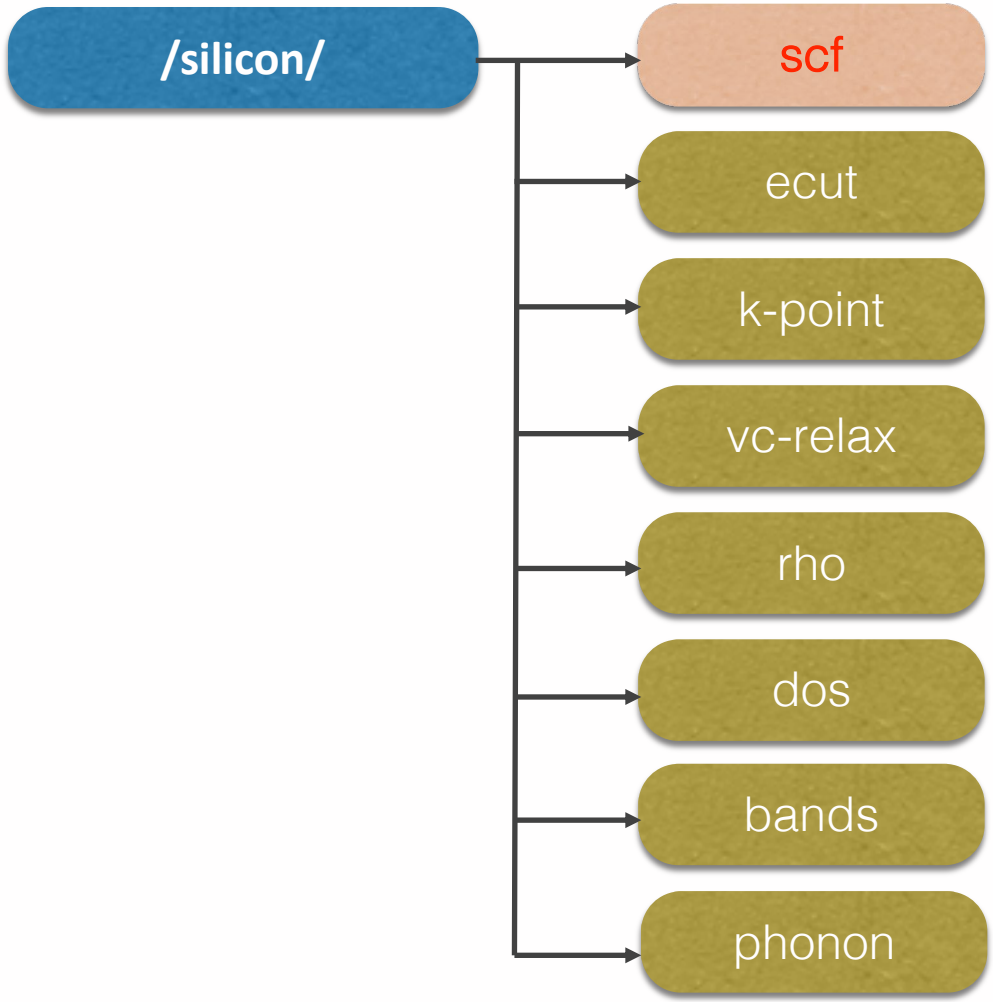
PART 3

MATERIAL DESIGN

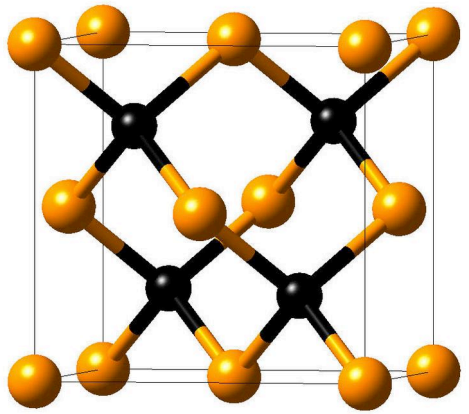
QUANTUM ESPRESSO STRUCTURE

HANDS-ON #1

Hands-on #1 Total energy & Relaxation for Silicon



- Basic self consistent calculation (**scf**)
- Convergence of total energy & plane waves cut-off (**ecut**)
- Convergence of total energy & BZ sampling (**k-point**)
- Lattice constant (**vc-relax**)



