PSlib100/QE

pslibrary.1.0.0 PAW dataset / QUANTUM ESPRESSO 5.1

`name and version of the code:` QUANTUM ESPRESSO 5.1
`type of basis set:` plane waves
`method:` projector-augmented wave (pslibrary.1.0.0)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see table
`basis set size`	see table (wave function cutoff e_{cut}^{wfc})
`k-mesh density`	$20 \times 20 \times 20$
`reciprocal-space integration method`	Marzari-Vanderbilt cold smearing with a fictitious temperature corresponding to 0.002 Ry (0.02 Ry when required to achieve convergence)

METHOD-SPECIFIC INFORMATION

`wave function cutoff`	see table (e_{cut}^{wfc})
`density cutoff`	see table (e_{cut}^{rho})

ADDITIONAL COMMENTS

Co and Tc do not converge.

REFERENCES

`PAW dataset`

[1] http://www.qe-forge.org/gf/project/pslibrary/frs
[2] A. Dal Corso, *Comput. Mater. Sci.* **95**, 337–350 (2014).

`code`

[3] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari and R. M. Wentzcovitch, *J. Phys.: Condens. Matter* **21**, 395502 (2009).

`scalar relativity`

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

`smearing`

[5] N. Marzari, D. Vanderbilt, A. De Vita and M. C. Payne, *Phys. Rev. Lett.* **82**, 3296 (1999).

Table I. Calculation settings and results per element: wave function cutoff e_{cut}^{wfc}, density cutoff e_{cut}^{rho}, valence, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	e_{cut}^{wfc} [Ry]	e_{cut}^{rho} [Ry]	valence	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	100	450	$1s^1$	17.420	10.298	2.701
He	100	410	$1s^2$	17.773	0.867	6.675
Li	210	820	$1s^2 2s^1 2p^0$	20.225	13.837	3.332
Be	170	780	$1s^2 2s^2 2p^0$	7.897	123.072	3.286
B	90	650	$2s^2 2p^1$	7.255	237.375	3.477
C	80	660	$2s^2 2p^2$	11.646	209.465	3.577
N	90	640	$2s^2 2p^3$	29.421	53.564	3.789
O	100	650	$2s^2 2p^4$	19.537	51.449	4.026
F	100	640	$2s^2 2p^5$	19.261	34.300	4.097
Ne	110	530	$2s^2 2p^6$	24.253	1.431	13.082
Na	140	650	$2s^2 2p^6 3s^1$	37.178	7.705	3.714
Mg	200	800	$2s^2 2p^6 3s^2 3p^0$	22.952	36.034	4.020
Al	60	290	$3s^2 3p^1$	16.476	77.977	4.664
Si	90	350	$3s^2 3p^2$	20.448	88.920	4.327
P	70	350	$3s^2 3p^3$	21.457	68.210	4.335
S	80	370	$3s^2 3p^4$	17.218	83.692	4.038
Cl	90	450	$3s^2 3p^5$	38.549	19.476	4.429
Ar	100	450	$3s^2 3p^6$	52.312	0.742	7.335
K	90	560	$3s^2 3p^6 4s^1 4p^0$	73.694	3.586	3.770
Ca	90	550	$3s^2 3p^6 4s^2 4p^0$	42.159	17.351	3.311
Sc	100	810	$3s^2 3p^6 3d^1 4s^2$	24.584	54.831	3.405
Ti	110	1150	$3s^2 3p^6 3d^2 4s^2$	17.453	111.307	3.549
V	100	1300	$3s^2 3p^6 3d^3 4s^2$	13.517	181.522	3.836
Cr	100	920	$3s^2 3p^6 3d^4 4s^2$	11.837	182.041	6.560
Mn	120	1410	$3s^2 3p^6 3d^5 4s^2$	11.443	115.696	2.712
Fe	150	1000	$3s^2 3p^6 3d^6 4s^2$	11.358	203.810	4.636
Co	150	960	$3s^2 3p^6 3d^7 4s^2$	N/A	N/A	N/A
Ni	150	960	$3s^2 3p^6 3d^8 4s^2$	10.928	197.978	4.903
Cu	150	660	$3s^2 3p^6 3d^{10} 4s^1$	11.988	140.068	5.060
Zn	150	800	$3s^2 3p^6 3d^{10} 4s^2$	15.261	73.058	5.414
Ga	120	490	$3d^{10} 4s^2 4p^1$	20.299	49.119	5.293
Ge	90	480	$3d^{10} 4s^2 4p^2$	23.905	59.055	4.823
As	90	580	$3d^{10} 4s^2 4p^3$	22.625	68.220	4.232
Se	110	500	$3d^{10} 4s^2 4p^4$	29.742	47.867	4.338
Br	120	580	$3d^{10} 4s^2 4p^5$	39.310	23.003	4.846
Kr	130	620	$3d^{10} 4s^2 4p^6$	66.107	0.636	3.324
Rb	70	520	$4s^2 4p^6 5s^1 5p^0$	90.994	2.789	3.763
Sr	80	530	$4s^2 4p^6 5s^2 5p^0$	54.920	11.825	3.262
Y	80	520	$4s^2 4p^6 4d^1 5s^2 5p^0$	32.847	40.821	3.013
Zr	100	540	$4s^2 4p^6 4d^2 5s^2 5p^0$	23.387	94.293	3.333
Nb	100	540	$4s^2 4p^6 4d^3 5s^2 5p^0$	18.150	170.260	3.710
Mo	100	620	$4s^2 4p^6 4d^4 5s^2 5p^0$	15.802	260.025	4.229
Tc	120	850	$4s^2 4p^6 4d^5 5s^2 5p^0$	N/A	N/A	N/A
Ru	110	720	$4s^2 4p^6 4d^6 5s^2$	13.774	313.121	4.892
Rh	110	730	$4s^2 4p^6 4d^7 5s^2$	14.051	257.621	5.205
Pd	120	1080	$4s^2 4p^6 4d^8 5s^2$	15.307	169.707	5.540
Ag	130	820	$4s^2 4p^6 4d^9 5s^2$	17.844	90.965	5.839
Cd	130	1070	$4s^2 4p^6 4d^{10} 5s^2$	22.855	44.097	6.445

