One-Day Workshop on Date: 18/02/2026

Descriptor and Machine Learning for Materials

Module 1:

Structure Optimization and Density of states calculation using Quantum Espresso (QE)

Tutor: ***Dr. Rohit Milind Babar,*** *(Email:* ***rohit.b@srmap.edu.in****)*

- **What we will learn in today's hands-on:**

  Exercise 1: Unit cell relaxation calculation for graphene.

  Exercise 2: Density of states (DOS) calculation for graphene.

  Exercise 3: Projected density of states (PDOS) calculation for graphene.

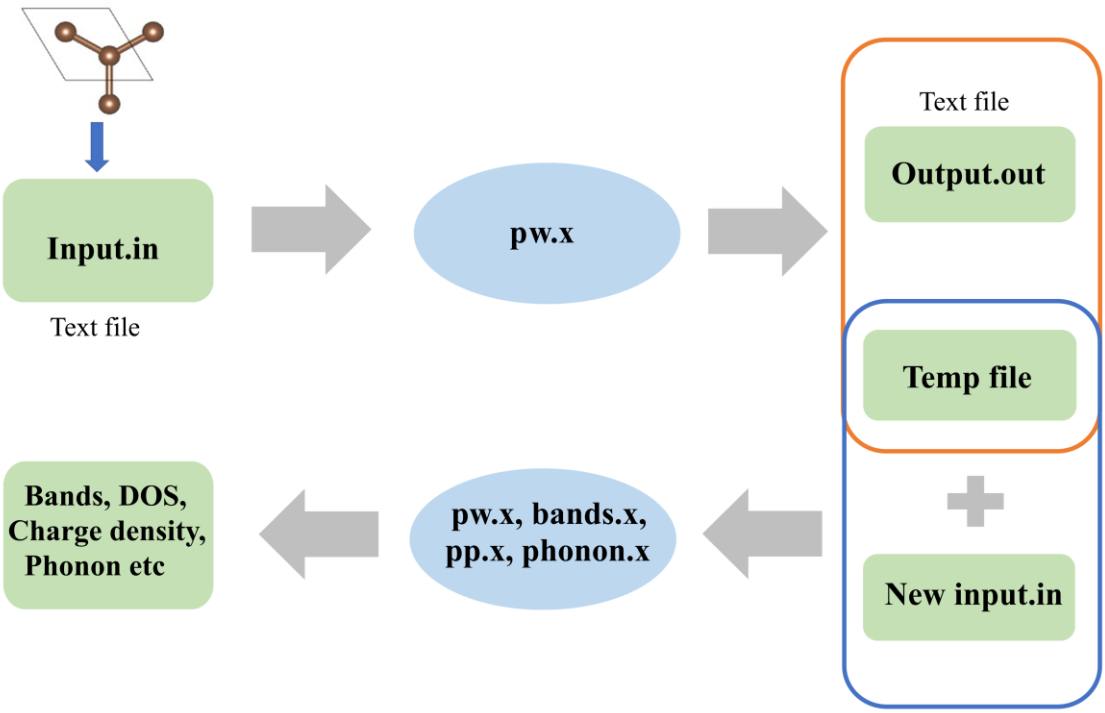
- **Requirement to run any QE calculation:**

  i) QE software package.

  ii) Relevant environment for QE calculation like HPC Cluster.

  iii) Model Structure (Geometric information like lattice vector, lattice type, atom positions & atom type).

- **Schematics steps for QE run:**



- **Structure of QE input file:**

&NAMELIST_1

Flag1 =.....,
Flag2 =……..,
.
FlagX =……,
/

&NAMELIST_2

Flag1 =.....,
Flag2 =……..,
.
FlagX =……,
/

Input_Card1
Input_Card2

For more details follow QE websites: https://www.quantumespresso.org/Doc/INPUT_PW.html

- **QE input file:**

&CONTROL (Here we define general variables that control the run)

calculation = "scf" (scf, nscf, realx, vc-relax, bands, dos, MD etc.).

pseudo_dir = "/home/samim/pseudo" (Location of pseudo potential file).

outdir = "/samim/temp" (Location where temporary output files i.e charge file wave files).

prefix = "graphene" (Name of the temporary files).

