ONCVPSP(SG15)1/QE

SG15 ONCVPSP 2015-01-24 NCPP dataset / QUANTUM ESPRESSO 5.1

`name and version of the code:` QUANTUM ESPRESSO 5.1
`type of basis set:` plane waves
`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 (Z_{val})
`basis set size`	wave function cutoff = 100 Ry
`k-mesh density`	see table (k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts*, and number of irreducible k-points # *k*)
`reciprocal-space integration method`	Gaussian smearing with a fictitious temperature corresponding to 0.01 eV

METHOD-SPECIFIC INFORMATION

`wave function cutoff`	100 Ry
`density cutoff`	400 Ry

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`

[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).

Table I. Calculation settings and results per element: valence Z_{val}, k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts* and number of irreducible k-points # k, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	Z_{val} [–]	*kpts* [–]	# k [–]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	1	28×28×20	6 020	17.356	10.288	2.666
He	2	40×40×22	4 620	17.708	0.882	6.528
Li	3	38×38×38	27 436	20.244	13.846	3.345
Be	4	52×52×28	9 828	7.931	123.706	3.308
B	3	26×26×24	12 324	7.18	235.366	3.428
C	4	48×48×12	10 512	11.586	207.537	3.728
N	5	16×16×16	688	28.773	53.217	3.662
O	6	26×24×24	7 488	18.594	50.245	3.779
F	7	16×28×14	3 136	19.284	33.755	4.001
Ne	8	22×22×22	286	24.259	1.352	7.255
Na	9	32×32×32	16 384	37.113	7.762	3.697
Mg	10	36×36×20	9 900	22.961	36.548	4.05
Al	11	24×24×24	364	16.528	77.801	4.976
Si	4	32×32×32	8 448	20.522	87.495	4.268
P	5	30×8×22	1 320	21.473	67.79	4.31
S	6	38×38×38	27 436	17.241	85.344	4.124
Cl	7	12×24×12	864	39.386	18.701	4.375
Ar	8	16×16×16	120	52.321	0.757	7.526
K	9	20×20×20	220	73.655	3.604	3.982
Ca	10	18×18×18	165	42.173	17.627	3.356
Sc	11	34×34×20	8 840	24.642	54.566	3.371
Ti	12	40×40×22	4 620	17.407	112.06	3.548
V	13	34×34×34	969	13.468	182.297	3.947
Cr	14	36×36×36	2 280	12.441	115.19	7.007
Mn	15	28×28×28	5 488	11.899	127.159	4.815
Fe	16	36×36×36	2 280	11.454	179.159	7.087
Co	17	46×46×24	13 248	10.923	211.276	4.755
Ni	18	28×28×28	1 120	10.943	195.413	5.085
Cu	19	28×28×28	560	11.986	138.944	5.102
Zn	20	44×44×20	14 740	15.172	75.771	5.369
Ga	13	22×12×22	1 452	20.344	48.728	4.88
Ge	14	30×30×30	6 975	23.981	58.974	4.894
As	5	30×30×10	6 825	22.688	68.597	4.285
Se	6	26×26×20	3 510	30.014	47.021	4.462
Br	7	12×24×12	864	39.67	22.377	4.835
Kr	8	16×16×16	120	65.983	0.647	7.29
Rb	9	18×18×18	165	91.02	2.794	3.749
Sr	10	16×16×16	120	54.406	11.237	5.299
Y	11	32×32×18	2 448	32.858	41.387	3.167
Zr	12	36×36×20	9 900	23.398	94.027	3.282
Nb	13	30×30×30	680	18.148	170.015	3.637
Mo	14	32×32×32	816	15.781	260.241	4.318
Tc	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Ru	16	42×42×24	5 544	13.77	312.145	4.85
Rh	17	26×26×26	455	14.05	256.947	5.173
Pd	18	26×26×26	455	15.311	169.625	5.548
Ag	19	24×24×24	364	17.825	91.083	6.047
Cd	20	38×38×18	9 918	22.95	43.617	6.942

In	13	30×30×20	1 200	27.515	35.993	4.969
Sn	14	26×26×26	4 563	36.878	35.784	4.921
Sb	15	26×26×8	4 108	31.762	50.339	4.542
Te	16	26×26×16	8 216	35.036	44.723	4.629
I	17	12×22×10	660	50.373	18.602	5.156
Xe	18	14×14×14	84	86.788	0.543	7.248
Cs	9	16×16×16	120	116.906	1.965	3.598
Ba	10	20×20×20	220	63.228	8.716	2.004
Lu	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Hf	26	36×36×20	3 420	22.596	108.619	3.44
Ta	27	30×30×30	680	18.325	195.013	3.621
W	28	32×32×32	816	16.15	301.071	4.122
Re	15	42×42×22	5 082	14.94	365.239	4.432
Os	16	42×42×24	5 544	14.255	398.979	4.812
Ir	17	26×26×26	455	14.472	349.218	5.119
Pt	18	26×26×26	455	15.687	246.036	5.475
Au	19	24×24×24	364	17.982	138.715	6.007
Hg	20	24×24×28	1 092	29.55	7.772	9.92
Tl	13	32×32×18	7 056	31.361	26.88	5.448
Pb	14	20×20×20	220	31.943	40.077	5.575
Bi	15	26×26×8	4 108	36.917	42.82	4.69
Po	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*