FHI98pp/ABINIT

Troullier-Martins FHI NCPP dataset / ABINIT 7.6.4

`name and version of the code:` ABINIT 7.6.4
`type of basis set:` plane waves
`method:` norm-conserving pseudopotentials (Troullier-Martins FHI)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see table (Z_{val})
`basis set size`	cut-off energy = 120 Ry
`k-mesh density`	see table (k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts*, and number of irreducible k-points # *k*)
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.01 eV

METHOD-SPECIFIC INFORMATION

`number of symmetry operations`	1

ADDITIONAL COMMENTS

The ASE script used to generate these data has been included after the table.

REFERENCES

`potentials`

[1] http://www.abinit.org/downloads/psp-links/psp-links/gga_fhi
[2] M. Fuchs and M. Scheffler, *Comput. Phys. Commun.* **119**, 67–98 (1999).

`code`

[3] X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, Ph. Ghosez, J.-Y. Raty and D. C. Allan, *Comput. Mater. Sci.* **25**, 478–492 (2002).
[4] X. Gonze, B. Amadon, P.-M. Anglade, J.-M. Beuken, F. Bottin, P. Boulanger, F. Bruneval, D. Caliste, R. Caracas, M. Côté, T. Deutsch, L. Genovese, Ph. Ghosez, M. Giantomassi, S. Goedecker, D. R. Hamann, P. Hermet, F. Jollet, G. Jomard, S. Leroux, M. Mancini, S. Mazevet, M. J. T. Oliveira, G. Onida, Y. Pouillon, T. Rangel, G.-M. Rignanese, D. Sangalli, R. Shaltaf, M. Torrent, M. J. Verstraete, G. Zerah and J. W. Zwanziger, *Comput. Phys. Commun.* **180**, 2582–2615 (2009).
[5] M. Torrent, F. Jollet, F. Bottin, G. Zérah, X. Gonze, *Comput. Mater. Sci.* **42**, 337–351, (2008).

`scalar relativity`

[6] D. D. Koelling and B. N. Harmon, *J. Phys. C: Solid State* **10**, 3107–3114 (1977).

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Table I. Calculation settings and results per element: valence Z_{val}, k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts* and number of irreducible k-points # k, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	Z_{val} [–]	*kpts* [–]	# k [–]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	1	28×28×20	7 840	16.888	10.154	2.630
He	2	40×40×22	17 600	17.811	0.815	6.207
Li	1	38×38×38	27 436	19.714	13.526	3.208
Be	2	52×52×28	37 856	7.633	122.833	3.201
B	3	26×26×24	8 112	7.152	237.409	3.529
C	4	48×48×12	13 824	11.510	208.889	3.539
N	5	16×16×16	2 048	28.316	53.653	3.524
O	6	26×24×24	7 488	18.428	50.928	3.899
F	7	16×28×14	3 136	19.213	33.913	3.969
Ne	8	22×22×22	5 324	24.296	1.784	14.844
Na	1	32×32×32	16 384	36.888	7.555	3.607
Mg	2	36×36×20	12 960	22.793	35.843	3.977
Al	3	24×24×24	6 912	16.562	76.366	4.888
Si	4	32×32×32	16 384	20.399	87.919	4.281
P	5	30×8×22	2 640	21.378	68.272	4.308
S	6	38×38×38	27 436	17.131	84.386	4.053
Cl	7	12×24×12	1 728	38.591	19.147	4.341
Ar	8	16×16×16	2 048	52.244	0.755	7.340
K	1	20×20×20	4 000	66.652	3.974	3.690
Ca	2	18×18×18	2 916	42.778	17.926	3.592
Sc	3	34×34×20	11 560	25.165	54.566	3.382
Ti	4	40×40×22	17 600	18.148	111.096	3.698
V	5	34×34×34	19 652	14.511	171.538	3.896
Cr	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Mn	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Fe	8	36×36×36	23 328	11.897	907.659	−9.882
Co	9	46×46×24	25 392	11.595	204.094	4.438
Ni	10	28×28×28	10 976	11.484	179.020	4.703
Cu	11	28×28×28	10 976	12.343	136.898	5.123
Zn	12	44×44×20	19 360	15.672	71.454	5.378
Ga	3	22×12×22	2 904	20.152	50.274	5.216
Ge	4	30×30×30	13 500	24.052	57.747	4.812
As	5	30×30×10	4 500	23.038	66.918	4.240
Se	6	26×26×20	6 760	30.092	46.474	4.443
Br	7	12×24×12	1 728	39.729	22.251	4.847
Kr	8	16×16×16	2 048	66.028	0.646	7.251
Rb	1	18×18×18	2 916	84.308	2.996	3.746
Sr	2	16×16×16	2 048	52.327	13.253	3.112
Y	3	32×32×18	9 216	32.679	42.006	3.141
Zr	4	36×36×20	12 960	23.803	97.703	3.418
Nb	5	30×30×30	13 500	18.501	175.198	3.635
Mo	6	32×32×32	16 384	15.930	266.027	4.283
Tc	7	42×42×22	19 404	14.572	313.700	4.555
Ru	8	42×42×24	21 168	13.931	322.583	4.929
Rh	9	26×26×26	8 788	14.188	267.769	5.262
Pd	10	26×26×26	8 788	15.674	170.009	5.670
Ag	11	24×24×24	6 912	18.651	85.846	6.131
Cd	12	38×38×18	12 996	23.717	40.160	7.136

