

computing a (partial) Density Of States

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. basicbands.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}
  0.5000000000000000  0.5000000000000000  0.0000000000000000
  0.5000000000000000  0.0000000000000000  0.5000000000000000
  0.0000000000000000  0.5000000000000000  0.5000000000000000

ATOMIC_SPECIES
  Si 28.08500 Si.pbe-n-kjpaw_psl.1.1.0.0.UPF

ATOMIC_POSITIONS {crystal}
Si 0.0000000000000000 0.0000000000000000 0.0000000000000000
Si 0.2500000000000000 0.2500000000000000 0.2500000000000000

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 projwfc.x program (call it, e.g., basicdos2.in):

```

&PROJWFC
  prefix='basic',
  outdir='.',
  Emin=-6,
  Emax=17,
  DeltaE=0.05,
  filpdos='silicon',
  filproj='silicon'
/

```

It is important that outdir and prefix have the same values as in the file you just used for pw.x. The file names in 'filpdos' and 'filproj' 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:

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

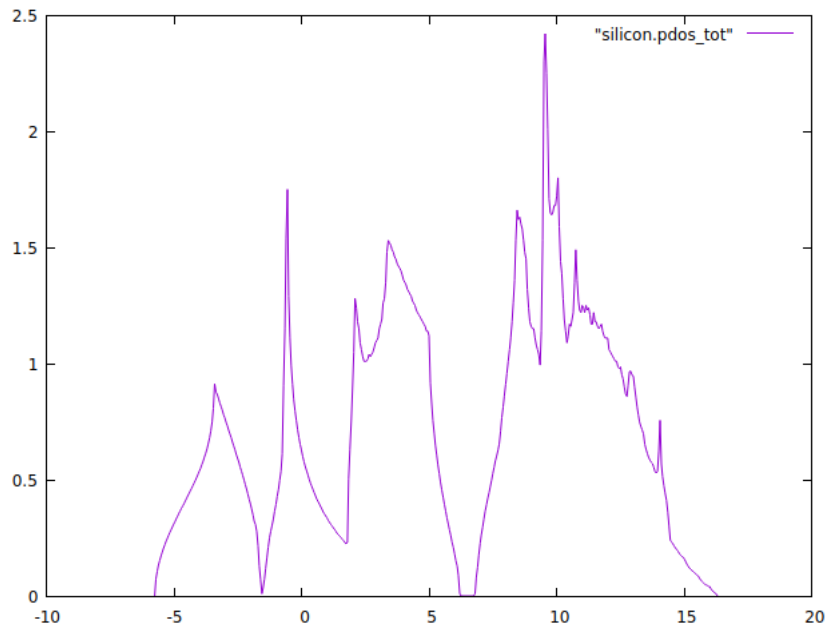
Visualizing the DOS can be done with gnuplot. In order to use gnuplot in the terminal window in which you are working, you should type first the command 'conda activate visualise'. Then type :

```
gnuplot
```

and then enter the command

```
plot "silicon.pdos_tot" 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
```

after which you can type

```
plot "silicon.pdos_tot" with lines
```

again to generate a new picture.

