computing a band structure

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 basicbands.in
```

open that file:

```
nano basicbands.in
```

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

In the &SYSTEM block, tell that you want to calculate 10 bands (at most):

```
nbnd=10,
```

Finally, replace the K_POINTS section by this:

```
K_POINTS {crystal_b}
11
  0.00  0.00  0.00  30 !G
  0.50  0.00  0.50  30 !X
  0.50  0.25  0.75  30 !W
  0.375 0.375 0.74  30 !K
  0.00  0.00  0.00  30 !G
  0.50  0.50  0.50  30 !L
  0.625 0.25  0.625 30 !U
  0.50  0.25  0.75  30 !W
  0.50  0.50  0.50  30 !L
  0.375 0.375 0.74  30 !K|U
  0.50  0.00  0.50  30 !X
```

To avoid a feeling of black magic happening, it is important to examine the meaning of the latter block. The '11' announces that 11 lines of coordinates will follow. Each line starts with three coordinates in reciprocal space, given as fractional coordinates:

- 0.5 means "one half of the edge of the first Brillouin zone along the x^* direction".
- 0.25 means "one quarter of the edge of the first Brillouin zone along the y^* direction".
- etc.

These 11 points define a path through the first Brillouin zone: you start at the position of the first point, go in a straight line to the second point, from there in a straight line to the third point,…, until you arrive at the 11th point. The number in the 4th column (here always 30) tells that along each of these straight segments 30 points will be taken at which eigenvalues will be calculated. The name that follows after the '!' is a (conventional) name given to each of the points. When two names are given (K|U) it indicates that these are two equivalent points, and you ‘jump’ from one to the other (a kind of ‘tunneling’ along the path).

The conventional names of these points are documented, for instance, in Setyawan & Curtarolo (http://dx.doi.org/10.1016/j.commatsci.2010.05.010). Their Tab. 3 applies to the space group of silicon:

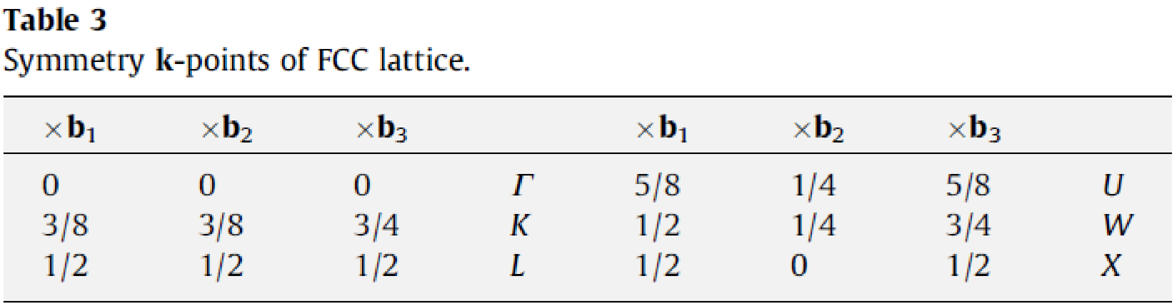


Table 3
Symmetry **k**-points of FCC lattice.

