Computational Physics Course

Learn to use software packages

Here we follow the tutorial made by Dr. Koretsune (RIKEN)

```
&control
 calculation = 'scf'
 prefix='graphene',
 tstress = .true.
 tprnfor = .true.
 pseudo_dir = './',
 outdir='./work/'
 disk_io='low'
 wf_collect=.true.
/
&system
 ibrav = 4,
 celldm(1) = 4.602,
 celldm(3) = 4,
 nat = 2,
 ntyp = 1,
 ecutwfc = 30.0,
 ecutrho = 150.0,
 occupations = 'smearing'
 smearing = 'm-p'
 degauss = 0.01
/
&electrons
 mixing_beta = 0.7
 conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C  12.0107  C.pz-van_ak.UPF
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00 0.57735026918962576451 0.00
K_POINTS {automatic}
12 12 1 0 0 0
```

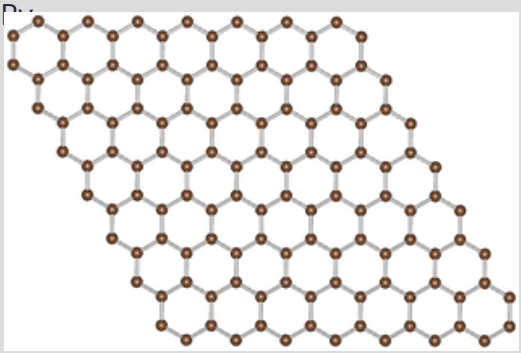
Prepare the input file

This is an input file for graphene.
Note that the Bravais lattice type is 4 (hexagonal) and
a1 = a(1,0,0), a2 = a(-1/2,sqrt(3)/2,0), a3 = a(0,0,c/a).

Here we have two cut-off energies; one for the wave function (namely the KS orbital) and the other for the electron density n(r). We need both when using the ultrasoft PP. We will use C.pz-van_ak.UPF, which can be downloaded from the site http://www.quantum-espresso.org/pseudo-search-results/?el_id=6&unp_id&fun_id&colum_k&origin_id or just by clicking the text.

Run the program (SCF)

After saving the input file as graphene.scf.in, run the program by typing
pw.x < graphene.scf.in > graphene.scf.out
You will find a line "convergence has been achieved" in the output file.
You will also find that the total energy is
! total energy = -22.84944326 Ry



```
&control
 calculation = 'bands'
 prefix='graphene',
 tstress = .true.
```

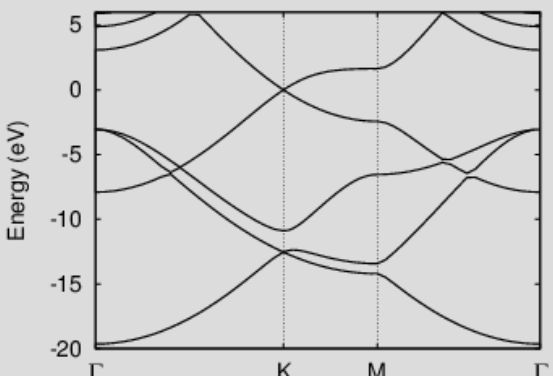
Run the program (band)

Having obtained the self-consistently determined density n(r), we then calculate the band dispersion by slightly changing the parameters. Here we specify the number of bands as 16, four for the occupied states and others for unoccupied states.

