OTFG19.1/CASTEP

CASTEP C19 USPP dataset / CASTEP 19.1

name and version of the code: CASTEP 19.1.1
type of basis set: plane waves
method: ultrasoft pseudopotentials ("On-The-Fly" Vanderbilt-type version C19)

GENERAL INFORMATION

exchange-correlation functional	PBE
relativistic scheme	scalar relativistic (Koelling-Harmon)
assignment of core / valence states	see table
basis set size	cutoff energy = 816 eV
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 "C19" library release (Mercurial changeset e8cf5c1713f6)
pseudopotential core radii	see table (r_c)
local channel	see table (l_{loc})
non-local core radii	$2.0\,a_0$ for 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	$1.0\,a_0$ (Fe, Co, Ni, Cu); $0.6\,a_0$ (V, Cr, Mn); $0.7\,r_c$ otherwise
pseudization radius for NLCC core charge	same as for augmentation functions
size of FFT grid for augmentation	3 × FFT grid for soft density ($E_{c,\rho} = 9\,E_{c,\phi}$) for magnetic elements, 1.5 × soft FFT grid ($E_{c,\rho} = 2.25\,E_{c,\phi}$) otherwise

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 C19 potential set is similar to C9 with revisions to O, Al, Bi, Po, Rn and the $3d$ transition metals.

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	25×25×17	585	17.428	10.284	2.677
He	$1s^2$	1.00	1	7	33×33×18	972	17.612	0.899	6.690
Li	$1s^2 2s^1$	1.00	1	7	32×32×4	1 056	20.233	13.772	4.261
Be	$1s^2 2s^2$	1.00	2	7	43×43×24	2 112	7.919	123.511	3.289
B	$2s^2 2p^1$	1.20	2	8	21×21×20	2 310	7.225	236.982	3.455
C	$2s^2 2p^2$	1.40	2	7	39×39×10	735	11.628	208.952	3.569
N	$2s^2 2p^3$	1.10	2	7	14×14×14	119	28.940	54.143	3.736
O	$2s^2 2p^4$	1.10	2	8	22×20×20	2 200	18.612	51.337	3.889
F	$2s^2 2p^5$	1.20	2	7	14×23×13	1 092	19.237	34.484	3.963
Ne	$2s^2 2p^6$	1.40	2	6	19×19×19	220	23.877	1.492	8.067
Na	$2s^2 2p^6 3s^1$	1.30	2	7	26×26×4	702	37.206	7.710	3.684
Mg	$2s^2 2p^6 3s^2$	1.80	3	–	31×31×17	864	22.900	35.933	4.408
Al	$3s^2 3p^1$	2.19	3	–	21×21×21	286	16.491	77.172	4.318
Si	$3s^2 3p^2$	1.80	3	–	27×27×27	560	20.441	88.568	4.306
P	$3s^2 3p^3$	1.81	3	–	26×8×19	520	21.428	68.203	4.322
S	$3s^2 3p^4$	1.80	3	–	33×33×33	3 281	17.177	86.274	3.887
Cl	$3s^2 3p^5$	1.81	3	–	11×20×10	300	38.739	19.081	4.379
Ar	$3s^2 3p^6$	1.60	2	–	15×15×15	120	51.661	0.788	7.267
K	$3s^2 3p^6 4s^1$	1.50	2	6	16×16×16	120	73.853	3.543	3.845
Ca	$3s^2 3p^6 4s^2$	2.00	3	–	16×16×16	120	42.188	17.417	3.322
Sc	$3s^2 3p^6 3d^1 4s^2$	1.80	3	6.5	29×29×17	765	24.690	53.938	3.362
Ti	$3s^2 3p^6 3d^2 4s^2$	1.79	3	5.5	33×33×18	972	17.392	111.647	3.586
V	$3s^2 3p^6 3d^3 4s^2$	1.80	3	7	28×28×28	560	13.467	181.562	3.895
Cr	$3s^2 3p^6 3d^5 4s^1$	1.80	3	7	30×30×30	680	11.749	179.010	6.633
Mn	$3s^2 3p^6 3d^5 4s^2$	1.80	3	7	24×24×24	936	11.450	120.822	2.072
Fe	$3d^6 4s^2$	2.40	3	5.5	30×30×30	680	11.350	193.093	5.060
Co	$3d^7 4s^2$	2.41	3	5.5	39×39×21	1 617	10.861	213.726	4.752
Ni	$3d^8 4s^2$	2.40	3	5.5	24×24×24	364	10.912	198.983	4.686
Cu	$3d^{10} 4s^1$	2.21	3	6	23×23×23	364	11.938	138.583	5.121
Zn	$3d^{10} 4s^2$	2.20	3	6	37×37×17	1 197	15.188	74.595	5.553
Ga	$3d^{10} 4s^2 4p^1$	2.00	3	6	19×11×19	600	20.311	48.644	5.390
Ge	$3d^{10} 4s^2 4p^2$	2.00	3	6	26×26×26	1 638	23.903	58.854	4.797
As	$3d^{10} 4s^2 4p^3$	2.00	3	6	26×26×8	1 404	22.614	68.179	4.135
Se	$3d^{10} 4s^2 4p^4$	1.99	3	6	22×22×17	2 156	29.808	47.016	4.454
Br	$4s^2 4p^5$	2.00	2	6	11×20×10	300	39.486	22.437	4.850
Kr	$4s^2 4p^6$	1.90	2	–	13×13×13	84	66.334	0.569	−19.406
Rb	$4s^2 4p^6 5s^1$	2.09	2	–	15×15×15	120	91.212	2.760	3.781
Sr	$4s^2 4p^6 5s^2$	2.00	3	–	14×14×14	84	55.011	11.756	3.213
Y	$4s^2 4p^6 4d^1 5s^2$	2.00	3	–	27×27×15	600	32.905	40.488	3.054
Zr	$4s^2 4p^6 4d^2 5s^2$	2.10	3	–	30×30×17	2 160	23.368	93.640	3.384
Nb	$4s^2 4p^6 4d^4 5s^1$	1.60	3	6	26×26×26	455	18.143	169.383	3.737
Mo	$4s^2 4p^6 4d^5 5s^1$	1.60	3	6	27×27×27	560	15.779	259.070	4.237
Tc	$4s^2 4p^6 4d^6 5s^1$	1.60	3	6	35×35×19	1 200	14.427	298.845	4.520
Ru	$4s^2 4p^6 4d^7 5s^1$	1.61	3	6	36×36×20	3 420	13.749	312.189	4.876
Rh	$4s^2 4p^6 4d^8 5s^1$	1.60	3	7	22×22×22	286	14.032	256.802	5.304
Pd	$4s^2 4p^6 4d^{10} 5s^0$	1.60	3	7	22×22×22	286	15.291	169.791	5.525

