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Computational Physics Course

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Density of states

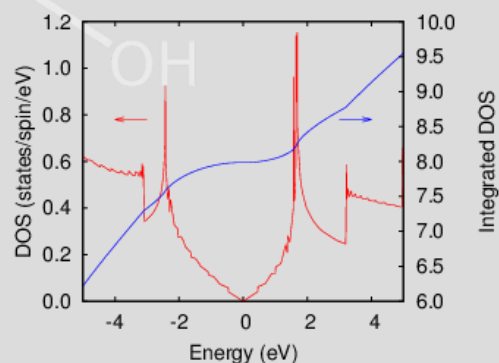
You can draw the density of states using the nscf option in pw.x.

```
&control
  calculation = 'nscf'
  prefix='graphene',
  tstress = .true.
  tprnfor = .true.
  pseudo_dir = './',
  outdir='./work/'
  disk_io='low'
  wf_collect=.true.
/
&system
 ibrav = 4,
  cellpar(1) = 4.602,
  cellpar(2) = 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
```

Use the lines shown in the left as the input file "graphene.nscf.in".

Here, we use a Brillouine zone integration scheme called 'tetrahedra'. This is more accurate than just by smearing the distribution function and applying the trapezoidal method.

In addition, we use finer mesh points as specified, in the last line, by 36 36 1 in our case.



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

After running pw.x, use the lines shown in the left to run dos.x. Then, you will get graphene.dos, as specified in the input file, which can be used in gnuplot. I do not provide you with the plt file as did in the above; prepare it yourselves. Try to make the figure shown above.

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The University of Tokyo

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

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