siesta
TM

Converge calculations:
Mesh, k-points and SCF convergence

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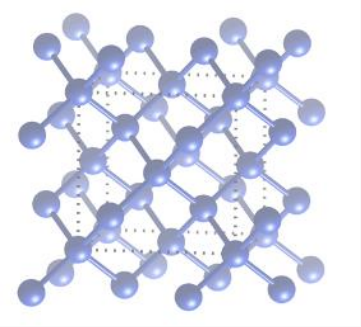
ICN2 Institut Català de Nanociència i Nanotecnologia
10 YEARS
BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación
CSIC
Consejo Superior de Investigaciones Científicas
MAX DRIVING THE EXASCALE TRANSITION
Ministerio de Ciencia, Innovación y Universidades
Financiado por la Unión Europea NextGenerationEU
Plan de Recuperación, Transformación y Resiliencia
AGENCIA ESTATAL DE INVESTIGACIÓN

Sampling

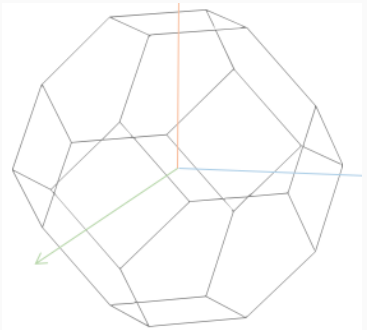
Real space

- **Potentials**
- **Densities**
- **Basis**

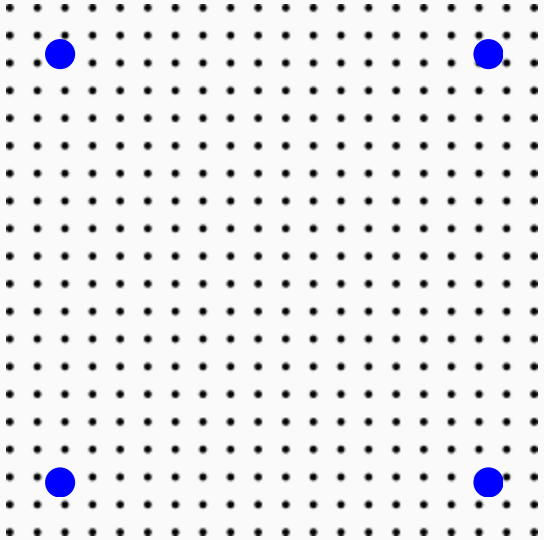


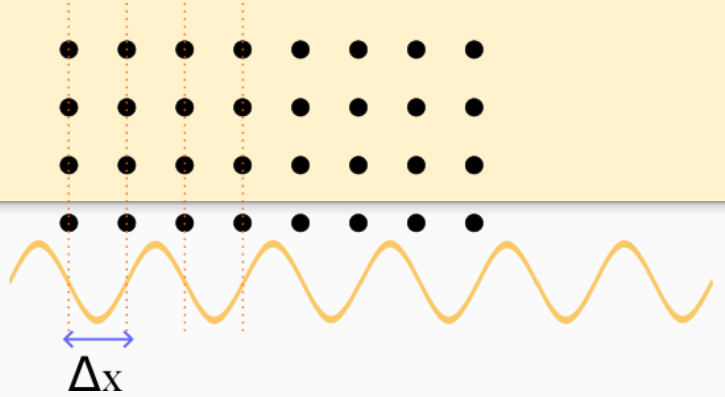
Reciprocal space

- **Density of states**
- **Bandstructure**



Real space grid





$$\Delta x \rightarrow k_c = \frac{\pi}{\Delta x} \rightarrow E_c = \frac{\hbar^2 k_c^2}{2m_e}$$

Fineness ↔ Maxim energy avoiding aliasing

$\Delta x \leftrightarrow E_c$ MeshCutoff

Energy units (Ry)

Real space grid: MeshCutoff

- What is it set by the user?

  Mesh.Cutoff 300 Ry (default)

```
Mesh.Cutoff  100 Ry
```

- What is set by siesta?

  MESH = 18 x 18 x 30 = 9720

  Mesh cutoff (required, used) = 100.000 101.039 Ry

- How can one decide the good value?

  Minimize the total energy.