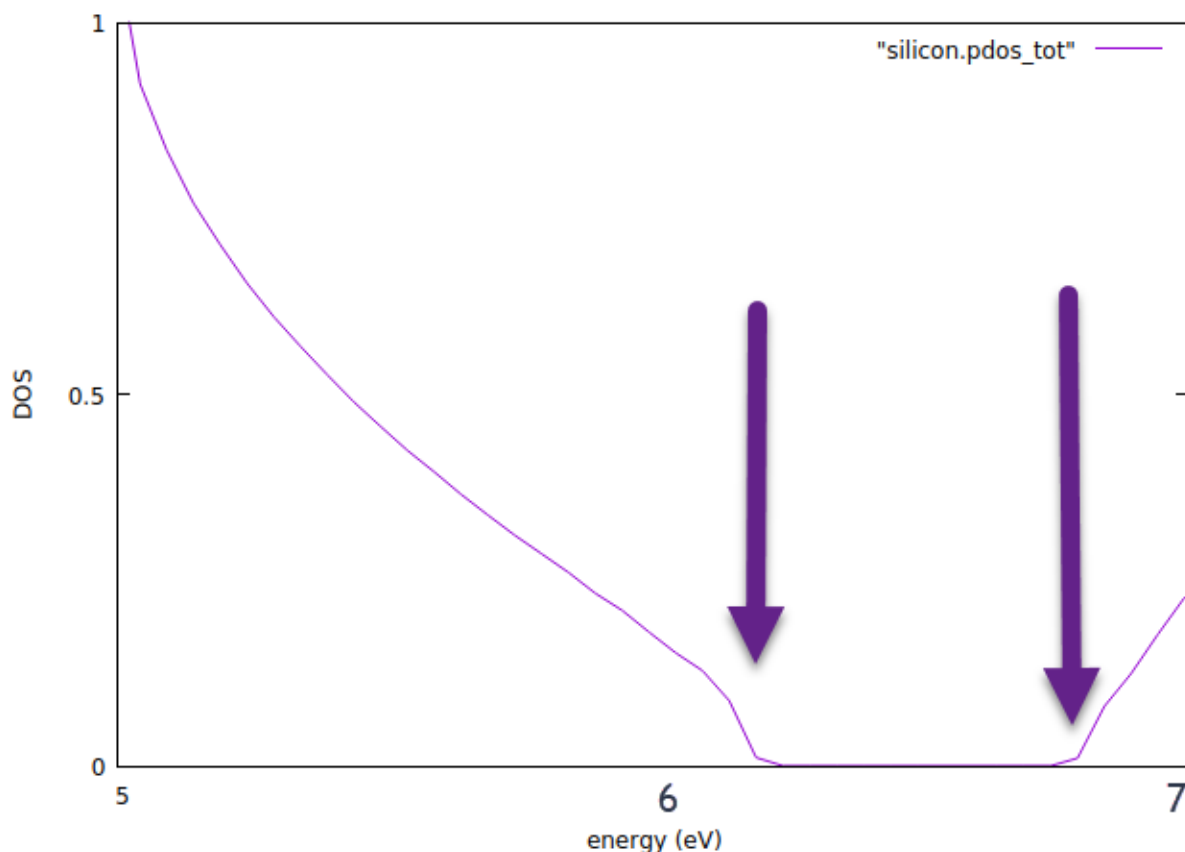
You can compare the DOS of silicon to the band structure, and see how they relate.

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

An important feature that is not directly visible on this plot yet, is the position of the Fermi energy. You can read the value of the Fermi energy in the output file of the initial scf calculation (basic.out) :

```
the Fermi energy is 6.2683 ev
! total energy = -93.45255564 Ry
  Harris-Foulkes estimate = -93.45255563 Ry
  estimated scf accuracy < 9.0E-09 Ry
total all-electron energy = -1160.144286 Ry
```

The following picture is a blow-up of the region from 5 to 7 eV. The short arrow shows the position of the Fermi energy, which appears to be at the top of a band (the valence band). The longer arrow shows the position of the next band (the first unoccupied band, known as the conduction band). This means that in this calculation the band gap is found to be about 0.6 eV (this is smaller than the actual band gap of silicon, and this underprediction of the band gap of semiconductors is one of the known deficiencies of DFT with LDA or GGA functionals) :



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 band structure of silicon. How can you tell aluminum is a metal ?

The DOS you have plot so far, is the 'total DOS' – this means: for all states, without specifying the character of the states. It is also possible to create several so-called *partial densities of states*. These are the total DOS

restricted to, for instance, s-electron character. The plot shows then the energies at which you find states with s-electron character.

Another way to visualize this: a crystal orbital is very different from a hydrogen-type orbital. But you could write a crystal orbital as a linear combination of s-, p-, d-,... hydrogen type orbitals. If the s-orbital is 17% of the crystal orbital, then this crystal orbital will contribute 0.17 to the partial s-DOS, whereas the same orbital will contribute 1.00 to the total DOS.

Let's now visualize these partial DOS.

