MBK2013/OpenMX

Morrison-Bylander-Kleinman 2013 NCPP dataset / OpenMX 3.7

`name and version of the code:` OpenMX 3.7
`type of basis set:` optimized numerical pseudo-atomic orbitals
`method:` norm-conserving pseudopotentials (Morrison-Bylander-Kleinman 2013)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see table I
`basis set size`	see table I
`k-mesh density`	see table I (number of k-points in the full 1st Brillouin zone of the primitive cell, # k)
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.026 eV

METHOD-SPECIFIC INFORMATION

`real-space mesh for integrations`	400 Rydberg
`real-space mesh for the Poisson solver by FFT`	400 Rydberg
`projector expansion for the neutral atom potentials`	OFF
`one-dimensional radial mesh in k-space (1DFFT.NumGridK)`	900
`one-dimensional radial mesh in r-space (1DFFT.NumGridR)`	900
`cutoff energy for the one-dimensional radial mesh in k-space (1DFFT.EnergyCutoff)`	3 600 Rydberg

ADDITIONAL COMMENTS

In the pseudopotential generation, unbound states were calculated by Hamann's scheme [2].

REFERENCES

`pseudopotentials`

[1] I. Morrison, D.M. Bylander and L. Kleinman, *Phys. Rev. B* **47**, 6728 (1993).
[2] D. R. Hamann, *Phys. Rev. B* **40**, 2980 (1989).

`code`

[3] T. Ozaki, *Phys. Rev. B* **67**, 155108 (2003).
[4] T. Ozaki and H. Kino, *Phys. Rev. B* **69**, 195113 (2004).
[5] T. Ozaki and H. Kino, *Phys. Rev. B* **72**, 045121 (2005).
[6] http://www.openmx-square.org/

`scalar relativity`

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

Table I. Calculation settings per element: basis set (BS), valence and unbound states included in the pseudopotential generation and the occupation, which is give by superscript, and cutoff radii in a.u., which is given in parentheses (States), and the number of k-points in the full 1st Brillouin zone of the primitive cell (# k).

