

# **Solid State Theory: Band Structure Methods**

**Lilia Boeri**

**Tues 13/5/2013**

**Computer room**

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

	12/3 Intro	19/3 DFT1	26/3 DFT2	
2/4 DFT3	9/4 DFT4	16/4 BREAK	23/4 BREAK	30/4 BREAK
7/5 ADV1	13/5 P1	21/5 ADV2	23/5 P2	
30/5 P3	4/6 ADV3	11/6 ADV4/ QA		

### 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.

# Silicon:

- **Crystal structure:**

FCC lattice, 2 atoms/unit cell.

**Primitive vectors (FCC):**

$$\mathbf{a}_1 = a(0, 1/2, 1/2)$$

$$\mathbf{a}_2 = a(1/2, 0, 1/2)$$

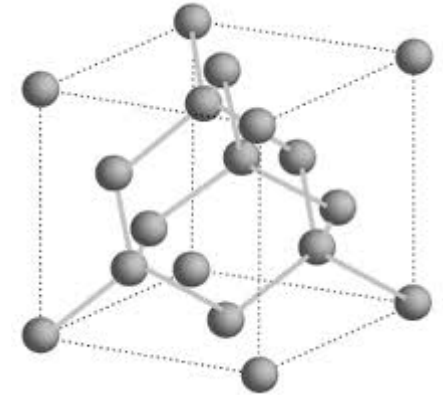
$$\mathbf{a}_3 = a(1/2, 1/2, 0)$$

**Basis vectors:**

Si1: 0.0,0.0,0.0

Si2:  $\frac{1}{4}$ ,  $\frac{1}{4}$ ,  $\frac{1}{4}$

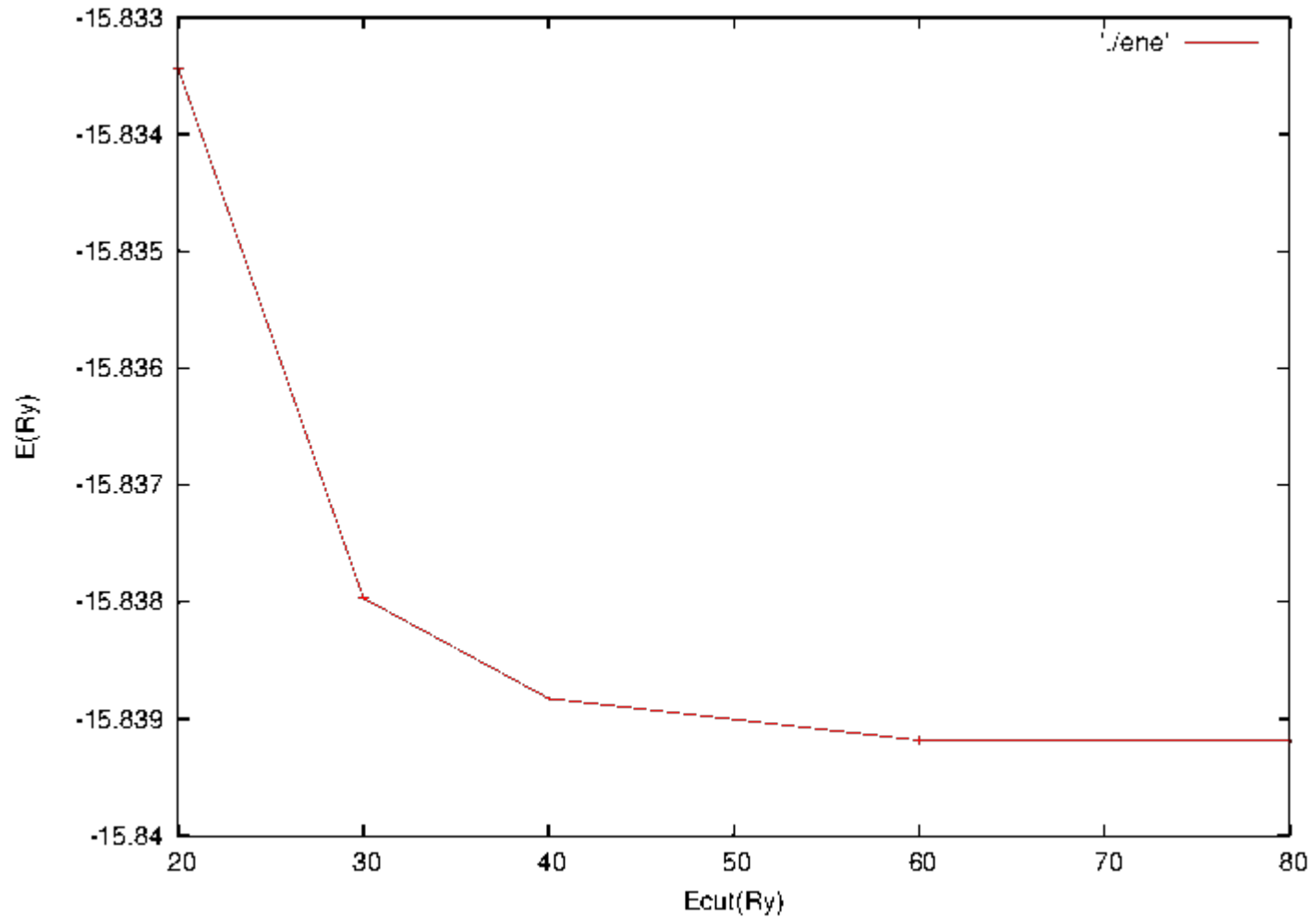
$a = 5.4309 \text{ \AA} = 10.262913 \text{ B (a.u.)}$