If you look at the content of your folder (by the command: `ls -l`), you see that not only `silicon.pdos_tot` has been generated, but several other `silicon.pdos_*` files as well:

```
max@qmobile:~/work/test/si$ ls -l
total 240584
-rw-r--r-- 1 max users      122 Dec 13 17:45 basicdos2.in
-rw-r--r-- 1 max users 1765513 Dec 13 17:59 basicdos2.out
-rw-r--r-- 1 max users   1473 Dec 13 17:44 basicdos.in
-rw-r--r-- 1 max users   7010 Dec 13 17:52 basicdos.out
-rw-r--r-- 1 max users   1467 Dec 13 17:36 basic.in
-rw-r--r-- 1 max users  14539 Dec 13 17:37 basic.out
drwxr-xr-x 2 max users  36864 Dec 13 17:59 basic.save
-rw-r--r-- 1 max users 239162880 Dec 13 17:51 basic.wfc1
-rw-r--r-- 1 max users  800034 Dec 13 17:52 basic.xml
-rw-r--r-- 1 max users   39570 Dec 13 18:03 silicon.jpg
-rw-r--r-- 1 max users     355 Dec 13 17:59 silicon.lowdin
-rw-r--r-- 1 max users   13734 Dec 13 17:59 'silicon.pdos_atm#1(Si)_wfc#1(s)'
-rw-r--r-- 1 max users   23480 Dec 13 17:59 'silicon.pdos_atm#1(Si)_wfc#2(p)'
-rw-r--r-- 1 max users   13734 Dec 13 17:59 'silicon.pdos_atm#2(Si)_wfc#1(s)'
-rw-r--r-- 1 max users   23480 Dec 13 17:59 'silicon.pdos_atm#2(Si)_wfc#2(p)'
-rw-r--r-- 1 max users   13730 Dec 13 17:59 silicon.pdos_tot
-rw-r--r-- 1 max users  2700494 Dec 13 17:59 silicon.projwfc_up
-rw-r--r-- 1 max users 1691876 Nov 16 2018 Si.pbe-n-kjpaw_psl.1.0.0.UPF
```

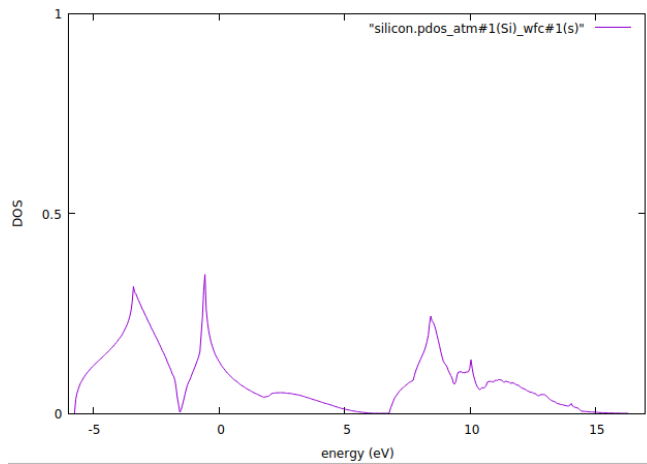
They contain the partial DOS. The first two for the first Si atom in the unit cell (they have `atom1 (Si)` in their name), the second two for the other Si atom (`atom2 (Si)`). The s-electron partial DOS has 1 (s) in the name, the p-electron partial DOS has 2 (p). As the two Si atoms in this crystal are crystallographically equivalent, we need to look at only one of them.

In order to plot the s-electron partial DOS for the first Si atom, do:

```
gnuplot
```

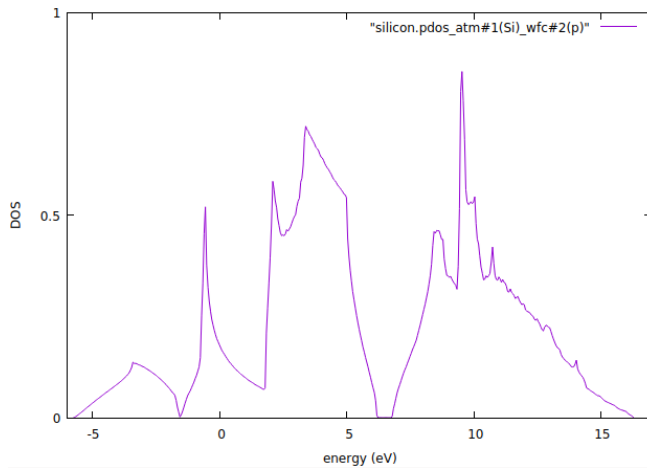
```
plot "silicon.pdos_atm#1(Si)_wfc#1(s)" with lines
```

which will give you:



The p-DOS is plot by

`plot "silicon.pdos_atm#1(Si)_wfc#2(p)" with lines`



For silicon, the difference between the s-DOS and p-DOS is not very large, as the chemical bond in silicon is a sp^3 hybrid that consists of s- and p-electrons alike. The largest difference that is visible is that the orbitals with s-character are dominant in the energy range [-6 eV, -1 eV], whereas in the range [1 eV, 6 eV] the orbitals with p-character are dominant. The unoccupied band (conduction band) that starts at about 7 eV is mostly of p-character too.