HGH-NLCC/BigDFT

HGHk-sc and NLCC NCPP dataset / BigDFT 1.7.6

`name and version of the code:` BigDFT 1.7.6
`type of basis set:` Daubechies wavelets
`method:` norm-conserving pseudopotentials (HGHk, HGHk-sc and NLCC)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	HGHk PSP generated with relativistic corrections
`assignment of core / valence states`	see table I (valence)
`basis set size`	full high-resolution grid, h_{grid} indicated in 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 $5 \cdot 10^{-5}$ Ry

METHOD-SPECIFIC INFORMATION

`pseudopotential families`	HGHk pseudopotentials generated by Krack and hard-coded in BigDFT HGHk-sc pseudopotentials generated by Krack with semi-core electrons and hard-coded in BigDFT NLCC pseudopotentials generated by Willand and later by S. Saha with non-linear core corrections and available in the BigDFT wiki

ADDITIONAL COMMENTS

In version 1.7.6, BigDFT cannot treat non orthorhombic systems. The six elements for which this is the case, are mentioned in table I.

REFERENCES

`potentials`

[1] S. Goedecker, M. Teter, and J. Hutter, *Phys. Rev. B* **54**, 1703–1710 (1996).
[2] C. Hartwigsen, S. Goedecker, and J. Hutter, *Phys. Rev. B* **58**, 3641–3662 (1998).
[3] M. Krack, *Theor. Chem. Acc.* **114**, 145–152 (2005).
[4] A. Willand, Y. O. Kvashnin, L. Genovese, A. Vázquez-Mayagoitia, A. K. Deb, A. Sadeghi, T. Deutsch and S. Goedecker, *J. Chem. Phys.* **138**, 104109 (2013).
[5] http://bigdft.org/Wiki/index.php?title=New_Soft-Accurate_NLCC_pseudopotentials

`code`

[6] L. Genovese, A. Neelov, S. Goedecker, T. Deutsch, S. A. Ghasemi, A. Willand, D. Caliste, O. Zilberberg, M. Rayson, A. Bergman and R. Schneider, *J. Chem. Phys.* **129**, 014109 (2008).
[7] S. Mohr, L. E. Ratcliff, P. Boulanger, L. Genovese, D. Caliste, T. Deutsch and S. Goedecker, *J. Chem. Phys.* **140**, 204110 (2014).

Table I. Calculation settings per element: potential type, real-space grid spacing h_{grid}, number of k-points in the full 1st Brillouin zone of the primitive cell # k, valence.

	potential	h_{grid} [bohr]	# k [–]	valence
H	NLCC-new	$0.3156 \times 0.3279 \times 0.3151$	1000	1
He	NLCC-new	$0.3193 \times 0.3072 \times 0.3225$	1728	2
Li		Rhombohedral		
Be	NLCC-new(QE)	$0.3086 \times 0.3054 \times 0.2813$	1728	4
B		Triclinic		
C	NLCC-new	$0.3332 \times 0.2886 \times 0.3341$	1000	4
N	NLCC-new	$0.3249 \times 0.3249 \times 0.3249$	1000	5
O		Monoclinic		
F		Monoclinic		
Ne	NLCC-new	$0.3013 \times 0.3013 \times 0.3013$	1728	8
Na		Rhombohedral		
Mg	NLCC-new	$0.3267 \times 0.3353 \times 0.3258$	1728	2
Al	NLCC-new	$0.3181 \times 0.3181 \times 0.3181$	1728	3
Si	NLCC-new	$0.323 \times 0.323 \times 0.323$	1000	4
P	NLCC-new	$0.3122 \times 0.3342 \times 0.3087$	1000	5
S		Rhombohedral		
Cl	NLCC-new	$0.4083 \times 0.411 \times 0.4265$	1000	7
Ar	HGHk	$0.3124 \times 0.3124 \times 0.3124$	1728	8
K	HGHk	$0.333 \times 0.333 \times 0.333$	3375	9
Ca	NLCC-new	$0.3263 \times 0.3263 \times 0.3263$	1728	10
Sc	NLCC-new	$0.302 \times 0.3138 \times 0.3252$	1728	11
Ti	HGHk	$0.3204 \times 0.3083 \times 0.314$	1728	12
V	HGHk	$0.3148 \times 0.3148 \times 0.3148$	3375	13
Cr	N/A	N/A	N/A	N/A
Mn	N/A	N/A	N/A	N/A
Fe	HGHk	$0.3347 \times 0.3347 \times 0.3347$	3375	16
Co	HGHk	$0.2919 \times 0.2949 \times 0.3174$	1728	17
Ni	N/A	N/A	N/A	N/A
Cu	HGHk	$0.2864 \times 0.2864 \times 0.2864$	1728	11
Zn	HGHk	$0.3111 \times 0.3144 \times 0.3152$	1728	12
Ga	HGHk	$0.4315 \times 0.407 \times 0.3622$	1000	3
Ge	HGHk	$0.3024 \times 0.3024 \times 0.3024$	1000	4
As	HGHk	$0.3008 \times 0.3126 \times 0.3186$	729	5
Se	HGHk	$0.3054 \times 0.3085 \times 0.3181$	1331	6
Br	HGHk	$0.4319 \times 0.3994 \times 0.4268$	1000	7
Kr	HGHk	$0.3037 \times 0.3037 \times 0.3037$	1728	8
Rb	HGHk	$0.335 \times 0.335 \times 0.335$	3375	9
Sr	NLCC-new	$0.316 \times 0.316 \times 0.316$	1728	10
Y	N/A	N/A	N/A	N/A
Zr	NLCC-new	$0.331 \times 0.3058 \times 0.3269$	1728	12
Nb	HGHk	$0.3139 \times 0.3139 \times 0.3139$	3375	13
Mo	HGHk	$0.3327 \times 0.3327 \times 0.3327$	3375	14
Tc	HGHk	$0.3229 \times 0.3262 \times 0.2982$	1728	15
Ru	HGHk-sc	$0.3187 \times 0.322 \times 0.2902$	1728	16
Rh	HGHk-sc	$0.3025 \times 0.3025 \times 0.3025$	1728	17
Pd	HGHk-sc	$0.3113 \times 0.3113 \times 0.3113$	1728	18
Ag	HGHk	$0.3279 \times 0.3279 \times 0.3279$	1728	11
Cd	HGHk	$0.3314 \times 0.3189 \times 0.3029$	1728	12
In	HGHk-sc	$0.3117 \times 0.3117 \times 0.3189$	3375	13

