FLEUR

FLEUR 0.26 / LAPW(+lo)

`name and version of the code:` FLEUR 0.26
`type of basis set:` linearized augmented plane waves (+ local orbitals)
`method:` all-electron

GENERAL INFORMATION

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

METHOD-SPECIFIC INFORMATION

`muffin-tin radii`	see table (R_{MT})
`radial mesh`	981 radial mesh points on a logarithmic 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`	6
`largest` ℓ`-value in expansion of density and potential`	12
`largest vector in Fourier expansion of charge density`	3 × the magnitude of $K_{\max}$

ADDITIONAL COMMENTS

if $R_{\mathrm{MT}} \leq 1.5$ an APW+lo basisset was used

REFERENCES

`code`

[1] http://www.flapw.de

`scalar relativity`

[2] D. D. Koelling and B. N. Harmon, *J. Phys. C: Solid State* **10**, 3107–3114 (1977).

Table I. Calculation settings and results per element: muffin-tin radius R_{MT}, maximum wavevector $K_{\max}$, number of k-points in the full 1st Brillouin zone of the primitive cell # k, semicore and valence shells, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	R_{MT} [b]	$K_{\max}$ [1/b]	# k [–]	semicore | valence	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	0.65	5.2	1 089	1s	17.487	10.326	1.524
He	2.00	5.0	10 935	1s	17.961	0.768	6.479
Li	2.30	4.7	4 913	1s 2s	20.252	13.768	3.349
Be	2.00	5.0	10 935	2s	7.907	123.263	3.316
B	1.50	4.5	600	2s 2p	7.241	237.280	3.459
C	1.30	5.2	1 350	2s 2p	11.636	209.379	3.663
N	1.00	6.0	216	2s 2p	28.878	52.302	2.530
O	1.10	6.2	064	2s 2p	18.546	49.833	3.019
F	1.30	5.0	600	2s 2p	19.180	35.016	5.626
Ne	2.20	5.0	3 375	2s 2p	24.938	1.261	10.672
Na	2.40	4.7	3 375	2s 2p | 3s	37.469	7.472	3.771
Mg	2.30	5.0	10 935	2p | 3s	22.938	36.107	4.063
Al	2.30	5.0	4 913	3s 3p	16.495	76.564	4.360
Si	2.10	5.0	4 913	3s 3p	20.463	88.518	4.340
P	2.00	5.5	1 680	3s 3p	21.470	74.223	3.384
S	2.30	5.0	15 625	3s 3p	17.233	83.410	4.163
Cl	1.80	5.0	240	3s 3p	38.918	18.987	4.570
Ar	2.50	4.5	3 375	3s 3p	52.601	0.712	8.863
K	2.50	4.5	6 859	3s 3p | 4s	73.669	3.589	3.789
Ca	2.40	4.7	9 261	3s 3p | 4s	42.234	17.333	3.469
Sc	2.30	5.0	10 935	3s 3p | 3d 4s	24.625	54.591	3.439
Ti	2.10	5.2	16 337	3s 3p | 3d 4s	17.395	112.192	3.590
V	2.10	5.2	29 791	3s 3p | 3d 4s	13.469	184.157	3.910
Cr	2.10	5.2	13 824	3s 3p | 3d 4s	11.810	184.128	7.278
Mn	2.10	5.2	15 680	3s 3p | 3d 4s	11.489	122.568	1.076
Fe	2.10	5.2	29 791	3s 3p | 3d 4s	11.385	197.580	3.644
Co	2.20	5.0	9 375	3p | 3d 4s	10.885	219.434	5.322
Ni	2.20	5.0	15 625	3p | 3d 4s	10.905	202.173	5.059
Cu	2.28	5.0	15 625	3d 4s	11.972	141.149	5.088
Zn	2.40	4.7	3 757	3d | 4s	15.220	75.199	5.358
Ga	2.30	5.0	1 152	3d | 4s 4p	20.311	48.302	5.271
Ge	2.30	5.0	4 913	3d | 4s 4p	23.926	59.091	4.991
As	2.30	5.0	2 197	3d | 4s 4p	22.617	68.500	4.296
Se	2.20	5.0	486	3d | 4s 4p	29.791	47.313	4.630
Br	2.10	5.0	360	3d | 4s 4p	39.483	22.434	4.779
Kr	2.50	4.5	3 375	4s 4p	66.261	0.620	10.392
Rb	2.50	4.5	6 859	4s 4p | 5s	91.066	2.799	3.806
Sr	2.40	5.0	9 261	4s 4p | 5s	54.493	11.282	4.542
Y	2.30	5.0	9 375	4s 4p | 4d 5s	32.861	41.027	1.790
Zr	2.30	5.0	9 375	4s 4p | 4d 5s	23.404	93.599	3.105
Nb	2.30	5.0	15 625	4s 4p | 4d 5s	18.163	168.662	3.233
Mo	2.20	5.0	15 625	4s 4p | 4d 5s	15.806	259.112	4.433
Tc	2.20	5.0	9 375	4s 4p | 4d 5s	14.450	300.101	4.553
Ru	2.20	5.0	9 375	4p | 4d 5s	13.783	313.162	4.916
Rh	2.20	5.0	15 625	4p | 4d 5s	14.061	258.234	5.246
Pd	2.30	5.0	15 625	4p | 4d 5s	15.332	169.300	5.735
Ag	2.30	5.0	15 625	4s 4p | 4d 5s	17.844	89.574	5.954

