



## First Principles Workshop

An introduction and hands-on tutorial with the  
Quantum ESPRESSO



# Quantum Espresso Hands-on Tutorial

by N. T. Hung, A. R. T. Nugraha and R. Saito group

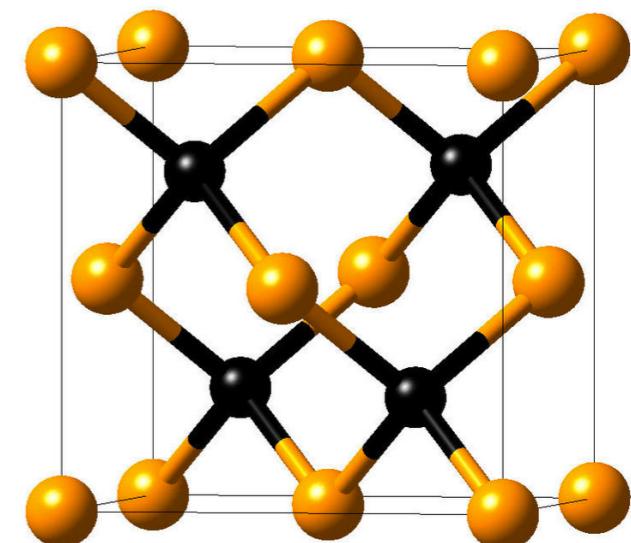
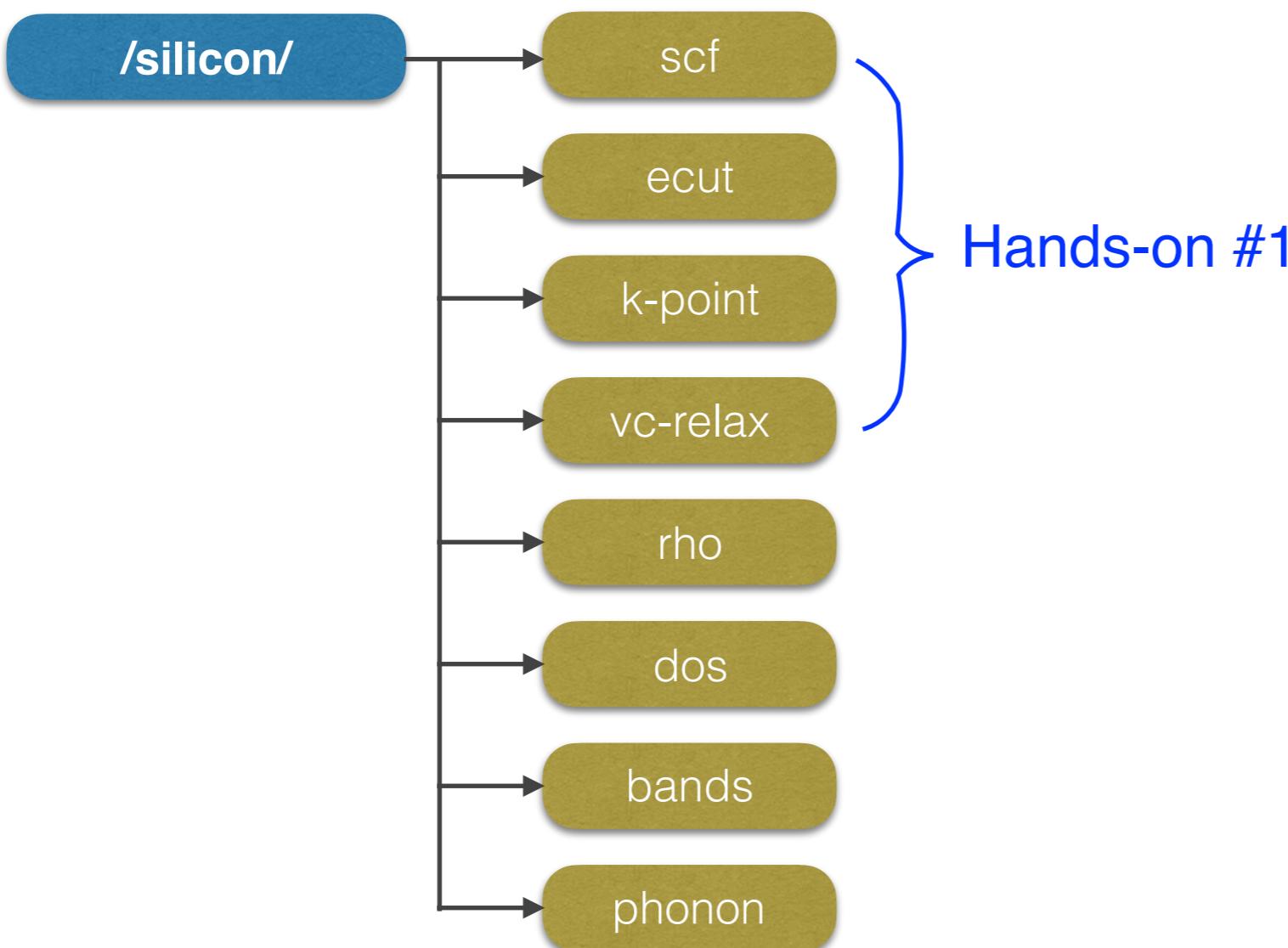
<http://flex.phys.tohoku.ac.jp>

# What we will do today

## Hands-on #1: Total energy and relaxations for Silicon

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

Files for practice



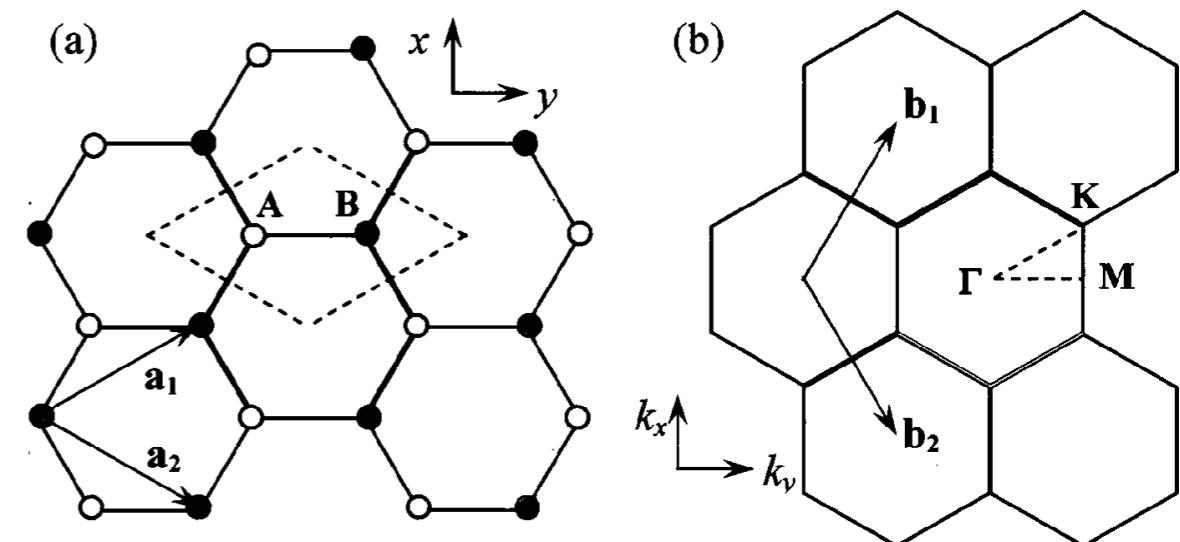
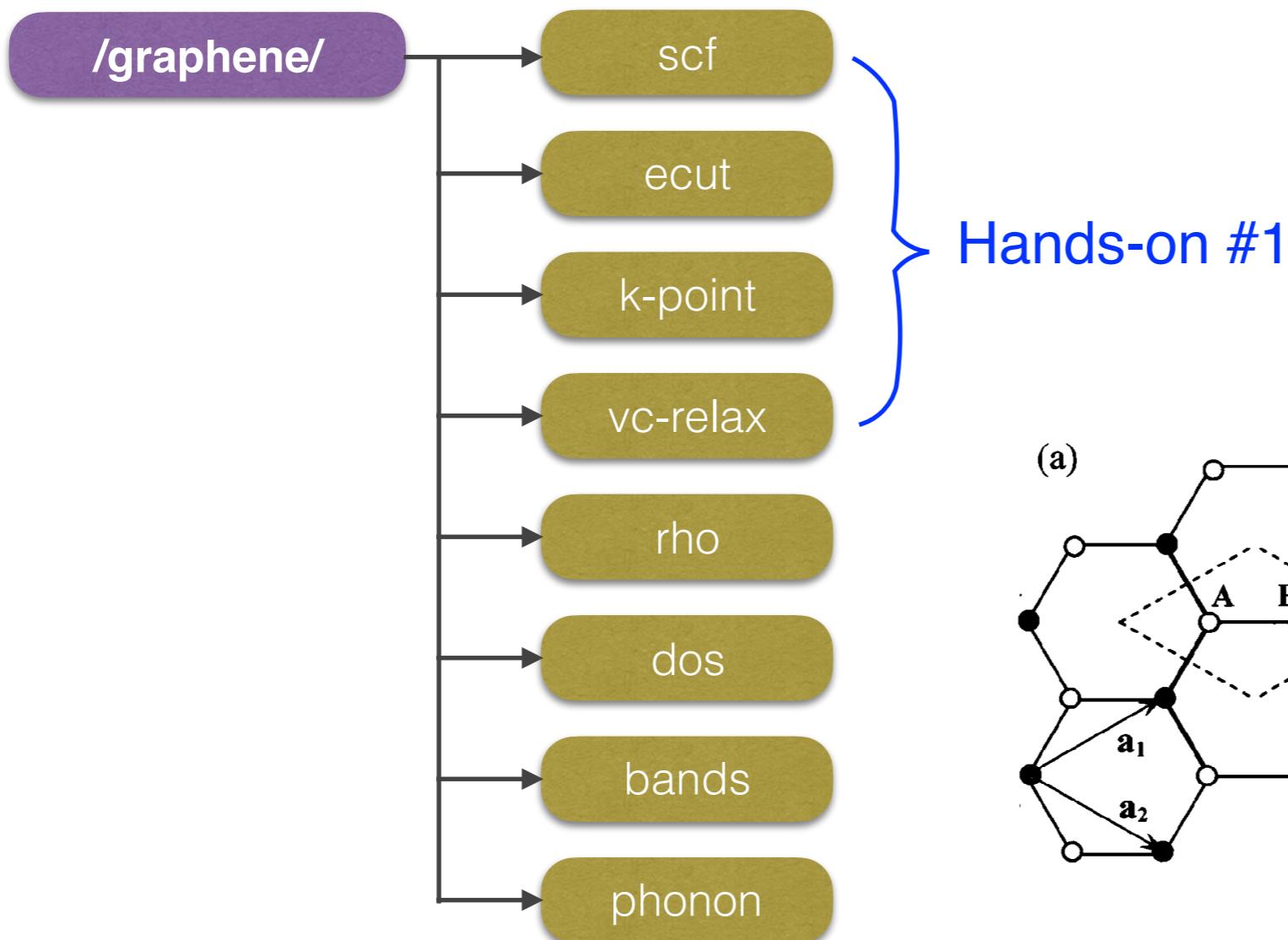
Silicon

# Exercise #1

Do it by yourself: Graphene's calculation!

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

Files for exercise

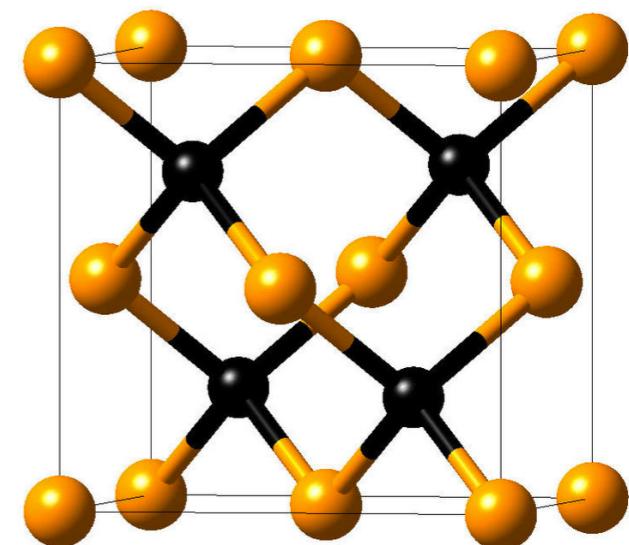
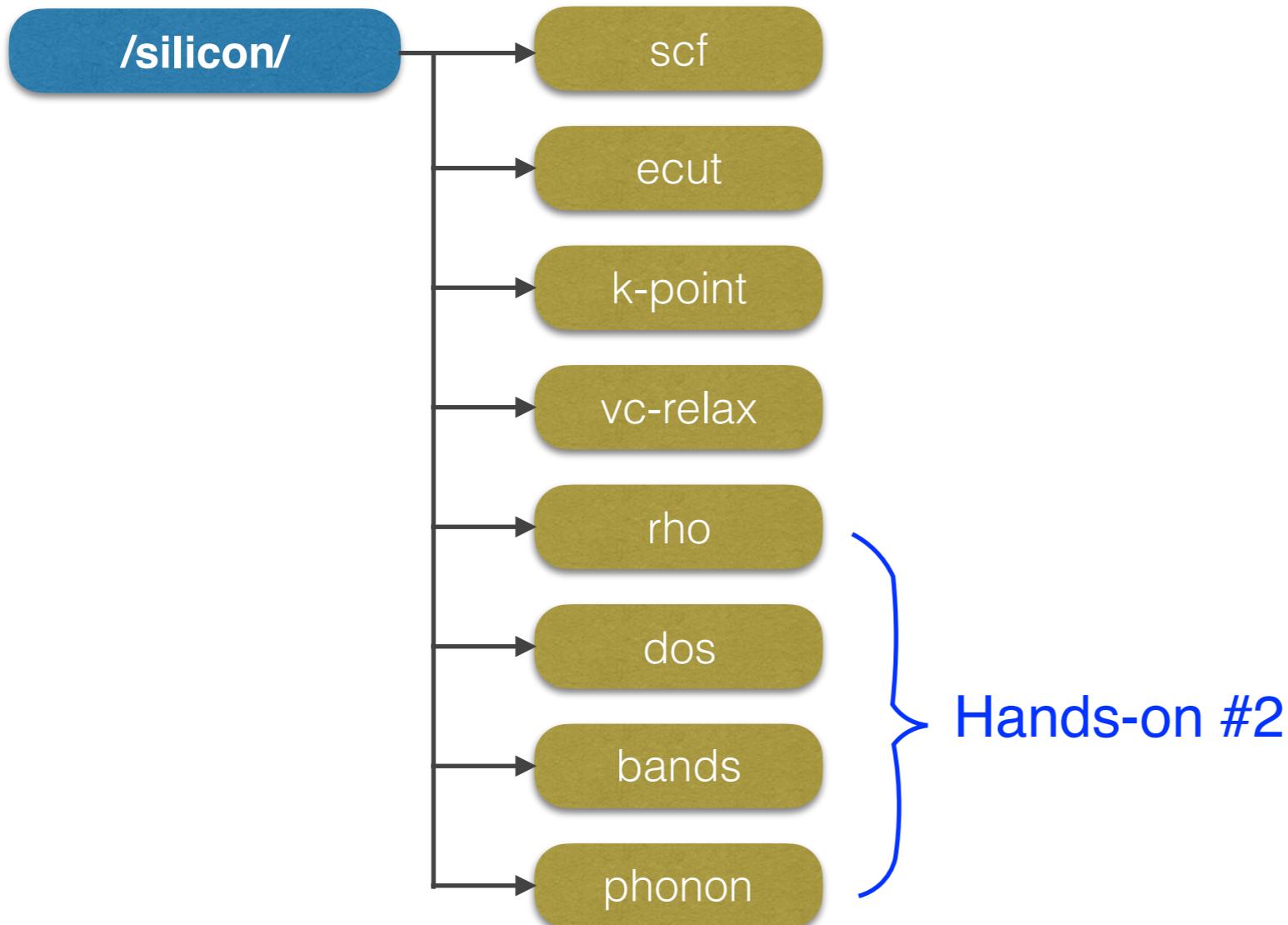


# What we will do today

## Hands-on #2: Charge density, Band structure, DOS, Phonon

- ▶ Charge density (rho)
- ▶ Density of states (dos)
- ▶ Band structure (bands), Phonon dispersion (phonon)

Files for practice

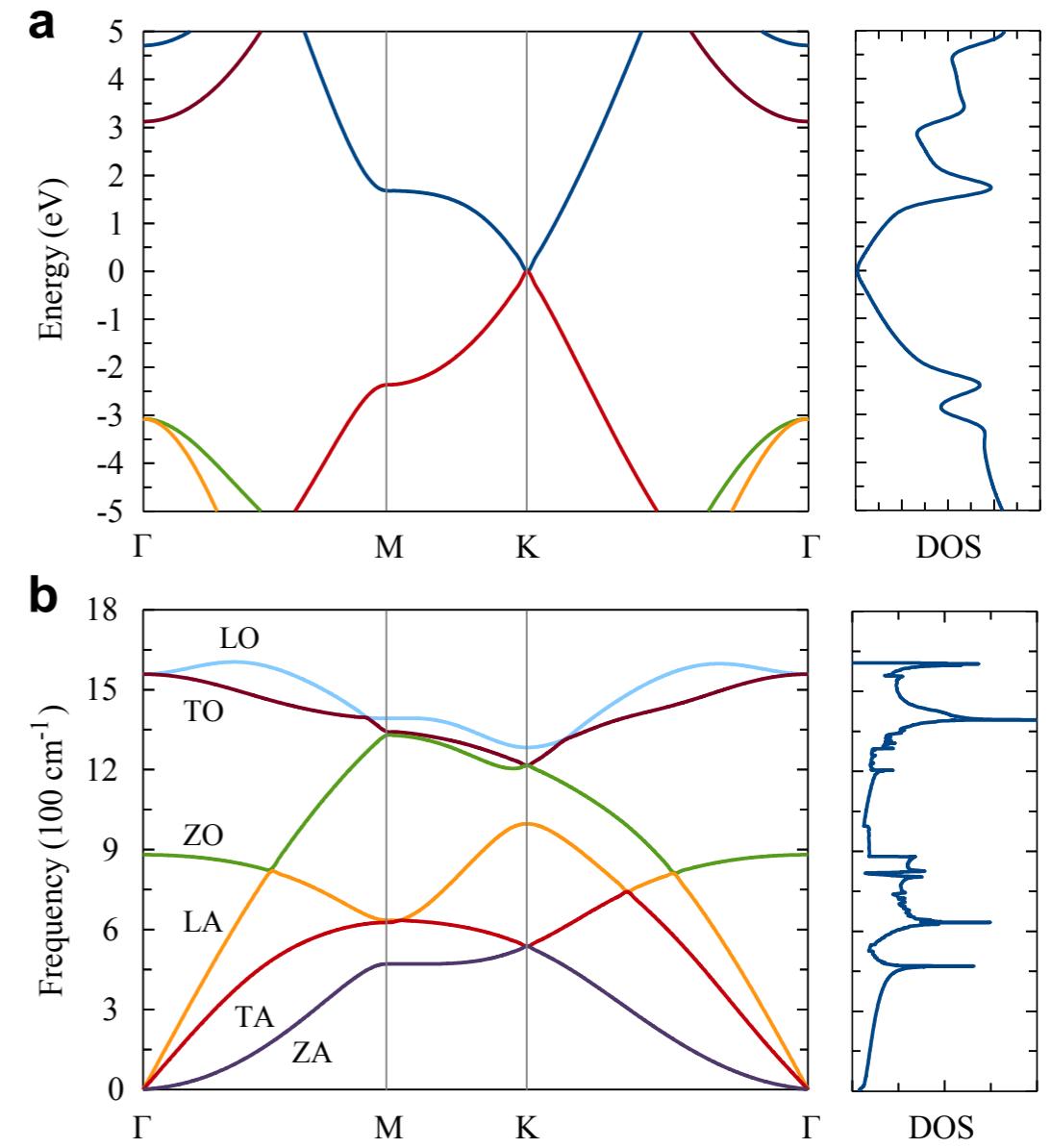
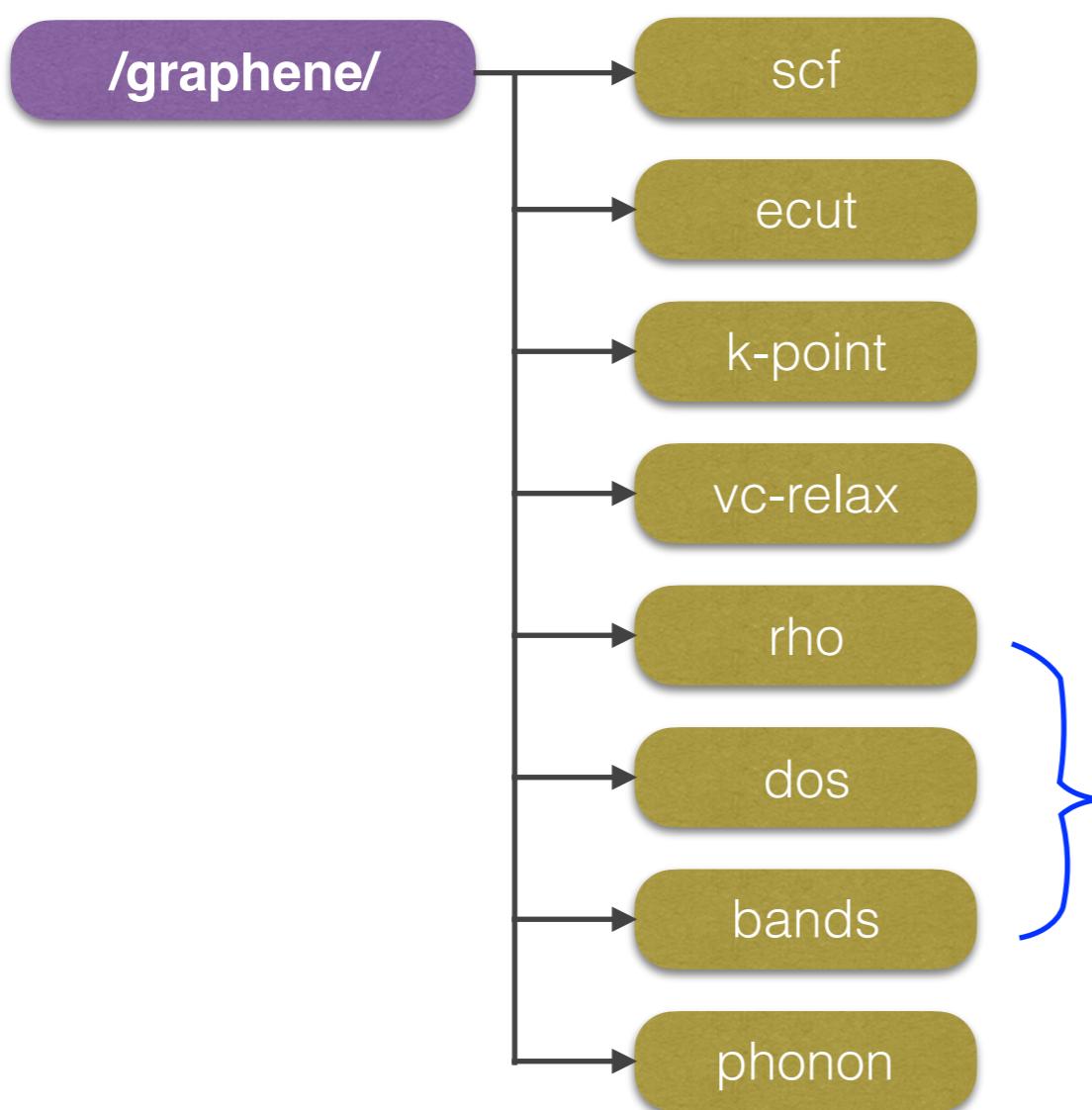


# Exercise #2

Do it by yourself: Graphene's calculation!

- ▶ Charge density (rho)
- ▶ Density of states (dos)
- ▶ Band structure (bands)

