Practical 2 – Band structure and DOS

Learning Objectives

- Gain awareness and familiarity with the tools available to produce band structure and density of states plots with CASTEP.
- Investigate how band structures differ for metallic and semiconductor systems differ.
- Running spin polarised calculations in CASTEP.

Introduction

The aim of this tutorial is to enable you to compute band structures using CASTEP and introduce you to a few of the tools which allow you to visualise the band structure and density of electronic states computed using CASTEP. The band structure of metals and semiconductors will be plotted so that you can look at the differences between different types of systems.

First you will look at the CASTEP input files (**`.cell`** and **`.param`**) used to produce band structure information.

Next you will use the perl script **`dispersion.pl`** that can be used to take CASTEP output and plot band structure diagrams.

Then you will use **`orbitals2bands`** – a tool that provides more information about the orbitals that contribute to different bands in your band structure diagram.

Finally you will look at the band structure of iron, to show how magnetic systems can be studied using CASTEP, you will also plot the density of states of iron using **`dos.pl`**.

Example files:

Download the input files

`wget` http://www-users.york.ac.uk/~mijp1/teaching/grad_FPMM/files/2.tar.gz

Then untar and unzip it using:

```
gunzip 2.tar.gz
tar -xvf 2.tar
```

Example 1 - Graphite

Move into the graphite directory, look at the CASTEP **.cell** and **.param** files and notice the differences from the previous single point energy runs.

The **.param** file needs to be changed so that CASTEP know which task you want to do:

```
task:              spectral
spectral_task:     bandstructure
```

The **.cell** file requires a path through the Brillouin Zone along which you want the bandstructure to be plotted:

```
%BLOCK SPECTRAL_KPOINT_PATH
 0.0000 0.00000 0.00000 ! G
 0.0000 0.00000 0.50000 ! A
-0.3333 0.66667 0.50000 ! H
-0.3333 0.66667 0.00000 ! K
 0.0000 0.00000 0.00000 ! G
 0.0000 0.50000 0.00000 ! M
 0.0000 0.50000 0.50000 ! L
-0.3333 0.66667 0.50000 ! H
%ENDBLOCK SPECTRAL_KPOINT_PATH
```

Run CASTEP using:

```
castep graphite
```

Once the CASTEP calculation has finished a **graphite.bands** file will be present in the directory. A band structure plot can be viewed by using the **dispersion.pl** tool.

```
dispersion.pl -xg -bs -symmetry hexagonal
graphite.bands
```

The **-xg** option tells **dispersion.pl** that you are using xmgrace to plot the band structure, the **-bs** option tells the script that you want to plot using CASTEP output files, the **-symmetry** hexagonal option labels the high symmetry points on the bands structure plot.

When you view this band structure plot you will notice the bands are coloured from lowest to highest energy. Using information about the wavefunction CASTEP can improve this band structure plot, so bands are

coloured due to the orbitals that contribute. This tool can be run in the same directory that you ran CASTEP in.

The program **orbitals2bands** overwrites your **.bands** file, so it's best to copy it to another file to preserve it before usage:

```
cp graphite.bands graphite.bands.orig
orbitals2bands graphite
```

Example 2 - Silicon and Aluminium

This example is very similar to example 1, but this time comparing a semiconductor and a metal, both with FCC crystal structures.

Go into the silicon and aluminium directories and compute the band structures as above.

The dispersion symmetry option needs to be told that these are FCC materials, not hexagonal, e.g.

```
dispersion.pl -xg -bs -symmetry fcc Al.bands
```

Compare the band structure of the Silicon and Aluminium crystals.

- *What are the main similarities and differences?*
- *Can you explain this using your knowledge of the bonding in these materials?*

Example 3 - Iron

In the iron directory there is a set of input files for iron. As iron is a magnetic system you need to instruct CASTEP that it is spin polarised. You also need to set up the calculation with the total spin set to a non-zero value, in order to find the magnetic ground state. (If you're interested you could try removing the **spin : 1** line from the **Fe.param** file and see what happens).

You set the spin in the **.param** file:

```
spin : 1
spin_polarised : true
```

The path through the Brillouin Zone is found in the **Fe.cell** file.

Run the iron computation using CASTEP and plot the band structure for iron using **dispersion.pl**. You might find the **-mono** option to **dispersion.pl** to be useful - it colours the bands by spin channel.

Density of States of Iron

To plot the density of states of iron, we need to run CASTEP again. Instead of computing the band structure along a high symmetry line, we compute it on a grid. Edit your **Fe.cell** file, remove the lines

```
%block spectral_kpoint_path
 ...
%endblock spectral_kpoint_path
```

and replace with the single line:

```
SPECTRAL_KPOINT_MP_GRID 12 12 12
```

Then edit your **Fe.param** file:

```
spectral_task:    DOS
```

Run CASTEP using these new input files then use the **dos.pl** plotting script:

```
dos.pl -xg -bs -w 0.2 Fe.bands
```

Can you relate the features in the DOS to those in the Bandstructure?
You might find the **-mirror** option useful. You should also experiment with the **-w** option to set the Gaussian broadening in eV - try smaller (0.05) and larger (0.5) values and explain what you see.

The DOS for the other crystals in this tutorial can be computed in a similar way.