OTFG-QC5/CASTEP

CASTEP QC5(19.1) USPP dataset / CASTEP 19.1.1

`name and version of the code:` CASTEP 19.1.1
`type of basis set:` plane waves
`method:` Ultrasoft pseudopotentials for "high-throughput" applications ("On-The-Fly" version QC5(19.1))

GENERAL INFORMATION

exchange-correlation functional	PBE
relativistic scheme	scalar relativistic (Koelling-Harmon)
assignment of core / valence states	see table
basis set size	cutoff energy = 500 eV (non-magnetic)/ 700 eV (magnetic)
k-mesh density	see table (grid values and number of k-points in the irreducible wedge of the 1st Brillouin zone (# k)); this choice achieves spacing $\Delta k < 0.0754\,\text{Å}^{-1}$.
reciprocal-space integration method	Gaussian smearing with a fictitious temperature corresponding to 0.2 eV

METHOD-SPECIFIC INFORMATION

pseudopotential library	CASTEP "on-the-fly" method. Settings for "QC5" library release (Mercurial changeset 74f52b43a4d7)
pseudopotential core radii	see table (r_c)
local channel	see table (l_{loc})
non-local core radii	$2.0\,a_0$ for Mn, Fe,Co, Ni, Cu; r_c otherwise
number of projectors	2 per valence l channel, plus 1 per semi-core state.
projector generation	KE-Optimized RRKJ with $q_c = 5.0$.
augmentation function pseudization radius	$1.0\,a_0$ (V-Zn); $0.7\,r_c$ otherwise
pseudization radius for NLCC core charge	same as for augmentation functions
size of FFT grid for augmentation	2 × FFT grid for soft density ($E_{c,\rho} = 4\,E_{c,\phi}$) for magnetic elements, 1.5 × soft FFT grid ($E_{c,\rho} = 2.25\,E_{c,\phi}$) otherwise

ADDITIONAL COMMENTS

This pseudopotential set is optimized using RRKJ KE tuning with $q_c = 5$ to give a reasonable level of convergence across the periodic table at constant cutoff of 340 eV for "high-throughput" applications. Full convergence is achieved at 500 eV cutoff, which was used for the non-magnetic tests here. Magnetic cases required a higher cutoff of 700 eV for full convergence. "Fine" FFT grid and k-point density were chosen uniformly across the periodic table to achieve high convergence.

REFERENCES

pseudopotential method

[1] D. Vanderbilt, *Phys. Rev. B* **41**(11), 7892–7895 (1990).

code

[2] S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. J. Probert, K. Refson and M. C. Payne, *Z. Kristall.*, **220**, 567–570 (2005).

scalar relativity

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

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Table I. Calculation settings and results per element: valence, pseudopotential core radius r_c, local channel l_{loc}, projector wave vector cutoff q_c, Monkhorst-Pack 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.

