JTH02/ABINIT

JTH2 PAW dataset / ABINIT 7.7.3

`name and version of the code:` ABINIT 7.7.3
`type of basis set:` plane waves
`method:` projector-augmented wave (JTH2)

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`	cutoff energy = 20 Ha
`k-mesh density`	$6\,750/N$ k-points in the full first Brillouin zone of an N-atom cell
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.002 Ha

METHOD-SPECIFIC INFORMATION

`PAW radii`	see table (R_{PAW})
`PAW cutoff energy`	20 Ha
`PAW cutoff augmentation energy`	40 Ha
`Partial-wave basis size`	2 elements per ℓ-value except for H, He, Li (one p element) and In, K, Kr, Pb, Rb and Sn (one d element)

ADDITIONAL COMMENTS

`PAW dataset generator`	ATOMPAW 4.0.0.8

REFERENCES

`PAW dataset`

[1] http://pwpaw.wfu.edu
[2] http://www.abinit.org/downloads/PAW2
[3] F. Jollet, M. Torrent and N. Holzwarth, *Comput. Phys. Commun.* **185**, 1246–1254 (2014).

`code`

[4] 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).
[5] 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).
[6] M. Torrent, F. Jollet, F. Bottin, G. Zérah, X. Gonze, *Comput. Mater. Sci.* **42**, 337–351, (2008).

`scalar relativity`

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

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

	valence	R_{PAW} [a.u.]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	$1s^1\ 2p^0$	0.9	17.49784	10.19793	3.158
He	$1s^2\ 2p^0$	1.3	17.82456	0.83536	6.413
Li	$1s^2\ 2s^1\ 2p^0$	1.6	20.23660	13.80609	3.344
Be	$1s^2\ 2s^2$	1.3	7.90864	122.23486	2.890
B	$2s^2\ 2p^1$	1.7	7.24518	237.25091	3.487
C	$2s^2\ 2p^2$	1.5	11.67933	212.34059	2.615
N	$2s^2\ 2p^3$	1.2	28.93191	55.07215	2.964
O	$2s^2\ 2p^4$	1.4	18.58084	51.38422	3.881
F	$2s^2\ 2p^5$	1.4	19.17107	35.54535	4.280
Ne	$2s^2\ 2p^6$	1.8	24.24011	1.32984	13.318
Na	$2s^2\ 2p^6\ 3s^1$	1.6	37.14517	7.96228	3.165
Mg	$2s^2\ 2p^6\ 3s^2$	1.9	22.99173	35.65411	4.272
Al	$3s^2\ 3p^1$	1.9	16.47447	77.74370	4.560
Si	$3s^2\ 3p^2$	1.9	20.43663	88.78771	4.362
P	$3s^2\ 3p^3$	1.9	21.43844	67.88073	4.375
S	$3s^2\ 3p^4$	1.9	17.16799	83.68796	4.129
Cl	$3s^2\ 3p^5$	1.8	38.88399	18.80925	4.305
Ar	$3s^2\ 3p^6$	1.8	52.20238	0.75000	6.572
K	$3s^2\ 3p^6\ 4s^1\ 3d^0$	2.1	73.78410	3.62429	3.657
Ca	$3s^2\ 3p^6\ 4s^2\ 3d^0$	1.9	42.13759	17.44248	3.821
Sc	$3s^2\ 3p^6\ 4s^2\ 3d^1$	2.4	24.62186	54.28881	3.361
Ti	$3s^2\ 3p^6\ 4s^1\ 3d^3$	2.3	17.44179	111.26898	3.586
V	$3s^2\ 3p^6\ 4s^2\ 3d^3$	2.2	13.49462	180.72451	3.812
Cr	$3s^2\ 3p^6\ 4s^1\ 3d^5$	2.1	11.76507	176.02398	6.499
Mn	$3s^2\ 3p^6\ 4s^1\ 3d^6$	2.1	11.46933	109.23894	1.795
Fe	$3s^2\ 3p^6\ 4s^1\ 3d^7$	2.1	11.35042	188.26412	4.337
Co	$3s^2\ 3p^6\ 4s^1\ 3d^8$	2.1	10.88408	212.91538	5.008
Ni	$3s^2\ 3p^6\ 4s^2\ 3d^8$	1.8	10.92726	195.27345	4.504
Cu	$3s^2\ 3p^6\ 4s^1\ 3d^{10}$	2.0	11.98367	143.88972	3.113
Zn	$4s^2\ 4p^0\ 3d^{10}$	2.3	15.17410	75.61000	5.861
Ga	$4s^2\ 4p^1\ 3d^{10}$	2.1	20.35737	48.97476	5.259
Ge	$4s^2\ 4p^2\ 3d^{10}$	2.3	23.95958	58.74576	4.844
As	$4s^2\ 4p^3$	2.1	22.62141	68.66612	4.408
Se	$4s^2\ 4p^4$	2.2	29.76678	47.18222	4.410
Br	$4s^2\ 4p^5$	2.2	39.42359	22.42968	4.955
Kr	$4s^2\ 4p^6\ 4d^0$	2.2	65.58856	0.66720	7.045
Rb	$4s^2\ 4p^6\ 5s^1\ 4d^0$	2.3	91.35346	2.76524	3.710
Sr	$4s^2\ 4p^6\ 5s^1\ 4d^1$	2.3	54.83515	11.56932	3.512
Y	$4s^2\ 4p^6\ 5s^2\ 4d^1$	2.21	32.87966	40.84792	3.095
Zr	$4s^2\ 4p^6\ 5s^1\ 4d^3$	2.21	23.39635	93.35861	3.307
Nb	$4s^2\ 4p^6\ 5s^1\ 4d^4$	2.21	18.13436	169.29464	3.675
Mo	$4s^2\ 4p^6\ 5s^1\ 4d^5$	2.2	15.81522	259.13798	4.065
Tc	$4s^2\ 4p^6\ 5s^1\ 4d^6$	2.2	14.42049	300.50292	4.496
Ru	$4s^2\ 4p^6\ 5s^1\ 4d^7$	2.2	13.75825	310.20598	4.882
Rh	$4s^2\ 4p^6\ 5s^1\ 4d^8$	2.4	14.02331	259.21608	5.199
Pd	$4s^2\ 4p^6\ 5s^1\ 4d^9$	2.5	15.34098	165.54672	5.834
Ag	$5s^1\ 5p^0\ 4d^{10}$	2.5	17.82774	91.16985	5.846
Cd	$5s^2\ 5p^0\ 4d^{9.5}$	2.5	22.83952	43.96281	6.457
In	$5s^2\ 5p^1\ 5d^0$	2.9	27.56008	36.89393	5.224

