ONCVPSP(SG15)1/Octopus

SG15 ONCVPSP 2015-01-24 NCPP dataset / Octopus 8.0

`name and version of the code:` Octopus 8.0
`type of basis set:` grid-based
`method:` norm-conserving pseudopotentials (Schlipf-Gygi ONCVPSP 2015-01-24)

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 ($\Delta_{\mathbf{r}}$)
`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

none

REFERENCES

`potentials`

[1] D. R. Hamann, *Phys. Rev. B* **88**, 085117 (2013).
[2] M. Schlipf and F. Gygi, *Comput. Phys. Commun.* (2015). doi: 10.1016/j.cpc.2015.05.011

`code`

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[4] X. Andrade, J. Alberdi-Rodriguez, D.A. Strubbe, M.J.T. Oliveira, F. Nogueira, A. Castro, J. Muguerza, A. Arruabarrena, S.G. Louie, A. Aspuru-Guzik, A. Rubio, M.A.L. Marques, *J. Phys.: Condens. Matter* **24**, 233202 (2012).
[5] X. Andrade, D.A. Strubbe, U. De Giovannini, A.H. Larsen, M.J.T. Oliveira, J. Alberdi-Rodriguez, A. Varas, I. Theophilou, N. Helbig, M. Verstraete, L. Stella, F. Nogueira, A. Aspuru-Guzik, A. Castro, M.A.L. Marques, A. Rubio, *Phys. Chem. Chem. Phys.* **17**, 31371–31396 (2015).

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Table I. Calculation settings per element: valence, grid spacing $\Delta_{\mathbf{r}}$, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	valence	$\Delta_{\mathbf{r}}$[Bohr]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	$1s^1$	0.35	17.35705	10.30363	1.838
He	$1s^2$	0.2	17.98743	0.72624	7.291
Li	$1s^2 2s^1$	0.2	20.30904	13.56652	3.193
Be	$1s^2 2s^2$	0.25	7.90810	124.97805	3.612
B	$2s^2 2p^1$	0.2	7.18504	234.70681	3.422
C	$2s^2 2p^2$	0.2	11.58684	207.83228	3.581
N	$2s^2 2p^3$	0.25	28.77555	53.02155	3.605
O	$2s^2 2p^4$	0.25	18.55891	47.04630	3.188
F	$2s^2 2p^5$	0.25	19.46356	33.00073	2.724
Ne	$2s^2 2p^6$	0.2	24.71548	1.20294	8.242
Na	$2s^2 2p^6 3s^1$	0.2	38.82111	58.73229	−1.997
Mg	$2s^2 2p^6 3s^2$	0.15	22.94293	36.57554	4.062
Al	$2s^2 2p^6 3s^2 3p^1$	0.2	16.51332	76.43611	4.838
Si	$3s^2 3p^2$	0.35	20.50880	87.46771	4.567
P	$3s^2 3p^3$	0.2	21.48447	67.78316	4.287
S	$3s^2 3p^4$	0.25	17.25770	83.48601	4.518
Cl	$3s^2 3p^5$	0.25	39.35430	18.70733	4.324
Ar	$3s^2 3p^6$	0.35	52.78677	0.73947	7.174
K	$3s^2 3p^6 4s^1$	0.2	73.44068	3.64218	3.797
Ca	$3s^2 3p^6 4s^2$	0.25	42.04012	17.23701	3.324
Sc	$3s^2 3p^6 3d^1 4s^2$	0.3	24.59188	54.56931	3.567
Ti	$3s^2 3p^6 3d^2 4s^2$	0.25	17.37629	113.07773	3.597
V	$3s^2 3p^6 3d^3 4s^2$	0.25	13.45137	181.79276	3.551
Cr	$3s^2 3p^6 3d^5 4s^1$	0.1	12.47184	117.71918	6.797
Mn	$3s^2 3p^6 3d^5 4s^2$	0.2	12.02863	116.79421	4.429
Fe	$3s^2 3p^6 3d^6 4s^2$	0.3	11.26645	223.90817	4.804
Co	$3s^2 3p^6 3d^7 4s^2$	0.25	10.84851	222.89490	5.329
Ni	$3s^2 3p^6 3d^8 4s^2$	0.25	10.98062	186.79687	4.849
Cu	$3s^2 3p^6 3d^{10} 4s^1$	0.15	11.99641	138.55508	5.107
Zn	$3s^2 3p^6 3d^{10} 4s^2$	0.15	15.20259	74.88503	5.363
Ga	$3d^{10} 4s^2 4p^1$	0.2	20.35082	51.94921	4.766
Ge	$3d^{10} 4s^2 4p^2$	0.15	23.98655	58.78066	4.837
As	$4s^2 4p^3$	0.3	22.69929	67.99218	4.164
Se	$4s^2 4p^4$	0.25	29.80470	46.74457	4.490
Br	$4s^2 4p^5$	0.3	39.66166	22.40336	4.844
Kr	$4s^2 4p^6$	0.35	65.54049	0.69114	9.749
Rb	$4s^2 4p^3 5s^1$	0.35	90.63407	2.82889	4.125
Sr	$4s^2 4p^3 5s^2$	0.3	54.59270	11.72212	3.503
Y	$4s^2 4p^3 4d^1 5s^2$	0.3	32.79323	40.83762	3.081
Zr	$4s^2 4p^3 4d^2 5s^2$	0.3	23.38387	94.85506	3.103
Nb	$4s^2 4p^3 4d^4 5s^1$	0.25	18.14151	169.50269	3.567
Mo	$4s^2 4p^3 4d^5 5s^1$	0.3	15.78981	259.05160	4.233
Tc	$4s^2 4p^3 4d^6 5s^1$	0.25	14.43282	297.24505	4.479
Ru	$4s^2 4p^3 4d^7 5s^1$	0.25	13.76807	311.24000	4.822
Rh	$4s^2 4p^3 4d^8 5s^1$	0.3	14.03624	259.47769	5.120
Pd	$4s^2 4p^3 4d^{10}$	0.2	15.31154	168.98122	5.540
Ag	$4s^2 4p^3 4d^{10} 5s^1$	0.2	17.85900	90.72193	5.838
Cd	$4s^2 4p^3 4d^{10} 5s^2$	0.15	22.97358	43.49941	6.499
In	$4d^{10} 5s^2 5p^1$	0.2	27.50568	35.29236	4.899