Silicon

Kohn-Sham equations

INPUT

Model:
unit cell
lattice vectors
basis

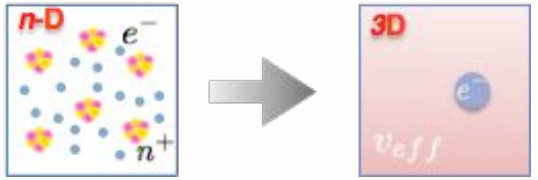
Physical approx:
xc-approximation
GGA, LDA, …

Numerical approx:
energy cut-off
k-points grid
SCF procedure

RUN

OUTPUT

Physical quantities:
charge density
total energy
KS wavefunctions
KS energies



Solve Kohn-Sham equations

$$\left[-\frac{1}{2}\nabla^2 + V_{ion}(r) + V_H[n(r)] + V_{XC}[n(r)] \right] \psi_i(r) = \varepsilon_i \psi_i(r)$$

External nuclear potential

Hartree potential

Exchange-correlation potential

Kohn-Sham equations

$$\underbrace{\left[-\frac{1}{2}\nabla^2 + V_{ion}(r) + V_H[n(r)] + V_{XC}[n(r)] \right]}_{H[n(r)]} \psi_i(r) = \varepsilon_i \psi_i(r)$$

Self-consistent field (SCF) method:

$$\psi_i(r) \rightarrow n(r) \rightarrow H[n(r)]$$

Structure of QE input file

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&ELECTRONS
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ATOMIC_POSITIONS (alat)
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K_POINTS automatic
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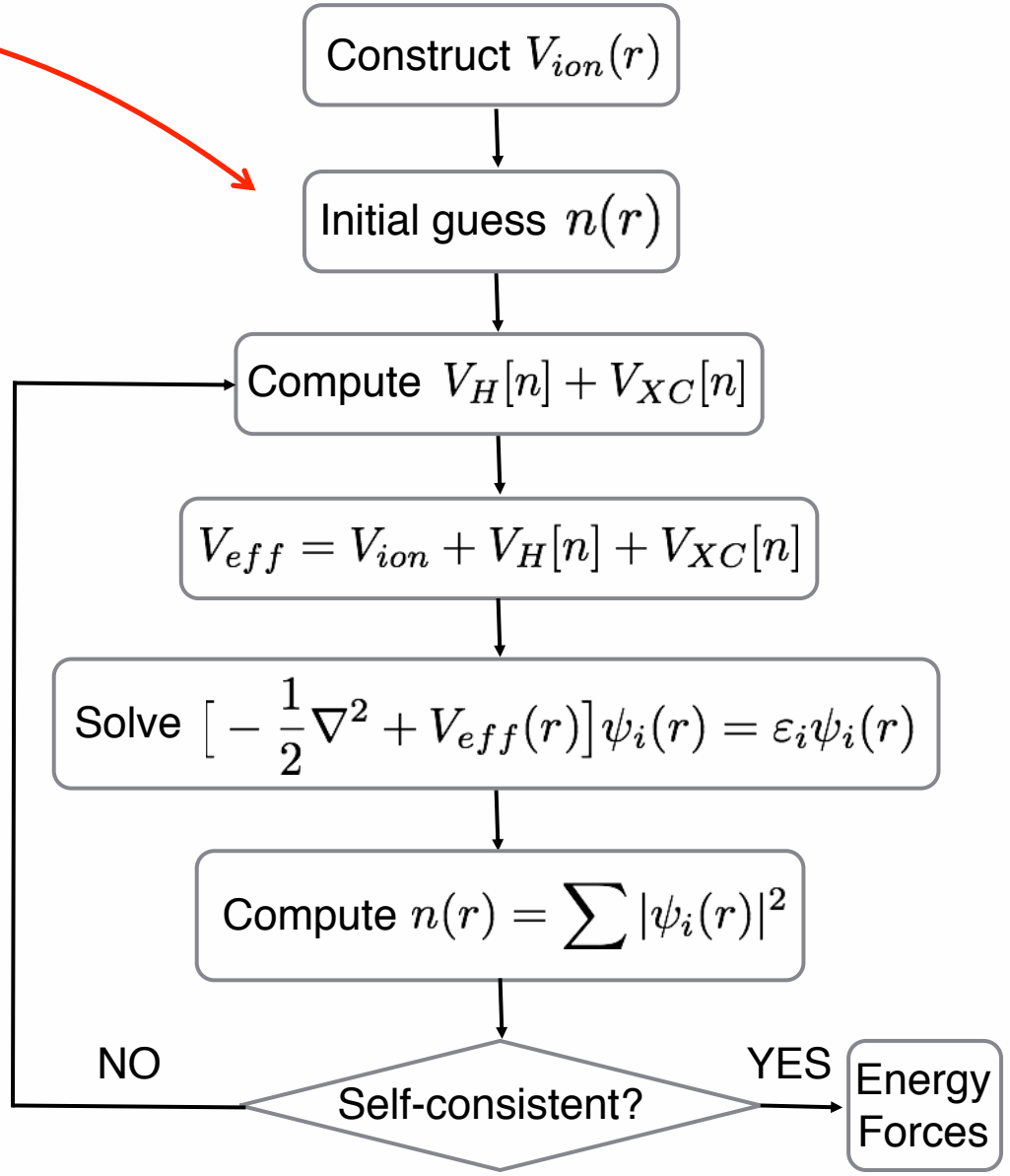