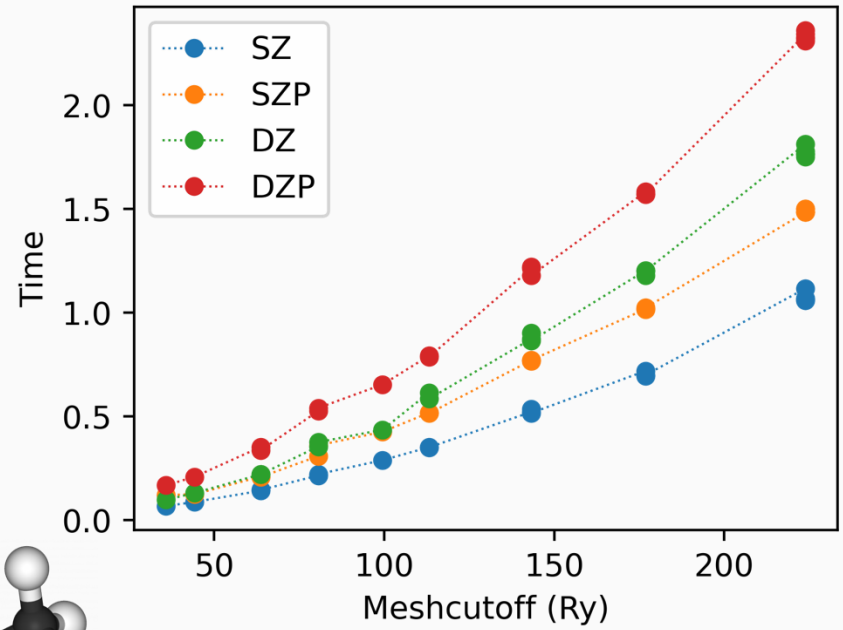
  Total force to zero.

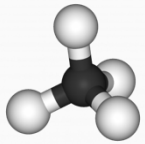
  Reasonable time (relatively small systems)

Real space grid: MeshCutoff

Time

`TIMES file`

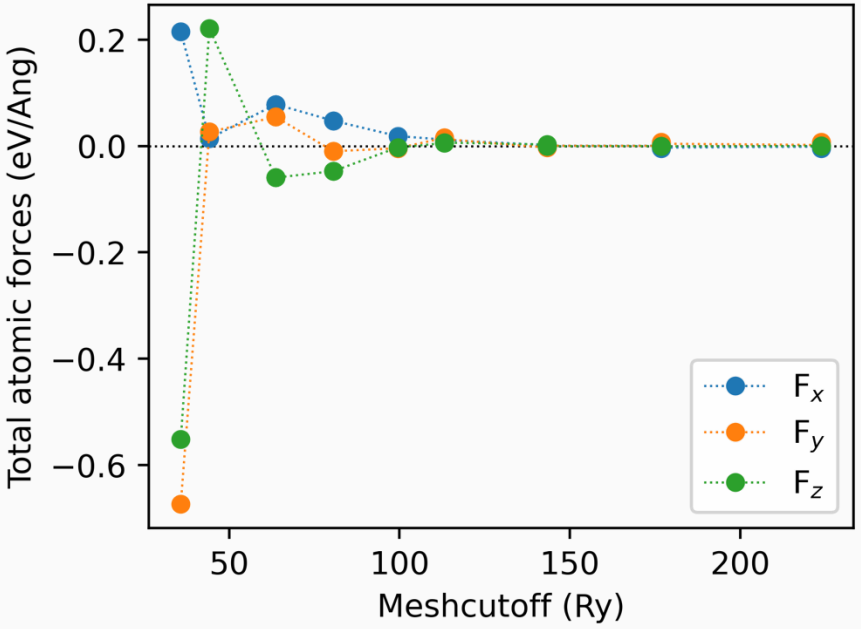




Results for methane (CH4)