Sn	$5s^2\ 5p^2\ 5d^0$	2.7	36.90498	36.06134	4.883
Sb	$5s^2\ 5p^3$	2.3	31.81108	50.69800	4.654
Te	$5s^2\ 5p^4$	2.3	34.97177	45.14244	4.735
I	$5s^2\ 5p^5$	2.3	50.40996	18.73037	5.018
Xe	$5s^2\ 5p^6$	2.4	86.82364	0.53258	3.803
Cs	$5s^2\ 5p^6\ 6s^1\ 5d^0$	2.2	117.24092	1.95497	4.664
Ba	$5s^2\ 5p^6\ 6s^2\ 5d^0$	2.3	63.61502	8.95960	1.790
Lu	$5s^2\ 5p^6\ 6s^2\ 5d^1\ 4f^{14}$	2.5	29.05320	47.69130	3.517
Hf	$5s^2\ 5p^6\ 6s^2\ 5d^2$	2.41	22.54152	107.55827	3.302
Ta	$5s^2\ 5p^6\ 6s^2\ 5d^3$	2.41	18.30307	195.82211	3.794
W	$5s^2\ 5p^6\ 6s^2\ 5d^4$	2.41	16.15981	304.55240	4.143
Re	$5s^2\ 5p^6\ 6s^2\ 5d^5$	2.4	14.96913	365.51908	4.377
Os	$5p^6\ 6s^1\ 5d^7$	2.5	14.29122	401.51823	4.791
Ir	$5p^6\ 6s^1\ 5d^8$	2.5	14.50797	349.66966	5.029
Pt	$6s^1\ 6p^0\ 5d^9$	2.5	15.67922	250.16206	5.560
Au	$6s^1\ 6p^0\ 5d^{10}$	2.5	18.01120	140.30086	5.501
Hg	$6s^2\ 6p^0\ 5d^{10}$	2.4	29.54526	9.07820	12.115
Tl	$6s^2\ 6p^1$	2.9	31.42148	27.79113	5.431
Pb	$6s^2\ 6p^2\ 6d^0$	2.9	32.01765	41.11989	5.147
Bi	$6s^2\ 6p^3$	2.9	36.92422	43.23146	4.717
Po	$6s^2\ 6p^4$	2.9	37.57022	46.08312	4.848
Rn	$6s^2\ 6p^6$	2.3	92.79747	0.61552	8.806