Hands-on session with siesta

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Where to find the course materials?

https://siesta-project.org/siesta/index.html

What is SIESTA?

Getting the code

Documentation

Support

News

Events

The Team

For Developers

https://siesta-project.org/siesta/index.html

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Home What is SIESTA? Getting the code Documentation Support News Events The Team For Developers

Events

Ongoing and future events

- Materials Science from First Principles: Materials Scientist Toolbox (3rd - 7th November 2025)
- SIESTA School 2025 (17th - 21th November 2025)

Past events

- Advanced SIESTA Workshop 2025 (2nd - 5th June 2025)
- SIESTA School 2024 (11th - 15th November 2024)
- The East-African School on Density Functional Theory and its Applications (8th - 10th July 2024)
- Efficient materials modelling on HPC with QUANTUM ESPRESSO, SIESTA and Yambo (11th - 15th March 2024)
- TranSIESTA School 2023 (13th - 17th November 2023)
- First steps with SIESTA: from zero to hero (2nd - 6th October 2023)
- First-principles simulations of materials with SIESTA (28th June - 2nd July 2021)
- Advanced school on Quantum Transport using SIESTA (17th May - 21st May 2021)
- Spin-orbit coupling in Siesta: Magnetism and other capabilities (20th June - 22nd June 2018)
- MaX SIESTA Tutorial 2017 (23rd May - 26th May 2017)

https://siesta-project.org/siesta/index.html

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Home What is SIESTA? Getting the code Documentation Support News Events The Team For Developers

Materials Science from First Principles: Materials Scientist Toolbox

Sorbonne University, 3rd - 7th November 2025

The Materials Science Work Package team of the HANAMI project is pleased to announce a five-day workshop to be held in the Pierre and Marie Curie campus of Sorbonne University (Paris), introducing the main computational tools widely used in materials science, along with their latest developments and applications.

The event is supported by HANAMI and by CECAM-FR-MOSER.

For more information, please visit the workshop website, which includes the agenda and the book of abstracts.

SIESTA Sessions

The first day, Monday 3rd November, will focus on SIESTA.

Introduction to Density Functional Theory

Lectures by Prof. Pablo Ordejón (CSIC and ICN2) [Slides].

Practical sessions with SIESTA

Practical sessions led by Prof. Pablo Ordejón (CSIC and ICN2) and Dr. Anthoni Alcaraz (ICN2) [Slides].

In these sessions, the following SIESTA tutorials will be covered:

- A First Encounter with SIESTA
- The real-space grid

How is the material organized?

/users/commun/seitsonen/HANAMI/siesta/

copy

```
siesta/
├──── plot_gnuplot.sh
├──── input_methane/
│     ├──── siesta.fdf
│     ├──── C.psml
│     └──── H.psml
├──── input_graphene/
│     ├──── siesta.fdf
│     └──── C.psf
└──── slides/
      └──── hands-on_session.pdf
```

```
siesta/
├──── exercise_1/
│   ├──── create_your_own_folders
├──── exercise_2/
├──── exercise_3/
├──── exercise_4/
├──── exercise_5/
└──── exercise_6/
```

How do we run siesta ?

Load de environment

source /users/commun/seitsonen/HANAMI/setup-modules.txt

module load siesta/5.4.1

#Verify siesta availability

$which siesta:

/users/commun/seitsonen/HANAMI/sw/target/app/siesta/siesta-5.4.1/bin/siesta

Exercise 1

INPUTS FOLDER

siesta/
├── input_methane/

OUTPUTS FOLDER

siesta/
├── exercise_1/

1. Copy all files from the input folder to the exercise folder.
2. In exercise_1 folder execute the following:

Exercise 1

```
mpiexec -n 4 siesta siesta.fdf > siesta.out
```

What did this command do?

Exercise 1

```
mpiexec -n 4 siesta siesta.fdf > siesta.out
```

What are the main ingredients?

For most basic SIESTA calculations, we need at least two inputs:

- Pseudo potential files (e.g. available in PSML format from http://www.pseudo-dojo.org, or a PSF created with ATOM).
- An fdf file with the input options.

```
├── input_methane/
│   ├── siesta.fdf
│   ├── C.psml
│   └── H.psml
```

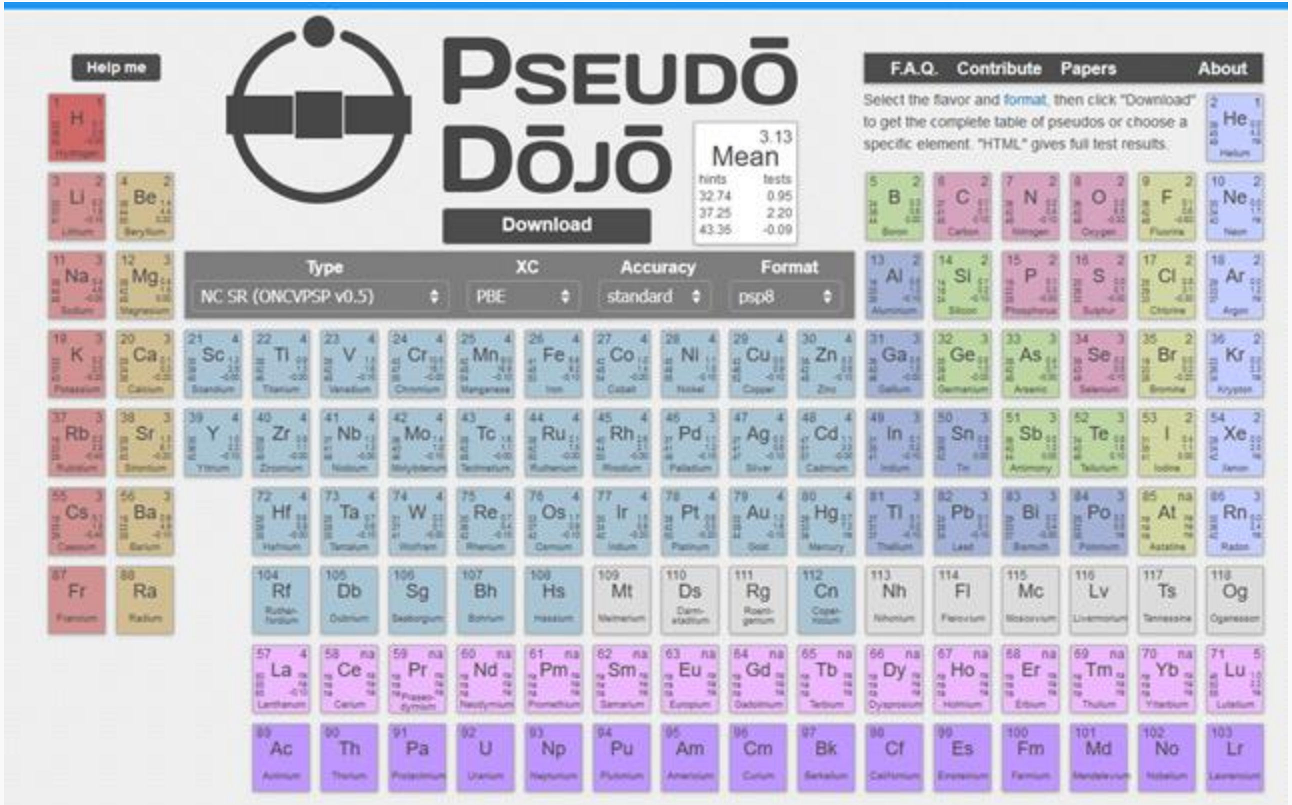
Exercise 1

```
mpiexec -n 4 siesta siesta.fdf > siesta.out
```

First ingredient: pseudopotential

Exercise 1

Recommended way: *get it from pseudo-dojo* (pseudo-dojo.org) *as a psml file.*



Exercise 1

Second ingredient: What's in the FDF?

The fdf file contains all relevant input options for our simulation:

- Geometry information
- Atomic species information
- Level of theory
- Basis set information
- and a plethora of fine-tuning options.

