FHI-aims/tier2

FHI-aims 081213 / NAO tier2 atomic ZORA

`name and version of the code:` FHI-aims 081213
`type of basis set:` numeric atom-centred orbital basis functions
`method:` all-electron

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	atomic zero-order regular approximation (ZORA) Eqs. (55)/(56) of [1]
`assignment of core / valence states`	treated on equal footing
`basis set size`	tier2 – see table I
`k-mesh density`	see table II (k-point grid *kpts*, and the number of irreducible k-points in the full 1st Brillouin zone of the primitive cell # k)
`reciprocal-space integration method`	Gaussian smearing with a fictitious broadening corresponding to 0.01 eV

METHOD-SPECIFIC INFORMATION

`Hartree potential multicentre expansion`	$l_{\mathrm{hartree}} = 8$
`logarithmic mesh for free-atom quantities`	see table I (number of points # $N_{\log}$ between $0.001/Z$ and 100.0 bohr)
`radial integration mesh`	see table I (number of shells per atom # N_{rad}, distributed according to Eq. (18) of [1])
`anchor distance of radial int. mesh`	7 Å
`smallest (innermost) Lebedev grid`	110 points
`largest (outermost) Lebedev grid`	590 points
`basis function confinement`	r_{onset} see table I, $w = 2.0$ Å Eq. (9) of [1]

ADDITIONAL COMMENTS

Radial integration mesh:
The "anchor distance of the radial mesh" is the radius of the second-most distant radial integration shell, specified by the "radial_base" keyword in FHI-aims. A detailed explanation of the construction of radial integration grids in FHI-aims can be found in the Appendix of [2].

Basis set character and angular momenta:
The set of radial functions used is characterized according to their angular momenta. Each basis set consists of the core and valence radial functions of a spherical free atom and further groups of radial functions, organized in "tiers" (levels). For each element, the table lists the closest noble gas configuration + valence shells included in the free atom + tier1 + tier2 radial functions.

The ASE script used to generate these data has been included after the tables.

REFERENCES

[1] V. Blum, R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter and M. Scheffler, *Comput. Phys. Commun.* **180**, 2175–2196 (2009).
[2] I. Y. Zhang, X. Ren, P. Rinke, V. Blum and M. Scheffler, *New J. Phys.* **15**, 123033 (2013).

Table I. Calculation settings per element: basis set size, number of logarithmic grid points $N_{\log}$, number of radial grid points N_{rad} and basis function onset radius r_{onset}.

