OTFG-ONCVPSP/CASTEP

CASTEP NCP19 dataset / CASTEP 19.1.1

name and version of the code: CASTEP 19.1.1
type of basis set: plane waves
method: Pseudopotentials ("On-The-Fly" ONCVPSP version 19)

GENERAL INFORMATION

exchange-correlation functional	PBE
relativistic scheme	scalar relativistic (Koelling-Harmon)
assignment of core / valence states	see table
basis set size	cutoff energy = 1280 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" optimized norm-conserving Vanderbilt (ONCVPSP). Settings for "NCP19" library release (Mercurial changeset 188025898a04)
pseudopotential core radii	see table (r_c)
local channel	see table (l_{loc})
non-local core radii	Same as r_c.
number of projectors	Mostly 1 per valence l channel plus 1 per semi-core state, except for O (2s and 2p) , Cr-Ni (3d), Nb (4d), W and Re (5p), Lu, Ir, Pt, Au (5p and 5d) and Pb (6s, 6p, 5d) where 2 per channel were used.
projector generation	KE-Optimized RRKJ.
pseudization radius for NLCC core charge	$0.7\,r_c$
size of FFT grid for core charge	1.5 × orbitals FFT grid ($E_{c,\rho} = 2.25\,E_{c,\phi}$)

ADDITIONAL COMMENTS

This pseudopotential set is generated using the Optimised Norm-Conserving Vanderbilt (ONCVPSP) method. Full convergence is achieved at 1280 eV cutoff, across the periodic table. 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.

REFERENCES

pseudopotential method

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

[2] D. Hamman, *Phys. Rev. B* **88**(8), 085117 (2013).

code

[3] 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`

[4] 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	8	25×25×17	585	17.345	10.301	2.657
He	$1s^2$	1.00	1	8	33×33×18	972	17.706	0.901	6.284
Li	$1s^2 2s^1$	1.20	1	8	32×32×4	1 056	20.216	13.827	3.323
Be	$1s^2 2s^2$	1.10	1	9	43×43×24	2 112	7.917	124.850	3.324
B	$2s^2 2p^1$	1.20	1	8	21×21×20	2 310	7.224	235.664	3.446
C	$2s^2 2p^2$	1.20	1	8	39×39×10	735	11.658	206.750	3.549
N	$2s^2 2p^3$	1.10	1	9	14×14×14	119	29.019	52.611	3.691
O	$2s^2 2p^4$	1.20	2	9	22×20×20	2 200	18.391	50.928	3.856
F	$2s^2 2p^5$	1.40	2	8	14×23×13	1 092	19.117	33.786	3.985
Ne	$2s^2 2p^6$	1.40	2	8	19×19×19	220	24.099	1.235	6.501
Na	$2s^2 2p^6 3s^1$	1.50	2	8	26×26×4	702	37.663	7.604	3.634
Mg	$3s^2$	1.80	1	–	31×31×17	864	22.773	36.343	4.333
Al	$3s^2 3p^1$	1.60	1	–	21×21×21	286	16.466	76.970	4.300
Si	$3s^2 3p^2$	1.60	1	–	27×27×27	560	20.415	88.326	4.299
P	$3s^2 3p^3$	1.59	1	–	26×8×19	520	21.414	68.104	4.328
S	$3s^2 3p^4$	1.80	1	–	33×33×33	3 281	17.089	86.599	3.876
Cl	$3s^2 3p^5$	1.59	1	6	11×20×10	300	38.573	19.122	4.376
Ar	$3s^2 3p^6$	1.60	2	6	15×15×15	120	51.734	0.779	7.292
K	$3s^2 3p^6 4s^1$	1.50	2	6	16×16×16	120	73.651	3.561	3.604
Ca	$3s^2 3p^6 4s^2$	2.00	3	6	16×16×16	120	42.227	17.479	3.334
Sc	$3s^2 3p^6 3d^1 4s^2$	1.80	3	7	29×29×17	765	24.697	54.195	3.354
Ti	$3s^2 3p^6 3d^2 4s^2$	1.79	3	7	33×33×18	972	17.467	112.052	3.563
V	$3s^2 3p^6 3d^3 4s^2$	1.60	3	7	28×28×28	560	13.461	182.590	3.864
Cr	$3s^2 3p^6 3d^5 4s^1$	1.30	3	10.5	30×30×30	680	11.888	157.036	5.795
Mn	$3s^2 3p^6 3d^5 4s^2$	1.30	3	10.5	24×24×24	936	11.795	133.157	2.800
Fe	$3s^2 3p^6 3d^6 4s^2$	1.29	3	10.5	30×30×30	680	11.370	163.553	9.389
Co	$3s^2 3p^6 3d^7 4s^2$	1.30	3	10.5	39×39×21	1 617	10.854	202.682	4.408
Ni	$3s^2 3p^6 3d^8 4s^2$	1.30	3	10.5	24×24×24	364	10.852	181.322	7.460
Cu	$3d^{10} 4s^1$	1.81	3	4.5	23×23×23	364	12.005	138.665	5.116
Zn	$3d^{10} 4s^2$	1.81	3	4.5	37×37×17	1 197	15.192	74.889	5.598
Ga	$3d^{10} 4s^2 4p^1$	1.81	3	4.5	19×11×19	600	20.378	48.309	5.383
Ge	$3d^{10} 4s^2 4p^2$	1.79	3	5	26×26×26	1 638	23.975	58.576	4.859
As	$3d^{10} 4s^2 4p^3$	1.80	3	5.5	26×26×8	1 404	22.750	68.024	4.288
Se	$3d^{10} 4s^2 4p^4$	1.80	3	6	22×22×17	2 156	30.086	46.607	4.516
Br	$3d^{10} 4s^2 4p^5$	1.80	3	6	11×20×10	300	39.999	22.169	4.794
Kr	$4s^2 4p^6$	1.90	2	–	13×13×13	84	65.935	0.654	7.210
Rb	$4s^2 4p^6 5s^1$	2.09	2	–	15×15×15	120	91.284	2.758	3.787
Sr	$4s^2 4p^6 5s^2$	2.00	3	–	14×14×14	84	54.810	11.953	3.185
Y	$4s^2 4p^6 4d^1 5s^2$	2.00	3	–	27×27×15	600	32.799	41.159	3.140
Zr	$4s^2 4p^6 4d^2 5s^2$	2.10	3	–	30×30×17	2 160	23.457	95.841	3.351
Nb	$4s^2 4p^6 4d^4 5s^1$	1.40	3	8	26×26×26	455	18.183	168.693	3.736
Mo	$4s^2 4p^6 4d^5 5s^1$	1.40	2	8	27×27×27	560	15.837	258.825	4.244
Tc	$4s^2 4p^6 4d^6 5s^1$	1.40	2	8	35×35×19	1 200	14.470	299.117	4.539
Ru	$4s^2 4p^6 4d^7 5s^1$	1.39	2	8	36×36×20	3 420	13.778	313.081	4.883
Rh	$4s^2 4p^6 4d^8 5s^1$	1.40	2	8	22×22×22	286	14.050	257.517	5.208
Pd	$4s^2 4p^6 4d^{10} 5s^0$	1.50	2	8	22×22×22	286	15.355	167.271	5.579