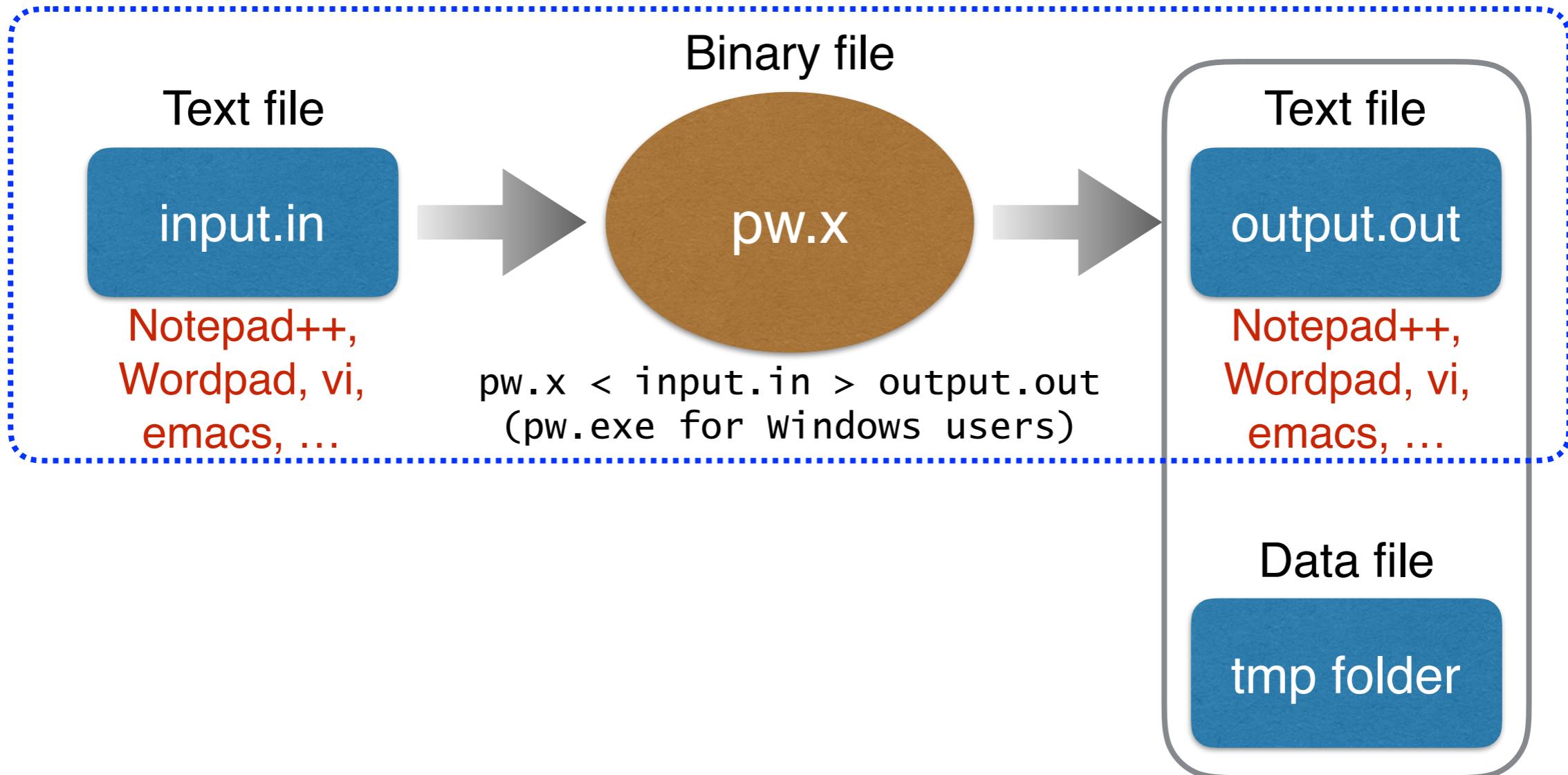
Files for exercise



Hands-on #2

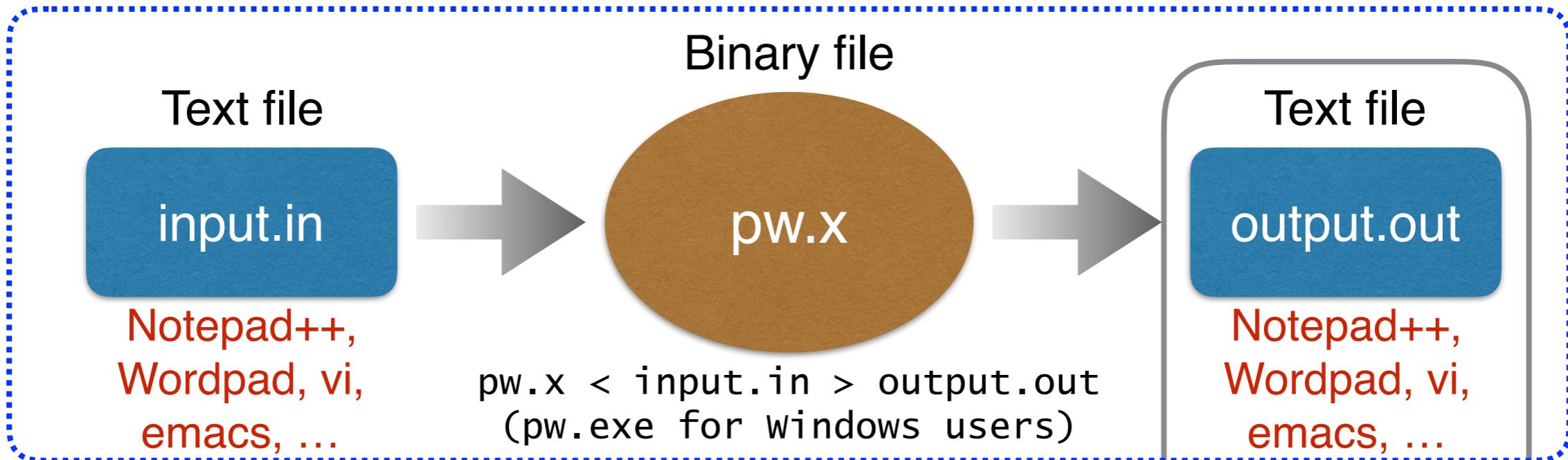
# Structure of QE I/O file

## Hands-on #1

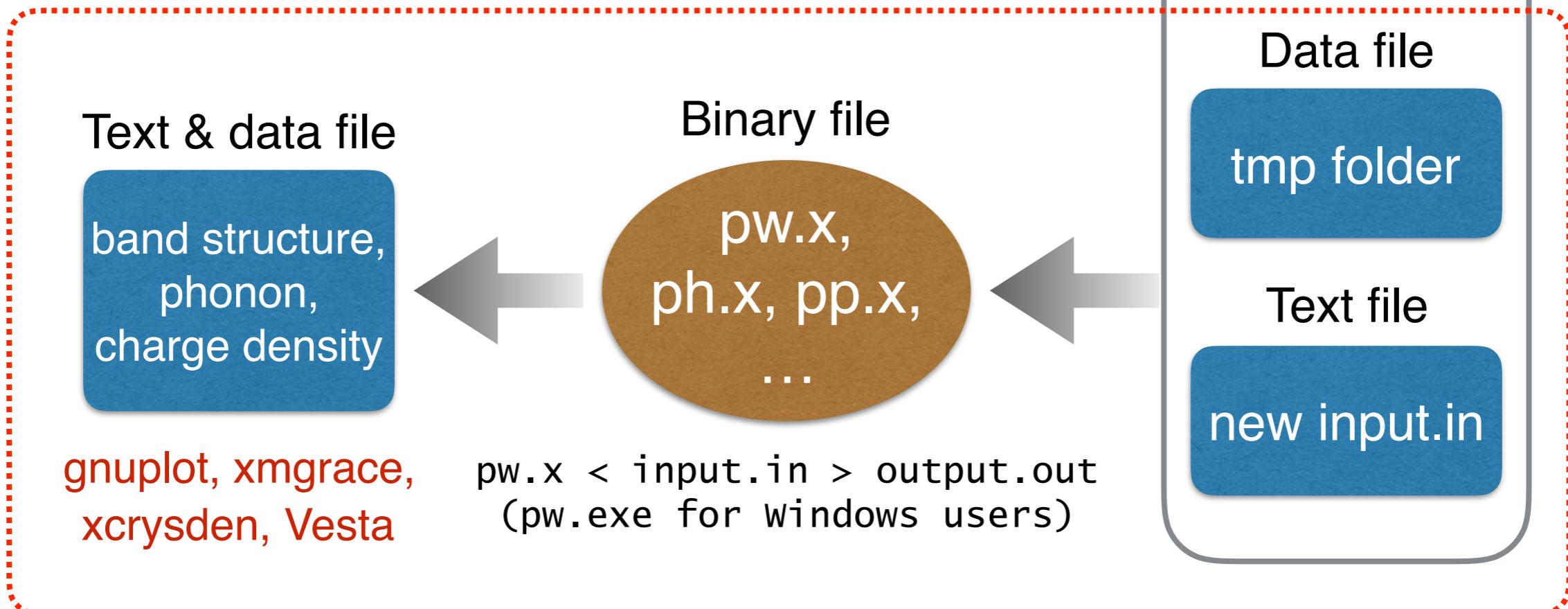


# Structure of QE I/O file

## Hands-on #1

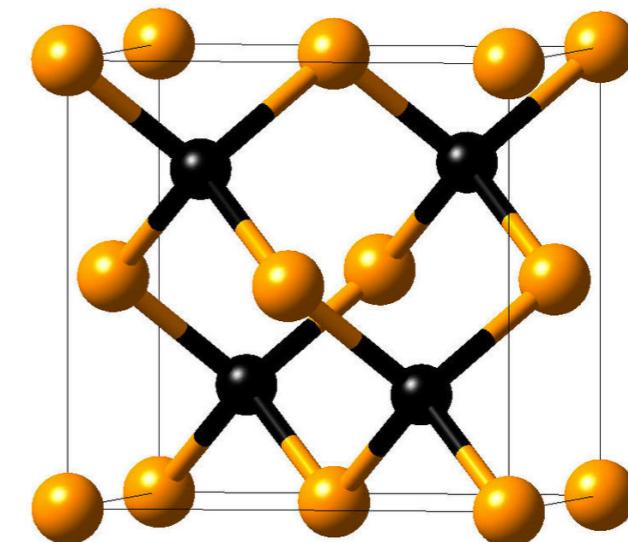


## Hands-on #2



# Structure of QE input file

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&ELECTRONS
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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
```



Silicon

# Kohn-Sham equations

IN

## Model:

unit cell  
lattice vectors  
basis

## Physical approx:

xc-approximation  
GGA, LDA, ...

## Numerical approx:

energy cut-off  
k-points grid  
SCF procedure

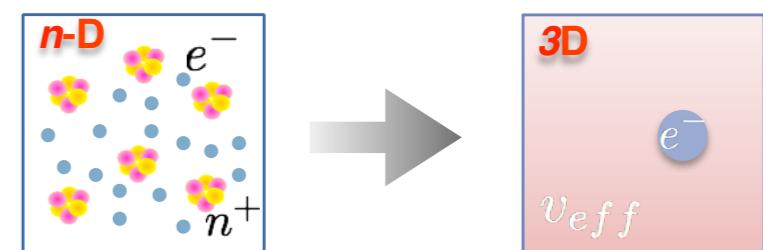
RUN



OUT

## 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

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

---

$$H[n(r)]$$

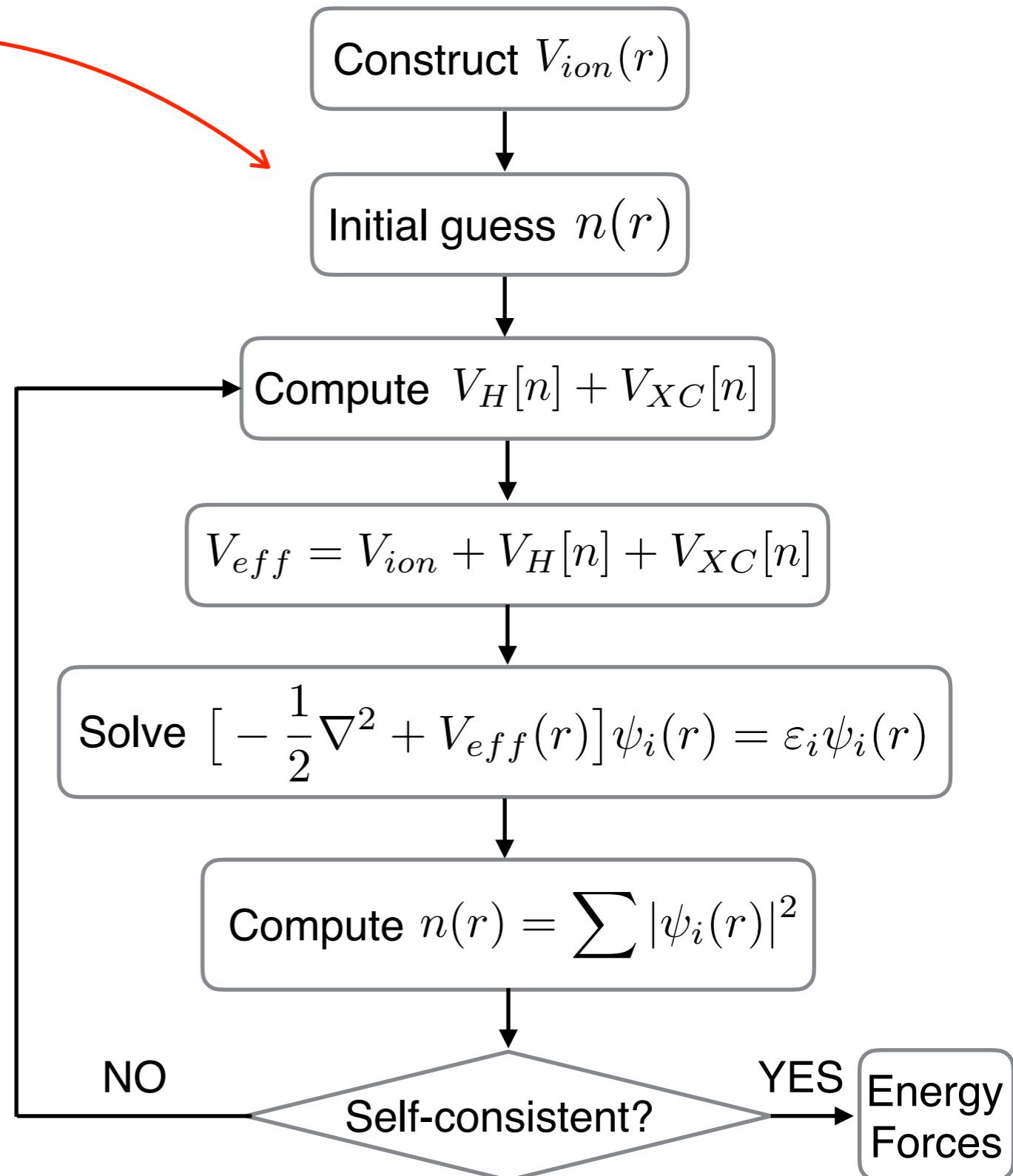
Self-consistent field (SCF) method:

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



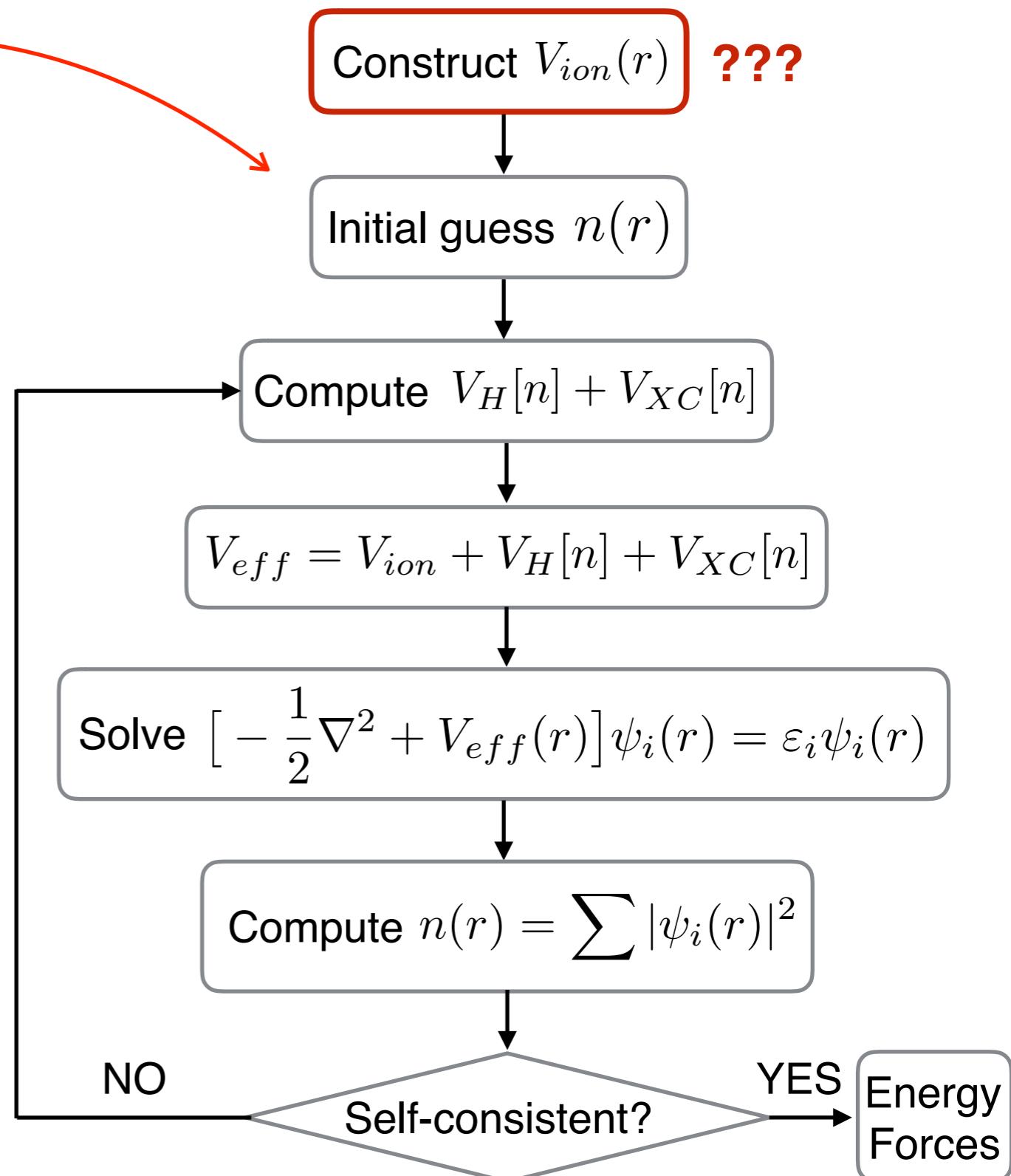
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ATOMIC_POSITIONS (alat)
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K_POINTS automatic
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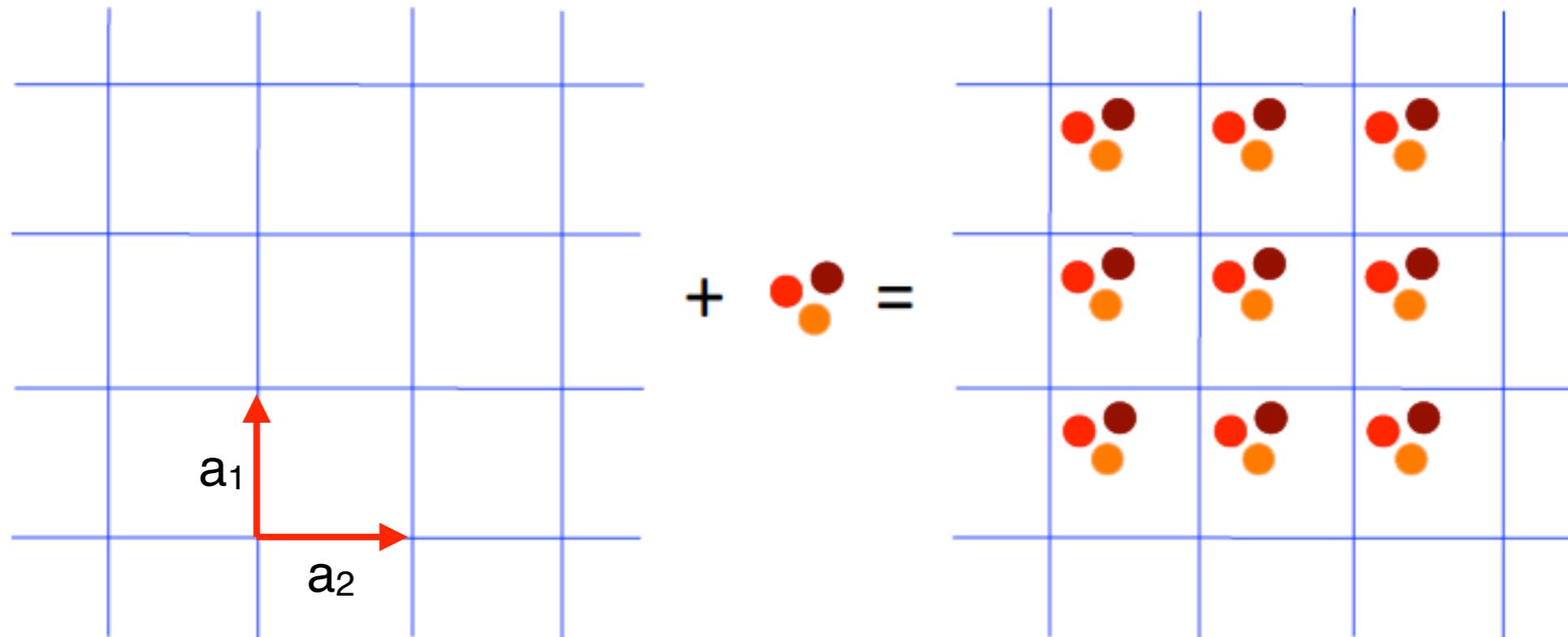
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  Si 0.25 0.25 0.25
K_POINTS automatic
  4 4 4 1 1 1
```



# Periodic boundary conditions

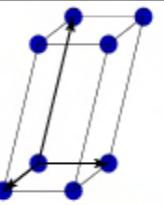
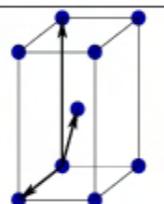
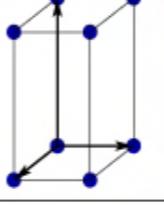
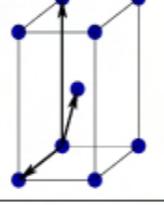
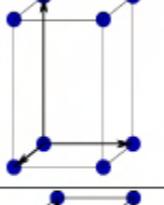
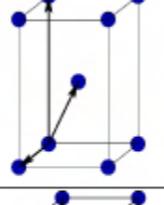
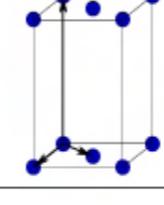
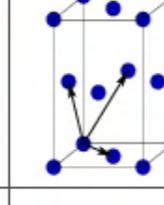
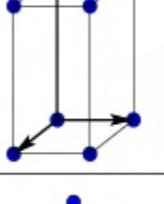
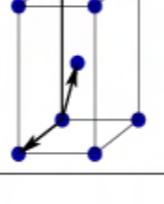
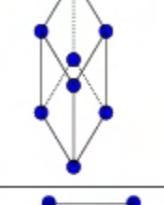
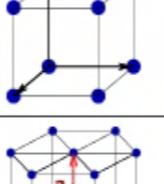
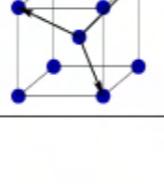
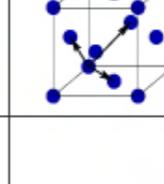
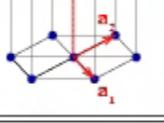
Crystal structure: Bravais lattice + Atomic basis



- ☞ **Bravais lattice:** (shape of unit cell & how it repeats). Specified by primitive lattice vectors  $a_1, a_2, a_3$   
 $R = n_1a_1 + n_2a_2 + n_3a_3$ , where  $n_1, n_2, n_3$  are integers.
- ☞ **Atomic basis:** how many atoms are in the unit cell, and how they are arranged.

# Periodic boundary conditions

4 Lattice types

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

7 Crystal classes

# Structure of QE input file

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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
```

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)

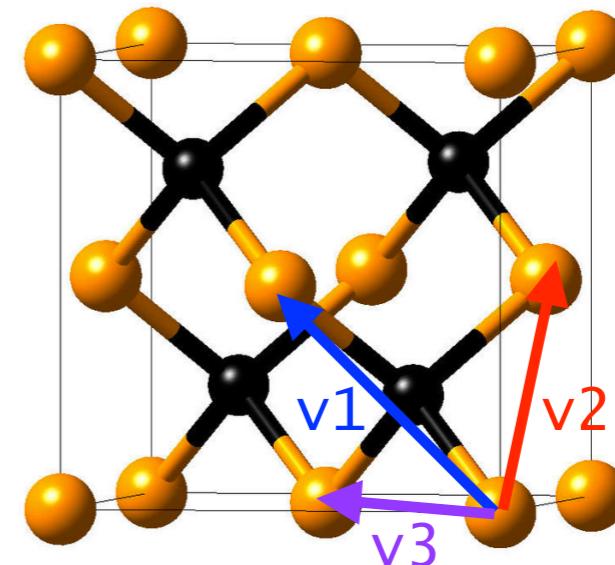
## face centered cubic:

v1 = (a/2)(-1,0,1)  
v2 = (a/2)(0,1,1)  
v3 = (a/2)(-1,1,0)

# Structure of QE input file

```
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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
```

FCC structure



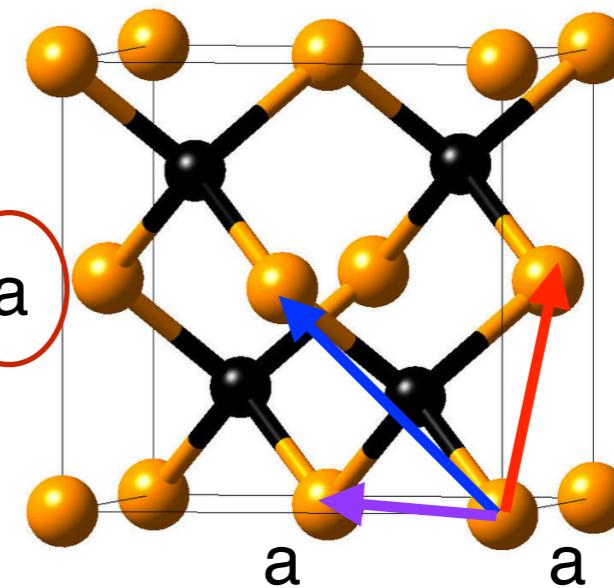
Silicon

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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K_POINTS automatic
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```

FCC structure

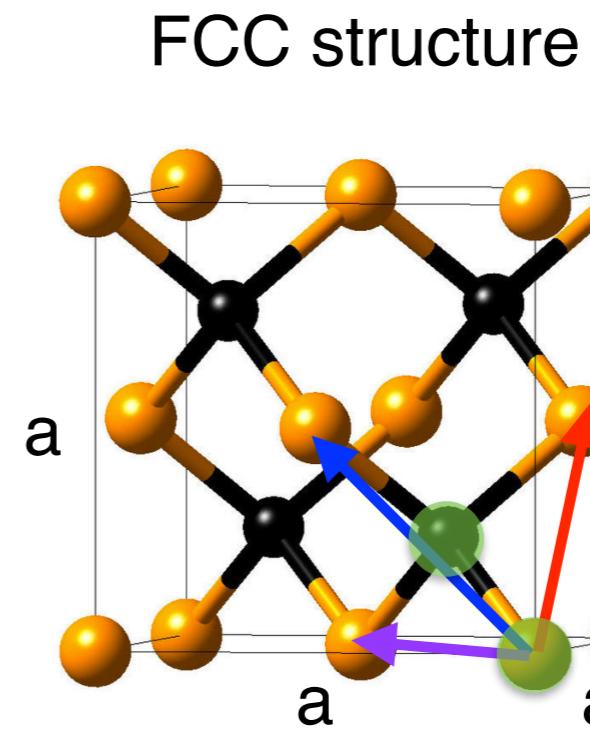


face centered cubic:  
v1 =  $(a/2)(-1,0,1)$   
v2 =  $(a/2)(0,1,1)$   
v3 =  $(a/2)(-1,1,0)$

$$1 \text{ bohr} = 0.529177 \text{ \AA}$$

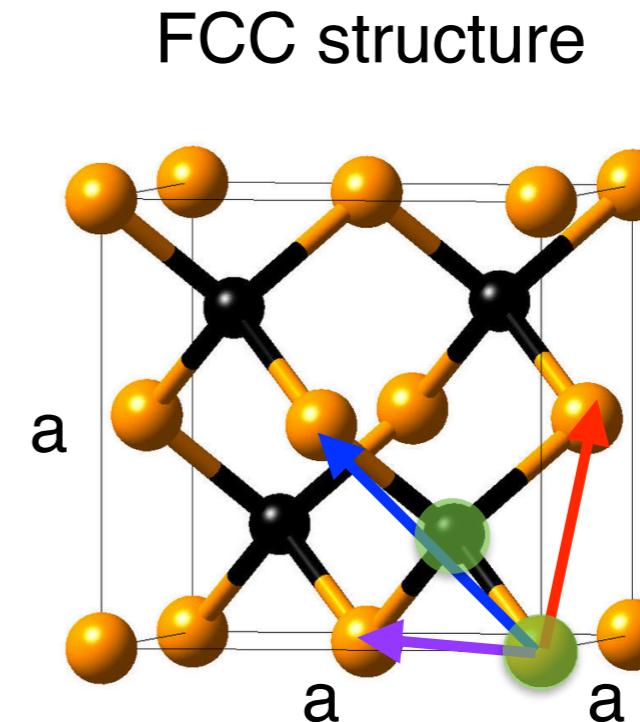
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  ecutwfc=60.0,
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/
ATOMIC_SPECIES
  Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```



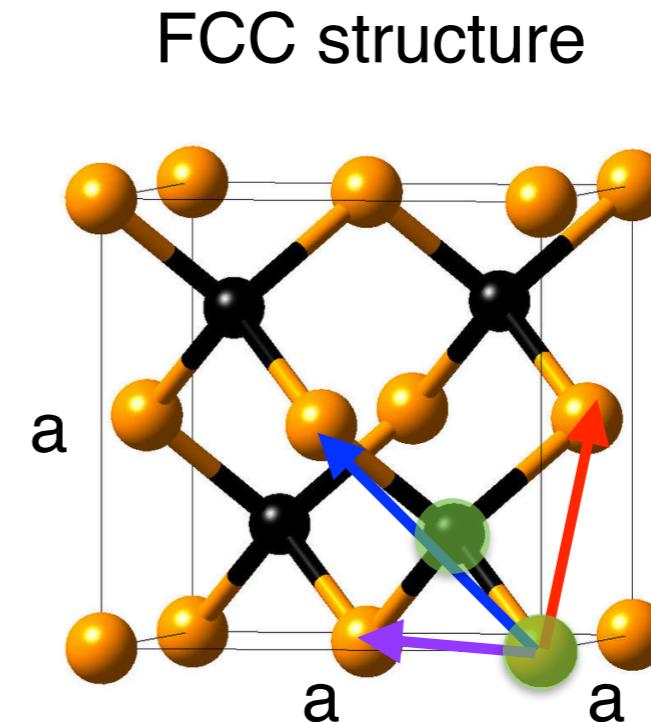
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  ecutwfc=60.0,
  ecutrho=720.0,
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&ELECTRONS
  mixing_beta=0.7,
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  Si 28.0855 Si.pbe-rrkj.UPF ←
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  Si  0.00  0.00  0.00
  Si  0.25  0.25  0.25
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  4 4 4 1 1 1
```