Force

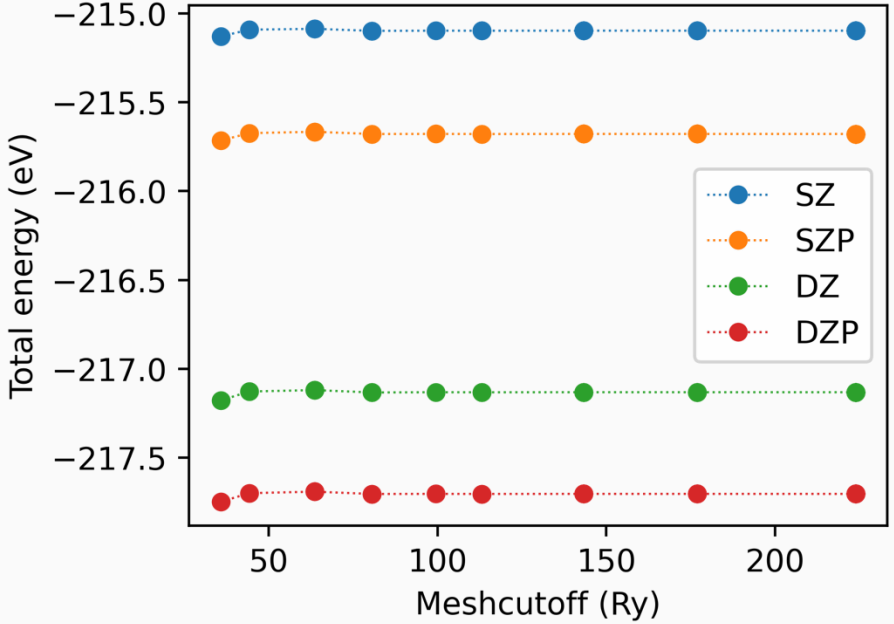
`siesta: Atomic forces (eV/Ang):`

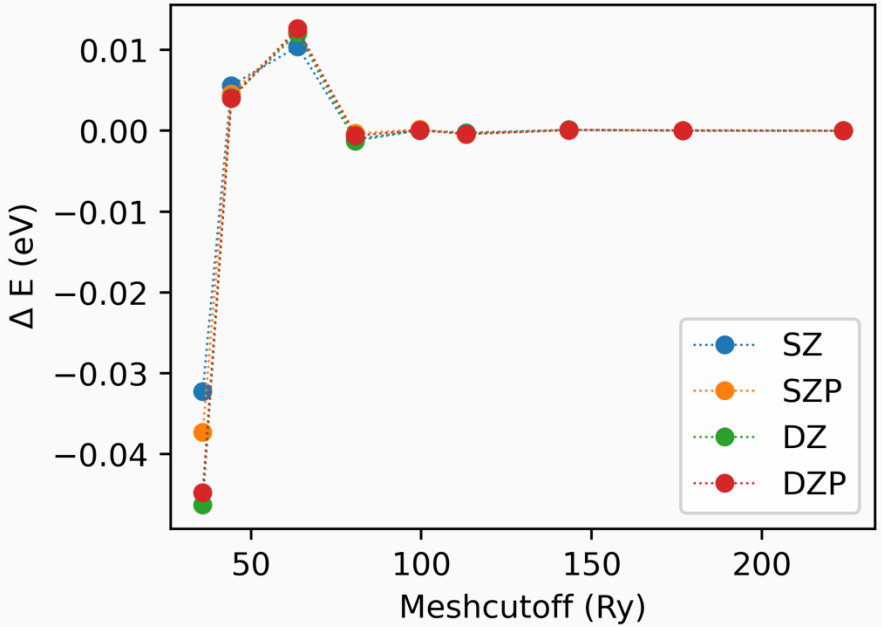


Real space grid: MeshCutoff

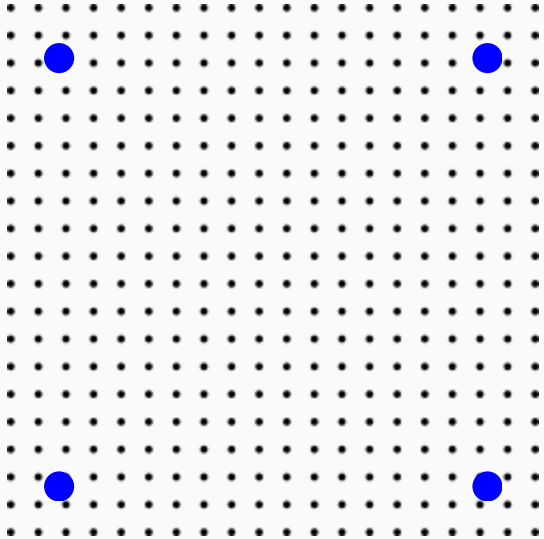
Energy

```
siesta: Final energy (eV):
```