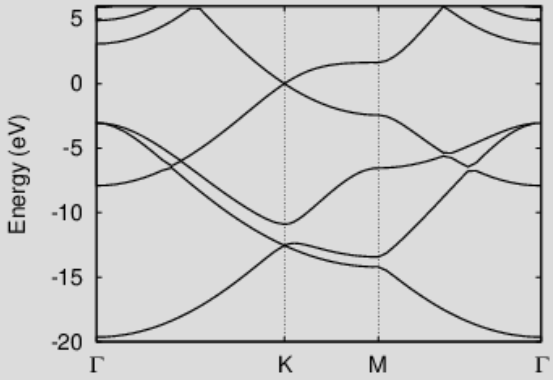
The KS energies are obtained along the line in the BZ connecting

```
 outdir='./work/'
 disk_io='low'
 wf_collect=.true.
/
&system
 ibrav = 4,
 celldm(1) = 4.602,
 celldm(3) = 4,
 nat = 2,
 ntyp = 1,
 ecutwfc = 30.0,
 ecutrho = 150.0,
 occupations = 'smearing'
 smearing = 'm-p'
 degauss = 0.01
nbnd = 16
/
&electrons
 mixing_beta = 0.7
 conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C  12.0107  C.pz-van_ak.UPF
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00 0.57735026918962576451 0.00
K_POINTS {tpiba_b}
4
0.00000000     0.00000000
0.00000000   20
0.66666667     0.00000000
0.00000000   20
0.50000000     0.28867500
0.00000000   20
0.00000000     0.00000000
0.00000000   20
```

```
&bands
  outdir = './work/',
  prefix='graphene',
  filband='graphene.band',
  lsym=.true.
/
```



Save this input file as graphene.nscf.in, run the program by pw.x < graphene.nscf.in > graphene.nscf.out



We need further efforts. Save the input file (left) as graphene.band.in.

Then run another program as
bands.x < graphene.band.in > graphene.band.out
The calculated results can be seen by using the following commands shown with brown, which are to be saved as band.plt

gnuplot band.plt

You will get the plot like this.

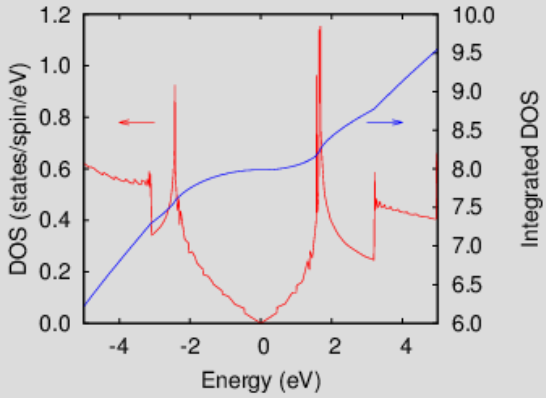
```
#!/usr/local/bin/gnuplot -persist
# Last modified: 2014/01/03 02:33
set terminal postscript eps enhanced 28
lw 2
set output "band.eps"
set ylabel 'Energy (eV)'

set xtics ("{/Symbol G}" 0, "K" 0.666666,
"M" 1, "{/Symbol G}" 1.5773)
set ytics 5

ymin=-20
ymax=6
set xrange [0:1.5773]
set yrange [ymin:ymax]
unset key

set arrow 1 nohead from 0.66666,ymin
to 0.66666,ymax lt 2
set arrow 2 nohead from 1,ymin to
1,ymax lt 2

plot graphene.band.gnu' using 1:2 w l
```

```
&control
 calculation = 'nscf'
 prefix='graphene',
 tstress = .true.
 tprnfor = .true.
 pseudo_dir = './',
 outdir='./work/'
 disk_io='low'
 wf_collect=.true.
/
&system
 ibrav = 4,
 celldm(1) = 4.602,
 celldm(3) = 4,
 nat = 2,
 ntyp = 1,
 ecutwfc = 30.0,
 ecutrho = 150.0,
 occupations = 'tetrahedra'
/
&electrons
 mixing_beta = 0.7
 conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C  12.0107  C.pz-van_ak.UPF
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00
0.57735026918962576451 0.00
K_POINTS {automatic}
36 36 1 0 0 0
```

The next task is to calculate the KS eigenvalues using a finer mesh and the result is used to draw the density of states.

