Day 3 Hands-on: Bandstructures, metals and XC functionals

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Today's Themes:

1) Performing band structure calculations
2) DFT calculations for metals: smearing parameters
3) XC functionals: LDA and PBE

Exercise 1

Performing band structure calculations

Exercise 1.1: band structure calculation

The scheme to compute the band structure is the following:

1. SCF pw.x calculation (calculation = 'scf')

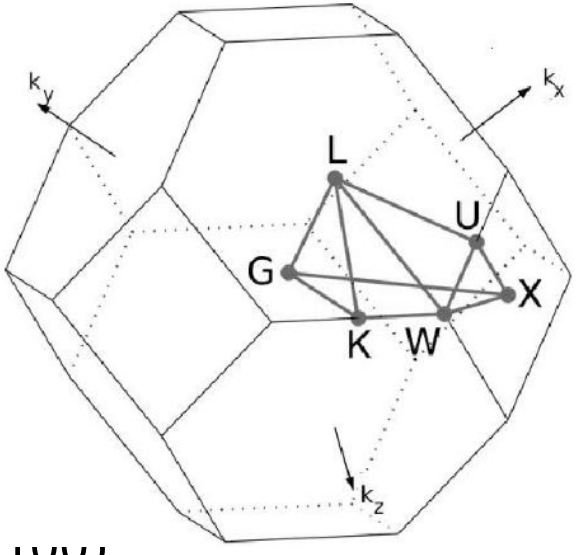
2. "bands"-type non-SCF pw.x calculation (fixed-potential) with:
   - calculation = 'bands'
   - number of bands (variable nbnd) is specified
   - a suitable path of k-points is specified in K-POINTS card. The k-point path must be continuous in k-space.

3. bands.x calculation, which, among others, produces data-files for the plot.

Important: we must keep the prefix same outdir and prefix for "nscf" and "scf" pw.x calculations and for the bands.x calculation.

Exercise 1.1: band structure calculation

The k-path in BZ for fcc crystal can be specified using xcrysden as follow:



1. Open the file si.scf.in with xcrysden.
2. Select: Tools → k-path selection
3. Select the path by clicking on a sequence of high
4. symmetry points: W – Γ – X – W – L – Γ
5. Specify how many k points to be calculated (Ex: 100)
6. save the k-path to file. (.pwscf extension is required for
7. formatting the file for pw.x)

Exercise 1.1: band structure calculation

Input file: si.scf.in

```
 &CONTROL
    calculation='scf'
    restart_mode='from_scratch',
    prefix = 'Si',
    pseudo_dir = '../../pseudo'
    outdir='./tmp'
 /

[...]

ATOMIC_SPECIES
   Si  28.086  Si.pbe-rrkj.UPF

ATOMIC_POSITIONS alat
   Si 0.00 0.00 0.00
   Si 0.25 0.25 0.25

K_POINTS automatic
   6 6 6   1 1 1
```

Input file: si.bands.in

```
 &CONTROL
    calculation='bands'
    restart_mode='from_scratch',
    prefix = 'Si',
    pseudo_dir = '../../../../pseudo'
    outdir='./tmp'
    verbosity = 'high'
 /
[...]
ATOMIC_SPECIES
   Si  28.086  Si.pbe-rrkj.UPF

ATOMIC_POSITIONS alat
   Si 0.00 0.00 0.00
   Si 0.25 0.25 0.25
K_POINTS {crystal_b}
  6
  0.50  0.25  0.75  30   !W
  0.00  0.00  0.00  30   !G
  0.50  0.00  0.50  30   !X
  0.50  0.25  0.75  30   !W
  0.50  0.50  0.50  30   !L
  0.00  0.00  0.00  30   !G
```

Exercise 1.1: band structure calculation

An input file for the data post processing program bands.x. This program print the eigenvalues to the file specified in ”filband”

```
&BANDS

outdir = ’./tmp’,
prefix=’Si’,
filband=’si_bands’,
/
```

