OTFG9/CASTEP

CASTEP C9 USPP dataset / CASTEP 9.0

`name and version of the code:` CASTEP 9.0
`type of basis set:` plane waves
`method:` ultrasoft pseudopotentials ("On-The-Fly" Vanderbilt-type version C9)

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 = 816 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 $\Delta k < 0.0754\,\text{Å}^{-1}$.
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. Proposed settings for "C9" library release (Mercurial changeset 6666)
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 - see table for q_c
augmentation function pseudization radius	$1.0\,a_0$ (V, Fe, Co, Ni, Cu, Zn); $0.7\,a_0$ (Cr, Mn); $0.7\,r_c$ otherwise
pseudization radius for NLCC core charge	same as for augmentation functions
size of FFT grid for augmentation	$2 \times$ FFT grid for soft density ($E_{c,\rho} = 16\,E_{c,\phi}$)

ADDITIONAL COMMENTS

Basis set, "fine" FFT grid, k-point density and plane-wave cutoff were chosen uniformly across the periodic table to achieve high convergence. Less stringent critera, determined individually per element will still give high convergence in almost all cases at a substantially reduced computational cost.

The C9 set of potentials is identical to C8 for the elements in the Delta test suite, except for Cr and Mn, for which the augmentation pseudization radius r_{inner} was reduced from $1.0\,a_0$ to $0.7\,a_0$.

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	$1s^1$	0.60	1	8	24×24×17	1 404	17.410	10.295	2.710
He	$1s^2$	1.00	1	7	33×33×18	972	17.601	0.917	6.736
Li	$1s^2 2s^1$	1.00	1	7	31×31×4	352	20.247	13.771	3.338
Be	$1s^2 2s^2$	1.00	2	7	42×42×23	5 544	7.919	123.382	3.295
B	$2s^2 2p^1$	1.20	2	8	21×21×20	2 310	7.225	237.104	3.450
C	$2s^2 2p^2$	1.40	2	7	39×39×10	735	11.629	208.972	3.569
N	$2s^2 2p^3$	1.10	2	7	14×14×14	119	28.941	54.101	3.726
O	$2s^2 2p^4$	1.10	2	7	21×20×20	2 100	18.664	51.111	3.869
F	$2s^2 2p^5$	1.20	2	7	14×23×12	1 008	19.235	34.233	4.072
Ne	$2s^2 2p^6$	1.40	2	6	18×18×18	165	23.825	1.456	7.597
Na	$2s^2 2p^6 3s^1$	1.30	2	7	26×26×3	533	37.203	7.708	3.690
Mg	$2s^2 2p^6 3s^2$	1.80	3	–	30×30×16	1 920	22.899	35.985	4.205
Al	$3s^2 3p^1$	2.00	3	–	21×21×21	286	16.483	76.821	4.587
Si	$3s^2 3p^2$	1.80	3	–	26×26×26	1 638	20.441	88.577	4.294
P	$3s^2 3p^3$	1.81	3	–	25×8×18	468	21.428	68.124	4.330
S	$3s^2 3p^4$	1.80	3	–	32×32×32	2 992	17.176	86.259	3.878
Cl	$3s^2 3p^5$	1.81	3	–	11×19×10	300	38.712	19.125	4.384
Ar	$3s^2 3p^6$	1.60	2	–	14×14×14	84	51.690	0.794	7.168
K	$3s^2 3p^6 4s^1$	1.50	2	6	16×16×16	120	73.863	3.548	3.609
Ca	$3s^2 3p^6 4s^2$	2.00	3	–	15×15×15	120	42.189	17.407	3.313
Sc	$3s^2 3p^6 3d^1 4s^2$	1.80	3	6.5	29×29×16	680	24.690	53.949	3.371
Ti	$3s^2 3p^6 3d^2 4s^2$	1.79	3	5.5	33×33×18	972	17.391	111.646	3.586
V	$3s^2 3p^6 3d^3 4s^2$	1.99	3	6	28×28×28	560	13.452	182.010	3.827
Cr	$3s^2 3p^6 3d^5 4s^1$	2.01	3	6	29×29×29	680	11.750	177.430	6.648
Mn	$3d^5 4s^2$	2.20	3	5.5	23×23×23	936	11.534	117.995	1.821
Fe	$3d^6 4s^2$	2.21	3	5.5	29×29×29	680	11.334	193.935	5.145
Co	$3d^7 4s^2$	2.20	3	5.5	38×38×21	4 180	10.853	214.714	4.823
Ni	$3d^8 4s^2$	2.19	3	6	24×24×24	364	10.898	199.722	4.896
Cu	$3d^{10} 4s^1$	2.21	3	6	23×23×23	364	11.938	138.398	5.060
Zn	$3d^{10} 4s^2$	2.00	3	6	36×36×17	3 078	15.169	74.744	5.447
Ga	$3d^{10} 4s^2 4p^1$	2.00	3	6	18×11×18	486	20.312	48.901	5.393
Ge	$3d^{10} 4s^2 4p^2$	2.00	3	6	25×25×25	455	23.903	58.828	4.840
As	$3d^{10} 4s^2 4p^3$	2.00	3	6	25×25×8	468	22.611	68.143	4.343
Se	$3d^{10} 4s^2 4p^4$	1.99	3	6	21×21×17	728	29.800	47.063	4.454
Br	$4s^2 4p^5$	2.00	2	6	10×20×10	250	39.468	22.447	4.848
Kr	$4s^2 4p^6$	1.90	2	–	13×13×13	84	65.527	0.740	5.506
Rb	$4s^2 4p^6 5s^1$	2.09	2	–	15×15×15	120	91.200	2.750	4.513
Sr	$4s^2 4p^6 5s^2$	2.00	3	–	14×14×14	84	55.011	11.754	3.264
Y	$4s^2 4p^6 4d^1 5s^2$	2.00	3	–	26×26×15	1 456	32.899	40.648	3.305
Zr	$4s^2 4p^6 4d^2 5s^2$	2.10	3	–	30×30×16	1 920	23.368	93.656	3.302
Nb	$4s^2 4p^6 4d^4 5s^1$	1.60	3	6	25×25×25	455	18.143	169.384	3.776
Mo	$4s^2 4p^6 4d^5 5s^1$	1.60	3	6	26×26×26	455	15.779	258.653	4.149
Tc	$4s^2 4p^6 4d^6 5s^1$	1.60	3	6	35×35×19	1 200	14.428	298.749	4.547
Ru	$4s^2 4p^6 4d^7 5s^1$	1.61	3	6	35×35×20	1 200	13.749	312.687	4.984
Rh	$4s^2 4p^6 4d^8 5s^1$	1.60	3	7	22×22×22	286	14.036	255.390	5.010
Pd	$4s^2 4p^6 4d^{10} 5s^0$	1.60	3	7	21×21×21	286	15.308	164.943	8.234

