Exercises on basis set generation

Full control on the definition of the basis set functions:

the PAO.Basis block

Javier Junquera

The PAO.Basis block

Full control on the definition of the basis set

```
%block PAO.Basis                        # Define Basis set
O     2  nodes  1.0                     # Label, number_of_l_shells, type (opt), ionic_charge (opt)
 n=2 0 2  E 50.0 2.5                    # n (opt if not using semicore levels),l,Nzeta,Softconf Prefactor(opt),Softconf inner radius(opt)
      3.50  3.50                        #     rc(izeta=1,Nzeta) (Bohr)
      0.95  1.00                        #     scaleFactor(izeta=1,Nzeta) (opt)
      1 1  P 2                          # l, Nzeta, PolOrb (opt), NzetaPol (opt)
      3.50                              #     rc(izeta=1,Nzeta) (Bohr)
Ba    5      0.70                       # Label, number_of_l_shells, type (opt), ionic_charge (opt)
 n=5    0    1   E     98.95      5.90  # n (opt if not using semicore levels),l,Nzeta,Softconf Prefactor(opt),Softconf inner radius(opt)
   6.40                                 #     rc(izeta=1,Nzeta) (Bohr)
   1.00                                 #     scaleFactor(izeta=1,Nzeta) (opt)
 n=6    0    2   E     97.95      6.50
   7.00   6.00
   1.00   1.00
 n=5    1    1   E     96.95      6.09
   6.60
   1.00
 n=5    2    1   E     95.95      6.60
   7.10
   1.00
 n=6    1    1   E     94.96      6.60
   7.10
   1.00
H     1                                 # Label, number_of_l_shells, type (opt), ionic_charge (opt)
      0 2 S 0.2                         # l, Nzeta, Per-shell split norm parameter
      5.00  0.00                        #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                     # End of definition of the basis set
```

Species label:
determines the species index according to the block ChemicalSpecieslabel

The PAO.Basis block

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     5.00  0.00                         #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                     # End of definition of the basis set
```

Number of shells of orbitals with different angular momentum for the corresponding chemical species

The PAO.Basis block

Full control on the definition of the basis set

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 n=5    0    1    E      98.95      5.90   # n (opt if not using semicore levels),l,Nzeta,Softconf Prefactor(opt),Softconf inner radius(opt)
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     0 2 S 0.2                          # l, Nzeta, Per-shell split norm parameter
     5.00  0.00                         #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                     # End of definition of the basis set
```

(O Oxygen)

