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## Pseudopotentials and basis sets available in QuantumATK

[PDF version](#)

The accuracy of the calculations with the LCAO model in QuantumATK depends on the pseudopotential and basis sets used for the calculations. In recent years we have put a large effort into providing a robust set which can provide good accuracy at reasonably computational resources. Thus, there is an evolution in quality of the pseudopotentials we provide, with the best sets being the [SG15](#) pseudopotentials available from the ATK-2016 release and PseudoDojo pseudopotentials available from the O-2018.06 release. The theoretical background of the basis sets and pseudopotentials are described in the [QuantumATK Manual](#), and the purpose of this note is to guide the user towards the best setting.

### Pseudopotentials

The pseudopotentials available for the QuantumATK software are listed in the below table. We see that it shows an evolution with quality of the pseudopotentials for each release. However, not all exchange correlation functionals are available for each type of pseudopotential. For [GGA](#) and [SOGGA](#) we recommend to use the [PseudoDojo](#) pseudopotential. For [LDA](#) we recommend the [FHI](#) pseudopotential. For [SOLDA](#) we recommend the [OMX](#), it can also give higher accuracy for LDA, however, the required mesh cutoff needs to be tested carefully.

Table 35 Pseudo- and PAW potential types available for the DFT calculators.<sup>¶</sup>

Name	Notes
FHI	Trouiller–Martins type.
HGH	Hartwigsen–Goedecker–Hutter type.
OMX	Fully relativistic. <a href="#">OMX webpage</a> .
SG15	ONCV type, scalar-relativistic (SG15) and fully relativistic (SG15-SO). <a href="#">SG15 webpage</a> .
PseudoDojo	ONCV type, scalar-relativistic (PseudoDojo) and fully relativistic (PseudoDojo-SO). <a href="#">PseudoDojo webpage</a> .
GPAW	PAW potentials. <a href="#">GPAW webpage</a> .
JTH	PAW potentials. <a href="#">JTH webpage</a> .
Suggested	A mixture of GPAW and JTH, chosen to give optimal results for each element.

Through the use of the keyword [NormConservingPseudoPotential](#), it is also possible to specify a

pseudopotential from a user-specified file. Not all pseudopotentials are available for all QuantumATK DFT calculators and exchange-correlation functional types. Please see the following table for details on each of the pseudopotential types:

Table 36 Details about the pseudo- and PAW potential types available for the QuantumATK DFT calculators.¶

Name	Introduced	Basis types	XC-types	Cutoff [Ha]	Accuracy	Efficiency
FHI	ATK-2008	LCAO, PW	LDA, GGA, MGGA, HGGA	30-100	Low	High
HGH	ATK-2011	LCAO, PW	LDA, GGA, MGGA, HGGA	75-500	Medium	Low
OMX	ATK-2015	LCAO	LDA, GGA, MGGA	75-500	High	Low
OMX-SO	ATK-2015	LCAO	SOLDA, SOGGA, SOMGGA	75-500	High	Low
SG15	ATK-2016	LCAO, PW	GGA, HGGA	30-220	High	Medium
SG15-SO	ATK-2016	LCAO, PW	GGA, SOGGA, HSOGGA	30-220	High	Medium
PseudoDojo	O-2018.06	LCAO, PW	GGA, HGGA	30-125	High	Medium
PseudoDojo-SO	P-2019.03	LCAO, PW	GGA, SOGGA, HSOGGA	30-125	High	Medium
PAW-GPAW	Q-2019.12	PW	LDA, GGA	N/A	High	Medium
PAW-JTH	Q-2019.12	PW	LDA, GGA	N/A	High	Medium
PAW-Suggested	Q-2019.12	PW	GGA	N/A	High	Medium

#### Warning

The higher values for OMX pseudopotentials, about 300 Hartree or more, are especially relevant for pseudopotentials with semi-core states. They often need these very high mesh cutoffs to give accurate forces.