In	3	30×30×20	9 000	26.429	38.473	4.877
Sn	4	26×26×26	8 788	36.610	35.423	4.756
Sb	5	26×26×8	2 704	31.496	51.162	4.523
Te	6	26×26×16	5 408	34.201	45.961	4.680
I	7	12×22×10	1 320	50.024	18.769	5.036
Xe	8	14×14×14	1 372	86.655	0.543	7.173
Cs	1	16×16×16	2 048	105.499	2.263	3.682
Ba	2	20×20×20	4 000	64.349	9.041	3.359
Lu	17	32×32×18	9 216	29.341	50.173	3.951
Hf	4	36×36×20	12 960	22.869	109.023	3.378
Ta	5	30×30×30	13 500	18.834	192.102	3.772
W	6	32×32×32	16 384	22.218	129.992	3.247
Re	7	42×42×22	19 404	15.305	366.796	4.462
Os	8	42×42×24	21 168	14.677	393.544	4.809
Ir	9	26×26×26	8 788	14.783	352.058	5.179
Pt	10	26×26×26	8 788	15.938	250.732	5.563
Au	11	24×24×24	6 912	18.298	138.991	6.103
Hg	12	24×24×28	8 064	31.522	−1.298	4.667
Tl	3	32×32×18	9 216	25.489	37.761	5.538
Pb	14	20×20×20	4 000	32.002	39.462	4.752
Bi	5	26×26×8	2 704	35.533	43.969	4.439
Po	6	30×30×30	13 500	36.472	47.179	5.014
Rn	8	14×14×14	1 372	91.436	0.587	16.798

script for the Atomic Simulation Environment (ASE)
S. R. Bahn, K. W. Jacobsen, *Comput. Sci. Eng.* **4**, 56–66 (2002)
https://wiki.fysik.dtu.dk/ase/

```
import os
import time

import numpy as np

import ase.db
from ase.units import Rydberg
from ase.utils import opencew
from ase.calculators.calculator import kpts2mp
from ase.io import Trajectory
from ase.calculators.abinit import Abinit
from ase.test.tasks.dcdft import DeltaCodesDFTCollection as Collection

c = ase.db.connect('dcdft_abinit_fhi.db')

ecut = 120

kptdensity = 16.0
width = 0.01

linspace = (0.98, 1.02, 5)  # eos numpy's linspace
linspacestr = ''.join([str(t) + 'x' for t in linspace])[:-1]

code = 'abinit' + '-' + '_c' + str(ecut) + '_e' + linspacestr
code = code + '_k' + str(kptdensity) + '_w' + str(width)

collection = Collection()

for name in collection.names:
    # save all steps in one traj file in addition to the database
    # we should only used the database c.reserve, but here
    # traj file is used as another lock ...
    fd = opencew(name + '_' + code + '.traj')
    if fd is None:
        continue
    traj = Trajectory(name + '_' + code + '.traj', 'w')
    atoms = collection[name]
    if name == 'Mn':  # fails to find the right magnetic state
        atoms.set_initial_magnetic_moments([10., 20., -10., -20.])
    if name == 'Co':  # fails to find the right magnetic state
        atoms.set_initial_magnetic_moments([10., 10.])
    if name == 'Ni':  # fails to find the right magnetic state
        atoms.set_initial_magnetic_moments([10., 10., 10., 10.])
    cell = atoms.get_cell()
    kpts = tuple(kpts2mp(atoms, kptdensity, even=True))
    kwargs = {}
    # loop over EOS linspace
    for n, x in enumerate(np.linspace(linspace[0], linspace[1], linspace[2])):
        id = c.reserve(name=name, ecut=ecut,
```

```
                linspacestr=linspacestr,
                kptdensity=kptdensity, width=width,
                x=x)
if id is None:
    continue
# perform EOS step
atoms.set_cell(cell * x, scale_atoms=True)
# set calculator
atoms.calc = Abinit(
    label=name + '_' + code + '_' + str(n),
    xc='PBE',
    kpts=kpts,
    ecut=ecut*Rydberg,
    occopt=3,
    tsmear=width,
    toldfe=1.0e-6,
    nstep=900,
    diemix=0.1,
    fband=0.95,
    # http://forum.abinit.org/viewtopic.php?f=8&t=35
    chksymbreak=0,
    nsym=1,  # various symmetry problems with various abinits ...
)
atoms.calc.set(**kwargs)  # remaining calc keywords
t = time.time()
atoms.get_potential_energy()
c.write(atoms,
        name=name, ecut=ecut,
        linspacestr=linspacestr,
        kptdensity=kptdensity, width=width,
        x=x,
        time=time.time()-t)
traj.write(atoms)
wfk = name + '_' + code + '_' + str(n) + 'o_WFK'
if os.path.exists(wfk): os.remove(wfk)
del c[id]
```