Save the input file as graphene.nscf.in and run the program

pw.x < graphene.nscf.in > graphene.nscf.out



Then, run the program using graphene.dos.in (left) as

dos.x < graphene.dos.in > graphene.dos.out

Try to make a plt file yourself, following the plt fie for band

```
&dos
  outdir = './work/',
  prefix='graphene',
  fildos='graphene.dos',
/
```

```
&inputpp
```

Run the program (charge density)

Now let us draw the spatial distribution of the density using

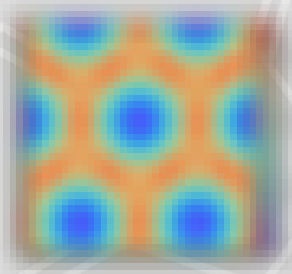
```
 plot_num=0
/
&plot
 iflag=2
 output_format=7
 fileout='charge.xsf'
 x0 = 0.0, 0.0, 0.0
 e1 = 2.0, 0.0, 0.0
 e2 = 0.0, 2.0, 0.0
 nx = 100
 ny = 100
/
```

pp.x < graphene.pp.in > graphene.pp.out

Here plot_num=0 corresponds to plotting the density. Here the density is calculated taking x0 as the origin. e1 and e2 specify the plane on which the density is calculated with the mesh points nx and ny. output_format=7 corresponds to generating output data for gnuplot.

Using the file charge.plt we can get the plot using gnuplot.

(When taking iflag=3 and output_format=5, we can get the output data for xcrysden.)



To use advanced routines, let us use more recent version of Quantum Espresso

1. cd ~
2. sudo apt-get install build-essential fftw3-dev gfortran — You can skip this if you have done once.
3. download quantum espresso from the site
4. tar -xzvf qe-6.0.tar.gz
5. cd qe-6.0
6. ./configure --enable-parallel=no --enable-openmp=yes — This will take long time
7. make all
8. cd ~
9. add the line “export PATH=$PATH:/home/username/qe-6.0/bin/” at the end of the file “.bashrc”.
10. source ~/.bashrc

For some reason, this newer version requires full path to start. That is, please type ./bin/pw.x instead of simply type pw.x when you are in the directory qe-6.0. Otherwise, older version will start.

Install wannier90 by following procedur — Let us learn the maximally localized Wannier orbitals

download wannier90 from http://www.wannier.org/

1. tar zxvf wannier90-2.0.1.tar.gz
2. cd wannier90-2.0.1
3. cp config/make.sys.gfort make.sys
4. make

Let us calculate the maximally localized Wannier orbitals and construct a tight-binding Hamiltonian.

As a preparation, we obtain the self-consistent density and then the bands using, respectively,
graphene.scf.in
graphene.nscf.in

Please copy&past the text shown below to make these input files

This can be done by typing
~/qe-6.0/bin/pw.x < graphene.scf.in > graphene.scf.in
~/qe-6.0/bin/pw.x < graphene.nscf.in > graphene.nscf.in

Then we convert the result to adapt to wannier90. Note that wannier90 is a package independent from quantum espresso; wannier90 is a build-in software that can be adapted to several different packages.

Please copy&past the text shown below to make this input

Use graphene.win for this purpose. This input file contains information on the following:

Number of bands and Wannier orbitals:
It should be reminded that num_bands should be equal to the number of bands used in the scf calculation.
- num_bands = 16
- num_wann = 5

Outer window, Inner window:
- dis_win_min = -30
- dis_win_max = 12
- dis_froz_min = -30
- dis_froz_max = 2.6

Inner window (dis_froz_min and dis_froz_max) indicates a range in the energy within which the original bands are reproduced accurately.
Outer window (dis_win_min, dis_win_max) is a range in the energy wherein the original bands to be reproduced are contained. Here we set inner bands as -30 eV to 2.6 eV to reproduce the sigma and pi bands near and below the Fermi level.
This setting of the window is technical in the sense that we need to exclude those bands above 2.6 eV because they have a different orbital character difficult to localize. Outer window, on the other hand, includes all the bands below 12 eV.

projection
- begin projections
- C: pz
- f= 0.167, 0.333, 0.00: s
- f=-0.333,-0.167, 0.00: s
- f= 0.167,-0.167, 0.00: s
- end projections

The bands are to be projected to pz orbital of carbon, which is represented initially by s-type orbitals located at the three positions indicated here.

specification of outputs
- hr_plot = .true.
- bands_plot = .true.
- wannier_plot = .true.

By this, plotted are the Wannier Hamiltonian, Wannier bands, and Wannier wave function. To plot the Wannier wave function, we need to set write_unk = .true. in doing the wannier90.x

Miscellaneous

The input also requires parameters used for the SCF calculation.