Sn	$4d^{10}5s^25p^2$	0.25	36.84614	35.83625	4.617
Sb	$4d^{10}5s^25p^3$	0.25	31.78261	50.29209	4.496
Te	$4d^{10}5s^25p^4$	0.25	35.07798	44.90330	4.641
I	$4d^{10}5s^25p^5$	0.25	50.45971	19.12220	4.081
Xe	$4d^{10}5s^25p^6$	0.25	89.77123	1.14650	−0.046
Cs	$5s^25p^66s^1$	0.3	116.91948	1.90554	3.097
Ba	$5s^25p^66s^2$	0.35	63.00362	8.84177	2.742
Lu	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Hf	$4f^{14}5s^25p^65d^26s^2$	0.25	22.61511	115.54352	2.959
Ta	$4f^{14}5s^25p^65d^36s^2$	0.2	18.30631	194.76300	4.007
W	$4f^{14}5s^25p^65d^46s^2$	0.15	16.17127	299.88374	4.105
Re	$5s^25p^65d^56s^2$	0.25	14.93809	363.01207	4.355
Os	$5s^25p^65d^66s^2$	0.15	14.25660	397.06100	4.774
Ir	$5s^25p^65d^76s^2$	0.25	14.46501	349.02794	5.052
Pt	$5s^25p^65d^96s^1$	0.2	15.60593	249.63320	5.470
Au	$5s^25p^65d^{10}6s^1$	0.3	17.95893	145.47578	6.046
Hg	$5s^25p^65d^{10}6s^2$	0.2	29.52762	7.90172	11.063
Tl	$5d^{10}6s^26p^1$	0.25	31.32545	27.30471	5.448
Pb	$5d^{10}6s^26p^2$	0.25	32.02484	39.05739	4.798
Bi	$5d^{10}6s^26p^3$	0.3	37.00529	44.60988	3.850
Po	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*