	BS	States	# k
H	H7.0-s3p2d1	$1s^{1}(0.80)2p^{0}(0.8)$	1 331
He	He8.0-s3p3d2f1	$1s^{2}(0.8)2s^{0}(1.0)2p^{0}(0.9)3d^{0}(0.9)$	1 152
Li	Li8.0-s3p3d2	$1s^{2}(0.6)2s^{0}(1.7)2p^{0}(0.6)$	392
Be	Be7.0-s3p2d1	$2s^{2}(1.45)2p^{0}(1.3)3p^{0}(1.9)3d^{0}(1.6)$	1 089
B	B7.0-s3p3d2	$2s^{2}(1.1)2p^{1}(0.9)3s^{0}(2.10)3d^{0}(0.9)$	343
C	C7.0-s3p3d2	$2s^{2}(1.42)2p^{2}(1.62)3d^{0}(1.3)$	726
N	N7.0-s3p3d2f1	$2s^{2}(1.0)2p^{3}(1.0)3d^{0}(1.0)3s^{0}(1.4)$	343
O	O7.0-s3p3d2f1	$2s^{2}(0.7)2p^{4}(1.2)3s^{0}(1.1)3p^{0}(1.2)3d^{0}(0.9)$	1 331
F	F7.0-s3p3d2f1	$2s^{2}(1.7)2p^{5}(1.1)3s^{0}(2.2)3p^{0}(2.2)3d^{0}(1.2)$	539
Ne	Ne9.0-s3p3d2f1	$2s^{2}(1.0)2p^{6}(1.3)3s^{0}(2.0)3p^{0}(2.4)3d^{0}(1.6)$	1 728
Na	Na9.0-s3p3d2f2	$2s^{2}(1.0)2p^{6}(1.3)3s^{1}(2.2)3p^{0}(2.2)3d^{0}(1.2)4s^{0}(2.5)$	392
Mg	Mg7.0-s4p3d3f1	$2p^{6}(1.1)3s^{2}(2.2)3p^{0}(2.0)3d^{0}(1.0)4s^{0}(2.6)$	726
Al	Al7.0-s4p4d2f1	$3s^{2}(2.2)3p^{1}(2.1)3d^{0}(1.4)4p^{0}(1.92)$	1 331
Si	Si7.0-s3p3d2f1	$3s^{2}(1.5)3p^{2}(1.7)3d^{0}(1.8)4s^{0}(2.2)4p^{0}(2.4)5d^{0}(2.4)$	1 331
P	P8.0-s4p3d3f2	$3s^{2}(1.4)3p^{3}(1.5)3d^{0}(1.5)4s^{0}(2.4)4p^{0}(2.7)$	369
S	S7.0-s4p3d3f2	$3s^{2}(1.4)3p^{4}(1.5)3d^{0}(1.4)4s^{0}(2.2)4p^{0}(2.4)$	1 331
Cl	Cl8.0-s4p3d3f1	$3s^{2}(1.3)3p^{5}(1.3)3d^{0}(1.3)4s^{0}(1.9)4p^{0}(1.9)4f^{0}(1.9)$	385
Ar	Ar11.0-s3p3d2f1	$3s^{2}(1.2)3p^{6}(1.25)3d^{0}(1.45)$	1 728
K	K10.0-s4p3d3f1	$3s^{2}(1.2)3p^{6}(1.7)3d^{0}(1.6)4s^{1}(2.9)4p^{0}(2.9)$	1 331
Ca	Ca9.0-s4p3d3f1	$3s^{2}(1.2)3p^{6}(1.7)3d^{0}(1.2)4s^{2}(2.8)4p^{0}(2.6)4f^{0}(1.2)$	1 728
Sc	Sc7.0-s4p3d3f1	$3s^{2}(1.2)3p^{6}(1.7)3d^{1}(1.6)4s^{2}(2.5)4p^{0}(2.4)4d^{0}(2.9)4f^{0}(1.2)$	1 296
Ti	Ti7.0-s3p3d3f1	$3s^{2}(1.3)3p^{6}(1.3)3d^{2}(1.3)4s^{2}(2.5)4p^{0}(2.4)4d^{0}(1.5)4f^{0}(1.0)$	1 296
V	V6.0-s3p3d3f1	$3s^{2}(1.1)3p^{6}(1.7)3d^{3}(1.45)4s^{2}(2.3)4p^{0}(2.4)4d^{0}(2.9)4f^{0}(1.2)$	1 728
Cr	Cr6.0-s3p3d3f1	$3s^{2}(1.1)3p^{6}(1.7)3d^{4}(1.45)4s^{2}(2.35)4p^{0}(2.4)4d^{0}(2.9)4f^{0}(1.2)$	1 331
Mn	Mn6.0-s3p3d3f1	$3s^{2}(0.8)3p^{6}(0.7)3d^{5}(0.8)4s^{2}(1.6)4p^{0}(1.8)4f^{0}(1.2)$	1 331