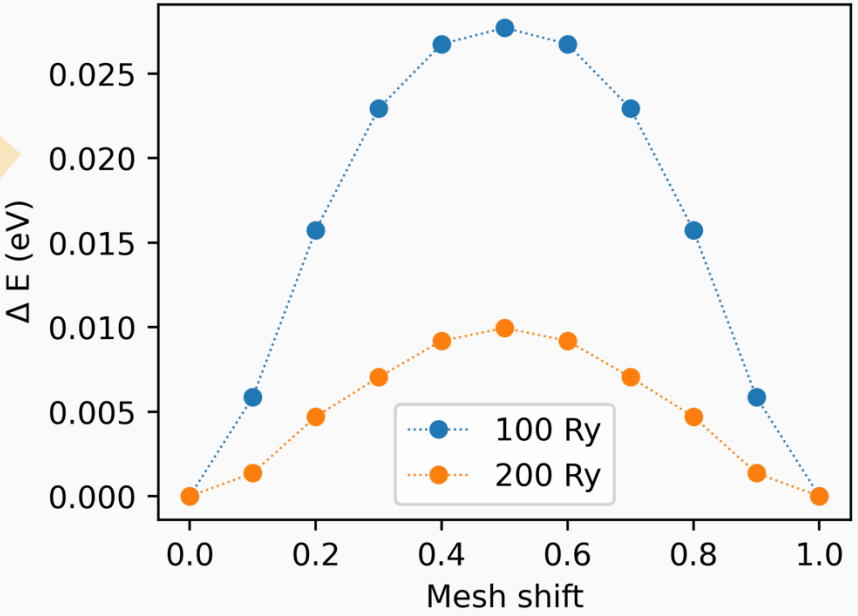




Egg-box effect

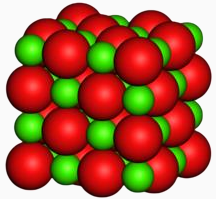


Invariant under any translation?




```
%block AtomicCoordinatesOrigin
 0.0 0.0 0.0
%endblock AtomicCoordinatesOrigin
```

$$\delta z_{shift} = \left(\frac{1}{M_z}\right)\frac{1}{10}$$



Solution:
- Increase Meshcutoff
- Use “grid-cell-sampling”

Results for magnesium oxide (MgO)

Let's try it

day2/03-RealSpaceGrid

Tutorials

This set of tutorials will guide you in the exploration of Siesta's features.

Before you do anything else, start here. You need to set up your local working environment to follow the tutorial.

- Setting up the local working environment for the tutorial exercises

Basics of Siesta

This section is recommended for all beginners, and also as a refresher for more experienced users.

- A first encounter with Siesta
- First crystals
- Pseudopotentials
- Basis sets
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Reciprocal space grid: k-mesh

- What is it set by the user?
  - k grid cut off
  - Monkhorst Pack grid
- What is set by siesta?
  - SystemLabel.KP
- How can one decide the good value?
  - Must consider the ratio between the lattice vectors.
  - Check:
    - DOS
    - Bandstructure
  - For metallic systems more k points will be needed.

```
kgrid_cutoff          10.0 Ang
```

```
%block kgrid_Monkhorst_Pack
  6  0  0    0.0
  0  6  0    0.0
  0  0  1    0.0
%endblock kgrid_Monkhorst_Pack
```

SystemLabel.KP

```
 22
 1 -0.447497E+00 -0.258363E+00  0.000000E+00   0.555556E-01
 2 -0.223749E+00 -0.129181E+00  0.000000E+00   0.555556E-01
 3  0.000000E+00  0.000000E+00  0.000000E+00   0.277778E-01
 4  0.671246E+00  0.387544E+00  0.000000E+00   0.277778E-01
 5 -0.447497E+00  0.111022E-15  0.000000E+00   0.555556E-01
 6 -0.223749E+00  0.129181E+00  0.000000E+00   0.555556E-01
 7  0.000000E+00  0.258363E+00  0.000000E+00   0.555556E-01
 8  0.223749E+00  0.387544E+00  0.000000E+00   0.555556E-01
 9  0.447497E+00  0.516726E+00  0.000000E+00   0.555556E-01
10  0.671246E+00  0.645907E+00  0.000000E+00   0.555556E-01
11 -0.447497E+00  0.258363E+00  0.000000E+00   0.555556E-01
12 -0.223749E+00  0.387544E+00  0.000000E+00   0.555556E-01
13  0.000000E+00  0.516726E+00  0.000000E+00   0.555556E-01
14  0.223749E+00  0.645907E+00  0.000000E+00   0.555556E-01
15  0.447497E+00  0.775088E+00  0.000000E+00   0.555556E-01
16  0.671246E+00  0.904270E+00  0.000000E+00   0.555556E-01
17 -0.447497E+00  0.516726E+00  0.000000E+00   0.277778E-01
18 -0.223749E+00  0.645907E+00  0.000000E+00   0.277778E-01
19  0.000000E+00  0.775088E+00  0.000000E+00   0.277778E-01
20  0.223749E+00  0.904270E+00  0.000000E+00   0.277778E-01
```