As many shells as indicated here

$(n = 2, l = 0, N_\zeta = 2)\ 2s$ with two ζ radial functions

$(n = 2, l = 1, N_\zeta = 1)\ 2p$ with one ζ radial function

The PAO.Basis block

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 n=6   1    1   E      94.96     6.60
   7.10
   1.00
H    1
     0 2 S 0.2
     5.00  0.00
%endblock PAO.Basis                     # End of definition of the basis set
```

(Ba Barium: semicore in valence)

$(n = 5, l = 0, N_\zeta = 1)$ $5s$ with one ζ radial function. semicore state

$(n = 6, l = 0, N_\zeta = 2)$ $6s$ with two ζ radial function.

$(n = 5, l = 1, N_\zeta = 1)$ $5p$ with one ζ radial function. semicore state

$(n = 5, l = 2, N_\zeta = 1)$ $5d$ with one ζ radial function.

$(n = 6, l = 1, N_\zeta = 1)$ $6p$ with one ζ radial function.

The PAO.Basis block

Full control on the definition of the basis set

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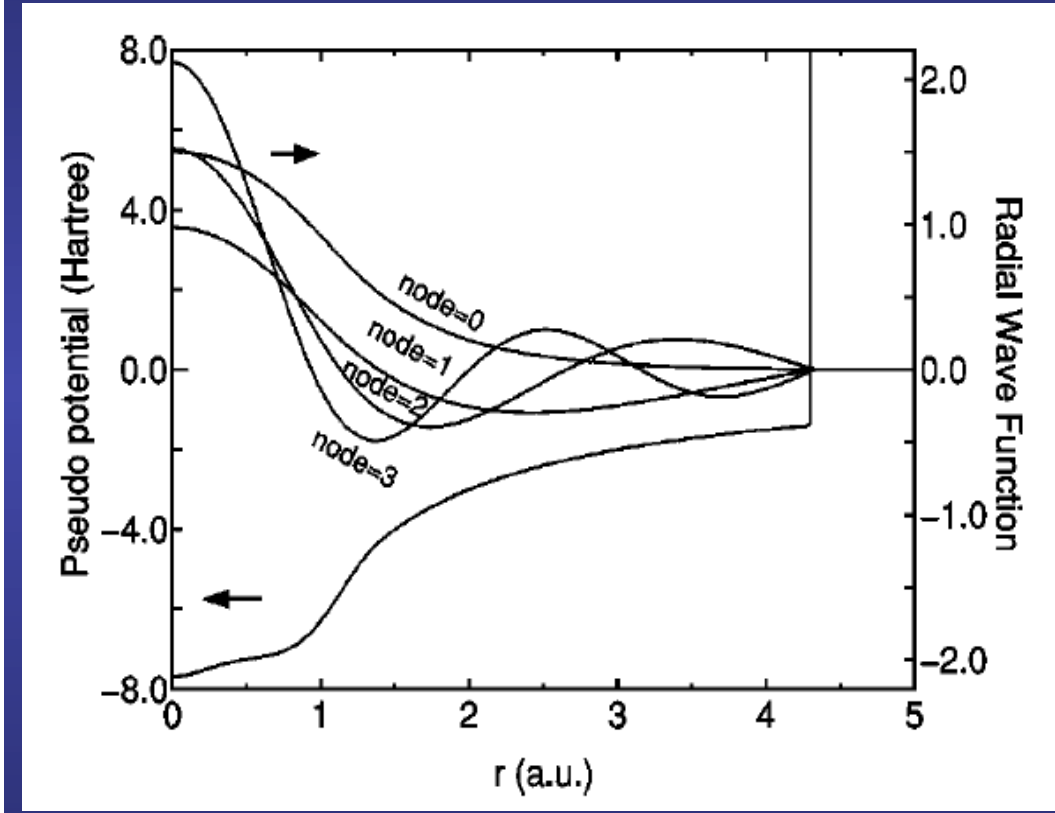
H    1                                # Label, number_of_l_shells, type (opt), ionic_charge (opt)
     0 2 S 0.2                        # l, Nzeta, Per-shell split norm parameter
     5.00  0.00                       #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                   # End of definition of the basis set
```

Kind of basis set generation procedure.

Default:
PAO.BasisType Split
(see the lecture on the SplitNorm)

Schemes to generate multiple-ζ basis sets
Use pseudopotential eigenfunctions with increasing number of nodes



T. Ozaki *et al.*, Phys. Rev. B 69, 195113 (2004)

http://www.openmx-square.org/

Advantages

Orthogonal

Asymptotically complete

Disadvantages

Excited states of the pseudopotentials, usually unbound

Efficient depends on localization radii

Availables in Siesta:

PAO.BasisType Nodes

The PAO.Basis block

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   1.00
H    1                                # Label, number_of_l_shells, type (opt), ionic_charge (opt)
     0 2 S 0.2                        # l, Nzeta, Per-shell split norm parameter
     5.00  0.00                       #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                   # End of definition of the basis set
```

Only used for the generation of the basis set

Default value 0.0 electrons

Solving the Schrödinger equation for an ion for the generation of the basis set

Extra charge δQ

Orbitals in **anions** tend to be more **delocalized**

Orbitals in **cations** tend to be more **localized**

(For instance, this parameter might be important in some oxides)

The PAO.Basis block

Full control on the definition of the basis set

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   1.00                                  #     scaleFactor(izeta=1,Nzeta) (opt)
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 n=6    1    1   E     94.96      6.60
   7.10
   1.00
H    1                                  # Label, number_of_l_shells, type (opt), ionic_charge (opt)
     0 2 S 0.2                          # l, Nzeta, Per-shell split norm parameter
     5.00  0.00                         #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                     # End of definition of the basis set
```

This flag determines whether the soft-confinement potential is used

V_0 (in Ry) r_i (in Bohr)

