exciting

exciting boron-9 / LAPW+xlo

name and version of the code: exciting boron-9
type of basis set: linearized augmented plane waves + several local orbitals
method: all-electron

GENERAL INFORMATION

exchange-correlation functional	PBE
relativistic scheme	core fully relativistic valence scalar relativistic (IORA)
assignment of core / valence states	see table
basis set size	see table ($R_{MT}^{min} K_{max}$)
k-mesh density	see table (number of k-points in the full 1st Brillouin zone of the primitive cell, # k)
reciprocal-space integration method	Gaussian smearing with a fictitious temperature corresponding to 0.001 Ry

METHOD-SPECIFIC INFORMATION

muffin-tin radii	see table (R_{MT})
radial mesh	400–1500 radial mesh points on an inverse cubic grid up to the muffin-tin radius
largest ℓ-value of wave function	12
largest ℓ-value of nonspherical Hamiltonian and overlap matrix elements inside the spheres	12
largest ℓ-value in expansion of density and potential	12
largest vector in Fourier expansion of charge density	$35 a_0^{-1}$ for I, $40 a_0^{-1}$ for H, He, O, Cl, Ar and Xe, $45 a_0^{-1}$ for Ne and $30 a_0^{-1}$ for remaining elements

ADDITIONAL COMMENTS

none

REFERENCES

code

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner and C. Draxl, *J. Phys.: Condens. Matter* **26**, 363202 (2014).

scalar relativity

[2] K. G. Dyall and E. van Lenthe, *J. Chem. Phys.* **111**, 1366–1372 (1999).

Table I. Calculation settings and results per element: muffin-tin radius R_{MT}, basis set size $R_{MT}^{min}K_{max}$, k-point mesh in the full 1st Brillouin zone of the primitive cell # k, valence, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	R_{MT} [b]	$R_{MT}^{min}K_{max}$ [–]	# k [–]	valence	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	0.5	8	5 x 5 x 5	1s	17.390	10.293	2.679
He	1.6	10	10 x 10 x 6	1s	17.766	0.858	6.543
Li	1.6	10	21 x 21 x 21	1s2s	20.221	13.852	3.361
Be	1.6	10	38 x 38 x 24	1s2s	7.904	123.142	3.266
B	1.2	10	5 x 5 x 5	1s2s2p	7.239	237.268	3.463
C	1.1	10	35 x 35 x 10	1s2s2p	11.631	208.981	3.570
N	0.9	10	3 x 3 x 3	1s2s2p	28.779	53.971	3.683
O	1.0	10	7 x 7 x 7	2s2p	18.505	51.214	3.860
F	1.1	10	3 x 5 x 3	2s2p	19.127	34.340	4.049
Ne	2.0	12	7 x 7 x 7	2s2p	24.292	1.264	7.196
Na	1.6	12	17 x 17 x 17	2s2p3s	37.079	7.732	3.681
Mg	1.6	12	27 x 27 x 17	2s2p3s	22.933	36.086	3.955
Al	1.8	12	32 x 32 x 32	2s2p3s3p	16.487	77.879	4.653
Si	1.6	12	24 x 24 x 24	2s2p3s3p	20.454	88.481	4.308
P	1.7	12	32 x 9 x 23	2s2p3s3p	21.447	68.108	4.334
S	1.6	12	32 x 32 x 32	2s2p3s3p	17.211	84.311	3.828
Cl	1.6	12	4 x 8 x 4	2s2p3s3p	38.779	18.987	4.375
Ar	2.0	12	7 x 7 x 7	3s3p	52.296	0.752	7.209
K	1.8	12	20 x 20 x 20	3s3p4s	73.681	3.594	3.773
Ca	1.6	12	24 x 24 x 24	3s3p4s	42.240	17.403	3.232
Sc	1.6	12	27 x 27 x 17	3s3p3d4s	24.617	54.821	3.405
Ti	1.6	12	29 x 29 x 19	3s3p3d4s	17.386	112.250	3.738
V	1.8	12	34 x 34 x 34	3s3p3d4s	13.449	182.314	3.605
Cr	1.6	12	29 x 29 x 29	3s3p3d4s	11.772	184.304	7.083
Mn	1.6	12	32 x 32 x 23	3s3p3d4s	11.444	121.093	0.907
Fe	1.6	12	48 x 48 x 48	3s3p3d4s	11.332	196.349	5.171
Co	1.6	12	35 x 35 x 22	3s3p3d4s	10.852	211.465	4.544
Ni	1.6	12	37 x 37 x 37	3s3p3d4s	10.882	198.724	5.229
Cu	1.8	12	36 x 36 x 36	3s3p3d4s	11.947	141.098	5.089
Zn	1.7	12	32 x 32 x 17	3s3p3d4s	15.192	74.341	5.247
Ga	2.0	12	23 x 13 x 23	3s3p3d4s4p	20.308	48.885	5.360
Ge	1.9	12	23 x 23 x 23	3s3p3d4s4p	23.899	58.988	4.945
As	1.8	12	22 x 22 x 8	3s3p3d4s4p	22.595	68.121	4.210
Se	1.7	12	10 x 10 x 9	3s3p3d4s4p	29.737	47.018	4.452
Br	1.6	12	4 x 8 x 4	3s3p3d4s4p	39.451	22.375	4.838
Kr	2.5	12	7 x 7 x 7	3d4s4p	66.039	0.646	7.238
Rb	1.9	12	18 x 18 x 18	3p3d4s4p5s	91.043	2.798	3.949
Sr	2.0	12	22 x 22 x 22	3d4s4p5s	54.407	11.618	5.334
Y	1.9	12	24 x 24 x 16	3d4s4p4d5s	32.852	41.391	3.267
Zr	1.8	12	27 x 27 x 17	3d4s4p4d5s	23.390	93.939	3.312
Nb	1.8	12	31 x 31 x 31	4s4p4d5s	18.126	168.449	3.665
Mo	1.6	12	33 x 33 x 33	4s4p4d5s	15.787	258.380	4.115
Tc	1.6	12	31 x 31 x 20	4s4p4d5s	14.436	299.401	4.557
Ru	1.6	12	32 x 32 x 20	4s4p4d5s	13.762	312.601	4.875
Rh	1.6	12	34 x 34 x 34	4s4p4d5s	14.040	257.642	5.197
Pd	1.6	12	33 x 33 x 33	4s4p4d5s	15.310	169.169	5.547
Ag	1.6	12	31 x 31 x 31	4s4p4d5s	17.842	91.486	5.772
Cd	1.6	12	28 x 28 x 15	4s4p4d5s	22.847	43.724	6.630

