Solid State Theory: Band Structure Methods

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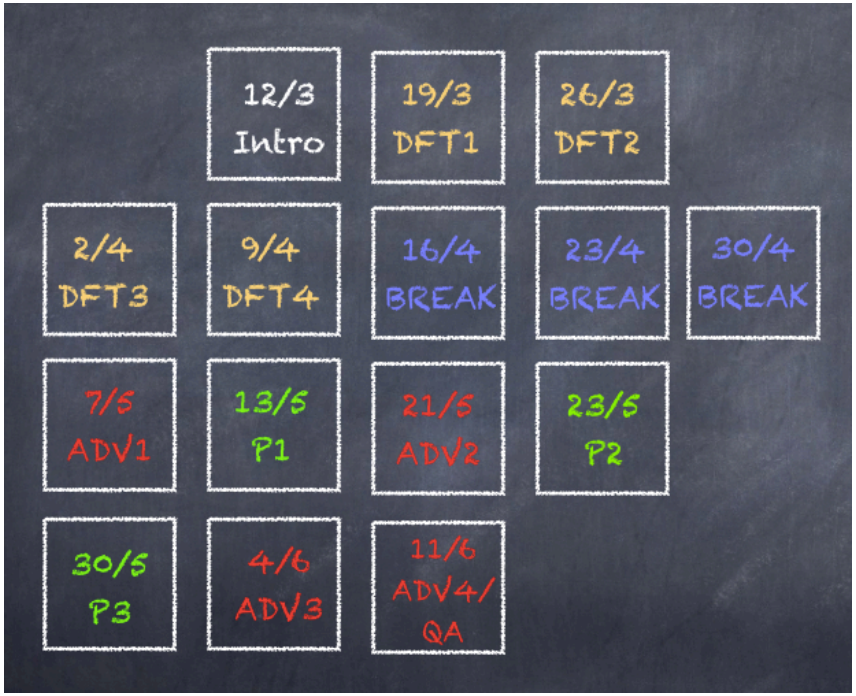
Tues 13/5/2013

Computer room

http://itp.tugraz.at/LV/boeri/ELE/



Important Dates (exercises):

13/5 (Tuesday, next week): 14-15:30 (Electronic structure, *pw.x*)
23/5 (Friday): 14-> 17 (Phonons, *ph.x*)
30/5 (Friday): 14-> 17 (Wannier Functions, *wannier90.x*).

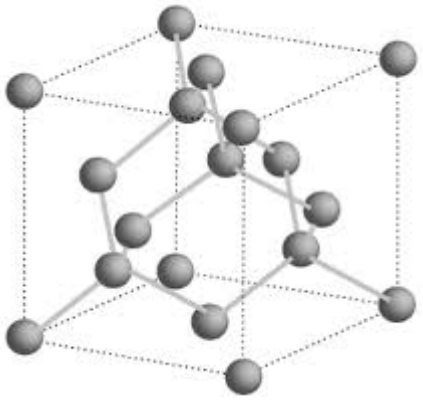
We will employ quantum espresso: http://www.quantum-espresso.org/

Outline:

- **Running a self-consistent calculation using a plane-wave pseudopotential code (*pw.x*).**
- **Convergence: cut-off energy (basis functions); k-space (reciprocal space integration).**
- **Plotting the charge density.**
- **Obtaining the equation of state.**
- **(Homework): studying stability of different crystal structures as a function of pressure.**

http://www.quantum-espresso.org/

Silicon:



- **Crystal structure:**

FCC lattice, 2 atoms/unit cell.

Primitive vectors (FCC):

$\mathbf{a_1}$**=** a(0,1/2,1/2)

$\mathbf{a_2}$= a(1/2,0,1/2)

$\mathbf{a_3}$**=** a(1/2,1/2,0)

Basis vectors:

Si1: 0.0,0.0,0.0

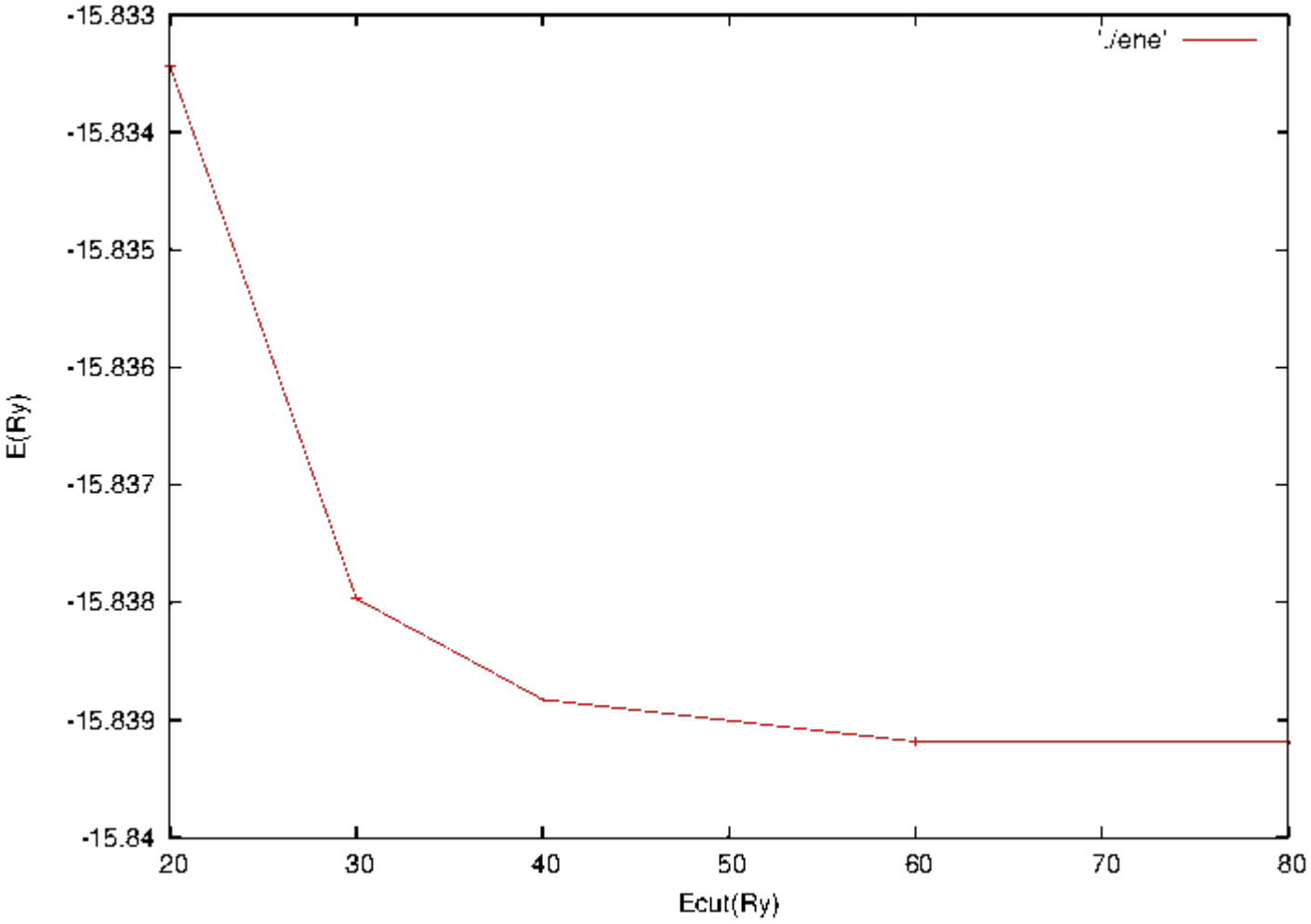
Si2: ¼ , ¼ , ¼

a=5.4309 A = 10.262913 B (*a.u.*)