To make input files, we first prepare nnkp files (graphene.nnkp) using wannier90.x and graphene.win

Please copy&past the text shown below to make this file

```
~/wannier90-2.0.1/wannier90.x -pp graphene
```

Then we use pw.x and graphene.pw2wan.in to convert the result of the nscf calculation to adapt to wannier90.

```
~/qe-6.0/bin/pw2wannier90.x < graphene.pw2wan.in > graphene.pw2wan.out
```

Final task is to make the most localized Wannier wave function by

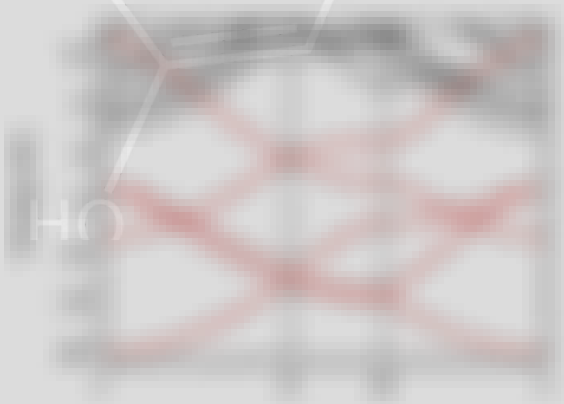
```
~/wannier90-2.0.1/wannier90.x graphene
```

We finally obtained “graphene_band.{gnu,dat,kpt}”, “graphene_hr.dat”, and “graphene_00001.xsf” – “graphene_00005.xsf”, which are, respectively, the Wannier band, Wannier Hamiltonian, and Wannier wave functions.

We can visualize the wave function by gnuplot

```
gnuplot
> load 'graphene_band.gnu'
```

The result (red) can be compared with the original band (black).

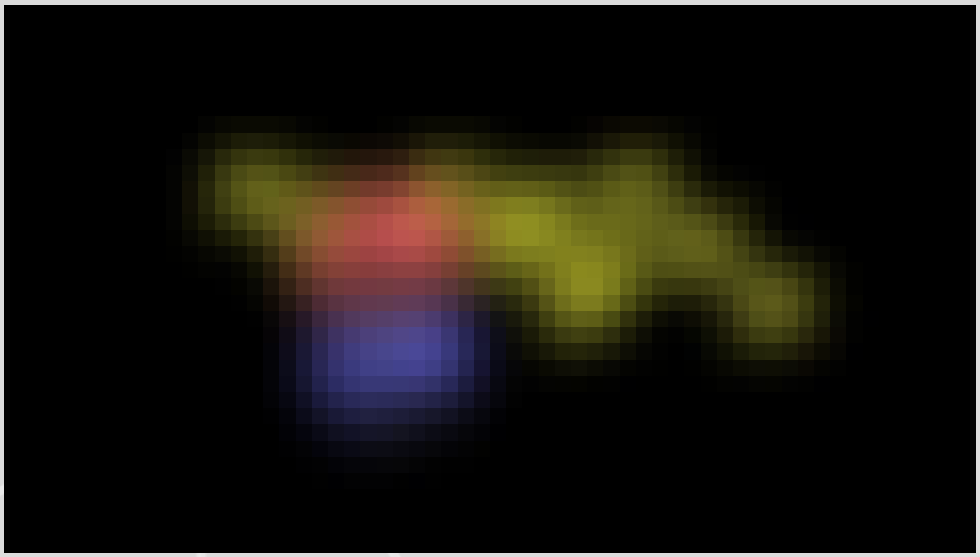


graphene_hr.dat indicates, for example, the neighboring transfer integrals as t = -3.00 eV, t’=0.23 eV

```
   0   0   0   5   1    0.000000   -0.000000
   0   0   0   1   2   -3.001042    0.000000
   0   0   0   2   2   -0.154412   -0.000000
   0   0   0   3   2   -0.000000    0.000000
   0   0   0   4   2   -0.000000   -0.000000
...
   0   0   0   5   5  -11.355711   -0.000000
   0   1   0   1   1    0.231742   -0.000000
   0   1   0   2   1   -3.001042   -0.000000
```

...