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  Si  0.25  0.25  0.25
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  4 4 4 1 1 1
```



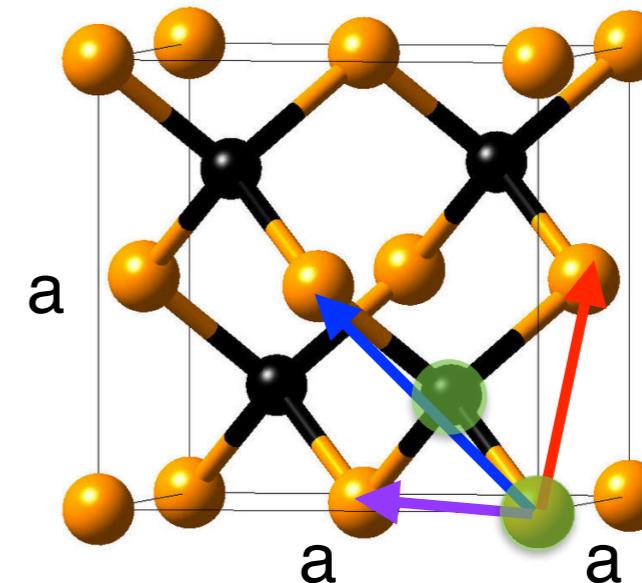
Mass of Si

# Structure of QE input file

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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
```

PP file

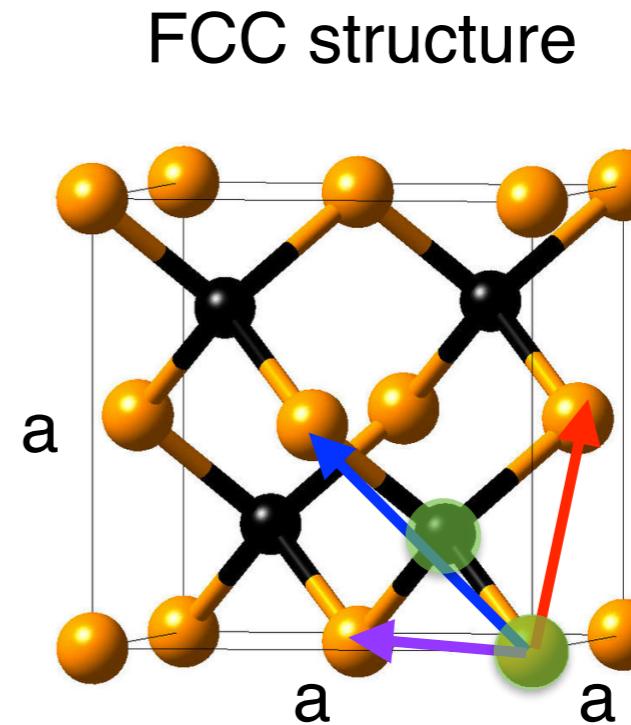
FCC structure



Silicon

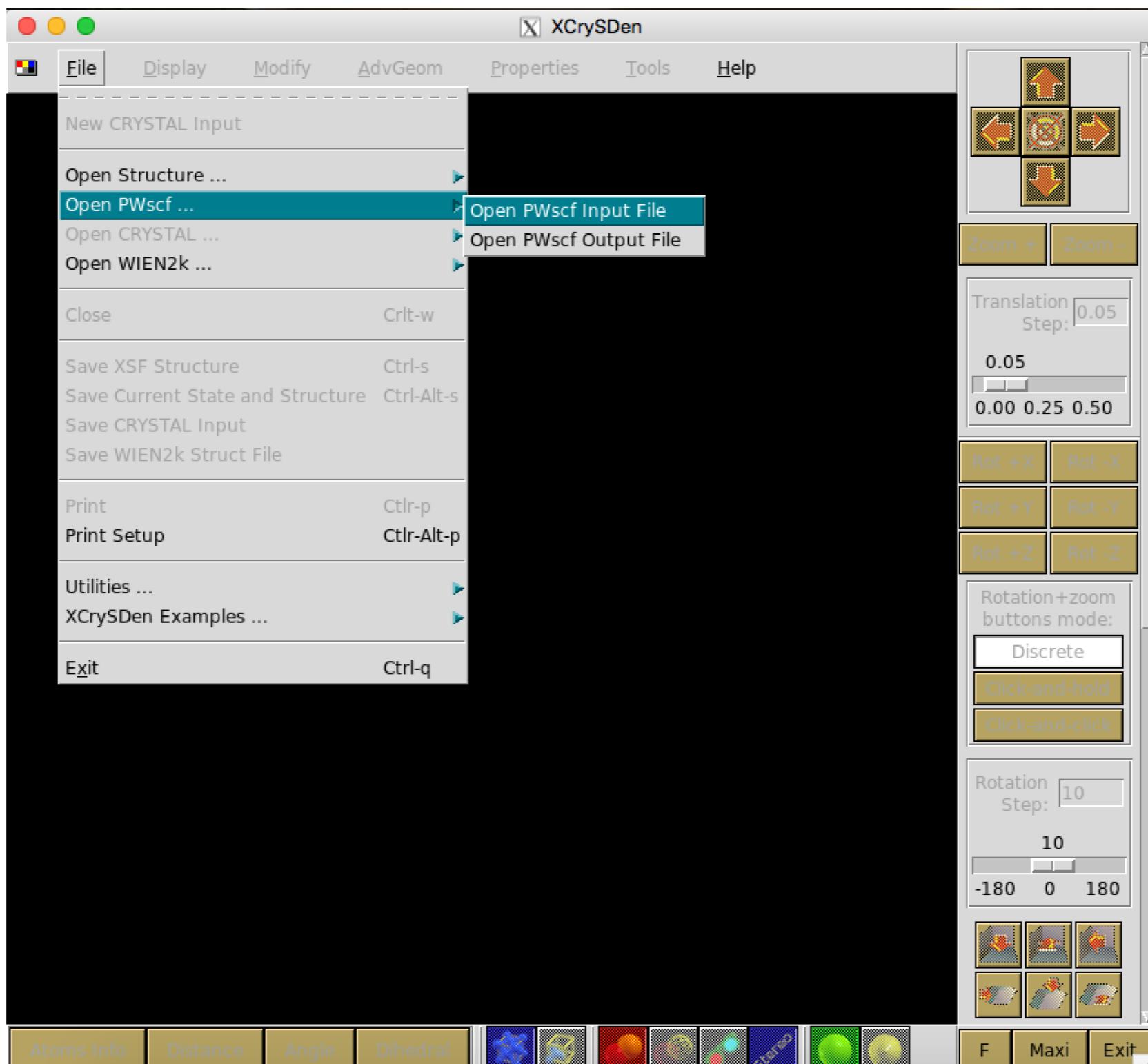
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  Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
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Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```



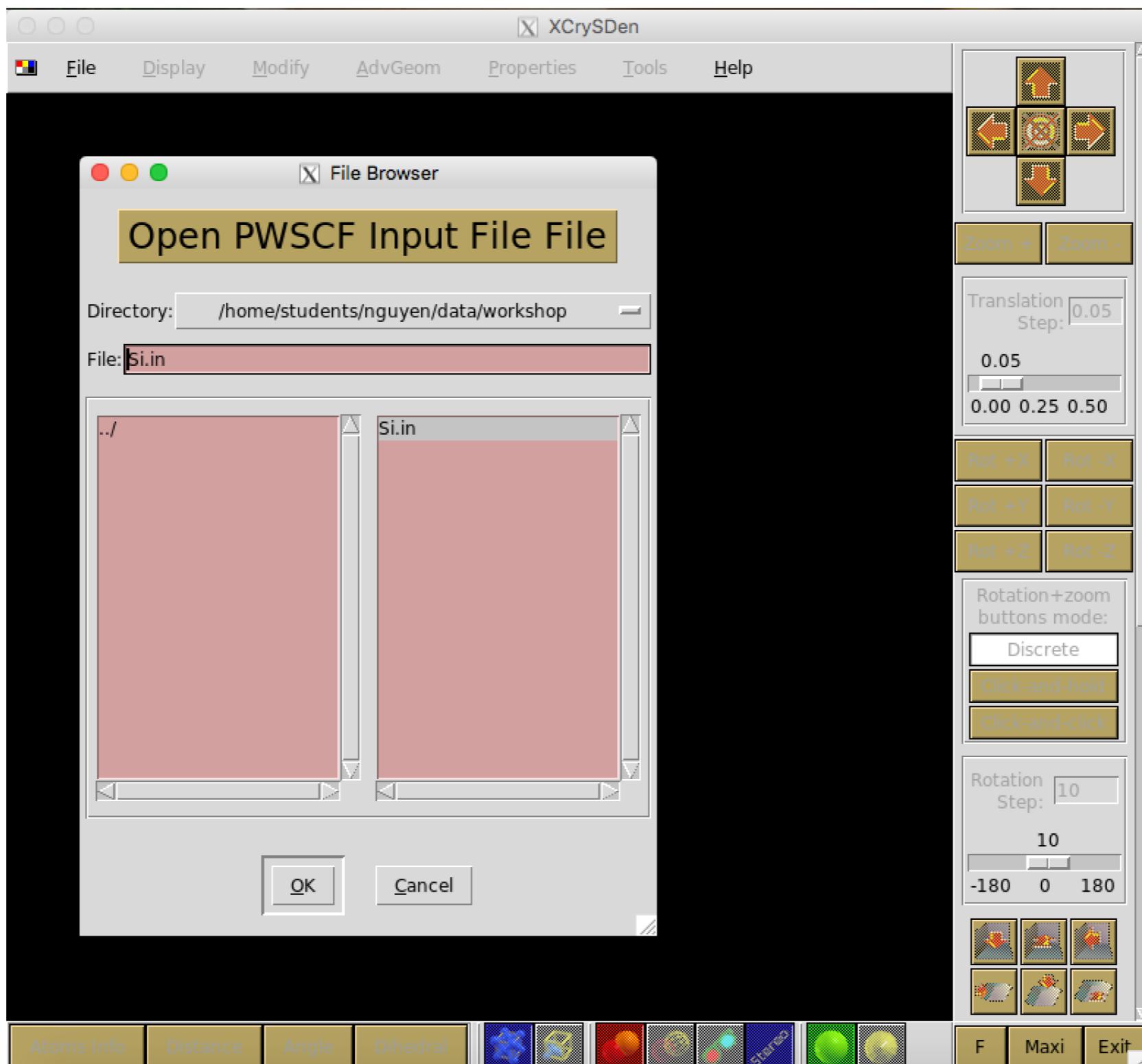
atomic positions are in cartesian coordinates, in units of the lattice parameter.

# How to check model structure

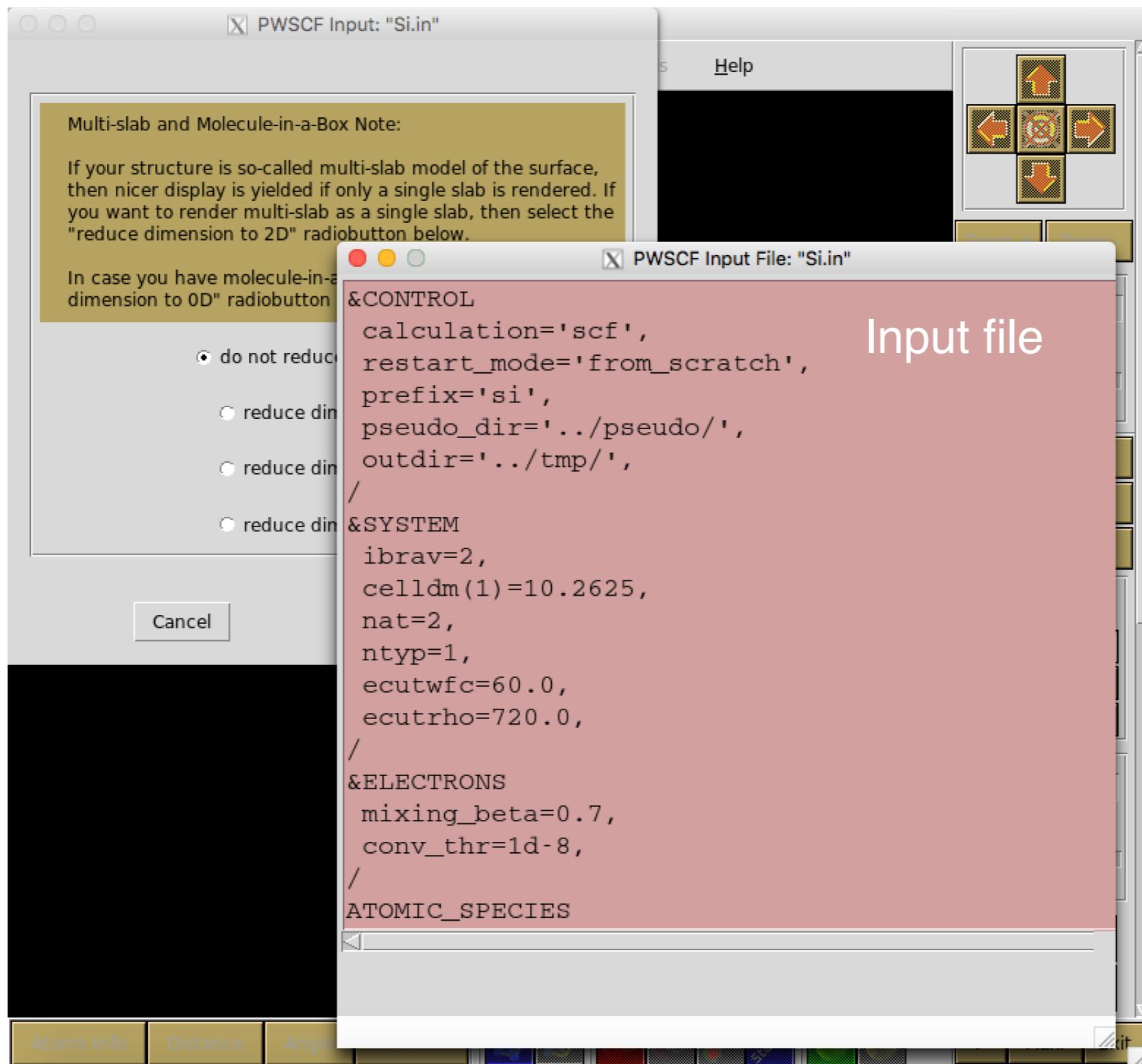


Xcrysden: <http://www.xcrysden.org/>

# How to check model structure



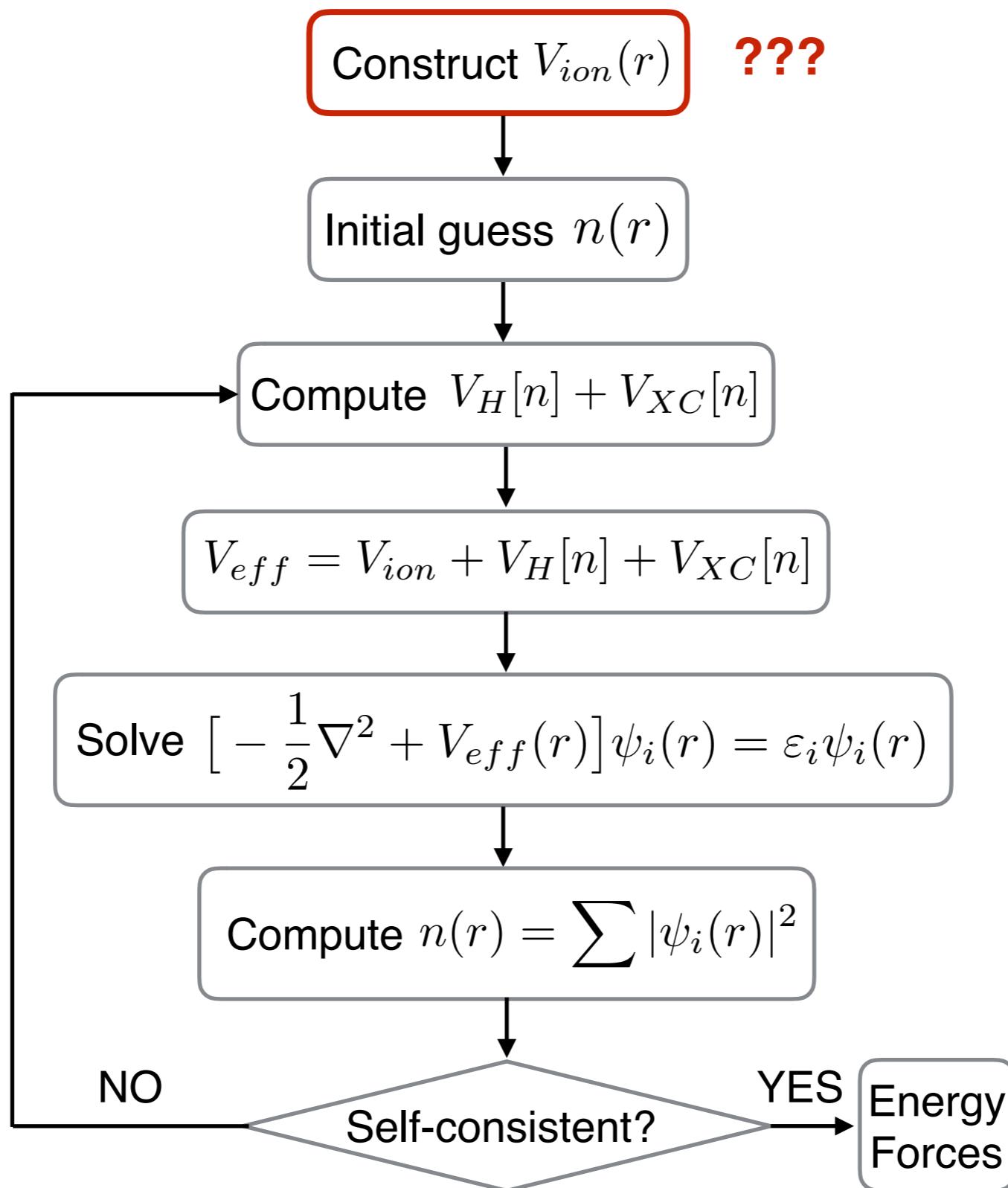
# How to check model structure



# How to check model structure



# External nuclear potential



# External nuclear potential

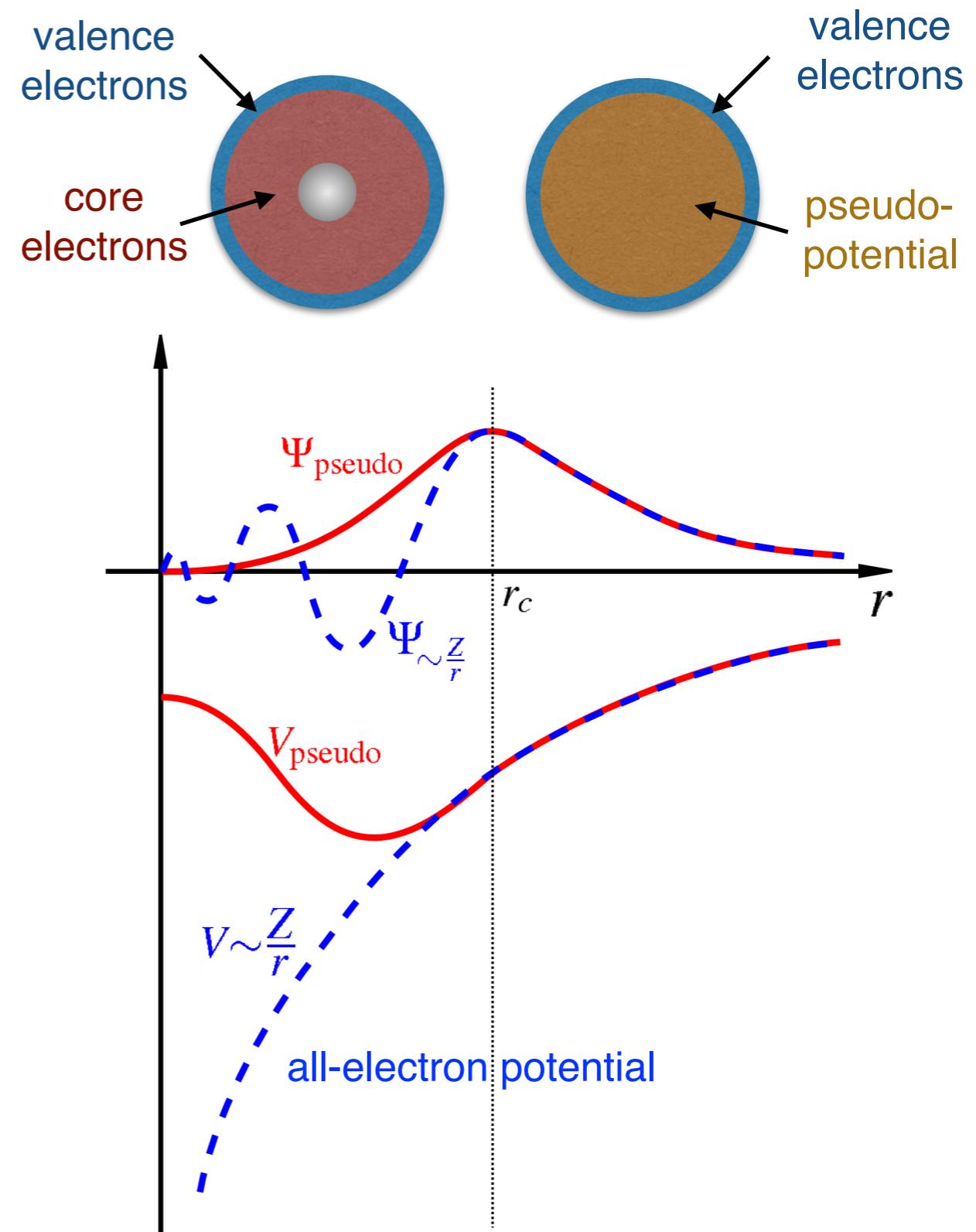
Electrons experience a Coulomb potential due to the nuclei with simple form:

$$V_{ion} = -\frac{Z}{r}$$

But this leads to computational problems!

## Pseudopotential (PP):

Replace the strong Coulomb potential of the nucleus and tightly bound core electrons by an effective ionic potential acting on the valence electrons.



# Pseudopotential

```
&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  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
```

← Name of the pseudopotential file

# How to get pseudopotential

<http://www.quantum-espresso.org/pseudopotentials/>

| ANY FUNCTIONAL |             | ANY TYPE      |           | Apply Filter |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
|----------------|-------------|---------------|-----------|--------------|-----------|-----------|-----------|-----------|-----------|----------|----------|----------|----------|-----------|-----------|-----------|----------|----------|
| ANY PP LIBRARY |             | OTHER OPTIONS |           |              |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
| 1<br>H         |             |               |           |              | 2<br>He   |           |           |           |           |          |          |          |          |           |           |           |          |          |
| 3<br>Li        | 4<br>Be     |               |           |              |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
| 11<br>Na       | 12<br>Mg    |               |           |              |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
| 19<br>K        | 20<br>Ca    |               |           |              |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
| 37<br>Rb       | 38<br>Sr    |               |           |              |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
| 55<br>Cs       | 56<br>Ba    | 57-70<br>*    |           |              |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
| 87<br>Fr       | 88<br>Ra    | 89-102<br>**  |           |              |           |           |           |           |           |          |          |          |          |           |           |           |          |          |
|                |             |               | 21<br>Sc  | 22<br>Ti     | 23<br>V   | 24<br>Cr  | 25<br>Mn  | 26<br>Fe  | 27<br>Co  | 28<br>Ni | 29<br>Cu | 30<br>Zn | 31<br>Ga | 32<br>Ge  | 33<br>As  | 34<br>Se  | 35<br>Br | 36<br>Kr |
|                |             |               | 39<br>Y   | 40<br>Zr     | 41<br>Nb  | 42<br>Mo  | 43<br>Tc  | 44<br>Ru  | 45<br>Rh  | 46<br>Pd | 47<br>Ag | 48<br>Cd | 49<br>In | 50<br>Sn  | 51<br>Sb  | 52<br>Te  | 53<br>I  | 54<br>Xe |
|                |             |               | 71<br>Lu  | 72<br>Hf     | 73<br>Ta  | 74<br>W   | 75<br>Re  | 76<br>Os  | 77<br>Ir  | 78<br>Pt | 79<br>Au | 80<br>Hg | 81<br>Tl | 82<br>Pb  | 83<br>Bi  | 84<br>Po  | 85<br>At | 86<br>Rn |
|                |             |               | 103<br>Lr | 104<br>Rf    | 105<br>Db | 106<br>Sg | 107<br>Bh | 108<br>Hs | 109<br>Mt |          |          |          |          |           |           |           |          |          |
| *              | Lanthanoids |               | 57<br>La  | 58<br>Ce     | 59<br>Pr  | 60<br>Nd  | 61<br>Pm  | 62<br>Sm  | 63<br>Eu  | 64<br>Gd | 65<br>Tb | 66<br>Dy | 67<br>Ho | 68<br>Er  | 69<br>Tm  | 70<br>Yb  |          |          |
| **             | Actinoids   |               | 89<br>Ac  | 90<br>Th     | 91<br>Pa  | 92<br>U   | 93<br>Np  | 94<br>Pu  | 95<br>Am  | 96<br>Cm | 97<br>Bk | 98<br>Cf | 99<br>Es | 100<br>Fm | 101<br>Md | 102<br>No |          |          |

PSEUDO SEARCH RESULTS

Pseudopotential File

**Si.blyp-hgh.UPF**

Pseudopotential type: NORMCONS  
Method: Goedecker-Hartwigsen-Hutter-Teter  
Functional type: Becke-Lee-Yang-Parr (BLYP) exch-corr  
non relativistic

Origin: Hartwigsen-Goedecker-Hutter PP  
Author: Goedecker/Hartwigsen/Hutter/Teter  
Generated in analytical, separable form. Converted from CPMD format using cpmd2upf v.5.0.1.  
Uploaded by marsamos  
Classification unverified

**Si.pbe-rrkj.UPF**

Pseudopotential type: NORMCONS  
Method: Rappe Rabe Kaxiras Joannopoulos  
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr  
scalar relativistic

Origin: Original QE PP library  
Author: Andrea Dal Corso  
Generated by Andrea Dal Corso code (rrkj3)  
Uploaded by Erica Vidal  
Classification controlled by Paolo Giannozzi

**Si.pbe-van\_gipaw.UPF**

Pseudopotential type: ULTRASOFT  
Method: Rappe Rabe Kaxiras Joannopoulos  
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr  
Is Gipaw  
scalar relativistic

Origin: Original QE PP library  
Generated by "atomic" code by A. Dal Corso (QE distribution)  
Uploaded by Erica Vidal  
Classification controlled by Paolo Giannozzi

## Si.pbe-rrkj.UPF

- ▶ type of exchange-correlation functional
- ▶ type of pseudopotential

# Pseudopotential

```

&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  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

```

Si.pbe-rrkj.UPF

```

<PP_INFO>
Generated using Andrea Dal Corso code (rrkj3)
Author: Andrea Dal Corso Generation date: unknown
Info: Si PBE 3s2 3p2 RRKJ3
      0 The Pseudo was generated with a Non-Relativistic calculation
      2.50000000000E+00 Local Potential cutoff radius
n1 pn 1 occ          Rcut          Rcut US          E pseu
3S 1 0 2.00          2.50000000000          2.60000000000          0.00000000000
3S 1 0 0.00          2.50000000000          2.60000000000          0.00000000000
3P 2 1 2.00          2.50000000000          2.70000000000          0.00000000000
3D 3 2 0.00          2.50000000000          2.50000000000          0.00000000000
</PP_INFO>

<PP_HEADER>
  0 Version Number
  Si Element
  NC Norm - Conserving pseudopotential
  F Nonlinear Core Correction
  SLA PW PBE PBE PBE Exchange-Correlation functional
  4.00000000000 Z valence
  -7.47480832270 Total energy
  0.0000000 0.0000000 Suggested cutoff for wfc and rho
  2 Max angular momentum component
  883 Number of points in mesh
  2 3 Number of Wavefunctions, Number of Projectors
  Wavefunctions
  n1 1 occ
  3S 0 2.00
  3P 1 2.00
</PP_HEADER>

<PP_MESH>
  <PP_R>
  1.77053726905E-04 1.79729551320E-04 1.82445815642E-04 1.85203131043E-04
  1.88002117930E-04 1.90843406086E-04 1.93727634813E-04 1.96655453076E-04
  1.99627519645E-04 2.02644503249E-04 2.05707082721E-04 2.08815947154E-04
  2.11971796056E-04 2.15175339506E-04 2.18427298316E-04 2.21728404189E-04
  2.25079399889E-04 2.28481039403E-04 2.31934088115E-04 2.35439322975E-04
  2.38997532677E-04 2.42609517831E-04 2.46276091150E-04 2.49998077629E-04
  2.53776314730E-04 2.57611652573E-04 2.61504954124E-04 2.65457095393E-04
  2.69468965628E-04 2.73541467517E-04 2.77675517391E-04 2.81872045428E-04
  2.86131995864E-04 2.90456327206E-04 2.94846012447E-04 2.99302039285E-04
  3.03825410344E-04 3.08417143402E-04 3.13078271619E-04 3.17809843768E-04
  3.22612924472E-04 3.27488594446E-04 3.32437950735E-04 3.37462106965E-04
  3.42562193593E-04 3.47739358159E-04 3.52994765549E-04 3.58329598249E-04

