FPLO/default

FPLO 14.00-49 / default LO basis and settings

`name and version of the code:` FPLO 14.00-49
`type of basis set:` numerical atom-centered local orbitals
`method:` all-electron

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see Section additional comments and table
`basis set size`	default (see below): 5-33 basis orbitals (typical basis set size of 20)
`k-mesh density`	see table (number of k-points in the full 1st Brillouin zone of the primitive cell, # k)
`reciprocal-space integration method`	linear tetrahedron method

METHOD-SPECIFIC INFORMATION

`numerical settings`	all settings are default settings except for k-mesh (see table)

ADDITIONAL COMMENTS

In the table below, the basis set is denoted in the following way: semi-core orbitals are separated by a /, Dnl means double basis orbitals, e.g. D3p = 3p4p. Ultra soft elements require a (non default) fixed compact support radius (as was used in the `FPLO/T+F+s` set of calculations). For this reason some of those elements (Xe, Rn, Hg) are excluded from the tables. The use of the linear tetrahedron method allows to keep the relatively small default k-mesh, except for the cases C, Al, Ag, where we used a higher k-point number for testing reasons.

REFERENCES

`code`

[1] K. Koepernik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999)
[2] www.fplo.de

`scalar relativity`

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

`reciprocal-space integration`

[4] G. Lehmann and M. Taut, *Phys. Status Solidi B* **54**, 469–477 (1972).

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Table I. Calculation settings and results per element: k-point mesh in the full 1st Brillouin zone of the primitive cell *kpts* and number of irreducible k-points # k, valence, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	kpts [–]	# k [–]	semi-core/valence	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	12 × 12 × 12	1 728	/ D1s 2p	17.814	10.242	2.733
He	12 × 12 × 12	1 728	/ D1s 2p	18.006	0.821	6.521
Li	12 × 12 × 12	1 728	1s / D2s D2p 3d	20.296	13.834	3.120
Be	12 × 12 × 12	1 728	1s / D2s D2p 3d	7.960	121.966	3.319
B	12 × 12 × 12	1 728	1s / D2s D2p 3d	7.363	232.928	3.469
C	12 × 12 × 30	4 320	1s / D2s D2p 3d	11.682	208.922	3.591
N	12 × 12 × 12	1 728	1s / D2s D2p 3d	29.250	54.097	3.779
O	12 × 12 × 12	1 728	1s / D2s D2p 3d	18.912	50.506	3.896
F	12 × 12 × 12	1 728	1s / D2s D2p 3d	19.479	33.690	4.080
Ne	12 × 12 × 12	1 728	1s / D2s D2p 3d	24.632	1.212	7.111
Na	12 × 12 × 12	1 728	2s 2p / D3s D3p 3d	37.269	7.732	3.648
Mg	12 × 12 × 12	1 728	2s 2p / D3s D3p 3d	22.958	36.094	4.040
Al	30 × 30 × 30	27 000	2s 2p / D3s D3p 3d	16.511	77.636	4.572
Si	12 × 12 × 12	1 728	2s 2p / D3s D3p 3d	20.563	87.877	4.293
P	12 × 12 × 12	1 728	2s 2p / D3s D3p 3d	21.710	65.989	4.346
S	12 × 12 × 12	1 728	2s 2p / D3s D3p 3d	17.506	82.463	4.066
Cl	12 × 12 × 12	1 728	2s 2p / D3s D3p 3d	40.005	17.915	4.425
Ar	12 × 12 × 12	1 728	2s 2p / D3s D3p 3d	53.005	0.707	8.199
K	12 × 12 × 12	1 728	3s 3p / D4s 4p D3d	73.927	3.550	4.271
Ca	12 × 12 × 12	1 728	3s 3p / D4s 4p D3d	42.376	17.676	2.763
Sc	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	24.700	54.659	3.483
Ti	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	17.487	111.484	3.577
V	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	13.475	181.755	3.911
Cr	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	11.807	181.337	7.401
Mn	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	11.136	139.431	7.920
Fe	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	11.339	194.220	5.085
Co	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	10.904	217.288	4.927
Ni	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	10.933	199.420	4.953
Cu	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	12.006	140.602	5.131
Zn	12 × 12 × 12	1 728	3s 3p / D4s D3d 4p	15.228	76.333	5.243
Ga	12 × 12 × 12	1 728	3s 3p 3d / D4s D4p 4d	20.624	47.270	5.055
Ge	12 × 12 × 12	1 728	3s 3p 3d / D4s D4p 4d	24.074	58.206	4.819
As	12 × 12 × 12	1 728	3s 3p 3d / D4s D4p 4d	22.844	67.087	3.977
Se	12 × 12 × 12	1 728	3s 3p 3d / D4s D4p 4d	30.411	45.391	4.449
Br	12 × 12 × 12	1 728	3s 3p 3d / D4s D4p 4d	40.571	21.231	4.758
Kr	12 × 12 × 12	1 728	3s 3p 3d / D4s D4p 4d	67.977	0.653	0.695
Rb	12 × 12 × 12	1 728	4s 4p / D5s 5p D4d	91.012	2.820	6.216
Sr	12 × 12 × 12	1 728	4s 4p / D5s 5p D4d	54.519	11.780	4.029
Y	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	32.972	41.360	3.493
Zr	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	23.564	93.640	3.559
Nb	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	18.248	169.905	3.789
Mo	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	15.959	257.816	4.163
Tc	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	14.604	295.456	4.472
Ru	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	13.908	310.410	4.914
Rh	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	14.221	252.623	5.199
Pd	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	15.530	163.813	5.388
Ag	30 × 30 × 30	27 000	4s 4p / D5s D4d 5p	18.064	89.425	5.818
Cd	12 × 12 × 12	1 728	4s 4p / D5s D4d 5p	22.980	42.652	7.573

In	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / D$5s$ $5d$ D$5p$	27.762	34.797	5.249
Sn	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / D$5s$ $5d$ D$5p$	37.371	34.251	4.851
Sb	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / D$5s$ $5d$ D$5p$	32.267	48.865	4.961
Te	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / D$5s$ $5d$ D$5p$	35.738	44.276	4.753
I	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / D$5s$ $5d$ D$5p$	52.230	17.377	4.847
Cs	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / D$6s$ D$5d$ $6p$	120.034	3.023	−1.799
Ba	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / D$6s$ $5d$ $6p$	64.746	5.905	4.374
Lu	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / D$6s$ D$5d$ $6p$ D$4f$	29.242	44.618	1.473
Hf	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / D$6s$ D$5d$ $6p$	22.687	107.319	2.917
Ta	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / D$6s$ D$5d$ $6p$	18.372	192.520	4.079
W	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / D$6s$ D$5d$ $6p$	16.281	299.936	4.293
Re	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / D$6s$ D$5d$ $6p$	15.104	350.456	4.364
Os	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / D$6s$ D$5d$ $6p$	14.421	386.707	5.033
Ir	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / D$6s$ D$5d$ $6p$	14.687	336.516	5.339
Pt	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / D$6s$ D$5d$ $6p$	15.861	248.654	4.888
Au	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / D$6s$ D$5d$ $6p$	18.201	136.117	5.586
Tl	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / D$6s$ $6d$ D$6p$	32.192	25.795	−0.186
Pb	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / D$6s$ $6d$ D$6p$	32.238	41.750	7.836
Bi	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / D$6s$ $6d$ D$6p$	37.260	41.671	7.016
Po	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / D$6s$ $6d$ D$6p$	37.996	44.318	5.586