Structure of QE input file

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&ELECTRONS
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 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
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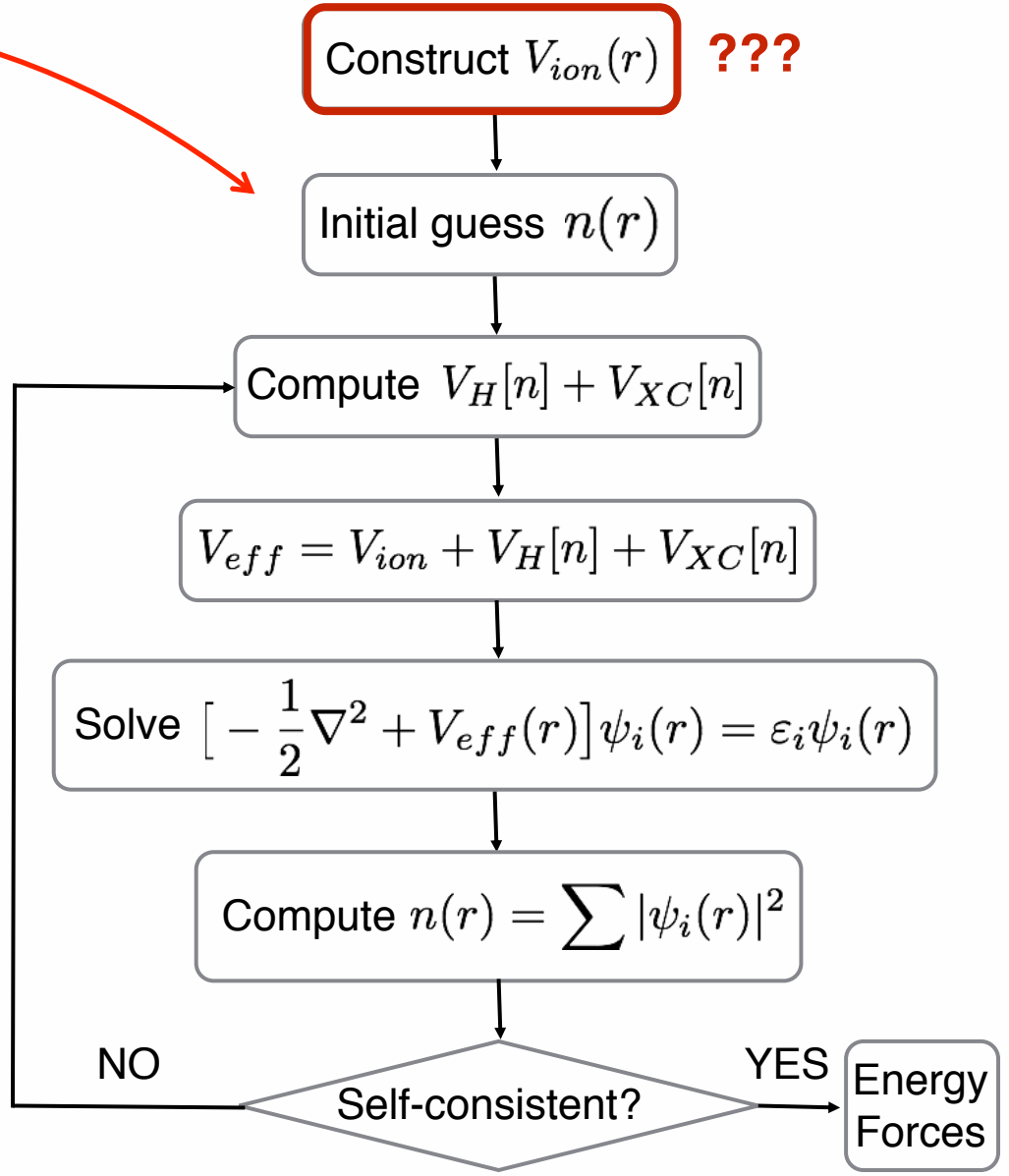
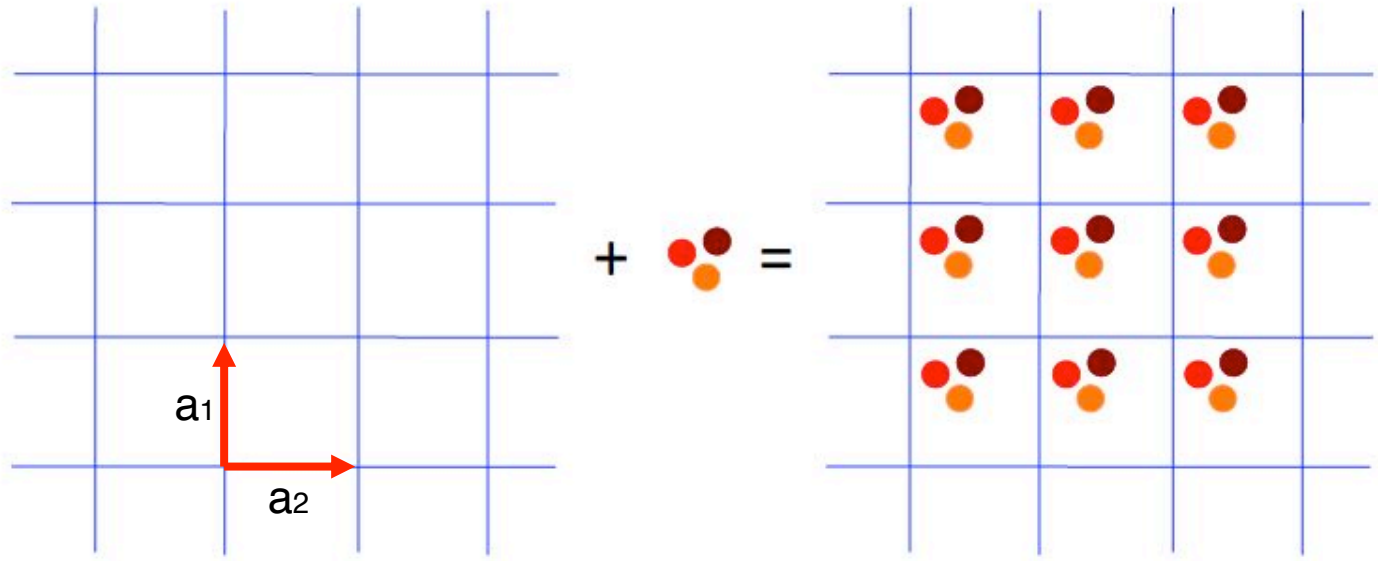
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```