/

&SYSTEM (Here we provide the input variables of the system)

ibrav = i (i = 0-14, -12 & -13)

0 = Free cell, 1 = simple cubic, 2 = FCC cubic, 3 = BCC cubic, 4 = Hexagonal …

a = x
b = y
c = z

cosAB = cosine of the angle between axis a and b (gamma).

cosAC = cosine of the angle between axis a and c (beta).

cosBC = cosine of the angle between axis b and c (alpha).

nat = n (Total numbers of atoms in system).

ntyp =m (Total number of types of atoms).

occupations = “smearing”.

smearing = “gaussian”

degauss= 0.02 (Smearing width in Ry unit).

ecutwfc=40 (kinetic energy cutoff (Ry) for plane wave).

ecutrho=400 (Kinetic energy cutoff (Ry) for charge density and potential).

/

&ELECTRONS (Here we provide the details of electronic calculations.)
conv_thr =1.0D-06 (Convergence threshold for self-consistency (desire accuracy).
electron_maxstep= 200 (maximum number of iterations for scf calculation.)
mixing_beta = 0.7 (mixing factor for self-consistency)
/
K_POINTS {automatic} (The Monkhosrt-Pack K- grid{automatic})
8 8 1 0 0 0

ATOMIC_SPECIES
C 12.01070 C.pbe-rrkjus.UPF
(atom mass pseudopotential)

ATOMIC_POSITIONS {angstrom}
C 0.000000 0.000000 3.950788
C -0.000012 1.424503 3.950788

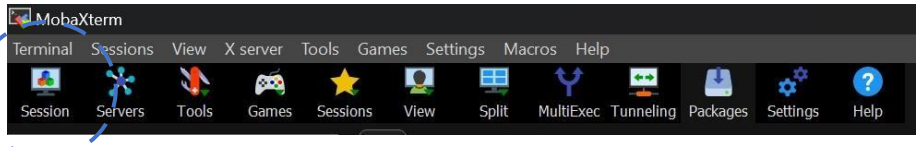
C.pbe-rrkjus.UPF
C : Atom name
Pbe : Type of exchange correlation function.
rrkj**us** : Type of pseudopotential. Here **us** means ultrasoft pseudopotential.
UPF : File formate

This is a QE preliminary QE input file.

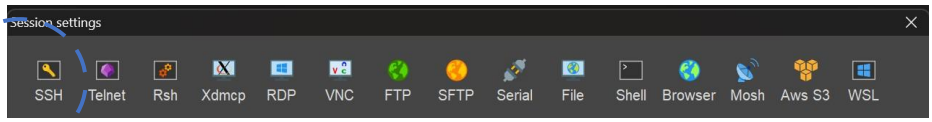
➢ How to access the server:

i) Open **mobaxterm** application.

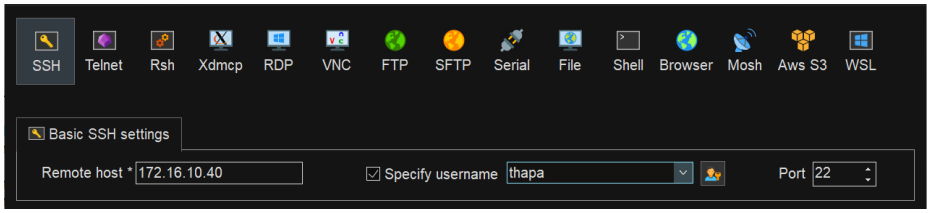
ii) Go to the session section.



iii) Click on SSH section.



iv) In the remote host give server address "**172.16.10.40**" ; Username "**thapa**" and port **22.**



v) Enter password :- workshop123

vi) Go to node02 for running calculation. Command: **ssh node05**. PW: workshop123

vii) Go to the folder "workshop_ANRF". Command: cd workshop_ANRF.

viii) Make a folder with your name in server. Command: mkdir your_name.
Ex:- mkdir samim.

ix) Enter to your folder. Command: cd your_folder_name.

x) Copy the relax and dos folder to your folder. Command: cp –r relax dos your_folder.

xi) Go to your folder. Command: cd your_folder. Where you can two folders **"relax" & "dos"**.

