Ground state of face-centered-cubic aluminum

This part of the tutorial can be performed on your laptop with a single cpu.

1. Build your own abinit input file for calculating the ground state energy of fcc-Al. Let's name it input. Use the template provided and fill it correctly using the following parameters:
   - 1-atom primitive cell.
   - **k**-point grid: $16 \times 16 \times 16$.
   - Cutoff energy: 20 Ha.
   - Cell parameter: 6.534 bohr.
   - Fermi-Dirac smearing of occupation levels with a thermal broadening of 0.001 Ha.
   - Print the density of states using the tetraedron method (prtdos 2).
2. To ensure you have the correct structure, run QAgate: qagate input. QAgate works just like the vi editor, you can type commands starting with ":" to get additional features. Try for example to type ": show id" then press Enter. Note that most of the basic functionalities (including the one you just typed) are available on the graphical user interface.
3. Run abinit in sequential: abinit < input.files. It should not take long.
4. Check several output parameters:
   - The convergence of the SCF cycle: grep ETOT output. Has everyting gone right?
   - The pressure in your system: grep Pressure output. How high is it?
   - Open your output file and check in the occupation section if you have enough empty bands.
   - You can easily plot the density of states with xmgrace: xmgrace output_DOS.
5. Now, modify your input file to allow for full geometry optimization. You just need five additional keywords: ionmov, ntime, optcell, ecutsm, and dilatmx. Put them in a separate section. Also, set the keyword prtfsurf to 1 in order to print the Fermi surface file at the end of each Broyden iteration.
6. Run abinit in sequential. It should take a bit longer. At the end of the calculation, check the files that have been created: you should have a bunch of files ending with .nc. That's netcdf files, which are useful for post-processing. You also have density files _DEN created at the end of each Broyden iteration, as well as a single wave function file _WFK that has been written at the end of the calculation (and at the end only, so if your job crashes before the end, you ain't got no wave function file!). One of the files is ending with _HIST.nc. It is the "history" file, which contains a lot of useful information about your calculation. Open it with QAgate: qagate output_HIST.nc.
7. Play a bit with QAgate:
   - Rotate the structure.
   - At the bottom of the main screen, you can read "Time step: 0/5". These are the Broyden iterations. If you press "Play", QAgate will quickly play all iterations. You can toggle the repeat mode to play them indefinitely and you can also decrease the playing speed.
   - Now, set QAgate in "Data" mode (top left corner. It is in "Plot" mode by default). It will plot any quantity you need to plot and will also create the corresponding data file.

- Plot the total energy with respect to the Broyden iterations. You should clearly see the convergence. QAgate has created a etotal.dat files with all the points.
- Plot the pressure with respect to the Broyden iterations. You should see it decrease up to 0 GPa. QAgate has created a pressure.dat files with all the points.
- Plot the cell parameters with respect to the Broyden iterations. You see that we somewhat underestimated the initial cell parameters. QAgate has created a file acell.dat with all the points. Open this file. What is the ground state cell parameter? We'll need it in the next part of this tutorial.
- Take a snapshot of your structure so that you can proudly display it at home.

8. Now, let's draw the Fermi surface. There should be files ending with _BXSF that have been created at the end of each Broyden iteration. These can be opened with XCrysDen. Open the last one using the following command: xcrysden --bxsf output_TIM6_BXSF. A window pops up and asks you to specify the Fermi energy. Just hit "OK" since abinit already provided it. You now have three windows:

   - One with data inside: it specifies the energy range of each band in your calculation. You can close this window.
   - One with a diagram that displays all bands of your calculation, their corresponding energy range, as well as the Fermi energy.
   - One with boxes to tick.

   From the second window, identify the bands that cross the Fermi energy. There should be only one, the band number 2. All other bands have their energy range outside the Fermi energy. Note that the band number 3 seems to cross the Fermi energy but that it not the case. It is just at the limit. Now, on the third window, tick the box corresponding to the band number 2 and hit "Selected". It opens a new windows that displays the Fermi surface of the band you have selected (band number 2 in our case). If you have additional bands that cross the Fermi level, just tick them and they will be shown in this new window.

   Play a bit with at the Fermi surface tool of xcrysden. You can for instance add the band number 3 in order to check that it indeed does not have a Fermi surface, that is, it does not cross the Fermi energy.

9. Now we going to analyze the charge density. For this, you need a charge density _DEN file, the cut3d utility, which is included in the abinit package, as well as the XCrysDen software:

   - Run cut3d by simply issuing the following command: cut3d. It will ask you which density file you want to analyze. Use the last density file: output_TIM6_DEN. Hit enter.
   - cut3d then shows a number of tasks it can perform. Here we want to create a density file for XCrysDen, so that's the choice number 9.
   - Choose a name for the XCrysDen file you will create. Let's call it Al_density.xsf.
   - cut3d asks if you want to shift the grid, answer no then type 0 to leave the program.
   - You now have a XCrysDen file that you can open with the following command: xcrsyden --xsf Al_density.xsf. At first it doesn't look any different than a regular crystal visualization. Don't be disappointed! Hit the following menus: Tools > Data Grid then "OK". There's a window that pops up with four tabs: "Isosurface", "Plane 1", "Plane 2", and "Plane 4". The isosurface tab is used to draw, well, isosurfaces... The three plane tabs are used to draw charge densities in three different planes, corresponding to the three directions of space.