## LCAO basis sets

QuantumATK mainly uses a numerical LCAO [basis sets](#). The accuracy depends on the number of orbitals and the range of the orbitals. Increasing the number of orbitals and their range decrease the efficiency and increase the memory requirement. For the latest [SG15](#) and [PseudoDojo](#) pseudopotentials we provide basis sets which systematically improve the accuracy. For the other pseudopotentials the improvement in accuracy is less systematic.

### SG15/PseudoDojo

Three different basis sets are available for each element when using the SG15/PseudoDojo pseudopotentials; **Medium**, **High**, and **Ultra**. All three derive from the numerical atom-centered basis sets of the [FHI-aims](#) package, but have been significantly modified and optimized with respect to

computational speed with the [DFT: LCAO](#) calculator.

The Medium basis set is default for the SG15/PseudoDojo pseudopotentials, and should be sufficient for most applications. However, if extreme accuracy is needed, the High and Ultra basis sets add more basis functions at the expense of increased computational load.

## OMX

The OMX basis sets were developed in Refs. [1] and [2], and are optimized towards maximum computational speed and accuracy with the OMX pseudopotentials. The [DFT: LCAO](#) calculator offers three different OMX basis set sizes for most elements; **Low**, **Medium**, and **High**, which include increasingly more pseudo-atomic orbitals in the basis set. More details are available on the website for the [OpenMX database \(2013\)](#).

## FHI

Four different types of basis functions can be used for the FHI pseudopotentials:


- [ConfinedOrbital](#)
- [AnalyticalSplit](#)
- [PolarizationOrbital](#)
- [HydrogenOrbital](#)

The basis sets available for FHI pseudopotentials are listed below. They are ordered with increasing number of basis orbitals – those with more orbitals are often more accurate, at the expense of increased computational load. The DZP basis set is default.

- SingleZeta: One [ConfinedOrbital](#) for each occupied valence orbital in the atom.
- DoubleZeta: One [ConfinedOrbital](#) and one [AnalyticalSplit](#) for each occupied valence orbital in the atom.
- SingleZetaPolarized: One [ConfinedOrbital](#) for each occupied valence orbital in the atom, and one [PolarizationOrbital](#) for the first unoccupied shell in the atom.
- DoubleZetaPolarized: One [ConfinedOrbital](#) and one [AnalyticalSplit](#) for each occupied valence orbital in the atom. One [PolarizationOrbital](#) for the first unoccupied shell in the atom.
- DoubleZetaDoublePolarized: One [ConfinedOrbital](#) and one [AnalyticalSplit](#) for each occupied valence orbital in the atom. One [PolarizationOrbital](#) and one [AnalyticalSplit](#) for the first unoccupied shell in the atom.

## Visualizing the basis functions

To see the type of the basis sets it is most easy to plot the basis functions, like this:

- Open the scripter
- Add an LCAOcalculator block from the Calculators section
- Go to the Basis set tab at click the plot widget  in the line where you define the basis set.

You will then get the following plot.



## Accuracy tests for elemental solids

To give an overall idea of the accuracy of each pseudopotential and basis sets we have performed so-called

$\Delta$ -tests [3] (see the web-site [Comparing Solid State DFT Codes, Basis Sets and Potentials](#)). These tests checks accuracy for the pseudopotential and basis set compared with state of the art all-electron calculations. The tests check the accuracy of the pseudopotential and basis sets in reproducing the equation of state of all the elemental solids in the periodic system using the GGA-PBE exchange-correlation functional.