Let's have a look…

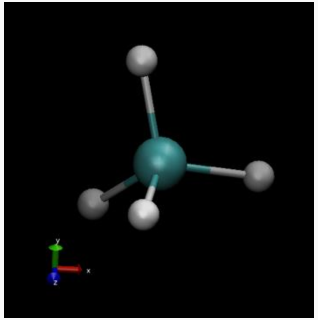
What’s in the FDF? System information

```
#General system specifications
SystemName          CH4 molecule
SystemLabel         ch4
NumberOfAtoms       5
NumberOfSpecies     2

%block ChemicalSpeciesLabel
 1  6 C   # Species index, atomic number, species label
 2  1 H   # Species index, atomic number, species label
%endblock ChemicalSpeciesLabel
```

All output filenames will begin with “ch4.”

Total number of atoms in the simulation box.

Different “kinds” of atoms present.



Note that we have to types of inputs: single variables, and blocks.

What’s in the FDF? System geometry

```
#Unit cell for the calculation
LatticeConstant 15 Ang
%block LatticeVectors
  1.000 0.000 0.000
  0.000 1.000 0.000
  0.000 0.000 1.000
%endblock LatticeVectors
```

Multiplies all lattice vectors by a constant. Note the units.

The lattice vectors themselves.

```
#Atomic coordinates
AtomicCoordinatesFormat  Ang

%block AtomicCoordinatesAndAtomicSpecies
  0.000      0.000      0.000    1   # C
  1.219     -0.284     -0.377    2   # H
 -0.284      1.219     -0.377    2   # H
 -0.140     -0.140      1.219    2   # H
 -0.833     -0.833     -0.503    2   # H
%endblock AtomicCoordinatesAndAtomicSpecies
```

Unit for the atomic coordinates block. Can also be “fractional”.

Atomic coordinates and species index (1 for C, 2 for H).

What’s in the FDF? Other options

```
# Type of solution
SolutionMethod diagon

# Basis set definition
PAO.BasisSize    SZ
PAO.EnergyShift 250 meV

#Real space grid
MeshCutoff 125.0 Ry

# Convergence of SCF
MaxSCFIterations    50
SCF.Mixer.Weight    0.4
SCF.Mixer.History   2
```

Solver options.

Basis Set Options

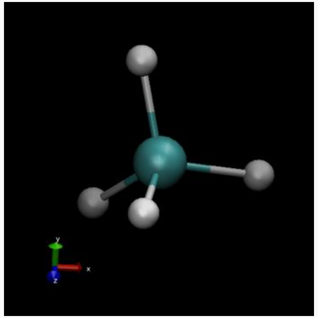
Relates to the amount of points for grid-based operations.

Options for SCF acceleration.

What about the outputs?

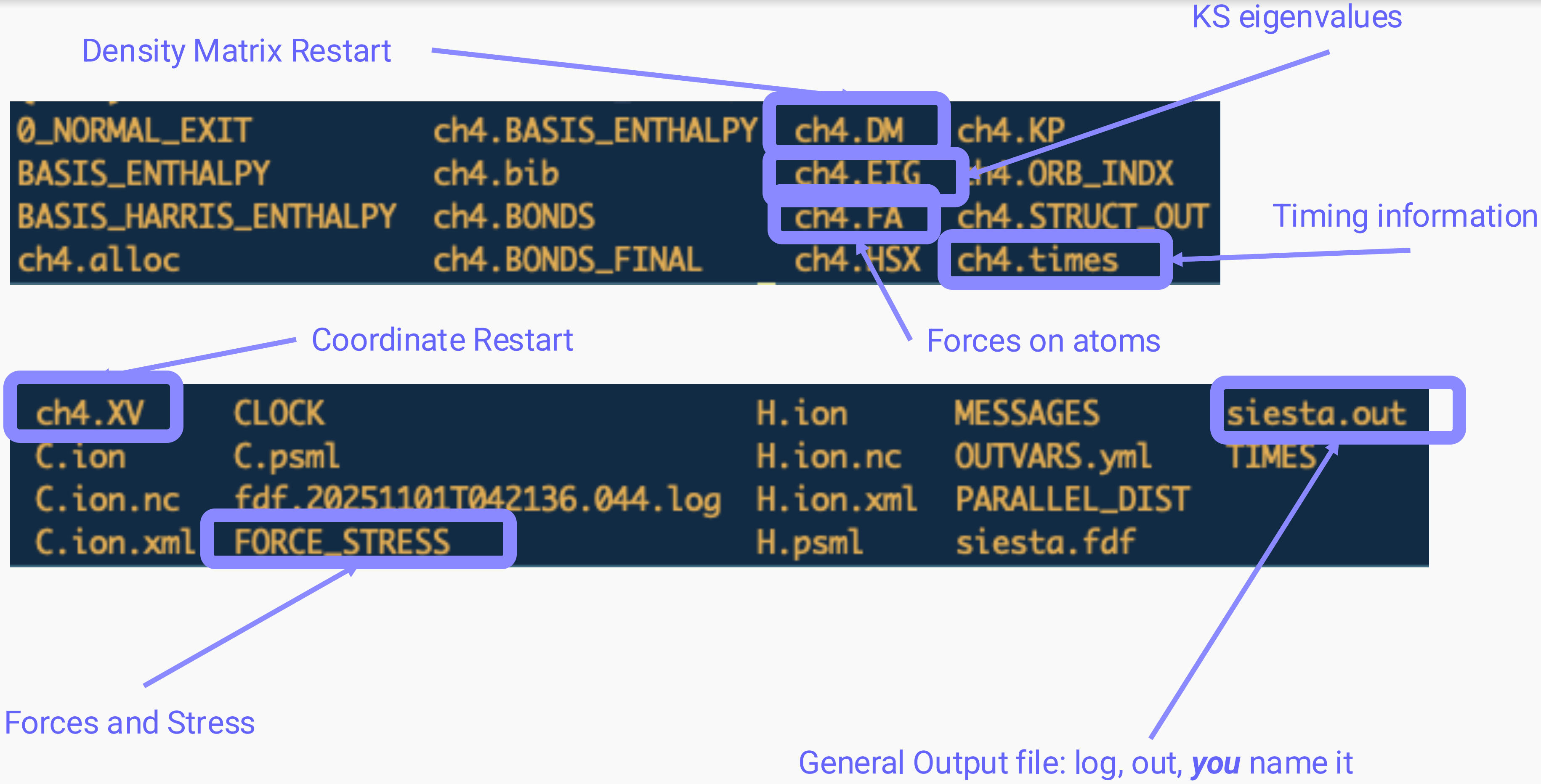
What are all of these files???

```
0_NORMAL_EXIT            ch4.BASIS_ENTHALPY   ch4.DM    ch4.KP
BASIS_ENTHALPY           ch4.bib              ch4.EIG   ch4.ORB_INDX
BASIS_HARRIS_ENTHALPY    ch4.BONDS            ch4.FA    ch4.STRUCT_OUT
ch4.alloc                ch4.BONDS_FINAL      ch4.HSX   ch4.times
```



```
ch4.XV      CLOCK                          H.ion       MESSAGES        siesta.out
C.ion       C.psml                         H.ion.nc    OUTVARS.yml     TIMES
C.ion.nc    fdf.20251101T042136.044.log    H.ion.xml   PARALLEL_DIST
C.ion.xml   FORCE_STRESS                   H.psml      siesta.fdf
```

What are all of these files???



Outputs: siesta.out

Installation and run info, Start Time

```
Executable       : siesta
Version          : unreleased a05b5f95a (2025-09-16)
Architecture     : x86_64
Compiler version: GNU-13.3.0
Compiler flags   : -fallow-argument-mismatch -O3 -march=native
Parallelisations: MPI
Lua support
ELSI support. Solvers:
   ELPA (internal)
   NTPoly
   OMM
DFT-D3 support

Runtime information:
* Directory : /users/ens/alcaraza/Siesta/siesta-docs/work-files/tutorials/basic/first-encounter/01-CH4-Basic
* Running on 4 nodes in parallel.
>> Start of run:  29-OCT-2025  17:43:57

                           ***********************
                           *  WELCOME TO SIESTA  *
                           ***********************
```

