MR308-Computational modeling of materials

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Hands-on session 8

In this hands-on session, we will be doing an exercise on metals. We have taken the example of aluminium (Al) in this hands-on. Here, we will perform the lattice optimization as well as convergence tests for Al.

The file `Al.scf.in` is slightly different from that used for insulators. This is because of the long-range interactions that exist in metals unlike in insulators. The file `Al.scf.in` is as follows:

```
 &control
    calculation='scf'
    restart_mode='from_scratch',
    prefix='Al',
    verbosity='low',
    pseudo_dir='./',
    outdir='./'
 /
 &system
    ibrav=2, celldm(1)=7.652445391, nat=1, ntyp=1,
    ecutwfc=30, occupations='smearing', smearing='gaussian',
    degauss=0.003
 /
 &electrons
    diagonalization = 'david'
    mixing_mode='plain'
    mixing_beta = 0.7
    conv_thr =  1.0d-7
 /

ATOMIC_SPECIES
 Al   26.9815385   Al.UPF

ATOMIC_POSITIONS
Al  0.00 0.00 0.00

K_POINTS  {automatic}
13 13 13 0 0 0
```

1. Lattice optimization:
First, we will perform lattice optimization. The script for the lattice optimization is in the `handson-8/latt_opt` directory.
Now run this script. On a successful run, a file called `en_conv` will be generated.
***Plot the energy with respect to lattice parameters by using `xmgrace` or `gnuplot` and send to us by e-mail.**

2. Convergence tests:

Now, we will perform convergence tests. The script for convergence is in the `handson-8/conv` directory. Look at the script carefully. The convergence test is with respect to variations in the **k**-mesh and the energy cut-off values.

****Plot the convergence of both energy cut-off and kpoints by using `xmgrace` or `gnuplot` and send to us by e-mail.**