*Table 37 Accuracy and performance of PBE pseudopotentials and basis types available for the DFT calculators. Performance is an approximate measure of time spent, relative to FHI-DZP. Lower numbers are faster. ¶*

Pseudo	Basis	$\Delta$ (meV)	Performance
FHI	SZP	39.4	0.5
FHI	DZP	18.2	1
FHI	DZDP	19.1	2
HGH	Tier4	12.8	6
OMX	Medium	8.0	3
OMX	High	2.2	10
SG15	Medium	3.45	2
SG15	High	1.88	6
SG15	Ultra	2.03	25
SG15	PW	1.32	N/A
PseudoDojo	Medium	4.53	2
PseudoDojo	High	1.52	6
PseudoDojo	Ultra	1.40	25
PseudoDojo	PW	1.04	N/A
PAW-GPAW	PW	1.44	N/A
PAW-JTH	PW	0.86	N/A
PAW-Suggested	PW	0.64	N/A

A

$\Delta$  value below 2 meV indicates a state of the art DFT calculation. *PAW-Suggested* is a combination of the two PAW sets where we have selected the best PAW potential for each element. The performance number given in the Table is an average indication of how much time a calculation of a 64 atom supercell takes, using the different models relative to the FHI-DZP model. Lower numbers are faster. There are large variations among the elements and the performance number should only be used as a rough guide.

## Accuracy tests for mixed solids

The

$\Delta$ -tests are done for ideal systems, in order to illustrate that these results are transferable to general systems we have performed a number of additional accuracy tests. The first test is for a number Rock Salt (RS) and Perovskite(P) structures provided in Ref. [4]. The reference points are FHI-aims all electron calculations. We see the deviations for the

$a$  (lattice constant),  
 $B$  (Bulk modulus) and  
 $E_f$  (formation energy) compared to the Ref. [4] in the below Table.

*Table 38 Accuracy of selected methods in QuantumATK on RockSalt (RS) geometries [4]. The formation energy is not available for the Ultra-soft and PAW plane-wave calculations. The reference is a fully converged all-electron calculation using FHI-aims.*

Pseudo	Basis	$a$ (%)	$B$ (%)	$E_f$ (%)	Source
Ultra-Soft	PW	0.13	5.0	N/A	[4]
PAW	PW	0.15	4.5	N/A	[4]
PseudoDojo	Ultra	0.15	1.90	1.83	QuantumATK
PseudoDojo	High	0.18	2.12	2.79	QuantumATK
PseudoDojo	Medium	0.5	5.32	15.59	QuantumATK
PseudoDojo	PW (40 Ha)	0.09	1.86	0.85	QuantumATK
SG15	High	0.3	8.6	4.6	QuantumATK
SG15	Medium	0.6	13.0	12.5	QuantumATK
FHI	DZP	3.0	23.2	15.5	QuantumATK

*Table 39 Accuracy of selected methods in QuantumATK on Perovskites (P) geometries from Ref. [4]*

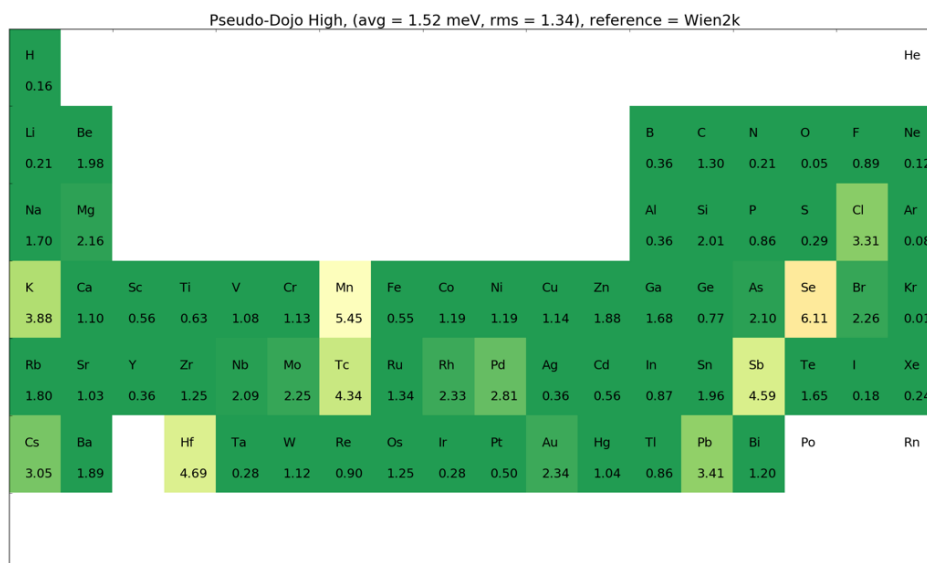
Pseudo	Basis	$a$ (%)	$B$ (%)	$E_f$ (%)	Source
Ultra-Soft	PW	0.08	5.5	N/A	[4]
PAW	PW	0.13	6.1	N/A	[4]
PseudoDojo	Ultra	0.13	1.87	0.91	QuantumATK
PseudoDojo	High	0.21	3.04	1.18	QuantumATK
PseudoDojo	Medium	0.35	3.68	2.73	QuantumATK
PseudoDojo	PW (40 Ha)	0.06	0.66	0.23	QuantumATK
SG15	High	0.3	5.7	1.4	QuantumATK
SG15	Medium	0.4	6.4	2.6	QuantumATK
FHI	DZP	3.5	18.3	12.8	QuantumATK