Let's try it

day2/04-KpointSampling

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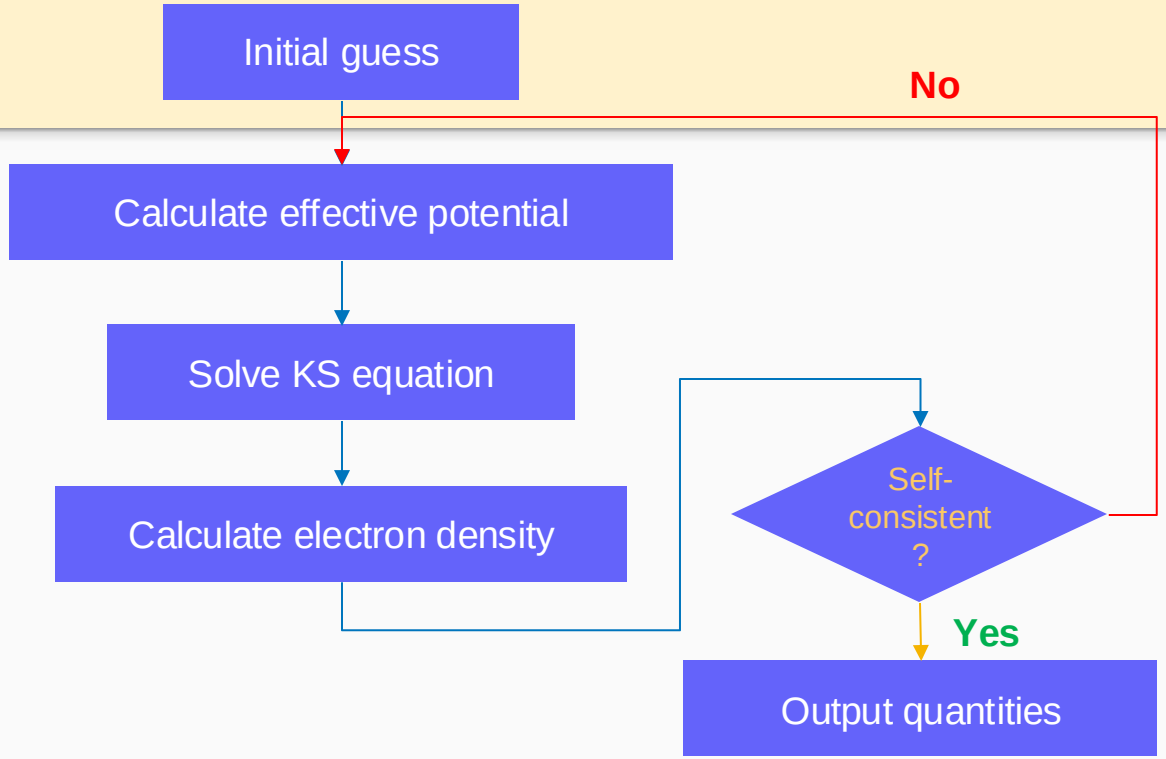
SCF Convergence



- The physical quantity that is mixed:
  - Density matrix
  - Hamiltonian matrix
- Mixing algorithm:
  - Linear
  - Broyden
  - Pulay

} N previous steps

SCF convergence

- SCF.Mix [default Hamiltonian]:
  - Density -> for systems hard to converge
  - Hamiltonian
- SCF.MixerMethod [default Pulay]
  - Linear
  - Pulay
  - Broyden
- SCF.Mixer.Weight [default 0.25]
  - 0.001 systems hard to converge ->a lot of steps
  - 0.4 systems easy to converge -> reduce steps
- SCF.Mixer.History [default 2]
- Max.SCF.Iterations [default 1000]
- SCF.DM.Converge F [default T]
- SCF.H.Converge F [default T]

All of them strongly dependent on the system!