```

# Plane wave expansion

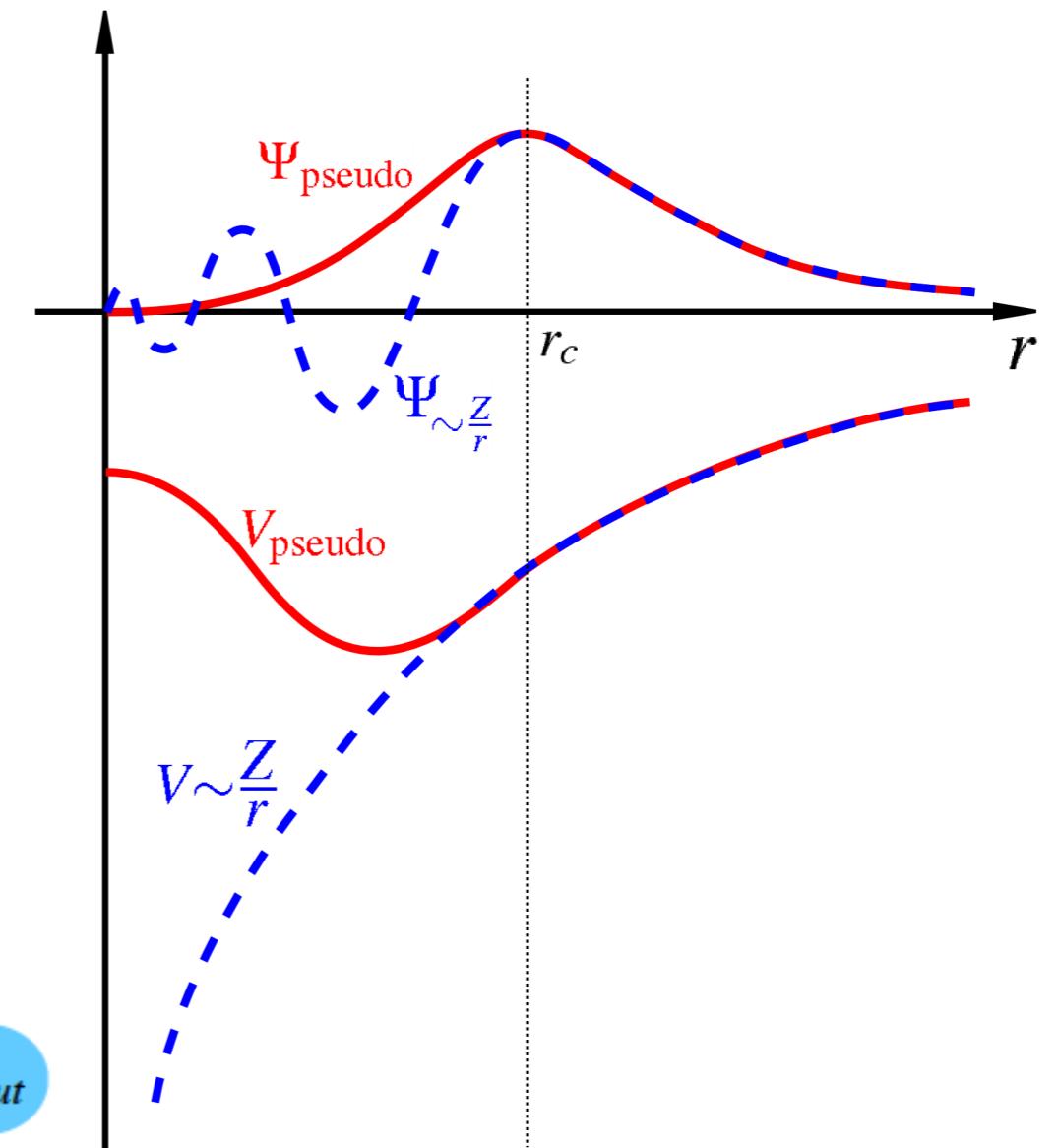
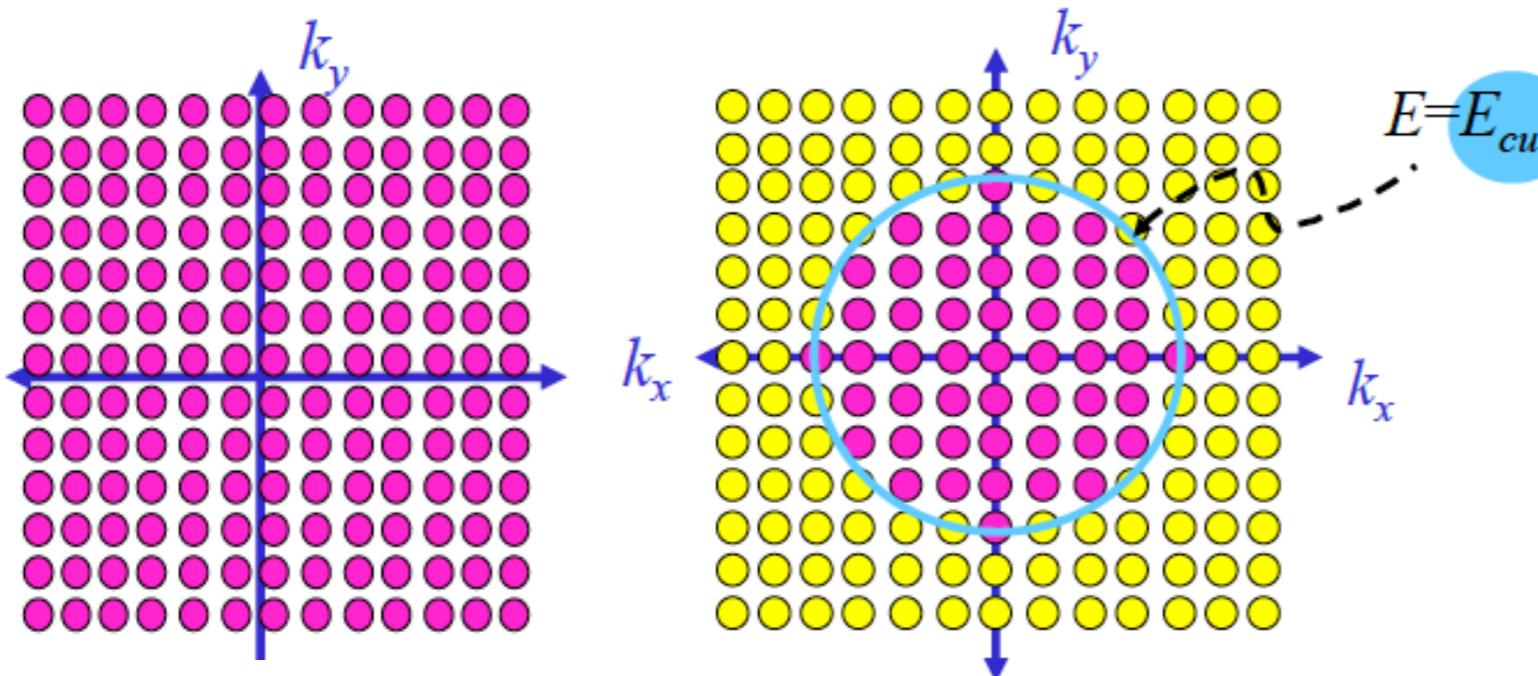
In a periodic system we can write the KS states as a superposition of plane waves:

$$\Psi_{k,n}(r) = \frac{1}{\Omega} \sum_G c_{k,n}^G e^{i(k+G) \cdot r}$$

$G$  are vectors in reciprocal space.

The sum, in principle infinite, can be truncated:

$$\frac{\hbar^2}{2m} |k + G|^2 \leq E_{cut}$$



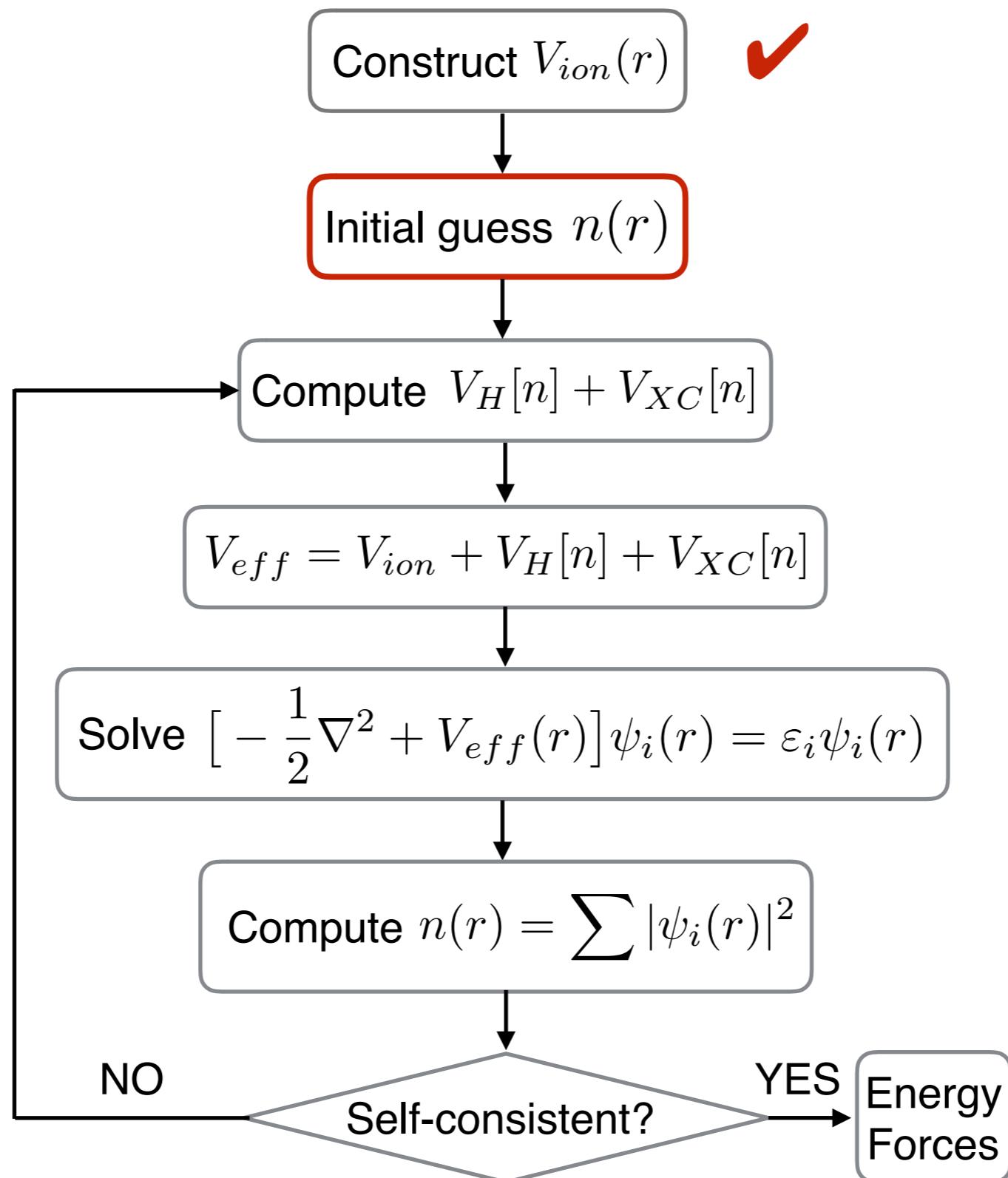
# Plane wave expansion

```
&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  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
```

$$\frac{\hbar^2}{2m} |k + G|^2 \leq E_{cut}$$

Units: Ry (1 Ry = 0.5 Ha = 13.6057 eV)  
For ultrasoft pseudopotentials we have also:  
**ecutrho = usually 8-12 × ecutwfc**

# Initial $n(r)$



# Initial n(r)

```
&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  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
```

startingwfc = 'atomic' (DEFAULT)  
= 'random'  
= 'file'

# Sampling of the Brillouin zone

Many quantities we need to compute involve an integral over the BZ:

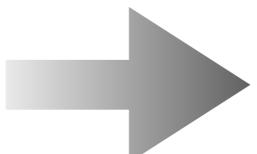
$$\bar{A} = \frac{1}{\Omega_{BZ}} \int_{BZ} A(k) d(k)$$

An example is the electronic density  $n(r)$ :

$$n(r) = \frac{1}{\Omega_{BZ}} \sum_i \int_{BZ} |\Psi_{i,k}(r)|^2 f(\epsilon_{i,k} - \epsilon_F) d(k)$$

In practice the integral is discretized:

$$\frac{1}{\Omega_{BZ}} \int_{BZ} d(k) \rightarrow \sum_k \omega_k$$



How do we choose the  $k$  points to include in the sum???

# Monkhorst and Pack (1976)

**Example:** square 2D lattice

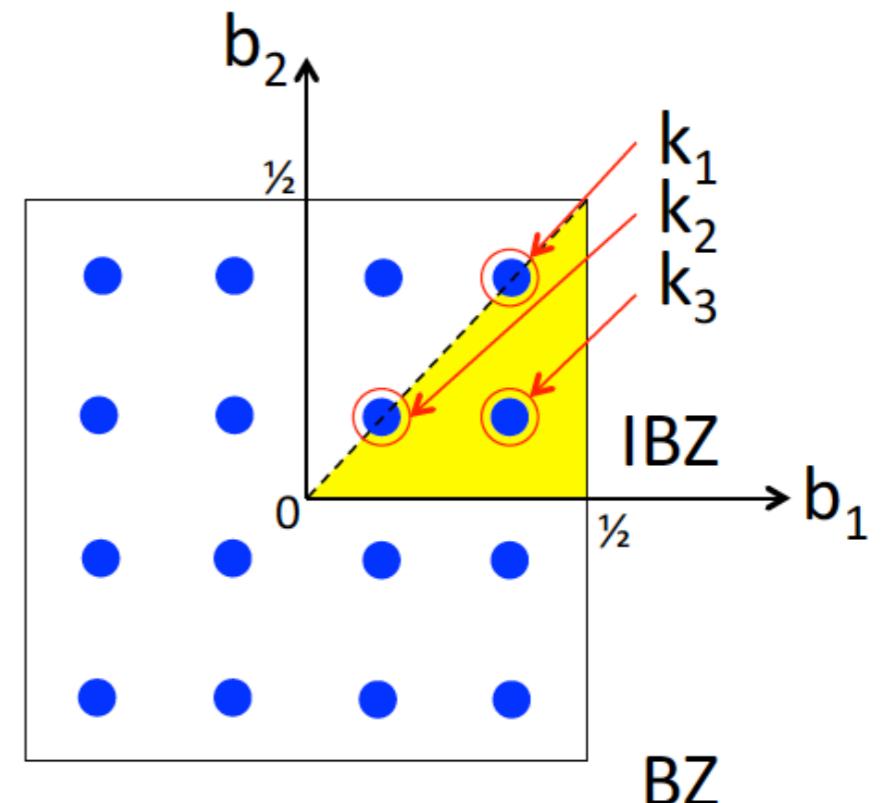
4×4 k-points grid (16 points)

3 inequivalent point (IBZ)

$$4 \times k_1 \rightarrow \omega_1 = 4/16 = 1/4$$

$$4 \times k_2 \rightarrow \omega_2 = 4/16 = 1/4$$

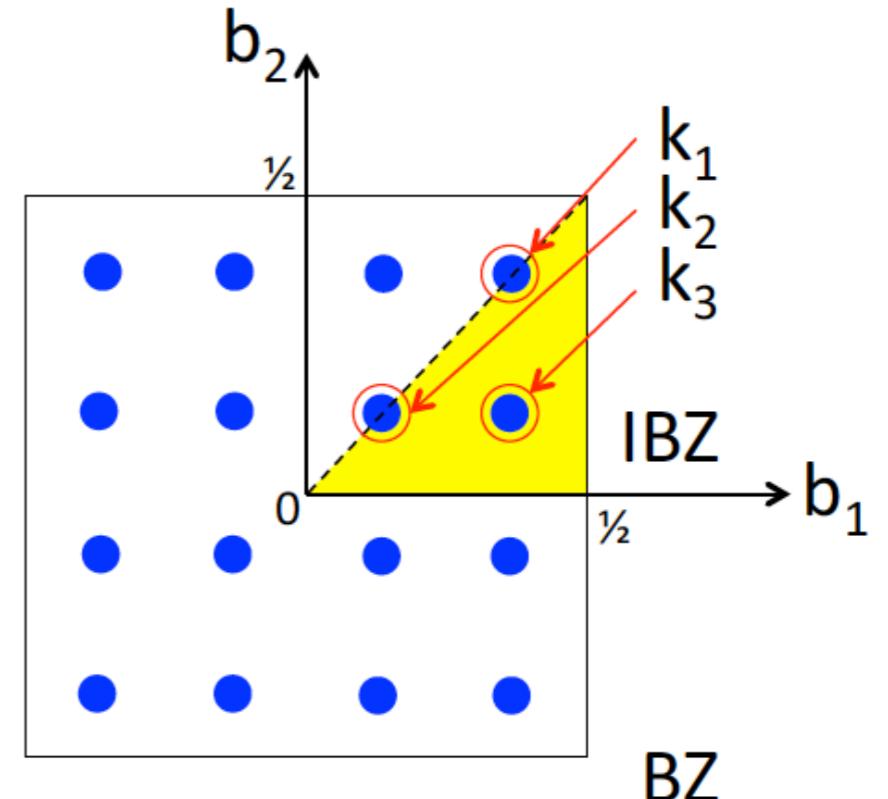
$$8 \times k_3 \rightarrow \omega_3 = 8/16 = 1/2$$



$$\frac{1}{\Omega_{BZ}} \int_{BZ} A(k) d(k) \simeq \frac{1}{4} A(k_1) + \frac{1}{4} A(k_2) + \frac{1}{2} A(k_3)$$

# Sampling of the Brillouin zone

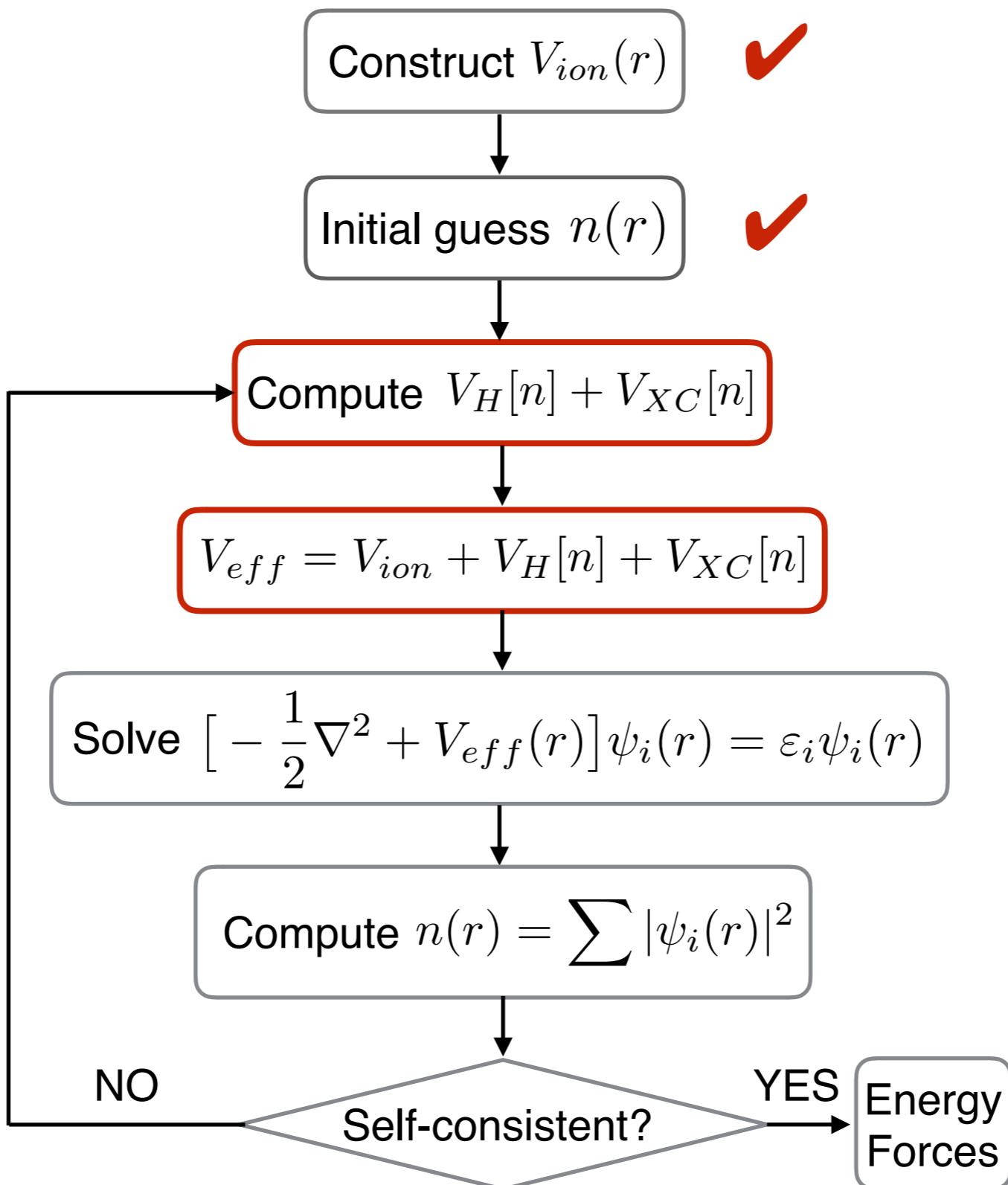
```
&CONTROL
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  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  nat=2,
  ntyp=1,
  ecutwfc=60.0,
  ecutrho=720.0,
/
&ELECTRONS
  mixing_beta=0.7,
  conv_thr=1d-8,
/
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
```



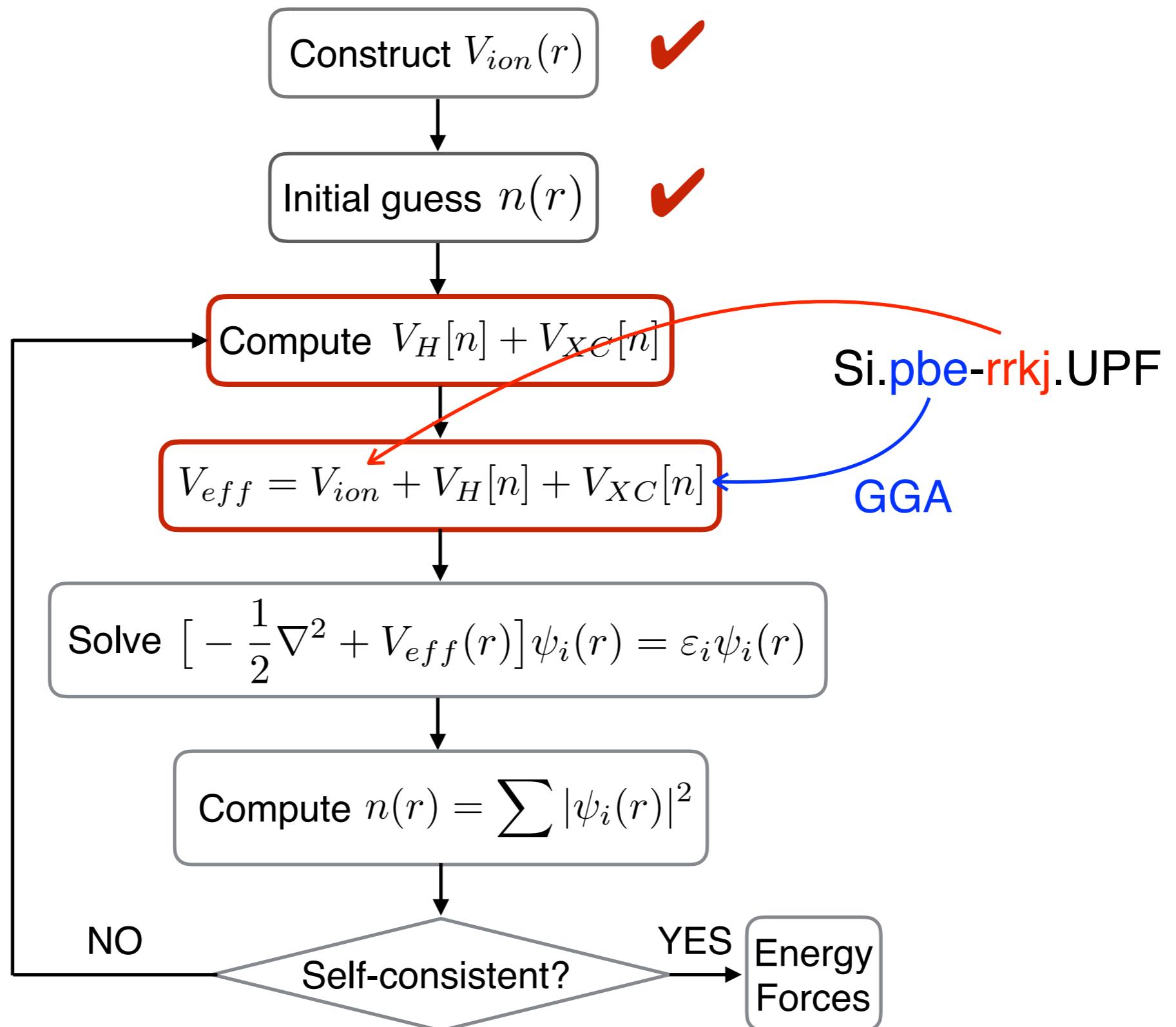
K\_POINTS automatic  
nk1, nk2, nk3, k1, k2, k3

nk1, nk2, nk3 as in Monkhorst-Pack  
grids k1, k2, k3 must be 0 ( no offset ) or  
1 ( grid displaced by half a grid step in  
the corresponding direction )