## Notes for each pseudopotential type

### PseudoDojo Pseudopotentials and basis sets

The PseudoDojo are state of the art norm-conserving pseudopotentials including multiple projectors, semi-core states and non-linear core correction [5]. They are only provided for the GGA-PBE functional, and comes in both a scalar relativistic and a fully relativistic version. The latter is used for calculations including spin-orbit. The pseudopotentials are smooth and all elements converge with a mesh cutoff below 125 Ha.

Below are given the  $\Delta$ -tests for the different elements.







SG15 Medium, 100 Ha, (avg = 3.45 meV, rms = 2.65)

SG15 Medium, 100 Ha, (avg = 3.45 meV, rms = 2.65)																			
H																	He		
0.96																	0.02		
Li	Be													B	C	N	O	F	Ne
0.64	1.75													1.65	0.66	6.57	9.37	3.79	0.06
Na	Mg													Al	Si	P	S	Cl	Ar
0.19	4.57													8.10	1.39	4.40	3.43	5.53	0.26
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
7.69	1.47	0.89	1.27	6.41			3.88	8.10	6.05	5.20	2.28	0.14	4.35	5.30	1.06	6.03	0.48		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
8.19	3.45		0.83	0.58	3.78	1.32	1.13	1.32	1.71	2.87	5.82	0.45	4.92	8.07	2.85	8.54	1.90		
Cs	Ba			Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	Rn		
10.78	2.96			3.43	2.86	2.74	3.01	1.34	6.31	5.17	5.50	2.11	4.78	1.68	2.36				

SG15 High, 100 Ha, (avg = 1.88 meV, rms = 1.74)

SG15 High, 100 Ha, (avg = 1.88 mev, rms = 1.74)																			
H																			He
0.19																			0.02
Li	Be													B	C	N	O	F	Ne
0.52	0.35													1.88	2.80	1.04	1.68	1.55	0.10
Na	Mg													Al	Si	P	S	Cl	Ar
0.43	0.42													2.70	1.29	0.43	0.34	1.74	0.11
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
4.96	0.38	0.20	1.44	2.18			7.01	5.40	4.84	3.37	3.21	1.28	3.09	1.84	1.58	1.78	0.30		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
6.73	0.50	0.68	0.22	1.31	1.54	2.60	0.33	1.94	0.47	2.64	2.88	1.57	3.42	1.22	4.02	2.73	0.60		
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po		Rn		
7.50	1.91		4.54	0.49	0.39	1.04	0.94	1.72	2.36	4.08	0.97	0.64	1.82	0.06					

SG15 Ultra, 100 Ha, (avg = 2.03 meV, rms = 1.80)

H																		He
0.22																		0.01
Li	Be											B	C	N	O	F	Ne	
0.72	0.26											1.92	2.64	1.62	1.05	1.95	0.07	
Na	Mg											Al	Si	P	S	Cl	Ar	
1.27	1.55											4.57	6.09	2.13	0.34	4.34	0.03	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
4.78	0.38	0.03	1.90	1.90			4.42	6.55	3.47	3.40	3.68	3.71	4.54	2.84	1.95	0.81	0.06	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6.45	0.67	0.67	0.57	0.75	1.26	0.57	0.75	2.08	0.98	3.15	2.83	1.02	2.20	0.91	3.99	1.52	0.59	
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po		Rn	
7.88	2.59		3.65	0.85	0.23	0.80	0.95	1.79	2.89	3.30	0.33	0.66	1.17	0.61				