	Basis set character (tier2) [–]	# $N_{\log}$ [–]	# N_{rad} [–]	r_{onset} [Å]
H	$1s{+}sp{+}spsd$	1131	49	4.0
He	$1s{+}sp{+}dspf$	1187	55	4.0
Li	[He]$+2s{+}psd{+}ppsdf$	1220	59	4.0
Be	[He]$+2s{+}psd{+}pdpsf$	1244	63	4.0
B	[He]$+2s2p{+}psd{+}fpsgd$	1262	65	4.0
C	[He]$+2s2p{+}psd{+}fpsgd$	1277	69	4.0
N	[He]$+2s2p{+}pds{+}fpsgd$	1290	71	4.0
O	[He]$+2s2p{+}pds{+}fpdgs$	1301	73	4.0
F	[He]$+2s2p{+}pds{+}fpsdg$	1310	75	4.0
Ne	[Ne]$+dps{+}fdsgp$	1319	77	4.0
Na	[Ne]$+3s{+}psd{+}psfd$	1327	81	5.0
Mg	[Ne]$+3s{+}pds{+}fpsd$	1334	81	5.0
Al	[Ne]$+3s3p{+}pdfs{+}gdsp$	1340	83	4.0
Si	[Ne]$+3s3p{+}dpfs{+}dgps$	1346	85	4.0
P	[Ne]$+3s3p{+}dpfgs{+}dpfsg$	1352	87	4.0
S	[Ne]$+3s3p{+}dpfs{+}dgpfs$	1357	89	4.0
Cl	[Ne]$+3s3p{+}dpfsg{+}dfsgp$	1362	91	4.0
Ar	[Ar]$+dpfs{+}dgps$	1367	93	4.0
K	[Ar]$+4s{+}dpsf{+}dsgp$	1371	93	6.0
Ca	[Ar]$+4s{+}dpdfs{+}gphsfpd$	1376	95	5.0
Sc	[Ar]$+4s3d{+}fpdgs{+}fdphds$	1380	95	4.0
Ti	[Ar]$+4s3d{+}fdpgs{+}dhfps$	1383	97	4.0
V	[Ar]$+4s3d{+}fdpgs{+}dfhdfpgs$	1387	99	4.0
Cr	[Ar]$+4s3d{+}fdpgs{+}fdhdfgsp$	1391	101	4.0
Mn	[Ar]$+4s3d{+}fdpgs{+}dhffpdgs$	1394	101	4.0
Fe	[Ar]$+4s3d{+}fpgds{+}dhffpgs$	1397	103	4.0
Co	[Ar]$+4s3d{+}pfdgs{+}phdfs$	1400	105	4.0
Ni	[Ar]$+4s3d{+}pfgds{+}pdhffs$	1403	105	4.0
Cu	[Ar]$+4s3d{+}pfsdg{+}pdhsf$	1406	107	4.0
Zn	[Ar]$+4s3d{+}pspfd{+}gpsd$	1409	107	4.0
Ga	[Ar]$+4s4p3d{+}pdfs{+}gpfhds$	1412	109	4.0
Ge	[Ar]$+4s4p3d{+}pdfs{+}gdpfhs$	1414	109	4.0
As	[Ar]$+4s4p3d{+}dpfs{+}ghpfds$	1417	111	4.0
Se	[Ar]$+4s4p3d{+}dpfs{+}gpdfsh$	1419	111	4.0
Br	[Ar]$+4s4p3d{+}dpfs{+}gdhpsf$	1421	113	4.0
Kr	[Kr]$+dpfs{+}gdphfs$	1424	113	4.0
Rb	[Kr]$+5s{+}dpfs{+}dgsp$	1426	115	6.0
Sr	[Kr]$+5s{+}dpfs{+}gdphsf$	1428	115	5.0
Y	[Kr]$+5s4d{+}fpdgs{+}fdhps$	1430	117	4.0
Zr	[Kr]$+5s4d{+}fdpgs{+}fhdpfs$	1432	117	4.0
Nb	[Kr]$+5s4d{+}fdpgs{+}fdhfps$	1434	119	4.0
Mo	[Kr]$+5s4d{+}fdpgs{+}fdhfps$	1436	119	4.0
Tc	[Kr]$+5s4d{+}fdpgs{+}fhfdpgs$	1438	121	4.0
Ru	[Kr]$+5s4d{+}fdpgs{+}fhfgdps$	1440	121	4.0
Rh	[Kr]$+5s4d{+}fpdgs{+}fhfdpgs$	1442	123	4.0
Pd	[Kr]$+5s4d{+}pfgsd{+}fgdhsp$	1444	125	4.0
Ag	[Kr]$+5s4d{+}pfsdg{+}fhpds$	1446	125	4.0
Cd	[Kr]$+5s4d{+}pfspgd{+}fhpsd$	1147	125	4.0
In	[Kr]$+5s5p4d{+}pfds{+}gpfhfds$	1449	125	4.0

