GBRV12/QE

GBRV 1.2 USPP dataset / QUANTUM ESPRESSO 5.1

`name and version of the code:` QUANTUM ESPRESSO 5.1
`type of basis set:` plane waves
`method:` ultrasoft pseudopotentials (GBRV 1.2)

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 = 50 Ry
`k-mesh density`	$20 \times 20 \times 20$
`reciprocal-space integration method`	Marzari-Vanderbilt cold smearing with a fictitious temperature corresponding to 0.002 Ry (0.02 Ry when required to achieve convergence)

METHOD-SPECIFIC INFORMATION

`wave function cutoff`	50 Ry
`density cutoff`	250 Ry

ADDITIONAL COMMENTS

none

REFERENCES

`potentials`

[1] http://www.physics.rutgers.edu/gbrv/
[2] K. F. Garrity, J. W. Bennett, K. M. Rabe and D. Vanderbilt, *Comput. Mater. Sci.* **81** 446–452 (2014).

`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).

`smearing`

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

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

	Z_{val} [–]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	1	17.932	10.488	2.746
He	*N/A*	*N/A*	*N/A*	*N/A*
Li	3	20.245	13.809	3.362
Be	4	7.957	123.035	3.374
B	3	7.247	235.781	3.448
C	4	11.633	207.935	3.551
N	5	29.272	54.662	3.771
O	6	18.739	50.533	3.936
F	7	19.539	34.202	4.453
Ne	*N/A*	*N/A*	*N/A*	*N/A*
Na	9	37.083	7.697	3.895
Mg	10	22.955	36.079	4.160
Al	3	16.498	76.956	4.785
Si	4	20.434	88.589	4.309
P	5	21.724	67.174	4.335
S	6	17.200	82.677	3.692
Cl	7	38.824	18.943	4.489
Ar	*N/A*	*N/A*	*N/A*	*N/A*
K	9	73.711	3.604	3.118
Ca	10	42.226	17.369	3.032
Sc	11	24.607	54.521	3.398
Ti	12	17.405	111.975	3.467
V	13	13.443	182.712	4.061
Cr	14	11.869	174.060	6.711
Mn	15	11.687	121.937	−0.485
Fe	16	11.426	174.765	7.580
Co	17	10.852	216.635	4.919
Ni	18	10.892	198.555	4.861
Cu	19	11.982	140.397	5.031
Zn	20	15.219	74.684	5.409
Ga	19	20.383	48.640	5.421
Ge	14	23.894	59.013	5.110
As	5	22.712	68.635	4.294
Se	6	29.737	47.281	4.516
Br	7	39.602	22.356	4.896
Kr	*N/A*	*N/A*	*N/A*	*N/A*
Rb	9	91.018	2.796	3.784
Sr	10	54.524	11.388	4.584
Y	11	32.856	41.199	3.007
Zr	12	23.381	94.498	3.430
Nb	13	18.115	169.439	3.256
Mo	14	15.775	261.446	4.246
Tc	15	14.425	300.141	4.533
Ru	16	13.744	312.974	4.875
Rh	15	14.072	258.886	5.184
Pd	16	15.322	171.293	5.590
Ag	19	17.877	90.607	5.627
Cd	12	22.942	43.690	6.955
In	13	27.632	35.670	4.911

Sn	14	36.849	35.709	4.957
Sb	15	31.780	50.204	4.715
Te	6	34.931	45.243	4.735
I	7	50.215	18.707	5.020
Xe	*N/A*	*N/A*	*N/A*	*N/A*
Cs	9	116.846	1.965	3.423
Ba	10	63.346	8.714	3.178
Lu	*N/A*	*N/A*	*N/A*	*N/A*
Hf	12	22.594	107.763	3.455
Ta	13	18.275	195.901	3.723
W	14	16.142	305.193	4.334
Re	15	14.951	364.312	4.428
Os	16	14.263	398.882	4.820
Ir	15	14.499	347.354	5.121
Pt	16	15.598	250.473	5.440
Au	11	17.922	140.426	6.049
Hg	12	29.922	7.435	2.338
Tl	13	31.383	26.719	5.708
Pb	14	31.965	39.033	3.774
Bi	15	36.828	42.720	4.636
Po	*N/A*	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*	*N/A*