Elk

Elk 3.1.5 / APW+lo

`Name and version of the code:` Elk 3.1.5 development version
`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 (k-mesh in the full 1st Brillouin zone of the primitive cell)
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.0005 Ha

METHOD-SPECIFIC INFORMATION

`muffin-tin radii`	see table (R_{MT})
`radial mesh`	200-700 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`	12
`largest` ℓ`-value in expansion of density and potential`	9

ADDITIONAL COMMENTS

Use elk version 3.1.5 or beyond. Set the internal flag *vhighq* to .True. for a highly accurate calculation together with the k-mesh and core-valence partition in the table in order to acquire the results described here.

REFERENCES

`code`

[1] http://elk.sourceforge.net/

`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 $R_{MT}^{min}K_{max}$, k-mesh in the full 1st Brillouin zone of the primitive cell $kpts$, valence, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	R_{MT} [b]	$R_{MT}^{min}K_{max}$ [–]	$kpts$	valence	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	1.00	5.0	10×10×8	$1s$	17.384	10.427	2.744
He	1.40	9.0	15×15×8	$1s$	17.779	0.866	6.040
Li	1.60	9.0	20×20×10	$1s$ $2s$	20.222	13.804	3.316
Be	1.90	9.0	27×27×15	$2s$	7.907	123.308	3.314
B	1.25	7.0	6×6×3	$2s$ $2p$	7.237	235.211	3.827
C	1.20	9.0	28×28×8	$2s$ $2p$	11.633	208.983	3.567
N	1.00	7.0	4×4×4	$2s$ $2p$	28.889	54.448	3.754
O	1.10	7.0	6×4×4	$2s$ $2p$	18.676	50.474	1.552
F	1.10	7.0	8×10×6	$2s$ $2p$	19.189	34.563	4.309
Ne	1.60	9.0	20×20×20	$2s$ $2p$	24.292	1.030	0.337
Na	2.00	9.0	24×24×24	$2s$ $2p$ $3s$	37.111	7.713	3.645
Mg	2.20	9.0	20×20×20	$2s$ $2p$ $3s$	22.959	35.887	3.785
Al	2.00	9.0	24×24×24	$2p$ $3s$ $3p$	16.475	77.319	4.461
Si	2.00	9.0	24×24×24	$3s$ $3p$	20.467	88.468	4.311
P	2.00	9.0	14×6×11	$3s$ $3p$	21.457	68.188	4.338
S	2.00	9.0	28×28×28	$3s$ $3p$	17.200	83.361	3.860
Cl	1.00	9.0	4×8×4	$3s$ $3p$	38.862	19.921	2.962
Ar	2.00	9.0	10×10×10	$3s$ $3p$	53.103	1.242	−12.069
K	2.20	9.0	24×24×24	$3s$ $3p$ $4s$	73.773	3.575	3.604
Ca	2.40	9.0	20×20×20	$3s$ $3p$ $4s$	42.252	16.637	3.686
Sc	2.00	9.0	26×26×16	$3s$ $3p$ $3d$ $4s$	24.645	54.346	3.375
Ti	1.90	9.0	20×20×20	$3s$ $3p$ $3d$ $4s$	17.388	109.212	3.955
V	1.80	9.0	26×26×26	$3s$ $3p$ $3d$ $4s$	13.453	182.886	3.886
Cr	2.00	9.0	26×26×26	$3s$ $3p$ $3d$ $4s$	11.774	182.677	7.260
Mn	2.00	9.0	16×16×16	$3s$ $3p$ $3d$ $4s$	11.440	117.306	0.755
Fe	2.10	9.0	32×32×32	$3s$ $3p$ $3d$ $4s$	11.340	195.057	4.982
Co	1.93	9.0	35×35×22	$3p$ $3d$ $4s$	10.851	212.235	4.785
Ni	2.00	9.0	18×18×18	$3p$ $3d$ $4s$	10.884	199.912	4.919
Cu	2.20	9.0	26×26×26	$3p$ $3d$ $4s$	11.935	141.094	5.157
Zn	2.20	9.0	24×24×20	$3p$ $3d$ $4s$	15.162	75.313	5.337
Ga	2.20	9.0	20×20×20	$3d$ $4s$ $4p$	20.271	49.586	6.295
Ge	1.60	9.0	20×20×20	$3d$ $4s$ $4p$	23.877	59.346	4.902
As	2.20	9.0	20×20×20	$3d$ $4s$ $4p$	22.589	67.586	5.753
Se	2.00	9.0	20×20×20	$3d$ $4s$ $4p$	29.768	47.069	4.655
Br	2.10	9.0	4×8×4	$3d$ $4s$ $4p$	39.467	22.398	4.649
Kr	3.00	9.0	20×20×20	$3d$ $4s$ $4p$	65.941	0.628	9.334
Rb	2.60	9.0	20×20×20	$4s$ $4p$ $5s$	91.216	2.788	3.757
Sr	2.60	9.0	20×20×20	$4s$ $4p$ $5s$	54.527	11.003	5.308
Y	2.30	9.0	28×28×20	$4s$ $4p$ $4d$ $5s$	32.891	41.133	3.183
Zr	2.20	9.0	28×28×16	$4s$ $4p$ $4d$ $5s$	23.407	93.791	3.354
Nb	2.00	9.0	24×24×24	$4s$ $4p$ $4d$ $5s$	18.139	170.922	3.837
Mo	2.00	9.0	24×24×24	$4s$ $4p$ $4d$ $5s$	15.787	259.067	4.215
Tc	2.00	9.0	20×20×20	$4s$ $4p$ $4d$ $5s$	14.441	299.311	4.482
Ru	1.70	9.0	26×26×14	$4s$ $4p$ $4d$ $5s$	13.756	312.566	4.899
Rh	2.00	9.0	31×31×31	$4s$ $4p$ $4d$ $5s$	14.029	257.177	5.226
Pd	2.20	9.0	24×24×24	$4s$ $4p$ $4d$	15.301	168.586	5.314
Ag	2.00	9.0	18×18×18	$4s$ $4p$ $4d$ $5s$	17.824	91.107	5.828
Cd	2.00	9.0	24×24×12	$4p$ $4d$ $5s$	22.584	45.833	7.265