## PAW data sets

For the Projector Augmented Wave (PAW) method, we need data describing the system inside the augmentation sphere (partial waves, projectors, core densities, ...). This is gathered in a PAW data set file. We support data set files in the .xml format, as specified on the [ESL website](#). We ship two different data sets, the [GPAW](#) and [JTH \[8\]](#) data sets, for which we found default wave function cutoffs that are as low as possible without losing accuracy. We made a combined PAW-Suggested data set for GGA, that gives the best results.

Below are given the  $\Delta$ -tests for the different elements.

GPAW, WFC=30.0 Ha (avg = 1.44 meV, rms = 1.71)

H																	He
0.18																	0.01
Li	Be											B	C	N	O	F	Ne
0.23	2.68											0.13	0.38	0.51	0.28	0.28	0.05
Na	Mg											Al	Si	P	S	Cl	Ar
0.48	0.11											1.06	1.24	0.88	0.89	0.30	0.01
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.01	0.76	0.43	1.80	4.10	1.62	0.23	5.74	3.32	5.15	4.33	0.51	1.36	0.75	0.74	0.18	1.51	0.05
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.18	2.02	0.47	0.90	2.64	1.11		1.34	6.61	1.01	0.49	0.36	1.82	1.10	1.47	2.56	1.41	0.02
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po		Rn
0.14	0.96		1.10	0.79	2.02	2.91	7.70	3.62	0.72	6.48	0.46	1.41	1.19	0.64			0.02

JTH, WFC=30.0 Ha (avg = 0.86 meV, rms = 0.95)

H																		He
0.06																		0.01
Li	Be											B	C	N	O	F	Ne	
0.10	0.14											0.14	0.87	0.74	0.58	0.23	0.04	
Na	Mg											Al	Si	P	S	Cl	Ar	
0.44	0.47											0.19		0.69	0.25	0.18	0.01	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
0.13	0.06	0.50	0.41	1.34	2.91	2.29	1.59	0.93	2.76	2.41	0.11	0.64	0.65	0.12		2.60	0.17	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
0.06	1.16	0.40	0.61	0.50	1.28	0.81	1.10	1.66	0.55	3.06	4.25	1.91	3.63	0.27	0.06	0.83	0.02	
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po		Rn	
0.08	0.95		0.29	0.62	1.04	2.00	0.35	0.50	2.48	0.47	0.28	0.64	1.09	0.28	0.71		0.03	

