PSlib031/QE

pslibrary.0.3.1 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.0.3.1)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valance scalar-relativistic (Koelling-Harmon 1977)
`assignment of core / valence states`	see table (Z_{val})
`basis set size`	see table (wave function cutoff e^{wfc})
`k-mesh density`	see table (shifted k-point mesh in the full 1st Brillouin zone of the primitive cell *kpts*, and number of irreducible k-points # k)
`reciprocal-space integration method`	see table [Gaussian (Marzari-Vanderbilt) smearing with a fictitious temperature corresponding to 0.02 Ry (0.05 Ry)]

METHOD-SPECIFIC INFORMATION

`wave function cutoff`	see table (e^{wfc})
`density cutoff`	$e^{wfc} \times 4$

ADDITIONAL COMMENTS

none

REFERENCES

`PAW dataset details`

- E. Kucukbenli, M. Monni, B. I. Adetunji, X. Ge, G. A. Adebayo, N. Marzari, S. de Gironcoli and A. Dal Corso, arXiv:1404.3015 (2014)
- http://www.qe-forge.org/gf/project/pslibrary/

`code`

- 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`

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

`smearing`

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

PSlib031/QE

pslibrary.0.3.1 PAW dataset / QUANTUM ESPRESSO 5.1

	Z_{val} [-]	e^{wfc} [Ry]	smear	# k[-]	*kpts* [-]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	1	60	G	12	4 4 4	17.42131	10.28519	2.775
He	2	40	G	108	6 6 4	17.68548	0.98328	0.101
Li	3	80	MV	500	10 10 10	20.23868	13.79499	3.279
Be	2	40	MV	3039	15 15 9	7.86339	124.29788	3.313
B	3	60	G	20	4 4 4	7.24347	235.55031	3.212
C	4	60	G	75	7 7 2	11.62797	209.22173	3.644
N	5	80	G	4	3 3 3	29.13421	54.21620	3.743
O	6	80	G	32	4 4 4	19.25778	51.80999	3.998
F	7	120	G	23	3 5 3	19.30412	34.13435	3.892
Ne	8	200	G	4	4 4 4	23.28520	3.60673	25.835
Na	9	60	MV	256	8 8 8	37.08232	7.72960	3.675
Mg	2	40	MV	1020	13 13 8	22.88271	36.56051	4.048
Al	3	40	MV	35	10 10 10	16.43746	77.51373	4.946
Si	4	40	G	39	5 5 5	20.41871	88.93774	4.290
P	5	40	G	20	7 2 5	21.32226	68.91312	4.326
S	6	40	G	3430	19 19 19	17.08679	84.17314	4.391
Cl	7	40	G	8	3 4 2	38.50371	19.07449	4.212
Ar	8	80	G	4	3 3 3	50.93585	2.85465	30.955
K	9	60	MV	20	7 7 7	73.86289	3.81905	0.227
Ca	10	60	MV	10	6 6 6	41.94199	17.55183	3.419
Sc	11	80	MV	288	8 8 5	24.59533	55.50824	3.280
Ti	12	100	MV	369	9 9 6	17.41080	110.90888	4.257
V	13	100	MV	35	9 9 9	13.51741	181.52541	3.781
Cr	14	100	MV	70	9 9 9	11.88121	179.04944	6.298
Mn	15	100	MV	80	7 7 7	11.56139	106.78915	−3.272
Fe	16	120	MV	112	12 12 12	11.36931	199.77832	6.108
Co	9	80	MV	1800	10 10 6	10.89105	221.80375	4.772
Ni	10	80	MV	70	10 10 10	10.92454	202.83198	4.938
Cu	11	60	MV	35	9 9 9	12.09346	127.85123	10.132
Zn	12	140	MV	288	16 16 8	15.18210	75.22894	5.426
Ga	13	80	MV	135	9 6 9	20.41631	49.89060	5.112
Ge	14	60	MV	63	6 6 6	23.95587	60.11917	1.339
As	5	40	MV	192	9 9 3	22.63885	68.81854	4.307
Se	6	40	G	52	4 4 4	29.92170	46.95624	4.493
Br	7	40	G	4	2 4 2	39.76096	22.22211	4.827
Kr	8	60	G	4	3 3 3	66.58636	0.68576	2.186
Rb	9	80	MV	20	8 8 8	91.26761	2.75054	2.530
Sr	10	60	MV	4	4 4 4	54.30192	12.09388	3.747
Y	11	60	MV	225	7 7 5	32.89100	41.99345	3.223
Zr	12	80	MV	288	8 8 5	23.46569	93.89028	3.349
Nb	13	80	MV	35	10 10 10	18.19888	168.89182	3.327
Mo	14	80	MV	56	11 11 11	15.80404	259.62998	4.315
Tc	15	100	MV	1695	15 15 10	14.44780	299.53214	4.600
Ru	16	200	MV	2916	18 18 12	13.78595	312.54189	4.877
Rh	17	100	MV	35	9 9 9	14.12612	257.26406	5.226
Pd	10	80	MV	35	9 9 9	15.39990	168.85100	5.550
Ag	11	80	MV	20	8 8 8	17.95772	88.33418	5.852
Cd	12	100	MV	549	11 11 6	22.84630	43.48633	6.486
In	13	80	MV	216	16 16 11	27.41502	35.65851	5.229
Sn	14	180	MV	63	6 6 6	36.96970	35.46094	4.963
Sb	5	60	MV	87	6 6 3	31.80131	50.73655	4.567
Te	16	160	G	16	4 4 3	35.12362	44.50574	4.600

I	7	60	G	4	2 4 2	50.19766	18.72793	5.125
Cs	9	40	MV	20	7 7 7	117.35555	1.98088	2.707
Ba	10	80	MV	20	7 7 7	63.44648	9.03233	4.305
Hf	12	80	MV	288	8 8 5	22.50211	107.15708	3.253
Ta	13	80	MV	20	8 8 8	18.18723	198.24772	4.180
W	14	80	MV	56	11 11 11	16.21792	302.54789	4.014
Re	15	120	MV	864	12 12 8	14.90006	364.94682	4.470
Os	8	60	MV	864	12 12 8	14.33109	402.27853	4.848
Ir	9	60	MV	84	13 13 13	14.63471	348.94637	5.159
Pt	10	60	MV	56	11 11 11	15.84272	248.04692	5.588
Au	11	60	MV	20	8 8 8	18.13404	136.02640	6.508
Hg	12	60	MV	50	8 8 10	29.27980	8.83168	8.874
Tl	13	80	MV	1470	14 14 9	31.34104	27.00735	5.411
Pb	14	80	MV	56	11 11 11	32.04736	38.91928	4.808
Bi	15	80	MV	57	6 6 2	36.91008	42.56608	4.652
Po	16	120	MV	286	21 21 21	37.53931	45.30648	4.855