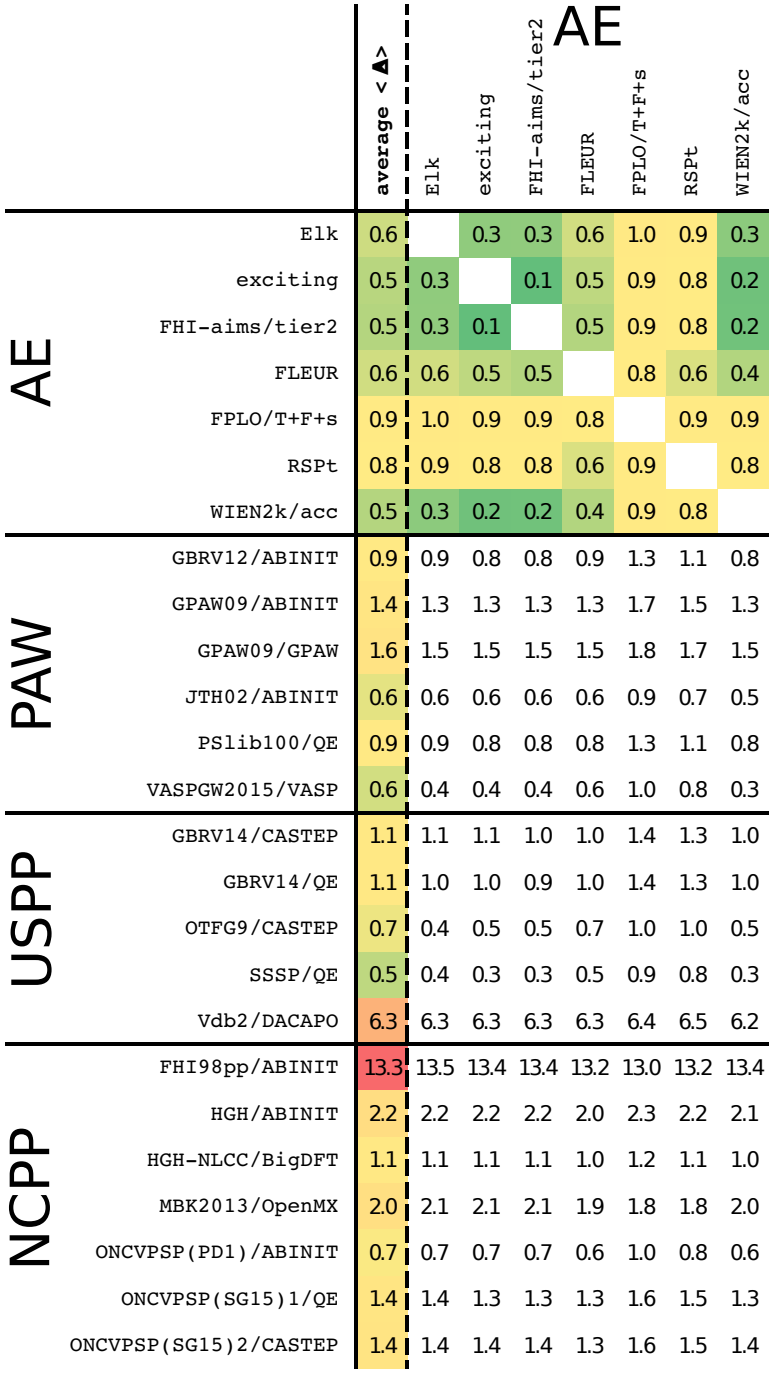

PBE lattice parameter of Si [Å]
5.51
5.49
5.47
5.45
5.43
5.41
1995
2000
2005
2010
year of publication
PBE (1996)
precision
accuracy
experiment