In	2.0	12	31 x 31 x 20	4s4p4d5s5p	27.474	35.693	5.141
Sn	1.9	12	20 x 20 x 20	4s4p4d5s5p	36.833	35.921	4.781
Sb	1.8	12	29 x 29 x 11	4s4p4d5s5p	31.750	50.351	4.528
Te	2.2	12	20 x 20 x 15	4s4p4d5s5p	34.971	44.698	4.680
I	2.1	12	4 x 8 x 4	4s4p4d5s5p	50.229	18.594	5.039
Xe	2.5	12	6 x 6 x 6	4d5s5p	87.016	0.541	6.953
Cs	1.9	12	17 x 17 x 17	4s4p4d5s5p6s	116.706	1.946	3.982
Ba	1.8	12	21 x 21 x 21	4s4p4d5s5p6s	63.294	8.853	0.788
Lu	1.8	12	25 x 25 x 16	4f5s5p5d6s	29.060	47.104	3.491
Hf	1.8	12	27 x 27 x 17	4f5s5p5d6s	22.534	106.671	3.563
Ta	1.8	12	31 x 31 x 31	4f5s5p5d6s	18.277	192.984	3.835
W	1.8	12	32 x 32 x 32	4f5s5p5d6s	16.145	302.786	4.226
Re	1.8	12	31 x 31 x 19	4f5s5p5d6s	14.960	363.074	4.336
Os	1.6	12	31 x 31 x 20	4f5s5p5d6s	14.279	397.148	4.803
Ir	1.6	12	34 x 34 x 34	4f5s5p5d6s	14.498	347.970	5.054
Pt	2.0	12	33 x 33 x 33	4f5s5p5d6s	15.642	248.632	5.440
Au	1.9	12	31 x 31 x 31	4f5s5p5d6s	17.980	139.241	5.799
Hg	2.1	12	25 x 25 x 29	4f5s5p5d6s	29.526	8.475	11.302
Tl	2.0	12	24 x 24 x 15	4f5s5p5d6s6p	31.427	26.461	5.338
Pb	1.9	12	26 x 26 x 26	4f5s5p5d6s6p	32.030	40.202	4.860
Bi	1.9	12	19 x 19 x 7	4f5s5p5d6s6p	36.923	42.539	4.632
Po	2.3	12	25 x 25 x 25	4f5s5p5d6s6p	37.566	45.342	4.553
Rn	2.5	12	6 x 6 x 6	5p5d6s6p	93.131	0.547	6.906