Outputs

```
initatom: Reading input for the pseudopotentials and atomic orbitals ----------
Species number:   1 Atomic number:    6 Label: C
Species number:   2 Atomic number:    1 Label: H

Ground state valence configuration (from tables):   2s02  2p02  3d00  4f00
Ground state valence configuration (from tables):   1s01  2p00  3d00  4f00

---- Processing specs for species: C
Reading pseudopotential information in PSML from:
  C.psml
PSML file version: 1.1
Using libxc ids:  116 133
GGA--PBEsol XC_GGA_X_PBE_SOL--XC_GGA_C_PBE_SOL ps
PSML uuid: 51a02af0-1d5f-11e8-49c3-12b9ebd99919

---- Processing specs for species: H
Reading pseudopotential information in PSML from:
  H.psml
PSML file version: 1.1
Using libxc ids:    1  12
LDA--PW92 XC_LDA_X--XC_LDA_C_PW pw
PSML uuid: c4d96a40-23d1-11e8-69b6-c18eff5d81ce

---- Pseudopotential check for C

Pseudized shells:
2s( 2.00) rc: 1.20
2p( 2.00) rc: 1.26
Valence configuration for ps generation: 2s:2p: Total charge:   4.000000

---- Pseudopotential check for H

Pseudized shells:
1s( 1.00) rc: 1.01
2p( 0.00) rc: 0.91
Valence configuration for ps generation: 1s: Total charge:   1.000000
For C, standard SIESTA heuristics set lmxkb to 2
 (one more than the basis l, including polarization orbitals).
Use PS.lmax or PS.KBprojectors blocks to override.
```

Species and pseudopotential information

Outputs

```
atom: ---------------------------------------------------------------------------

atom: SANKEY-TYPE ORBITALS:

SPLIT: Orbitals with angular momentum L= 0

SPLIT: Basis orbitals for state 2s

SPLIT: PAO cut-off radius determined from an
SPLIT: energy shift=  0.018375 Ry
Split based on tail norm

   izeta = 1
                 lambda =    1.000000
                     rc =    4.188930
                 energy =   -0.981019
                kinetic =    0.980783
    potential(screened) =   -1.961802
       potential(ionic) =   -5.541734

SPLIT: Orbitals with angular momentum L= 1

SPLIT: Basis orbitals for state 2p

SPLIT: PAO cut-off radius determined from an
SPLIT: energy shift=  0.018375 Ry
Split based on tail norm

   izeta = 1
                 lambda =    1.000000
                     rc =    4.967013
                 energy =   -0.365210
                kinetic =    2.559078
    potential(screened) =   -2.924288
       potential(ionic) =   -6.383934
atom: Total number of Sankey-type orbitals:  4

atm_pop: Valence configuration (for local Pseudopot. screening):
 2s( 2.00)
 2p( 2.00)
Vna: chval, zval:    4.00000    4.00000
```

Basis set generation

Outputs

Coordinates and selected options

```
coor:   Atomic-coordinates input format  =     Cartesian coordinates
coor:                                          (in Angstroms)

siesta: Atomic coordinates (Bohr) and species
siesta:      0.00000   0.00000   0.00000  1        1
siesta:      2.30358  -0.53668  -0.71243  2        2
siesta:     -0.53668   2.30358  -0.71243  2        3
siesta:     -0.26456  -0.26456   2.30358  2        4
siesta:     -1.57414  -1.57414  -0.95053  2        5

siesta: System type = molecule

initatomlists: Number of atoms, orbitals, and projectors:      5     8    28

siesta: ******************** Simulation parameters ****************************
siesta:
siesta: The following are some of the parameters of the simulation.
siesta: A complete list of the parameters used, including default values,
siesta: can be found in file out.fdf
siesta:
redata: Spin configuration                          = none
redata: Number of spin components                   = 1
redata: Time-Reversal Symmetry                      = T
redata: Spin spiral                                 = F
redata: Long output                                 =   F
redata: Number of Atomic Species                    =        2
redata: Charge density info will appear in .RHO file
redata: Write Mulliken charges (when)               = none
redata: Write Mulliken Pop.                         = NO
redata: Write Hirshfeld charges (when)              = none
redata: Write Voronoi charges (when)                = none
redata: Write spin charge (when)                    = none
redata: Matel table size (NRTAB)                    =     1024
redata: Mesh Cutoff                                 =   125.0000 Ry
redata: Net charge of the system                    =     0.0000 |e|
redata: Min. number of SCF Iter                     =        0
redata: Max. number of SCF Iter                     =       50
redata: SCF convergence failure will abort job
redata: SCF mix quantity                            = Hamiltonian
redata: Mix DM or H after convergence               =   F
redata: Recompute H after scf cycle                 =   F
```

Outputs

```
                    ====================================
                       Single-point calculation
                    ====================================

outcell: Unit cell vectors (Ang):
       15.000000    0.000000    0.000000
        0.000000   15.000000    0.000000
        0.000000    0.000000   15.000000

outcell: Cell vector modules (Ang)   :   15.000000   15.000000   15.000000
outcell: Cell angles (23,13,12) (deg):     90.0000     90.0000     90.0000
outcell: Cell volume (Ang**3)        :   3375.0000
<dSpData1D:S at geom step 0
  <sparsity:sparsity for geom step 0
    nrows_g=8 nrows=2 sparsity=.2500 nnzs=16, refcount: 7>
  <dData1D:(new from dSpData1D) n=16, refcount: 1>
refcount: 1>
new_DM -- step:     1
Initializing Density Matrix...

Attempting to read DM from file... Failed...
DM filled with atomic data:
<dSpData2D:DM initialized from atoms
  <sparsity:sparsity for geom step 0
    nrows_g=8 nrows=2 sparsity=.2500 nnzs=16, refcount: 8>
  <dData2D:DM n=16 m=1, refcount: 1>
refcount: 1>
No. of atoms with KB's overlaping orbs in proc 0. Max # of overlaps:      5       8

InitMesh: MESH = 108 x 108 x 108 = 1259712
InitMesh: Mesh cutoff (required, used) =   125.000   143.274 Ry
New grid distribution [1]: sub = 2
New grid distribution [2]: sub = 2
New grid distribution [3]: sub = 2
Setting up quadratic distribution...

stepf: Fermi-Dirac step function

siesta: Program's energy decomposition (eV):
siesta: Ebs     =       -87.057890
```

Type of run, cell information.

Sparsity information.

Mesh information.

Outputs

```
siesta: Program's energy decomposition (eV):
siesta: Ebs     =       -87.057890
siesta: Eions   =       407.435544
siesta: Ena     =       134.583366
siesta: Ekin    =       143.164339
siesta: Enl     =       -10.642485
siesta: Eso     =         0.000000
siesta: Edftu   =         0.000000
siesta: DEna    =         3.582210
siesta: DUscf   =         0.299525
siesta: DUext   =         0.000000
siesta: Ex      =       -74.401564
siesta: Ec      =       -11.671706
siesta: Exc     =       -86.073270
siesta: EbV     =         0.000000
siesta: eta*DQ  =         0.000000
siesta: Emadel  =         0.000000
siesta: Emeta   =         0.000000
siesta: Emolmec =         0.000000
siesta: Ekinion =         0.000000
siesta: Eharris =      -232.130754
siesta: Etot    =      -222.521860
siesta: FreeEng =      -222.521860
```

Initial, non-SCF energy decomposition.

Outputs

```
      iscf     Eharris(eV)        E_KS(eV)     FreeEng(eV)     dDmax    Ef(eV) dHmax(eV)
   scf:    1     -232.130754     -222.521860     -222.521860  1.101199 -6.841474  1.028330
timer: Routine,Calls,Time,% = IterSCF        1       0.155  24.53
   scf:    2     -222.542289     -222.538095     -222.538095  0.022736 -6.524821  0.232074
   scf:    3     -222.538153     -222.538197     -222.538197  0.002707 -6.429279  0.141576
   scf:    4     -222.538205     -222.538216     -222.538216  0.001493 -6.290235  0.047798
   scf:    5     -222.538224     -222.538221     -222.538221  0.000478 -6.324841  0.001216
   scf:    6     -222.538221     -222.538221     -222.538221  0.000031 -6.324150  0.000384

SCF Convergence by DM+H criterion
max |DM_out - DM_in|         :     0.0000305952
max |H_out - H_in|      (eV) :     0.0003842923
SCF cycle converged after 6 iterations

Using DM_out to compute the final energy and forces
No. of atoms with KB's overlaping orbs in proc 0. Max # of overlaps:      5       8

siesta: E_KS(eV) =             -222.5382

siesta: E_KS - E_eggbox =      -222.5382

siesta: Atomic forces (eV/Ang):
----------------------------------------
   Tot    0.002408    0.002408   -0.001498
----------------------------------------
   Max    2.338422
   Res    1.118414    sqrt( Sum f_i^2 / 3N )
----------------------------------------
   Max    2.338422    constrained

Stress tensor Voigt[x,y,z,yz,xz,xy] (kbar):        1.98        1.98        0.92       -0.21       -0.21       -0.03
(Free)E + p*V (eV/cell)     -225.9574
Target enthalpy (eV/cell)     -222.5382
```

