computing a Density Of States (DOS)

Use the same input file you created for the basic silicon example (e.g. basic.in, which was how we called it before). Rerun that calculation with pw.x in an empty folder.

Then copy basic.in to a new name, e.g. basicdos.in :

```
cp basic.in basicdos.in
```

open that file:

```
nano basicdos.in
```

and replace `calculation='scf'` by `calculation='nscf'`

In the `&SYSTEM` block, change the line 'occupations' from 'smearing' to 'tetrahedra' :

```
occupations='tetrahedra',
```

Finally, increase the density of k-mesh considerably, for instance by a factor of 5:

```
K_POINTS {automatic}
35 35 35 0 0 0
```

The input file you have created, is this one:

```
#*********************************************************************************
#* Generated by cif2cell 1.2.10 2018-09-17 14:27 *
#* T. Bjorkman, Comp. Phys. Commun. 182, 1183-1186 (2011). Please cite generously. *
#* *
#* Data obtained from COD. Reference number : 9008566 *
#* () *
#* Wyckoff, R. W. G., Crystal Structures 1, 7-83 (1963) *
#*********************************************************************************

&CONTROL
calculation='nscf',
outdir='.',
prefix='basic',
pseudo_dir='.',
verbosity='low',
tprnfor=.true.,
tstress=.true.,
/

&SYSTEM
ibrav = 0
A = 5.43070
nat = 2
ntyp = 1
ecutwfc=50,
ecutrho=200,
input_dft='pbe',
occupations='tetrahedra',
smearing='mv',
degauss=0.005d0,
/
```

```
&ELECTRONS
conv_thr=1d-08,
mixing_beta=0.7d0,
/

CELL_PARAMETERS {alat}
0.500000000000000 0.500000000000000 0.000000000000000
0.500000000000000 0.000000000000000 0.500000000000000
0.000000000000000 0.500000000000000 0.500000000000000

ATOMIC_SPECIES
Si 28.08500 Si.pbe-n-kjpaw_psl.1.0.0.UPF

ATOMIC_POSITIONS {crystal}
Si 0.000000000000000 0.000000000000000 0.000000000000000
Si 0.250000000000000 0.250000000000000 0.250000000000000

K_POINTS {automatic}
35 35 35 0 0 0
```

Now run pw.x again, using this input file:

```
pw.x -input basicdos.in > basicdos.out
```

Next, prepare a new short input file for the dos.x program (call it, e.g., `basicdos2.in`) :

```
&DOS
outdir='.',
prefix='basic',
Emin= -6,
Emax=17,
DeltaE=0.05,
fildos='silicon.dos',
/
```

It is important that outdir and prefix have the same values as in the file you just used for `pw.x` . The file name in 'fildos' can be freely chosen. The ranges of the energies can be taken based on what you saw during the band structure plotting (if you did not do band structure plotting before calculating the DOS, then it will be some trial and error: start with large values, and then zoom in to the relevant region in a second calculation).

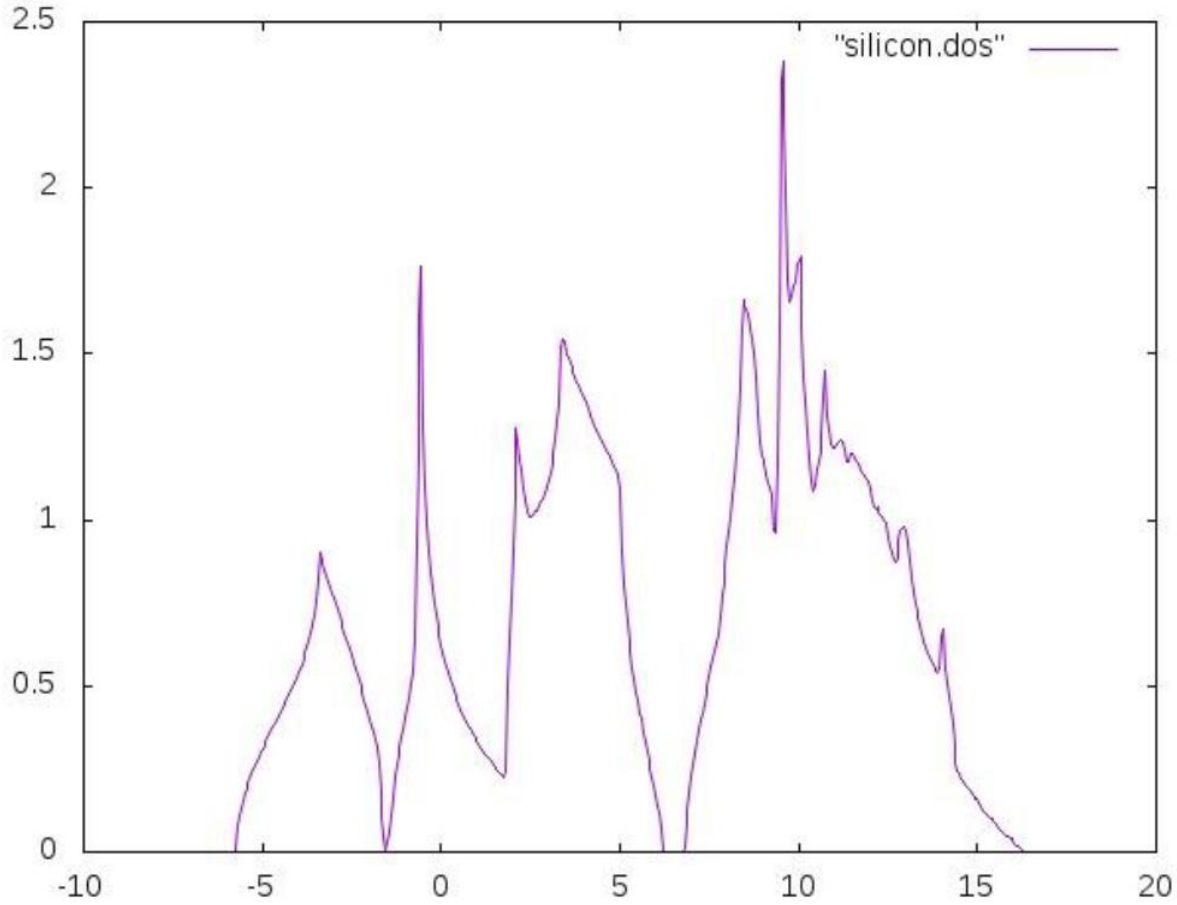
Now run the dos.x program with this input:

```
dos.x -input basicdos2.in > basicdos2.out
```

Visualizing the DOS can be done with gnuplot. Type '`gnuplot`', and then enter the command

```
plot "silicon.dos" with lines
```

You'll see the DOS on your screen.



In order to export the picture as jpg, type

```
set term jpeg
set output "silicon.jpg"
replot
set term x11
```

(similarly for png and pdf)

You leave gnuplot by 'q'.

A few useful commands to ameliorate your plot:

```
set title "silicon DOS"
set xlabel "energy (eV)"
set ylabel "DOS"
set xrange [-6:17]
set yrange [0:2.5]
set xtics 5
set ytics 0.5
```

A quick course on using gnuplot is available at https://alvinalexander.com/technology/gnuplot-charts-graphs-examples

As you have the DOS of silicon now, you can compare it to the band structure, and see how they relate.

As an optional task, you might want to calculate the DOS for aluminum (fcc). The same Γ-X-W-K-Γ-L-U-W-L-K|U-X route can be used. The fcc-Al DOS will be qualitatively different from the DOS of silicon. How can you tell aluminum is a metal ?