OTFG-MS/CASTEP

CASTEP MS 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 Materials Studio)

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. "Materials Studio" OTFG set, available as "MS" library in 8.0 and 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; $2.15\,a_0$ for Cu; $2.3\,a_0$ for Ag; $2.5\,a_0$ for Ba; $2.4\,a_0$ for Pt; $2.34\,a_0$ for Pb; 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	MP grid	$\#\ k$	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	$1s^1$	0.80	1	6.4	15×15×10	135	17.466	10.325	2.755
He	$1s^2$	0.80	1	7	20×20×11	660	17.389	0.973	7.833
Li	$1s^2 2s^1$	1.20	1	5.5	19×19×19	670	20.205	13.777	3.872
Be	$1s^2 2s^2$	1.40	1	–	26×26×14	1 274	7.783	113.861	0.135
B	$2s^2 2p^1$	1.41	2	5.5	13×13×12	546	7.212	237.134	3.460
C	$2s^2 2p^2$	1.40	2	6	24×24×6	468	11.639	209.296	3.568
N	$2s^2 2p^3$	1.50	2	6	9×9×9	45	30.263	53.506	3.710
O	$2s^2 2p^4$	1.30	2	7.5	13×12×12	468	*N/A*	*N/A*	*N/A*
F	$2s^2 2p^5$	1.40	2	7.5	9×14×8	252	19.236	34.191	4.040
Ne	$2s^2 2p^6$	1.60	2	6	11×11×11	56	23.844	1.380	6.939
Na	$2s^2 2p^6 3s^1$	1.30	2	–	16×16×16	408	37.273	7.664	3.781
Mg	$2p^6 3s^2$	1.60	2	4.5	19×19×10	200	22.905	35.645	2.230
Al	$3s^2 3p^1$	2.00	2	–	13×13×13	84	16.383	78.452	4.654
Si	$3s^2 3p^2$	1.80	2	–	16×16×16	408	20.367	88.913	4.321
P	$3s^2 3p^3$	1.81	2	–	16×5×11	144	21.199	68.951	4.405
S	$3s^2 3p^4$	1.69	2	–	20×20×20	770	17.040	83.598	4.119
Cl	$3s^2 3p^5$	1.71	2	–	7×12×6	72	37.958	19.411	4.376
Ar	$3s^2 3p^6$	1.71	2	–	9×9×9	35	51.694	0.788	6.892
K	$3s^2 3p^6 4s^1$	1.80	2	5.5	10×10×10	35	73.746	3.563	3.779
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	–	18×18×10	450	24.692	53.951	3.356
Ti	$3s^2 3p^6 3d^2 4s^2$	1.79	3	–	20×20×11	660	17.411	111.535	3.576
V	$3s^2 3p^6 3d^3 4s^2$	1.99	3	–	17×17×17	165	13.082	192.587	3.860
Cr	$3s^2 3p^6 3d^5 4s^1$	1.80	3	–	18×18×18	165	*N/A*	*N/A*	*N/A*
Mn	$3d^5 4s^{0.75} 4p^{0.25}$	2.30	3	4.	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	–	24×24×13	1 092	11.118	203.370	4.023
Ni	$3d^8 4s^2$	2.00	1	–	15×15×15	120	11.110	196.344	4.916
Cu	$3d^{10} 4s^{0.5} 4p^{0.001}$	2.21	3	–	14×14×14	84	11.966	136.475	4.557
Zn	$3d^{10} 4s^2$	2.00	3	6	22×22×10	660	15.161	79.714	8.419
Ga	$3d^{10} 4s^2 4p^1$	2.00	3	–	11×7×11	144	20.425	49.450	3.177
Ge	$4s^2 4p^2$	2.30	2	–	16×16×16	408	23.812	59.806	5.099
As	$4s^2 4p^3$	1.60	2	–	16×16×5	344	22.349	69.724	4.250
Se	$4s^2 4p^4$	1.61	2	–	13×13×10	175	29.581	47.354	4.454
Br	$4s^2 4p^5$	2.00	2	–	7×12×6	72	39.468	22.441	4.903
Kr	$4s^2 4p^6$	1.90	2	–	8×8×8	20	65.283	0.792	18.828
Rb	$4s^2 4p^6 5s^1$	2.49	2	3.75	9×9×9	35	91.095	2.768	3.773
Sr	$4s^2 4p^6 5s^2$	2.00	3	–	9×9×9	35	55.012	11.777	3.226
Y	$4s^2 4p^6 4d^1 5s^2$	2.00	3	–	16×16×9	360	32.896	40.513	3.062
Zr	$4s^2 4p^6 4d^2 5s^2$	2.10	3	–	18×18×10	450	23.369	93.604	3.239
Nb	$4s^2 4p^6 4d^4 5s^1$	2.19	3	–	16×16×16	120	18.090	169.497	3.953
Mo	$4s^2 4p^6 4d^5 5s^1$	2.00	3	–	16×16×16	120	15.740	261.695	4.487
Tc	$4s^2 4p^6 4d^6 5s^1$	2.01	3	–	21×21×12	288	14.408	299.426	4.537
Ru	$4s^2 4p^6 4d^7 5s^1$	2.00	3	–	22×22×12	792	13.709	314.924	4.878
Rh	$4d^8 5s^1$	2.19	1	–	14×14×14	84	14.280	267.672	5.434
Pd	$4s^2 4p^6 4d^{10} 5s^{0.05}$	2.01	3	5.5	13×13×13	84	15.266	169.583	5.565