Fe	Fe6.0H-s3p3d3f1	$3s^{2}(0.8)3p^{6}(0.8)3d^{6.5}(0.88)4s^{1.5}(1.9)4p^{0}(1.9)4f^{0}(1.7)$	1 331
Co	Co6.0S-s3p4d3f2	$3p^{6}(1.4)3d^{8}(1.6)4s^{1}(2.2)4p^{0}(2.2)4d^{0}(2.4)4f^{0}(2.4)5s^{0}(2.7)$	1 352
Ni	Ni6.0S-s3p3d2f1	$3p^{6}(1.2)3d^{8}(1.6)4s^{2}(2.3)4p^{0}(2.3)4d^{0}(2.2)4f^{0}(1.7)5s^{0}(2.9)$	1 728
Cu	Cu6.0H-s3p3d3f1	$3s^{2}(0.6)3p^{6}(0.7)3d^{9}(1.05)4s^{2}(2.0)4p^{0}(1.7)4d^{0}(2.1)4f^{0}(1.2)$	1 728
Zn	Zn6.0H-s4p3d2f1	$3s^{2}(1.3)3p^{6}(1.4)3d^{10}(1.4)4s^{2}(1.7)4p^{0}(2.2)4d^{0}(2.0)4f^{0}(1.2)$	1 152
Ga	Ga8.0-s3p3d3f1	$3d^{10}(1.5)4s^{2}(1.7)4p^{1}(1.8)4d^{0}(2.2)4f^{0}(1.5)$	847
Ge	Ge7.0-s4p4d3f2	$4s^{2}(1.6)4p^{2}(1.8)4d^{0}(2.4)4f^{0}(1.5)5p^{0}(2.8)5d^{0}(2.7)$	1 000
As	As9.0-s4p4d3f2	$3d^{10}(1.6)4s^{2}(1.4)4p^{3}(1.5)4d^{0}(1.7)5p^{0}(2.3)$	864
Se	Se9.0-s4p3d3f2	$4s^{2}(1.4)4p^{4}(1.7)4d^{0}(1.9)4f^{0}(1.7)5s^{0}(1.7)$	1 584
Br	Br8.0-s3p3d3f1	$4s^{2}(1.5)4p^{5}(1.5)4d^{0}(1.9)4f^{0}(1.9)5s^{0}(2.1)$	330
Kr	Kr10.0-s3p3d2f1	$4s^{2}(1.2)4p^{6}(1.4)4d^{0}(1.7)4f^{0}(1.5)5p^{0}(2.3)$	1 728
Rb	Rb11.0-s4p3d3f2	$4s^{2}(1.4)4p^{6}(1.4)4d^{0}(1.5)4f^{0}(1.7)5s^{1}(2.7)5p^{0}(3.1)6s^{0}(3.1)$	1 728
Sr	Sr10.0-s3p3d3f2	$4s^{2}(1.4)4p^{6}(1.4)4d^{0}(1.5)4f^{0}(1.7)5s^{2}(2.6)5p^{0}(3.1)$	1 728
Y	Y8.0-s4p3d3f2	$4s^{2}(1.5)4p^{6}(1.5)4d^{1}(1.5)4f^{0}(1.7)5s^{2}(2.3)5p^{0}(3.1)6s^{0}(3.1)$	1 152
Zr	Zr7.0-s3p3d3f1	$4s^{2}(1.2)4p^{6}(1.3)4d^{2}(1.4)4f^{0}(1.3)5s^{2}(2.5)5p^{0}(2.5)5d^{0}(2.7)$	1 152
Nb	Nb7.0-s3p3d3f1	$4s^{2}(1.3)4p^{6}(1.3)4d^{3}(1.3)4f^{0}(1.4)5s^{2}(2.6)5p^{0}(2.6)5d^{0}(2.2)$	1 728
Mo	Mo7.0-s3p3d2f1	$4s^{2}(1.1)4p^{6}(1.2)4d^{5}(1.6)4f^{0}(1.5)5s^{1}(2.3)5p^{0}(2.8)$	1 728
Tc	Tc7.0-s3p3d3f1	$4s^{2}(1.2)4p^{6}(1.2)4d^{6}(1.6)5s^{1}(2.3)5p^{0}(2.8)$	1 152
Ru	Ru7.0-s3p3d2f1	$4p^{6}(1.1)4d^{7}(1.6)4f^{0}(1.5)5s^{1}(2.3)5p^{0}(2.6)6s^{0}(3.0)$	1 152
Rh	Rh7.0-s3p3d2f1	$4p^{6}(1.1)4d^{8}(1.6)4f^{0}(1.4)5s^{1}(2.5)5p^{0}(2.6)6s^{0}(3.0)$	1 728
Pd	Pd7.0-s3p3d2f1	$4p^{6}(1.1)4d^{9}(1.6)4f^{0}(1.4)5s^{1}(2.5)5p^{0}(2.8)6s^{0}(3.0)$	1 728
Ag	Ag7.0-s3p3d2f2	$4p^{6}(1.0)4d^{10}(1.6)4f^{0}(1.4)5s^{1}(2.3)5p^{0}(2.4)6s^{0}(3.0)$	1 728