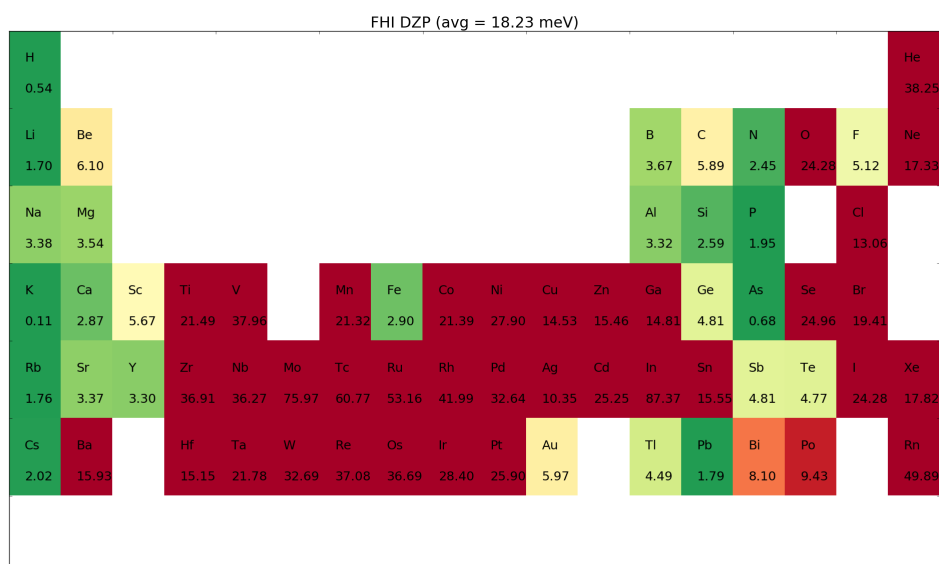
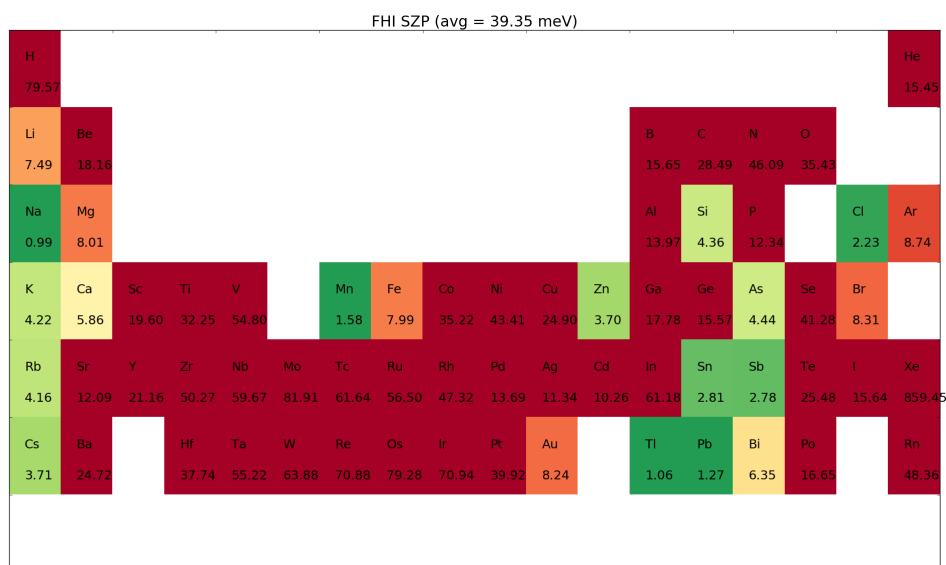
H																	He
0.14																	0.04
Li	Be											B	C	N	O	F	Ne
0.25	0.09											0.22	0.61	0.21	0.70	0.35	0.12
Na	Mg											Al	Si	P	S	Cl	Ar
0.42	0.08											0.04	1.31	0.96	0.70	0.27	0.05
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.07	0.08	0.50	0.57	1.68	1.79	0.51	1.51	0.91	2.07	2.07	0.07	0.58	0.86	0.15	0.18	1.44	0.03
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.26	1.20	0.60	0.71	0.17	1.22	0.80	0.93	1.34	1.18	0.21	0.14	1.21	1.19	0.36	0.06	0.92	0.08
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po		Rn
0.07	0.90		0.46	0.86	1.16	2.59	0.28	0.33	0.75	0.67	0.16	0.51	0.96	0.31	0.15		0.01

## FHI pseudopotentials and basis sets

The FHI pseudopotentials are the oldest pseudopotentials in QuantumATK. These pseudopotentials are generated with the Fritz-Haber Institute (FHI) pseudopotential code. They are numerical norm-conserving pseudopotentials with a single projector for each angular momentum and without semicore states. For a number of elements the exclusion of semi-core states gives a low accuracy.

The basis sets provided with the FHI pseudopotentials use generic parameters, which are not optimized for each element and generally not of high accuracy. However, the basis sets and pseudopotentials are rather efficient and for some elements can give satisfactory accuracy. We only recommend the SZP and DZP basis sets. Below are given

$\Delta$  values for these settings and the table can be used to estimate the accuracy of the model for various elements.



