ONCVPSP(SG15)1/CASTEP

SG15 ONCVPSP 2015-01-24 NCPP dataset / CASTEP 9.0

`name and version of the code:` CASTEP 9.0 (Hg revision 6666 Jun 05 2015)
`type of basis set:` plane waves
`method:` norm-conserving pseudopotentials (Schlipf-Gygi ONCVPSP 2015-01-24)

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 = 952 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

`size of FFT grid for augmentation`	N/A

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 criteria, determined individually per element will still give high convergence in almost all cases at substantially reduced computational cost.

REFERENCES

`potentials`

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[2] M. Schlipf and F. Gygi, *Comput. Phys. Commun.* (2015). doi: 10.1016/j.cpc.2015.05.011

`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).

ONCVPSP(SG15)1/CASTEP

SG15 ONCVPSP 2015-01-24 NCPP dataset / CASTEP 9.0

Table I. Calculation settings and results per element: valence, 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	*kpts*	# k	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	$1s^1$	24×24×17	1 404	17.357	10.297	2.691
He	$1s^2$	33×33×18	972	17.711	0.882	6.404
Li	$1s^2\ 2s^1$	31×31×4	352	20.264	13.798	3.366
Be	$1s^2\ 2s^2$	42×42×23	5 544	7.933	124.158	3.309
B	$2s^2\ 2p^1$	21×21×20	2 310	7.180	235.389	3.405
C	$2s^2\ 2p^2$	39×39×10	735	11.587	208.587	3.549
N	$2s^2\ 2p^3$	14×14×14	119	28.777	53.174	3.663
O	$2s^2\ 2p^4$	21×20×20	2 100	18.607	50.062	3.649
F	$2s^2\ 2p^5$	14×23×12	1 008	19.281	33.791	4.081
Ne	$2s^2\ 2p^6$	18×18×18	165	24.271	1.344	7.261
Na	$2s^2\ 2p^6\ 3s^1$	26×26×3	533	37.174	7.739	3.684
Mg	$2s^2\ 2p^6\ 3s^2$	30×30×16	1 920	22.973	36.398	4.344
Al	$2s^2\ 2p^6\ 3s^2\ 3p^1$	21×21×21	286	16.542	77.143	4.264
Si	$3s^2\ 3p^2$	26×26×26	1 638	20.522	87.493	4.266
P	$3s^2\ 3p^3$	25×8×18	468	21.474	67.776	4.313
S	$3s^2\ 3p^4$	32×32×32	2 992	17.231	87.583	3.958
Cl	$3s^2\ 3p^5$	11×19×10	300	39.399	18.682	4.369
Ar	$3s^2\ 3p^6$	14×14×14	84	52.304	0.759	7.704
K	$3s^2\ 3p^6\ 4s^1$	16×16×16	120	73.844	3.581	3.133
Ca	$3s^2\ 3p^6\ 4s^2$	15×15×15	120	42.150	17.405	3.318
Sc	$3s^2\ 3p^6\ 3d^1\ 4s^2$	29×29×16	680	24.716	53.956	3.349
Ti	$3s^2\ 3p^6\ 3d^2\ 4s^2$	33×33×18	972	17.422	111.583	3.504
V	$3s^2\ 3p^6\ 3d^3\ 4s^2$	28×28×28	560	13.489	181.719	3.864
Cr	$3s^2\ 3p^6\ 3d^5\ 4s^1$	29×29×29	680	12.430	116.331	6.841
Mn	$3s^2\ 3p^6\ 3d^5\ 4s^2$	23×23×23	936	11.912	124.007	3.996
Fe	$3s^2\ 3p^6\ 3d^6\ 4s^2$	29×29×29	680	11.463	171.168	8.576
Co	$3s^2\ 3p^6\ 3d^7\ 4s^2$	38×38×21	4 180	10.932	209.487	4.731
Ni	$3s^2\ 3p^6\ 3d^8\ 4s^2$	24×24×24	364	10.960	194.124	4.866
Cu	$3s^2\ 3p^6\ 3d^{10}\ 4s^1$	23×23×23	364	11.971	135.520	5.366
Zn	$3s^2\ 3p^6\ 3d^{10}\ 4s^2$	36×36×17	3 078	15.177	75.431	5.622
Ga	$3d^{10}\ 4s^2\ 4p^1$	18×11×18	486	20.341	49.091	5.378
Ge	$3d^{10}\ 4s^2\ 4p^2$	25×25×25	455	23.992	58.657	4.849
As	$4s^2\ 4p^3$	25×25×8	468	22.687	68.424	4.223
Se	$4s^2\ 4p^4$	21×21×17	728	30.015	47.026	4.461
Br	$4s^2\ 4p^5$	10×20×10	250	39.671	22.387	4.837
Kr	$4s^2\ 4p^6$	13×13×13	84	65.975	0.645	7.299
Rb	$4s^2\ 4p^6\ 5s^1$	15×15×15	120	91.165	2.764	3.769
Sr	$4s^2\ 4p^6\ 5s^2$	14×14×14	84	54.942	11.778	3.213
Y	$4s^2\ 4p^6\ 4d^1\ 5s^2$	26×26×15	1 456	32.919	40.516	3.072
Zr	$4s^2\ 4p^6\ 4d^2\ 5s^2$	30×30×16	1 920	23.400	93.780	3.342
Nb	$4s^2\ 4p^6\ 4d^4\ 5s^1$	25×25×25	455	18.166	169.438	3.743
Mo	$4s^2\ 4p^6\ 4d^5\ 5s^1$	26×26×26	455	15.784	259.481	4.239
Tc	$4s^2\ 4p^6\ 4d^6\ 5s^1$	35×35×19	1 200	14.443	297.773	4.491
Ru	$4s^2\ 4p^6\ 4d^7\ 5s^1$	35×35×20	1 200	13.776	311.240	4.841
Rh	$4s^2\ 4p^6\ 4d^8\ 5s^1$	22×22×22	286	14.065	255.184	5.188
Pd	$4s^2\ 4p^6\ 4d^{10}$	21×21×21	286	15.342	167.685	5.585
Ag	$4s^2\ 4p^6\ 4d^{10}\ 5s^1$	20×20×20	220	17.833	90.812	5.848

