Questaal

Questaal v7.14.1 / FP-LMTO

`name and version of the code:` Questaal version v7.14.1
`type of basis set:` Linear Muffin-Tin Orbitals
`method:` all-electron

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon [1])
`assignment of core / valence states`	see table
`basis set`	augmented smoothed Hankel functions [2]
`k-mesh density`	see table
`reciprocal-space integration method`	linear tetrahedron method

METHOD-SPECIFIC INFORMATION

`muffin-tin radii`	touching spheres at the smallest volume tested
`basis set size`	2 basis functions per l, m (2-κ basis) with $l \leq$`LMX` partial wave expansion with $l \leq$`LMXA` (see table)
`local orbitals and LAPW`	extended local orbitals for semi-core states combined LMTO/APW basis for molecular cases local orbitals for higher n (see comments and table)
`core treatment`	overlapping frozen atomic core density

ADDITIONAL COMMENTS

1. Each LMTO basis function is defined by two parameters, the smoothing radius (`RSMH`) and the Hankel energy (`EH`). The two basis functions per l are constructed with different `RSMH` using an automatic system in which the Hankel energy is a free parameter – `EH=-0.5` Ryd is used here for all systems.

2. The criteria for inclusion of states as semi-core are the leaked charge or atomic eigenvalue: $q(r > R_{mt})$ >2e-3 or $e > -2.2$Ryd. "Extended" local orbitals include smoothed Hankel tails fitted to the semi-core K.E at the muffin-tin radius.

3. Some high-lying local orbitals are included: e.g., the 3d transition elements are treated with the 4d states as local orbitals.

4. An additional LAPW basis is used in combination with the LMTO basis when the (touching) muffin-tin spheres fill < 30% of the cell.

5. Full details of the calculations can be found in the source distribution.

REFERENCES

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

[2] E. Bott, M. Methfessel, W. Krabs and P. C. Schmidt, *J. Math. Phys.* **39**, 3393–3425 (1998).

Table I. Calculation settings and fitted equation of state results for each element: k-point grid, muffin-tin radius, l cut-offs for basis and augmentation, specification of semi-core and *high-lying* local orbitals and the plane-wave cut-off for additional LAPW basis, if present.

