ONCVPSP/ABINIT

ONCVPSP 3.2.1 Pseudo-Dojo v0.1 NCPP dataset / ABINIT 7.11.8

`name and version of the code:` ABINIT 7.11.8
`type of basis set:` plane waves
`method:` norm-conserving pseudopotentials (ONCVPSP 3.2.1 Pseudo-Dojo v0.1)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic
`assignment of core / valence states`	see table
`basis set size`	see table (E_{cut})
`k-mesh density`	6750 / N k-points in the first Brillouin zone of a N-atom cell
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.0036 Ha

METHOD-SPECIFIC INFORMATION

none

ADDITIONAL COMMENTS

RC_{min} and RC_{max} are the minimum and maximum core radii used to pseudize the all-electron wave-functions

The E_{cut} provided in the table are the values at which the Δ value is converged well within 0.1 meV/atom. For many practical applications, a much smaller cutoff energy is already sufficient (usually 20 Ha less than the value of E_{cut} reported in the table).

REFERENCES

`potentials`

[1] D. R. Hamann, *Phys. Rev. B* **88**, 085117 (2013).
[2] www.mat-simresearch.com

`pseudo-dojo`

[3] www.pseudo-dojo.org
[4] www.pseudo-dojo.org/datasets/pseudos_deltafactor_paper.tgz

`code`

[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] www.abinit.org

Table I. Calculation settings and results per element: minimum and maximum core radii RC_{min} and RC_{max}, plane-wave cutoff E_{cut}, valence, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	RC_{min} [b]	RC_{max} [b]	E_{cut} [Ha]	valence	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	0.70	1.00	65	$1s^1$	17.358	10.272	2.667
He	1.00	1.25	75	$1s^2$	17.663	0.888	6.418
Li	1.00	1.20	68	$1s^2 2s^1$	20.266	13.769	3.336
Be	1.05	1.20	73	$1s^2 2s^2$	7.943	123.595	3.331
B	1.20	1.20	60	$2s^2 2p^1$	7.221	235.844	3.449
C	1.20	1.25	63	$2s^2 2p^2$	11.626	207.914	3.594
N	1.20	1.35	60	$2s^2 2p^3$	28.907	53.609	3.985
O	1.25	1.35	64	$2s^2 2p^4$	18.471	50.671	3.823
F	1.15	1.30	70	$2s^2 2p^5$	19.225	33.909	1.176
Ne	1.30	1.50	60	$2s^2 2p^6$	24.325	1.084	1.835
Na	1.20	1.55	48	$2s^2 2p^6 3s^1$	37.200	7.659	3.688
Mg	1.15	1.55	60	$2s^2 2p^6 3s^2$	22.982	35.891	4.030
Al	1.70	1.75	40	$3s^2 3p^1$	16.455	77.065	4.578
Si	1.60	1.71	44	$3s^2 3p^2$	20.401	88.196	4.287
P	1.45	1.55	43	$3s^2 3p^3$	21.458	67.941	4.313
S	1.45	1.50	41	$3s^2 3p^4$	17.187	83.225	4.189
Cl	1.35	1.55	45	$3s^2 3p^5$	38.714	18.936	4.518
Ar	1.55	1.55	49	$3s^2 3p^6$	52.278	0.758	9.158
K	1.35	1.60	54	$3s^2 3p^6 4s^1$	73.935	3.510	3.797
Ca	1.45	1.85	52	$3s^2 3p^6 4s^2$	42.179	17.450	3.346
Sc	1.35	1.65	59	$3s^2 3p^6 3d^1 4s^2$	24.723	53.284	3.688
Ti	1.30	1.65	60	$3s^2 3p^6 3d^2 4s^2$	17.428	111.105	3.556
V	1.30	1.65	60	$3s^2 3p^6 3d^3 4s^2$	13.483	184.486	3.671
Cr	1.10	1.40	80	$3s^2 3p^6 3d^5 4s^1$	11.802	171.884	6.586
Mn	1.10	1.35	83	$3s^2 3p^6 3d^5 4s^2$	11.392	119.895	3.254
Fe	1.10	1.20	85	$3s^2 3p^6 3d^6 4s^2$	11.389	182.963	6.329
Co	1.20	1.55	70	$3s^2 3p^6 3d^7 4s^2$	10.880	211.182	4.756
Ni	1.20	1.55	75	$3s^2 3p^6 3d^8 4s^2$	10.915	193.669	5.034
Cu	1.20	1.60	72	$3s^2 3p^6 3d^{10} 4s^1$	11.979	141.886	4.706
Zn	1.35	1.85	58	$3s^2 3p^6 3d^{10} 4s^2$	15.176	74.223	5.537
Ga	1.65	1.90	58	$3d^{10} 4s^2 4p^1$	20.341	49.148	4.897
Ge	1.80	1.90	57	$3d^{10} 4s^2 4p^2$	23.935	58.812	4.857
As	1.60	1.80	60	$3d^{10} 4s^2 4p^3$	22.597	68.127	4.183
Se	1.50	1.90	59	$3d^{10} 4s^2 4p^4$	29.759	46.886	4.553
Br	1.50	1.90	56	$3d^{10} 4s^2 4p^5$	39.446	22.234	5.053
Kr	1.50	1.80	44	$4s^2 4p^6$	65.929	0.648	7.087
Rb	1.70	1.85	41	$4s^2 4p^6 5s^1$	91.353	2.717	3.667
Sr	1.30	1.60	52	$4s^2 4p^6 5s^2$	55.055	11.783	3.106
Y	1.50	1.60	54	$4s^2 4p^6 4d^1 5s^2$	32.960	40.398	2.995
Zr	1.50	1.55	51	$4s^2 4p^6 4d^2 5s^2$	23.423	93.577	3.304
Nb	1.35	1.45	61	$4s^2 4p^6 4d^4 5s^1$	18.175	168.661	3.662
Mo	1.35	1.45	58	$4s^2 4p^6 4d^5 5s^1$	15.812	258.833	4.224
Tc	1.30	1.35	64	$4s^2 4p^6 4d^5 5s^2$	14.462	298.037	4.576
Ru	1.30	1.35	60	$4s^2 4p^6 4d^7 5s^1$	13.789	311.286	4.868
Rh	1.30	1.35	60	$4s^2 4p^6 4d^8 5s^1$	14.076	255.055	5.223
Pd	1.40	1.55	59	$4s^2 4p^6 4d^{10}$	15.343	168.170	5.512
Ag	1.40	1.60	59	$4s^2 4p^6 4d^{10} 5s^1$	17.817	90.242	6.029
Cd	1.70	2.10	59	$4d^{10} 5s^2$	22.824	43.918	6.385

