WIEN2k/acc

WIEN2k 13.1 / APW+lo

`name and version of the code:` WIEN2k 13.1
`type of basis set:` 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 ($R_{MT}^{min} K_{max}$)
`k-mesh density`	see table (number of k-points in the full 1st Brillouin zone of the primitive cell, # k)
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.001 Ry

METHOD-SPECIFIC INFORMATION

`muffin-tin radii`	see table (R_{MT})
`radial mesh`	781 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`	6
`largest vector in Fourier expansion of charge density`	3 × the magnitude of the smallest vector
`IFFT-factor`	4

ADDITIONAL COMMENTS

none

REFERENCES

`code`

[1] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka and J. Luitz, "WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties" (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2.

`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}, basis set size $R_{MT}^{min}K_{max}$, number of k-points 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	0.50	5.0	7 260	1s	17.388	10.284	2.711
He	1.60	10.0	15 376	1s	17.771	0.847	7.708
Li	1.60	10.0	8 000	1s 2s	20.219	13.839	3.336
Be	1.80	10.0	31 941	2s	7.910	122.903	3.036
B	1.18	7.5	6 859	2s 2p	7.240	237.290	3.468
C	1.10	7.5	10 890	2s 2p	11.637	208.991	3.579
N	0.99	7.5	2 197	2s 2p	28.885	54.220	3.724
O	1.00	7.5	7 581	2s 2p	18.559	51.378	3.895
F	1.10	8.0	6 336	2s 2p	19.167	34.325	3.935
Ne	1.60	10.0	21 952	2s 2p	24.249	1.406	14.437
Na	1.60	10.0	4 913	2s 2p 3s	37.469	7.472	3.771
Mg	1.60	10.0	11 760	2s 2p 3s	22.936	35.933	4.067
Al	1.75	10.0	32 768	2p 3s 3p	16.480	78.077	4.570
Si	1.57	10.0	13 824	2p 3s 3p	20.453	88.545	4.306
P	1.73	10.0	6 174	3s 3p	21.471	68.208	4.348
S	1.60	10.0	29 791	3s 3p	17.184	83.407	4.261
Cl	1.60	10.0	3 528	3s 3p	38.889	19.081	4.343
Ar	1.60	10.0	10 648	3s 3p	52.385	0.743	7.256
K	1.60	10.0	8 000	3s 3p 4s	73.679	3.574	4.593
Ca	1.60	10.0	12 167	3s 3p 4s	42.199	17.114	3.312
Sc	1.60	10.0	10 935	3s 3p 3d 4s	24.620	54.393	3.424
Ti	1.60	10.0	14 400	3s 3p 3d 4s	17.390	112.213	3.583
V	1.60	10.0	39 304	3s 3p 3d 4s	13.452	181.674	3.745
Cr	1.60	10.0	21 952	3s 3p 3d 4s	11.773	183.899	7.158
Mn	1.60	10.0	22 528	3s 3p 3d 4s	11.447	118.632	−0.206
Fe	1.60	10.0	46 656	3s 3p 3d 4s	11.344	197.652	5.801
Co	1.93	10.0	24 624	3s 3p 3d 4s	10.864	216.489	4.363
Ni	1.85	10.0	46 656	3s 3p 3d 4s	10.891	199.970	5.006
Cu	1.78	10.0	42 875	3s 3p 3d 4s	11.957	141.121	4.845
Zn	1.70	10.0	16 335	3s 3p 3d 4s	15.195	74.572	5.271
Ga	2.04	10.0	6 800	3d 4s 4p	20.307	49.223	5.384
Ge	1.93	10.0	10 648	3d 4s 4p	23.915	59.128	4.988
As	1.82	10.0	3 703	3d 4s 4p	22.589	68.285	4.225
Se	1.72	10.0	6 400	3d 4s 4p	29.744	47.070	4.441
Br	1.64	10.0	3 200	3d 4s 4p	39.447	22.415	4.870
Kr	1.60	10.0	8 000	3d 4s 4p	65.658	0.671	9.857
Rb	1.89	10.0	5 832	4s 4p 5s	90.809	2.787	5.798
Sr	1.76	10.0	9 261	4s 4p 5s	54.527	11.256	3.490
Y	1.67	10.0	8 750	4s 4p 4d 5s	32.844	41.593	3.016
Zr	1.60	10.0	11 760	4s 4p 4d 5s	23.385	93.684	3.207
Nb	1.60	10.0	29 791	4s 4p 4d 5s	18.137	171.270	3.548
Mo	1.60	10.0	32 768	4s 4p 4d 5s	15.786	258.928	4.332
Tc	1.60	10.0	17 408	4s 4p 4d 5s	14.437	299.149	4.459
Ru	1.60	10.0	19 602	4s 4p 4d 5s	13.762	312.502	4.953
Rh	1.60	10.0	39 304	4s 4p 4d 5s	14.040	257.824	5.321
Pd	1.60	10.0	35 937	4s 4p 4d 5s	15.310	168.629	5.562
Ag	1.60	10.0	29 791	4s 4p 4d 5s	17.847	90.148	5.420
Cd	1.60	10.0	10 933	4s 4p 4d 5s	22.835	44.082	6.969

In	1.98	10.0	19 683	4p 4d 5s 5p	27.471	34.937	4.781
Sn	1.88	10.0	8 000	4p 4d 5s 5p	36.817	36.030	4.637
Sb	1.80	10.0	8 000	4p 4d 5s 5p	31.730	50.367	4.516
Te	2.17	10.0	5 200	4d 5s 5p	34.977	44.787	4.691
I	2.06	10.0	2 527	4d 5s 5p	50.233	18.654	5.046
Xe	2.00	10.0	6 859	4d 5s 5p	86.681	0.548	6.344
Cs	1.90	10.0	4 913	4d 5s 5p 6s	117.080	1.982	2.141
Ba	1.83	10.0	8 000	4d 5s 5p 6s	63.140	8.677	3.771
Lu	1.60	12.0	9 464	4f 5s 5p 5d 6s	29.054	46.384	2.943
Hf	1.60	12.0	11 760	4f 5s 5p 5d 6s	22.532	107.004	3.498
Ta	1.60	12.0	29 791	4f 5s 5p 5d 6s	18.286	195.147	3.714
W	1.60	12.0	32 768	4f 5s 5p 5d 6s	16.139	301.622	4.279
Re	1.60	12.0	17 408	4f 5s 5p 5d 6s	14.958	362.850	4.517
Os	1.60	12.0	17 408	4f 5s 5p 5d 6s	14.280	397.259	4.844
Ir	1.60	12.0	35 937	4f 5s 5p 5d 6s	14.500	347.680	5.179
Pt	1.97	12.0	32 768	5s 5p 5d 6s	15.642	248.711	5.465
Au	1.87	12.0	29 791	5s 5p 5d 6s	17.975	139.109	5.757
Hg	2.06	12.0	17 576	5s 5p 5d 6s	29.612	8.055	8.899
Tl	1.98	12.0	8 125	5p 5d 6s 6p	31.390	26.865	5.489
Pb	1.91	12.0	15 625	5p 5d 6s 6p	32.003	39.544	4.533
Bi	1.85	12.0	2 166	5p 5d 6s 6p	36.905	42.630	4.705
Po	2.31	12.0	13 824	5d 6s 6p	37.587	45.458	4.926
Rn	2.16	12.0	5 832	5d 6s 6p	92.685	0.564	8.618