Wannier wave function can be shown with XCrysden. graphen_00001.xsf is like



graphene.scf.in

```
&control
 calculation = 'scf'
 prefix='graphene',
 tstress = .true.
 tprnfor = .true.
 pseudo_dir = './',
 outdir='./work/'
 disk_io='low'
 wf_collect=.true.
/
&system
 ibrav = 4,
 celldm(1) = 4.602,
 celldm(3) = 4,
 nat = 2,
 ntyp = 1,
 ecutwfc = 30.0,
 ecutrho = 150.0,
 occupations = 'smearing'
 smearing = 'm-p'
 degauss = 0.01
/
&electrons
 mixing_beta = 0.7
 conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C  12.0107  C.pz-van_ak.UPF
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00 0.57735026918962576451
0.00
K_POINTS {automatic}
```

graphene.nscf.in

```
&control
 calculation = 'nscf'
 prefix='graphene',
 tstress = .true.
 tprnfor = .true.
 pseudo_dir = './',
 outdir='./work/'
 disk_io='low'
 wf_collect=.true.
/
&system
 ibrav = 4,
 celldm(1) = 4.602,
 celldm(3) = 4,
 nat = 2,
 ntyp = 1,
 ecutwfc = 30.0,
 ecutrho = 150.0,
 occupations = 'smearing'
 smearing = 'm-p'
 degauss = 0.01
 nbnd = 16
/
&electrons
 mixing_beta = 0.7
 conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C  12.0107  C.pz-van_ak.UPF
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00 0.57735026918962576451 0.00
K_POINTS {crystal}
```

graphene.win

num_bands = 16
num_wann = 5

dis_win_min = -30
dis_win_max = 12
dis_froz_min = -30
dis_froz_max = 2.6

begin projections
C: pz
f= 0.167, 0.333, 0.00: s
f=-0.333,-0.167, 0.00: s
f= 0.167,-0.167, 0.00: s
end projections

hr_plot = .true.
bands_plot = .true.
wannier_plot = .true.

wannier_plot_supercell = 3

!exclude_bands=

begin kpoint_path
G 0.00000 0.00000 0.00000 K 0.33333 0.33333 0.00000
K 0.33333 0.33333 0.00000 M 0.50000 0.00000 0.00000
M 0.50000 0.00000 0.00000 G 0.00000 0.00000 0.00000
end kpoint_path

begin unit_cell_cart
bohr
4.602 0.0000000000 0.0000000000
-2.301 3.9854489082159866 5238 0.0000000000
0.0000000000 0.0000000000 18.408
end unit_cell_cart

begin atoms_frac
C 0.0000000 0.0000000 0.00
C 0.3333333 0.6666667 0.00
end atoms_frac

mp_grid = 12 12 1

begin kpoints
0.00000000 0.00000000 0.00000000 0.00694444
0.00000000 0.08333333 0.00000000 0.00694444
0.00000000 0.16666667 0.00000000 0.00694444
0.00000000 0.25000000 0.00000000 0.00694444
0.00000000 0.33333333 0.00000000 0.00694444
0.00000000 0.41666667 0.00000000 0.00694444
0.00000000 0.50000000 0.00000000 0.00694444
0.00000000 0.58333333 0.00000000 0.00694444
0.00000000 0.66666667 0.00000000 0.00694444
0.00000000 0.75000000 0.00000000 0.00694444
0.00000000 0.83333333 0.00000000 0.00694444
0.00000000 0.91666667 0.00000000 0.00694444
0.08333333 0.00000000 0.00000000 0.00694444
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0.08333333 0.16666667 0.00000000 0.00694444
0.08333333 0.25000000 0.00000000 0.00694444
0.08333333 0.33333333 0.00000000 0.00694444
0.08333333 0.41666667 0.00000000 0.00694444
0.08333333 0.50000000 0.00000000 0.00694444
0.08333333 0.58333333 0.00000000 0.00694444
0.08333333 0.66666667 0.00000000 0.00694444
0.08333333 0.75000000 0.00000000 0.00694444
0.08333333 0.83333333 0.00000000 0.00694444
0.08333333 0.91666667 0.00000000 0.00694444
0.16666667 0.00000000 0.00000000 0.00694444
0.16666667 0.08333333 0.00000000 0.00694444
0.16666667 0.16666667 0.00000000 0.00694444
0.16666667 0.25000000 0.00000000 0.00694444