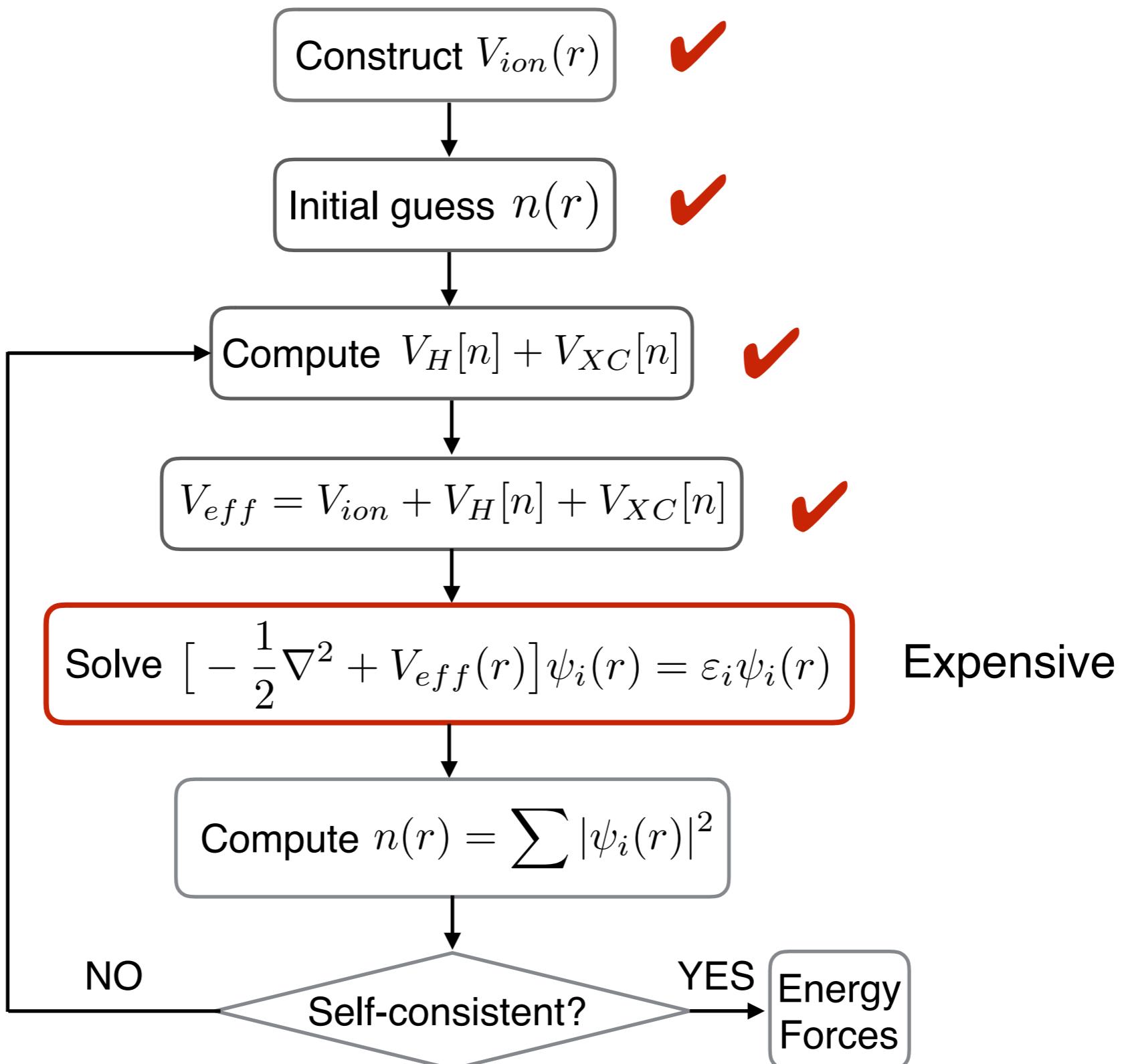
# QE run



# QE run



# QE run

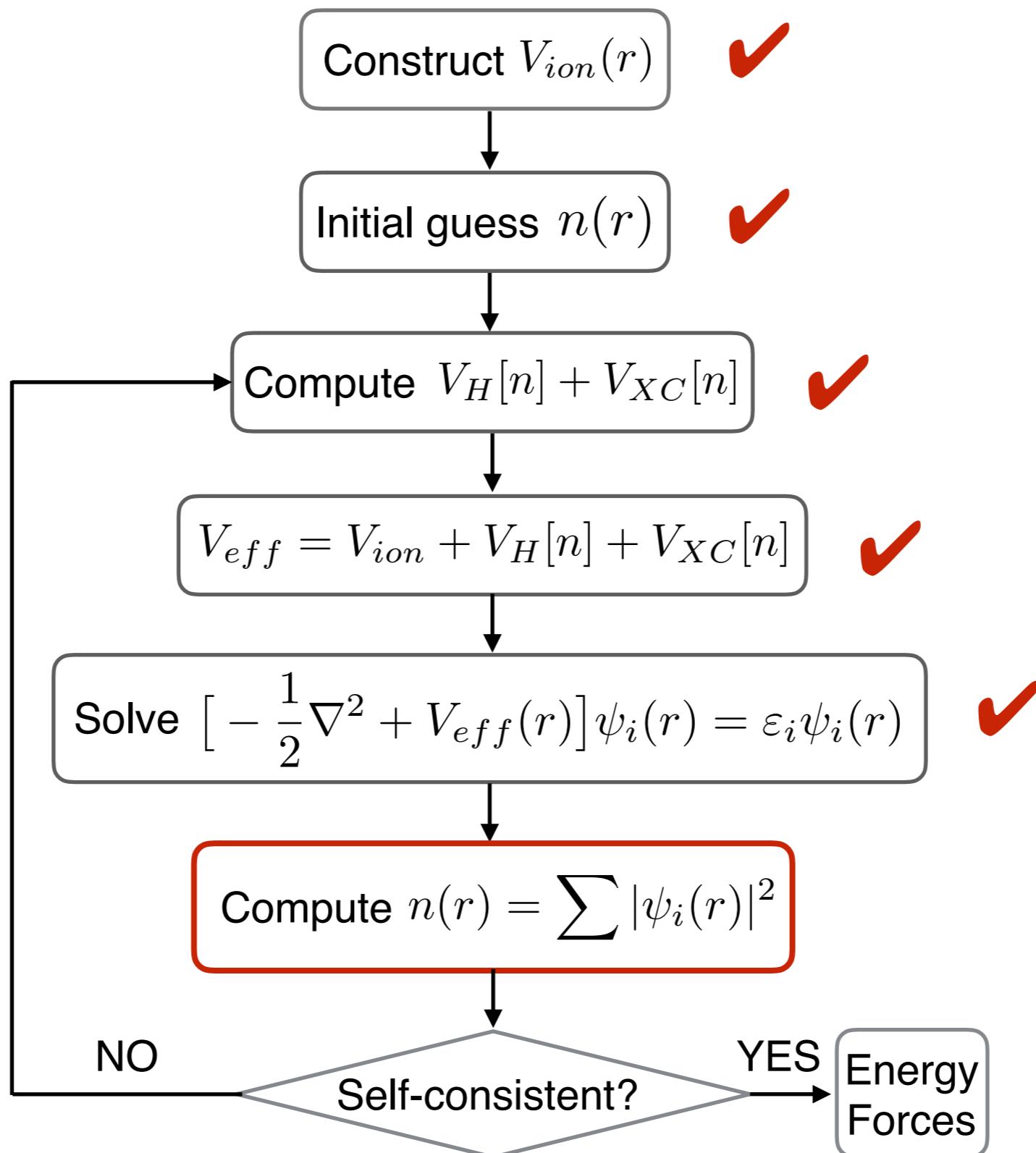


# Solve wave equation

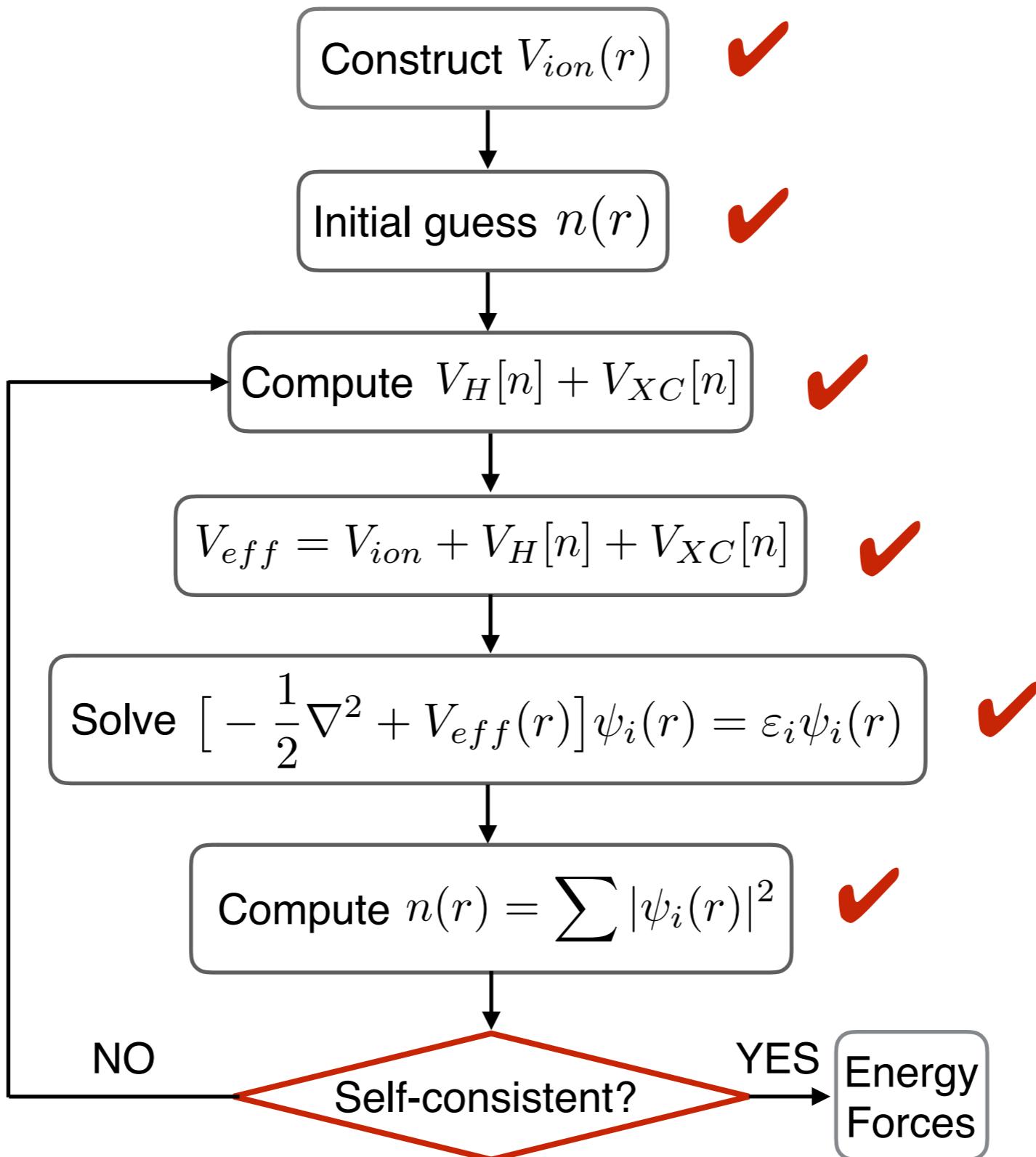
```
&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  nat=2,
  ntyp=1,
  ecutwfc=60.0,
  ecutrho=720.0,
/
&ELECTRONS
  mixing_beta=0.7,
  conv_thr=1d-8,
/
ATOMIC_SPECIES
  Si 28.0855 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
```

diagonalization = 'david' (DEFAULT)  
= 'cg'

# QE run



# QE run

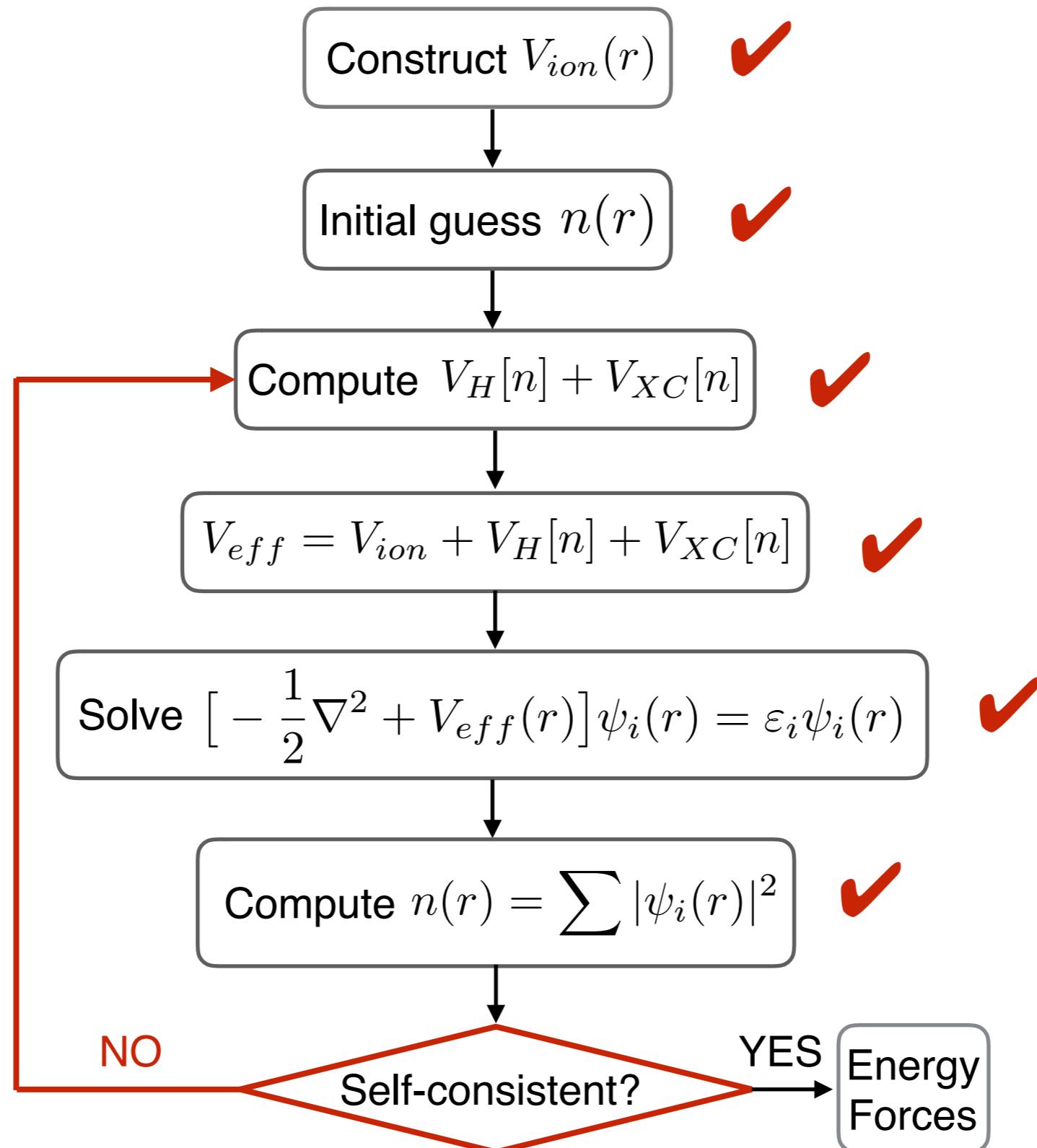


# Self-consistency

```
&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  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
```

Convergence threshold for self-consistency:  
estimated energy error > conv\_thr (NO)  
or energy error < conv\_thr (YES)

# QE run

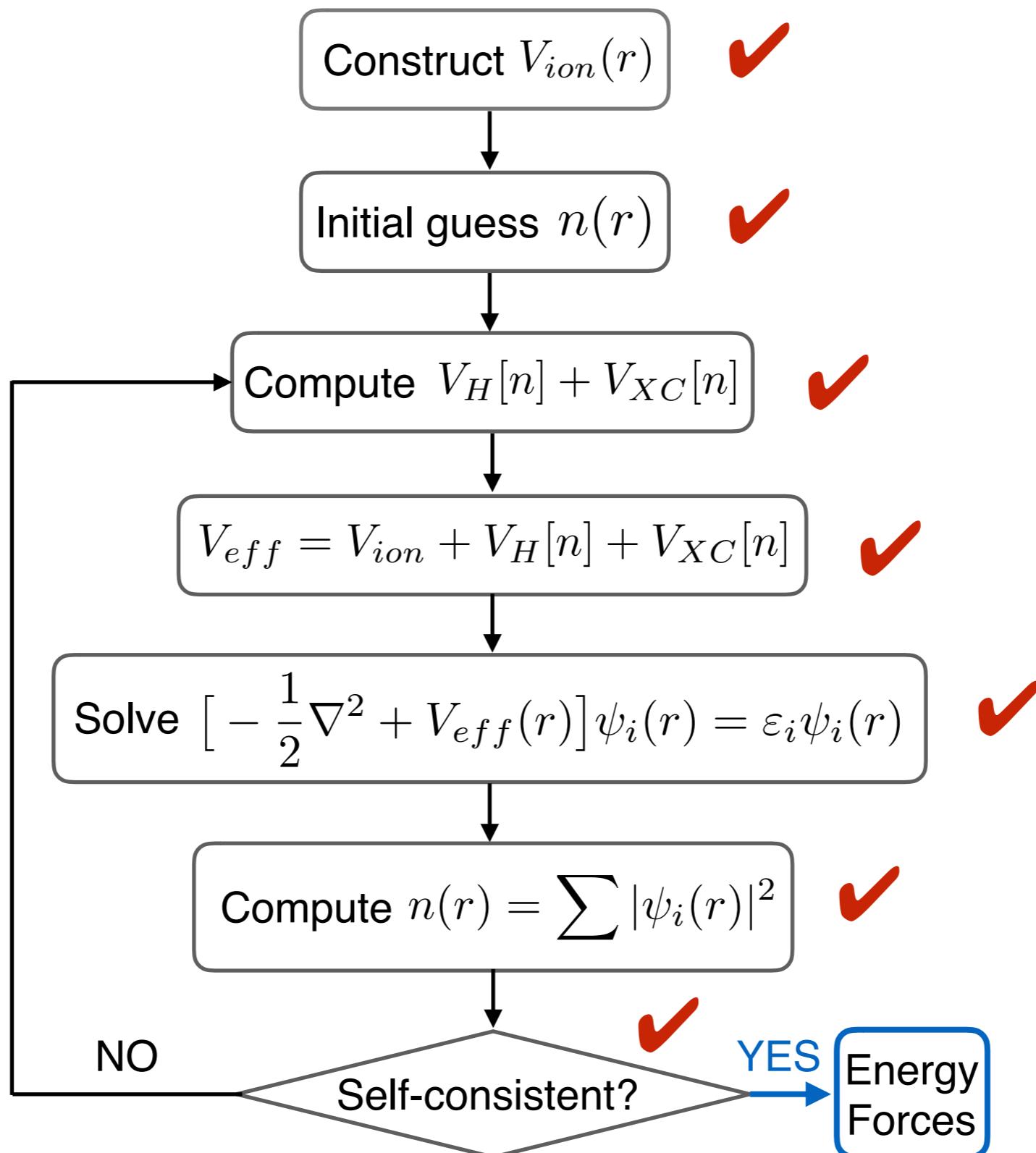


# new n(r)

```
&CONTROL
  calculation='scf',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../../pseudo/',
  outdir='../../tmp/',
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  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
```

Mix new and old density:  
0.7 = 70% of the **new density** and  
30% of **old density** at first step

# QE run



# Total energy

```
$ pw.x <Si.scf.in> Si.scf.out &
$ vi Si.scf.out
or
$ grep ! Si.scf.out
```

```
highest occupied level (ev):      5.9399

! total energy                  = -15.74122935 Ry
Harris-Foulkes estimate        = -15.74122935 Ry
estimated scf accuracy         <      8.8E-09 Ry

The total energy is the sum of the following terms:

one-electron contribution =      4.77318714 Ry
hartree contribution       =      1.09508506 Ry
xc contribution             =     -4.81266477 Ry
ewald contribution          =    -16.79683678 Ry

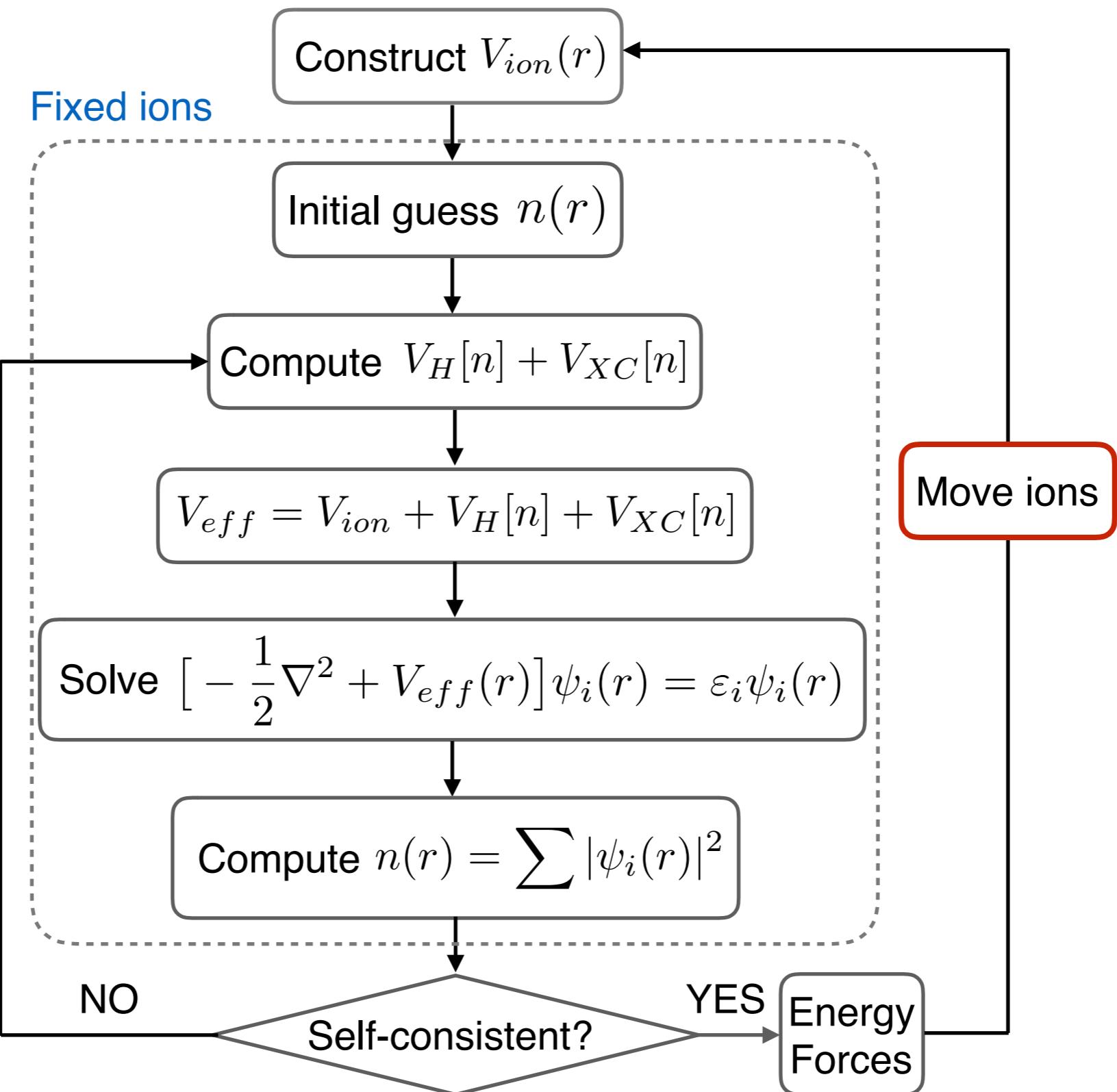
convergence has been achieved in   6 iterations

Writing output data file si.save

init_run      :      0.59s CPU      0.88s WALL (      1 calls)
electrons     :      1.24s CPU      1.52s WALL (      1 calls)

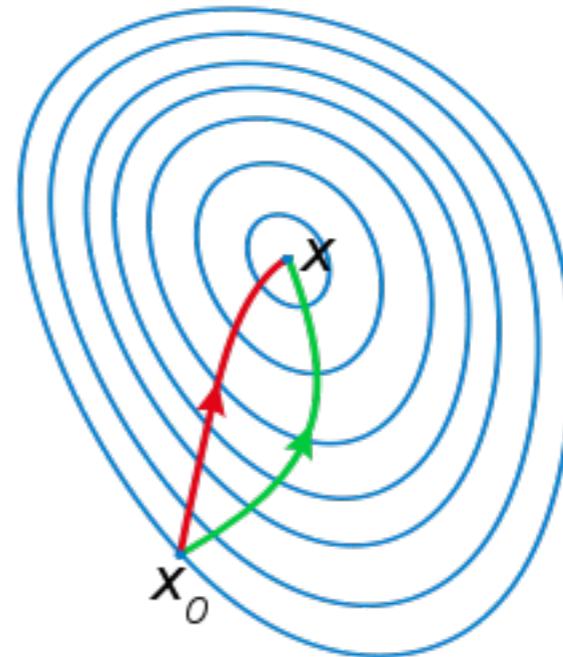
Called by init_run:
wfcinit      :      0.08s CPU      0.22s WALL (      1 calls)
potinit      :      0.06s CPU      0.07s WALL (      1 calls)
```

# QE run



# Structure optimization

```
&CONTROL
  calculation='vc-relax',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../pseudo/',
  outdir='./tmp/',
  forc_conv_thr=1d-5,
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  nat=2,
  ntyp=1,
  ecutwfc=60.0,
  ecutrho=720.0,
/
&ELECTRONS
  mixing_beta=0.7,
  conv_thr=1d-8,
/
&IONS
  ion_dynamics='bfgs', ←
/
&CELL
  cell_dynamics='bfgs',
  press=0.0,
  press_conv_thr=0.5,
/
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
```



Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm is an **iterative method** for solving unconstrained **nonlinear optimization problems**.

# Structure optimization

```
&CONTROL
  calculation='vc-relax',
  restart_mode='from_scratch',
  prefix='si',
  pseudo_dir='../pseudo/',
  outdir='./tmp/',
  forc_conv_thr=1d-5,
/
&SYSTEM
  ibrav=2,
  celldm(1)=10.2625,
  nat=2,
  ntyp=1,
  ecutwfc=60.0,
  ecutrho=720.0,
/
&ELECTRONS
  mixing_beta=0.7,
  conv_thr=1d-8,
/
&IONS
  ion_dynamics='bfgs',
/
&CELL
  cell_dynamics='bfgs',
  press=0.0,
  press_conv_thr=0.5,
/
ATOMIC_SPECIES
  Si 28.0855 Si.pbe-rrkj.UPF
ATOMC_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
```

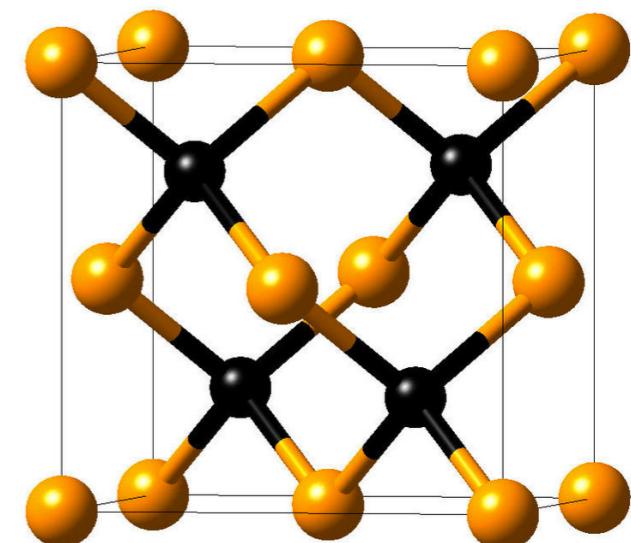
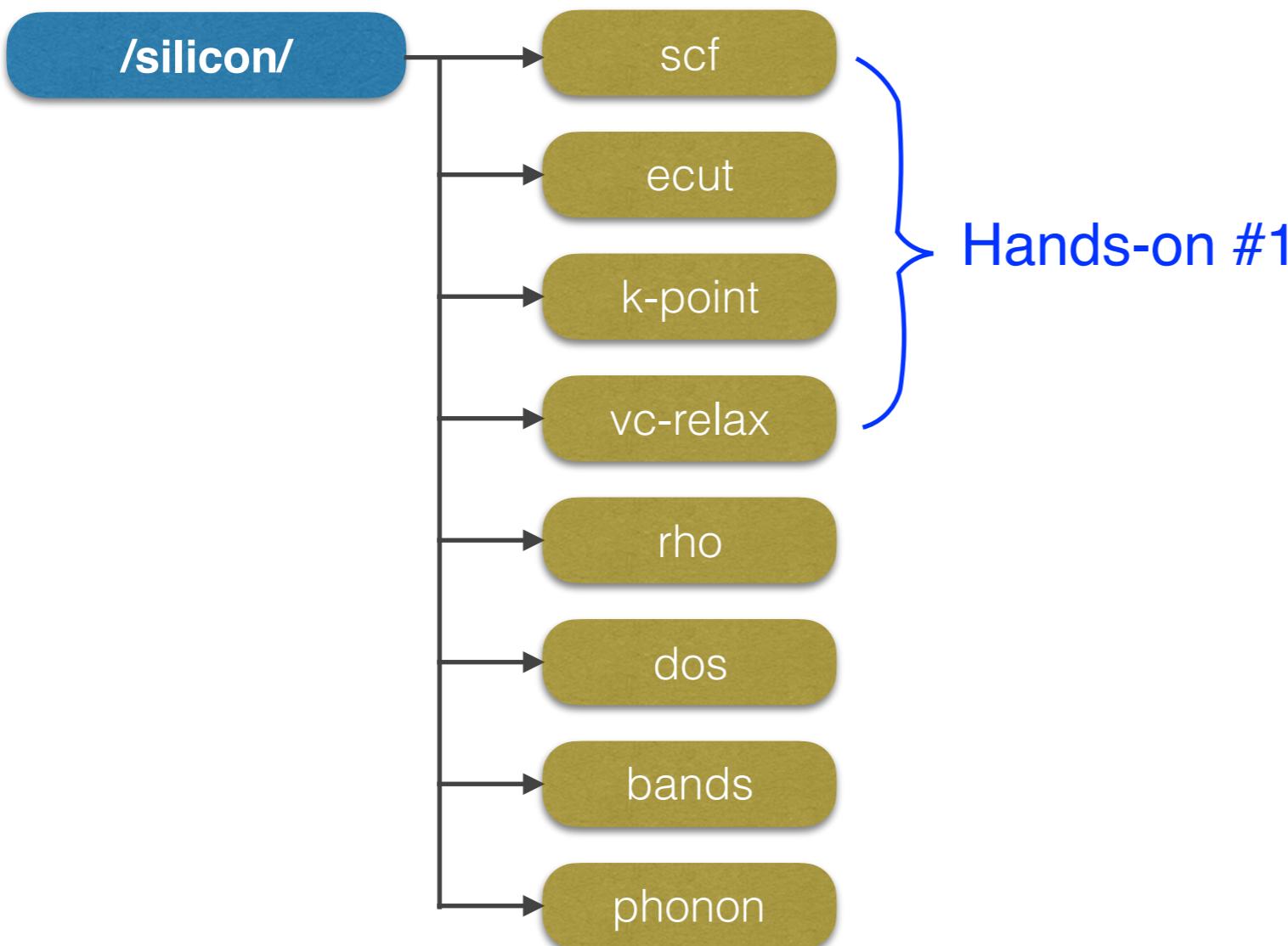
Cell lattice parameters and free (internal) coordinates of the atoms may be changed by relaxation