Sn	HGHk	$0.3144 \times 0.3144 \times 0.3144$	1000	4
Sb	N/A	N/A	N/A	N/A
Te	HGHk	$0.3042 \times 0.3074 \times 0.313$	1331	6
I	HGHk	$0.3242 \times 0.3074 \times 0.3207$	1000	7
Xe	HGHk	$0.3333 \times 0.3333 \times 0.3333$	1728	8
Cs	N/A	N/A	N/A	N/A
Ba	HGHk	$0.3167 \times 0.3167 \times 0.3167$	3375	10
Lu	N/A	N/A	N/A	N/A
Hf	HGHk	$0.3276 \times 0.3362 \times 0.319$	1728	12
Ta	N/A	N/A	N/A	N/A
W	N/A	N/A	N/A	N/A
Re	N/A	N/A	N/A	N/A
Os	N/A	N/A	N/A	N/A
Ir	N/A	N/A	N/A	N/A
Pt	HGHk-sc	$0.3131 \times 0.3131 \times 0.3131$	1728	18
Au	HGHk-sc	$0.3287 \times 0.3287 \times 0.3287$	1728	9
Hg	HGHk	$0.3231 \times 0.3231 \times 0.3353$	3375	2
Tl	HGHk-sc	$0.3266 \times 0.2829 \times 0.3332$	1728	13
Pb	HGHk	$0.3177 \times 0.3177 \times 0.3177$	1728	4
Bi	HGHk	$0.3097 \times 0.3129 \times 0.3289$	729	5
Po	HGHk	$0.3164 \times 0.3164 \times 0.3164$	6859	6
Rn	HGHk	$0.3237 \times 0.3237 \times 0.3237$	1728	8

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	17.419	10.320	2.707
He	17.787	0.856	6.449
Li	*N/A*	*N/A*	*N/A*
Be	7.898	123.156	3.321
B	*N/A*	*N/A*	*N/A*
C	11.638	209.724	3.587
N	28.884	53.817	3.692
O	*N/A*	*N/A*	*N/A*
F	*N/A*	*N/A*	*N/A*
Ne	24.243	1.280	7.149
Na	*N/A*	*N/A*	*N/A*
Mg	22.922	36.253	3.951
Al	16.481	75.000	4.678
Si	20.456	87.441	4.257
P	21.478	68.243	4.320
S	*N/A*	*N/A*	*N/A*
Cl	38.904	18.924	4.378
Ar	52.251	0.784	6.644
K	73.533	3.603	3.764
Ca	42.196	17.200	3.000
Sc	24.617	54.023	3.329
Ti	17.286	117.112	3.440
V	13.354	192.394	3.681
Cr	*N/A*	*N/A*	*N/A*
Mn	*N/A*	*N/A*	*N/A*
Fe	11.403	169.200	6.695
Co	10.804	228.322	4.347
Ni	*N/A*	*N/A*	*N/A*
Cu	11.943	151.945	4.698
Zn	14.933	88.604	4.838
Ga	20.375	47.024	4.877
Ge	24.078	57.391	4.687
As	22.561	68.485	4.178
Se	29.728	47.127	4.402
Br	39.346	22.501	4.773
Kr	65.777	0.658	7.259
Rb	90.569	2.883	3.718
Sr	54.525	11.533	3.880
Y	*N/A*	*N/A*	*N/A*
Zr	23.386	92.952	3.322
Nb	18.146	169.256	3.697
Mo	15.818	258.970	4.179
Tc	14.477	298.905	4.454
Ru	13.806	311.588	4.755
Rh	14.072	256.467	5.548
Pd	15.372	168.551	5.525
Ag	17.961	90.563	5.725
Cd	22.864	44.755	6.380
In	27.605	35.490	5.210

Sn	37.097	34.262	4.617
Sb	N/A	N/A	N/A
Te	35.166	44.640	4.643
I	50.553	18.548	4.997
Xe	86.782	0.546	7.258
Cs	N/A	N/A	N/A
Ba	63.291	8.667	3.125
Lu	N/A	N/A	N/A
Hf	22.449	107.444	3.384
Ta	N/A	N/A	N/A
W	N/A	N/A	N/A
Re	N/A	N/A	N/A
Os	N/A	N/A	N/A
Ir	N/A	N/A	N/A
Pt	15.605	253.369	5.395
Au	17.879	143.855	5.959
Hg	29.310	8.761	11.165
Tl	31.473	26.984	5.408
Pb	31.614	39.478	4.793
Bi	36.805	42.795	4.578
Po	37.618	45.741	4.855
Rn	93.303	0.542	7.344