GBRV14/CASTEP

GBRV 1.4 USPP 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:` ultrasoft pseudopotentials (GBRV 1.4)

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

`size of FFT grid for augmentation`	2 × 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.

REFERENCES

`pseudopotential method`

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

[2] K. F. Garrity, J. W. Bennett, K. M. Rabe and D. Vanderbilt, *Comput. Mater. Sci.* **81** 446–452 (2014).

`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).

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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	18.178	10.381	2.796
He	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Li	$1s^2\ 2s^1$	31×31×4	352	20.225	14.201	3.362
Be	$1s^2\ 2s^2$	42×42×23	5 544	7.942	123.928	3.322
B	$2s^2\ 2p^1$	21×21×20	2 310	7.226	236.701	3.457
C	$2s^2\ 2p^2$	39×39×10	735	11.634	207.932	3.563
N	$2s^2\ 2p^3$	14×14×14	119	29.269	54.718	3.807
O	$2s^2\ 2p^4$	21×20×20	2 100	18.784	50.761	3.975
F	$2s^2\ 2p^5$	14×23×12	1 008	19.355	34.125	4.081
Ne	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Na	$2s^2\ 2p^6\ 3s^1$	26×26×3	533	37.185	7.713	3.705
Mg	$2s^2\ 2p^6\ 3s^2$	30×30×16	1 920	22.946	35.879	4.322
Al	$3s^2\ 3p^1$	21×21×21	286	16.505	76.727	4.293
Si	$3s^2\ 3p^2$	26×26×26	1 638	20.434	88.595	4.308
P	$3s^2\ 3p^3$	25×8×18	468	21.722	67.178	4.331
S	$3s^2\ 3p^4$	32×32×32	2 992	17.176	86.243	3.875
Cl	$3s^2\ 3p^5$	11×19×10	300	38.768	19.014	4.376
Ar	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
K	$3s^2\ 3p^6\ 4s^1$	16×16×16	120	73.905	3.546	3.604
Ca	$3s^2\ 3p^6\ 4s^2$	15×15×15	120	42.216	17.398	3.317
Sc	$3s^2\ 3p^6\ 3d^1\ 4s^2$	29×29×16	680	24.679	53.977	3.364
Ti	$3s^2\ 3p^6\ 3d^2\ 4s^2$	33×33×18	972	17.402	111.536	3.582
V	$3s^2\ 3p^6\ 3d^3\ 4s^2$	28×28×28	560	13.459	181.463	3.831
Cr	$3s^2\ 3p^6\ 3d^5\ 4s^1$	29×29×29	680	11.847	169.679	6.717
Mn	$3s^2\ 3p^6\ 3d^5\ 4s^2$	23×23×23	936	11.657	116.061	1.641
Fe	$3s^2\ 3p^6\ 3d^6\ 4s^2$	29×29×29	680	11.444	170.016	8.434
Co	$3s^2\ 3p^6\ 3d^7\ 4s^2$	38×38×21	4 180	10.872	211.657	4.797
Ni	$3s^2\ 3p^6\ 3d^8\ 4s^2$	24×24×24	364	10.903	197.636	4.903
Cu	$3s^2\ 3p^6\ 3d^{10}\ 4s^1$	23×23×23	364	11.989	140.875	5.113
Zn	$3s^2\ 3p^6\ 3d^{10}\ 4s^2$	36×36×17	3 078	15.210	74.572	5.579
Ga	$3p^6\ 3d^{10}\ 4s^2\ 4p^1$	18×11×18	486	20.353	48.441	5.365
Ge	$3d^{10}\ 4s^2\ 4p^2$	25×25×25	455	23.875	58.996	4.842
As	$4s^2\ 4p^3$	25×25×8	468	22.705	68.555	4.248
Se	$4s^2\ 4p^4$	21×21×17	728	29.735	47.287	4.471
Br	$4s^2\ 4p^5$	10×20×10	250	39.602	22.376	4.851
Kr	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Rb	$4s^2\ 4p^6\ 5s^1$	15×15×15	120	91.201	2.761	3.782
Sr	$4s^2\ 4p^6\ 5s^2$	14×14×14	84	55.638	11.702	2.940
Y	$4s^2\ 4p^6\ 4d^1\ 5s^2$	26×26×15	1 456	32.918	40.494	3.068
Zr	$4s^2\ 4p^6\ 4d^2\ 5s^2$	30×30×16	1 920	23.390	93.647	3.333
Nb	$4s^2\ 4p^6\ 4d^4\ 5s^1$	25×25×25	455	18.124	169.582	3.738
Mo	$4s^2\ 4p^6\ 4d^5\ 5s^1$	26×26×26	455	15.772	259.156	4.231
Tc	$4s^2\ 4p^6\ 4d^6\ 5s^1$	35×35×19	1 200	14.430	298.648	4.526
Ru	$4s^2\ 4p^6\ 4d^7\ 5s^1$	35×35×20	1 200	13.751	312.098	4.861
Rh	$4p^6\ 4d^8\ 5s^1$	22×22×22	286	14.086	256.398	5.213
Pd	$4p^6\ 4d^{10}$	21×21×21	286	15.388	168.165	5.589
Ag	$4s^2\ 4p^6\ 4d^{10}\ 5s^1$	20×20×20	220	17.875	91.036	5.828

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Cd	$4d^{10}\ 5s^2$	32×32×15	2 176	22.976	43.300	5.358
In	$4d^{10}\ 5s^2\ 5p^1$	25×25×17	819	27.512	35.110	5.148
Sn	$4d^{10}\ 5s^2\ 5p^2$	22×22×22	1 012	36.785	35.789	4.879
Sb	$4d^{10}\ 5s^2\ 5p^3$	22×22×8	1 012	31.774	50.420	4.359
Te	$5s^2\ 5p^4$	21×21×14	595	34.829	45.724	4.982
I	$5s^2\ 5p^5$	10×18×9	225	50.191	15.027	12.869
Xe	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Cs	$5s^2\ 5p^6\ 6s^1$	14×14×14	84	116.809	1.946	3.516
Ba	$5s^2\ 5p^6\ 6s^2$	17×17×17	165	63.466	8.717	2.900
Lu	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Hf	$5s^2\ 5p^6\ 5d^2\ 6s^2$	30×30×17	2 160	22.601	107.641	3.423
Ta	$5s^2\ 5p^6\ 5d^3\ 6s^2$	25×25×25	455	18.280	194.863	3.771
W	$5s^2\ 5p^6\ 5d^4\ 6s^2$	26×26×26	455	16.145	304.810	4.227
Re	$5s^2\ 5p^6\ 5d^5\ 6s^2$	35×35×19	1 200	14.957	365.128	4.451
Os	$5s^2\ 5p^6\ 5d^6\ 6s^2$	35×35×19	1 200	14.269	398.233	4.836
Ir	$5p^6\ 5d^7\ 6s^2$	22×22×22	286	14.508	346.326	5.044
Pt	$5p^6\ 5d^9\ 6s^1$	21×21×21	286	15.620	248.687	5.495
Au	$5d^{10}\ 6s^1$	20×20×20	220	17.921	140.684	6.024
Hg	$5d^{10}\ 6s^2$	20×20×24	660	29.583	8.068	8.578
Tl	$5d^{10}\ 6s^2\ 6p^1$	27×27×15	600	31.422	26.489	5.258
Pb	$5d^{10}\ 6s^2\ 6p^2$	17×17×17	165	31.922	39.532	4.755
Bi	$5d^{10}\ 6s^2\ 6p^3$	21×21×7	303	36.811	42.720	4.890
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*