## OMX Pseudopotentials and basis sets

The OMX pseudopotentials are from the [OpenMX packages](#). They are fully relativistic, multiple projectors and with semi-core states. Thus, these are generally high accuracy pseudopotentials which can be used for both LDA, GGA and spin-orbit calculations. The drawback of the pseudopotentials is that they for some elements require very high mesh cutoffs.

The basis sets provided are from the original openMX package. This means that they are not calculated on the fly, and therefore only accurate for the exchange-correlation potential for which they were calculated. Thus, if other exchange-correlation functionals than LDA-PZ or GGA-PBE are used, the accuracy will be lower. For our other pseudopotentials the basis sets are generated on the fly with the selected exchange-correlation potential, thus, even if the pseudopotential is not generated for the exchange-correlation functional the basis set will conform to the exchange-correlation functional.

For the OMX pseudopotentials, we have defined two basis set types, Medium and High. It is also possible for the user to define custom basis sets through the `atomic_species` keyword, see [OpenMXBasisSet](#).

The basis sets was pre-calculated using GGA-PBE or LDA-PZ and included together with the

pseudopotential. Thus, if other exchange-correlation functionals than LDA-PZ or GGA-PBE are used, the accuracy will be low.

For the other pseudo potentials the basis sets are calculated on the fly, using the selected exchange-correlation potential. i.e. only core electrons are treated with the GGA-PBE functional, while valence electrons are treated with the selected exchange-correlation functional.

Below we provide the

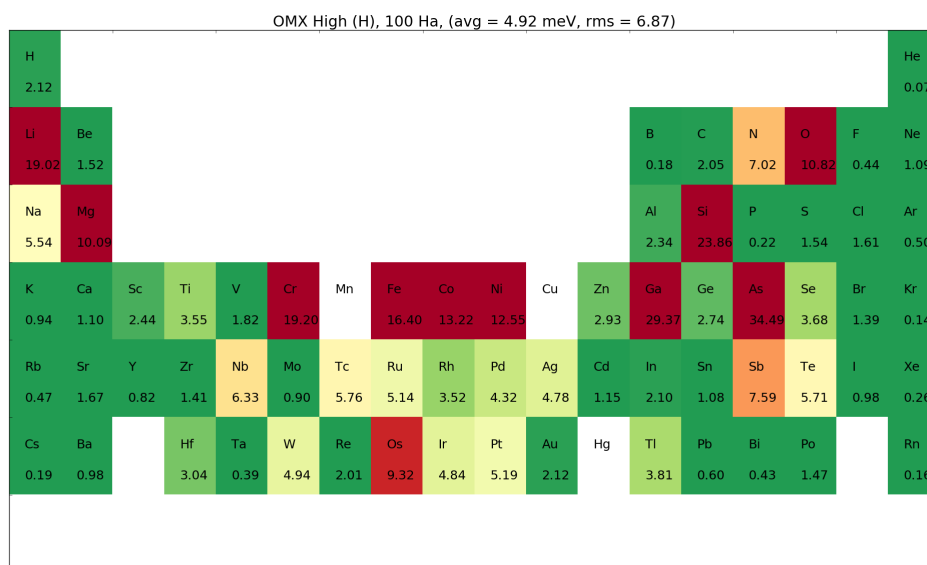
$\Delta$  values for the Medium and High basis sets. For the High basis set we also provide the  $\Delta$  value when a 100 Ha mesh cutoff is used. This, gives an indication for which elements the default mesh cutoff needs to be increased.