The same as in the scf and bands input

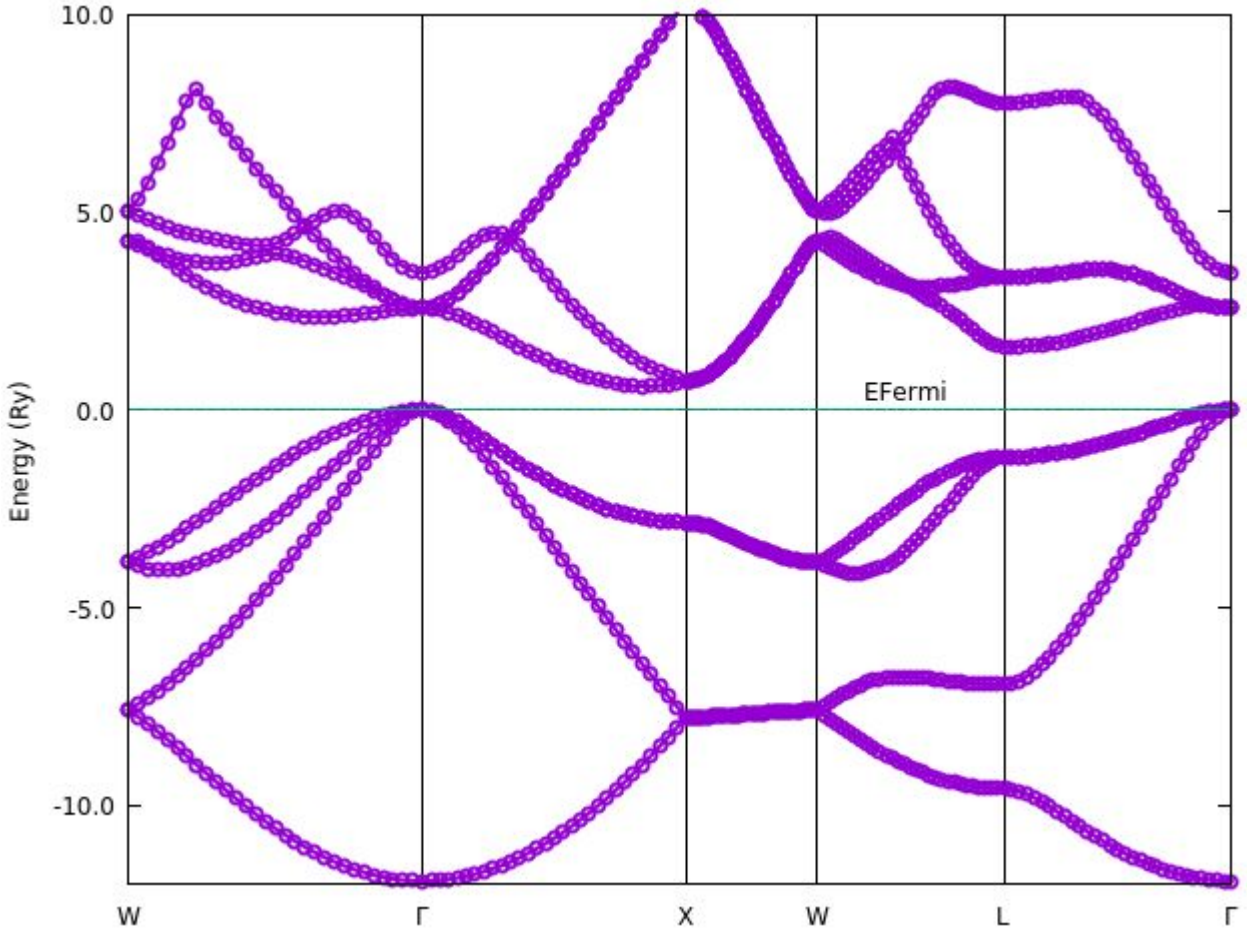
Contains data for bands

Run the postprocessing calculation (bands.x):

```
$ bands.x < bands.in | tee  bands.out
```

bands data are stored in three files with different formats, among which we have bands.dat.gnu (can be plotted with gnuplot) and bands.dat can be visualized using the program plotband.x.