Sn	[Kr]+5s5p4d+$pdfs$+$gpfdhfs$	1451	127	4.0
Sb	[Kr]+5s5p4d+$dpfs$+$gfhdfps$	1452	127	4.0
Te	[Kr]+5s5p4d+$dfps$+$gfhpfds$	1454	129	4.0
I	[Kr]+5s5p4d+$dfps$+$gfhpds$	1455	129	4.0
Xe	[Xe]+$dfps$+$gfdfhps$	1457	129	4.0
Cs	[Xe]+6s+$dfps$+$dfgfhps$	1458	131	6.0
Ba	[Xe]+6s+$dfps$+$fgdhps$	1460	131	8.0
Lu	[Xe]+6s5d4f+$pdfgs$+$ppdhfdgs$	1479	141	4.0
Hf	[Xe]+6s5d4f+$fdpgs$+$fdhpds$	1480	143	4.0
Ta	[Xe]+6s5d4f+$fdpgs$+$dhfgps$	1482	143	4.0
W	[Xe]+6s5d4f+$fdpgs$+$hdfgdps$	1483	143	4.0
Re	[Xe]+6s5d4f+$fdpgs$+$hdfgpds$	1484	145	4.0
Os	[Xe]+6s5d4f+$fpdgs$+$hpfdgs$	1485	145	4.0
Ir	[Xe]+6s5d4f+$fpgds$+$hffgpds$	1486	145	4.0
Pt	[Xe]+6s5d4f+$fpgsd$+$hfdpgs$	1487	145	4.0
Au	[Xe]+6s5d4f+$pfsghd$+$fdpsgh$	1488	147	4.0
Hg	[Xe]+6s5d4f+$pfsgpd$+$hfpsdg$	1489	147	4.0
Tl	[Xe]+6s6p5d4f+$pfdsg$+$phfds$	1490	147	4.0
Pb	[Xe]+6s6p5d4f+$pfdgs$+$hdffps$	1491	149	4.0
Bi	[Xe]+6s6p5d4f+$pdfsg$+$dphffs$	1492	149	4.0
Po	[Xe]+6s6p5d4f+$dfpsg$+$fhpds$	1493	149	4.0
Rn	[Rn]+$dfpgs$+$fdhfsg$	1495	151	4.0

Table II. 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, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	kpts [–]	# k [–]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	28 x 28 x 20	7840	17.3955	10.3244	2.7385
He	40 x 40 x 22	17600	18.0461	0.8494	1.1724
Li	38 x 38 x 38	27436	20.2584	13.8120	3.4520
Be	52 x 52 x 28	37856	7.9069	123.7151	3.4723
B	26 x 26 x 24	8112	7.2393	237.3241	3.4365
C	48 x 48 x 12	13824	11.6300	209.1781	3.5981
N	16 x 16 x 16	2048	28.8025	54.0466	3.6934
O	26 x 24 x 24	7488	18.5125	51.3380	3.9259
F	16 x 28 x 14	3136	19.1427	34.2735	4.0643
Ne	22 x 22 x 22	5324	24.4391	1.1878	6.9161
Na	32 x 32 x 32	16384	37.0854	7.7625	3.7955
Mg	36 x 36 x 20	12960	22.9569	35.9978	3.9894
Al	24 x 24 x 24	6912	16.4921	77.7749	5.0377
Si	32 x 32 x 32	16384	20.4535	88.6201	4.2489
P	30 x 8 x 22	2640	21.4435	68.1001	4.3366
S	38 x 38 x 38	27436	17.2125	83.9136	4.0230
Cl	12 x 24 x 12	1728	38.8211	18.9341	4.3405
Ar	16 x 16 x 16	2048	52.4645	0.7327	8.6099
K	20 x 20 x 20	4000	73.8148	3.5802	3.6558
Ca	18 x 18 x 18	2916	42.2161	17.6892	3.4734
Sc	34 x 34 x 20	11560	24.6089	54.6364	3.3974
Ti	40 x 40 x 22	17600	17.3902	111.5900	3.6297
V	34 x 34 x 34	19652	13.4479	182.2043	3.9567
Cr	36 x 36 x 36	23328	11.7715	185.0625	6.9532
Mn	28 x 28 x 28	10976	11.4777	119.6118	0.0802
Fe	36 x 36 x 36	23328	11.3392	194.4014	4.6849
Co	46 x 46 x 24	25392	10.8513	214.1797	4.6796
Ni	28 x 28 x 28	10976	10.8872	198.1638	4.9449
Cu	28 x 28 x 28	10976	11.9615	140.0409	5.2277
Zn	44 x 44 x 20	19360	15.1941	75.4154	5.5155
Ga	22 x 12 x 22	2904	20.3013	49.1819	5.4723
Ge	30 x 30 x 30	13500	23.8905	59.3238	4.9369
As	30 x 30 x 10	4500	22.5901	68.2982	4.2925
Se	26 x 26 x 20	6760	29.7404	47.0304	4.4686
Br	12 x 24 x 12	1728	39.4566	22.3752	4.8436
Kr	16 x 16 x 16	2048	66.2448	0.6297	6.6440
Rb	18 x 18 x 18	2916	91.1656	2.8045	3.5574
Sr	16 x 16 x 16	2048	54.3677	11.4507	5.3802
Y	32 x 32 x 18	9216	32.8355	41.4725	3.1396
Zr	36 x 36 x 20	12960	23.3940	93.7535	3.2944
Nb	30 x 30 x 30	13500	18.1270	170.4048	3.7274
Mo	32 x 32 x 32	16384	15.7887	259.4884	4.3507
Tc	42 x 42 x 22	19404	14.4381	299.1265	4.5298
Ru	42 x 42 x 24	21168	13.7635	312.1158	4.8757
Rh	26 x 26 x 26	8788	14.0431	257.0866	5.1885
Pd	26 x 26 x 26	8788	15.3106	168.8863	5.5095
Ag	24 x 24 x 24	6912	17.8455	91.0431	5.9975
Cd	38 x 38 x 18	12996	22.8392	43.9964	6.9580