# What we will do today

## Hands-on #1: Total energy and relaxations for Silicon

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

Files for practice



Silicon

# Result

## Hands-on #1

- ▶ Basic self consistent calculation (scf)

/silicon/

scf

Command: \$ pw.x <Si.scf.in> Si.scf.out  
(pw.exe for windows users)

```
highest occupied level (ev):      5.9399
```

```
! total energy          = -15.74122935 Ry
Harris-Foulkes estimate = -15.74122935 Ry
estimated scf accuracy <     8.8E-09 Ry
```

```
The total energy is the sum of the following terms:
```

```
Parallel routines
fft_scatter :    0.16s CPU      0.24s WALL (    2061 calls)
PWSCF       :    1.96s CPU      4.47s WALL
```

```
This run was terminated on: 19: 3:24 14Feb2016
```

```
=-----  
| JOB DONE.  
=-----
```

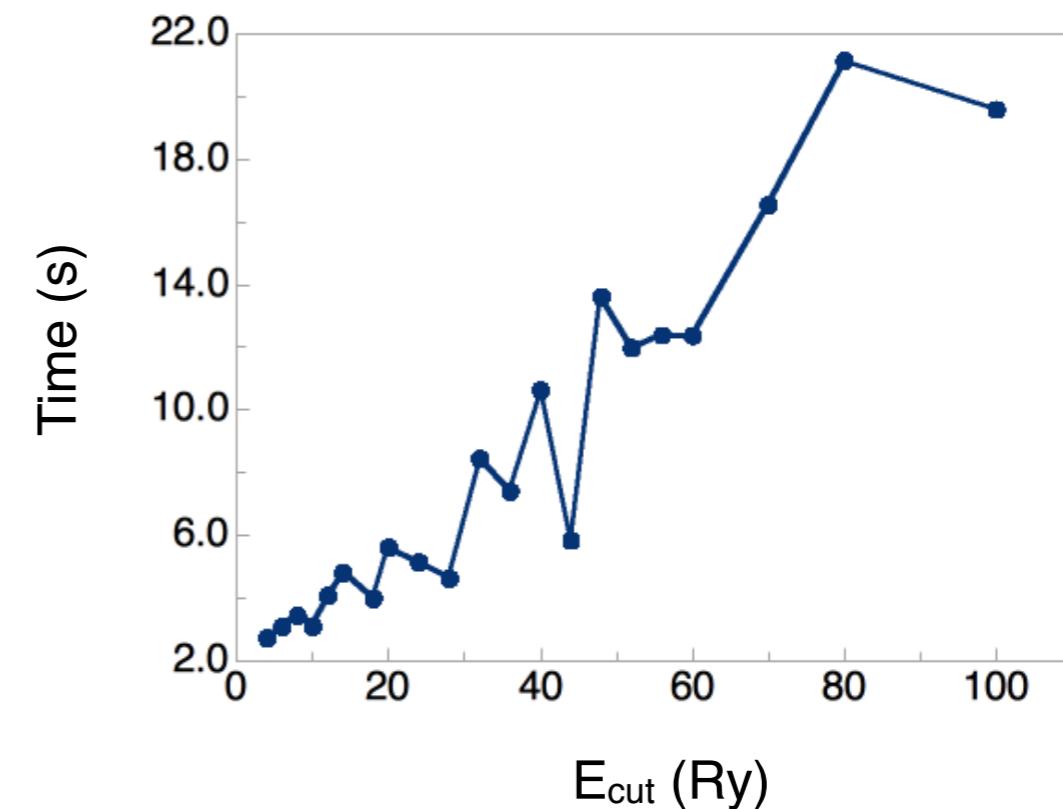
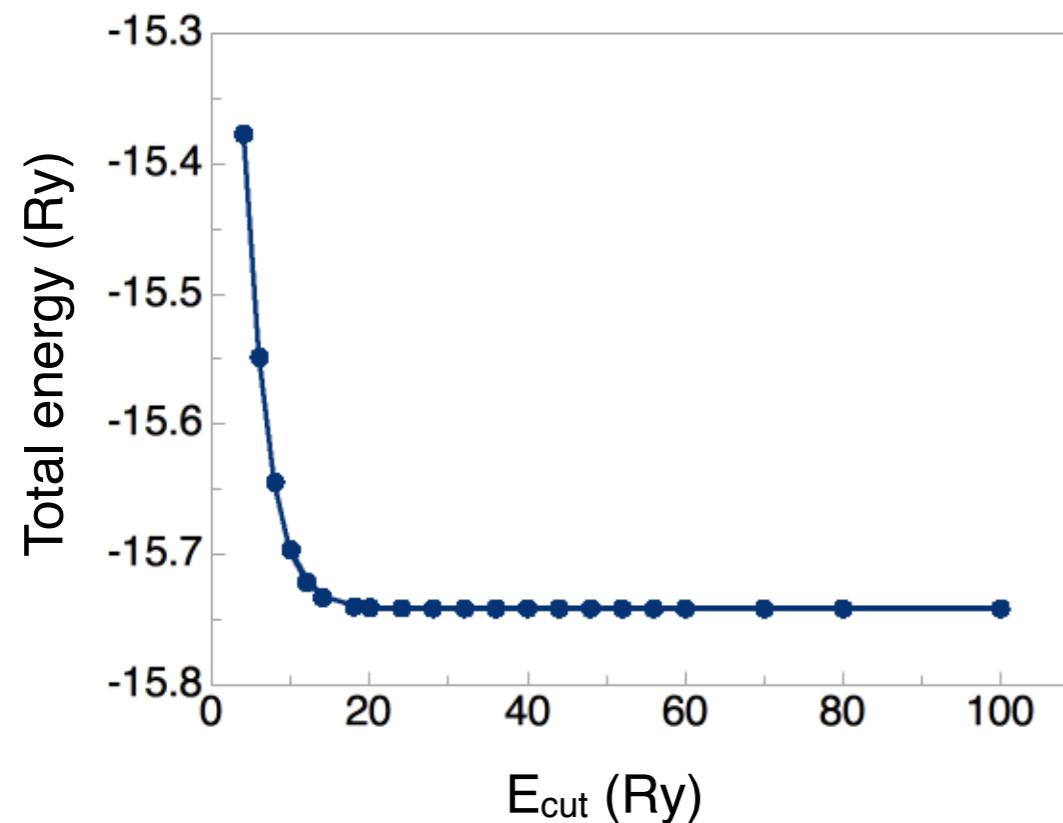
# Result

## Hands-on #1

- ▶ Convergence of total energy & plane waves cutoff (ecut)



Command: `$ pw.x <Si.ecut.#.in> Si.ecut.#.out`  
(pw.exe for windows users)



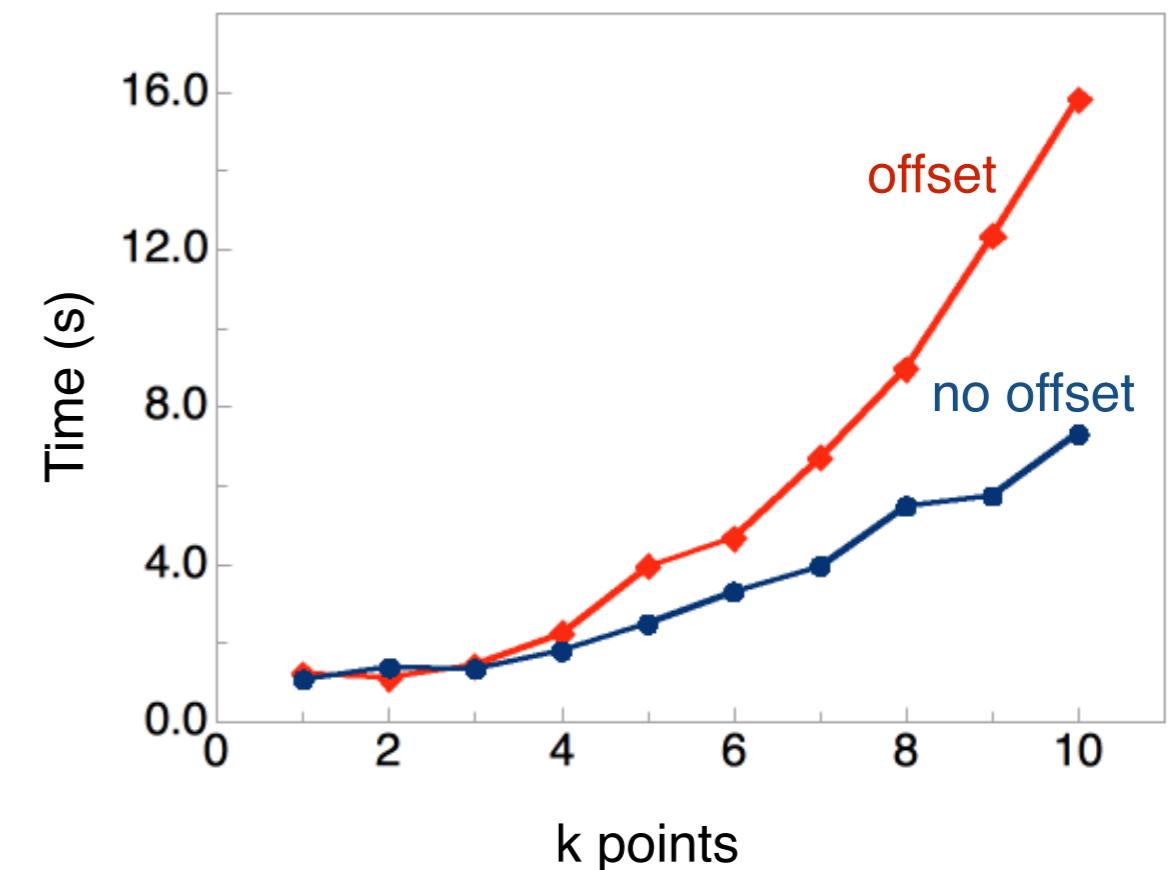
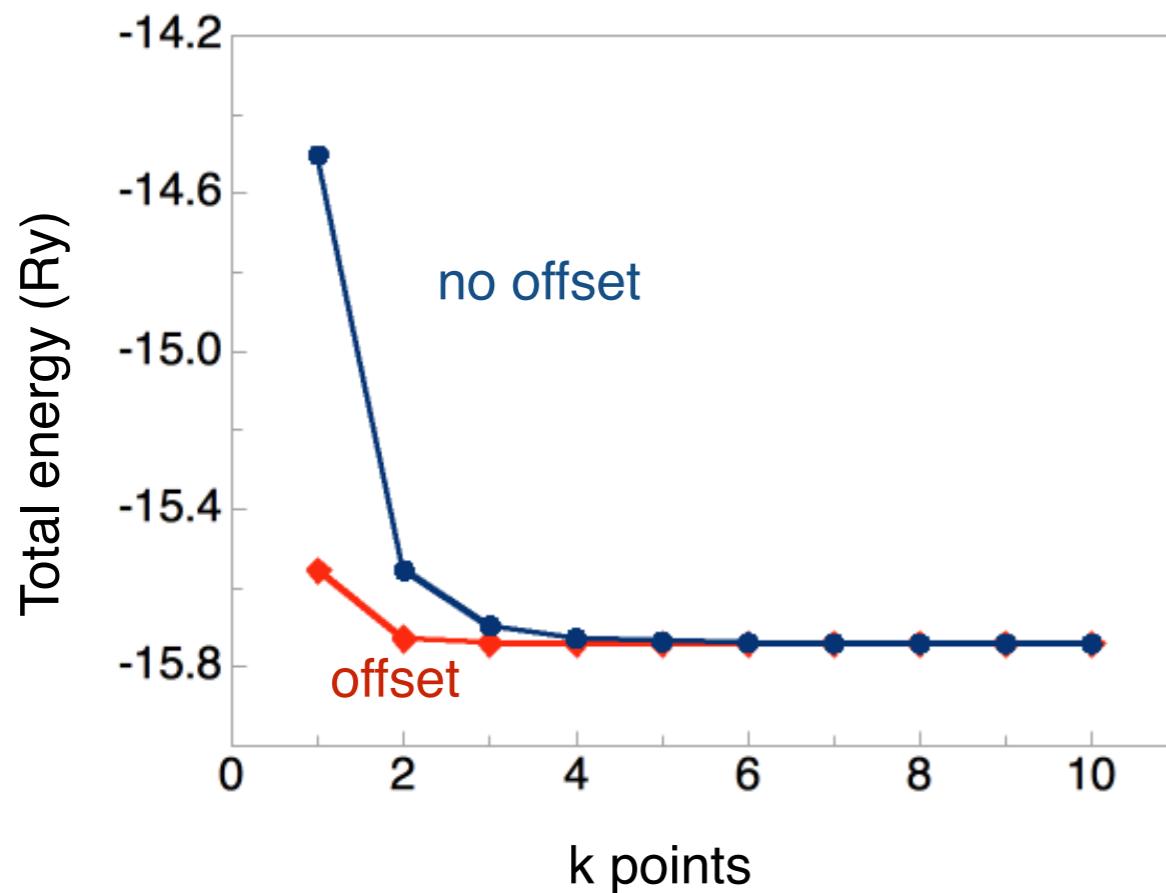
# Result

## Hands-on #1

- ▶ Convergence of total energy & BZ sampling (k-point)



Command: `$ pw.x <Si.k-point.#.#.in> si.k-point.#.#.out`  
(pw.exe for windows users)



# Result

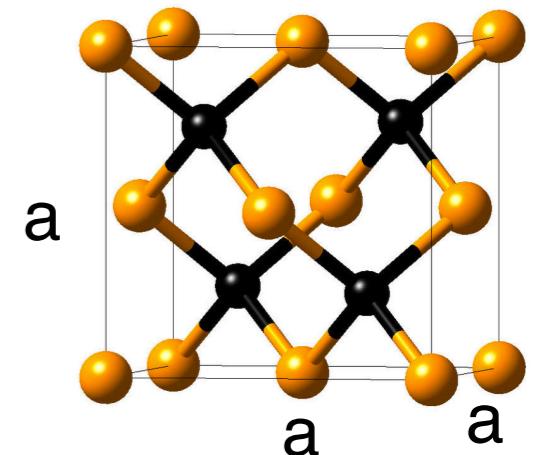
## Hands-on #1

### ► Lattice constant (vc-relax)

/silicon/

vc-relax

Command: \$ pw.x <Si.vc-relax.in> si.vc-relax.out a = 10.2500 Bohr  
(pw.exe for windows users)



Input:

a = 10.2500 Bohr

Output:

a = 10.3464 Bohr

```
bfgs converged in    4 scf cycles and    3 bfgs steps
(criteria: energy <  1.0E-04, force <  1.0E-05, cell <  5.0E-01)

End of BFGS Geometry Optimization

Final enthalpy =      -15.7417268079 Ry
Begin final coordinates
  new unit-cell volume =      276.89334 a.u.^3 (      41.03136 Ang^3 )

CELL_PARAMETERS (alat= 10.25000000)
-0.504704263  0.000000000  0.504704263
-0.000000000  0.504704263  0.504704263
-0.504704263  0.504704263  0.000000000

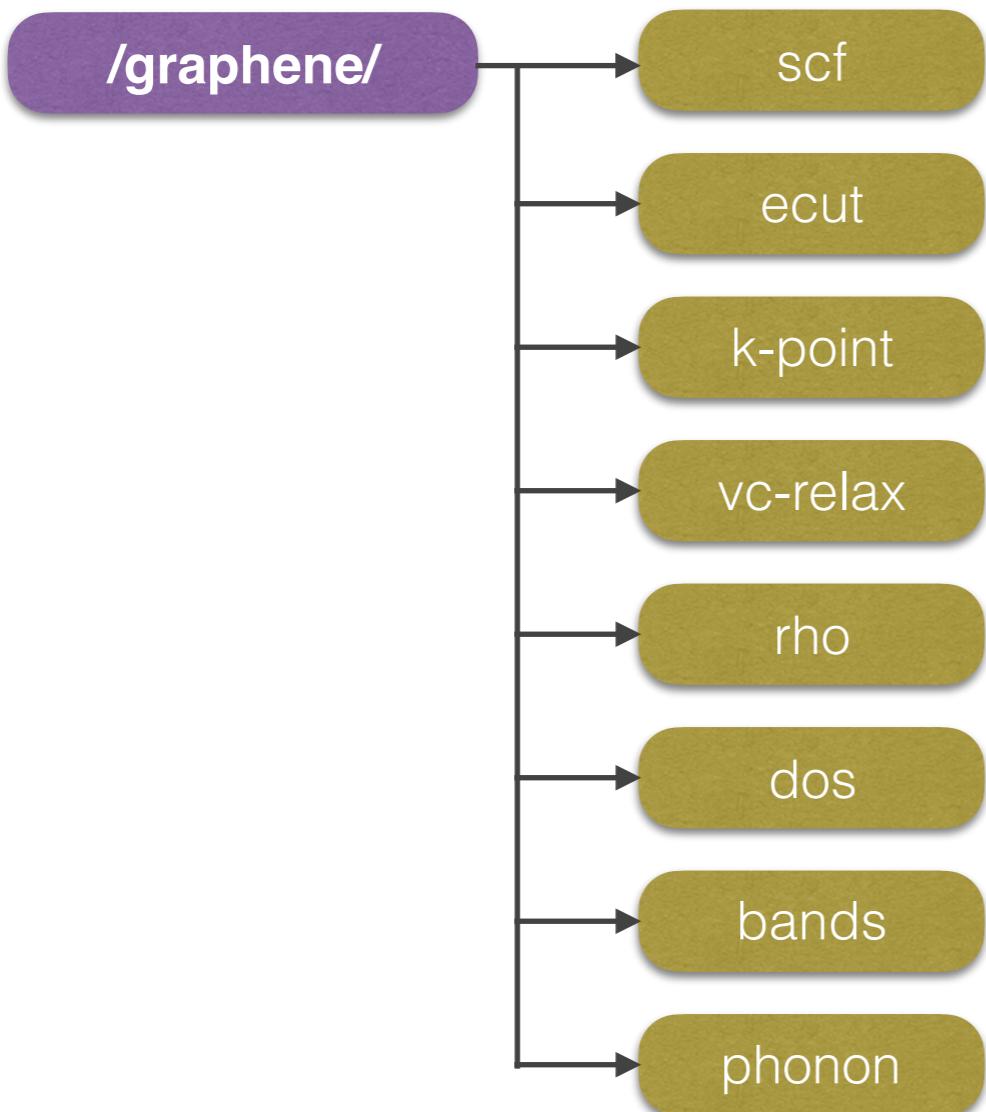
ATOMIC_POSITIONS (alat)
Si      -0.000000000  -0.000000000  -0.000000000
Si      0.252352132  0.252352132  0.252352132
End final coordinates
```

# Exercise #1

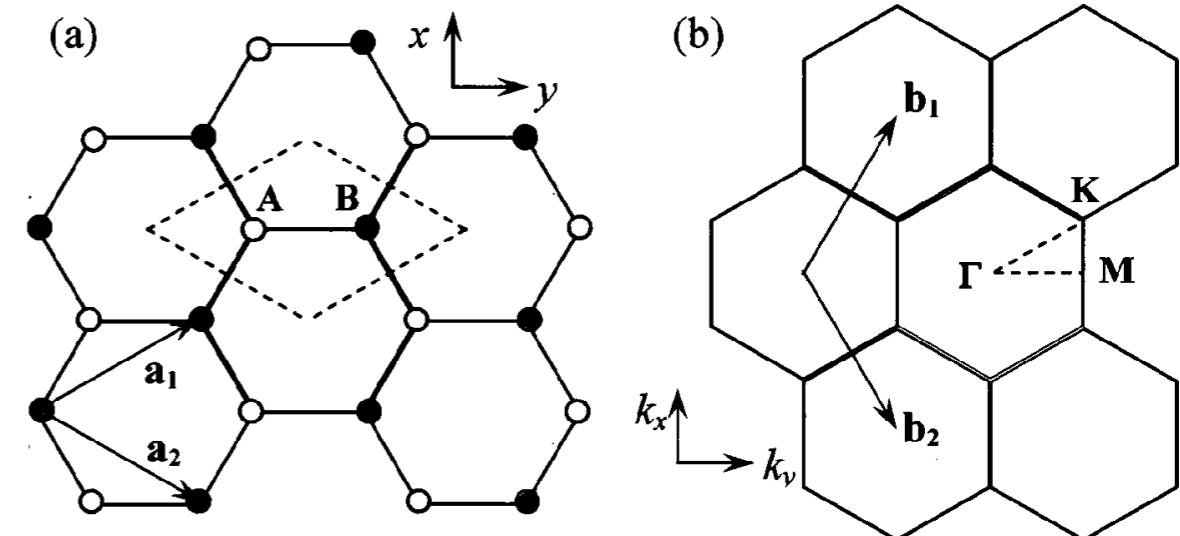
Do it by yourself: Graphene's calculation!