Cd	Cd7.0-s3p2d3f1	$4d^{10}(1.0)5s^{2}(1.9)5p^{0}(2.5)6s^{0}(3.0)$	1 008
In	In7.0-s3p3d3f1	$4d^{10}(1.1)5s^{2}(2.0)5p^{1}(2.4)6s^{0}(3.0)6p^{0}(3.0)$	1 152
Sn	Sn7.0-s2p3d3f2	$4d^{10}(1.4)4f^{0}(1.2)5s^{2}(2.0)5p^{2}(2.0)6s^{0}(2.7)6p^{0}(2.6)$	1 000
Sb	Sb7.0-s3p3d3f2	$4d^{10}(1.4)4f^{0}(1.2)5s^{2}(2.0)5p^{3}(2.0)5d^{0}(2.2)6s^{0}(2.5)6p^{0}(2.5)$	600
Te	Te7.0-s4p3d3f2	$4d^{10}(1.5)4f^{0}(2.0)5s^{2}(2.0)5p^{4}(2.0)5d^{0}(2.4)6s^{0}(2.4)6p^{0}(2.5)$	1 089
I	I9.0-s3p3d3f2	$4f^{0}(2.2)5s^{2}(2.0)5p^{5}(1.8)5d^{0}(2.2)6s^{0}(2.4)$	330
Xe	Xe11.0-s3p3d2f1	$4f^{0}(2.0)5s^{2}(1.8)5p^{6}(1.8)5d^{0}(2.2)6s^{0}(2.1)$	1 728
Cs	Cs12.0-s3p3d3f2	$4f^{0}(2.0)5s^{2}(1.6)5p^{6}(2.0)5d^{0}(2.5)6s^{1}(3.4)$	1 728
Ba	Ba10.0-s3p3d3f2	$4f^{0}(2.01)5s^{2}(1.7)5p^{6}(1.9)5d^{0}(2.5)5f^{0}(2.9)6s^{2}(3.2)$	1 728
Lu	Lu8.0-s4p4d3f2g1	$5s^{2}(1.3)5p^{6}(1.35)5d^{1}(1.5)5f^{0}(2.4)6s^{2}(2.3)6p^{0}(2.7)$	1 152
Hf	Hf7.0-s3p3d3f1	$5s^{2}(1.3)5p^{6}(1.35)5d^{2}(1.5)6s^{2}(2.3)6p^{0}(2.7)$	1 152
Ta	Ta7.0-s3p3d3f2	$5s^{2}(1.2)5p^{6}(1.2)5d^{3}(1.53)6s^{2}(2.2)6p^{0}(2.8)$	1 331
W	W7.0-s3p3d3f1	$5p^{6}(1.3)5d^{4}(2.0)6s^{2}(2.6)6p^{0}(2.8)$	1 331
Re	Re7.0-s3p3d3f1	$5s^{2}(1.2)5p^{6}(1.3)5d^{5}(1.6)6s^{2}(2.7)6p^{0}(2.8)$	1 331
Os	Os7.0-s3p3d2f1	$5p^{6}(1.1)5d^{6}(1.7)6s^{2}(2.4)6p^{0}(2.8)7s^{0}(3.0)$	1 331
Ir	Ir7.0-s3p3d2f1	$5p^{6}(1.1)5d^{7}(1.7)5f^{0}(2.0)6s^{2}(2.6)6p^{0}(2.7)7s^{0}(3.1)$	1 331
Pt	Pt7.0-s4p3d2f2	$5p^{6}(1.1)5d^{9}(1.7)6s^{1}(2.0)6p^{0}(2.8)7s^{0}(2.9)$	1 331
Au	Au7.0-s4p3d2f2	$5p^{6}(1.2)5d^{10}(1.7)5f^{0}(2.0)6s^{1}(2.1)6p^{0}(3.2)7s^{0}(3.1)$	1 331
Hg	Hg8.0-s3p3d2f1	$5p^{6}(1.2)5d^{10}(1.6)5f^{0}(2.1)6s^{2}(2.2)6p^{0}(3.1)7s^{0}(2.9)$	1 200
Tl	Tl8.0-s4p4d3f2	$5p^{6}(1.2)5d^{10}(1.6)5f^{0}(2.1)6s^{2}(2.2)6p^{1}(2.6)7s^{0}(2.5)$	1 152
Pb	Pb8.0-s4p4d3f2	$5d^{10}(1.3)5f^{0}(1.7)6s^{2}(2.1)6p^{2}(2.3)7s^{0}(2.5)7p^{0}(3.2)$	1 728
Bi	Bi8.0-s4p4d3f2	$5d^{10}(1.1)5f^{0}(1.9)6s^{2}(2.0)6p^{3}(2.2)7s^{0}(2.3)7p^{0}(2.8)$	720
Po	Po8.0-s3p3d3f2	$5d^{10}(1.3)5f^{0}(1.9)6s^{2}(1.8)6p^{4}(2.4)$	1 728
Rn	Rn11.0-s3p3d2f1	$5f^{0}(1.9)6s^{2}(1.7)6p^{6}(2.0)6d^{0}(2.6)7s^{0}(2.2)$	1 728

