

GBRV15/CASTEP

GBRV 1.5 USPP dataset/ CASTEP 17.2.1

name and version of the code: CASTEP 17.2.1 (Hg revision 7269 (056e886bd5a1) May 15 2017)
type of basis set: plane waves
method: ultrasoft pseudopotentials (GBRV 1.5)

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 \AA^{-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	$2 \times$ FFT grid for soft density ($E_{c,\rho} = 16 E_{c,\phi}$)
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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 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 [$\text{\AA}^3/\text{atom}$]	B_0 [GPa]	B_1 [-]
H	$1s^1$	$24 \times 24 \times 17$	1 404	18.178	10.381	2.796
He	N/A	N/A	N/A	N/A	N/A	N/A
Li	$1s^2 2s^1$	$31 \times 31 \times 4$	352	20.225	14.201	3.362
Be	$1s^2 2s^2$	$42 \times 42 \times 23$	5 544	7.942	123.928	3.322
B	$2s^2 2p^1$	$21 \times 21 \times 20$	2 310	7.226	236.701	3.457
C	$2s^2 2p^2$	$39 \times 39 \times 10$	735	11.634	207.932	3.563
N	$2s^2 2p^3$	$14 \times 14 \times 14$	119	29.269	54.718	3.807
O	$2s^2 2p^4$	$21 \times 20 \times 20$	2 100	18.784	50.761	3.975
F	$2s^2 2p^5$	$14 \times 23 \times 12$	1 008	19.355	34.125	4.081
Ne	N/A	N/A	N/A	N/A	N/A	N/A
Na	$2s^2 2p^6 3s^1$	$26 \times 26 \times 3$	533	37.216	7.698	3.680
Mg	$2s^2 2p^6 3s^2$	$30 \times 30 \times 16$	1 920	22.946	35.879	4.322
Al	$3s^2 3p^1$	$21 \times 21 \times 21$	286	16.505	76.727	4.293
Si	$3s^2 3p^2$	$26 \times 26 \times 26$	1 638	20.434	88.595	4.308
P	$3s^2 3p^3$	$25 \times 8 \times 18$	468	21.435	68.141	4.332
S	$3s^2 3p^4$	$32 \times 32 \times 32$	2 992	17.176	86.243	3.875
Cl	$3s^2 3p^5$	$11 \times 19 \times 10$	300	38.768	19.014	4.376
Ar	N/A	N/A	N/A	N/A	N/A	N/A
K	$3s^2 3p^6 4s^1$	$16 \times 16 \times 16$	120	73.905	3.546	3.604
Ca	$3s^2 3p^6 4s^2$	$15 \times 15 \times 15$	120	42.216	17.398	3.317
Sc	$3s^2 3p^6 3d^1 4s^2$	$29 \times 29 \times 16$	680	24.679	53.977	3.364
Ti	$3s^2 3p^6 3d^2 4s^2$	$33 \times 33 \times 18$	972	17.402	111.536	3.582
V	$3s^2 3p^6 3d^3 4s^2$	$28 \times 28 \times 28$	560	13.459	181.463	3.831
Cr	$3s^2 3p^6 3d^5 4s^1$	$29 \times 29 \times 29$	680	11.805	171.895	6.726
Mn	$3s^2 3p^6 3d^5 4s^2$	$23 \times 23 \times 23$	936	11.500	115.074	1.764
Fe	$3s^2 3p^6 3d^6 4s^2$	$29 \times 29 \times 29$	680	11.407	181.905	6.693
Co	$3s^2 3p^6 3d^7 4s^2$	$38 \times 38 \times 21$	4 180	10.872	211.657	4.797
Ni	$3s^2 3p^6 3d^8 4s^2$	$24 \times 24 \times 24$	364	10.903	197.636	4.903
Cu	$3s^2 3p^6 3d^{10} 4s^1$	$23 \times 23 \times 23$	364	11.989	140.875	5.113
Zn	$3s^2 3p^6 3d^{10} 4s^2$	$36 \times 36 \times 17$	3 078	15.210	74.572	5.579
Ga	$3p^6 3d^{10} 4s^2 4p^1$	$18 \times 11 \times 18$	486	20.353	48.441	5.365
Ge	$3d^{10} 4s^2 4p^2$	$25 \times 25 \times 25$	455	23.875	58.998	4.844
As	$4s^2 4p^3$	$25 \times 25 \times 8$	468	22.705	68.555	4.248
Se	$4s^2 4p^4$	$21 \times 21 \times 17$	728	29.735	47.287	4.471
Br	$4s^2 4p^5$	$10 \times 20 \times 10$	250	39.602	22.376	4.851
Kr	N/A	N/A	N/A	N/A	N/A	N/A
Rb	$4s^2 4p^6 5s^1$	$15 \times 15 \times 15$	120	91.201	2.761	3.782
Sr	$4s^2 4p^6 5s^2$	$14 \times 14 \times 14$	84	55.638	11.702	2.940
Y	$4s^2 4p^6 4d^1 5s^2$	$26 \times 26 \times 15$	1 456	32.918	40.494	3.068
Zr	$4s^2 4p^6 4d^2 5s^2$	$30 \times 30 \times 16$	1 920	23.390	93.647	3.333
Nb	$4s^2 4p^6 4d^4 5s^1$	$25 \times 25 \times 25$	455	18.124	169.582	3.738
Mo	$4s^2 4p^6 4d^5 5s^1$	$26 \times 26 \times 26$	455	15.772	259.156	4.231
Tc	$4s^2 4p^6 4d^6 5s^1$	$35 \times 35 \times 19$	1 200	14.430	298.648	4.526
Ru	$4s^2 4p^6 4d^7 5s^1$	$35 \times 35 \times 20$	1 200	13.751	312.098	4.861
Rh	$4p^6 4d^8 5s^1$	$22 \times 22 \times 22$	286	14.086	256.398	5.213
Pd	$4p^6 4d^{10}$	$21 \times 21 \times 21$	286	15.388	168.165	5.589
Ag	$4s^2 4p^6 4d^{10} 5s^1$	$20 \times 20 \times 20$	220	17.875	91.036	5.828