×$\mathbf{b}_1$	×$\mathbf{b}_2$	×$\mathbf{b}_3$		×$\mathbf{b}_1$	×$\mathbf{b}_2$	×$\mathbf{b}_3$	
0	0	0	*Γ*	5/8	1/4	5/8	*U*
3/8	3/8	3/4	*K*	1/2	1/4	3/4	*W*
1/2	1/2	1/2	*L*	1/2	0	1/2	*X*

You recognize exactly these coordinates in the input file we are constructing.

These points are visualized in Fig. 2 of Setyawan & Curtarolo:

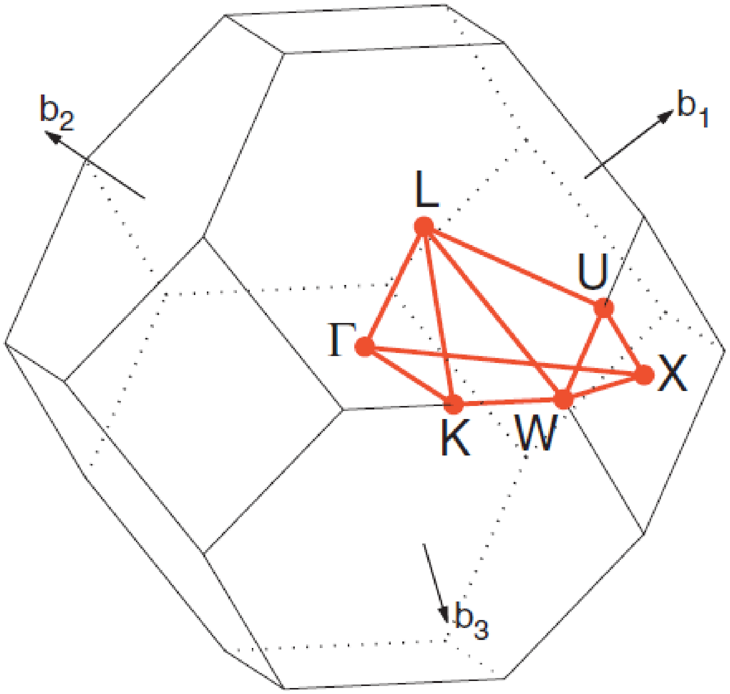


Fig. 2. Brillouin zone of FCC lattice. Path: *Γ*–*X*–*W*–*K*–*Γ*–*L*–*U*–*W*–*L*–*K*|*U*–*X*. An example of band structure using this path is given in Fig. 27.

You can plot a band structure for any path you want. Conventionally, however, for every space group a default path is used. This makes is easier to compare band structure plots (two plots for the same crystal

Another way to get to such visual information, is via the Bilbao Crystallographic Server.

space Group Symmetry
kvec
choose (take here nr. 227 or Fd-3m for silicon)
optimized listing (ITA)
then click on the word ‘Brillouin zone’ above the table.

but along a different path can look very different, whereas they still reflect the same information). You can look up the conventional path for every space group in Setyawan & Curtarolo (http://dx.doi.org/10.1016/j.commatsci.2010.05.010). In the above Fig. 2, they list the path (Γ-X-W-K-Γ-L-U-W-L-K|U-X) and refer to Fig. 27 as an example for the path for this space group:

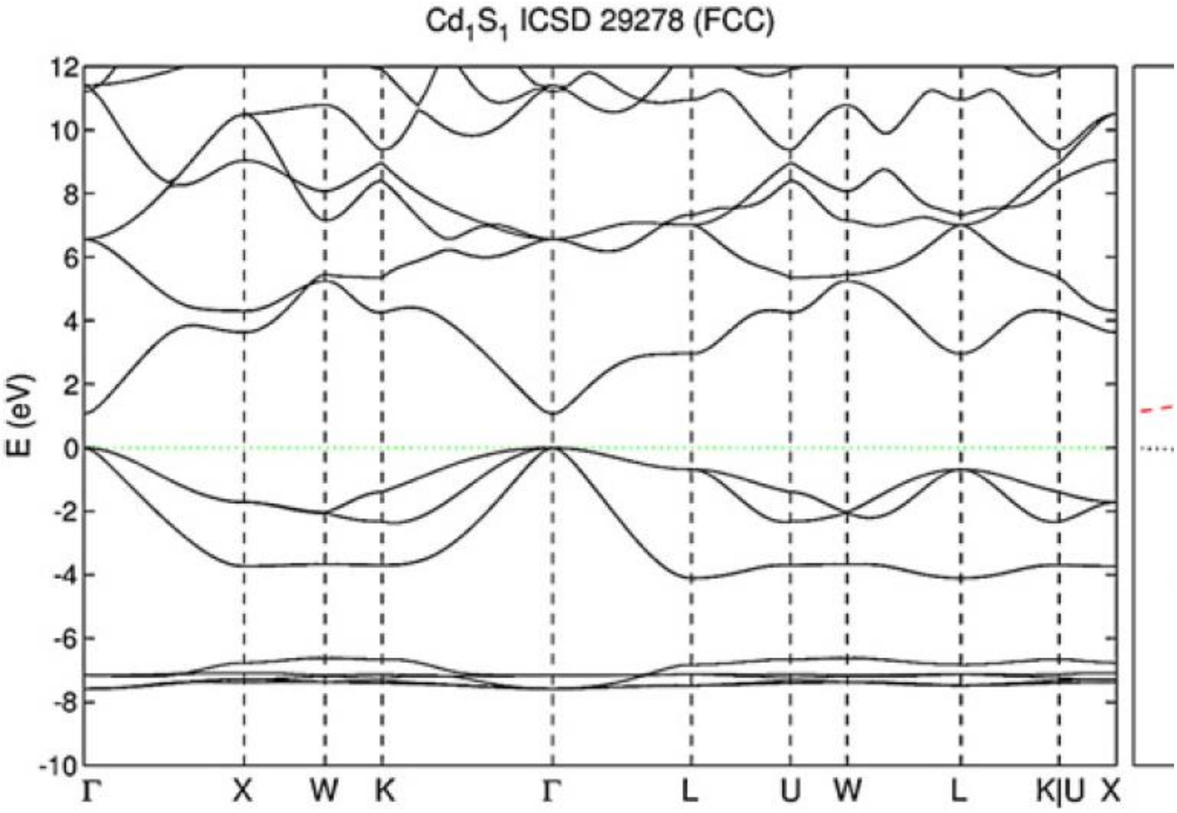


Fig. 27. Band structure of CdS in FCC lattice.

The path Γ-X-W-K-Γ-L-U-W-L-K|U-X is exactly the one we specified in the input file above.

After all of this, you finally have your input file, which should read:

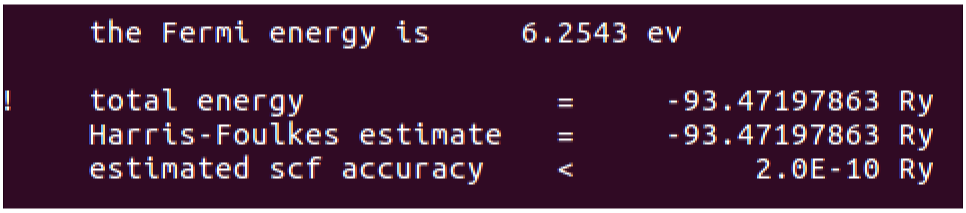
```
#************************************************************************************
#*                  Generated by cif2cell 1.2.10 2018-09-17 14:27                   *
#*  T. Bjorkman, Comp. Phys. Commun. 182, 1183-1186 (2011). Please cite generously. *
#*                                    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