In	30 x 30 x 20	9000	27.5167	35.8699	4.8709
Sn	26 x 26 x 26	8788	36.8318	35.8545	5.0021
Sb	26 x 26 x 8	2704	31.7533	50.3972	4.5283
Te	26 x 26 x 16	5408	34.9740	44.7145	4.6885
I	12 x 22 x 10	1320	50.2501	18.6164	5.0436
Xe	14 x 14 x 14	1372	86.8790	0.5681	7.2531
Cs	16 x 16 x 16	2048	116.7703	2.0044	4.1222
Ba	20 x 20 x 20	4000	63.0761	8.8520	2.2069
Lu	32 x 32 x 18	9216	29.0652	47.0124	3.5308
Hf	36 x 36 x 20	12960	22.5418	107.5910	3.4407
Ta	30 x 30 x 30	13500	18.2835	193.6651	3.5015
W	32 x 32 x 32	16384	16.1399	301.5926	4.2144
Re	42 x 42 x 22	19404	14.9559	363.3583	4.4155
Os	42 x 42 x 24	21168	14.2799	396.7276	4.8143
Ir	26 x 26 x 26	8788	14.4993	347.6047	5.2287
Pt	26 x 26 x 26	8788	15.6401	248.0916	5.4707
Au	24 x 24 x 24	6912	17.9752	138.6731	6.1054
Hg	24 x 24 x 28	8064	29.5950	7.7226	9.8983
Tl	32 x 32 x 18	9216	31.4374	26.6619	5.5187
Pb	20 x 20 x 20	4000	31.9622	39.9991	5.6218
Bi	26 x 26 x 8	2704	36.9073	42.5965	4.6508
Po	30 x 30 x 30	13500	37.5659	45.4307	5.0102
Rn	14 x 14 x 14	1372	93.0392	0.5344	6.8771

