FPLO/T+F+s

FPLO 14.00-49 / enhanced LO basis + fixed compact support

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, the compact support 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. The compact support radius was fixed for all volumes to its default value at the equilibrium volume. This option is only needed for very soft elements. We use it for all elements for consistency. 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. D$3p$ = $3p4p$, Tnl means triple basis orbitals, e.g. T$3p$ = $3p4p5p$. The additional nominal $5f$ orbital for Lu is of course not identical to the $5f$ part of its T$4f$ basis states but rather an effective $7f$ state. 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	/ T1*s* D2*p* 4*f* 3*d*	17.416	10.230	2.787
He	12 × 12 × 12	1 728	/ T1*s* D2*p* 4*f* 3*d*	17.907	0.721	6.620
Li	12 × 12 × 12	1 728	1*s* / T2*s* T2*p* D3*d* 4*f*	20.187	14.044	3.204
Be	12 × 12 × 12	1 728	1*s* / T2*s* T2*p* D3*d* 4*f*	7.875	128.283	2.983
B	12 × 12 × 12	1 728	1*s* / T2*s* T2*p* D3*d* 4*f*	7.151	251.656	3.253
C	12 × 12 × 30	4 320	1*s* / T2*s* T2*p* D3*d* 4*f*	11.612	210.856	3.464
N	12 × 12 × 12	1 728	1*s* / T2*s* T2*p* D3*d* 4*f*	28.869	53.468	3.696
O	12 × 12 × 12	1 728	1*s* / T2*s* T2*p* D3*d* 4*f*	18.670	49.820	3.972
F	12 × 12 × 12	1 728	1*s* / T2*s* T2*p* D3*d* 4*f*	19.327	33.714	4.038
Ne	12 × 12 × 12	1 728	1*s* / T2*s* T2*p* D3*d* 4*f*	24.473	1.320	6.856
Na	12 × 12 × 12	1 728	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	36.671	8.485	3.166
Mg	12 × 12 × 12	1 728	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	22.857	36.700	4.009
Al	30 × 30 × 30	27 000	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	16.460	78.338	4.699
Si	12 × 12 × 12	1 728	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	20.448	89.612	4.316
P	12 × 12 × 12	1 728	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	21.439	69.231	4.278
S	12 × 12 × 12	1 728	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	17.171	85.775	4.033
Cl	12 × 12 × 12	1 728	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	39.117	18.691	4.401
Ar	12 × 12 × 12	1 728	2*s* 2*p* / T3*s* T3*p* D3*d* 4*f*	52.751	0.668	4.416
K	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* D4*p* T3*d* 4*f*	73.618	3.634	3.674
Ca	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* D4*p* T3*d* 4*f*	42.049	18.471	2.626
Sc	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	24.594	55.191	3.388
Ti	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	17.385	113.098	3.476
V	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	13.435	183.541	3.783
Cr	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	11.763	187.691	7.436
Mn	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	11.469	101.103	8.298
Fe	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	11.351	193.245	5.231
Co	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	10.880	217.588	5.055
Ni	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	10.910	199.949	4.840
Cu	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	11.976	141.049	4.912
Zn	12 × 12 × 12	1 728	3*s* 3*p* / T4*s* T3*d* D4*p* 4*f*	15.205	75.275	5.178
Ga	12 × 12 × 12	1 728	3*s* 3*p* 3*d* / T4*s* T4*p* D4*d* 4*f*	20.144	53.313	4.927
Ge	12 × 12 × 12	1 728	3*s* 3*p* 3*d* / T4*s* T4*p* D4*d* 4*f*	23.932	58.748	4.903
As	12 × 12 × 12	1 728	3*s* 3*p* 3*d* / T4*s* T4*p* D4*d* 4*f*	22.599	68.041	4.117
Se	12 × 12 × 12	1 728	3*s* 3*p* 3*d* / T4*s* T4*p* D4*d* 4*f*	29.730	47.950	4.356
Br	12 × 12 × 12	1 728	3*s* 3*p* 3*d* / T4*s* T4*p* D4*d* 4*f*	39.560	22.399	4.801
Kr	12 × 12 × 12	1 728	3*s* 3*p* 3*d* / T4*s* T4*p* D4*d* 4*f*	66.250	0.685	6.981
Rb	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* D5*p* T4*d* 4*f*	90.498	2.925	3.551
Sr	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* D5*p* T4*d* 4*f*	54.421	11.754	4.369
Y	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	32.761	42.457	3.021
Zr	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	23.355	95.945	3.286
Nb	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	18.112	170.838	3.714
Mo	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	15.790	262.153	4.249
Tc	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	14.475	297.705	4.348
Ru	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	13.802	311.999	4.809
Rh	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	14.095	258.215	4.981
Pd	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	15.349	173.757	5.380
Ag	30 × 30 × 30	27 000	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	17.876	91.828	5.729
Cd	12 × 12 × 12	1 728	4*s* 4*p* / T5*s* T4*d* D5*p* 4*f*	22.877	44.230	6.688

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In	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T$5s$ D$5d$ T$5p$ $4f$	27.474	36.355	5.227
Sn	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T$5s$ D$5d$ T$5p$ $4f$	36.748	37.120	4.718
Sb	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T$5s$ D$5d$ T$5p$ $4f$	31.701	51.432	4.495
Te	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T$5s$ D$5d$ T$5p$ $4f$	35.074	44.726	4.656
I	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T$5s$ D$5d$ T$5p$ $4f$	50.758	18.094	5.013
Xe	$12 \times 12 \times 12$	1 728	$4s$ $4p$ $4d$ / T$5s$ D$5d$ T$5p$ $4f$	88.064	0.484	9.704
Cs	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T$6s$ T$5d$ D$6p$ $4f$	116.596	1.968	3.455
Ba	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T$6s$ D$5d$ D$6p$ $4f$	63.231	8.927	3.873
Lu	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T$6s$ T$5d$ D$6p$ T$4f$ $5f$	29.065	47.356	3.411
Hf	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	22.514	108.991	3.395
Ta	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	18.289	193.127	3.695
W	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	16.165	303.073	4.203
Re	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	14.989	361.595	4.402
Os	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	14.313	395.763	4.793
Ir	$12 \times 12 \times 12$	1 728	$4f$ $5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	14.545	345.626	4.945
Pt	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	15.703	245.707	5.290
Au	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	18.062	138.811	5.251
Hg	$12 \times 12 \times 12$	1 728	$5s$ $5p$ / T$6s$ T$5d$ D$6p$ $5f$	29.925	7.571	8.395
Tl	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T$6s$ D$6d$ T$6p$ $5f$	31.424	27.221	5.134
Pb	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T$6s$ D$6d$ T$6p$ $5f$	31.985	40.331	4.575
Bi	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T$6s$ D$6d$ T$6p$ $5f$	36.868	42.959	4.691
Po	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T$6s$ D$6d$ T$6p$ $5f$	37.558	45.949	4.855
Rn	$12 \times 12 \times 12$	1 728	$5s$ $5p$ $5d$ / T$6s$ D$6d$ T$6p$ $5f$	94.269	0.537	7.620