



Computational Physics Course

Learn to use software packages

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

Then we use the left ([graphene.pw2wan.in](#)) to convert the result of the nscf calculation to wannier90's format.

```
$pw2wannier90.x < graphene.pw2wan.in > graphene.pw2wan.out
```

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

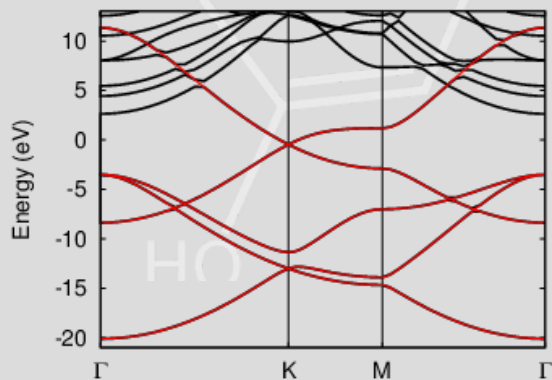
```
$wannier90.x graphene
```

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).



Report (2)

Follow this HP to draw the above figure. Then, reading the paper shown below to construct the minimal tight-binding Hamiltonian using the output of wannier90.x, thereby showing how you got the result. By diagonalizing the Minimal Hamiltonian, draw the band and compare the result with the above figure. It is sufficient to just calculate the eigenvalues at one of the k-points, such as gamma, K, or M.

PDF





The University of Tokyo

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

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