SCF cycle information

Converged KS energy

Converged total forces and cell stress

Outputs

Final energy decomposition

```
siesta: Program's energy decomposition (eV):
siesta: Ebs     =       -88.949134
siesta: Eions   =       407.435544
siesta: Ena     =       134.583366
siesta: Ekin    =       141.825781
siesta: Enl     =       -10.477008
siesta: Eso     =         0.000000
siesta: Edftu   =         0.000000
siesta: DEna    =         4.466002
siesta: DUscf   =         0.266389
siesta: DUext   =         0.000000
siesta: Ex      =       -74.112598
siesta: Ec      =       -11.654609
siesta: Exc     =       -85.767207
siesta: EbV     =         0.000000
siesta: eta*DQ  =         0.000000
siesta: Emadel  =         0.000000
siesta: Emeta   =         0.000000
siesta: Emolmec =         0.000000
siesta: Ekinion =         0.000000
siesta: Eharris =      -222.538221
siesta: Etot    =      -222.538221
siesta: FreeEng =      -222.538221

siesta: Final energy (eV):
siesta:  Band Struct. =     -88.949134
siesta:       Kinetic =     141.825781
siesta:       Hartree =     282.961698
siesta:         Edftu =       0.000000
siesta:       Eso     =       0.000000
siesta:    Ext. field =       0.000000
siesta:         Exch. =     -74.112598
siesta:         Corr. =     -11.654609
siesta:     Bulk bias =       0.000000
siesta:   Exch.-corr. =     -85.767207
siesta:  Ion-electron =    -696.354718
siesta:       Ion-ion =     134.796225
siesta:       Ekinion =       0.000000
siesta: D3 dispersion =       0.000000
siesta:         Total =    -222.538221
siesta:         Fermi =      -6.324150
```

Outputs

Final forces

Final stress/pressure

Electric dipole

```
siesta: Atomic forces (eV/Ang):
siesta:      1    0.164966    0.164966   -1.084421
siesta:      2   -2.338422    0.480063    0.757120
siesta:      3    0.480063   -2.338422    0.757120
siesta:      4    0.338967    0.338967   -0.916986
siesta:      5    1.356834    1.356834    0.485668
siesta: ----------------------------------------
siesta:    Tot    0.002408    0.002408   -0.001498

siesta: Stress tensor (static) (eV/Ang**3):
siesta:     0.001233   -0.000021   -0.000128
siesta:    -0.000021    0.001233   -0.000128
siesta:    -0.000128   -0.000128    0.000572

siesta: Cell volume =       3375.000000 Ang**3

siesta: Pressure (static):
siesta:                Solid            Molecule  Units
siesta:          -0.00001103          0.00000000  Ry/Bohr**3
siesta:          -0.00101308          0.00000045  eV/Ang**3
siesta:          -1.62314011          0.00072877  kBar

Basis Enthalpy Calculation:
    Basis Pressure for species 1(C) :      0.2000000 GPa
    Basis Pressure for species 2(H) :      0.2000000 GPa

    Orbital volume contribution        =          0.496873 eV
    (Free)E + p_basis*V_orbitals       =       -222.041348 eV
    (Free)Eharris+ p_basis*V_orbitals  =       -222.041349 eV
WARNING: BASIS_ENTHALPY and BASIS_HARRIS_ENTHALPY files are deprecated. They will be removed in future releases.
Please use system_label.BASIS_ENTHALPY in your scripts instead.

siesta: Electric dipole (a.u.)  =   -0.011465   -0.011465    0.009499
siesta: Electric dipole (Debye) =   -0.029140   -0.029140    0.024144
```

Outputs

Primary bibliography, and end-of-run time

```
cite: Please indicate the Siesta version in published work: unreleased a05b5f95a (2025-09-16)
cite: This calculation has made use of features in the following articles
cite: which we encourage you to cite in published work.
cite: (Please see "ch4.bib" for a BibTeX file.)
        Primary SIESTA paper
          DOI: www.doi.org/10.1088/0953-8984/14/11/302
        PSML pseudopotential format
          DOI: www.doi.org/10.1016/j.cpc.2018.02.011


>> End of run:  29-OCT-2025  17:43:59
Job completed
```

Other things to choose

1. Pseudopotentials
2. Functional
3. Basis set

Choosing a DFT functional

SIESTA offers different families of DFT functionals:

- LDA (CA, PW92)
- GGA (PW91,BLYP, PBE, PBESol, RevPBE)
- Van der Waals functionals (DRSLL, VV)

A peek into basis sets

For now, we will only concern ourselves with:

- Exploring the basis set cardinality (SZ,DZ, SZP, DZP,TZP), i.e. *the amount of basis functions per atom*. In principle, more functions imply a better quality, but also an increase in computational costs.

- Playing with the *energy shift*, which essentially modifies the cut-off radius of the basis set. The lower the energy shift, the larger the cut-off radius of the orbitals.

Exercise 2 (We will improve our input)

INPUTS FOLDER

```
siesta/
├── input_methane/
```

OUTPUTS FOLDER

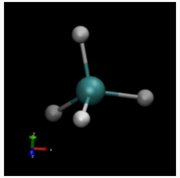
```
siesta/
├── exercise_2/
│   ├── create_your_own_folders
```

1. Copy all files from the input folder to the exercise folder.
2. In this exercise you will do a scan modifying the basis set and the energy shift value.

```
# Basis set definition
PAO.BasisSize    SZ
PAO.EnergyShift 250 meV
```

SZ DZ SZP DZP TZP

Energy Shifts (meV): 10 50 100 150 200 250 300



Everything depends on how you organize it

siesta: Total = -221.815381

Exercise 2

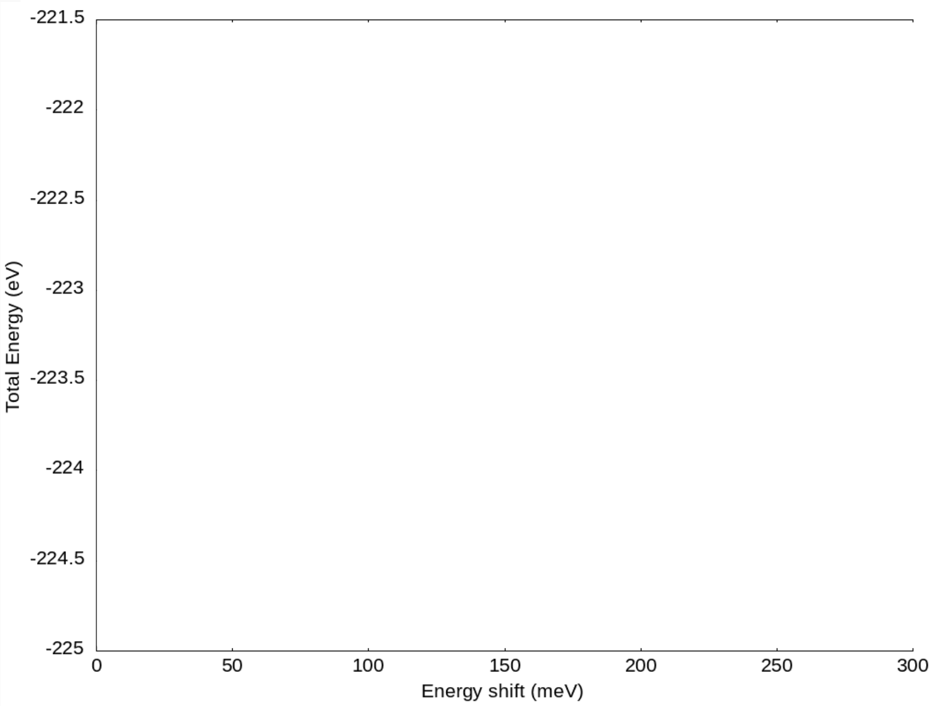
(We will improve our input)

siesta/

├── plot_gnuplot.sh

Basis set

```
bash ../siesta/plot_gnuplot.sh -x "Energy shift (meV)" \
-y "Total Energy (eV)" -l "SZ, SZP, DZ, DZP, TZP" \
-f bes_1.dat bes_2.dat bes_3.dat bes_4.dat bes_5.dat
```