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

Files for exercise

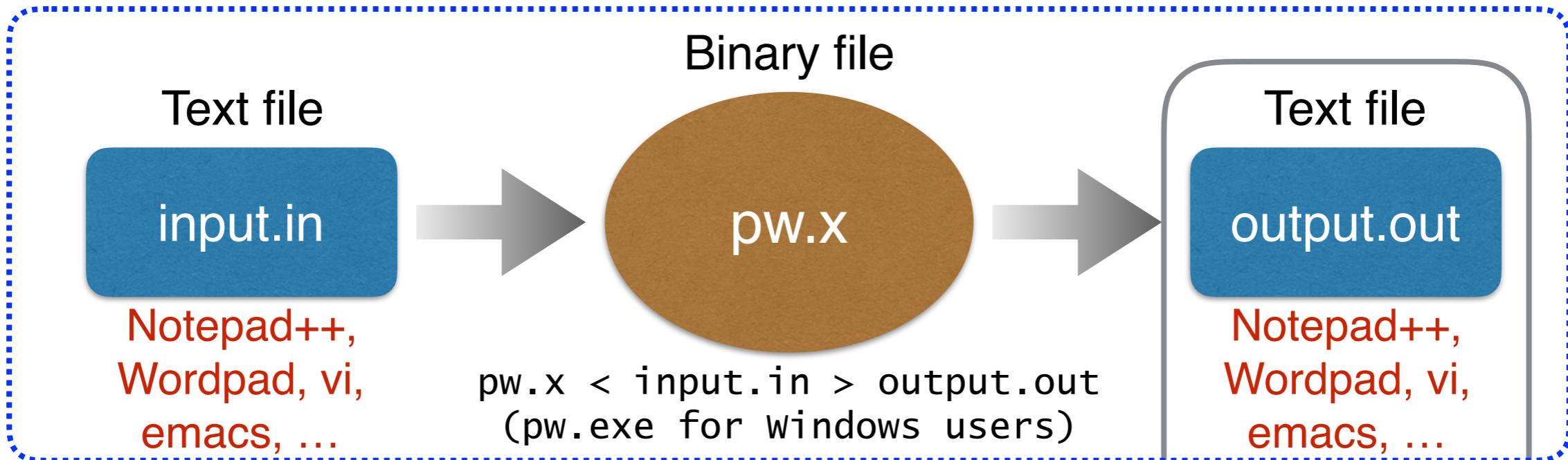


Hands-on #1

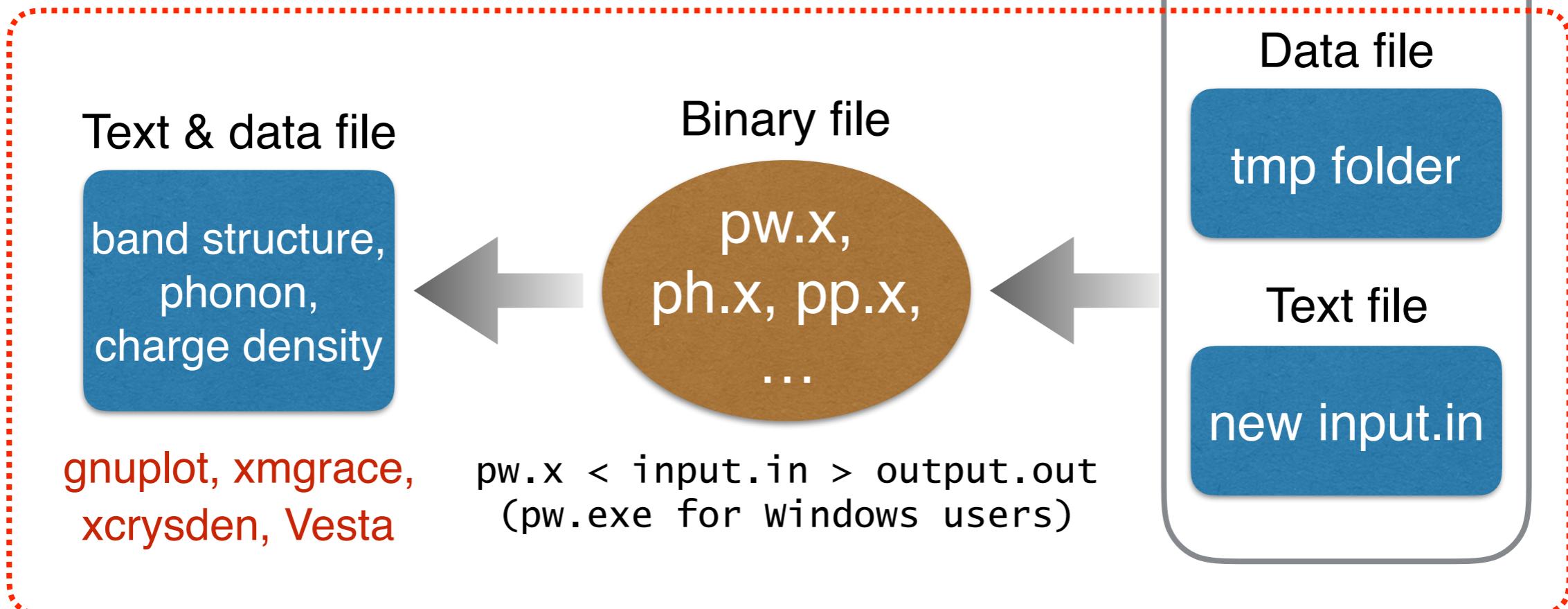


# Structure of QE I/O file

## Hands-on #1



## Hands-on #2



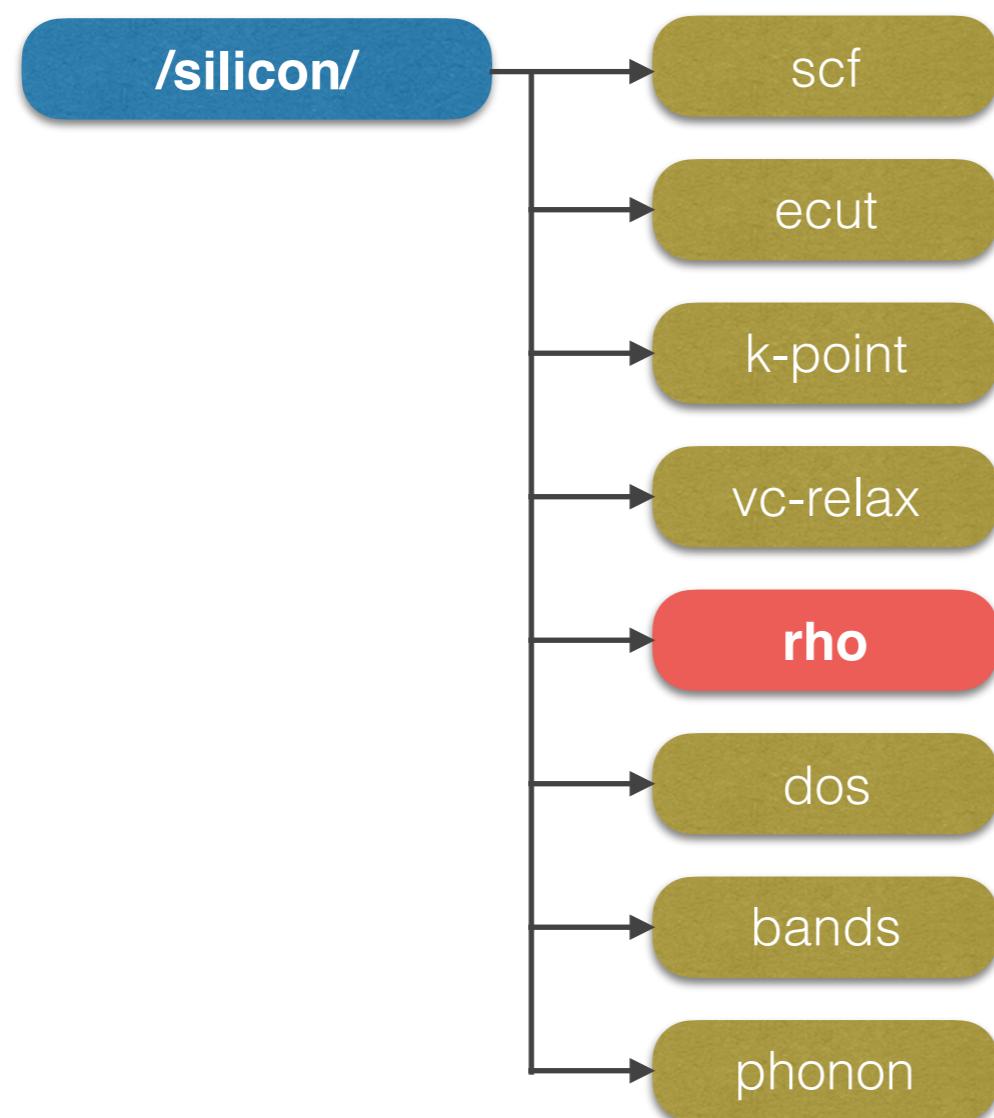
# Charge density

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ pp.x < Si.pp.in > Si.pp.out  
(* .exe for windows users)
```

Step 1: SCF calculation (Hands-on #1)  
Step 2: Visual charge density

Files for charge density



# Charge density

Command:

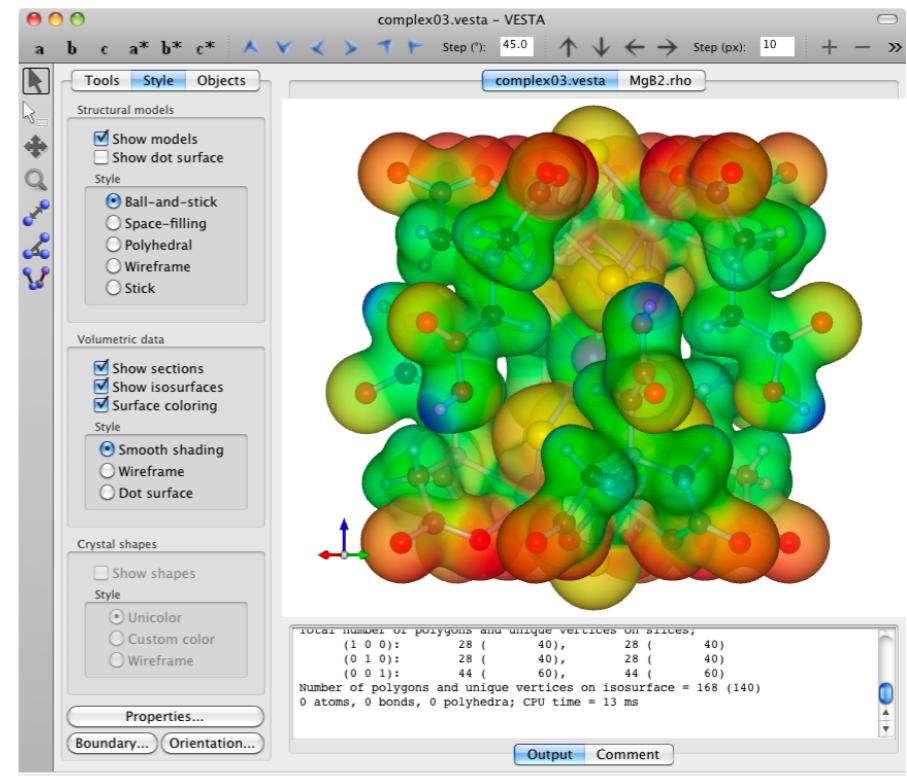
```
$ pw.x < Si.scf.in > Si.scf.out  
$ pp.x < Si.pp.in > Si.pp.out  
(* .exe for windows users)
```

**Si.pp.in**

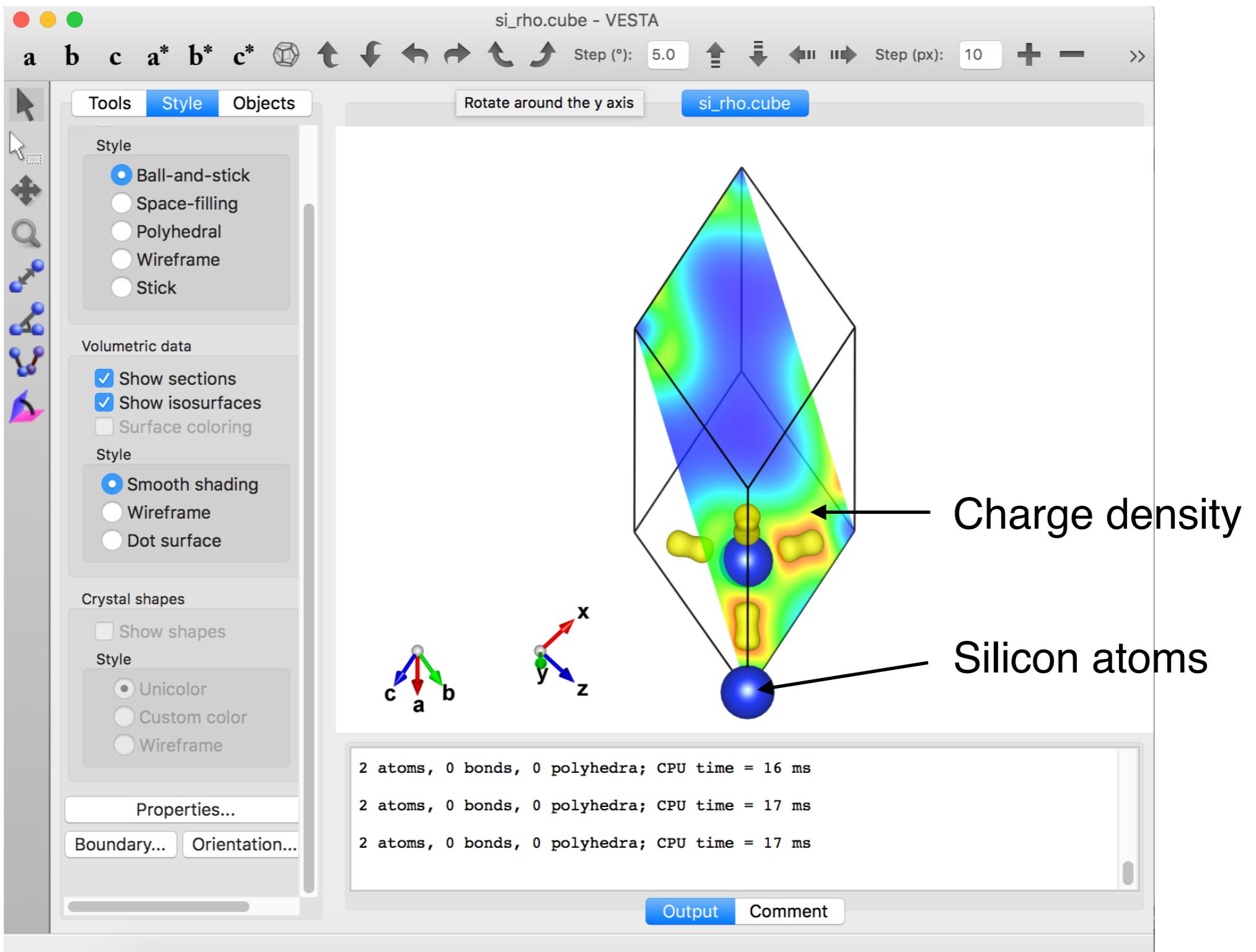
```
&INPUTPP  
outdir='../../tmp/' , ← Data of wavefunctions in step SCF  
prefix='si' ,  
plot_num=0 ,  
/  
&PLOT  
iflag=3 ,  
output_format=6 ,  
fileout='si_rho.cube' , → Data of  
nx=64,ny=64,nz=64 ,  
/
```

Step 1: SCF calculation (Hands-on #1)  
Step 2: Visual charge density

VESTA: <http://jp-minerals.org/vesta/en/>



# Charge density



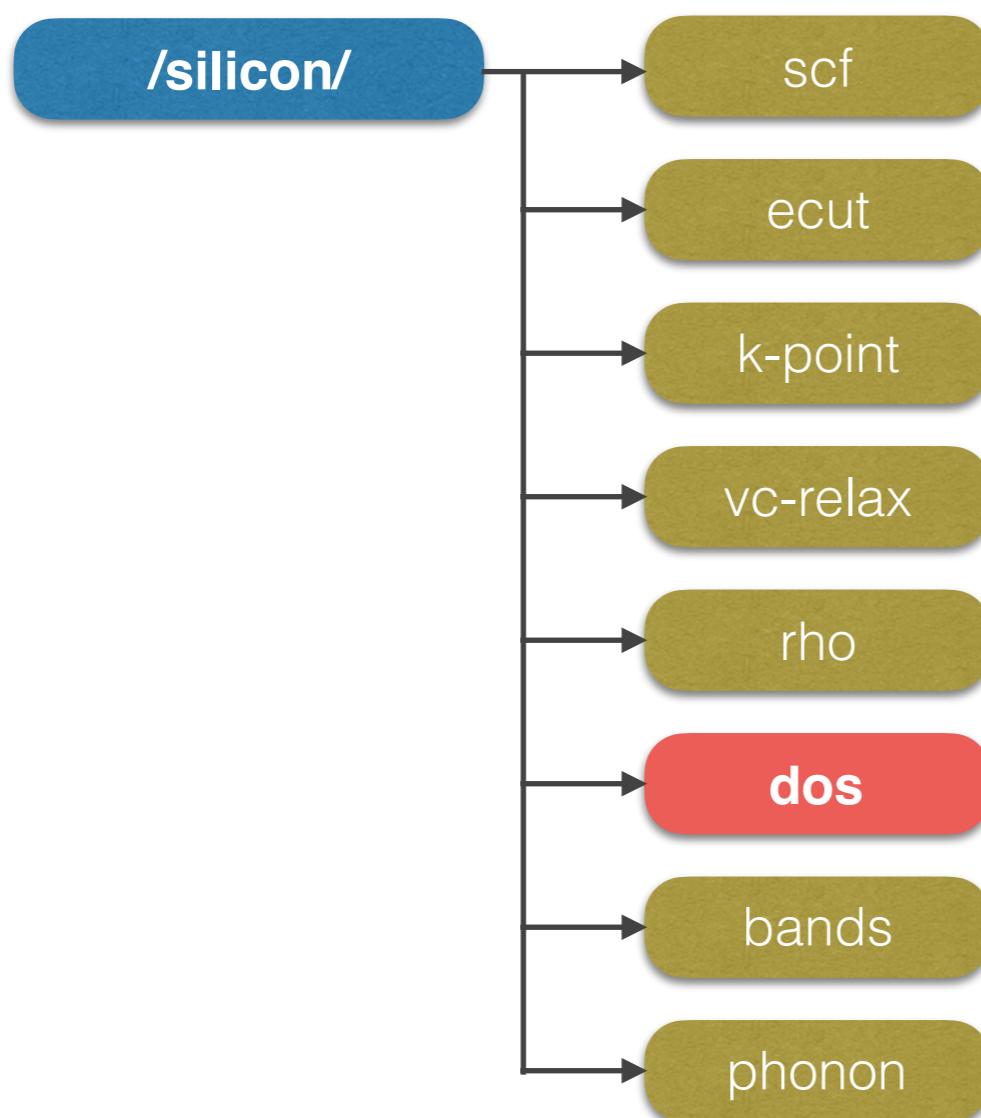
# Density of states (DOS)

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ pw.x < Si.nscf.in > Si.nscf.out  
$ dos.x < Si.dos.in > Si.dos.out  
(* .exe for windows users)
```

Step 1: SCF calculation (Hands-on #1)  
Step 2: Non-SCF calculation  
Step 3: Plot DOS

Files for density of states



# Density of states (DOS)

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ pw.x < Si.nscf.in > Si.nscf.out  
$ dos.x < Si.dos.in > Si.dos.out  
          (*.exe for windows users)
```

Si.nscf.in

```
&CONTROL  
calculation='nscf',           ← non-SCF calculation  
restart_mode='from_scratch',  
prefix='si',  
pseudo_dir='../../pseudo/',  
outdir='../../tmp/',  
/  
&SYSTEM  
ibrav=2,  
celldm(1)=10.2625,  
nat=2,  
ntyp=1,  
ecutwfc=60.0,  
ecutrho=720.0,  
nbnd=8,  
occupations='tetrahedra',      ← Linear tetrahedron method  
/  
&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  
12 12 12 1 1 1           ← High density k-point
```

Step 1: SCF calculation (Hands-on #1)  
Step 2: Non-SCF calculation  
Step 3: Plot DOS

# Density of states (DOS)

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ pw.x < Si.nscf.in > Si.nscf.out  
$ dos.x < Si.dos.in > Si.dos.out
```

(\* .exe for windows users)

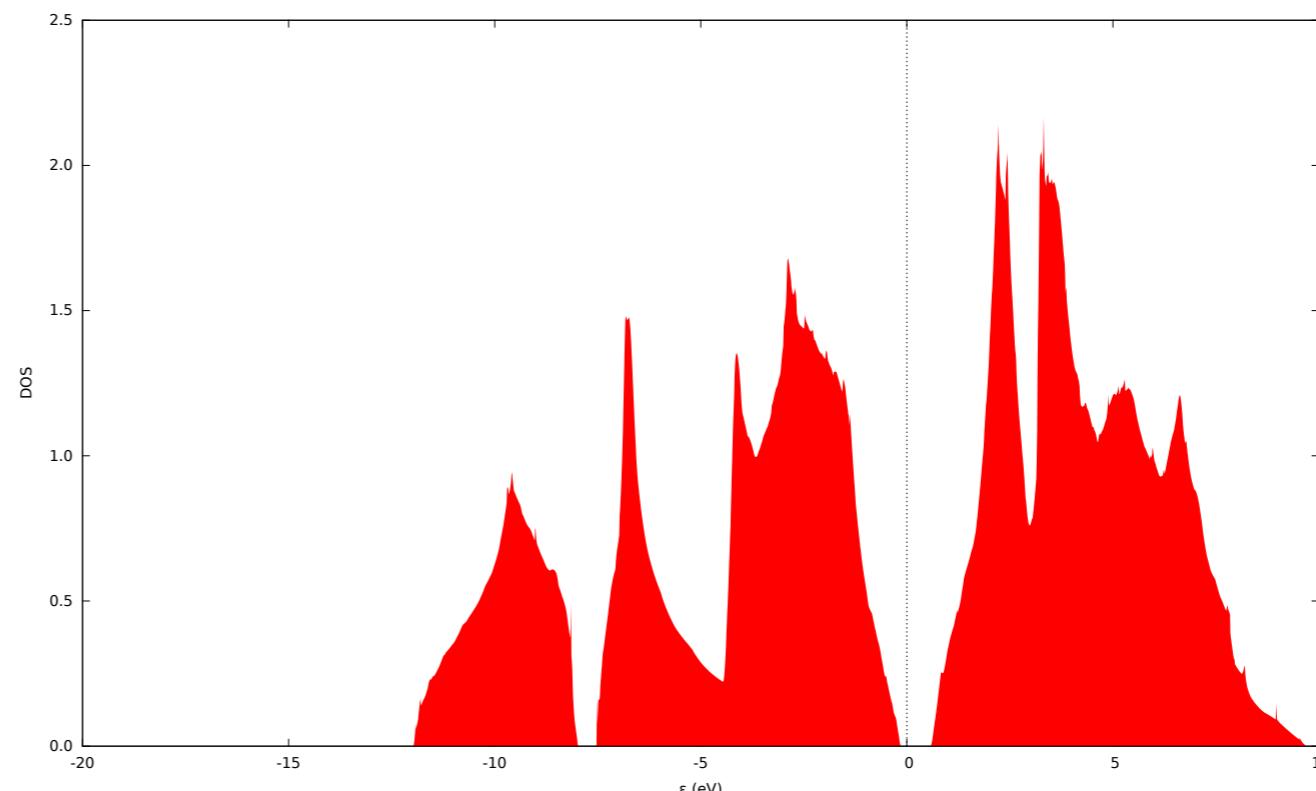
Step 1: SCF calculation (Hands-on #1)  
Step 2: Non-SCF calculation  
**Step 3: Plot DOS**

**Si.dos.in**

```
&DOS  
prefix='si',  
outdir='../../tmp/',  
fildos='si.dos'  
emin=-9.0,  
emax=16.0,  
/
```

→ Data file of DOS (state/eV)

Command:  
\$ gnuplot < si\_dos.gnu



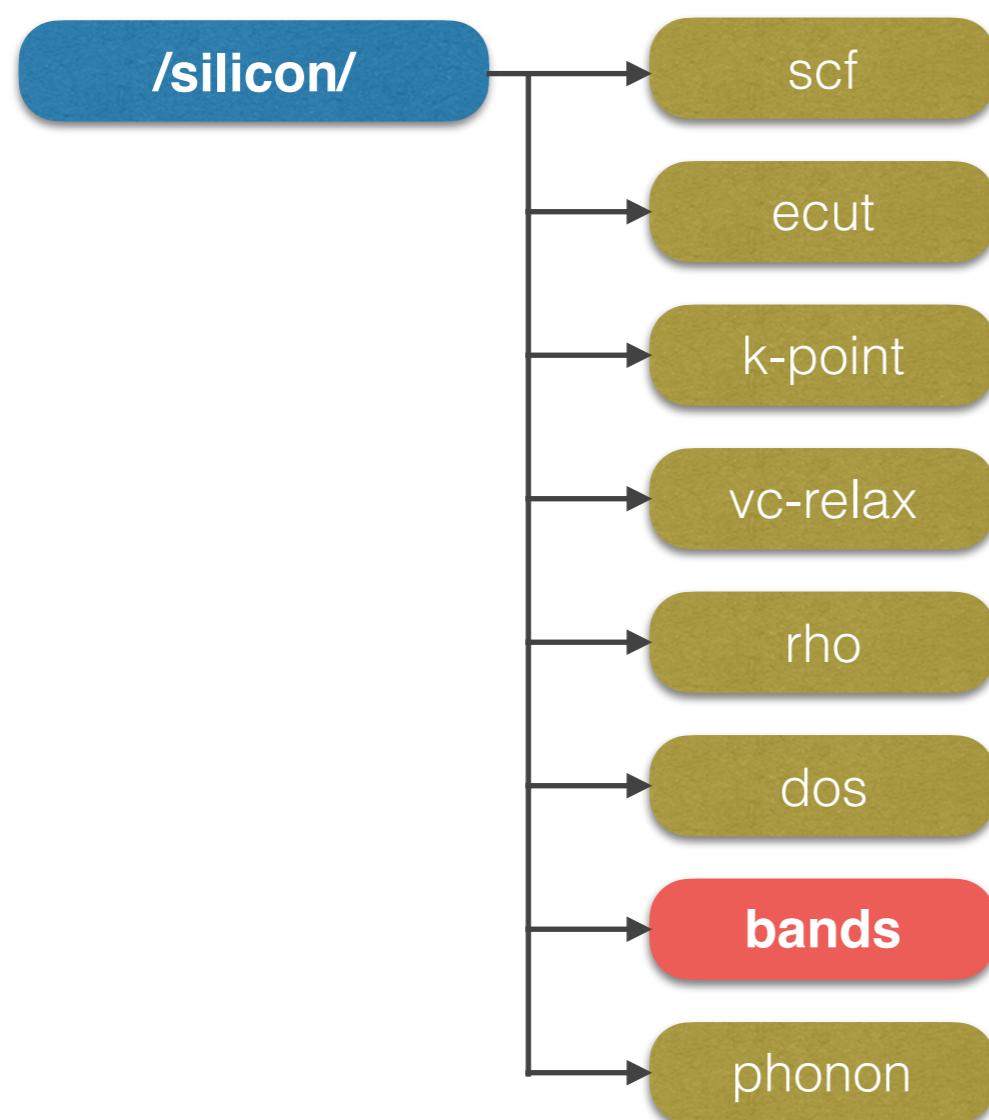
# Band structure

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ pw.x < Si.nscf.in > Si.nscf.out  
$ bands.x <Si.bands.in > Si.bands.out  
$ plotband.x <Si.plotband  
(*.exe for windows users)
```

- Step 1: SCF calculation (Hands-on #1)
- Step 2: Non-SCF calculation
- Step 3: Data of bands structure
- Step 4: Plot band structure

## Files for band structure



# Band structure

Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ pw.x < Si.nscf.in > Si.nscf.out
$ bands.x <Si.bands.in > Si.bands.out
$ plotband.x <Si.plotband
```

**Si.nscf.in** (\*.exe for windows users)

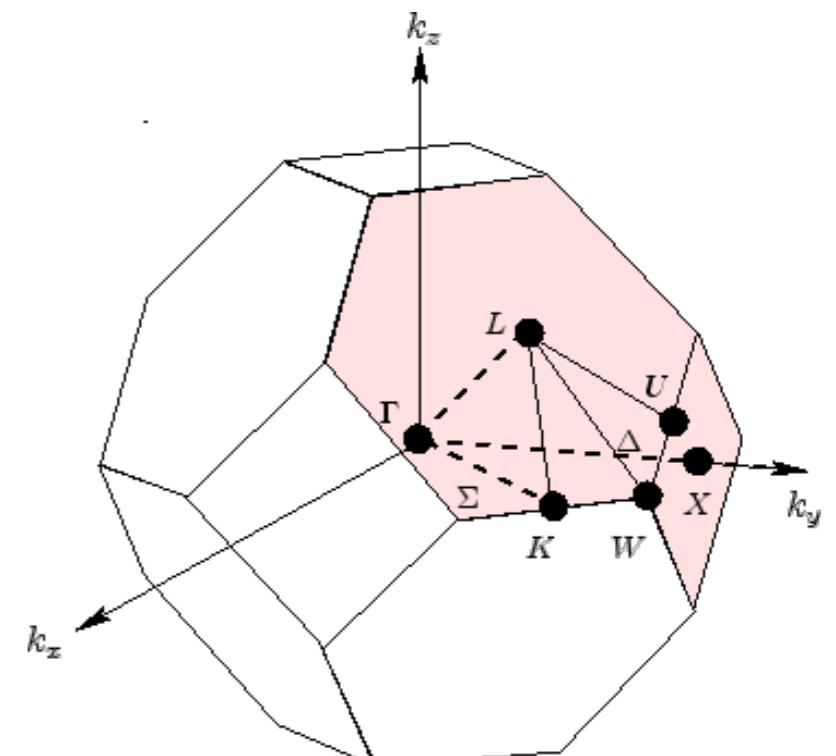
```
&CONTROL
calculation='bands', ← non-SCF calculation
restart_mode='from_scratch',
prefix='si',
pseudo_dir='../../pseudo/',
outdir='../../tmp/',
/
&SYSTEM
ibrav=2,
celldm(1)=10.2625,
nat=2,
ntyp=1,
ecutwfc=60.0,
ecutrho=720.0,
nbnd=8,
/
&ELECTRONS
mixing_beta=0.7,
conv_thr=1d-8,
/
ATOMIC_SPECIES
Si 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
K_POINTS {crystal_b} ← Selected special k-point coordinates
5
0.0000000000 0.0000000000 -0.5000000000 20 ← L
0.0000000000 0.0000000000 0.0000000000 30 ← Γ
-0.5000000000 0.0000000000 -0.5000000000 10 ← X
-0.3750000000 0.0000000000 -0.6250000000 30 ← U
0.0000000000 0.0000000000 0.0000000000 20 ← Γ
```

Step 1: SCF calculation (Hands-on #1)