Exercise 1.1: Si band structure



Si is an insulator, what about metallic systems?

Exercise 1.2: band structure of a metal

Let us consider Aluminum, in the fcc phase. It is a metal, only valence bands and a few k-points will not suffice.

- move to the Day3/example1.bandstructure/ex2.Al directory
- read the pw.x input file al.scf.in
- notice the presence of new variables: occupations, smearing, degauss;
- run pw.x as:

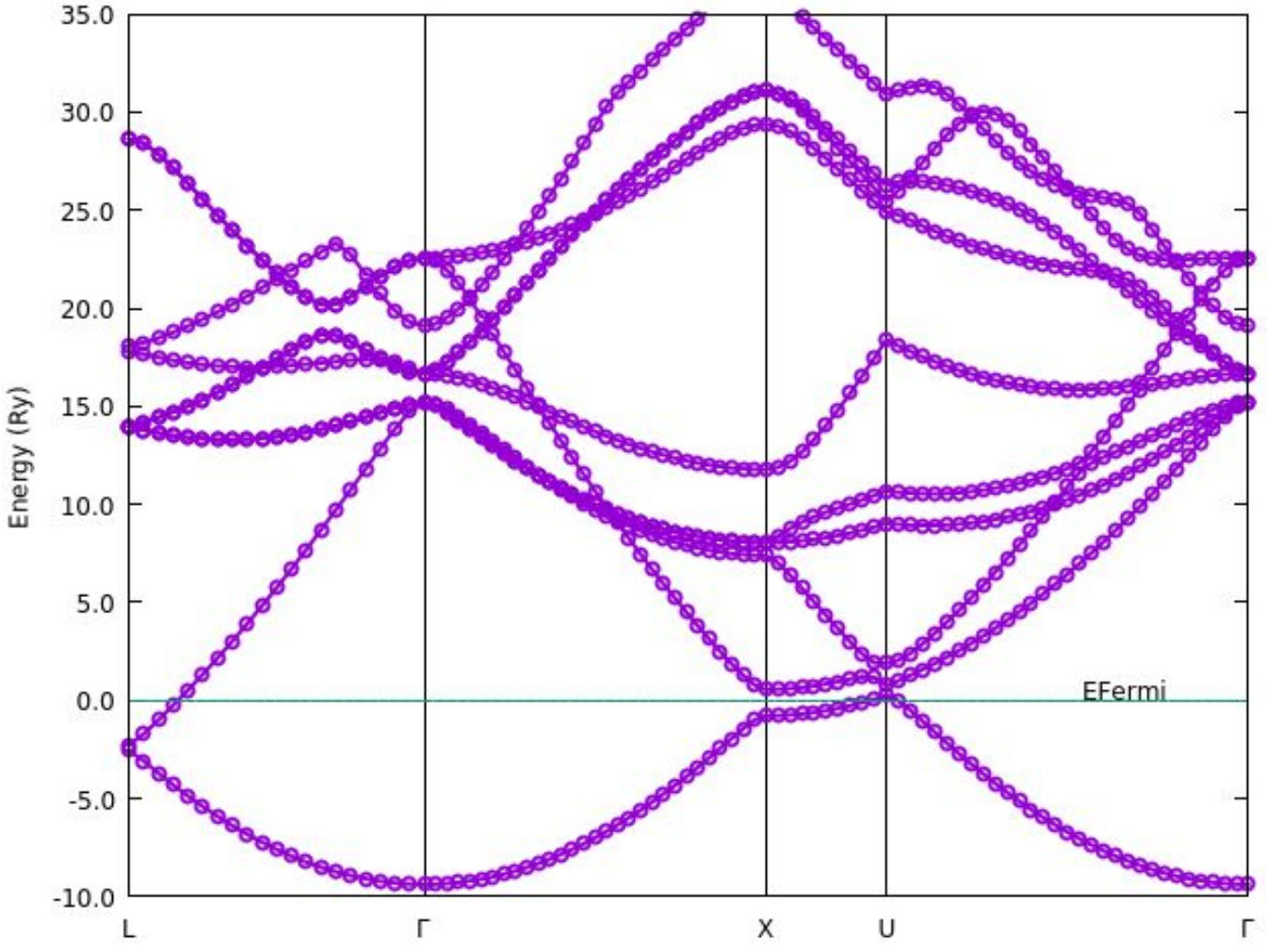
```
$ pw.x < al.scf.in | tee al.scf.out
```