	Calculation type	Folder name
Exercise 1	Structure Optimisation	relax
Exercise 2	DOS	dos
Exercise 3	PDOS	dos

Note: To go to a directory command: **cd directory_name**

To go out from the from a directory command: **cd ..**

To view an input file command: **vi input_file_name**

To go out from an input file command: **esc(button) :q**

To edit input file command: **" I (button)" then edit**

After editing to save the input file command: **esc(button):wq**

To run QE calculations command: **mpirun –np 2 pw.x -i input.in | tee output.out**

➢ **Exercise 1: Relaxation calculation for Graphene unit cell.**

i) For optimised calculation go to relax directory. Command: **cd relax**

ii) Here we have provided the sample input file for a primitive graphene cell using experimental lattice constant. To view input file Command **vi relax.in**

Input file:

```
&CONTROL
    calculation = "relax"
    outdir = './',
    pseudo_dir = '/home/samim/quantum_base/upf_files',
    prefix = 'graphene' ,
    etot_conv_thr = 1.0D-5
    forc_conv_thr = 1.0D-4
/

&SYSTEM
    a           = 2.463
    c           = 20
    degauss     = 0.01
    ecutrho     = 400
    ecutwfc     = 40
    ibrav       = 4
    nspin       = 2
    nat         = 2
    ntyp        = 1
    occupations = "smearing"
    smearing    = "mv"
    starting_magnetization(1) =  0.0
/

&ELECTRONS
    conv_thr         = 1.0D-07
    electron_maxstep = 100
    mixing_beta      = 0.7
/

&IONS
ion_dynamics = "bfgs"
/

K_POINTS {automatic}
12  12  1  0 0 0

ATOMIC_SPECIES
C      12.01070  C.pbe-n-rrkjus_psl.0.1.UPF

ATOMIC_POSITIONS {angstrom}
C               1.2334917809        0.7145164034        9.7637700000
C               0.0020482191        1.4254935966        9.7637700000
```

Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm is an iterative method for solving unconstrained nonlinear optimization problems.

iii) To go out from the input file. Command: **esc(button):q**

iv) Run the calculation with this command: **mpirun -np 2 pw.x -i relax.in | tee relax.out**

Output file:

```
   -16.1744 -14.3157 -12.0431  -3.6997  -1.0411   8.5366   8.9592   9.8779

         k =-0.3333 0.4811 0.0000 (  3001 PWs)   bands (ev):

   -16.1746 -14.3150 -12.0437  -3.7001  -1.0405   8.5361   8.9591   9.8763

     the Fermi energy is    -2.3224 ev

!    total energy              =     -23.90891377 Ry
     estimated scf accuracy    <       0.00000003 Ry
     smearing contrib. (-TS)   =      -0.00009116 Ry
     internal energy E=F+TS    =     -23.90882261 Ry

     The total energy is F=E-TS. E is the sum of the following terms:
     one-electron contribution =    -224.64975224 Ry
     hartree contribution      =     113.60282081 Ry
     xc contribution           =      -8.30502890 Ry
     ewald contribution        =      95.44313771 Ry

     total magnetization       =     0.00 Bohr mag/cell
     absolute magnetization    =     0.00 Bohr mag/cell

     convergence has been achieved in   1 iterations

     negative rho (up, down):  1.408E-05 1.408E-05

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =    -0.00007184    0.00004147    0.00000000
     atom    2 type  1   force =     0.00007184   -0.00004147    0.00000000

     Total force =     0.000117     Total SCF correction =     0.000650
     SCF correction compared to forces is large: reduce conv_thr to get better values
     Energy error              =      1.0E-06 Ry
     Gradient error            =      7.2E-05 Ry/Bohr

     bfgs converged in   2 scf cycles and   1 bfgs steps
     (criteria: energy <  1.0E-05 Ry, force <  1.0E-04 Ry/Bohr)

     End of BFGS Geometry Optimization

     Final energy              =     -23.9089137698 Ry

     File ./graphene.bfgs deleted, as requested
Begin final coordinates

ATOMIC_POSITIONS (angstrom)
C               1.2335485661        0.7144836184        9.7637700000
C               0.0019914339        1.4255263816        9.7637700000
End final coordinates
```