Ag	$4d^{10}5s^{1}$	2.21	1	–	13×13×13	84	17.916	94.677	5.892
Cd	$4d^{10}5s^{2}$	2.20	1	5	20×20×9	550	22.675	48.099	7.659
In	$4d^{10}5s^{2}5p^{1}$	2.30	3	–	16×16×10	180	27.505	35.257	5.195
Sn	$5s^{2}5p^{2}$	2.01	2	–	14×14×14	280	36.402	36.706	4.635
Sb	$5s^{2}5p^{3}$	2.00	2	–	14×14×5	266	31.414	51.132	6.986
Te	$5s^{2}5p^{4}$	2.20	2	–	13×13×9	161	34.968	44.958	4.995
I	$5s^{2}5p^{5}$	2.01	2	–	6×11×5	54	50.412	18.688	5.029
Xe	$5s^{2}5p^{6}$	2.00	2	–	8×8×8	20	86.230	0.574	9.665
Cs	$5s^{2}5p^{6}6s^{1}$	2.70	2	3.5	9×9×9	35	116.997	2.056	0.326
Ba	$5s^{2}5p^{6}6s^{2}$	3.00	2	3.5	10×10×10	35	63.926	8.724	3.574
Lu	$5s^{2}5p^{6}5d^{1}6s^{2}$	2.11	2	–	17×17×10	165	29.249	46.375	3.278
Hf	$5d^{2}6s^{2}$	2.40	1	–	19×19×10	200	21.544	127.054	3.747
Ta	$5d^{3}6s^{2}$	2.40	1	–	16×16×16	120	17.903	223.750	4.301
W	$5s^{2}5p^{6}5d^{4}6s^{2}$	2.11	3	–	16×16×16	120	16.082	306.883	4.554
Re	$5s^{2}5p^{6}5d^{5}6s^{2}$	2.10	3	–	21×21×12	288	14.902	367.224	4.409
Os	$5s^{2}5p^{6}5d^{6}6s^{2}$	2.00	3	–	21×21×12	288	14.229	399.974	5.296
Ir	$5s^{2}5p^{6}5d^{7}6s^{2}$	1.99	3	5.5	13×13×13	84	14.454	351.739	4.960
Pt	$5d^{9}6s^{1}$	2.31	1	–	13×13×13	84	16.055	250.611	5.699
Au	$5s^{2}5p^{6}5d^{10}6s^{1}$	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	$5d^{10}6s^{2}6p^{1}$	2.39	3	4.5	17×17×9	165	31.418	26.012	4.629
Pb	$5d^{10}6s^{2}6p^{2}$	2.40	3	–	10×10×10	35	31.883	34.443	4.194
Bi	$6s^{2}6p^{3}$	2.10	2	–	13×13×5	91	36.513	43.160	4.382
Po	$6s^{2}6p^{4}$	2.00	2	–	15×15×15	120	37.513	47.606	−1.063
Rn	$6s^{2}6p^{6}$	2.00	2	–	7×7×7	20	92.385	0.563	6.867