Vdb2/DACAPO

Vanderbilt-type USPP dataset version 2 / Dacapo 2.7.16

`name and version of the code:` Dacapo 2.7.16
`type of basis set:` plane waves
`method:` ultrasoft pseudopotentials (Vanderbilt-type v2)

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`	plane-wave cutoff = 700 eV
`k-mesh density`	8 k-points per Å^{-1}
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.06 eV

METHOD-SPECIFIC INFORMATION

`plane-wave cutoff`	700 eV
`density cutoff`	1000 eV

ADDITIONAL COMMENTS

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

REFERENCES

`potentials`

[1] D. Vanderbilt, *Phys. Rev. B* **41**, 7892–7895 (1990).
[2] https://wiki.fysik.dtu.dk/dacapo/Pseudopotential_Library

`code`

[3] https://wiki.fysik.dtu.dk/dacapo/dacapo.

`scalar relativity`

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

Table I. Calculation settings and results per element: potential, valence Z_{val}, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	potential	Z_{val} [–]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	ch_e9g4.pseudo	1	17.683	10.617	2.728
He	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Li	Li_us_cc.pseudo	1	22.156	12.196	3.532
Be	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
B	B_us_cc.pseudo	3	7.228	236.231	3.45
C	C_us_gga.pseudo	4	11.573	211.609	3.598
N	N_us.pseudo	5	30.218	55.628	3.389
O	co_gef_e13_gga.pseudo	6	19.338	53.354	3.722
F	F_pw91_us_7.3.4.pseudo	7	19.872	35.781	4.621
Ne	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Na	Na_tm_lda_cc.pseudo	1	35.524	8.072	3.724
Mg	mg_us_gga.pseudo	8	23.058	35.951	4.052
Al	Al_us_gga_org.pseudo	3	16.455	77.26	5.027
Si	csi_e8ag4.pseudo	4	20.403	88.872	4.307
P	P_us.pseudo	5	21.427	67.695	4.196
S	S_tm.pseudo	6	17.037	83.932	4.452
Cl	Cl_us_gga.pseudo	7	38.077	19.69	6.753
Ar	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
K	k_us_gga.pseudo	9	73.872	3.893	1.431
Ca	Ca_us_cc_pw91.pseudo	10	42.217	17.175	1.979
Sc	Sc_us_cc_pw91.pseudo	11	24.643	54.266	3.418
Ti	ti_us_gga.pseudo	12	17.404	111.643	3.831
V	V_us_pw91_13elec.pseudo	13	13.47	180.486	3.601
Cr	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Mn	Mn_us_gga.pseudo	7	10.748	277.287	4.329
Fe	Fe_us_gga_d2.1.8.pseudo	8	11.626	162.557	8.238
Co	Co_us_gga.pseudo	9	10.973	214.957	5.157
Ni	Ni_us_gga.pseudo	10	10.954	203.148	4.772
Cu	Cu_us_gga.pseudo	11	12.306	133.614	5.029
Zn	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Ga	ga_pw91_us_13elec.pseudo	13	20.345	49.928	3.377
Ge	ge_pw91_us_14elec.pseudo	14	23.907	59.757	4.804
As	as_pw91_us_15elec.pseudo	15	22.548	69.623	4.089
Se	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Br	Br_us.pseudo	17	39.468	22.404	4.667
Kr	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Rb	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Sr	Sr_us_cc_pw91.pseudo	10	54.752	11.506	3.321
Y	Y_us_cc_pw91.pseudo	11	32.899	40.972	3.065
Zr	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Nb	Nb_us_pw91_13elec.pseudo	13	18.093	170.578	3.971
Mo	Mo_us.pseudo	6	16.182	267.884	4.531
Tc	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Ru	Ru_us_gga.pseudo	8	14.12	344.792	5.059
Rh	Rh_us_gga_fl.pseudo	9	13.985	259.049	5.12
Pd	pd_us_gga.pseudo	10	15.82	170.298	5.644
Ag	ag_us.pseudo	11	17.744	92.462	5.863
Cd	Cd_us_gga.pseudo	12	22.766	44.499	6.813
In	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*

Sn	sn_us_f.pseudo	14	36.792	35.194	4.237
Sb	sb_us_gga.pseudo	15	31.192	54.089	4.649
Te	te_tm.pseudo	16	38.558	41.165	4.833
I	I_us.pseudo	17	49.319	19.099	5.063
Xe	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Cs	cs_tm_7el.pseudo	7	123.835	1.793	3.432
Ba	Ba_us_cc_pw91.pseudo	10	62.41	8.497	2.585
Lu	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Hf	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Ta	Ta_us_pw91_13elec.pseudo	13	18.21	194.071	3.724
W	W_us_pw91_6elec.pseudo	6	16.12	306.074	4.283
Re	re_us_gga_7elec.pseudo	7	14.689	371.713	4.44
Os	os_us_gga_7elec_7.3.4.pseudo	8	14.177	408.197	4.723
Ir	ir_us_gga_flocal.pseudo	9	14.296	352.89	5.15
Pt	pt_us_gga.pseudo	10	15.971	243.678	5.562
Au	Au_us_gga.pseudo	11	18.227	138.628	5.811
Hg	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Tl	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Pb	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Bi	Bi_us_gga.pseudo	15	36.777	43.893	4.081
Po	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*

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/

```
from ase.calculators.jacapo.pw91_psp import defaultpseudopotentials as psp
from ase.tasks.calcfactory import calculator_factory
from ase.test.tasks.dcdft import DeltaCodesDFTTask as Task

xc = 'PBE'

fit = (5, 0.02)

w = 0.06
pw = 700
dw = 1000
kd = 8.0

tag = 'dcdft_%s_jacapo' % xc.lower()

calcfactory = calculator_factory('jacapo',
                                 pw=pw,
                                 dw=dw,
                                 xc='PBE',
                                 ft=w,
                                 symmetry=True,
                                 spinpol=True, # must set explicitly
                                 calculate_stress=False,
                                 deletenc=True,  # start fresh every time
                                 kptdensity=kd,
                                 )

taskopts = {}

task = Task(
    calcfactory=calcfactory,
    tag=tag,
    fit=fit,
    use_lock_files=True,
    **taskopts)

if __name__ == '__main__':
    keys = set(psp.keys()).intersection(set(task.collection.names))
    for m in ['Be', 'Cr', 'Kr', 'Xe']:
        keys.remove(m)  # EOS fails: maybe need higher ecut?
    for m in ['Zn', 'Zr']:
        keys.remove(m)  # do not converge
    task.run(keys)
```