OMX Medium (H)(avg = 7.98 meV, rms = 10.12)

H																	He
1.18																	0.06
Li	Be											B	C	N	O	F	Ne
6.08	0.68											0.09	2.24	13.42	13.97	7.83	0.50
Na	Mg											Al	Si	P	S	Cl	Ar
3.07	2.04											4.38	6.22	14.52	8.40	14.71	0.17
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.18	2.27	0.50	2.74	1.89	5.95	13.56	2.95	2.83	5.54	4.42	3.54	7.01	10.84	5.56	17.75	11.34	0.23
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.89	3.62	0.98	1.10	1.47	19.26	23.36	32.11	25.81	4.55	2.03	1.22	4.25	3.61	9.72	15.90	5.56	0.29
Cs	Ba	Hf		Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	Rn	
0.16	2.26	7.19		11.60	21.81	33.17	52.67	34.63	27.23	3.69	0.61	0.48	1.28	7.16	0.18	0.21	

OMX High (Optimal)(avg = 2.16 meV, rms = 1.97)

H																	He
2.16																	0.04
Li	Be											B	C	N	O	F	Ne
0.55	1.53											0.14	1.63	5.99	4.69	0.49	0.44
Na	Mg											Al	Si	P	S	Cl	Ar
2.54	1.55											2.44	1.46	0.17	1.85	1.39	0.09
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.07	0.30	0.21	1.82	1.82	6.41	7.88	3.15	2.50	2.44	3.72	3.17	2.54	2.69	4.26	3.68	1.35	0.16
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.09	0.99	1.03	0.81	1.36	1.63	4.96	5.18	4.49	3.30	1.09	2.62	1.68	1.12	1.43	1.93	1.01	0.17
Cs	Ba			Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	Rn
0.36	1.11			3.75	3.94	4.32	2.66	9.25	5.32	4.95	1.50	0.18	0.34	0.25	0.64	0.54	0.16

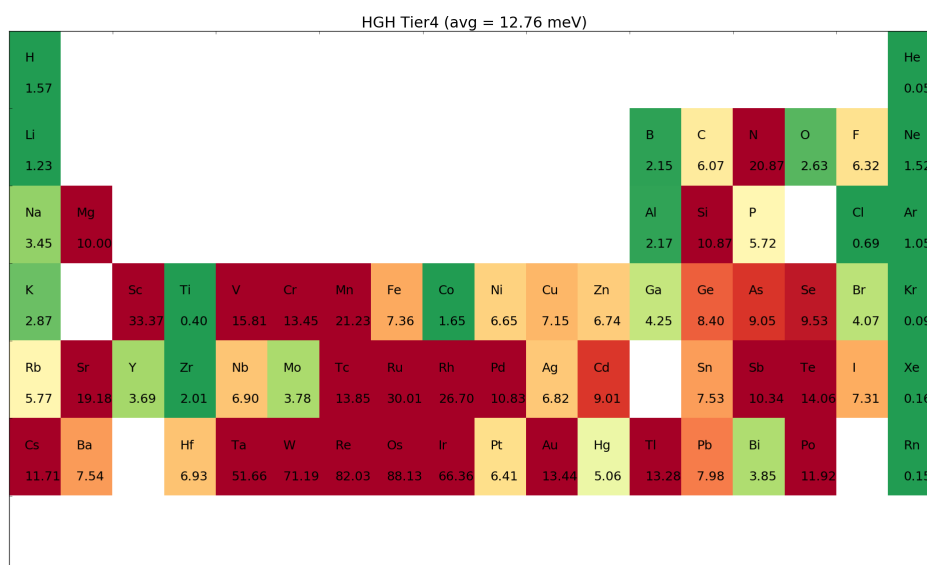


## HGH Pseudopotentials and basis sets

The Hartwigsen–Goedecker–Hutter (HGH) type pseudopotentials are also norm-conserving pseudopotentials, however, include multiple projectors and semi-core states. The pseudopotentials use analytical functions which are slightly lower accuracy than numerical pseudopotentials. These pseudopotentials require high values for the mesh cutoff for some elements.

For each pseudopotential we provide a hierarchy of basis sets. The basis sets were optimized to describe the total energy of dimers with different bondlengths. This was an early version of our basis set optimization tool and not all elements are well described.

Generally the pseudopotentials and basis sets have better accuracy than the FHI pseudopotentials but can be computationally heavy and require high mesh cutoffs. The sets are only provided for backwards compatibility and are no longer recommended.



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