     We'll leave the isosurfaces for now and we'll first look into the charge density planes. Untick the "Display Isosurface" option in the first tab and move to the second tab "Plane 1":

- Tick the box "display color-plane" and hit "Submit". The plane will appear in your main window. There's not much to see...
- Tick the box "display thermometer" and hit "Submit". You now have a scale, which makes easier quantitative analysis. You see that most of the plane is white, and there's a little bit of gray. Since there is no black area, it means that there are electrons everywhere in the plane. There's no space without electrons. It is consistent with the fact that Al is a free electron metal. Electrons are delocalized.
- At the bottom of the property window, there are several arrows that you can use to make the density plane move. Move it up to the slide number 12. The plane should be in the middle of the cell. You see that there are less electrons here but it is still gray, not black. As we said, there are electrons everywhere!
- If you are more into colors than just black and white, you can change the plane colors with the "Select color basis" menu. Try "Geographic" for instance.

That's it for the charge density! Play around with XCrysDen, it takes some practice :)

Band structure of fcc-Al

This part of the tutorial can be performed on your laptop with a single cpu.

1. We'll start from the input file template. Fill it correctly with the same parameters as in previous section, except that now we'll use the ground state cell parameters (you should have the file acell.dat from previous section that tells you the correct value).

2. Run abinit: abinit < input.files. Check the pressure in order to verify that you have the correct cell parameters: grep Pressure output. It should be around 10^{-2} or 10^{-3} GPa.

3. We will now modify the input file to create two datasets (ndtset 2). The first dataset is the ground state calculation we just made, the second dataset will compute the band structure as follows (it is adviced to check the meaning of these variables on the website):

   - Read the charge density from the previous ground state calculation: getden -1.
   - Perform a non self-consistent calculation: iscf -2. We need very accurate wave functions to calculate the band structure tolwfr 1e-20.
   - Calculate the band structure at 10 specific points in the Brillouin Zone, so that makes 9 divisons of the BZ: kptopt -9.
   - The band structure will be calculated along this path in the BZ: L-Γ-X-W-K-L-W-X-K-Γ. This can be achieved by setting the keyword kptbounds with the following values:

     1/2 0 0
     0 0 0
     0 1/2 1/2
     1/4 1/2 3/4
     3/8 3/8 3/4
     1/2 1/2 1/2
     1/4 1/2 3/4
     1/2 1/2 1
     3/8 3/8 3/4
     0 0 0

     These values correspond to the coordinates of the 10 points in the BZ.
   - Each segment is divided in 50 points where the band structure will be calculated: ndivk2 9*50.

4. Run abinit: abinit < input.files.

5. Check the output files. You should have output files for each dataset, which can be identified with the _DS1 or _DS2 extension. The band structure information is located in the output_DS2_EIG.nc file.

6. Open your input file with QAgate: qagate input. Let's now plot the band structure:

   - In the main window, type :plot band output_DS2_EIG.nc. You obtain a very simple band structure that can be slightly improved.
   - You can add the Fermi level on the diagram. First get the value of the Fermi energy from your abinit output file : grep Fermi output. Add this value to your band structure diagram by typing :plot band output_DS2_EIG.nc fermi 0.34529. Now the bands have been shifted so that the Fermi level is set to

the zero energy. You can see that the first band does not cross the Fermi energy, the second band does, the third band is at the limit and the fourth band does not. This is consistent with the Fermi surface we had in the previous section.

- You can also add the kpoint labels and segment divisions on the diagram :plot band output_DS2_EIG.nc fermi 0.34529 labels L:G:X:W:K:L:W:X:K:G ndiv 50:50:50:50:50:50:50:50:50. However, we are lazy and the command line is getting pretty long to type... Therefore we are going to create a configuration file in which we will write all the instructions we want QAgate to perform, and we will run QAgate with this configuration file.
  - Create a file config.qagate and edit it.
  - Write the first instruction: we want QAgate to open the input file, so it will be :o input.
  - On the second line, write the next instruction: we want the band structure, so it will be :plot band output_DS2_EIG.nc fermi 0.34529 labels L:G:X:W:K:L:W:X:K:G ndiv 50:50:50:50:50:50:50:50:50.
  - Run QAgate and tell it to read the configuration file: qagate -c config.qagate.
  - You now have a magnificient band structure.

Templates

- **Input file for Al ground state:**

```
# SCF Cycle Parameters
nstep
ecut
pawecutdg
tolvrs
nband

# Structural Parameters and Spin
natom
ntypat
typat
znucl

acell

rprim


xred

occopt
tsmear

# K-Point Grid
kptopt 1
ngkpt
nshiftk 1
shiftk 0 0 0

# Output files
prtdos
```

- **Files file for Al ground state:**

```
input
output
input
output
tmp
Al.LDA_PW-JTH.xml
```