INSTRUCTIONS EXERCISE 4

Note that the following color code has been used in this instruction sheet:
Broad headings are in red.
File names are in magenta.
Phrases to be typed into the command line are in blue.
Input parameters are in dark green.

In this exercise, you will use post-processing tools to calculate density of states (dos) and electronic band structure of Al.

- STEP 1:

    You will see the following files:
    exercise4_instructions.pdf this file!
    Al.scf.in this is a sample input file, for a primitive Al cell.
    Al.nscf.in this is a sample input file to perform non-self-consistent calculations.
    Al.dos.in this is a sample input file to perform density of states calculations.
    Al.bands.in this is an input file for collecting bands.
- k-point-path this is a file containing list of k-points along symmetry directions in Brillouin zone.
- Al.plotband.in this is an input file for putting band structure data into a plottable format.

- STEP 2: Open and read the sample file Al.scf.in

- Change the degauss and K_POINTS values to those at which the convergence is achieved in exercise 1

- STEP 3: Run an scf calculation:

- ~/pw.x < Al.sample.in > Al.sample.out

- STEP 4: Non-self-consistent calculations:

- Open Si.nscf.in file
- Note differences between scf to nscf -
- ---> 1. the flag calculation='nscf'
- ---> 2. occupations='tetrahedra' in the namelist &SYSTEM.
- ---> 3. K_POINTS card is hanged from "6 6 6 1 1 1" to "12 12 12 1 1 1", this is because we now want to compute eigenvalues on a finer mesh in k-space.
- Remember that the same wavefunctions (as obtained from scf calculations) have to be used, so the SAME prefix as scf calculations!!
- Run the nscf calculations:
    ~/pw.x < Al.nscf.in > Al.nscf.out

- STEP 5: DOS calculations:

- Open Al.dos.in

- Make sure that it has the same prefix as used in the scf calculations.
- Check the energy range of the eigen values obtained in the nscf output file Si.nscf.out. Emin and Emax gives this range.
- The DOS results are written in fildos = dos.dat

- Run density of states calculations:
  ~/dos.x < Al.dos.in > Al.dos.out
- Have a look at dos.out and the data file Al.dos.dat.
- Plot dos.dat to see the DOS plot (you can use gnuplot or xmgrace programs).

- STEP 6: Band structure calculations for Al

- Follow the same procedure as was used for Si example. (Input files for Al are given in this folder.)