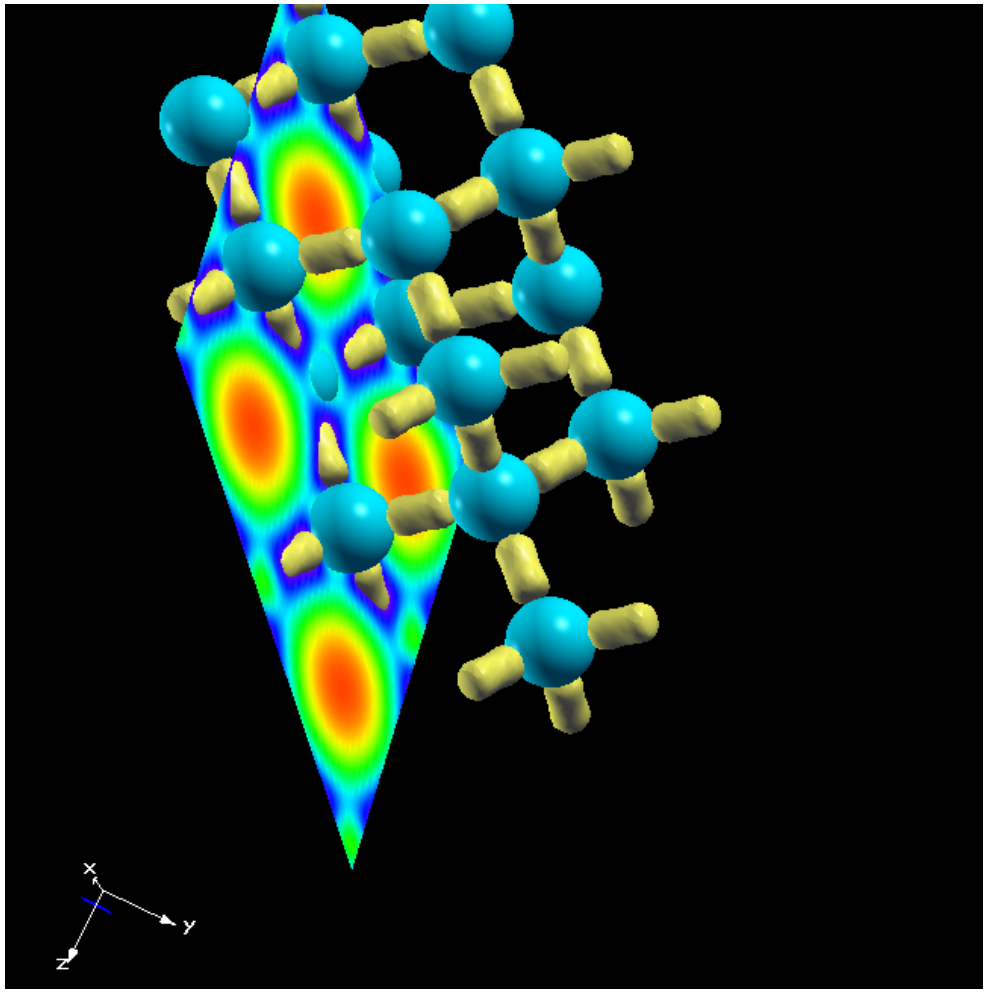
Input file (si.scf.in):

```
&control
   calculation= 'scf'
   prefix= 'SI'
   pseudo_dir = './pseudo/'
   outdir= './tmp/'
   tprnfor = .true.,
   tstress = .true.,
 /
 &system
   ibrav= 2, celldm(1)=10.262913,
   nat=  2, ntyp= 1,
   ecutwfc= 40,
 /
 &electrons
  conv_thr = 1.0D-6
  mixing_beta = 0.4
/
ATOMIC_SPECIES
Si 28.085 Si.pz-vbc.UPF
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS automatic
4 4 4 0 0 0
```

Converging the basis set:

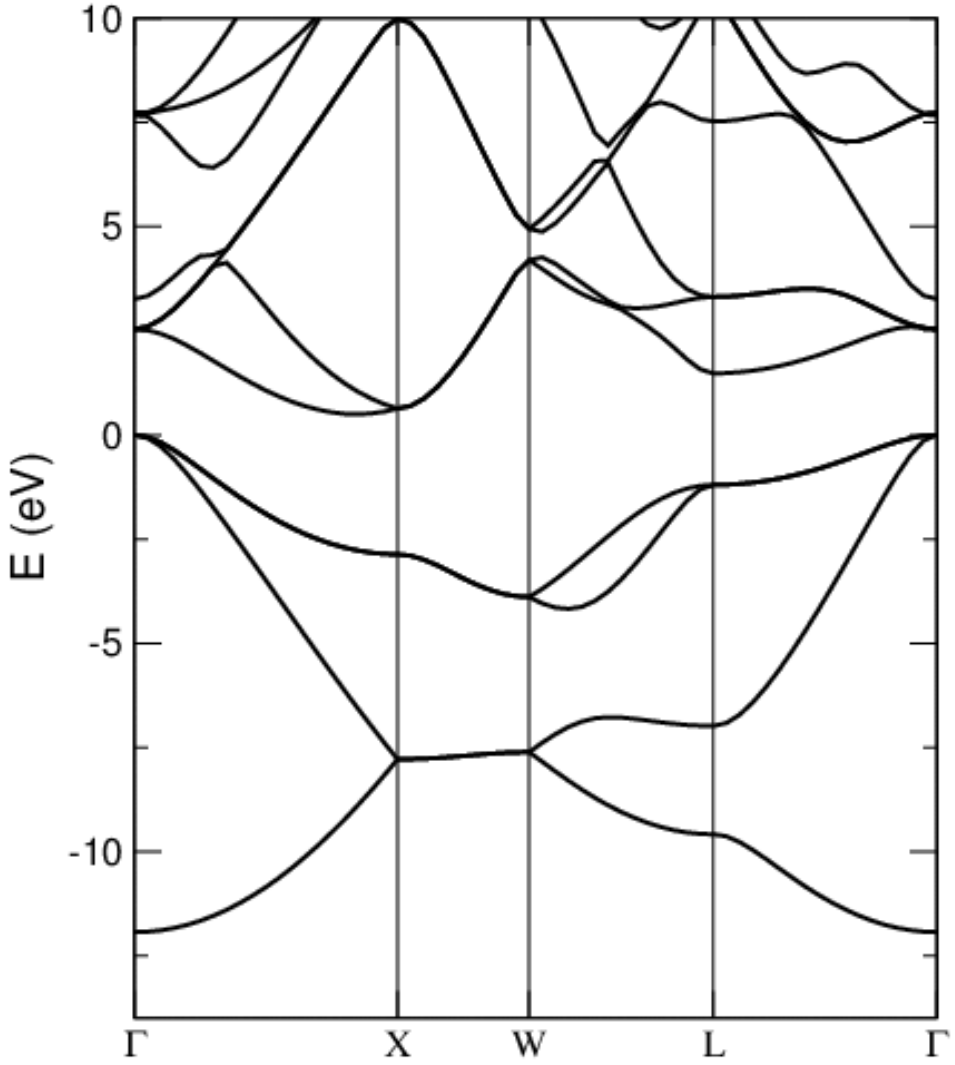


Charge Density (si.charge.in):

