FPLO/T+F

FPLO 14.00-49 / enhanced LO basis

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	enhanced (see below): 21-56 basis orbitals (typical basis set size of 35)
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 the basis and k-mesh (see below and table).

ADDITIONAL COMMENTS

We enhanced the default basis according to the following scheme. The core and semi-core orbitals stay untouched. A double valence basis orbital (e.g. $3d4d$) becomes a triple basis orbital (e.g. $3d4d5d$) with the charge parameter $Q_3 = Q_2 + 2$ and compression parameter $P_3 = \max(0.85, P_2)$. A single valence basis orbital becomes a double basis orbital with $Q_2 = Q_1 + 2$ and $P_2 = \max(0.85, P_1)$. An additional f-orbital is added with $Q = 4$ and $P = 1$. For H and He additionally a single d-orbital ($Q = 5$, $P = 1$) is added to the default basis. 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 = $3p4p$, Tnl means triple basis orbitals, e.g. T3p = $3p4p5p$. The additional nominal $5f$ orbital for Lu is of course not identical to the $5f$ part of its T4f basis states but rather an effective $7f$ state. 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).

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	/ T1s D2p 4f 3d	17.427	10.245	2.612
He	12 × 12 × 12	1 728	/ T1s D2p 4f 3d	17.892	0.836	6.491
Li	12 × 12 × 12	1 728	1s / T2s T2p D3d 4f	20.302	13.721	3.142
Be	12 × 12 × 12	1 728	1s / T2s T2p D3d 4f	7.911	123.155	3.311
B	12 × 12 × 12	1 728	1s / T2s T2p D3d 4f	7.274	235.966	3.464
C	12 × 12 × 30	4 320	1s / T2s T2p D3d 4f	11.652	207.885	3.572
N	12 × 12 × 12	1 728	1s / T2s T2p D3d 4f	28.870	53.512	3.756
O	12 × 12 × 12	1 728	1s / T2s T2p D3d 4f	18.695	49.733	3.844
F	12 × 12 × 12	1 728	1s / T2s T2p D3d 4f	19.331	33.727	4.041
Ne	12 × 12 × 12	1 728	1s / T2s T2p D3d 4f	24.480	1.221	7.123
Na	12 × 12 × 12	1 728	2s 2p / T3s T3p D3d 4f	37.179	7.715	3.670
Mg	12 × 12 × 12	1 728	2s 2p / T3s T3p D3d 4f	22.936	35.882	4.141
Al	30 × 30 × 30	27 000	2s 2p / T3s T3p D3d 4f	16.488	77.482	4.593
Si	12 × 12 × 12	1 728	2s 2p / T3s T3p D3d 4f	20.483	88.289	4.297
P	12 × 12 × 12	1 728	2s 2p / T3s T3p D3d 4f	21.496	67.764	4.332
S	12 × 12 × 12	1 728	2s 2p / T3s T3p D3d 4f	17.260	84.276	4.129
Cl	12 × 12 × 12	1 728	2s 2p / T3s T3p D3d 4f	39.134	18.579	4.403
Ar	12 × 12 × 12	1 728	2s 2p / T3s T3p D3d 4f	52.686	0.719	8.192
K	12 × 12 × 12	1 728	3s 3p / T4s D4p T3d 4f	73.926	3.527	4.289
Ca	12 × 12 × 12	1 728	3s 3p / T4s D4p T3d 4f	42.320	17.476	2.595
Sc	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	24.618	54.688	3.413
Ti	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	17.396	111.947	3.551
V	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	13.447	181.646	3.880
Cr	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	11.785	184.253	7.314
Mn	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	11.468	100.527	8.437
Fe	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	11.359	191.502	5.356
Co	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	10.878	216.897	4.965
Ni	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	10.908	199.051	4.972
Cu	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	11.974	140.348	5.146
Zn	12 × 12 × 12	1 728	3s 3p / T4s T3d D4p 4f	15.207	75.445	5.292
Ga	12 × 12 × 12	1 728	3s 3p 3d / T4s T4p D4d 4f	20.383	48.761	5.182
Ge	12 × 12 × 12	1 728	3s 3p 3d / T4s T4p D4d 4f	23.924	58.958	4.915
As	12 × 12 × 12	1 728	3s 3p 3d / T4s T4p D4d 4f	22.633	67.560	4.039
Se	12 × 12 × 12	1 728	3s 3p 3d / T4s T4p D4d 4f	29.856	46.692	4.446
Br	12 × 12 × 12	1 728	3s 3p 3d / T4s T4p D4d 4f	39.636	22.145	4.752
Kr	12 × 12 × 12	1 728	3s 3p 3d / T4s T4p D4d 4f	67.564	0.635	0.529
Rb	12 × 12 × 12	1 728	4s 4p / T5s D5p T4d 4f	90.955	2.805	6.262
Sr	12 × 12 × 12	1 728	4s 4p / T5s D5p T4d 4f	54.443	11.700	4.070
Y	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	32.862	41.364	3.525
Zr	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	23.403	94.148	3.428
Nb	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	18.117	169.586	3.694
Mo	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	15.806	259.205	4.263
Tc	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	14.467	297.489	4.445
Ru	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	13.793	310.576	4.937
Rh	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	14.078	255.504	5.197
Pd	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	15.350	166.938	5.306
Ag	30 × 30 × 30	27 000	4s 4p / T5s T4d D5p 4f	17.883	90.451	5.784
Cd	12 × 12 × 12	1 728	4s 4p / T5s T4d D5p 4f	22.835	43.273	7.811

In	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T5s D5d T5p $4f$	27.588	35.164	5.243
Sn	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T5s D5d T5p $4f$	36.922	35.119	4.834
Sb	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T5s D5d T5p $4f$	31.824	50.010	4.952
Te	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T5s D5d T5p $4f$	35.169	45.240	4.734
I	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T5s D5d T5p $4f$	50.976	18.078	3.423
Cs	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T6s T5d D6p $5f$	120.111	3.015	−1.820
Ba	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T6s D5d D6p $4f$	63.901	6.052	6.146
Lu	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T6s T5d D6p T4f $5f$	29.183	44.303	1.445
Hf	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T6s T5d D6p $5f$	22.584	106.895	2.931
Ta	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T6s T5d D6p $5f$	18.279	192.499	4.046
W	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T6s T5d D6p $5f$	16.178	301.300	4.285
Re	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T6s T5d D6p $5f$	14.994	352.329	4.370
Os	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T6s T5d D6p $5f$	14.314	389.219	5.053
Ir	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T6s T5d D6p $5f$	14.532	342.719	5.373
Pt	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T6s T5d D6p $5f$	15.691	254.342	4.624
Au	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T6s T5d D6p $5f$	18.021	138.071	4.300
Tl	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T6s D6d T6p $5f$	31.889	24.827	−0.475
Pb	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T6s D6d T6p $5f$	31.972	43.115	7.784
Bi	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T6s D6d T6p $5f$	36.734	43.808	6.951
Po	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T6s D6d T6p $5f$	37.458	45.587	5.567