The origin of the problem

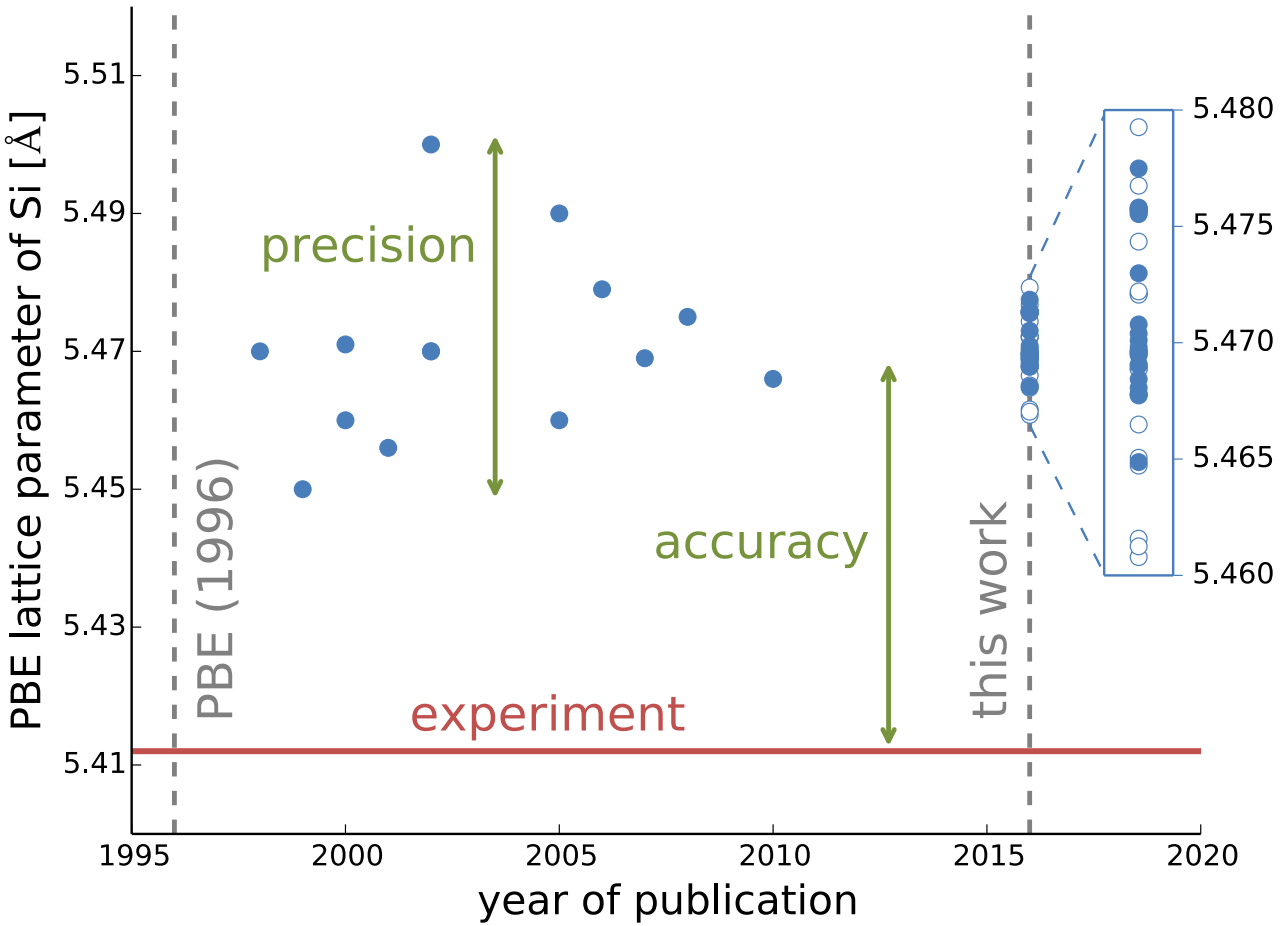


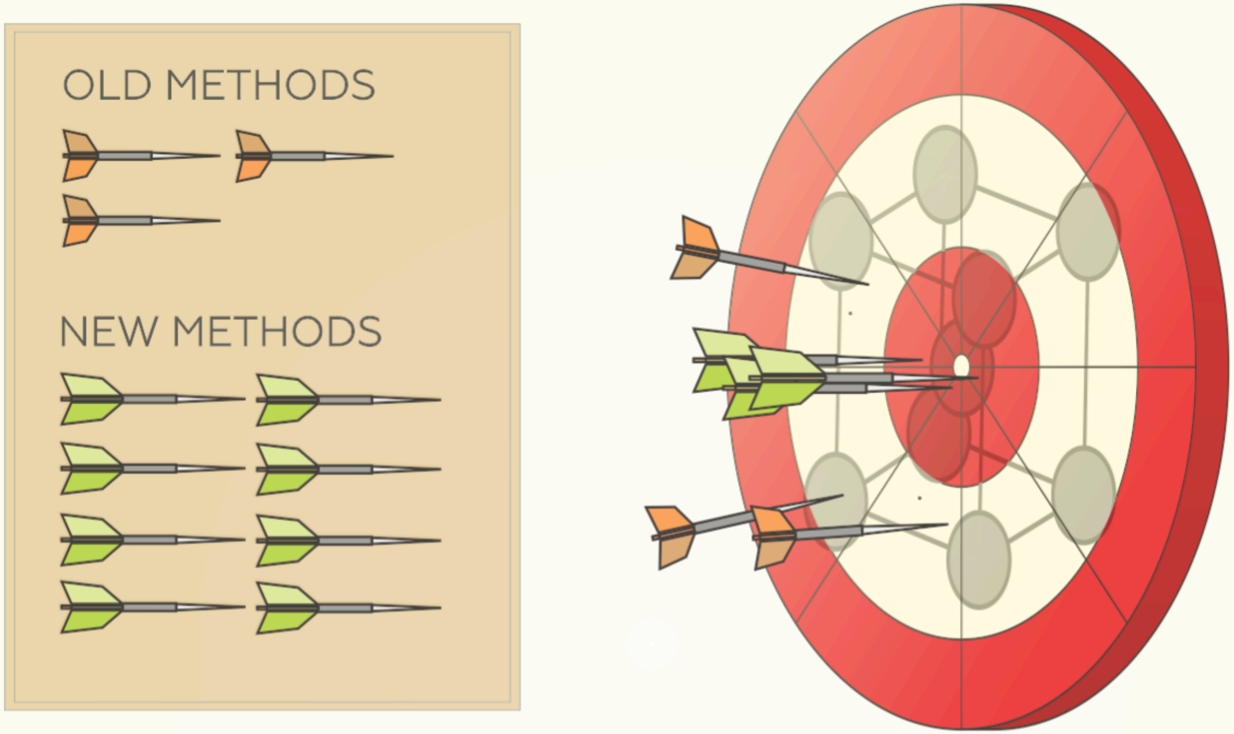
Delta Gauge (f.k.a. Delta factor)




AE
average <Δ>
Elk
exciting
FHI-aims/tier2
FLEUR
FPLO/T+F+s
RSPt
WIEN2k/acc
AE
Elk 0.6 0.3 0.3 0.6 1.0 0.9 0.3
exciting 0.5 0.3 0.1 0.5 0.9 0.8 0.2
FHI-aims/tier2 0.5 0.3 0.1 0.5 0.9 0.8 0.2
FLEUR 0.6 0.6 0.5 0.5 0.8 0.6 0.4
FPLO/T+F+s 0.9 1.0 0.9 0.9 0.8 0.9 0.9
RSPt 0.8 0.9 0.8 0.8 0.6 0.9 0.8
WIEN2k/acc 0.5 0.3 0.2 0.2 0.4 0.9 0.8
PAW
GBRV12/ABINIT 0.9 0.9 0.8 0.8 0.9 1.3 1.1 0.8
GPAW09/ABINIT 1.4 1.3 1.3 1.3 1.3 1.7 1.5 1.3
GPAW09/GPAW 1.6 1.5 1.5 1.5 1.5 1.8 1.7 1.5
JTH02/ABINIT 0.6 0.6 0.6 0.6 0.6 0.9 0.7 0.5