	NKABC	R_{mt} (Bohr)	LMAX	LMAXA	local orbitals	LAPW (Ryd)	V_0 (Å^3/at)	B_0 (GPa)	B_1
H	6 6 4	0.695	1	2		4.0	17.401	10.286	2.91
He	6 6 3	2.708	1	2					
Li	23 23 23	2.821	2	3			20.201	13.853	3.35
Be	23 23 13	2.048	2	3			7.895	123.443	3.32
B	7 7 7	1.597	2	3			7.205	239.564	3.46
C	16 16 4	1.319	2	3		2.0	11.635	206.530	4.01
N	5 5 5	1.030	2	3		4.0	28.833	52.396	1.97
O	6 6 6	1.140	2	3		4.0	18.679	50.849	3.83
F	5 9 5	1.320	2	3		4.0	19.219	38.000	4.75
Ne	5 5 5	3.025	2	3			24.532	0.855	-2.45
Na	18 18 18	3.463	2	3	2p		37.106	7.793	3.72
Mg	30 30 16	2.939	2	3			22.959	36.582	4.03
Al	12 12 12	2.644	2	3			16.491	77.908	4.99
Si	13 13 13	2.191	2	3			20.454	87.341	4.33
P	17 5 12	2.058	2	3		2.0	21.640	66.466	4.27
S	22 22 22	2.389	2	3			17.072	89.015	4.19
Cl	4 8 4	1.848	2	3		4.0	39.393	19.787	3.50
Ar	5 5 5	3.895	2	3	3s		56.226	0.810	-0.53
K	13 13 13	4.237	3	4	3p,*4d*		73.768	3.616	3.75
Ca	19 19 19	3.616	3	4	3p,*4d*		42.289	17.504	3.28
Sc	21 21 12	2.976	3	4	3p,*4d*		24.646	55.135	3.44
Ti	15 15 8	2.664	3	4	3p,*4d*		17.406	113.080	3.63
V	15 15 15	2.403	3	4	3p,*4d*		13.461	183.653	3.90
Cr	19 19 19	2.301	3	4	3p,*4d*		11.759	184.827	7.11
Mn	15 15 15	2.353	3	4	3p,*4d*		11.443	120.279	0.66
Fe	9 9 9	2.271	3	4	3p,*4d*		11.355	201.389	5.63
Co	16 16 9	2.293	3	4	*4d*		10.884	213.286	3.92
Ni	13 13 13	2.306	3	4	*4d*		10.909	200.088	5.14
Cu	21 21 21	2.380	3	4	*4d*		11.942	139.805	4.94
Zn	27 27 13	2.463	3	4	*4d*		15.185	74.744	5.29
Ga	32 19 32	2.349	3	4	3d		20.313	48.649	5.28
Ge	17 17 17	2.309	3	4	3d		23.914	58.045	4.89
As	27 27 8	2.366	3	4			22.652	69.459	4.28
Se	10 10 8	2.225	3	4		2.0	29.906	47.059	4.39
Br	5 10 5	2.187	3	4		2.0	39.414	26.195	2.13
Kr	5 5 5	4.207	3	4	4s		67.096	0.509	-5.04
Rb	10 10 10	4.546	3	4	4p,*5d*		91.114	2.809	3.74
Sr	21 21 21	3.939	3	4	4p,*5d*		54.554	11.432	4.41
Y	17 17 9	3.274	3	4	4p,*5d*		32.905	41.934	3.31
Zr	20 20 11	2.959	3	4	4p,*5d*		23.427	94.614	3.22
Nb	15 15 15	2.663	3	4	4p,*5d*		18.122	171.090	3.90
Mo	14 14 14	2.540	3	4	4p,*5d*		15.787	261.711	4.24
Tc	22 22 12	2.522	3	4	4p,*5d*		14.449	300.855	4.55
Ru	27 27 15	2.466	3	4	4p,*5d*		13.757	313.631	4.90
Rh	13 13 13	2.514	3	4	4p,*5d*		14.039	258.728	5.23
Pd	24 24 24	2.587	3	4	4p,*5d*		15.294	170.649	5.62
Ag	24 24 24	2.725	3	4	*5d*		17.796	91.658	5.92

Cd	26 26 12	2.811	3	4	*5d*		22.796	44.354	7.04
In	14 14 9	3.052	3	4	*5d*		27.440	35.913	5.22
Sn	16 16 16	2.667	3	4	4d		36.899	35.007	4.75
Sb	17 17 6	2.735	3	4	4d		31.716	50.810	4.48
Te	14 14 9	2.680	3	4			34.804	46.791	4.67
I	5 10 4	2.560	3	4		2.0	50.493	19.387	3.98
Xe	5 5 5	4.617	3	4	5s		86.475	0.257	-13.02
Cs	12 12 12	4.939	3	4	5s,5p,*6d*		117.081	1.963	3.36
Ba	13 13 13	4.029	3	4	5p,*6d*		63.431	8.764	3.13
Lu	17 17 9	3.158	3	4	5p,*6d*,*5f*		29.076	47.184	3.48
Hf	15 15 8	2.902	3	4	5p,*6d*,*5f*		22.538	107.760	3.42
Ta	22 22 22	2.662	3	4	5p,*6d*,*5f*		18.280	194.171	3.86
W	23 23 23	2.556	3	4	5p,*6d*,*5f*		16.141	303.169	4.23
Re	21 21 11	2.549	3	4	5p,*6d*		14.967	366.638	4.55
Os	23 23 13	2.497	3	4	5p,*6d*		14.282	399.010	4.85
Ir	21 21 21	2.537	3	4	5p,*6d*		14.501	349.274	5.15
Pt	19 19 19	2.602	3	4	5p,*6d*		15.633	250.112	5.53
Au	18 18 18	2.731	3	4	*6d*		17.926	141.311	5.93
Hg	11 11 13	3.147	3	4	*6d*		29.102	10.750	10.11
Tl	30 30 17	3.240	3	4	5d		31.426	27.114	5.34
Pb	24 24 24	3.301	3	4	5d		32.014	40.648	4.74
Bi	26 26 9	2.881	3	4	5d		36.651	44.295	4.50
Po	18 18 18	3.099	3	4			37.405	48.502	4.49
Rn	5 5 5	4.708	3	4	6s		83.371	0.151	-6.33