Computational Physics Course

Learn to use software packages

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3. Day 4-5 (simulation of graphene)

Here we learn how to use Quantum Espresso. We calculate the electronic structure of graphene and draw the particle density, band structure, and density of states. We then extract a tight-binding parameter.

1. Structure of 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).

```
&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
```

Here I show the first input file used by Quantum espresso. This input file, to be saved as "graphene.scf.in" for example, consists of &control, &system, &electrons, and other parts.

&control consists of type of calculation and indication to computer. You can see the Quantum Espresso HP for detail, but the most important is 'scf'. With this, we will get the electron density by performing the scf (= self consistent field) calculation.

&system characterizes the structure of graphene. We specify the information on the primitive cell, number of atoms, number of elements, basis function, and electron occupation.
   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
   The larger the value for the cut-off is, the more accurate is the calculation. At the same time, the more time is required.

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for the calculation. You need to find a best compromise between the numerical accuracy and the numerical cost.

&electrons specifies the parameter mixing_beta, which controls the speed of scf calculation; the larger the parameter is, the faster is the speed but the less the numerical stability is. Here conv_thr is also specified, which is the threshold for the scf convergence; the smaller the value is, the more accurate is the calculation.

I the last part, we specify the atomic element, the atomic mass, and the pseudopotential used for the calculation. Then we set the position of the atoms within the primitive cell. Finally, we specify the number of mesh points used to do the Brillouine zone integration.

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

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