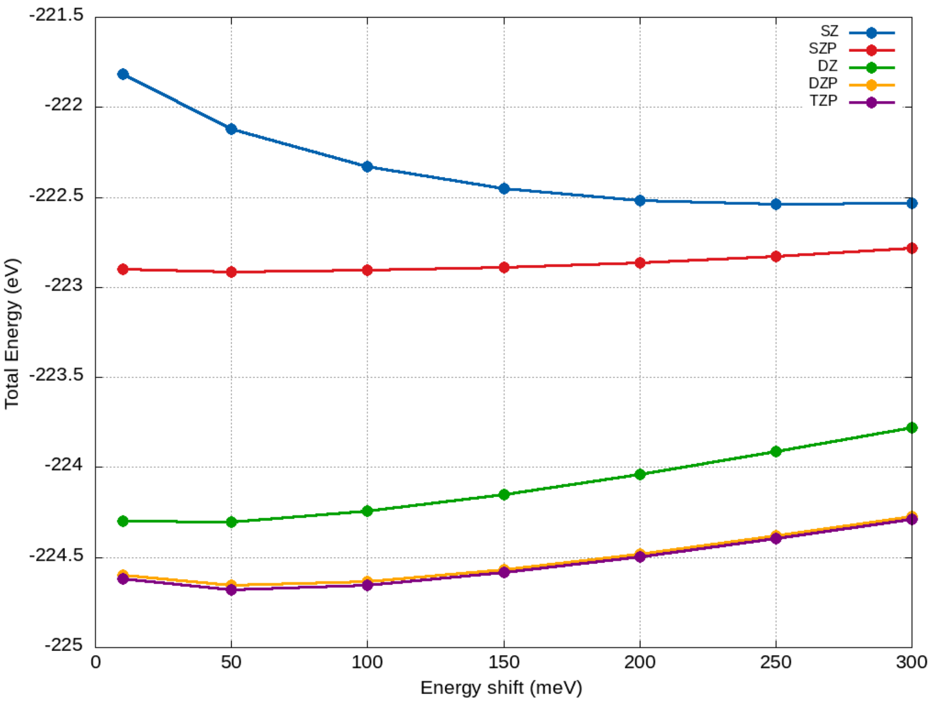


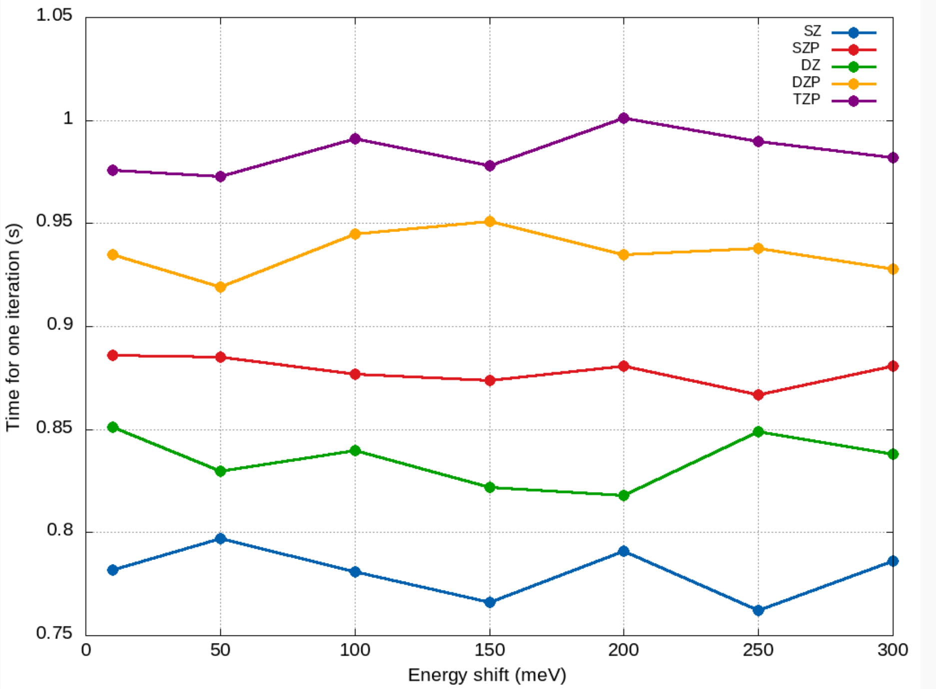
Exercise 2 (We will improve our input)

siesta/
├── plot_gnuplot.sh

Basis set

```
bash ../siesta/plot_gnuplot.sh -x "Energy shift (meV)" \
-y "Total Energy (eV)" -l "SZ, SZP, DZ, DZP, TZP" \
-f bes_1.dat bes_2.dat bes_3.dat bes_4.dat bes_5.dat
```





Exercise 3 (We will improve our input)

INPUTS FOLDER

```
siesta/
├── input_methane/
```

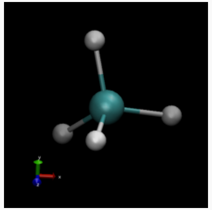
OUTPUTS FOLDER

```
siesta/
├──── exercise_3/
│   ├──── create_your_own_folders
```

1. Copy all files from the input folder to the exercise folder.
2. In this exercise you will do a scan modifying the mesh cutoff value.

```
#Real space grid
MeshCutoff 125.0 Ry
```

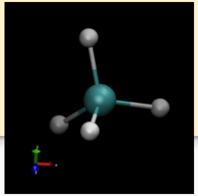
Mesh cutoff: 30 60 90 120 150 180 210 240 270 300