- in the output file notice that

  – the number of bands (Kohn-Sham states) is automatically set to a value larger than the number of electrons divided by 2

  – the Fermi energy is computed.

Exercise 1.2: band structure of a metal



Exercise 2

Performing metallic calculations: smearing

Exercise 2: smearing

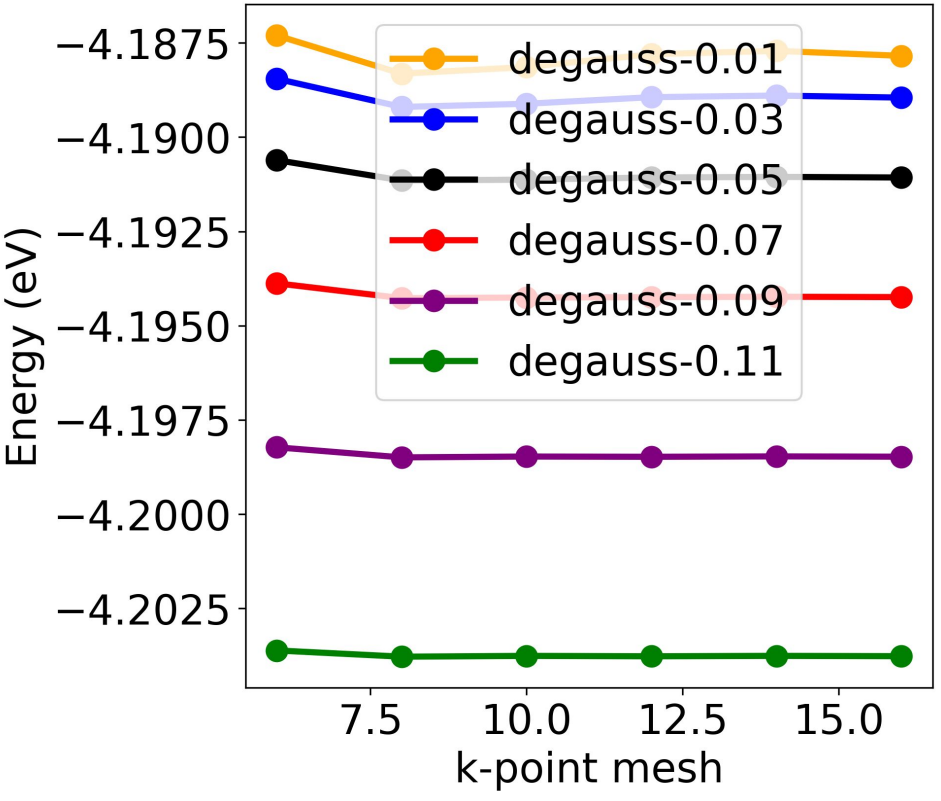
In this exercise we will compute the total energy for this fcc Al with the following values for degauss, k-point meshes and different smearing variables:

- degauss variable, in range from 0.01 to 0.11
- k-points: N×N×N (1×1×1) with N=6,8,10, …, 16
- smearing variable, possible values: 'gauss' (or 'g'), 'marzari-vanderbilt'
- (or 'm-v'), 'methfessel-paxton' (or 'm-p')
- Follow the instructions in example2.smearing:

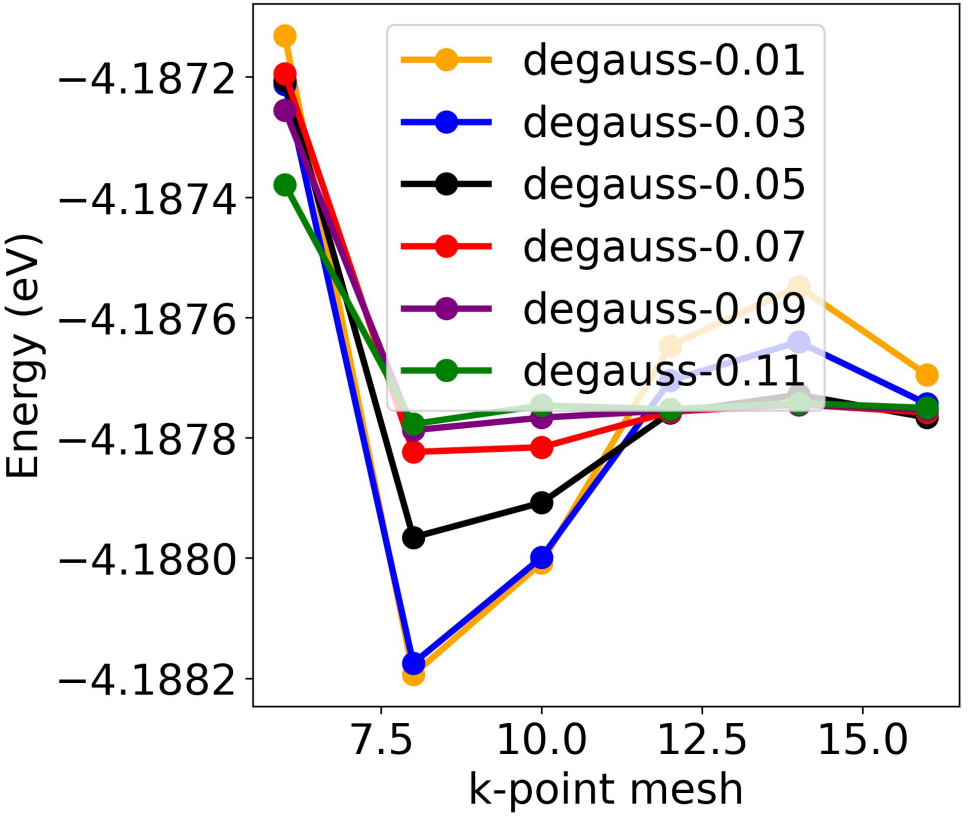
Plot the convergence of the total energy with respect to the number of k-points for the different smearing values.

Exercise 2: smearing

Gaussian

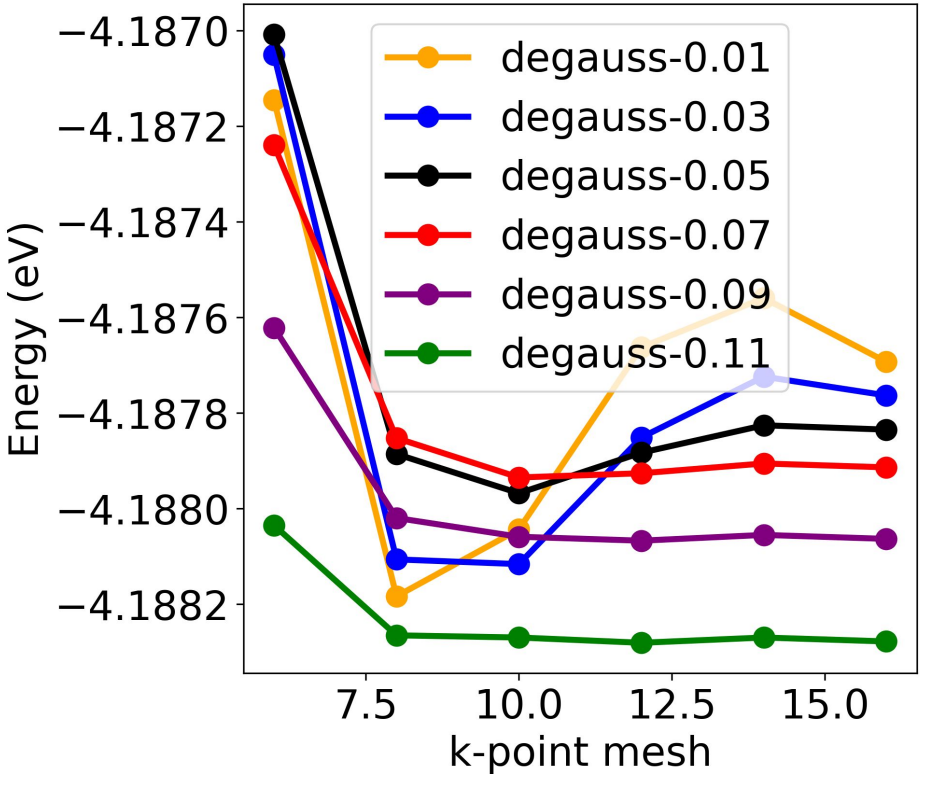


Methfessel-Paxton

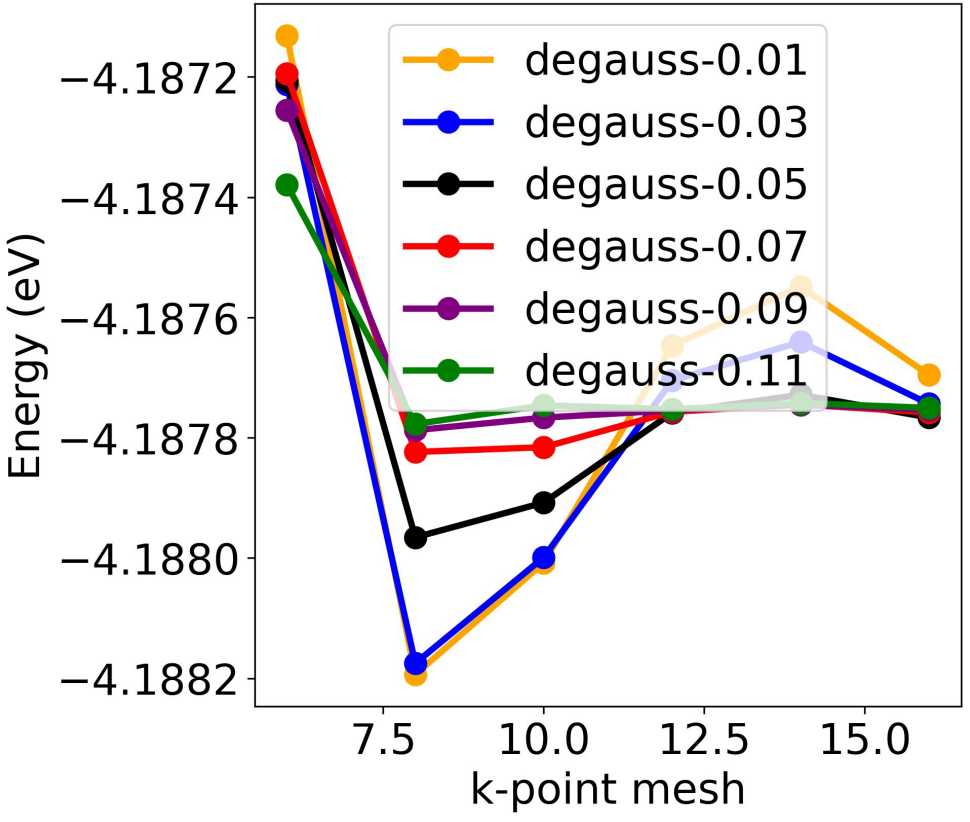


Exercise 2: smearing

Marzari-vanderbilt



Methfessel-Paxton



Exercise 2: smearing

Choose a suitable k-point mesh and plot the total energy as a function of degauss for Marzari-Vanderbilt and Gaussean smearing.