Periodic boundary conditions

Crystal structure: Bravais lattice + Atomic basis



☞ Bravais lattice: (shape of unit cell & how it repeats). Specified by primitive lattice vectors a_1, a_2, a_3

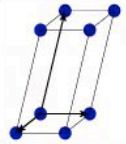
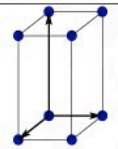
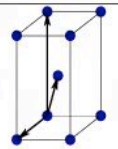
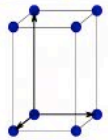
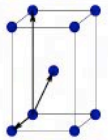
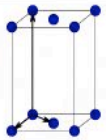
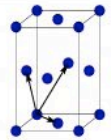
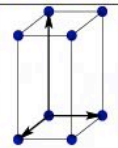
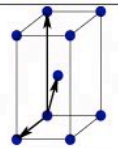
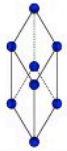
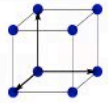
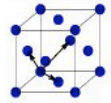
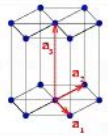
$$R = n_1a_1 + n_2a_2 + n_3a_3, \text{ where } n_1, n_2, n_3 \text{ are integers.}$$

☞ Atomic basis: how many atoms are in the unit cell, and how they are arranged.

Periodic boundary conditions

4 Lattice types

7 Crystal classes

Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

Structure of QE input file

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 outdir='../tmp/',
/
&SYSTEM
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 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&ELECTRONS
 mixing_beta=0.7,
 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```

```
ibrav = 1 (SC)
ibrav = 2 (FCC)
ibrav = 4 (Hexagonal)
…
```

```
simple cubic:
v1 = a(1,0,0)
v2 = a(0,1,0)
v3 = a(0,0,1)

face centered cubic:
v1 = (a/2)(-1,0,1)
v2 = (a/2)(0,1,1)
v3 = (a/2)(-1,1,0)
```

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 conv_thr=1d-8,
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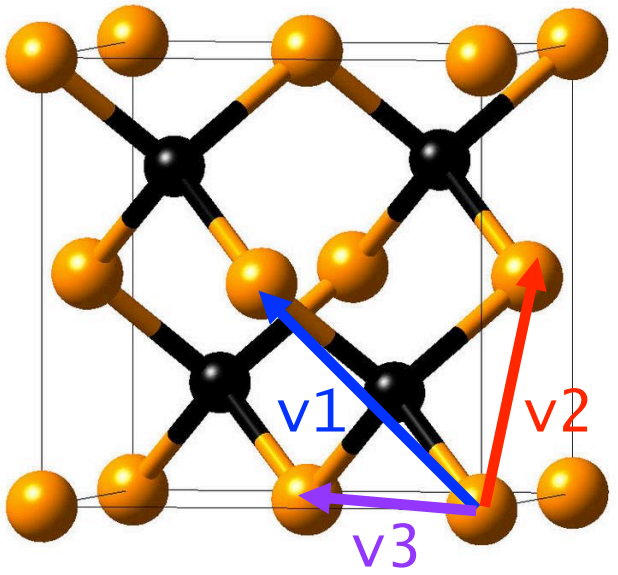
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```

FCC structure



face centered cubic:
v1 = (a/2)(-1,0,1)
v2 = (a/2)(0,1,1)
v3 = (a/2)(-1,1,0)