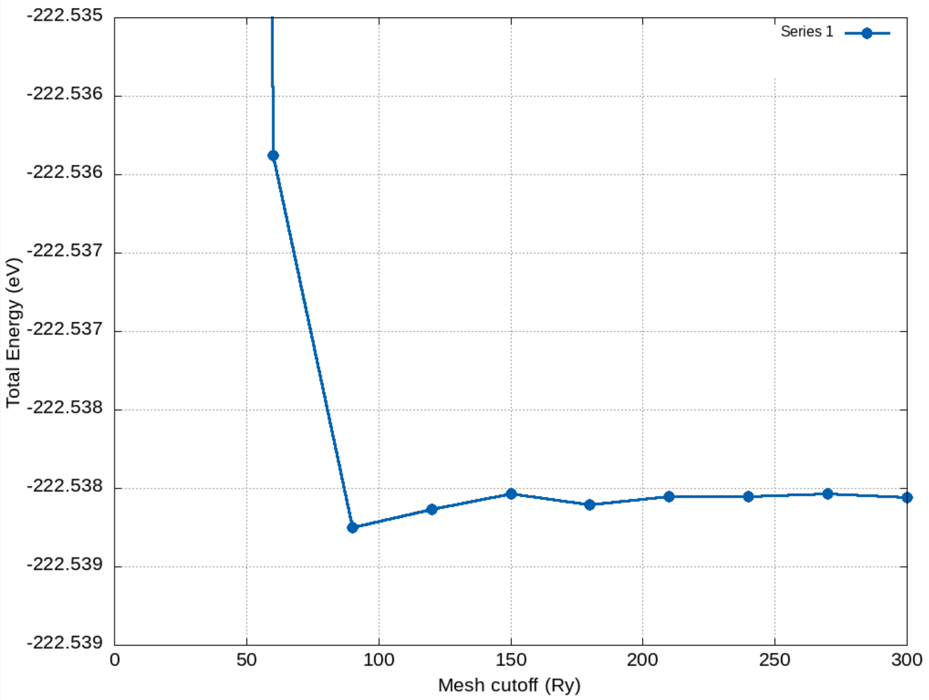


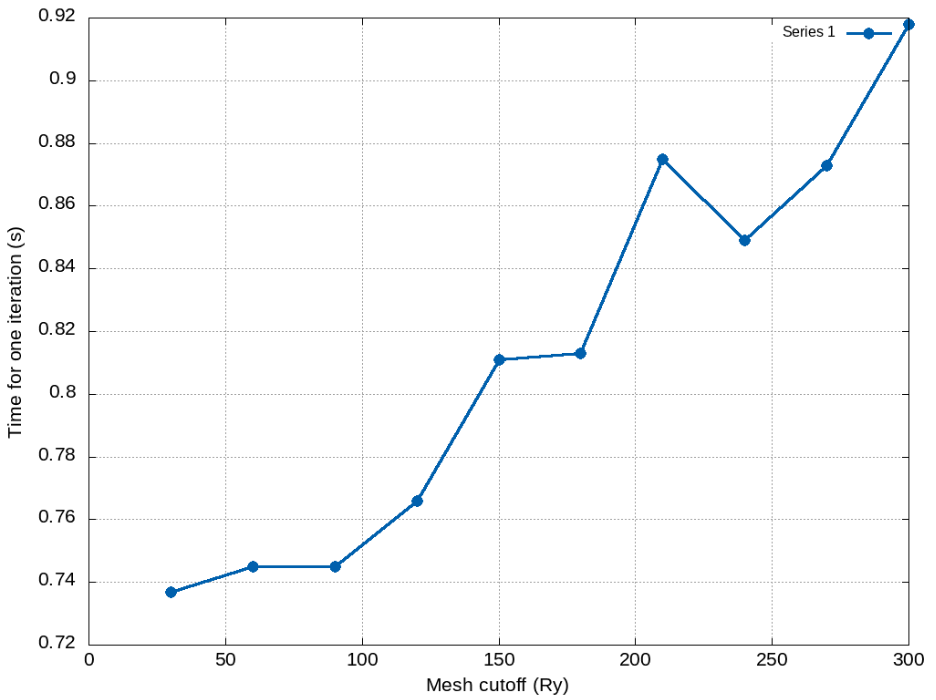
Everything depends on how you organize it

siesta: Total = -221.815381

Exercise 3 (We will improve our input)







Exercise 3

(Best options for CH_4)

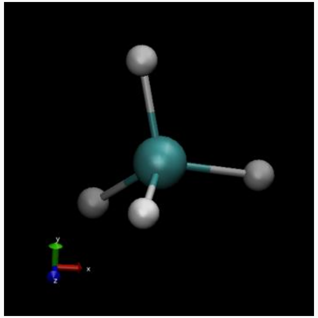
```
# Basis set definition
PAO.BasisSize    SZ
PAO.EnergyShift 250 meV
```

DZP

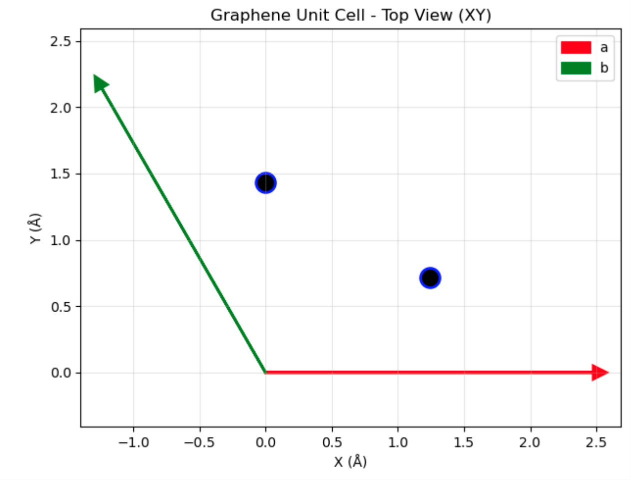
50-100 meV

```
#Real space grid
MeshCutoff 125.0 Ry
```

150 Ry



Exercise 4 (Graphene)




```
#Atomic coordinates
AtomicCoordinatesFormat fractional

%block AtomicCoordinatesAndAtomicSpecies
  0.33333333  0.66666667  0.5         1     # C
  0.66666667  0.33333333  0.5         1     # C
%endblock AtomicCoordinatesAndAtomicSpecies

#Unit cell for the calculation
LatticeConstant 2.476675 Ang
%block LatticeParameters
1.000  1.000  10.0  90.0  90.0  120.0
%endblock LatticeParameters
```

Exercise 4 (k-point sampling)

INPUTS FOLDER

siesta/
├── input_graphene/

OUTPUTS FOLDER

siesta/
├── exercise_4/
│ ├── create_your_own_folders

1. Copy all files from the input folder to the exercise folder.
2. In this exercise you will do a scan modifying the Monkhorst_pack block.

```
# K-sampling
%block kgrid_Monkhorst_Pack
     0  0     0.0
  0     0     0.0
  0  0  1     0.0
%endblock kgrid_Monkhorst_Pack
```

Monkhorst block: 1, 2, 3, 4, …

siesta: k-grid: Number of k-points = 22

Y	0	0
0	Y	0
0	0	1

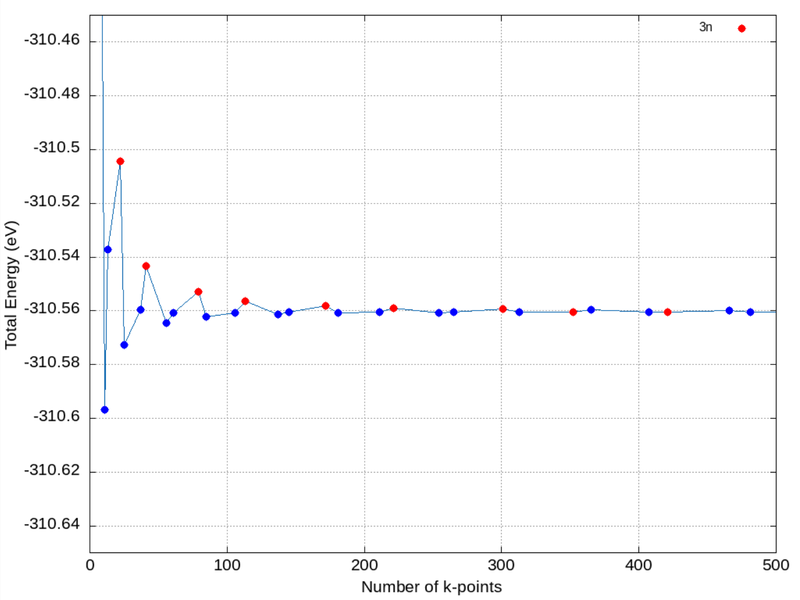
Using: Y=1

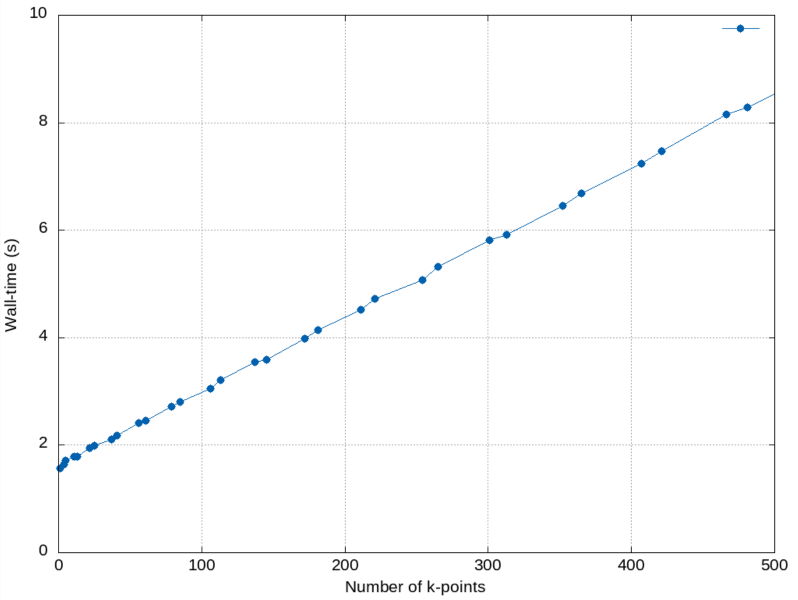
1	0	0
0	1	0
0	0	1

Using: Y=2

2	0	0
0	2	0
0	0	1

Exercise 4 (k-point sampling)





Exercise 5 (Plot the bands)

