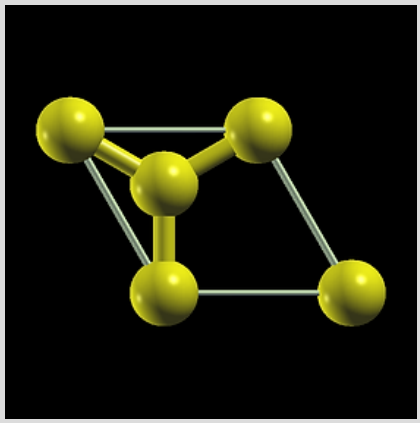
Computational Physics Course

Learn to use software packages

Save the input file as "graphene.scf.in" and then check the file using the following procedure.



Use PWGui: To implement this software, visit the Quantum Espresso HP
http://www.quantum-espresso.org/tools/
and download the PWGui. After installing this software, open the input file "graphene.scf.in". You can check all the parameters. In ths PWGui, you can show the structure of graphene, as shown the figure.

Then, do the scf calculation by typing
$mpirun -np 4 pw.x < graphene.scf.in

```
iteration #  5     ecut=    30.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  8.38E-09,  avg # of iterations =  2.9

negative rho (up, down):  1.646E-04 0.000E+00

total cpu time spent up to now is        1.6 secs

total energy              =     -22.84944326 Ry
Harris-Foulkes estimate   =     -22.84944326 Ry
estimated scf accuracy    <       0.00000001 Ry
```

You will find the sentences as shown in left delivered to the standard output. It says that, the self consistency is estimated here as 0.00000001 Ry. On this basis, scf is recognized to be achieved and the calculation stops. After this, the eigenvalues are calculated at the k-points generated and are shown; those results are not appropriate for drawing the band structure, so that the band structure is calculated separately afterwards.

Finally, you will see the atomic force and the stress tensor. The atomic force will be exactly zero, indicating that the structure is stable. The stress, on the other hand, will not be zero, indicating that the primitive cell needs to be slightly changed to obtain the most stable one.

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

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