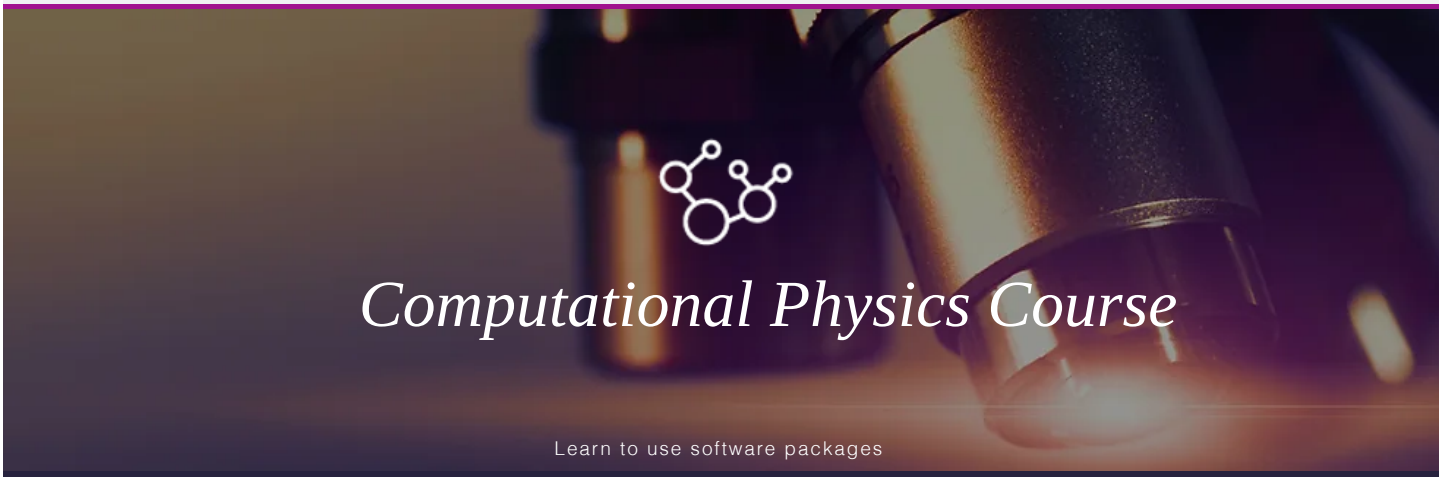


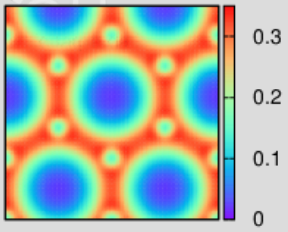

```
&inputpp
 prefix='graphene',
 outdir='./work/'
 plot_num=0
/
&plot
 iflag=2
 output_format=7
 fileout='charge.xsf'
 x0 = 0.0, 0.0, 0.0
 e1 = 2.0, 0.0, 0.0
 e2 = 0.0, 2.0, 0.0
 nx = 100
 ny = 100
/
```

Charge density

To get the charge density, we can reuse the nscf calculation, which was done in the last page. We need to do pp.x calculation, or the post processing run, using the lines shown in the left. You can use the input (plt file) as shown below. You can obtain the figure as shown below.

Note that, when taking iflag=3 and output_format=5, we can get the output data for xcrysden.

```
#!/usr/local/bin/gnuplot -persist
# Last modified: 2014/02/20 20:33
set terminal postscript eps enhanced color 28 lw 2
set output "charge.eps"
set pm3d map
set size square unset xtics unset ytics set cbtics 0.1 s
et cbrange [0:0.35]
set palette rgbformulae 33,13,10
splot 'charge.dat'
```



Show where are carbon atoms located in this figure. Where is the C=C bond?

次へ

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

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