INPUTS FOLDER

siesta/
├── input_graphene/

OUTPUTS FOLDER

siesta/
├── exercise_5/
│   ├── create_your_own_folders

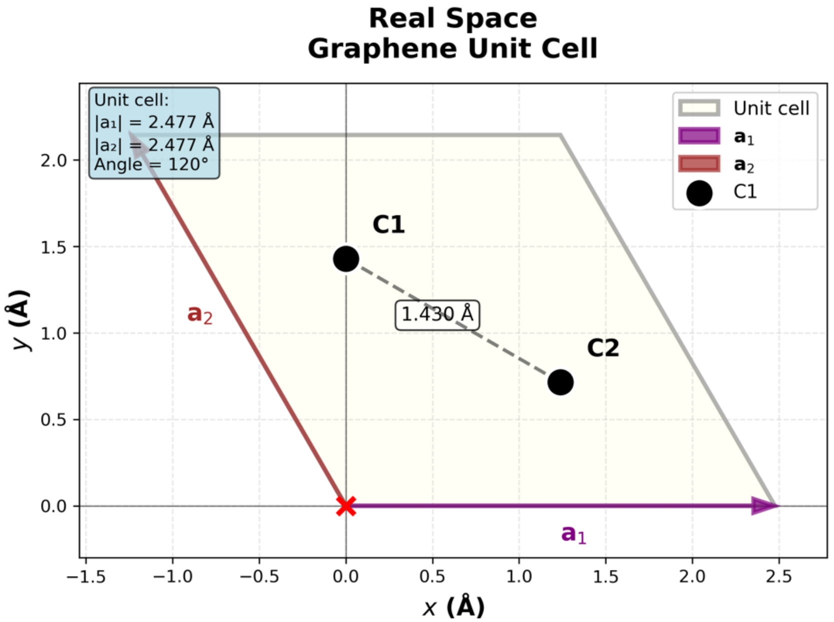
1. Copy all files from exercise 4 folder to the exercise 5 folder.
2. In this exercise you will redo the Graphene exercise 4 but this time uncomment the following options:

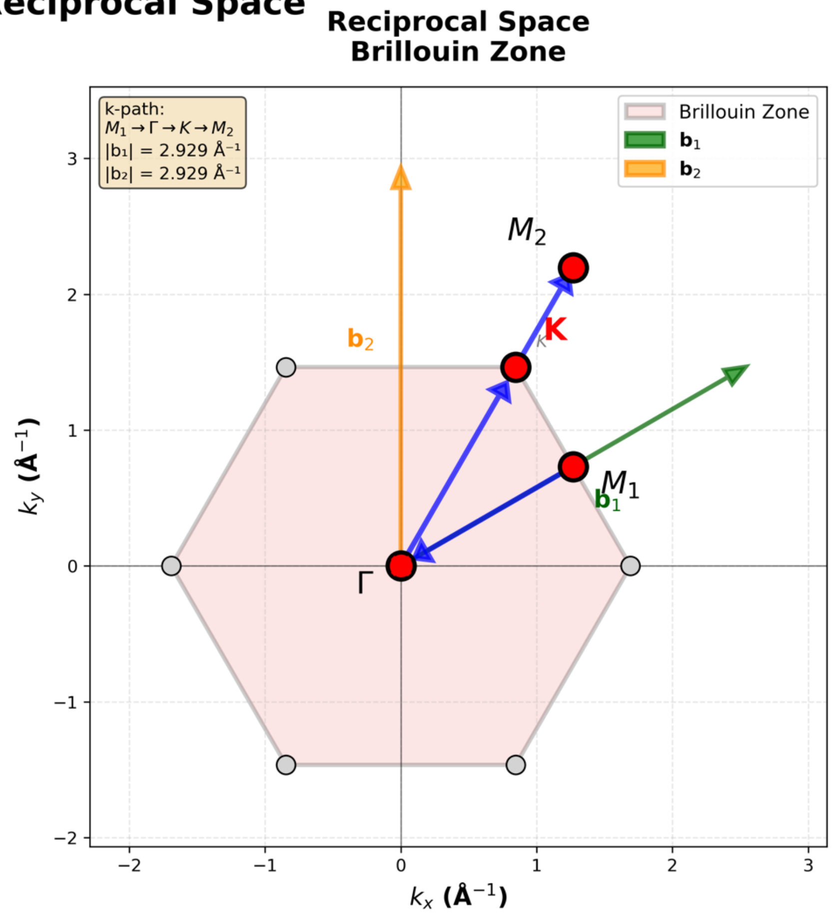
```
#WriteKbands         T
#WriteBands          T
#BandLinesScale      ReciprocalLatticeVectors

#%block Bandlines
#  1   0.5000000000   0.000000000   0.0000   M
# 30   0.0000000000   0.000000000   0.0000   \Gamma
# 45   0.3333333333   0.333333333   0.0000   K
# 30   0.5000000000   0.500000000   0.0000   M
#%endblock BandLines
```

Exercise 5

(what did we do in these calculations?)

Graphene: Real and Reciprocal Space






```
%block Bandlines
  1   0.5000000000   0.000000000   0.0000   M
 30   0.0000000000   0.000000000   0.0000   \Gamma
 45   0.3333333333   0.333333333   0.0000   K
 30   0.5000000000   0.500000000   0.0000   M
%endblock BandLines
```

How do I plot the bands?

What else is there?

/users/commun/seitsonen/HANAMI/sw/target/app/siesta/siesta-5.4.1/bin/

Utilities and others

A look at the SIESTA suite:

cdf2dm	dmbs2dm	fat	gnubands	hsx2hs	ol-stm	pipes_serial	rho2xsf	tbtrans	wfsx2wfs
cdf2grid	dm_creator	fcbuild	grid1d	ioncat	optical	plstm	runJobs	ts2ts	xv2vesta
cdf2xsf	dmfilter	fdf2grimme	grid2cdf	ionplot.sh	optical_input	plsts	sies2arc	tscontour	xv2xsf
cdf_diff	dm_noncol_sign_flip4	fmixmd-driver	grid2cube	lindhard	orbmol_proj	protoNEB	siesta	unfold	
cdf_fft	dmUnblock	fmpdos	grid2d	lwf2cdf	pdosxml	psml2psf	siesta_qmmm	vib2vesta	
cdf_get_cell	eig2bxsf	fractional	grid2val	macroave	permute	psop	simplex	vib2xsf	
cdf_laplacian	Eig2DOS	g2c_ng	grid_rotate	md2axsf	phonons	pvtsp	sockets_parallel	vibra	
countJobs	eigfat2plot	gen-basis	grid_supercell	mixps	phonons-f08	read_spin_texture	sockets_serial	v_info	
denchar	f2fmaster	get_chem_labels	horizontal	mpi_driver	phtrans	readwf	spin_texture	wfs2wfsx	
dm2cdf	f2fslave	getResults	hs2hsx	mprop	pipes_parallel	readwfx	swarm	wfsnc2wfsx	

Utilities and others

gnubands

```
cdf2dm         dmbs2dm               fat              gnubands        hsx2hs      ol-stm          pipes_serial       rho2xsf           tbtrans     wfsx2wfs
cdf2grid       dm_creator            fcbuild          grid1d          ioncat      optical         plstm              runJobs           ts2ts       xv2vesta
cdf2xsf        dmfilter              fdf2grimme       grid2cdf        ionplot.sh  optical_input   plsts              sies2arc          tscontour   xv2xsf
cdf_diff       dm_noncol_sign_flip4  fmixmd-driver    grid2cube       lindhard    orbmol_proj     protoNEB           siesta            unfold
cdf_fft        dmUnblock             fmpdos           grid2d          lwf2cdf     pdosxml         psml2psf           siesta_qmmm       vib2vesta
cdf_get_cell   eig2bxsf              fractional       grid2val        macroave    permute         psop               simplex           vib2xsf
cdf_laplacian  Eig2DOS               g2c_ng           grid_rotate     md2axsf     phonons         pvtsp              sockets_parallel  vibra
countJobs      eigfat2plot           gen-basis        grid_supercell  mixps       phonons-f08     read_spin_texture  sockets_serial    v_info
denchar        f2fmaster             get_chem_labels  horizontal      mpi_driver  phtrans         readwf             spin_texture      wfs2wfsx
dm2cdf         f2fslave              getResults       hs2hsx          mprop       pipes_parallel  readwfx            swarm             wfsnc2wfsx
```

Utilities and others

```
gnubands

$ gnubands -h
 Usage: gnubands [options] [bandsfile|PIPE]

   bandsfile   : SystemLabel.bands
        PIPE   : < SystemLabel.bands

 Options:

     -h         : print help
     -G         : print GNUplot commands for correct labels to stderr
                  Suggested usage: prog options 2> bands.gplot 1> bands.dat
                     gnubands [options] 1> bands.dat 2> bands.gplot
                  and then:
                     gnuplot -persist bands.gplot
     -s arg     : only plot selected spin bands [1,nspin]
     -F         : shift energy to Fermi-level
     -b arg     : first band to write
     -B arg     : last band to write
     -e arg     : minimum energy to write
                :   If -F set, will be with respect
                :   to Fermi level
     -E arg     : maximum energy to write
                :   Note, see -e
     -o file    : specify output file (instead of piping)
                : if used with -G a file name file.gplot will be created
```