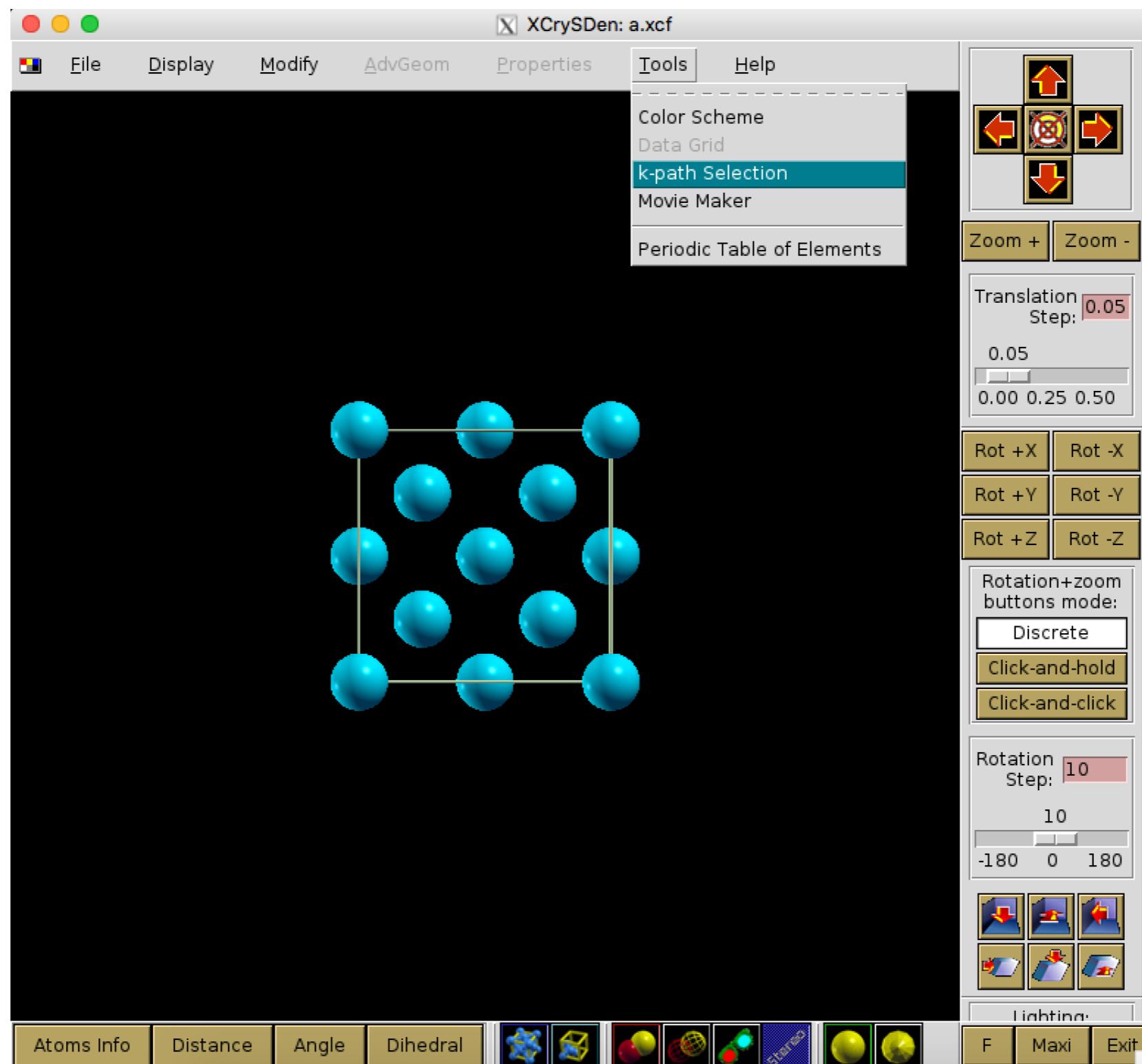
Step 2: Non-SCF calculation

Step 3: Data of bands structure

Step 4: Plot band structure

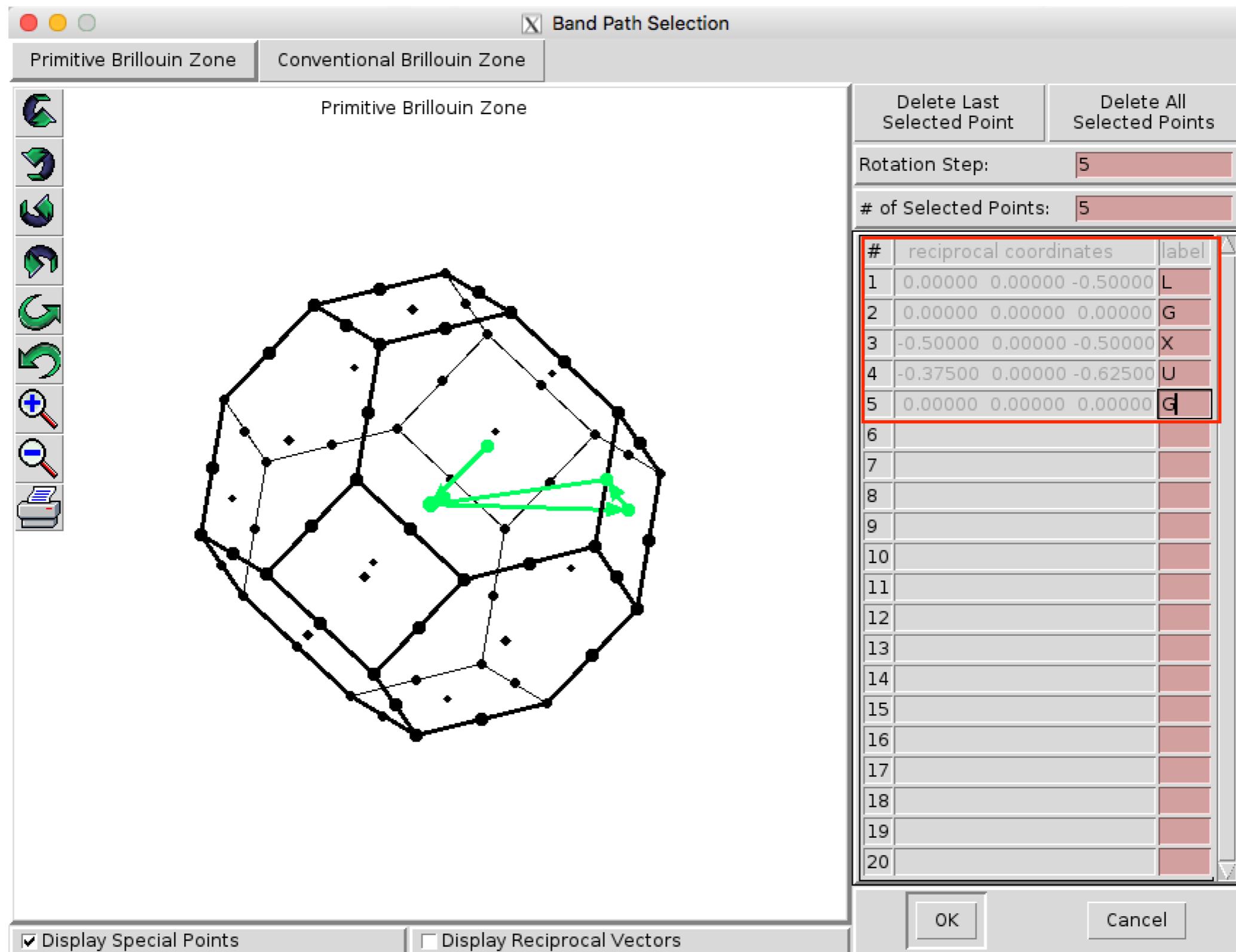


# XCrySDen k-Path



Xcrysden: <http://www.xcrysden.org/>

# XCrySDen k-Path



# Band structure

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ pw.x < Si.nscf.in > Si.nscf.out  
$ bands.x <Si.bands.in> Si.bands.out  
$ plotband.x <Si.plotband  
          (*.exe for windows users)
```

Si.bands.in

```
&BANDS  
 outdir='..tmp/' ,  
  prefix='si' ,  
  filband='si.bands' , → Name of data file  
 /
```

- Step 1: SCF calculation (Hands-on #1)
- Step 2: Non-SCF calculation
- Step 3: Data of bands structure**
- Step 4: Plot band structure

# Band structure

Command:

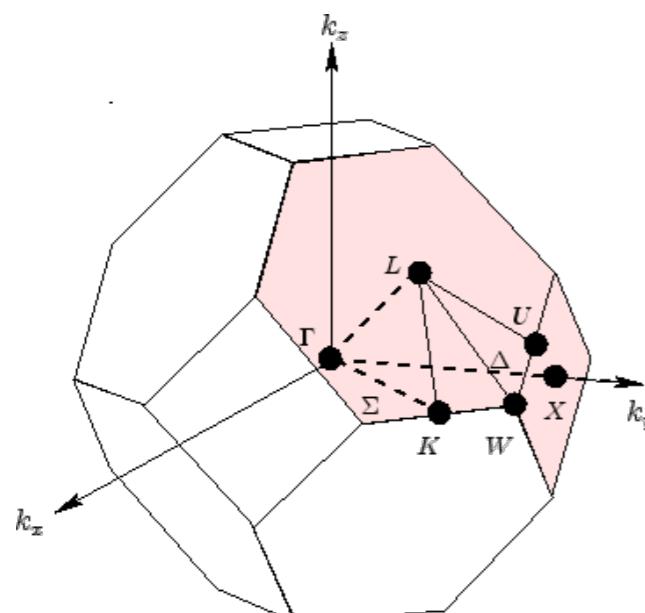
```
$ pw.x < Si.scf.in > Si.scf.out  
$ pw.x < Si.nscf.in > Si.nscf.out  
$ bands.x <Si.bands.in > Si.bands.out  
$ plotband.x <Si.plotband
```

(\* .exe for windows users)

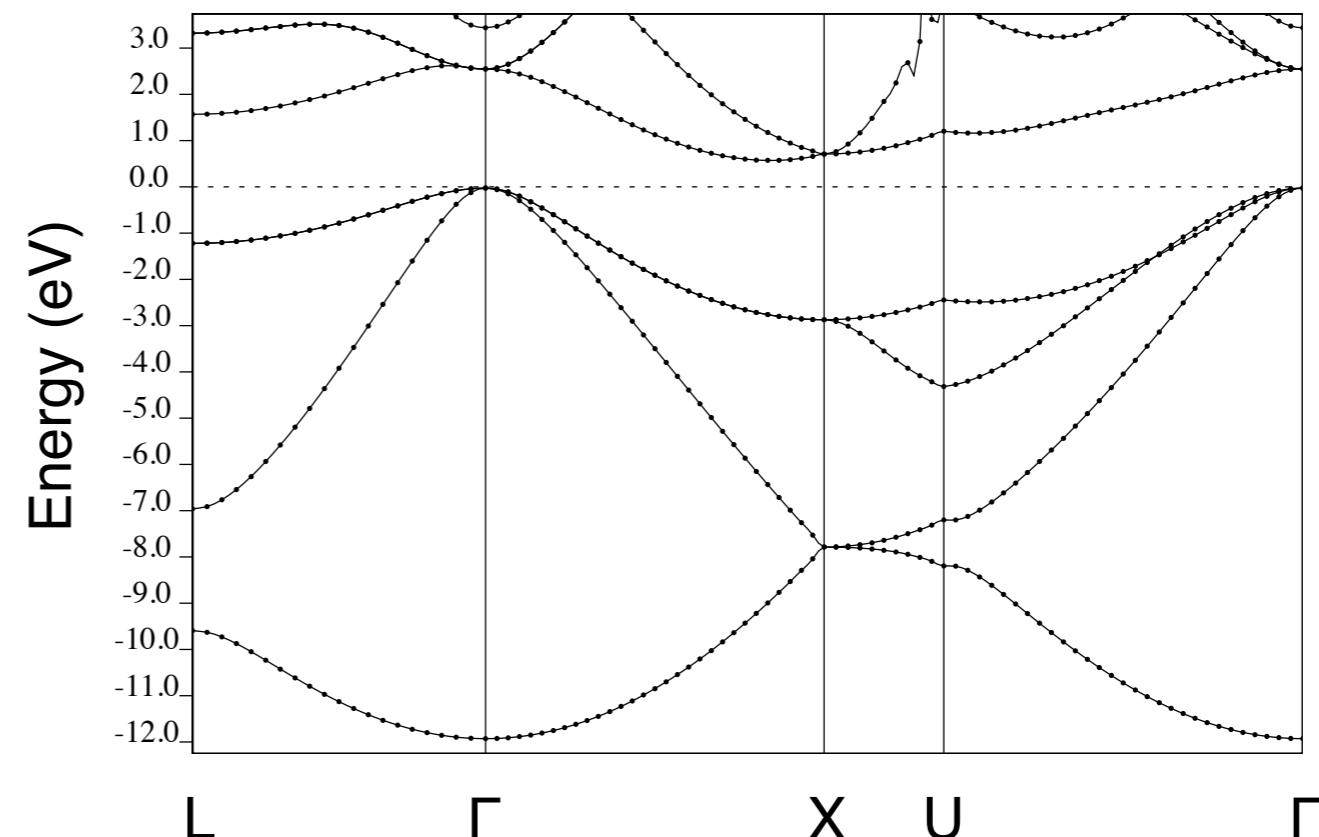
- Step 1: SCF calculation (Hands-on #1)
- Step 2: Non-SCF calculation
- Step 3: Data of bands structure
- Step 4: Plot band structure

**si.plotband**

```
si.bands          ←  
-6.0 10  
si.bands.xmgr    ←  
si.bands.ps      →  
6.255  
1.0 6.255
```



Data file



# Phonon

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ ph.x < Si.ph.in > Si.ph.out  
$ q2r.x <Si.q2r.in > Si.q2r.out  
$ matdyn.x <Si.matdyn.in > Si.matdyn.out  
(* .exe for windows users)
```

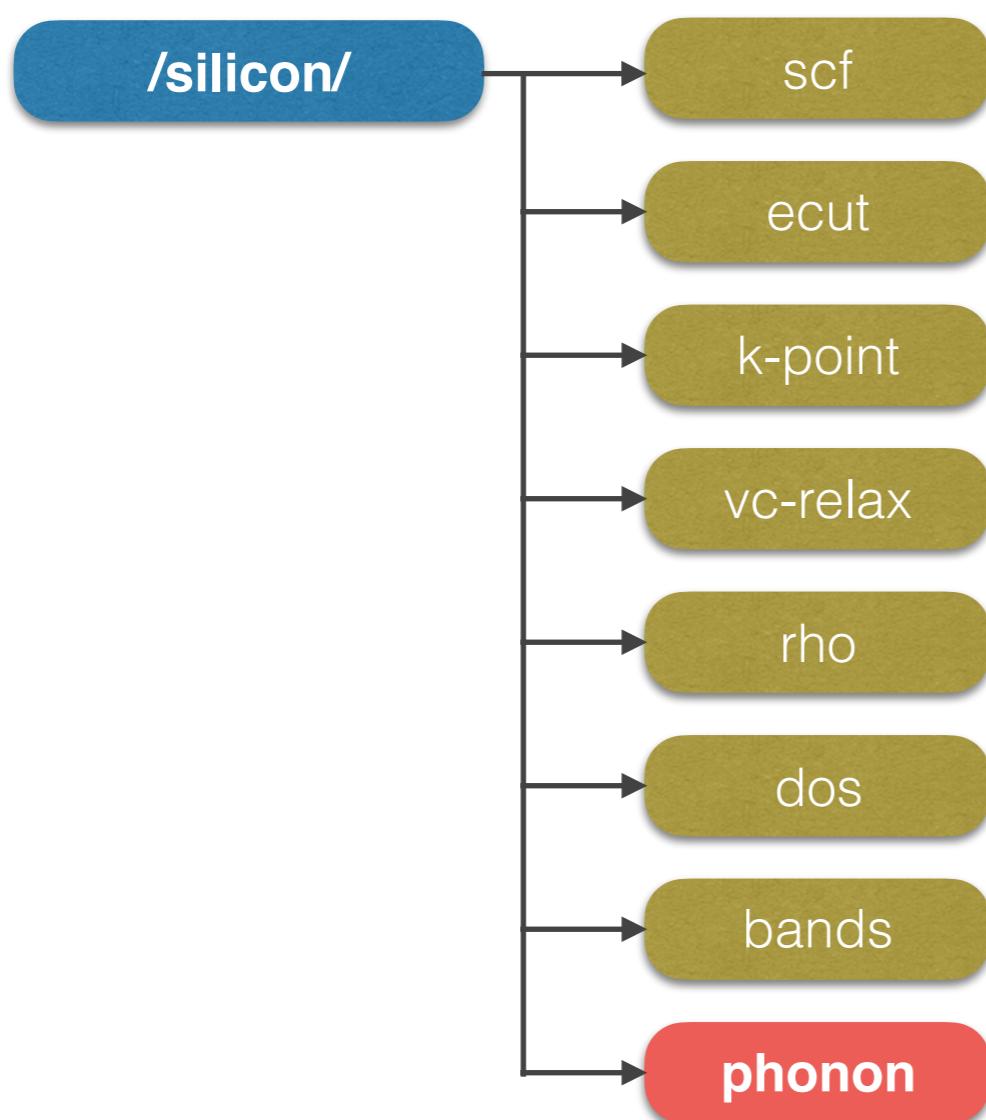
Step 1: SCF calculation (Hands-on #1)

Step 2: Calculation of dynamical matrices on q-vectors

Step 3: Calculation of IFC's in real space

Step 4: A plot of the phonon DOS

## Files for phonon



# Phonon

Command:

```
$ pw.x < Si.scf.in > Si.scf.out
$ ph.x < Si.ph.in > Si.ph.out
$ q2r.x < Si.q2r.in > Si.q2r.out
$ matdyn.x < Si.matdyn.in > Si.matdyn.out
```

*(\*.exe for windows users)*

**Si.pp.in**

```
phonon calc.
&inputph
 outdir="..tmp/",
  prefix="si",
  tr2_ph = 1d-14,
  ldisp = .true.,
  nq1=4, nq2=4, nq3=4,
  amass(1)=28.0855,
  fildyn='si.dyn',
/
```

**Si.q2r.in**

```
&input
  fildyn='si.dyn',
  zasr='simple',
  flfrc='si.fc',
/
```

**Density functional perturbation theory (DFPT):**  
direct calculation of second-order derivatives of the energy

Step 1: SCF calculation (Hands-on #1)

Step 2: Calculation of dynamical matrices on q-vectors

Step 3: Calculation of IFC's in real space

Step 4: A plot of the phonon DOS

## Interatomic force constants (IFC's) in real space

$$C_{st}^{ab}(\mathbf{R}) = \frac{\partial^2 E}{\partial u_s^a(\mathbf{0}) \partial u_t^b(\mathbf{R})} = \frac{1}{N_c} \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{R}} \tilde{C}_{st}^{ab}(\mathbf{q})$$

- Calculation of  $C_{s,t}^{a,b}(\mathbf{q})$  on a suitable grid of  $\mathbf{q}$ -vectors
- Fourier transform to real space

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Phonons and related crystal properties from density-functional perturbation theory

Stefano Baroni, Stefano de Gironcoli, Andrea Dal Corso, and Paolo Giannozzi  
Rev. Mod. Phys. 73, 515 – Published 6 July 2001

# Phonon

Command:

```
$ pw.x < Si.scf.in > Si.scf.out  
$ ph.x < Si.ph.in > Si.ph.out  
$ q2r.x <Si.q2r.in > Si.q2r.out  
$ matdyn.x <Si.matdyn.in > Si.matdyn.out
```

**Si.matdyn.in** (\*.exe for windows users)

```
&input  
asr='simple',  
dos=.true.,  
amass(1)=28.0855,  
flfrc='si.fc',  
fldos='si.phdos',  
nk1=50,nk2=50,nk3=50,  
/
```

Step 1: SCF calculation (Hands-on #1)

Step 2: Calculation of dynamical matrices on q-vectors

Step 3: Calculation of IFC's in real space

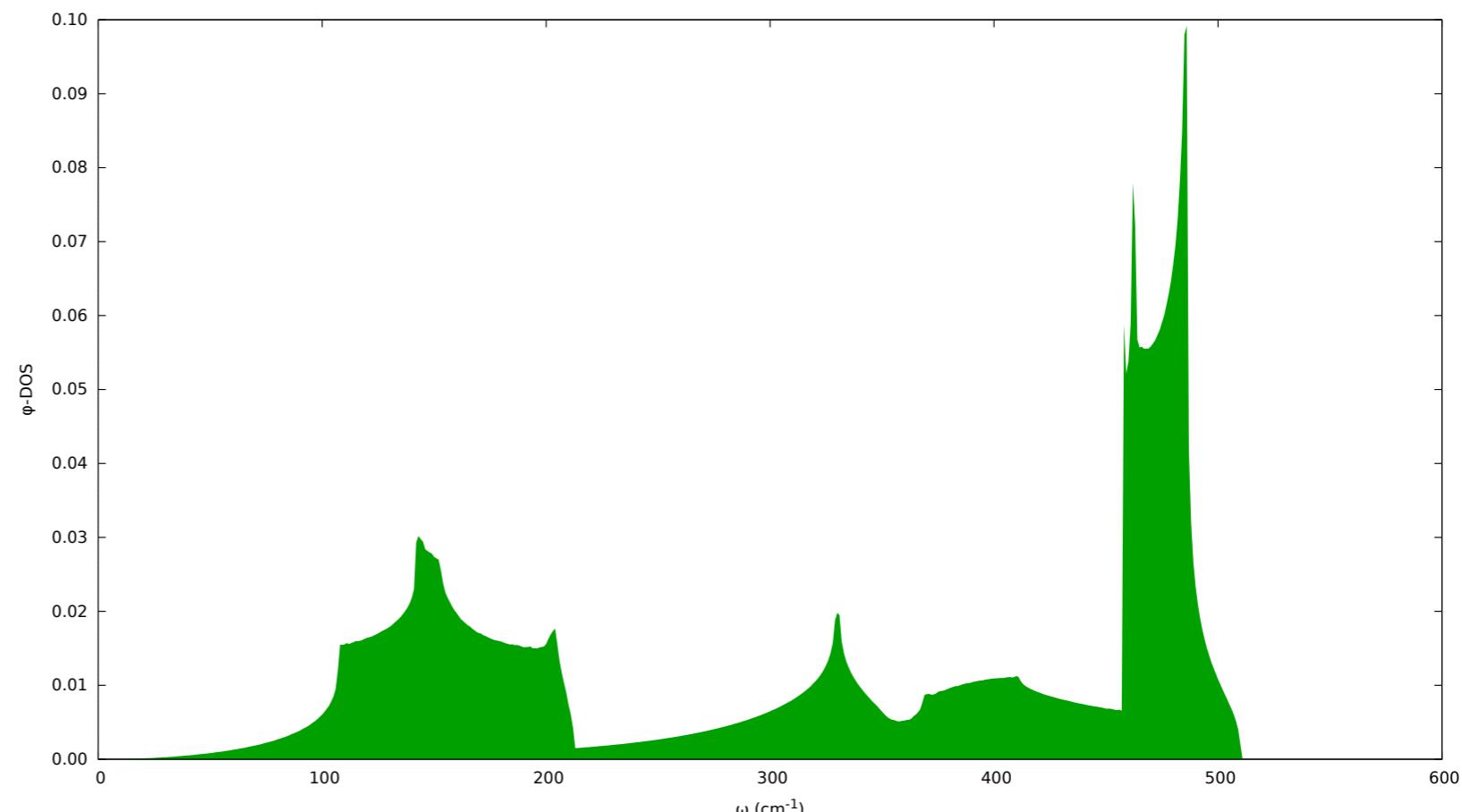
Step 4: A plot of the phonon DOS

Interatomic force constants (IFC's) in real space

Data file of phonon DOS

Command:

```
$ gnuplot < si_phdos.gnu
```

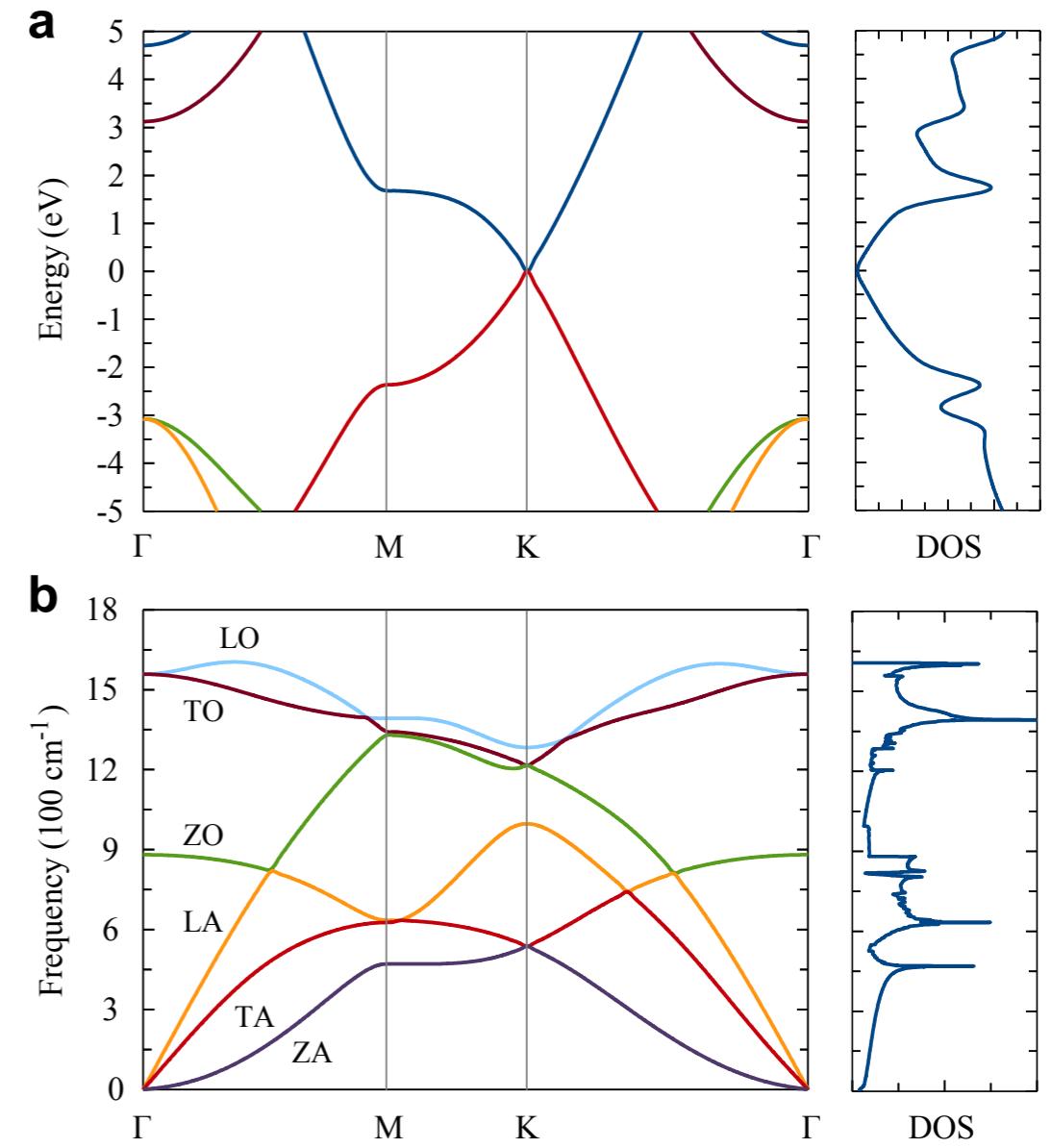
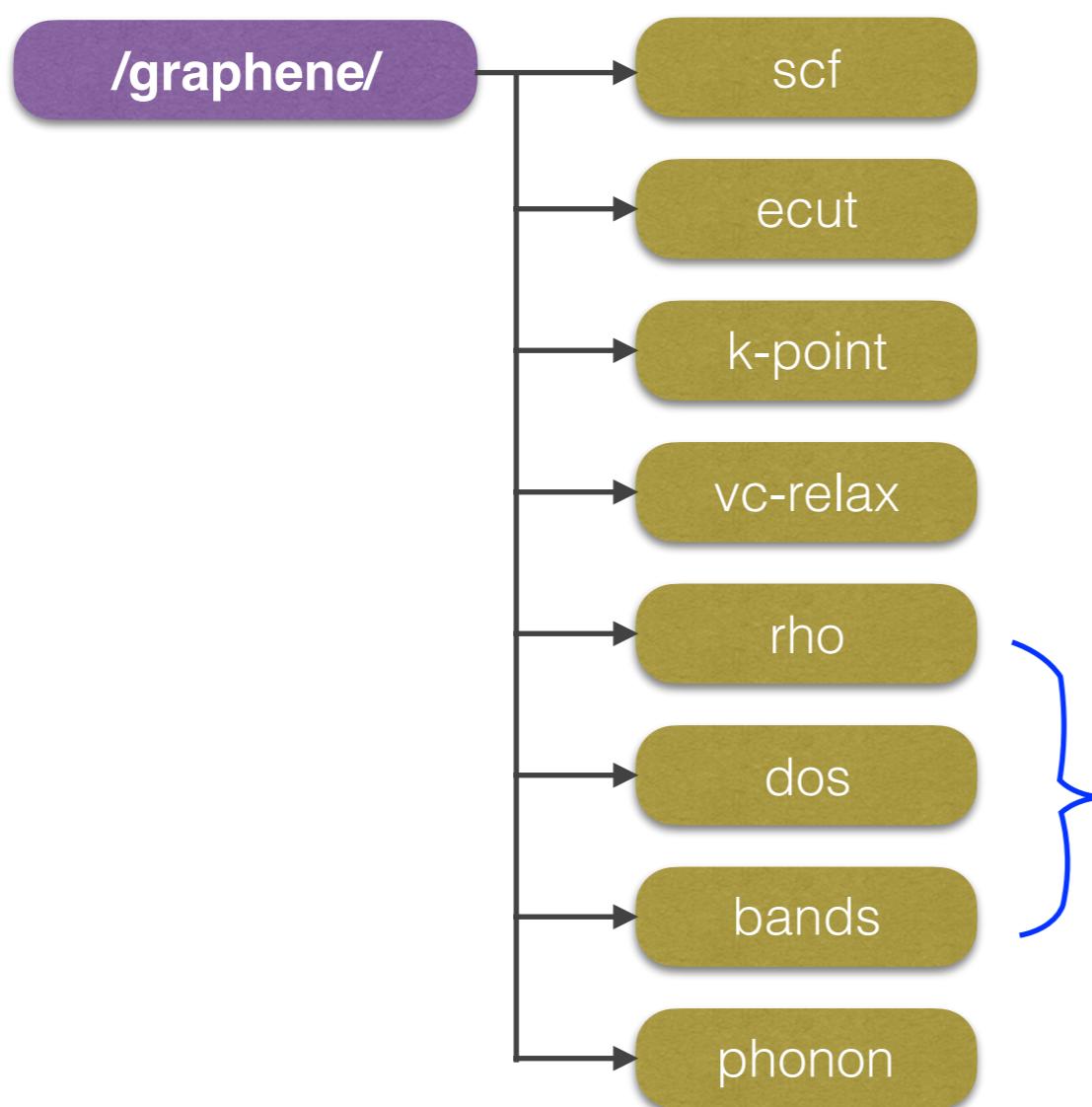


# Exercise #2

Do it by yourself: Graphene's calculation!

- ▶ Charge density (rho)
- ▶ Density of states (dos)
- ▶ Band structure (bands)

Files for exercise



Hands-on #2

thank you!