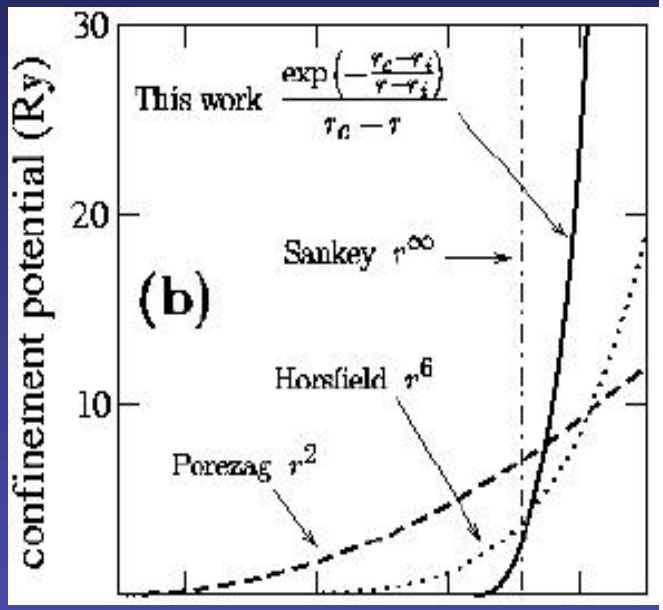
Default value: 0.0 Ry **Default value: 0.0 Bohr**

If negative, computed as the given fraction of the PAO cutoff radius.

Soft-confinement potential

Available in SIESTA

$$V(r) = V_0 \frac{e^{-\frac{r_c - r_i}{r - r_i}}}{r_c - r}$$



J. Junquera *et al.*, Phys. Rev. B 64, 235111 (2001)

V_0 Prefactor of the soft-confinement potential

r_i Inner radius where the shoft-confinement potential starts off

Advantages: orbital continuous with all the derivatives continuous

diverges at r_c (orbital exactly vanishes there)