Utilities and others

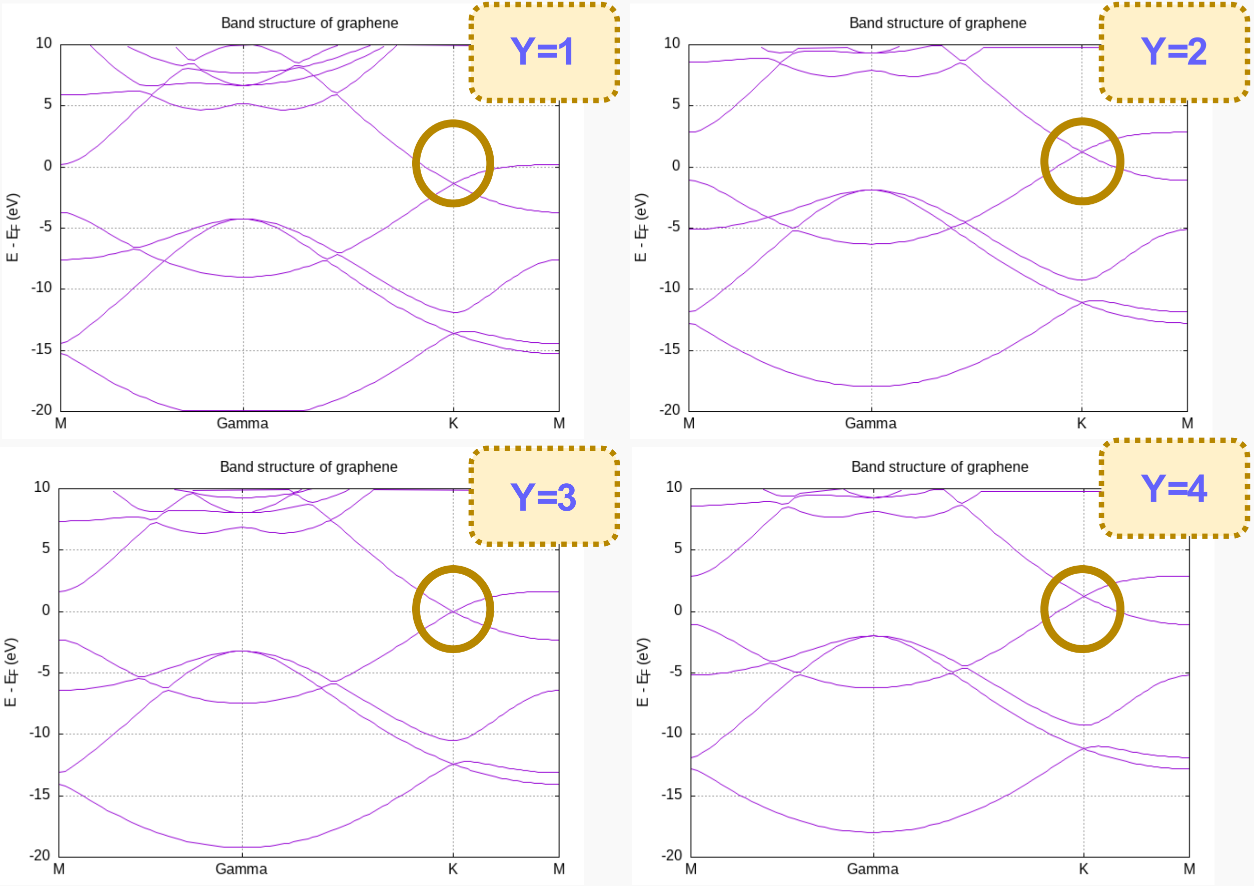
gnubands

Graphene bands

```
gnubands -F -G -o bands -E 10 -e -20 graphene.bands

gnuplot -e "set grid; set ylabel 'E - E_{F} (eV)'; set title 'Band structure of graphene'; set terminal png; set output 'bandstructure.png'; set key noautotitle; load 'bands.gplot'"
```

Exercise 5

(Plot the bands)



$$\begin{matrix} Y & 0 & 0 \\ 0 & Y & 0 \\ 0 & 0 & 1 \end{matrix}$$

Exercise 6 (SCF convergence)

INPUTS FOLDER

```
siesta/
├── input_methane/
```

OUTPUTS FOLDER

```
siesta/
├── exercise_6/
│   ├── create_your_own_folders
```

1. Copy all files from input folder to the exercise 6 folder.
2. In this exercise you will scan three keywords:

Add these lines in the input file

- **SCF.mix** **density** → { density | hamiltonian }
- **SCF.mixer.method** **linear** → { linear | Pulay | Broyden }
- **SCF.mixer.weight** **0.6** → { 0 | 0.1 | 0.2 | … | 1 }

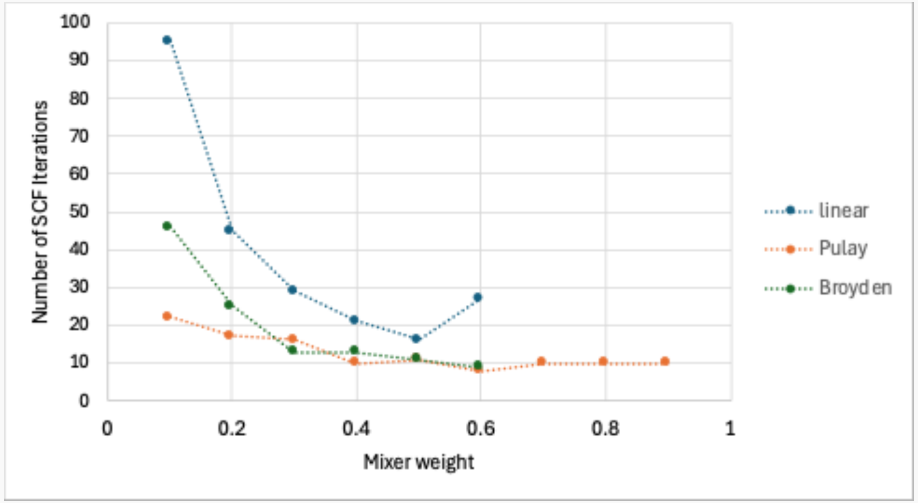
0: New DM is the same as in the previous step
1: New DM is totally different from the previos step

comment:

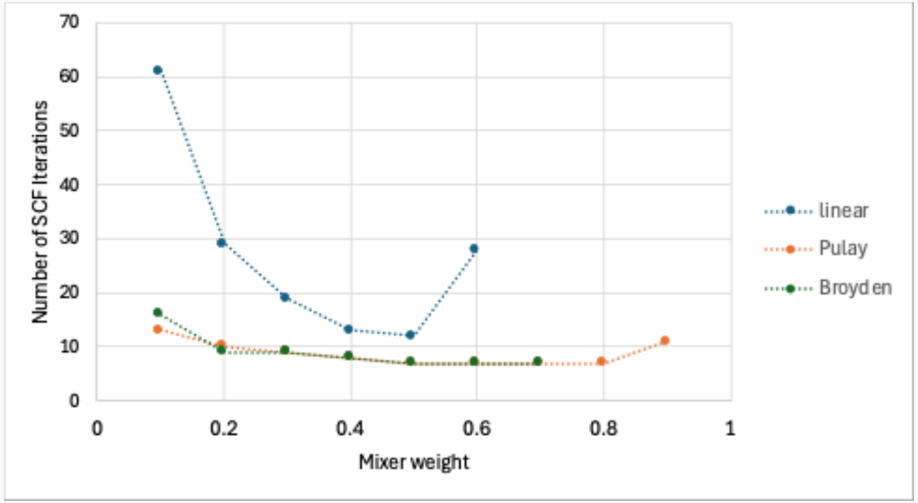
#MaxSCFIterations 50

Exercise 6 (SCF convergence)

Mixing Density Matrix



Mixing Hamiltonian



Questions?

Useful material

https://docs.siesta-project.org/projects/siesta

- Installing Siesta
- Manuals
- Tutorials
- Inputs for tutorials