Ag	$4s^24p^64d^{10}5s^1$	1.50	3	7	21×21×21	286	17.827	90.562	5.459
Cd	$4s^24p^64d^{10}5s^2$	1.50	3	7	32×32×15	2 176	22.853	43.567	6.197
In	$4d^{10}5s^25p^1$	2.50	3	–	26×26×17	819	27.474	35.231	5.078
Sn	$4d^{10}5s^25p^2$	2.49	3	–	22×22×22	1 012	36.803	35.707	4.883
Sb	$4d^{10}5s^25p^3$	2.50	3	–	22×22×8	1 012	31.774	50.370	4.343
Te	$5s^25p^4$	2.20	2	–	22×22×14	1 771	34.974	45.273	4.695
I	$5s^25p^5$	2.01	2	–	10×19×9	250	50.489	17.853	5.427
Xe	$5s^25p^6$	2.19	2	–	12×12×12	56	86.885	0.504	−2.086
Cs	$5s^25p^66s^1$	2.19	2	5	14×14×14	84	116.834	1.958	2.602
Ba	$5s^25p^66s^2$	2.00	2	5.5	17×17×17	165	63.212	8.782	2.943
Lu	$4f^{14}5s^25p^65d^16s^2$	2.11	2	6	28×28×16	1 680	29.102	46.253	3.465
Hf	$4f^{14}5s^25p^65d^26s^2$	2.10	3	6	31×31×17	864	22.494	107.847	3.721
Ta	$4f^{14}5s^25p^65d^36s^2$	2.40	3	6	26×26×26	455	18.252	193.296	5.246
W	$4f^{14}5s^25p^65d^46s^2$	2.41	3	6	27×27×27	560	16.129	304.823	3.675
Re	$4f^{14}5s^25p^65d^56s^2$	2.40	3	6	35×35×19	1 200	14.949	366.034	4.461
Os	$4f^{14}5s^25p^65d^66s^2$	2.41	3	6	35×35×20	1 200	14.277	400.732	5.039
Ir	$4f^{14}5s^25p^65d^76s^2$	2.39	3	6	22×22×22	286	14.498	349.828	5.134
Pt	$4f^{14}5s^25p^65d^96s^1$	2.40	3	6	21×21×21	286	15.636	248.599	5.461
Au	$4f^{14}5s^25p^65d^{10}6s^1$	2.39	3	6	20×20×20	220	17.932	141.017	6.004
Hg	$5s^25p^65d^{10}6s^2$	2.19	3	–	21×21×24	792	29.052	8.690	8.355
Tl	$5s^25p^65d^{10}6s^26p^1$	2.20	3	–	27×27×15	600	31.365	26.528	5.078
Pb	$5s^25p^65d^{10}6s^26p^2$	2.19	3	–	17×17×17	165	31.922	39.613	4.773
Bi	$6s^26p^3$	2.80	2	–	21×21×7	303	36.966	43.135	4.934
Po	$6s^26p^4$	2.41	2	–	25×25×25	455	37.509	46.337	4.343
Rn	$6s^26p^6$	2.41	2	–	12×12×12	56	92.465	0.607	10.721