SCF.Mix Hamiltonian
SCF.MixerMethod Pulay
SCF.Mixer.Weight 0.3

SCF.DM.Tolerance 10^{-4}
SCF.H.Tolerance 10^{-3} eV

Max.SCF.Iterations 75

SCF.MixerMethod pulay
SCF.Mixer.Weight 0.2

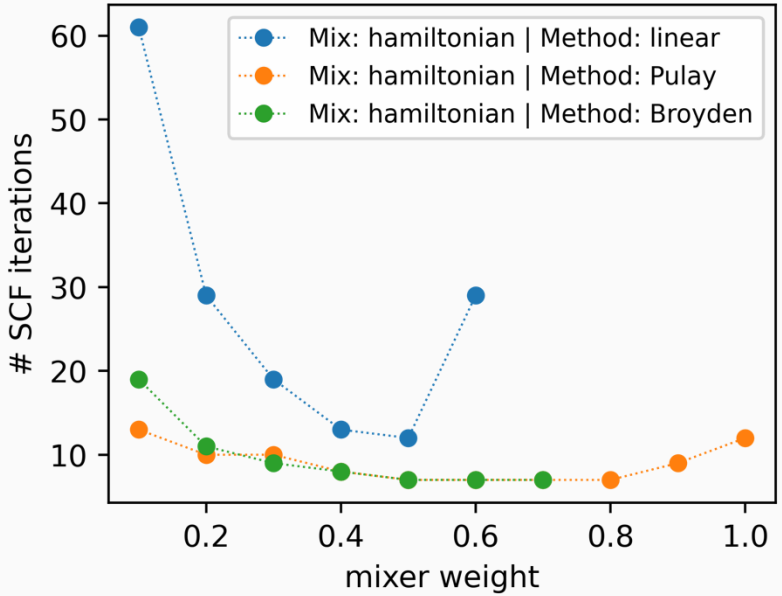
SCF.Mixer.History 5

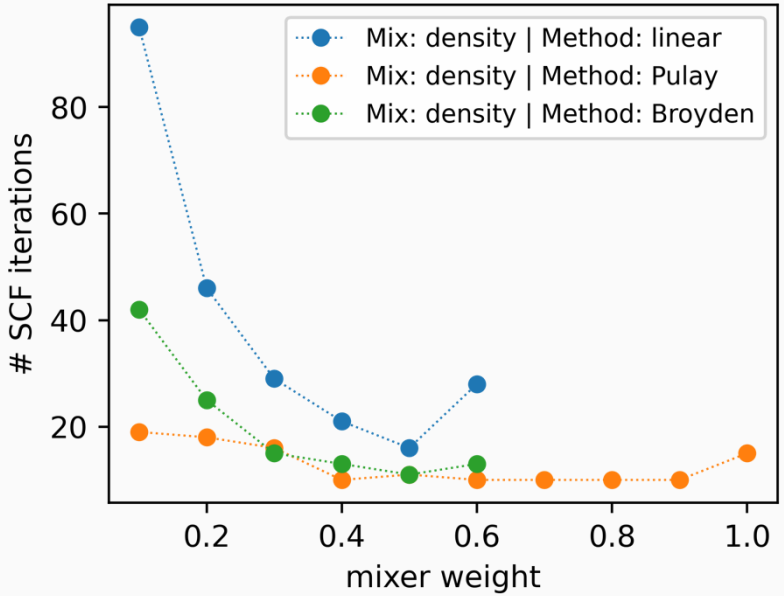
More advanced options … (manual)

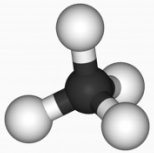
SCF convergence

```
SCF cycle converged
```

```
SCF_NOT_CONV:
```







Results for methane (CH4)

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day2/05-SCF-Options

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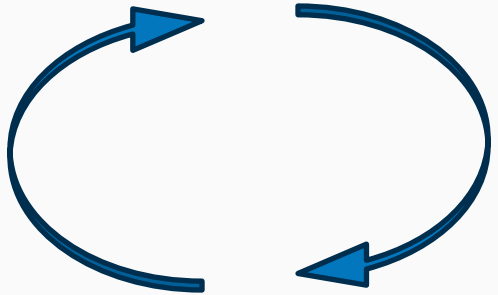
How do I converge the whole calculation?

1. Optimize the Basis set
2. Converge real space mesh: Energy
3. (Converge K grid: increase it for metallic systems)
4. SCF mixing



siesta
TM

Thank you

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