Ag	$4s^2 4p^6 4d^{10} 5s^1$	1.50	2	8	21×21×21	286	17.843	91.041	5.863
Cd	$4s^2 4p^6 4d^{10} 5s^2$	1.50	2	9	32×32×15	2 176	22.613	46.179	6.480
In	$4d^{10} 5s^2 5p^1$	2.61	3	6	26×26×17	819	27.686	35.151	5.082
Sn	$4d^{10} 5s^2 5p^2$	2.60	3	6	22×22×22	1 012	37.013	35.392	4.881
Sb	$5s^2 5p^3$	2.59	2	6	22×22×8	1 012	31.845	50.752	4.395
Te	$5s^2 5p^4$	2.20	2	–	22×22×14	1 771	35.011	45.000	4.734
I	$5s^2 5p^5$	2.20	2	–	10×19×9	250	50.543	18.607	5.097
Xe	$5s^2 5p^6$	2.19	2	–	12×12×12	56	86.397	0.553	7.177
Cs	$5s^2 5p^6 6s^1$	2.19	2	5	14×14×14	84	116.524	1.954	3.497
Ba	$5s^2 5p^6 6s^2$	2.00	2	5.5	17×17×17	165	63.143	8.815	2.937
Lu	$5s^2 5p^6 5d^1 6s^2$	1.80	2	8	28×28×16	1 680	29.332	46.265	3.351
Hf	$5s^2 5p^6 5d^2 6s^2$	1.80	2	8	31×31×17	864	22.562	104.063	3.365
Ta	$5s^2 5p^6 5d^3 6s^2$	1.79	2	8	26×26×26	455	18.273	187.763	3.693
W	$5s^2 5p^6 5d^4 6s^2$	1.60	3	8	27×27×27	560	16.137	302.279	4.190
Re	$5s^2 5p^6 5d^5 6s^2$	1.81	3	8	35×35×19	1 200	14.962	363.236	4.441
Os	$5s^2 5p^6 5d^6 6s^2$	1.80	2	8	35×35×20	1 200	14.298	389.497	4.795
Ir	$5s^2 5p^6 5d^7 6s^2$	1.60	3	7	22×22×22	286	14.502	346.312	5.112
Pt	$5s^2 5p^6 5d^9 6s^1$	1.60	3	7	21×21×21	286	15.642	247.097	5.457
Au	$5s^2 5p^6 5d^{10} 6s^1$	1.60	3	7	20×20×20	220	17.955	139.479	6.008
Hg	$5d^{10} 6s^2$	2.79	3	5	21×21×24	792	29.402	8.443	8.523
Tl	$5d^{10} 6s^2 6p^1$	2.80	3	5	27×27×15	600	31.511	26.584	5.227
Pb	$5d^{10} 6s^2 6p^2$	2.40	3	7	17×17×17	165	31.959	39.508	4.775
Bi	$6s^2 6p^3$	2.20	2	7	21×21×7	303	36.704	43.213	4.944
Po	$6s^2 6p^4$	2.19	2	7	25×25×25	455	37.603	45.942	4.351
Rn	$6s^2 6p^6$	2.20	2	7	12×12×12	56	93.362	0.543	7.221