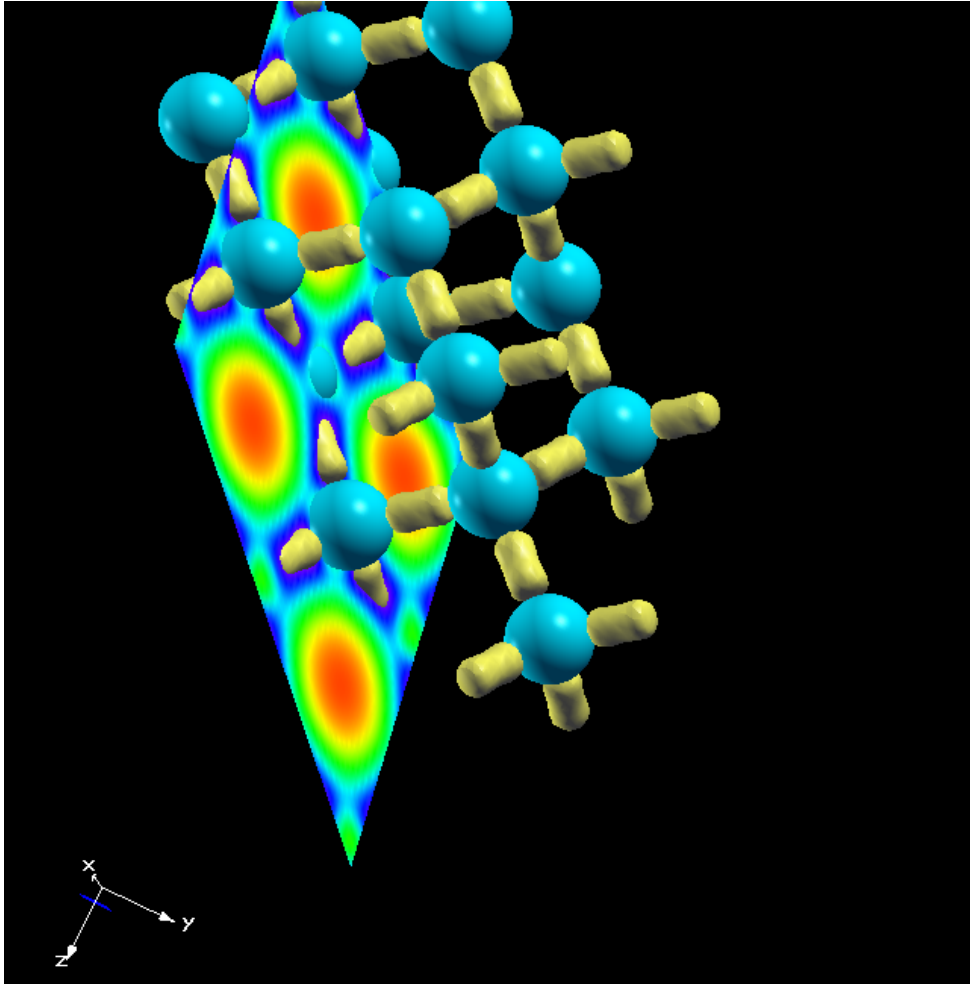
# Input file (si.scf.in):

```
&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:

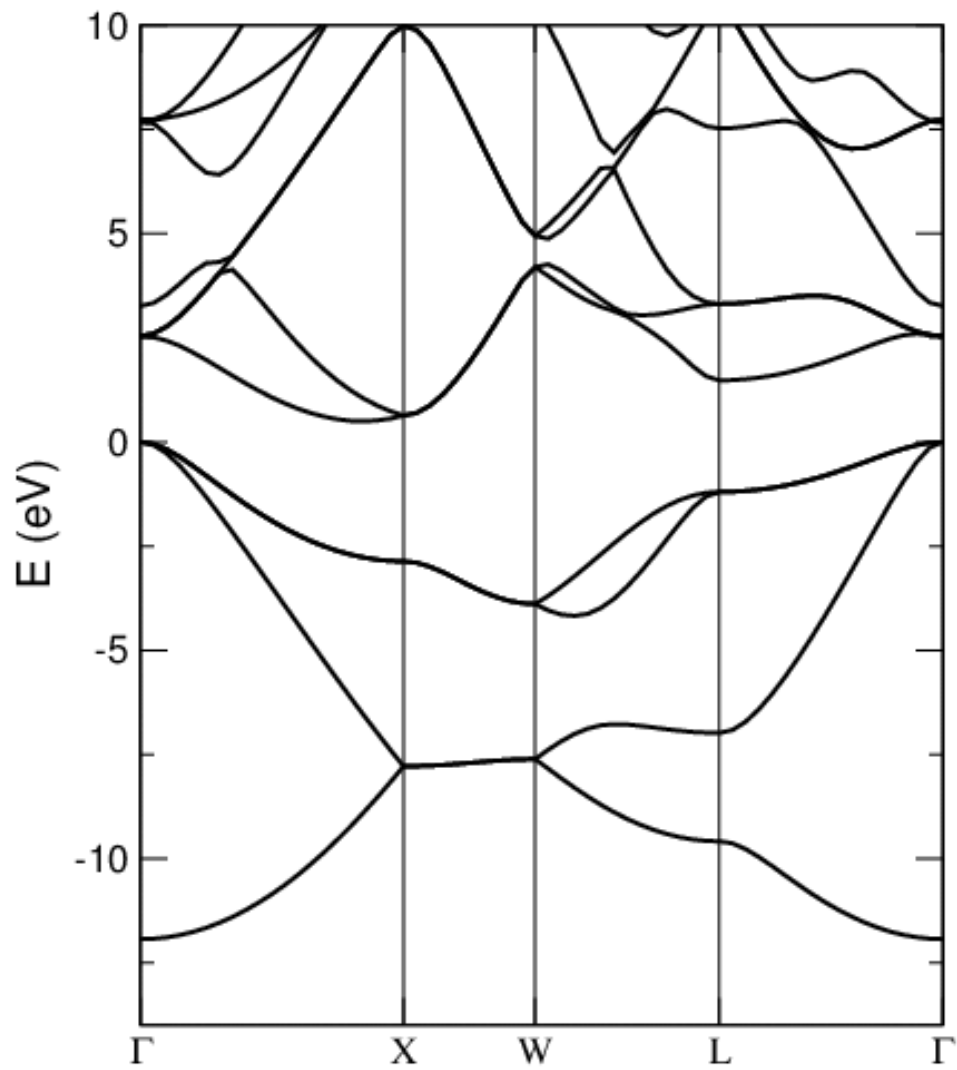


# Charge Density (si.charge.in):



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

# Band Structure:





# Special k points (FCC structure):

Band Path Selection

Primitive Brillouin Zone    Conventional Brillouin Zone

