RSPt

RSPt revision 1904 / FP-LMTO

`name and version of the code:` RSPt repository revision 1904
`type of basis set:` linear muffin-tin 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-mesh density`	see table (number of k-points in the full 1st Brillouin zone of the primitive cell, # k)
`reciprocal-space integration method`	modified tetrahedron method on a Fourier quadrature mesh [3]

METHOD-SPECIFIC INFORMATION

`muffin-tin radii`	95% of touching, rescaled with volume, except for O and Xe, which had fixed radii of 1.10 and 2.70 bohr radii, respectively
`radial mesh`	450-600 radial mesh points on a logarithmic grid, selected automatically.
`wave function` ℓ `cutoff`	8
`potential and density` ℓ `cutoff`	8
`interstitial Fourier mesh`	see table

`basis set specification`

The default choice (repository revision 1904) is described by the letter 'V', indicating 'valence', i.e. basis functions corresponding to the selected valence electrons, always including s, p and d basis functions above the completely filled semi-core shells. Basis functions for the interstitial are spherical Hankel functions at kinetic energies 0.3, -0.6 and -2.3 Ry, the first one being replaced by the average kinetic energy over the interstitial. s and p basis functions are by default attached to all three tails, d functions, occupied f functions and semi-core states to tails 1 and 2 and higher polarization functions are attached to only the "interstitial average" tail. The most common basis setting is then describable as V+4f, indicating that f electrons were added to the normal setting.
More complex variations are denoted by specifically singling out the modified shells and describe them separately after the 'V+' symbol, specifying the choice of linearization energy in parentheses () and attached tails in square brackets []. For example, the Na basis (V+4f, including $2s$, $2p$ and $3s$ electrons) could explicitly be given as:
2s(0)[1,2] 2p(0)[1,2] 3s(20)[1,2,3] 3s(21)[1,2,3] 3d(0)[1,2] 4f(0)[1]
The meaning of the choices of linearization energies are explained in the RSPt manual.

ADDITIONAL COMMENTS

The LMTO basis set required for high accuracy varies predictably across the periodic table, with the notable exception of Cl, which required a very large basis. The reason for this anomaly is not clear, but good convergence was nevertheless achievable. This appears to be a special feature of the Cl dimeric crystal which has not been observed in other Cl compounds. A very large basis was also required for the 5d series, where a crossover of the 4f and 5p semi-core bands occur.

REFERENCES

`code`

[1] J. M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, and O. Grechnyev, *Full-Potential Electronic Structure Method, Energy and Force Calculations with Density Functional and Dynamical Mean Field Theory*, volume 167 of Springer Series in Solid-State Sciences. Springer-Verlag, Berlin Heidelberg (2010).

`scalar relativity`

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

`Brillouin zone integration`

[3] S. Froyen, *Phys. Rev. B*, **39** 3168–3172 (1989).

Table I. Calculation settings and results per element: basis (see explanation under 'basis set specification'), interstitial Fourier mesh, 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.

	Basis	FFT grid	# k [–]	Valence	V_0 [$\frac{\mathring{A}^3}{atom}$]	B_0 [GPa]	B_1 [–]
H	V	(42,42,64)	3 888	1s	17.348	10.504	2.580
He	V	(24,24,40)	4 000	1s	17.865	0.824	6.457
Li	V	(30,30,30)	8 000	1s 2s	20.248	13.748	3.129
Be	V	(24,24,40)	2 000	1s 2s	7.906	123.165	3.309
B	V+4f	(45,45,48)	576	2s 2p	7.246	236.771	3.269
C	V+4f	(20,20,72)	4 608	2s 2p	11.649	207.772	3.572
N	V	(64,64,64)	1 000	2s 2p	28.894	53.658	3.683
O	V	(96,96,96)	216	2s 2p	18.566	49.923	3.796
F	V	(96,64,96)	144	2s 2p	19.251	34.415	4.039
Ne	V	(32,32,32)	1 728	2s 2p	27.716	0.496	11.006
Na	V+4f	(30,30,30)	4 608	2s 2p 3s	37.022	7.799	3.759
Mg	V+4f	(24,24,40)	4 000	2s 2p 3s	22.923	36.225	4.024
Al	V+4f	(20,20,20)	6 912	2p 3s 3p	16.493	78.166	4.854
Si	V+4f	(25,25,25)	2 048	2p 3s 3p	20.492	87.962	4.319
P	V+4f	(24,90,36)	560	2p 3s 3p	21.571	67.049	4.338
S	V+4f	(20,20,20)	7 942	3s 3p	17.223	83.465	4.115
Cl	V+4f+5g1 4d[3] 4s[1,2] 4p[1,2]	(48,27,60)	1 024	3s 3p	38.938	24.938	0.106
Ar	V+4f	(32,32,32)	4 096	3s 3p	54.467	0.613	8.809
K	V+4f	(25,25,25)	5 832	3s 3p 4s	73.708	3.601	3.646
Ca	V+4f	(20,20,20)	6 912	3s 3p 4s	42.247	17.565	3.210
Sc	V+4f	(24,24,40)	4 000	3s 3p 3d 4s	24.650	54.649	3.291
Ti	V+4f	(24,24,40)	4 000	3s 3p 3d 4s	17.415	111.675	3.615
V	V+4f	(25,25,25)	4 096	3s 3p 3d 4s	13.470	182.345	3.857
Cr	V+4f	(25,25,25)	32 768	3s 3p 3d 4s	11.838	183.708	−1.489
Mn	V+4f	(24,24,36)	9 216	3s 3p 3d 4s	11.461	118.129	0.173
Fe	V+4f	(25,25,25)	32 768	3s 3p 3d 4s	11.344	195.786	5.599
Co	V+4f	(24,24,40)	20 480	3s 3p 3d 4s	10.866	213.590	4.849
Ni	V+4f	(32,32,32)	16 384	3s 3p 3d 4s	10.898	198.488	4.891
Cu	V+4f	(20,20,20)	16 384	3s 3p 3d 4s	11.965	140.904	5.046
Zn	V+4f	(20,20,40)	4 000	3s 3p 3d 4s	15.214	74.774	5.409
Ga	V+4f	(36,64,36)	864	3d 4s 4p	20.402	48.421	4.979
Ge	V+4f	(25,24,25)	4 000	3d 4s 4p	24.029	58.900	4.572
As	V+4f	(36,36,108)	1 944	3d 4s 4p	22.666	68.064	4.156
Se	V+4f 4d[3]	(36,36,45)	3 375	3d 4s 4p	29.932	46.243	4.363
Br	V+4f 4d[3]	(81,54,96)	1 024	3d 4s 4p	39.875	21.933	4.828
Kr	V+4f	(48,48,48)	4 096	3d 4s 4p	66.723	0.632	6.257
Rb	V+4f	(25,25,25)	4 097	4s 4p 5s	90.905	2.798	3.730
Sr	V+4f	(20,20,20)	6 912	4s 4p 5s	54.449	6.989	9.328
Y	V+4f	(24,24,40)	4 000	4s 4p 4d 5s	32.886	41.158	3.078
Zr	V+4f	(24,24,40)	4 000	4s 4p 4d 5s	23.422	93.632	3.357
Nb	V+4f	(25,25,25)	4 096	4s 4p 4d 5s	18.156	169.960	3.551
Mo	V+4f	(25,25,25)	13 824	4s 4p 4d 5s	15.813	258.382	4.198
Tc	V+4f	(24,24,40)	4 000	4s 4p 4d 5s	14.460	299.496	5.134
Ru	V+4f	(24,24,40)	4 000	4s 4p 4d 5s	13.791	310.790	4.907
Rh	V+4f	(20,20,20)	6 912	4s 4p 4d 5s	14.071	256.396	5.221

