A tutorial on practical density functional calculations using plane wave basis set

Fadjar Fathurrahman

Part I. Basic Theory

1 Introduction

This is a tutorial explaining basic density functional theory calculations for (mainly) condensed matter systems using plane wave basis set.

Example equations:

$$\int_0^\infty \frac{\alpha}{\beta} \mathrm{d}\Gamma$$

2 Atomic structure specification

We need to specify unit cell and basis (atomic positions within the unit cell)

cif file

xyz file

cif2cell

GUI tools: avogadro

ASE

assumption: the softwares are already installed in your systems.

Part II. Silicon crystal: total energy and electronic structure

A tutorial about input file

3 Using Quantum ESPRESSO

Using ONCV PBE pspot

```
$ grep ! LOG1
!    total energy              =     -15.71919101 Ry
```

or -7.859595505 Ha

Using GTH pspot and VWN xc

```
$ grep ! LOG1
!    total energy              =     -15.82201747 Ry
```

or -7.911008735 Ha

4 Using ABINIT

Using ONCV PBE pspot

```
$ grep Etotal LOG1
    >>>>>>>>> Etotal= -8.43967410558013E+00
```

Using GTH vwn pspot

```
$ grep Etotal LOG1
    >>>>>>>>> Etotal= -7.91100879337138E+00
```

5 Using JDFTX

```
jdftx -c 1 < INPUT
```

```
$ grep "Etot =" LOG1
     Etot =       -7.8595945951064721
```

6 PW codes how to

6.1 Specifying unit cell

6.1.1 PWSCF

```
&SYSTEM
  ibrav = 0
/

CELL_PARAMETERS bohr
  -5.1315500000   0.0000000000   5.1315500000
   0.0000000000   5.1315500000   5.1315500000
  -5.1315500000   5.1315500000   0.0000000000
```

6.1.2 ABINIT

```
acell 1.0 1.0 1.0
rprim
  -5.1315500000   0.0000000000   5.1315500000
   0.0000000000   5.1315500000   5.1315500000
  -5.1315500000   5.1315500000   0.0000000000
```

6.1.3 JDFTX

Example:

```
lattice \
  3.61496   3.61496   0.00000 \
  3.61496   0.00000   3.61496 \
  0.00000   3.61496   3.61496
```

The lattice matrix is arranged by column.

6.2 Specifying metallic occupation

6.2.1 PWSCF

6.2.2 ABINIT

6.2.3 JDFTX

- `elec-smearing Fermi 0.001`
- `elec-smearing Cold 0.001`