INSTRUCTIONS FOR EXERCISE 6

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 perform simple relax calculation for a molecule.

- STEP 1:

  You will see the following files:
  exercise6_instructions.pdf this file!
  c2h2.scf.in this is a sample scf input file, for an acetylene molecule containing two C and two H atoms .
  c2h2.bfgs.in this is a sample input file for relax calculation .

- STEP 2: Open and read the sample file c2h2.scf.in

- Note that in the namelist &control, we have specified tprnfor = .true. to print the forces on each atom.
- K_POINTS is set as gamma. Is it sufficient?
- Open the structure in xcrysden. Acetylene is a linear molecule, but here we have a structure that is not in its ground state..

- STEP 3: Run an scf calculation:

- Run the scf calculation

  pw.x < c2h2.scf.in > c2h2.scf.out

- STEP 4: Read the output, and answer the following questions:

- Check the forces on each atom (at the end of the output file).
- What are the values of Total force and Total scf correction? (you can use grep)
- To visualize the forces, open c2h2.scf.out in xcrysden (xcrysden --pwo c2h2.scf.out)
- Do you think the forces are large?

- STEP 5: Now optimize the structure of the acetylene molecule

- Open c2h2.bfgs.in file. Notice that in the namelist &control, calculation = “relax” and forc_conv_thr = 1.0D-3 Ry/bohr have been specified for the structural optimization. The convergence criteria for the ionic minimization will be satisfied when all the of all forces are smaller than forc_conv_thr.

- Also a new namelist “ions” has been added.
- Note that in the card ATOMIC_POSITION, 3 more columns have been added for each atomic species. These columns can take values either 0 or 1. The values of these three columns denote the allowed relaxation of a atom along x, y and z direction, respectively. If one wants to fix the position of a atom along x direaction and allow it to relax along y and z directions, then the values can be specified by 0 1 1.

- STEP 6: Run the relax calculation:

- To get the optimized structure, run the following command,
  pw.x < c2h2.bfgs.in > c2h2.bfgs.out &

- STEP 7: Read the output, and answer the following questions:
- Now check the total energy changes. Do
  grep ! c2h2.bfgs.out | nl
- you can also check the value of the forces at each bfgs step. Do,
  grep "Total force" c2h2.bfgs.out | nl
- Are the forces smaller than the specified threshold values at convergence?
- Use XCrySDen to visualize the dynamics:
  xcrysden --pwo c2h2.bfgs.out
  (remember to select “reduce dimension to 0D” and “Display All Coordinates as Animation”; type “f” to visualize the forces)
  Do you see the forces to vanish at convergence?