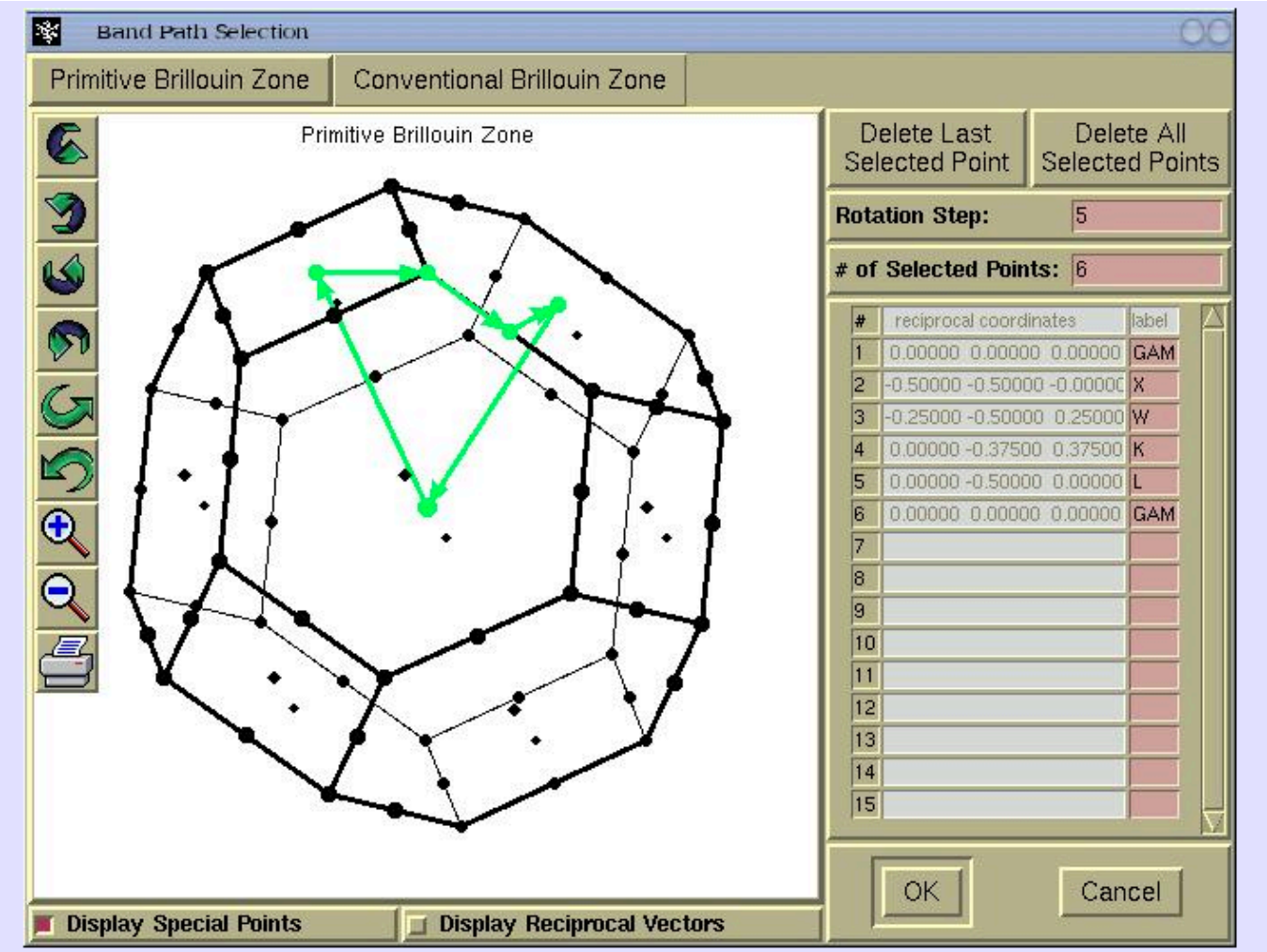


For this plot you need xcrysden (http://www.xcrysden.org/)

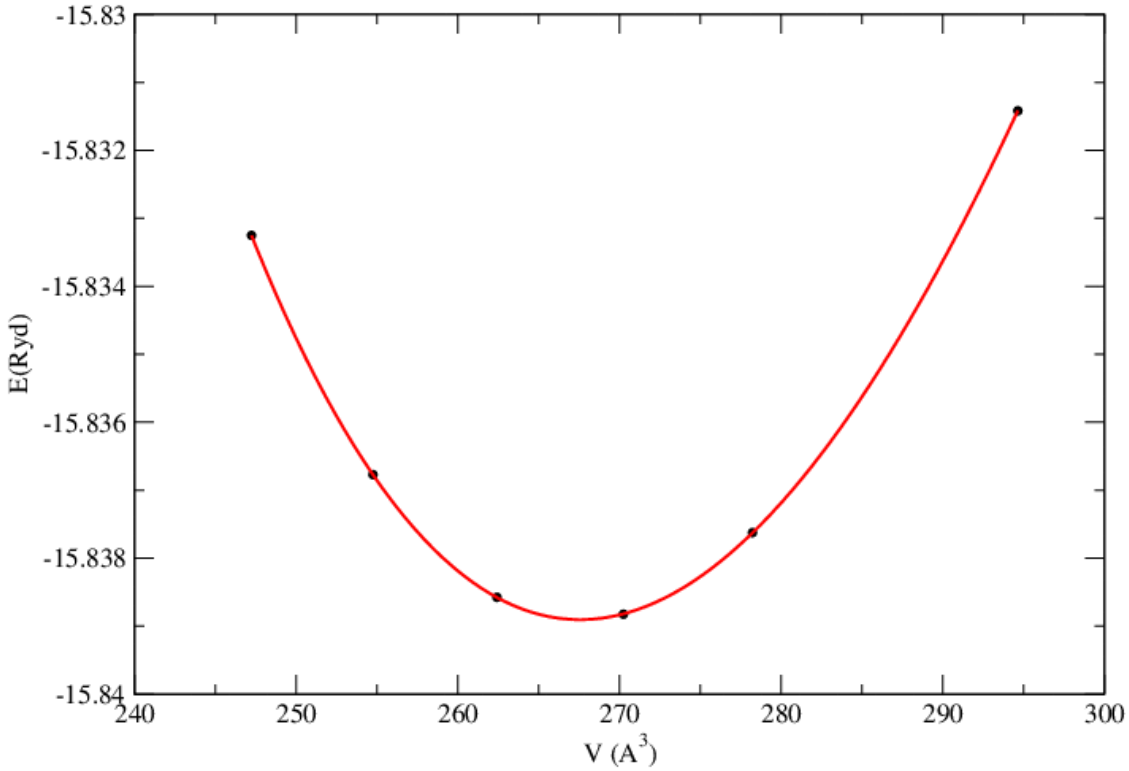
Band Structure:



Special k points (FCC structure):



Equation of state:



Equation of state: EOS2 (PRB52,8064)

a,b,c,d -15.977229 52.489842 -659.228070 2105.431619

V0,B(GPa),BP,E0 267.5514 94.4139 4.0179

Equation of state: Murnaghan

V0,B(GPa),BP,E0 267.5519 94.1350 4.0339 -15.838904

Experiment:

V0,B(GPa): 270.24 97.6