&CONTROL
  calculation='bands',
  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,
  nbnd=10,
  input_dft='pbe',
  occupations='smearing',
  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 {crystal_b}
11
  0.00  0.00  0.00  30 !G
  0.50  0.00  0.50  30 !X
  0.50  0.25  0.75  30 !W
  0.375 0.375 0.74  30 !K
  0.00  0.00  0.00  30 !G
  0.50  0.50  0.50  30 !L
  0.625 0.25  0.625 30 !U
  0.50  0.25  0.75  30 !W
  0.50  0.50  0.50  30 !L
  0.375 0.375 0.74  30 !K|U
  0.50  0.00  0.50  30 !X
```

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

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

For later reference, open the file basic.out from the regular scf-calculation you did at the start of this excercis, and search for the Fermi energy:



```
     the Fermi energy is     6.2543 ev

!    total energy              =     -93.47197863 Ry
     Harris-Foulkes estimate   =     -93.47197863 Ry
     estimated scf accuracy    <          2.0E-10 Ry
```

Next, prepare a new short input file for the bands.x program (call it, e.g., `basicbands2.in`) :

```
&BANDS
  outdir='.',
  prefix='basic',
  filband='siliconbands.dat',
/
```

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 'filband' can be freely chosen.

Now run the bands.x program with this input:

```
bands.x -input basicbands2.in > basicbands2.out
```

Then run the `plotband.x` program, which will ask you a set of question:

- Input file: this is the value you gave for filband (here: siliconbands.dat)
- Range: you get as information the lowest and highest eigenvalue in the dataset. Choose now which region you want to plot. If you want to plot everthing, chose a minimal/maximal value that are slightly below/above the lowest/highest values (e.g. for min=-5.75 and max=16.31, choose -6 and 17). You can type both values on the same line, then press enter.
- Output file: gnuplot
- Output file (ps): type any name, preferably with .ps as suffix (e.g. siliconbands.ps)
- Efermi : write here the value you have written down from `basicbands.out` (or however you called that file) (6.2543 in the present example).
- Delta E, reference E: this is for plotting labels and tick marks on the vertical axis. Delta E gives the distance between labels (e.g. 5 eV), while reference E gives one energy value for which a label surely will be printed (e.g. 0 eV) . Example input is '5 0' (on one line, then enter)

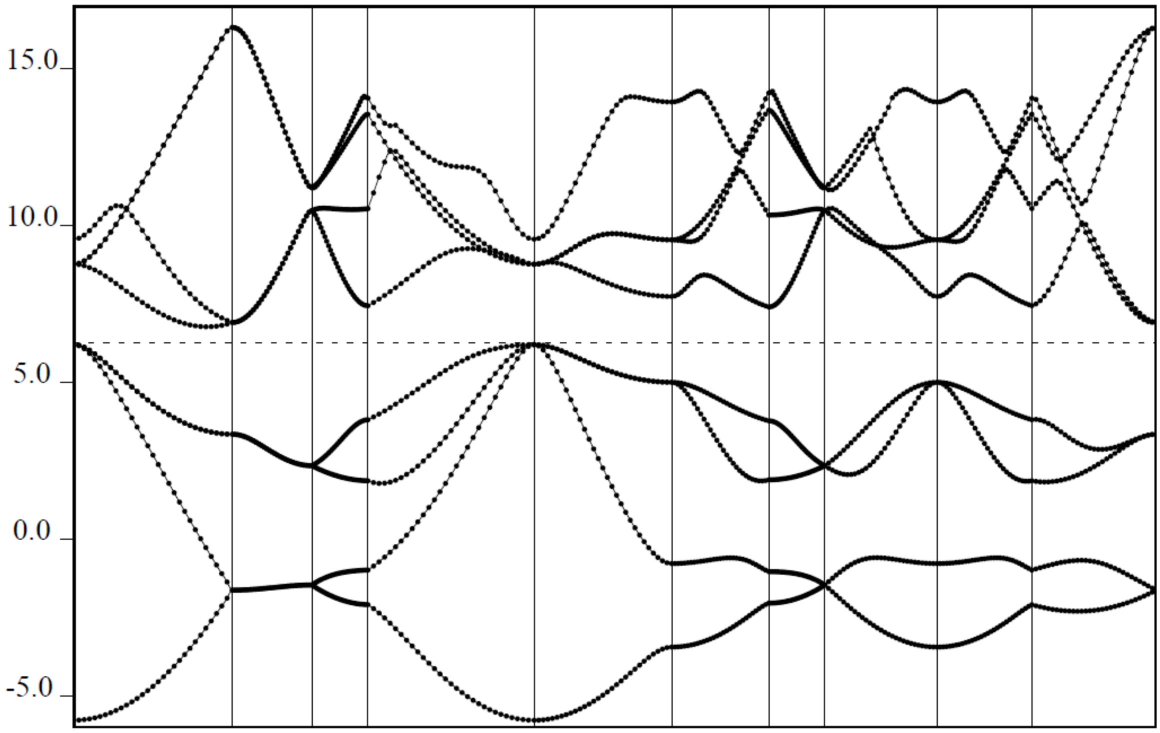
A file in postscript format has now been created, with the name you choose (siliconbands.ps).
Convert that file to pdf:

```
ps2pdf siliconbands.ps
```

The put the pdf file into the shared folder of your virtual machine:

```
cp siliconbands.pdf /media/sf_host
```

Go to your normal computer and use your regular pdf viewer to look at the picture:



The horizontal line is at the Fermi energy, and the labels on the vertical axis are there where we asked them to be.

The horizontal axis is not labeled in this simple plotting procedure. For reporting/publishing purposes, you can add the labels manually using your favourite graphics editing software. Wherever there is a vertical line (there are 11 of them here), there is one of the points you specified in the list of `K_POINTS`.

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