Cd	2.50	4.7	3 757	4d | 5s	22.895	43.604	7.093
In	2.40	5.0	1 089	4d | 5s 5p	27.582	34.820	5.579
Sn	2.30	5.0	4 913	4d | 5s 5p	36.855	35.856	4.720
Sb	2.40	5.0	2 197	4d | 5s 5p	31.756	50.566	4.570
Te	2.30	5.0	405	4d | 5s 5p	34.999	44.735	4.676
I	2.50	4.5	480	4d | 5s 5p	50.274	18.717	5.223
Xe	2.50	4.5	3 375	4d | 5s 5p	86.920	0.563	7.631
Cs	2.40	4.5	15 625	5s 5p | 6s	116.618	1.959	3.306
Ba	2.40	4.5	15 625	5s 5p | 6s	63.209	8.883	3.167
Lu	2.30	5.0	9 375	4f 5s 5p | 5d 6s	29.052	47.001	3.775
Hf	2.30	5.0	9 375	4f 5s 5p | 5d 6s	22.544	107.882	3.124
Ta	2.30	5.0	15 625	4f 5s 5p | 5d 6s	18.290	189.938	3.421
W	2.30	5.0	15 625	5s 5p | 5d 6s	16.153	303.713	4.465
Re	2.30	5.0	9 375	5s 5p | 5d 6s	14.972	364.930	4.596
Os	2.30	5.0	9 375	5p | 5d 6s	14.295	399.584	4.766
Ir	2.30	5.0	15 625	5p | 5d 6s	14.505	349.950	5.100
Pt	2.30	5.0	15 625	5p | 5d 6s	15.627	250.406	5.834
Au	2.30	5.0	15 625	5p | 5d 6s	18.007	140.321	6.015
Hg	2.30	5.0	6 859	5p 5d | 6s	29.612	8.055	8.899
Tl	2.30	5.0	4 693	5d | 6s 6p	31.352	27.379	5.404
Pb	2.30	5.0	15 625	5d | 6s 6p	31.987	39.651	4.823
Bi	2.40	5.0	2 197	5d | 6s 6p	36.922	42.647	4.822
Po	2.40	5.0	13 824	5d | 6s 6p	37.598	45.146	5.365
Rn	2.50	4.5	3 375	5d | 6s 6p	93.218	0.500	8.101