In	1.85	2.35	53	$4d^{10}5s^25p^1$	27.458	35.033	5.180
Sn	1.85	2.60	54	$4d^{10}5s^25p^2$	36.874	35.729	4.902
Sb	2.15	2.60	32	$5s^25p^3$	31.680	50.573	4.530
Te	2.20	2.60	33	$5s^25p^4$	35.019	44.697	4.701
I	2.00	2.25	53	$5s^25p^5$	50.400	18.507	5.082
Xe	1.70	2.00	62	$4d^{10}5s^25p^6$	87.034	0.526	5.360
Cs	1.85	2.25	58	$5s^25p^66s^1$	116.766	1.935	3.562
Ba	1.90	2.15	40	$5s^25p^66s^2$	63.663	8.693	2.828
Lu	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Hf	1.40	1.60	84	$5s^25p^64f^{14}5d^26s^2$	22.549	106.760	3.430
Ta	1.95	2.55	39	$5p^65d^36s^2$	18.302	191.011	3.700
W	2.20	2.60	39	$5p^65d^46s^2$	16.135	300.330	4.154
Re	2.15	2.55	40	$5p^65d^56s^2$	14.950	363.302	4.482
Os	2.15	2.55	40	$5p^65d^66s^2$	14.290	397.370	4.834
Ir	1.85	2.50	45	$5p^65d^76s^2$	14.482	347.507	5.269
Pt	1.85	2.50	47	$5p^65d^96s^1$	15.609	245.191	5.347
Au	1.90	2.60	47	$5p^65d^{10}6s^1$	17.995	138.191	5.621
Hg	2.10	2.60	45	$5d^{10}6s^2$	29.308	9.510	10.049
Tl	2.00	2.60	49	$5d^{10}6s^26p^1$	31.427	26.450	5.413
Pb	2.10	2.60	46	$5d^{10}6s^26p^2$	32.016	39.930	4.835
Bi	2.10	2.50	51	$5d^{10}6s^26p^3$	36.929	42.498	4.642
Po	1.90	2.20	50	$5d^{10}6s^26p^4$	37.617	45.170	4.849
Rn	2.10	2.85	35	$6s^26p^6$	93.164	0.544	6.039