Pd	V+4f	(20,20,20)	6 912	4s 4p 4d 5s	15.339	168.636	5.534
Ag	V+4f	(25,25,25)	6 912	4s 4p 4d 5s	17.870	90.926	5.774
Cd	V+4f	(20,20,40)	4 000	4s 4p 4d 5s	22.904	42.213	4.704
In	V+4f 4d[3]	(24,24,36)	3 888	4p 4d 5s 5p	27.512	35.448	4.948
Sn	V+4f 4d[3]	(25,25,25)	4 000	4p 4d 5s 5p	37.019	35.578	4.576
Sb	V+4f 4d[3]	(36,36,96)	1 125	4p 4d 5s 5p	31.829	49.781	4.567
Te	V+4f 4d[3]	(27,27,36)	3 072	4d 5s 5p	35.186	43.951	4.589
I	V+4f 4d[3]	(96,56,128)	1 024	4d 5s 5p	50.795	17.952	5.295
Xe	V+4f 4d[3]	(48,48,48)	4 096	4d 5s 5p	92.929	0.539	2.652
Cs	V+4f[1,2]	(25,25,25)	4 096	4d 5s 5p 6s	117.168	1.887	1.462
Ba	V+4f[1,2]	(25,25,25)	4 096	4d 5s 5p 6s	63.267	9.097	2.649
Lu	V+5p(-1)[1,2,3] 4f(-1)[1,2,3]	(24,24,40)	4 000	4f 5s 5p 5d 6s	29.090	47.059	3.622
Hf	V+5p(-1)[1,2,3] 4f(-1)[1,2,3]	(24,24,40)	4 000	4f 5s 5p 5d 6s	22.540	106.803	3.426
Ta	V+5p(-1)[1,2,3] 4f(-1)[1,2,3]	(20,20,20)	13 824	4f 5s 5p 5d 6s	18.299	193.397	3.456
W	V+5p(-1)[1,2,3] 4f(-1)[1,2,3]	(20,20,20)	3 456	4f 5s 5p 5d 6s	16.156	299.772	4.338
Re	V+5p(-1)[1,2,3] 4f(-1)[1,2,3]	(24,24,40)	4 000	4f 5s 5p 5d 6s	14.979	362.519	4.325
Os	V+5p(-1)[1,2,3] 4f(-1)[1,2,3]	(24,24,40)	6 912	4f 5s 5p 5d 6s	14.297	396.392	4.735
Ir	V+5p(-1)[1,2,3] 4f(-1)[1,2,3]	(20,20,20)	6 912	4f 5s 5p 5d 6s	14.516	347.483	5.125
Pt	V+5f	(20,20,20)	6 912	5s 5p 5d 6s	15.666	247.747	5.421
Au	V+5f	(20,20,20)	6 912	5s 5p 5d 6s	18.005	139.347	6.081
Hg	V+5f	(27,27,24)	8 000	5s 5p 5d 6s	30.003	6.958	10.265
Tl	V+5f	(24,24,40)	4 000	5p 5d 6s 6p	31.475	26.455	5.771
Pb	V+5f 5d(-1)[1,2,3]	(20,20,20)	6 912	5p 5d 6s 6p	31.995	38.841	6.350
Bi	V+5f 5d(-1)[1,2,3]	(27,27,72)	4 693	5p 5d 6s 6p	37.021	43.647	7.254
Po	V+5f 5d(-1)[1,2,3]	(20,20,20)	13 824	5d 6s 6p	37.694	45.007	4.887
Rn	V+5f 5d(-1)[1,2,3]	(20,20,20)	6 912	5d 6s 6p	92.476	0.704	5.013