0.00000000 0.41666667 0.00000000 0.00694444
0.00000000 0.50000000 0.00000000 0.00694444
0.00000000 0.58333333 0.00000000 0.00694444

0.00000000 0.66666667 0.00000000 0.00694444
0.00000000 0.75000000 0.00000000 0.00694444
0.00000000 0.83333333 0.00000000 0.00694444
0.00000000 0.91666667 0.00000000 0.00694444
0.08333333 0.00000000 0.00000000 0.00694444
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0.08333333 0.25000000 0.00000000 0.00694444
0.08333333 0.33333333 0.00000000 0.00694444
0.08333333 0.41666667 0.00000000 0.00694444
0.08333333 0.50000000 0.00000000 0.00694444
0.08333333 0.58333333 0.00000000 0.00694444
0.08333333 0.66666667 0.00000000 0.00694444
0.08333333 0.75000000 0.00000000 0.00694444
0.08333333 0.83333333 0.00000000 0.00694444
0.08333333 0.91666667 0.00000000 0.00694444
0.16666667 0.00000000 0.00000000 0.00694444
0.16666667 0.08333333 0.00000000 0.00694444
0.16666667 0.16666667 0.00000000 0.00694444
0.16666667 0.25000000 0.00000000 0.00694444
0.16666667 0.33333333 0.00000000 0.00694444
0.16666667 0.41666667 0.00000000 0.00694444
0.16666667 0.50000000 0.00000000 0.00694444
0.16666667 0.58333333 0.00000000 0.00694444
0.16666667 0.66666667 0.00000000 0.00694444
0.16666667 0.75000000 0.00000000 0.00694444
0.16666667 0.83333333 0.00000000 0.00694444
0.16666667 0.91666667 0.00000000 0.00694444
0.25000000 0.00000000 0.00000000 0.00694444
0.25000000 0.08333333 0.00000000 0.00694444
0.25000000 0.16666667 0.00000000 0.00694444
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0.25000000 0.33333333 0.00000000 0.00694444
0.25000000 0.41666667 0.00000000 0.00694444
0.25000000 0.50000000 0.00000000 0.00694444
0.25000000 0.58333333 0.00000000 0.00694444
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0.33333333 0.25000000 0.00000000 0.00694444
0.33333333 0.33333333 0.00000000 0.00694444
0.33333333 0.41666667 0.00000000 0.00694444
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0.33333333 0.58333333 0.00000000 0.00694444
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0.33333333 0.75000000 0.00000000 0.00694444
0.33333333 0.83333333 0.00000000 0.00694444
0.33333333 0.91666667 0.00000000 0.00694444
0.41666667 0.00000000 0.00000000 0.00694444

0.16666667 0.41666667 0.00000000 0.00694444

0.16666667 0.50000000 0.00000000 0.00694444
0.16666667 0.58333333 0.00000000 0.00694444
0.16666667 0.66666667 0.00000000 0.00694444
0.16666667 0.75000000 0.00000000 0.00694444
0.16666667 0.83333333 0.00000000 0.00694444
0.16666667 0.91666667 0.00000000 0.00694444
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0.25000000 0.41666667 0.00000000 0.00694444
0.25000000 0.50000000 0.00000000 0.00694444
0.25000000 0.58333333 0.00000000 0.00694444
0.25000000 0.66666667 0.00000000 0.00694444
0.25000000 0.75000000 0.00000000 0.00694444
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0.33333333 0.16666667 0.00000000 0.00694444
0.33333333 0.25000000 0.00000000 0.00694444
0.33333333 0.33333333 0.00000000 0.00694444
0.33333333 0.41666667 0.00000000 0.00694444
0.33333333 0.50000000 0.00000000 0.00694444
0.33333333 0.58333333 0.00000000 0.00694444
0.33333333 0.66666667 0.00000000