	Valence	r_c	l_{loc}	q_c	*kpts*	$\#k$	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	$1s^1$	0.90	1	5	25×25×17	585	17.951	10.137	2.848
He	$1s^2$	1.20	1	5	33×33×18	972	17.327	1.250	19.148
Li	$1s^2 2s^1$	1.30	1	5	32×32×4	1 056	20.203	13.761	3.917
Be	$1s^2 2s^2$	1.30	2	5	43×43×24	2 112	7.937	124.877	2.839
B	$2s^2 2p^1$	1.41	2	5	21×21×20	2 310	7.213	237.256	3.464
C	$2s^2 2p^2$	1.40	2	5	39×39×10	735	11.645	209.095	3.597
N	$2s^2 2p^3$	1.40	2	5	14×14×14	119	31.066	54.969	3.789
O	$2s^2 2p^4$	1.50	2	5	22×20×20	2 200	20.351	54.389	4.253
F	$2s^2 2p^5$	1.60	2	5	14×23×13	1 092	19.874	36.011	4.438
Ne	$2s^2 2p^6$	1.70	2	5	19×19×19	220	23.689	1.448	7.515
Na	$2s^2 2p^6 3s^1$	1.80	2	5	26×26×4	702	37.259	7.707	3.626
Mg	$2s^2 2p^6 3s^2$	1.80	3	5	31×31×17	864	22.904	35.932	4.308
Al	$3s^2 3p^1$	2.00	0	5	21×21×21	286	16.549	76.983	4.330
Si	$3s^2 3p^2$	1.80	3	5	27×27×27	560	20.441	88.566	4.309
P	$3s^2 3p^3$	1.81	3	5	26×8×19	520	21.428	68.142	4.327
S	$3s^2 3p^4$	1.80	3	5	33×33×33	3 281	17.177	86.260	3.878
Cl	$3s^2 3p^5$	1.81	3	5	11×20×10	300	38.739	19.083	4.386
Ar	$3s^2 3p^6$	1.60	2	5	15×15×15	120	51.600	0.795	6.642
K	$3s^2 3p^6 4s^1$	1.70	2	5	16×16×16	120	73.815	3.547	3.633
Ca	$3s^2 3p^6 4s^2$	2.00	3	5	16×16×16	120	42.186	17.410	3.328
Sc	$3s^2 3p^6 3d^1 4s^2$	1.89	3	5	29×29×17	765	24.698	53.948	3.361
Ti	$3s^2 3p^6 3d^2 4s^2$	1.90	3	5	33×33×18	972	17.415	111.335	3.598
V	$3s^2 3p^6 3d^3 4s^2$	1.99	3	5	28×28×28	560	13.457	181.508	3.839
Cr	$3s^2 3p^6 3d^5 4s^1$	2.01	3	5	30×30×30	680	12.079	137.978	6.832
Mn	$3p^6 3d^5 4s^2$	2.20	4	5	24×24×24	936	11.887	120.834	2.083
Fe	$3d^6 4s^2$	2.21	3	5	30×30×30	680	11.343	193.485	5.127
Co	$3d^7 4s^2$	2.20	3	5	39×39×21	1 617	10.861	214.321	4.828
Ni	$3d^8 4s^2$	2.19	3	5	24×24×24	364	10.910	199.479	4.901
Cu	$3d^{10} 4s^1$	2.21	3	5	23×23×23	364	11.946	137.823	5.073
Zn	$3d^{10} 4s^2$	2.00	3	5	37×37×17	1 197	15.214	74.376	5.562
Ga	$3d^{10} 4s^2 4p^1$	2.10	3	5	19×11×19	600	20.511	47.870	5.393
Ge	$3d^{10} 4s^2 4p^2$	2.10	3	5	26×26×26	1 638	24.058	58.256	4.837
As	$3d^{10} 4s^2 4p^3$	2.11	3	5	26×26×8	1 404	22.733	68.008	4.211
Se	$3d^{10} 4s^2 4p^4$	2.10	3	5	22×22×17	2 156	29.958	46.832	4.437
Br	$4s^2 4p^5$	1.91	2	5	11×20×10	300	39.457	22.440	4.845
Kr	$4s^2 4p^6$	1.90	2	5	13×13×13	84	65.376	0.680	7.236
Rb	$4s^2 4p^6 5s^1$	2.09	2	5	15×15×15	120	91.213	2.760	3.779
Sr	$4s^2 4p^6 5s^2$	2.00	3	5	14×14×14	84	55.009	11.757	3.214
Y	$4s^2 4p^6 4d^1 5s^2$	2.00	3	5	27×27×15	600	32.905	40.491	3.072
Zr	$4s^2 4p^6 4d^2 5s^2$	2.10	3	5	30×30×17	2 160	23.373	93.985	2.917
Nb	$4s^2 4p^6 4d^4 5s^1$	1.91	3	5	26×26×26	455	18.121	169.506	3.738
Mo	$4s^2 4p^6 4d^5 5s^1$	2.00	3	5	27×27×27	560	15.759	259.405	4.226
Tc	$4s^2 4p^6 4d^6 5s^1$	2.09	3	5	35×35×19	1 200	14.401	299.150	4.522
Ru	$4s^2 4p^6 4d^7 5s^1$	2.10	3	5	36×36×20	3 420	13.721	312.693	4.857
Rh	$4s^2 4p^6 4d^8 5s^1$	2.10	3	5	22×22×22	286	14.000	257.209	5.182
Pd	$4s^2 4p^6 4d^{10} 5s^0$	2.20	3	5	22×22×22	286	15.271	168.527	5.552