- ❑ Going down you can find this section where final coordinates from your DFT calculation. Use these atomic positions for further calculation.
- ❑ For visualization of the optimised structure, you can use **Avogadro or XCrysden**.

➢ Exercise 2: Density of state calculations:

For total DOS calculation first go into dos folder. Command cd ../dos

For DOS calculation we need to perform

i) 1st SCF calculation.

ii) 2nd NSCF calculation.

iii) 3rd DOS calculation.

Open the "scf.in" file using vi editor and make the following changes:

a) Set calculation='scf'

b) Replace the atomic positions with the optimized positions obtained from the relax calculation.

c) To save the input file command esc(button):wq

Open the "nscf.in" file using vi editor and make the following changes:

a) Set calculation='nscf'

b) In &SYSTEM part set occupations='tetrahedra'

c) Remove the flag degauss & smearing

d) Increase the k-grid to 24×24×1. Note we are using a much denser k-grid.

e) Replace the atomic positions with the optimized positions obtained from the relax calculation.

To save the input file command esc(button):wq

Running SCF and NSCF calculations:

To run the SCF calculation command: **mpirun -np 2 pw.x -i scf.in |tee scf.out**

To run NSCF calculation command: **mpirun –np 2 pw.x –i nscf.in |tee nscf.out**

scf.in file

```
&CONTROL
    calculation = "scf"
    outdir = './',
    pseudo_dir = '/home/samim/quantum_base/upf_files',
    prefix = 'graphene' ,
/

&SYSTEM
    a           = 2.463
    c           = 20
    degauss     = 0.01
    ecutrho     = 400
    ecutwfc     = 40
    ibrav       = 4
    nat         = 2
    ntyp        = 1
    nspin       = 2
    occupations = "smearing"
    smearing    = "mv"
    starting_magnetization(1) = 0.0
/

&ELECTRONS
    conv_thr         = 1.D-07
    electron_maxstep = 200
    mixing_beta      = 0.7
/


K_POINTS {automatic}
12  12  1  0 0 0

ATOMIC_SPECIES
C      12.01070  C.pbe-n-rrkjus_psl.0.1.UPF

ATOMIC_POSITIONS {angstrom}
C               1.2335485661        0.7144836184        9.7637700000
C               0.0019914339        1.4255263816        9.7637700000
```

nscf.in file

```
&CONTROL
    calculation = "nscf"
    outdir = './',
    pseudo_dir = '/home/samim/quantum_base/upf_files',
    prefix = 'graphene' ,
/

&SYSTEM
    a           = 2.463
    c           = 20
    ecutrho     = 400
    ecutwfc     = 40
    ibrav       = 4
    nat         = 2
    ntyp        = 1
    nspin       = 2
    occupations = "tetrahedra"
    starting_magnetization(1) = 0.0
/

&ELECTRONS
    conv_thr         = 1.D-07
    electron_maxstep = 200
    mixing_beta      = 0.7
/


K_POINTS {automatic}
24  24  1  0 0 0

ATOMIC_SPECIES
C      12.01070  C.pbe-n-rrkjus_psl.0.1.UPF

ATOMIC_POSITIONS {angstrom}
C               1.2335485661        0.7144836184        9.7637700000
C               0.0019914339        1.4255263816        9.7637700000
```

DOS calculation:

dos.in input file is given already in this directory.