Ag	$4s^2 4p^6 4d^{10} 5s^1$	1.59	3	7	20×20×20	220	17.821	91.245	5.774
Cd	$4d^{10} 5s^2$	2.20	1	5	32×32×15	2 176	22.699	46.379	6.461
In	$4d^{10} 5s^2 5p^1$	2.30	3	–	25×25×17	819	27.509	35.248	4.927
Sn	$4d^{10} 5s^2 5p^2$	2.20	3	–	22×22×22	1 012	36.777	35.701	5.126
Sb	$4d^{10} 5s^2 5p^3$	2.19	3	–	22×22×8	1 012	31.704	50.423	4.338
Te	$5s^2 5p^4$	2.20	2	–	21×21×14	595	34.970	45.193	5.042
I	$5s^2 5p^5$	2.01	2	–	10×18×9	225	50.421	18.580	5.081
Xe	$5s^2 5p^6$	2.19	2	–	12×12×12	56	85.748	0.519	9.059
Cs	$5s^2 5p^6 6s^1$	2.19	2	5	14×14×14	84	116.636	1.933	5.731
Ba	$5s^2 5p^6 6s^2$	2.00	2	5.5	17×17×17	165	63.211	8.781	2.931
Lu	$4f^{14} 5s^2 5p^6 5d^1 6s^2$	2.11	2	6	27×27×15	600	29.103	46.301	3.405
Hf	$4f^{14} 5s^2 5p^6 5d^2 6s^2$	2.10	3	6	30×30×17	2 160	22.495	107.483	3.551
Ta	$4f^{14} 5s^2 5p^6 5d^3 6s^2$	2.40	3	6	25×25×25	455	18.268	195.230	3.289
W	$4f^{14} 5s^2 5p^6 5d^4 6s^2$	2.41	3	6	26×26×26	455	16.123	303.940	4.334
Re	$4f^{14} 5s^2 5p^6 5d^5 6s^2$	2.40	3	6	35×35×19	1 200	14.949	365.817	4.409
Os	$4f^{14} 5s^2 5p^6 5d^6 6s^2$	2.41	3	6	35×35×19	1 200	14.277	401.335	4.826
Ir	$4f^{14} 5s^2 5p^6 5d^7 6s^2$	2.39	3	6	22×22×22	286	14.498	349.836	5.133
Pt	$4f^{14} 5s^2 5p^6 5d^9 6s^1$	2.40	3	6	21×21×21	286	15.637	248.932	5.468
Au	$4f^{14} 5s^2 5p^6 5d^{10} 6s^1$	2.39	3	6	20×20×20	220	17.932	143.007	6.517
Hg	$5s^2 5p^6 5d^{10} 6s^2$	2.19	3	–	20×20×24	660	29.062	8.665	8.245
Tl	$5s^2 5p^6 5d^{10} 6s^2 6p^1$	2.20	3	–	27×27×15	600	31.365	26.502	5.141
Pb	$5s^2 5p^6 5d^{10} 6s^2 6p^2$	2.19	3	–	17×17×17	165	31.925	39.560	4.535
Bi	$5d^{10} 6s^2 6p^3$	2.30	3	–	21×21×7	303	36.785	42.645	4.909
Po	$5d^{10} 6s^2 6p^4$	2.31	3	–	25×25×25	455	37.491	45.752	4.291
Rn	$5d^{10} 6s^2 6p^6$	2.29	3	–	12×12×12	56	91.823	0.564	3.973