In	90	430	$4d^{10}5s^25p^1$	27.538	35.509	5.065
Sn	100	500	$4d^{10}5s^25p^2$	36.845	35.871	4.909
Sb	100	500	$4d^{10}5s^25p^3$	31.818	50.348	4.514
Te	170	660	$4d^{10}5s^25p^4$	35.066	45.025	4.615
I	140	560	$4d^{10}5s^25p^5$	49.996	19.177	5.066
Xe	90	430	$4d^{10}5s^25p^6$	87.000	0.536	6.634
Cs	70	520	$5s^25p^66s^1$	116.498	1.975	3.568
Ba	80	360	$5s^25p^66s^2$	63.551	8.658	2.910
Lu	346	1382	$4d^{10}4f^{14}5s^25p^65d^16s^2$	29.039	46.988	3.447
Hf	100	640	$4d^{10}4f^{14}5s^25p^65d^26s^2$	22.521	107.118	4.290
Ta	110	1060	$4f^{14}5s^25p^65d^36s^2$	18.260	194.192	3.730
W	110	760	$4f^{14}5s^25p^65d^46s^2$	16.118	302.789	4.187
Re	110	880	$4f^{14}5s^25p^65d^56s^2$	14.935	364.693	4.458
Os	140	900	$4f^{14}5s^25p^65d^66s^26p^0$	14.257	398.320	4.812
Ir	130	900	$4f^{14}5s^25p^65d^76s^2$	14.492	348.622	5.111
Pt	160	800	$4f^{14}5s^25p^65d^86s^2$	15.627	249.162	5.481
Au	140	760	$4f^{14}5s^25p^65d^{10}6s^16p^0$	17.939	140.383	5.988
Hg	150	850	$5s^25p^65d^{10}6s^2$	29.373	7.879	9.958
Tl	90	420	$5d^{10}6s^26p^1$	31.381	26.834	5.361
Pb	100	430	$5d^{10}6s^26p^2$	32.010	39.624	4.767
Bi	90	910	$5d^{10}6s^26p^3$	36.909	42.773	4.641
Po	100	910	$5d^{10}6s^26p^4$	37.589	45.723	4.877
Rn	100	430	$5d^{10}6s^26p^6$	93.380	0.539	3.228