Dos input file:

```
&DOS
 outdir= "./"
 prefix = 'graphene'
 fildos='graphene.dos'
/
```

Prefix and outdir must be same as SCF & NSCF calculations.

→ DOS data file.

Run the calculation with this command: **mpirun -np 4 dos.x -i dos.in |tee dos.out**

➢ Exercise 3: PDOS Calculation

PDOS calculation is same as dos calculations.

For DOS calculation we need to perform

i) 1st SCF calculation.

ii) 2nd NSCF calculation.

iii) 3rd PDOS calculation.

As we have already performed SCF & NSCF calculations.

Now we just need to perform PDOS calculation.

pdos.in input file is given already in this directory.

PDOS input file:

```
&PROJWFC
prefix  = "graphene",
outdir  = "./",
filproj = 'pdos.dat',
/
```

Prefix and outdir must be same as SCF & NSCF calculations.

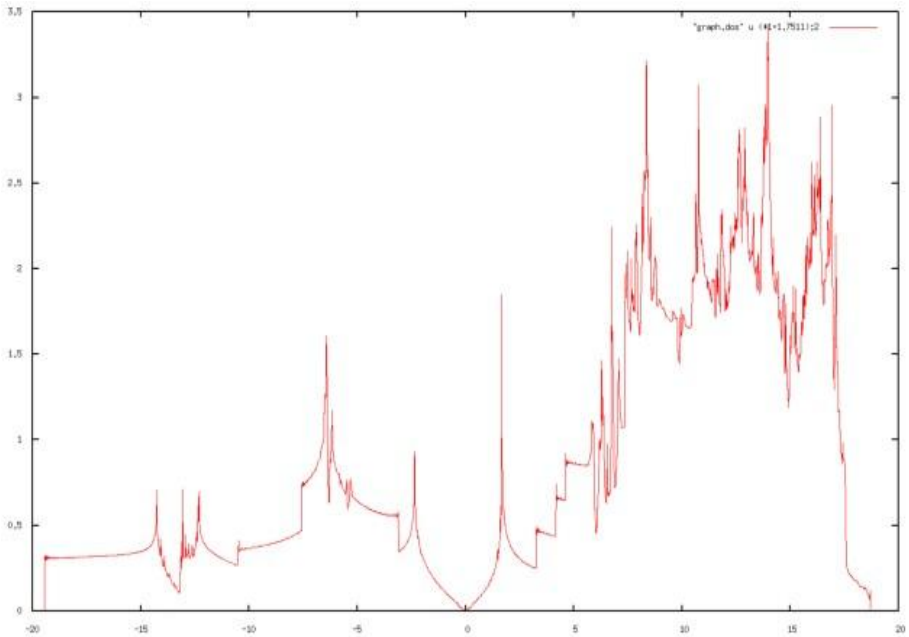
→ PDOS data file.

➢ For plotting DOS

Use any plotting software such as gnuplot (origin, qtiplot, matlab etc.)
We use here gnuplot. First note the Fermi energy value which is required for DOS plotting. You can find this value in scf output file. Check with this command vi scf.out and note down the Fermi energy value. For plotting in gnuplot you need to come to masternode**. Command exit**. Then again go to your working directory. Command cd your_name/hands_on_1/dos

Now plot DOS with these Commands:

i) gnuplot
ii) plot “graphene.dos” u ($1-fermi energy value):2 w l
iii) To come out from gnuplot command is exit



Part- 2

Follow the link below

https://github.com/CoderOnTheRoad/Descriptor_to_ML_workshop

Download as Zip

Follow the Instructor's Instruction