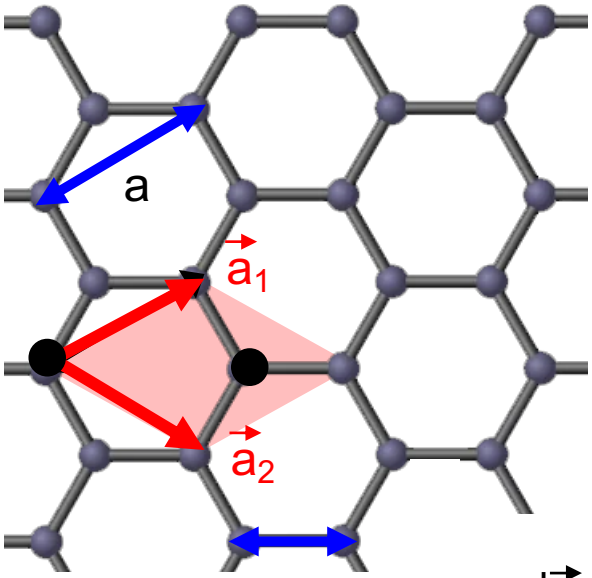
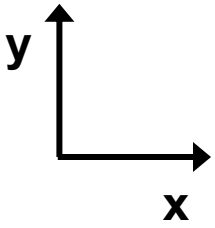
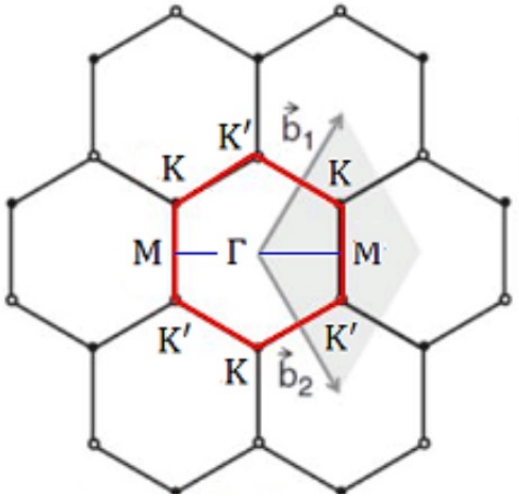
Exercise 2: graphene (2D system)

Real space





Reciprocal space



a_{cc} = 1.42Å

$|\vec{a}_1| = |\vec{a}_2| = a = \sqrt{3}a_{cc}$

$$\vec{a}_1 = \frac{a_{cc}}{2}(3, \sqrt{3})$$
$$\vec{a}_2 = \frac{a_{cc}}{2}(3, -\sqrt{3})$$

$$\vec{b}_1 = \frac{2\pi}{3a_{cc}}(1, \sqrt{3})$$
$$\vec{b}_2 = \frac{2\pi}{3a_{cc}}(1, -\sqrt{3})$$

$$\Gamma = \frac{2\pi}{3a_{cc}}(0,0)$$
$$M = \frac{2\pi}{3a_{cc}}(1,0)$$
$$K = \frac{2\pi}{3a_{cc}}\left(1, \frac{1}{\sqrt{3}}\right)$$
$$K' = \frac{2\pi}{3a_{cc}}\left(1, -\frac{1}{\sqrt{3}}\right)$$

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE**

0_Kconvergence →	Explore convergence wrt k-points
1_SCF →	Obtain electronic structure for converged k-grid
2_BAND_STRUCTURE →	Calculate electronic band structure
3_FATBANDS →	Calculate bands projected onto atomic orbitals
4_PDOS →	Calculate projected density of states

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/0_Kconvergence**

TODO

- Graphene's Brillouin zone is 2D. How must the k-grid be?
- Run several calculations for different k-point samplings
- What does the *Graphene.EIG* output file *c*ontain?
- Use the **Eig2DOS** utility to obtain the density of states for each k-grid
- Plot the density of states wrt to the energy for the different k-grids
- When are the calculations converged with respect to k-points?

Note: always use Fermi level as energy reference

Exercise 2: graphene (2D system)

How to calculate/plot DOS using Eig2DOS

- Load SIESTA so its utilities are also loaded

  > module load SIESTA

- Eig2DOS should be ready to use. You can get help on its usage by typing:

  > Eig2DOS -h

- Use Eig2DOS to get the DOS in the energy range of interest

  > Eig2DOS -m -5 -M 5 –s 0.1 – n 500 -f > DOS.dat

Energy defined wrt Fermi

- DOS.dat contains 4 columns:

  Energy, DOS(spin up), DOS(spin down), total DOS (up+down)

- Plot the total DOS with respect to E

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/1_SCF**

TODO

- Using the converged k-grid rerun the electronic structure calculation
- Siesta prints several output files. What do *Graphene.KP, Graphene.FA, Graphene.EIG, Graphene.XV, Graphene.DM* contain?
- This calculation will be used to run several post-processing calculations. Which of the above-mentioned output files will be useful in order to save time/resources? Store those files.