Primitive Brillouin Zone

Delete Last Selected Point    Delete All Selected Points

Rotation Step: 5

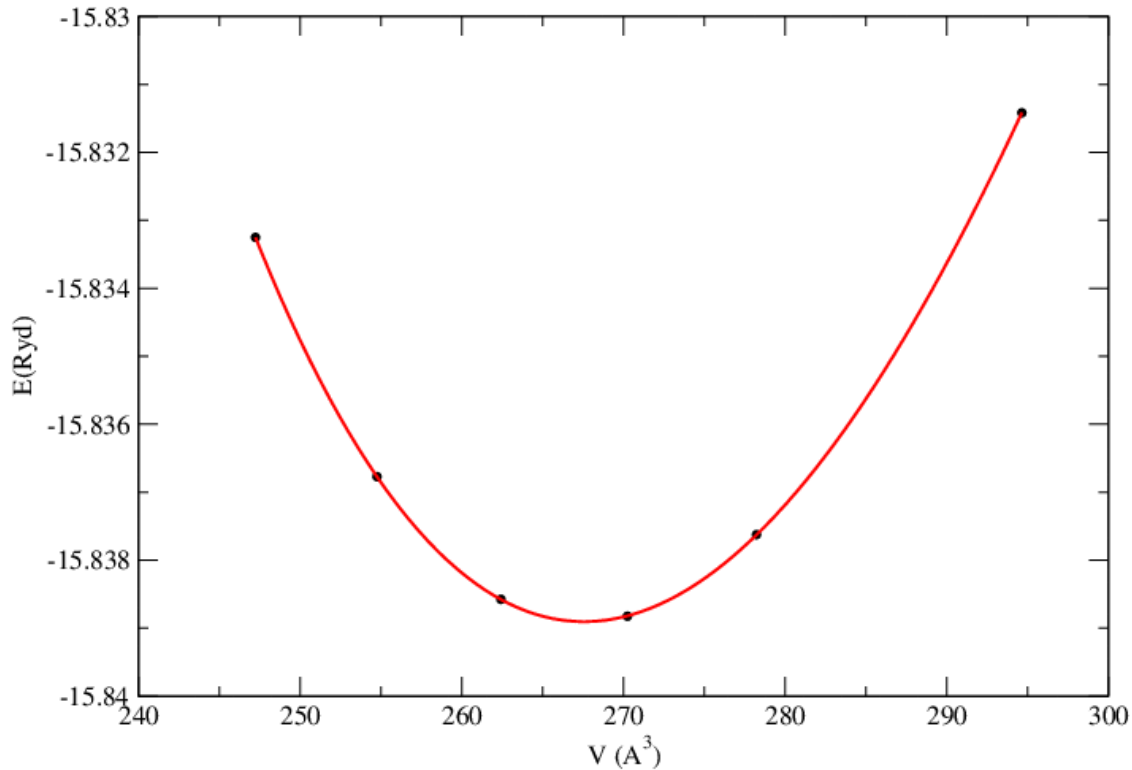
# of Selected Points: 6

#	reciprocal coordinates	label
1	0.00000 0.00000 0.00000	GAM
2	-0.50000 -0.50000 -0.00000	X
3	-0.25000 -0.50000 0.25000	W
4	0.00000 -0.37500 0.37500	K
5	0.00000 -0.50000 0.00000	L
6	0.00000 0.00000 0.00000	GAM
7		
8		
9		
10		
11		
12		
13		
14		
15		

Display Special Points     Display Reciprocal Vectors

OK    Cancel

# Equation of state:



Equation of state: EOS2 (PRB52,8064)

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

$V_0, B(\text{GPa}), BP, E_0$  267.5514 94.4139 4.0179

Equation of state: Murnaghan

$V_0, B(\text{GPa}), BP, E_0$  267.5519 94.1350 4.0339 -15.838904

Experiment:

$V_0, B(\text{GPa}): 270.24 \ 97.6$