zero at the core region

The PAO.Basis block

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     3.50                                 #     rc(izeta=1,Nzeta) (Bohr)
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 n=5    0    1   E     98.95      5.90    # n (opt if not using semicore levels),l,Nzeta,Softconf Prefactor(opt),Softconf inner radius(opt)
   6.40                                   #     rc(izeta=1,Nzeta) (Bohr)
   1.00                                   #     scaleFactor(izeta=1,Nzeta) (opt)
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   1.00   1.00
 n=5    1    1   E     96.95      6.09
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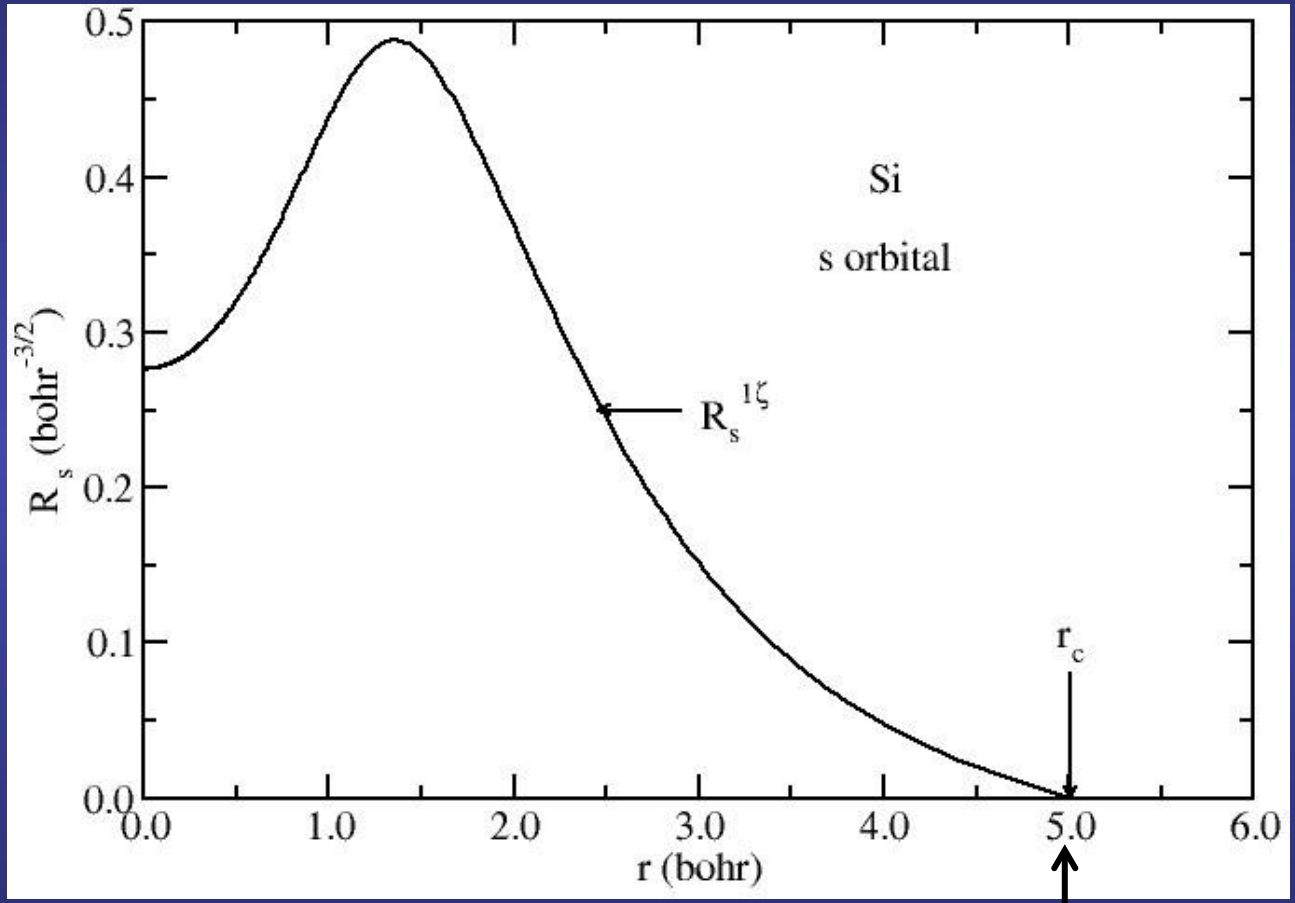
   7.10
   1.00
 n=6    1    1   E     94.96      6.60
   7.10
   1.00
H    1                                    # Label, number_of_l_shells, type (opt), ionic_charge (opt)
     0 2 S 0.2                            # l, Nzeta, Per-shell split norm parameter
     5.00  0.00                           #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                       # End of definition of the basis set
```

As many columns as zetas in the shell

Cutoff radius of ech zeta for a given shell (in Bohr)

The numerical atomic orbitals are strictly localized: they are zero beyond a given cutoff radius



This is the cutoff that might be explicitly included in the PAO.Basis block

The PAO.Basis block

Full control on the definition of the basis set

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     5.00  0.00                         #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                     # End of definition of the basis set
```

If some of these are zero, then the PAO.EnergyShift or PAO.SplitNorm will be used to determine the cutoff

For the secon-zeta onwards, if some of these are negative, then the actual rc used will be the given fraction of the first

The PAO.Basis block

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```

As many columns as zetas in the shell

Constraint factor of each zeta.
Default value 1.0

The PAO.Basis block

Full control on the definition of the basis set

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```

A shell of polarization functions (with angular momentum $l+1$) will be constructed from the first-zeta of angular mometum l (Default value: blank no polarization orbitals)

Number of zetas of the polarization shell

The PAO.Basis block

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   1.00                                  #     scaleFactor(izeta=1,Nzeta) (opt)
 n=6    0    2   E     97.95      6.50
   7.00   6.00
   1.00   1.00
 n=5    1    1   E     96.95      6.09
   6.60
   1.00
 n=5    2    1   E     95.95      6.60
   7.10
   1.00
 n=6    1    1   E     94.96      6.60
   7.10
   1.00
H    1                                  # Label, number_of_l_shells, type (opt), ionic_charge (opt)
     0 2 S 0.2                          # l, Nzeta, Per-shell split norm parameter
     5.00  0.00                         #     rc(izeta=1,Nzeta) (Bohr)
%endblock PAO.Basis                     # End of definition of the basis set
```

If this flag is set to S, the following numbers sets the split-norm parameter for that shell

Split Norm Parameter for the shell