Structure of QE input file

```
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 prefix='si',
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/
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 ecutrho=720.0,
/
&ELECTRONS
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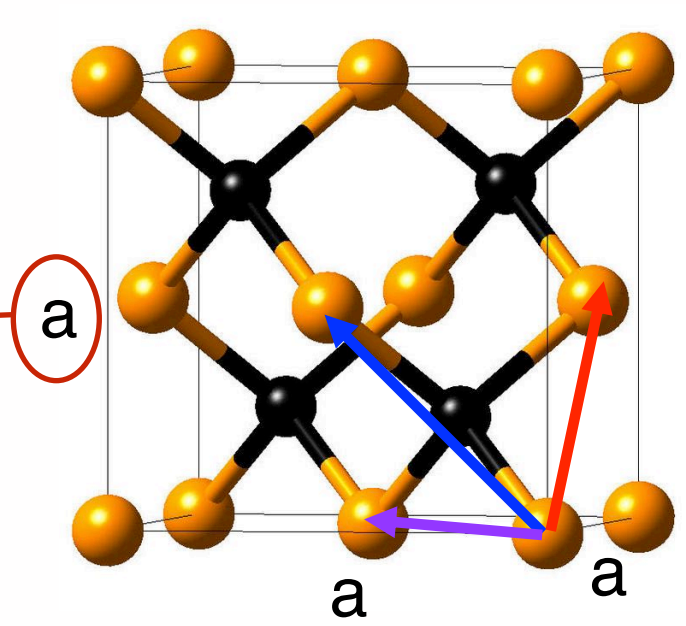
 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```

unit bohr

FCC structure



face centered cubic:
v1 = (a/2)(-1,0,1)
v2 = (a/2)(0,1,1)
v3 = (a/2)(-1,1,0)

1 bohr = 0.529177 Å

Structure of QE input file

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ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
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Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
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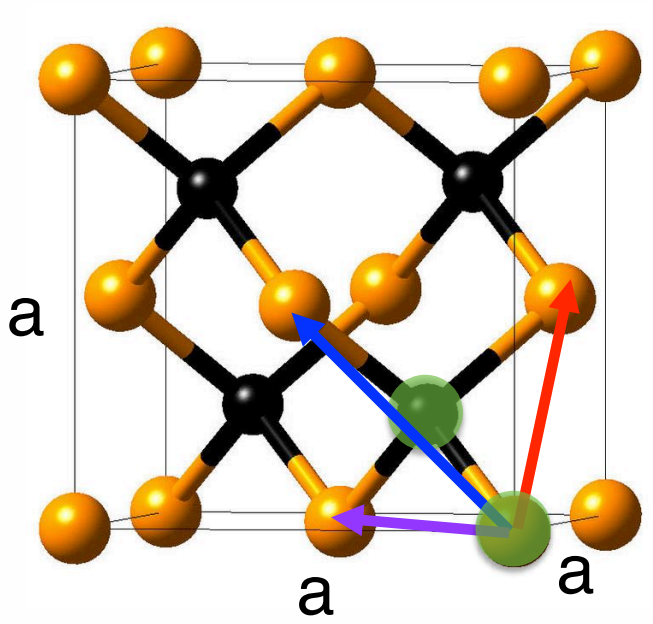
FCC structure



atomic positions are in cartesian coordinates, in units of the lattice parameter.

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ATOMIC_POSITIONS (alat)
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Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```
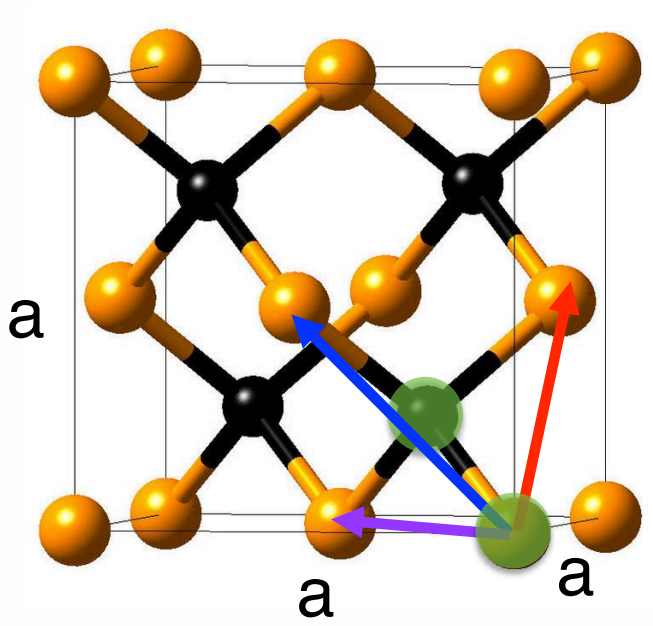

Silicon

Mass of Si

FCC structure



How to check the structure

XCrySDen: http://www.xcrysden.org