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SG15 ONCVPSP 2015-01-24 NCPP dataset / CASTEP 9.0

Cd	$4s^2\ 4p^6\ 4d^{10}\ 5s^2$	32×32×15	2 176	22.988	43.302	6.493
In	$4d^{10}\ 5s^2\ 5p^1$	25×25×17	819	27.519	35.044	4.806
Sn	$4d^{10}\ 5s^2\ 5p^2$	22×22×22	1 012	36.898	35.565	5.070
Sb	$4d^{10}\ 5s^2\ 5p^3$	22×22×8	1 012	31.762	50.252	4.330
Te	$4d^{10}\ 5s^2\ 5p^4$	21×21×14	595	35.023	44.640	5.076
I	$4d^{10}\ 5s^2\ 5p^5$	10×18×9	225	50.383	18.584	4.609
Xe	$4d^{10}\ 5s^2\ 5p^6$	12×12×12	56	87.780	0.812	−15.919
Cs	$5s^2\ 5p^6\ 6s^1$	14×14×14	84	116.758	1.947	3.518
Ba	$5s^2\ 5p^6\ 6s^2$	17×17×17	165	63.288	8.671	2.876
Lu	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Hf	$4f^{14}\ 5s^2\ 5p^6\ 5d^2\ 6s^2$	30×30×17	2 160	22.604	108.327	3.432
Ta	$4f^{14}\ 5s^2\ 5p^6\ 5d^3\ 6s^2$	25×25×25	455	18.337	193.936	3.741
W	$4f^{14}\ 5s^2\ 5p^6\ 5d^4\ 6s^2$	26×26×26	455	16.151	301.023	4.180
Re	$5s^2\ 5p^6\ 5d^5\ 6s^2$	35×35×19	1 200	14.945	364.752	4.418
Os	$5s^2\ 5p^6\ 5d^6\ 6s^2$	35×35×19	1 200	14.258	398.558	4.827
Ir	$5s^2\ 5p^6\ 5d^7\ 6s^2$	22×22×22	286	14.480	348.100	5.111
Pt	$5s^2\ 5p^6\ 5d^9\ 6s^1$	21×21×21	286	15.708	244.268	5.476
Au	$5s^2\ 5p^6\ 5d^{10}\ 6s^1$	20×20×20	220	17.983	139.001	6.011
Hg	$5s^2\ 5p^6\ 5d^{10}\ 6s^2$	20×20×24	660	29.462	8.036	8.600
Tl	$5d^{10}\ 6s^2\ 6p^1$	27×27×15	600	31.389	26.608	5.252
Pb	$5d^{10}\ 6s^2\ 6p^2$	17×17×17	165	32.002	39.699	4.883
Bi	$5d^{10}\ 6s^2\ 6p^3$	21×21×7	303	36.913	42.720	4.910
Po	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*