Ag	$4s^2 4p^6 4d^{10} 5s^1$	2.21	3	5	21×21×21	286	17.816	91.069	5.819
Cd	$4s^2 4p^6 4d^{10} 5s^2$	2.20	3	5	32×32×15	2 176	22.933	42.998	6.483
In	$4d^{10} 5s^2 5p^1$	2.30	1	5	26×26×17	819	27.744	34.952	5.117
Sn	$4d^{10} 5s^2 5p^2$	2.20	1	5	22×22×22	1 012	37.109	35.515	4.908
Sb	$4d^{10} 5s^2 5p^3$	2.19	1	5	22×22×8	1 012	32.041	50.332	4.380
Te	$5s^2 5p^4$	2.20	2	5	22×22×14	1 771	34.973	45.129	4.741
I	$5s^2 5p^5$	2.01	2	5	10×19×9	250	50.419	18.645	5.093
Xe	$5s^2 5p^6$	2.19	2	5	12×12×12	56	86.409	0.561	7.115
Cs	$5s^2 5p^6 6s^1$	2.19	2	5	14×14×14	84	116.783	1.946	3.505
Ba	$5s^2 5p^6 6s^2$	2.00	2	5	17×17×17	165	63.212	8.778	2.939
Lu	$4f^{14} 5s^2 5p^6 5d^1 6s^2$	2.29	2	5	28×28×16	1 680	29.063	46.340	3.443
Hf	$4f^{14} 5s^2 5p^6 5d^2 6s^2$	2.30	3	5	31×31×17	864	22.522	108.003	3.473
Ta	$4f^{14} 5s^2 5p^6 5d^3 6s^2$	2.30	3	5	26×26×26	455	18.288	194.989	3.796
W	$4f^{14} 5s^2 5p^6 5d^4 6s^2$	2.29	3	5	27×27×27	560	16.146	304.922	4.229
Re	$4f^{14} 5s^2 5p^6 5d^5 6s^2$	2.30	3	5	35×35×19	1 200	14.973	366.676	4.478
Os	$4f^{14} 5s^2 5p^6 5d^6 6s^2$	2.31	3	5	35×35×20	1 200	14.301	400.786	4.862
Ir	$4f^{14} 5s^2 5p^6 5d^7 6s^2$	2.30	3	5	22×22×22	286	14.518	350.222	5.145
Pt	$4f^{14} 5s^2 5p^6 5d^9 6s^1$	2.31	3	5	21×21×21	286	15.656	249.070	5.478
Au	$4f^{14} 5s^2 5p^6 5d^{10} 6s^1$	2.29	3	5	20×20×20	220	17.943	141.072	5.989
Hg	$5s^2 5p^6 5d^{10} 6s^2$	2.19	3	5	21×21×24	792	29.052	8.727	8.498
Tl	$5s^2 5p^6 5d^{10} 6s^2 6p^1$	2.20	3	5	27×27×15	600	31.361	26.557	5.209
Pb	$5s^2 5p^6 5d^{10} 6s^2 6p^2$	2.19	3	5	17×17×17	165	31.920	39.624	4.786
Bi	$5d^{10} 6s^2 6p^3$	2.30	1	5	21×21×7	303	37.187	42.492	4.923
Po	$5d^{10} 6s^2 6p^4$	2.31	1	5	25×25×25	455	37.945	45.949	4.165
Rn	$5d^{10} 6s^2 6p^6$	2.29	0	5	12×12×12	56	92.108	0.585	7.520