0.41666667 0.25000000 0.00000000 0.00694444
0.41666667 0.33333333 0.00000000 0.00694444

0.41666667 0.41666667 0.00000000 0.00694444
0.41666667 0.50000000 0.00000000 0.00694444
0.41666667 0.58333333 0.00000000 0.00694444
0.41666667 0.66666667 0.00000000 0.00694444
0.41666667 0.75000000 0.00000000 0.00694444
0.41666667 0.83333333 0.00000000 0.00694444
0.41666667 0.91666667 0.00000000 0.00694444
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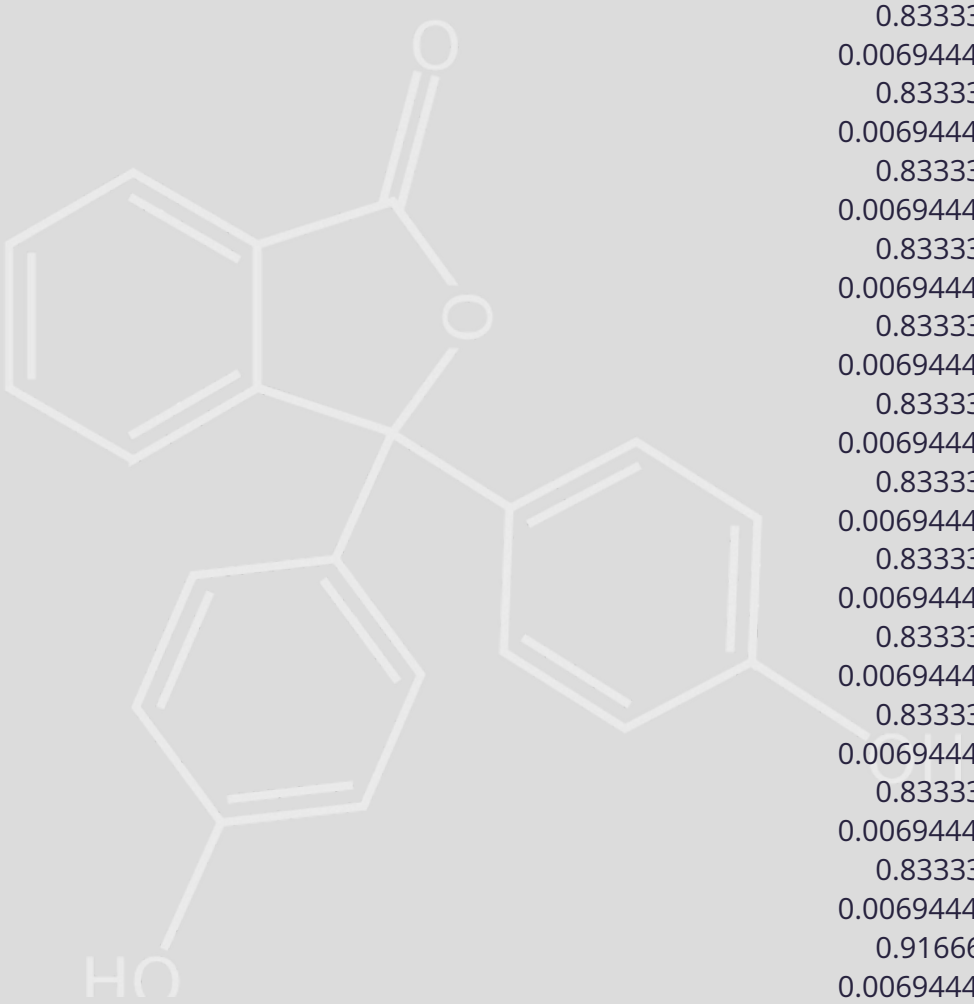

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graphene.pw2wan.in

```
&inputpp
   outdir='./work'
   prefix='graphene',
   seedname = 'graphene'
   write_unk = .true.
/
```

Problem (II)

Following this tutorial to construct a minimal tight-binding Hamiltonian, or the Hamiltonian consisting of the nearest-neighbor transfer only. And then do the followings:

1. Show the matrix element
2. Show the band structure

Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso