OTFG7/CASTEP

CASTEP C7 USPP dataset / CASTEP 8.0

`name and version of the code:` CASTEP 8.0
`type of basis set:` plane waves
`method:` ultrasoft pseudopotentials ("On-The-Fly" Vanderbilt-type version C7)

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`	cutoff energy = 700 eV
`k-mesh density`	see table for grid values and number of k-points in the irreducible wedge of the 1st Brillouin zone (# k); this choice achieves spacing $\Delta k < 0.0125\,\text{Å}^{-1}$
`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. Default in 7.0, available as "C7" library in later releases
`pseudopotential core radii`	see table (r_c)
`local channel`	see table (l_{loc})
`non-local core radii`	$2.0\,a_0$ for Mg, Ca, Ni; $2.61\,a_0$ for Li; $1.6\,a_0$ for N; $1.3\,a_0$ for O; $2.15\,a_0$ for Cu;$2.3\,a_0$ for Ag; r_c otherwise
`number of projectors`	mostly 2 per valence l channel, plus 1 per semi-core state
`projector generation`	KE-Optimized RRKJ - see table for q_c
`augmentation function pseudization radius`	between $0.5\,r_c$ and r_c dependent on element
`pseudization radius for NLCC core charge`	same as for augmentation functions
`size of FFT grid for augmentation`	1.5 × FFT grid for soft density ($E_{c,\rho} = 9\,E_{c,\phi}$)

ADDITIONAL COMMENTS

none

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).

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	$1s^1$	0.80	1	6.0	15×15×10	135	17.504	10.375	2.752
He	$1s^2$	0.80	1	7.0	20×20×11	660	17.445	0.938	6.977
Li	$1s^2 2s^1$	1.90	1	4.5	19×19×19	670	20.367	13.618	3.329
Be	$1s^2 2s^2 2p^{0.05}$	1.40	2	-	26×26×14	1 274	8.030	125.648	2.586
B	$2s^2 2p^1$	1.41	2	-	13×13×12	546	7.213	237.164	3.461
C	$2s^2 2p^2$	1.40	2	6.0	24×24×6	468	11.603	208.967	3.557
N	$2s^2 2p^3$	1.40	2	-	9×9×9	45	32.998	51.696	3.507
O	$2s^2 2p^4$	1.00	2	7.0	13×12×12	468	*N/A*	*N/A*	*N/A*
F	$2s^2 2p^5$	1.40	2	6.5	9×14×8	252	19.290	34.267	4.079
Ne	$2s^2 2p^6$	1.60	2	6.0	11×11×11	56	23.844	1.387	7.155
Na	$2s^2 2p^6 3s^1$	1.30	2	7.0	16×16×16	408	37.217	7.684	3.709
Mg	$2p^6 3s^2$	1.60	2	4.5	19×19×10	200	22.906	35.835	2.117
Al	$3s^2 3p^1$	2.00	2	3.0	13×13×13	84	16.382	78.155	4.630
Si	$3s^2 3p^2$	1.80	2	4.0	16×16×16	408	20.364	88.843	4.292
P	$3s^2 3p^3$	1.81	2	-	16×5×11	144	21.218	68.994	4.412
S	$3s^2 3p^4$	1.69	2	-	20×20×20	770	17.041	83.594	4.038
Cl	$3s^2 3p^5$	1.71	2	-	7×12×6	72	37.955	19.424	4.417
Ar	$3s^2 3p^6$	1.71	2	-	9×9×9	35	51.694	0.788	6.892
K	$3s^2 3p^6 4s^1$	2.50	2	3.0	10×10×10	35	73.385	3.570	3.743
Ca	$3s^2 3p^6 4s^2$	1.60	3	-	10×10×10	35	42.225	17.403	2.912
Sc	$3s^2 3p^6 3d^1 4s^2$	1.80	3	6.5	18×18×10	450	24.683	53.963	3.352
Ti	$3s^2 3p^6 3d^2 4s^2$	1.79	3	6.0	20×20×11	660	17.402	111.554	3.588
V	$3s^2 3p^6 3d^3 4s^2$	1.99	3	6.0	17×17×17	165	13.457	181.455	3.765
Cr	$3s^2 3p^6 3d^5 4s^1$	1.80	3	6.0	18×18×18	165	*N/A*	*N/A*	*N/A*
Mn	$3d^5 4s^{0.75} 4p^{0.25}$	2.30	3	4.5	14×14×14	84	*N/A*	*N/A*	*N/A*
Fe	$3d^6 4s^{1.75}$	2.00	1	-	18×18×18	165	11.768	184.590	3.002
Co	$3d^7 4s^{1.95} 4p^{0.05}$	2.49	3	4.0	24×24×13	1 092	11.118	203.370	4.023
Ni	$3d^8 4s^2$	2.19	3	-	15×15×15	120	10.946	197.586	4.838
Cu	$3d^{10} 4s^{0.5} 4p^{0.001}$	2.21	3	-	14×14×14	84	11.965	136.322	4.572
Zn	$3d^{10} 4s^2$	2.00	3	6.0	22×22×10	660	15.160	79.874	8.400
Ga	$3d^{10} 4s^2 4p^1$	2.00	3	6.0	11×7×11	144	20.359	49.424	3.079
Ge	$3d^{10} 4s^2 4p^2$	2.00	3	6.0	16×16×16	408	23.906	58.661	4.897
As	$4s^2 4p^3$	1.60	2	-	16×16×5	344	22.348	69.674	4.247
Se	$4s^2 4p^4$	1.61	2	-	13×13×10	175	29.581	47.635	4.617
Br	$4s^2 4p^5$	2.00	2	4.0	7×12×6	72	39.478	22.448	4.857
Kr	$4s^2 4p^6$	1.90	2	-	8×8×8	20	65.637	0.270	−21.298
Rb	$4s^2 4p^6 5s^2$	2.60	2	3.0	9×9×9	35	91.018	2.769	3.777
Sr	$4s^2 4p^6 5s^2$	2.00	3	-	9×9×9	35	55.013	11.787	3.191
Y	$4s^2 4p^6 4d^1 5s^2$	2.00	3	-	16×16×9	360	32.897	40.532	3.058
Zr	$4s^2 4p^6 4d^2 5s^2$	2.10	3	-	18×18×10	450	23.367	93.694	3.325
Nb	$4s^2 4p^6 4d^4 5s^1$	2.19	3	-	16×16×16	120	18.090	169.545	3.951
Mo	$4s^2 4p^6 4d^5 5s^1$	2.00	3	-	16×16×16	120	15.740	261.878	4.530
Tc	$4s^2 4p^6 4d^6 5s^1$	2.01	3	-	21×21×12	288	14.408	299.347	4.530
Ru	$4s^2 4p^6 4d^7 5s^1$	2.00	3	6.0	22×22×12	792	13.739	313.077	4.849
Rh	$4s^2 4p^6 4d^8 5s^1$	2.00	3	6.0	14×14×14	84	14.017	256.924	5.200
Pd	$4s^2 4p^6 4d^{10} 5s^{0.05}$	2.01	3	5.5	13×13×13	84	15.266	169.574	5.547

Ag	$4d^{10}5s^1$	2.21	1	5.0	13×13×13	84	17.922	94.580	5.891
Cd	$4d^{10}5s^2$	2.20	1	5.0	20×20×9	550	22.674	48.311	7.818
In	$4d^{10}5s^25p^1$	2.30	3	-	16×16×10	180	27.505	35.257	5.195
Sn	$4d^{10}5s^25p^2$	2.29	3	-	14×14×14	280	36.804	35.655	4.293
Sb	$5s^25p^3$	2.00	2	-	14×14×5	266	31.417	51.086	6.778
Te	$5s^25p^4$	2.20	2	-	13×13×9	161	34.972	45.035	4.788
I	$5s^25p^5$	2.01	2	-	6×11×5	54	50.410	18.667	5.083
Xe	$5s^25p^6$	2.00	2	-	8×8×8	20	86.383	0.533	4.293
Cs	$5s^25p^66s^1$	2.8	2	3.0	8×8×8	20	117.019	2.107	−0.824
Ba	$5s^25p^66s^2$	2.00	2	5.5	10×10×10	35	63.175	8.790	3.456
Lu	$5s^25p^65d^16s^2$	2.11	3	-	17×17×10	165	29.449	46.845	3.396
Hf	$5s^25p^65d^26s^2$	2.10	3	-	19×19×10	200	22.523	108.258	3.448
Ta	$5s^25p^65d^36s^2$	2.10	3	-	16×16×16	120	18.244	194.873	3.864
W	$5s^25p^65d^46s^2$	2.11	3	-	16×16×16	120	16.082	306.876	4.555
Re	$5s^25p^65d^56s^2$	2.10	3	-	21×21×12	288	14.904	367.009	4.413
Os	$5s^25p^65d^66s^2$	2.00	3	5.0	21×21×12	288	14.232	399.733	5.295
Ir	$5s^25p^65d^76s^2$	1.99	3	5.5	13×13×13	84	14.454	351.611	4.959
Pt	$5s^25p^65d^96s^1$	2.00	3	5.5	13×13×13	84	15.602	248.953	5.466
Au	$5s^25p^65d^{10}6s^1$	2.01	3	5.5	12×12×12	56	17.911	140.087	5.208
Hg	$5d^{10}6s^2$	2.19	1	-	13×13×15	224	28.143	6.768	−4.068
Tl	$6s^26p^1$	3.10	3	-	16×16×9	360	31.561	26.088	4.657
Pb	$6s^26p^2$	2.20	3	-	10×10×10	35	*N/A*	*N/A*	*N/A*
Bi	$6s^26p^3$	2.10	2	4.0	13×13×5	91	36.512	43.699	4.715
Po	$6s^26p^4$	2.00	2	-	15×15×15	120	37.513	47.606	−1.063
Rn	$6s^26p^6$	2.00	2	-	7×7×7	20	92.388	0.563	6.869