PSlib100/QE 0.9 0.9 0.8 0.8 0.8 1.3 1.1 0.8
VASPGW2015/VASP 0.6 0.4 0.4 0.4 0.6 1.0 0.8 0.3
USPP
GBRV14/CASTEP 1.1 1.1 1.1 1.0 1.0 1.4 1.3 1.0
GBRV14/QE 1.1 1.0 1.0 0.9 1.0 1.4 1.3 1.0
OTFG9/CASTEP 0.7 0.4 0.5 0.5 0.7 1.0 1.0 0.5
SSSP/QE 0.5 0.4 0.3 0.3 0.5 0.9 0.8 0.3
Vdb2/DACAPO 6.3 6.3 6.3 6.3 6.3 6.4 6.5 6.2
NCPP
FHI98pp/ABINIT 13.3 13.5 13.4 13.4 13.2 13.0 13.2 13.4
HGH/ABINIT 2.2 2.2 2.2 2.2 2.0 2.3 2.2 2.1
HGH-NLCC/BigDFT 1.1 1.1 1.1 1.1 1.0 1.2 1.1 1.0
MBK2013/OpenMX 2.0 2.1 2.1 2.1 1.9 1.8 1.8 2.0
ONCVPSP(PD1)/ABINIT 0.7 0.7 0.7 0.7 0.6 1.0 0.8 0.6
ONCVPSP(SG15)1/QE 1.4 1.4 1.3 1.3 1.3 1.6 1.5 1.3
ONCVPSP(SG15)2/CASTEP 1.4 1.4 1.4 1.4 1.3 1.6 1.5 1.4

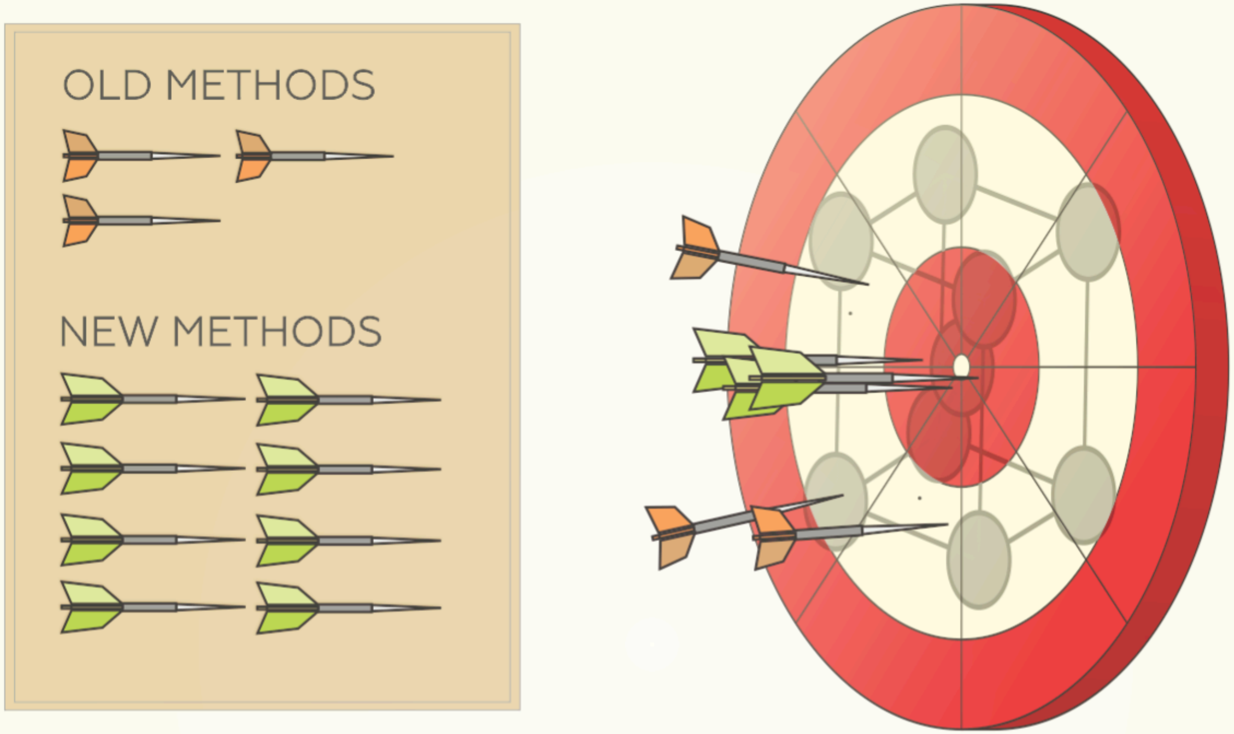
The problem


PBE lattice parameter of Si [Å]
5.51
5.49
5.47
5.45
5.43
5.41
5.480
5.475
5.470
5.465
5.460
precision
accuracy
experiment
PBE (1996)
this work
1995
2000
2005
2010
2015
2020
year of publication



SCOREBOARD

	0.3	0.6	0.6	0.3	0.6	3.9	1.0	1.0	0.9	1.7	1.8	0.3	0.9	3.8	1.3	1.5	1.2	0.6	1.6	0.9	2.1	0.7	0.4	1.1	1.1	1.0	2.5	0.4	0.4	6.4	6.3	13.5	2.2	1.1	2.1	0.7	1.5	1.4	1.4
0.3		0.5	0.5	0.1	0.5	3.9	1.0	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	2.1	0.6	0.4	1.0	1.1	1.0	2.5	0.5	0.3	6.4	6.3	13.4	2.2	1.1	2.1	0.7	1.4	1.3	1.4
0.6	0.5		0.0	0.5	0.7	3.8	0.9	1.1	0.7	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.4	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
0.6	0.5	0.0		0.5	0.7	3.8	0.9	1.1	0.8	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.5	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
0.3	0.1	0.5	0.5		0.5	3.9	0.9	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	2.0	0.6	0.4	0.9	1.0	0.9	2.5	0.5	0.3	6.4	6.3	13.4	2.2	1.1	2.1	0.7	1.4	1.3	1.4
0.6	0.5	0.7	0.7	0.5		3.6	0.8	0.8	0.6	1.4	1.5	0.4	0.9	3.5	1.3	1.5	1.0	0.6	1.5	0.8	1.9	0.7	0.6	1.0	1.0	1.0	2.6	0.7	0.5	6.5	6.3	13.2	2.0	1.0	1.9	0.6	1.3	1.3	1.3
3.9	3.9	3.8	3.8	3.9	3.6		3.1	3.6	3.3	2.9	2.5	3.9	4.0	3.1	4.1	4.1	3.4	3.6	3.3	3.9	2.8	3.9	4.0	4.0	4.0	4.1	5.8	4.1	3.9	7.9	7.2	13.0	4.9	3.6	3.2	3.7	4.1	4.1	4.1
1.0	1.0	0.9	0.9	0.9	0.8	3.1		0.8	0.7	1.4	1.4	0.9	1.3	3.4	1.7	1.9	1.0	0.9	1.5	1.3	1.9	1.2	1.0	1.3	1.3	1.3	3.1	1.1	1.0	6.6	6.4	13.7	2.4	1.2	1.8	1.0	1.6	1.6	1.6
1.0	0.9	1.1	1.1	0.9	0.8	3.6	0.8		0.9	1.5	1.5	0.9	1.3	3.5	1.7	1.8	1.2	0.9	1.4	1.3	1.9	1.2	1.0	1.4	1.4	1.4	2.9	1.0	0.9	6.4	6.4	13.0	2.3	1.2	1.8	1.0	1.6	1.6	1.6
0.9	0.8	0.7	0.8	0.8	0.6	3.3	0.7	0.9		1.3	1.3	0.8	1.1	3.4	1.5	1.7	0.9	0.7	1.6	1.1	1.9	1.0	0.8	1.2	1.3	1.3	3.0	1.0	0.8	6.7	6.5	13.2	2.2	1.1	1.8	0.8	1.5	1.5	1.5
1.7	1.7	1.8	1.8	1.7	1.4	2.9	1.4	1.5	1.3		0.9	1.7	1.9	3.2	2.2	2.3	1.3	1.5	1.8	1.8	1.7	1.8	1.8	1.9	1.9	1.9	3.8	1.8	1.6	7.1	7.0	13.0	2.8	1.7	1.9	1.6	2.1	2.1	2.1
1.8	1.8	1.8	1.8	1.8	1.5	2.5	1.4	1.5	1.3	0.9		1.8	2.0	2.6	2.1	2.2	1.1	1.5	1.6	1.8	1.4	1.9	2.0	2.0	2.0	2.0	3.8	2.0	1.7	6.9	6.9	12.3	2.8	1.6	1.5	1.7	1.9	1.9	1.9
0.3	0.2	0.5	0.5	0.2	0.4	3.9	0.9	0.9	0.8	1.7	1.8		0.8	3.8	1.3	1.5	1.2	0.5	1.6	0.8	2.0	0.7	0.3	0.9	1.0	1.0	2.5	0.5	0.3	6.4	6.2	13.4	2.1	1.0	2.0	0.6	1.4	1.3	1.4