In	2.75	9.0	20×20×20	$4p\ 4d\ 5s\ 5p$	27.519	36.312	4.859
Sn	2.60	9.0	20×20×20	$4p\ 4d\ 5s\ 5p$	36.863	35.285	4.509
Sb	2.60	9.0	20×20×20	$4d\ 5s\ 5p$	31.748	50.760	4.419
Te	2.60	9.0	20×20×20	$4d\ 5s\ 5p$	34.989	44.798	5.000
I	2.50	9.0	4×8×4	$4d\ 5s\ 5p$	50.256	18.718	4.861
Xe	2.40	9.0	16×16×16	$4d\ 5s\ 5p$	87.094	0.543	4.640
Cs	2.00	9.0	16×16×16	$4d\ 5s\ 5p\ 6s$	116.896	1.953	1.156
Ba	2.20	9.0	16×16×16	$4d\ 5s\ 5p\ 6s$	63.407	8.693	2.783
Lu	2.30	9.0	28×28×20	$4f\ 5s\ 5p\ 5d\ 6s$	29.039	46.680	3.474
Hf	2.00	9.0	20×20×20	$4f\ 5s\ 5p\ 5d\ 6s$	22.522	107.716	4.095
Ta	2.00	9.0	16×16×16	$4f\ 5s\ 5p\ 5d\ 6s$	18.302	193.210	3.913
W	2.00	9.0	20×20×20	$4f\ 5s\ 5p\ 5d\ 6s$	16.141	303.515	4.436
Re	1.80	9.0	28×28×18	$4f\ 5s\ 5p\ 5d\ 6s$	14.955	360.879	4.790
Os	2.40	9.0	24×24×13	$4f\ 5s\ 5p\ 5d\ 6s$	14.279	397.158	4.623
Ir	2.51	9.0	20×20×20	$4f\ 5p\ 5d\ 6s$	14.497	348.995	5.136
Pt	2.40	9.0	16×16×16	$4f\ 5p\ 5d\ 6s$	15.636	248.371	5.468
Au	2.20	9.0	28×28×28	$4f\ 5p\ 5d\ 6s$	17.969	140.419	5.945
Hg	2.00	9.0	28×28×31	$5p\ 5d\ 6s$	29.300	8.098	8.767
Tl	1.90	9.0	28×28×20	$5p\ 5d\ 6s\ 6p$	31.338	26.720	5.138
Pb	2.60	9.0	16×16×16	$5d\ 6s\ 6p$	31.973	39.380	4.335
Bi	2.60	9.0	20×20×8	$5d\ 6s\ 6p$	36.878	42.650	4.824
Po	2.60	9.0	37×37×37	$5d\ 6s\ 6p$	37.528	45.480	5.045
Rn	2.60	9.0	10×10×10	$5d\ 6s\ 6p$	92.709	0.560	4.085