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

	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	17.334	10.251	2.227
He	16.437	1.215	6.762
Li	19.943	14.719	3.900
Be	7.852	126.156	3.273
B	7.234	236.297	3.405
C	11.656	210.013	3.585
N	29.499	54.725	3.559
O	18.947	50.146	3.860
F	19.323	32.960	3.648
Ne	24.118	1.287	6.759
Na	37.232	8.238	2.672
Mg	23.104	36.052	3.981
Al	16.356	76.493	4.150
Si	20.524	89.302	4.380
P	21.441	68.790	4.206
S	17.231	86.014	4.063
Cl	39.211	18.857	4.349
Ar	48.559	2.464	11.119
K	73.486	3.550	4.456
Ca	42.190	17.130	3.331
Sc	24.633	54.814	3.279
Ti	17.329	115.575	3.969
V	13.454	193.477	3.947
Cr	11.915	167.075	7.939
Mn	11.733	126.605	−1.022
Fe	11.420	186.257	8.095
Co	10.929	214.191	4.807
Ni	10.960	201.770	4.822
Cu	12.058	138.499	4.779
Zn	15.293	74.375	5.440
Ga	20.506	47.242	4.917
Ge	24.080	56.656	6.167
As	22.818	68.087	4.896
Se	29.412	47.320	4.575
Br	39.675	22.296	4.613
Kr	65.732	0.801	9.878
Rb	90.508	2.674	4.958
Sr	54.791	11.440	2.212
Y	32.801	42.920	3.225
Zr	23.420	95.861	3.253
Nb	18.146	179.901	4.798
Mo	15.820	263.805	4.363
Tc	14.530	302.326	4.004
Ru	13.857	315.034	4.938
Rh	14.141	262.221	4.686
Pd	15.435	168.458	5.274
Ag	17.983	91.874	6.581
Cd	22.547	53.581	7.952
In	27.574	36.728	2.350

Sn	36.831	36.910	4.603
Sb	32.007	49.043	4.604
Te	35.179	44.421	4.506
I	50.890	18.253	4.910
Xe	88.907	0.497	7.823
Cs	118.844	1.923	4.786
Ba	63.672	9.099	3.373
Lu	29.070	49.294	4.041
Hf	22.400	109.783	3.855
Ta	18.238	199.819	4.233
W	16.150	305.293	4.670
Re	14.942	369.686	4.579
Os	14.368	398.124	4.787
Ir	14.578	356.806	4.829
Pt	15.742	256.315	5.190
Au	18.045	147.161	6.982
Hg	29.365	10.588	25.163
Tl	31.472	26.618	6.254
Pb	32.018	39.992	6.211
Bi	37.053	42.867	4.673
Po	37.566	44.965	5.680
Rn	91.382	0.556	7.446