SCOREBOARD

	0.3	0.6	0.6	0.3	0.6	3.9	1.0	1.0	0.9	1.7	1.8	0.3	0.9	3.8	1.3	1.5	1.2	0.6	1.6	0.9	2.1	0.7	0.4	1.1	1.1	1.0	2.5	0.4	0.4	6.4	6.3	13.5	2.2	1.1	2.1	0.7	1.5	1.4	1.4
0.3		0.5	0.5	0.1	0.5	3.9	1.0	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	2.1	0.6	0.4	1.0	1.1	1.0	2.5	0.5	0.3	6.4	6.3	13.4	2.2	1.1	2.1	0.7	1.4	1.3	1.4
0.6	0.5		0.0	0.5	0.7	3.8	0.9	1.1	0.7	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.4	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
0.6	0.5	0.0		0.5	0.7	3.8	0.9	1.1	0.8	1.8	1.8	0.5	1.0	3.8	1.3	1.6	1.3	0.7	1.7	1.0	2.2	0.8	0.6	1.1	1.2	1.1	2.6	0.7	0.6	6.5	6.3	13.6	2.2	1.2	2.0	0.8	1.5	1.4	1.5
0.3	0.1	0.5	0.5		0.5	3.9	0.9	0.9	0.8	1.7	1.8	0.2	0.8	3.8	1.3	1.5	1.2	0.6	1.6	0.8	2.0	0.6	0.4	0.9	1.0	0.9	2.5	0.5	0.3	6.4	6.3	13.4	2.2	1.1	2.1	0.7	1.4	1.3	1.4
0.6	0.5	0.7	0.7	0.5		3.6	0.8	0.8	0.6	1.4	1.5	0.4	0.9	3.5	1.3	1.5	1.0	0.6	1.5	0.8	1.9	0.7	0.6	1.0	1.0	1.0	2.6	0.7	0.5	6.5	6.3	13.2	2.0	1.0	1.9	0.6	1.3	1.3	1.3
3.9	3.9	3.8	3.8	3.9	3.6		3.1	3.6	3.3	2.9	2.5	3.9	4.0	3.1	4.1	4.1	3.4	3.6	3.3	3.9	2.8	3.9	4.0	4.0	4.0	4.1	5.8	4.1	3.9	7.9	7.2	13.0	4.9	3.6	3.2	3.7	4.1	4.1	4.1
1.0	1.0	0.9	0.9	0.9	0.8	3.1		0.8	0.7	1.4	1.4	0.9	1.3	3.4	1.7	1.9	1.0	0.9	1.5	1.3	1.9	1.2	1.0	1.3	1.3	1.3	3.1	1.1	1.0	6.6	6.4	13.7	2.4	1.2	1.8	1.0	1.6	1.6	1.6
1.0	0.9	1.1	1.1	0.9	0.8	3.6	0.8		0.9	1.5	1.5	0.9	1.3	3.5	1.7	1.8	1.2	0.9	1.4	1.3	1.9	1.2	1.0	1.4	1.4	1.4	2.9	1.0	0.9	6.4	6.4	13.0	2.3	1.2	1.8	1.0	1.6	1.6	1.6
0.9	0.8	0.7	0.8	0.8	0.6	3.3	0.7	0.9		1.3	1.3	0.8	1.1	3.4	1.5	1.7	0.9	0.7	1.6	1.1	1.9	1.0	0.8	1.2	1.3	1.3	3.0	1.0	0.8	6.7	6.5	13.2	2.2	1.1	1.8	0.8	1.5	1.5	1.5
1.7	1.7	1.8	1.8	1.7	1.4	2.9	1.4	1.5	1.3		0.9	1.7	1.9	3.2	2.2	2.3	1.3	1.5	1.8	1.8	1.7	1.8	1.8	1.9	1.9	1.9	3.8	1.8	1.6	7.1	7.0	13.0	2.8	1.7	1.9	1.6	2.1	2.1	2.1
1.8	1.8	1.8	1.8	1.8	1.5	2.5	1.4	1.5	1.3	0.9		1.8	2.0	2.6	2.1	2.2	1.1	1.5	1.6	1.8	1.4	1.9	2.0	2.0	2.0	2.0	3.8	2.0	1.7	6.9	6.9	12.3	2.8	1.6	1.5	1.7	1.9	1.9	1.9
0.3	0.2	0.5	0.5	0.2	0.4	3.9	0.9	0.9	0.8	1.7	1.8		0.8	3.8	1.3	1.5	1.2	0.5	1.6	0.8	2.0	0.7	0.3	0.9	1.0	1.0	2.5	0.5	0.3	6.4	6.2	13.4	2.1	1.0	2.0	0.6	1.4	1.3	1.4