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script for the Atomic Simulation Environment (ASE)
S. R. Bahn, K. W. Jacobsen, *Comput. Sci. Eng.* **4**, 56–66 (2002)
https://wiki.fysik.dtu.dk/ase/

```
import os
import sys
import time

import numpy as np

import ase.db
from ase.utils import opencew
from ase.calculators.calculator import kpts2mp
from ase.io.trajectory import PickleTrajectory
from ase.calculators.aims import Aims
from ase.test.tasks.dcdft import DeltaCodesDFTCollection as Collection

collection = Collection()

if len(sys.argv) == 1:
    names = collection.names
else:
    names = [sys.argv[1]]

c = ase.db.connect('dcdft_aims.db')

# select the basis set
basis = 'tier2'

kptdensity = 16.0  # this is converged
width = 0.01

basis_threshold = 0.00001
relativistic = 'scalar'

sc_accuracy_rho = 1.e-4
sc_accuracy_eev = 5.e-3

if relativistic == 'none':
    linspace = (0.92, 1.08, 7)  # eos numpy's linspace
else:
    linspace = (0.98, 1.02, 5)  # eos numpy's linspace
linspacestr = ''.join([str(t) + 'x' for t in linspace])[:-1]

code = 'aims' + '-' + basis + '_e' + linspacestr
code = code + '_k' + str(kptdensity) + '_w' + str(width)
code = code + '_t' + str(basis_threshold) + '_r' + str(relativistic)

collection = Collection()

for name in names:
    # save all steps in one traj file in addition to the database
    # we should only used the database c.reserve, but here
```

```
# traj file is used as another lock ...
fd = opencew(name + '_' + code + '.traj')
if fd is None:
    continue
traj = PickleTrajectory(name + '_' + code + '.traj', 'w')
atoms = collection[name]
cell = atoms.get_cell()
kpts = tuple(kpts2mp(atoms, kptdensity, even=True))
kwargs = {}
if relativistic == 'scalar':
    kwargs.update({'relativistic': ['atomic_zora', relativistic]})
elif relativistic == 'none':
    kwargs.update({'relativistic': 'none'})
else:  # e.g. 1.0e-12
    kwargs.update({'relativistic': ['zora', 'scalar', relativistic]})
if atoms.get_initial_magnetic_moments().any():  # spin-polarization
    magmom = atoms.get_initial_magnetic_moments().sum() / len(atoms)
    kwargs.update({'spin': 'collinear'})
# convergence problems for tier2
charge_mix_param = 0.01
basis_threshold = 0.00001
if basis in ['tier2']:
    if name in ['Cr', 'Fe'] and relativistic == 'none':
        basis_threshold = 0.00005
        sc_accuracy_rho=2.5e-3
        sc_accuracy_eev=5.e-3
    if name in ['Mn']:
        charge_mix_param = 0.01
        basis_threshold = 0.00005
        sc_accuracy_rho=2.5e-3
        sc_accuracy_eev=5.e-3
        if relativistic == 'none':
            sc_accuracy_rho=3.0e-3
# loop over EOS linspace
for n, x in enumerate(np.linspace(linspace[0], linspace[1], linspace[2])):
    id = c.reserve(name=name, basis=basis, linspacestr=linspacestr,
                   kptdensity=kptdensity, width=width,
                   basis_threshold=basis_threshold,
                   relativistic=relativistic,
                   x=x)
    if id is None:
        continue
    # perform EOS step
    atoms.set_cell(cell * x, scale_atoms=True)
    # set calculator
    atoms.calc = Aims(
        label=name + '_' + code + '_' + str(n),
        species_dir=os.path.join(os.environ['AIMS_SPECIES_DIR'], basis),
        xc='PBE',
        kpts=kpts,
        KS_method='elpa',
        sc_accuracy_rho=sc_accuracy_rho,
        sc_accuracy_eev=sc_accuracy_eev,
        occupation_type=['gaussian', width],
```

```
    override_relativity=True,
    override_illconditioning=True,
    basis_threshold=basis_threshold,
    charge_mix_param=charge_mix_param,
    sc_iter_limit=9000,
    )
atoms.calc.set(**kwargs)  # remaining calc keywords
t = time.time()
atoms.get_potential_energy()
c.write(atoms,
        name=name, basis=basis, linspacestr=linspacestr,
        kptdensity=kptdensity, width=width,
        basis_threshold=basis_threshold,
        relativistic=relativistic,
        x=x,
        time=time.time()-t)
traj.write(atoms)
del c[id]
```