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/2_BAND_STRUCTURE**

A post-processing calculation will be performed to get the electronic band structure

A new flag must be included in RUN.fdf: **`UseSaveData T`**

Reads in all data saved from previous calculations
(must be in the same directory)

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/2_BAND_STRUCTURE**

For the band structure calculation a new block must be included in RUN.fdf

```
####################
#                  #
# Band structure #
#                  #
####################

BandLinesScale pi/a
%block BandLines
1  0.0000000000      0.0000000000      0.0000000000  !G
100 1.15470053838    0.0000000000      0.0000000000  !M
100 1.15470053838    0.6666666666      0.0000000000  !K
100 0.0000000000     0.0000000000      0.0000000000
%endblock BandLines
```

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/2_BAND_STRUCTURE**

TODO

- Perform a SIESTA run (restart from 1_SCF step)
- Inspect the *Graphene.bands* file. What does it contain?
- Use the **gnubands** utility to obtain the band structure
- Plot the electronic band structure of graphene, and identify the most interesting features.
- Compare the band structure with the DOS obtained in the 0_Kconvergence step. Do they fit together?

Note: always use Fermi level as energy reference

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/3_PDOS**

Density of States:

The density of states (DOS) is essentially the number of different states at a particular energy level that electrons are allowed to occupy, i.e. the number of electron states per unit volume per unit energy.

Projected/Partial Density of States:

The projected/partial density of states (PDOS) is the relative contribution of a particular atom/orbital to the total DOS

DOS vs PDOS

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/3_PDOS**

For the PDOS calculation a new block must be included in RUN.fdf

```
########
#      #
# PDOS #
#      #
########

%block ProjectedDensityOfStates
-15.00 5.00 0.100 500 eV
%endblock ProjectedDensityOfStates
```

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/3_PDOS**

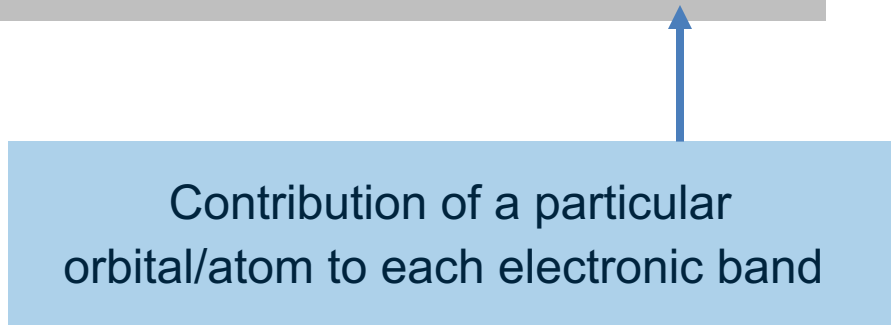
TODO

- Perform a SIESTA run (restart from 1_SCF step)
- Inspect the *Graphene.PDOS* file. What does it contain?
- Use the **fmpdos** utility to obtain the DOS projected onto the relevant orbitals of carbon (2s, 2px, 2py, 2pz)
- Plot the PDOS for the different orbitals. Which are the relevant orbitals around Fermi level? Compare with the total DOS (obtained previously)

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/4_FATBANDS**

A post-processing calculation will be performed to get the so-called fatbands




```
#############
#           #
# Fat Bands #
#           #
#############

COOP.Write T
WFS.Write.For.Bands T
```

New block must be included in RUN.fdf
besides the block for the band structure

Exercise 2: graphene (2D system)

Go to: **/scratch/esc#/EXERCISE_2_GRAPHENE/4_FATBANDS**

TODO

- Perform a SIESTA run (restart from 1_SCF step)
- What does the *Graphene.bands.WFSX* file contain?
- In order to plot the fatbands, we will make use of two SIESTA utilities: **fat** and **eigfat2plot.** The **fat** utility code requires an input file. Check fatbands.mpr in the corresponding directory, and comment on its content.
- Execute the following:

```
> cp Graphene.bands.WFSX Graphene.WFSX
> fat fatbands
```

- Which are the output files printed out by **fat**? These files must be converted to a plotting format. Use **eigfat2plot** for this purpose.
- Which orbitals contribute more to the bands in each energy region? Compare the fatbands with the PDOS obtained previously.