

Quantum Espresso code



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

Quantum Espresso code

- Different executables for different tasks in QEDIR/**bin**
- Documentation in QEDIR/**Doc/INPUT_XX.txt** or online at http://www.quantum-espresso.org/wp-content/uploads/Doc/INPUT_PW.html

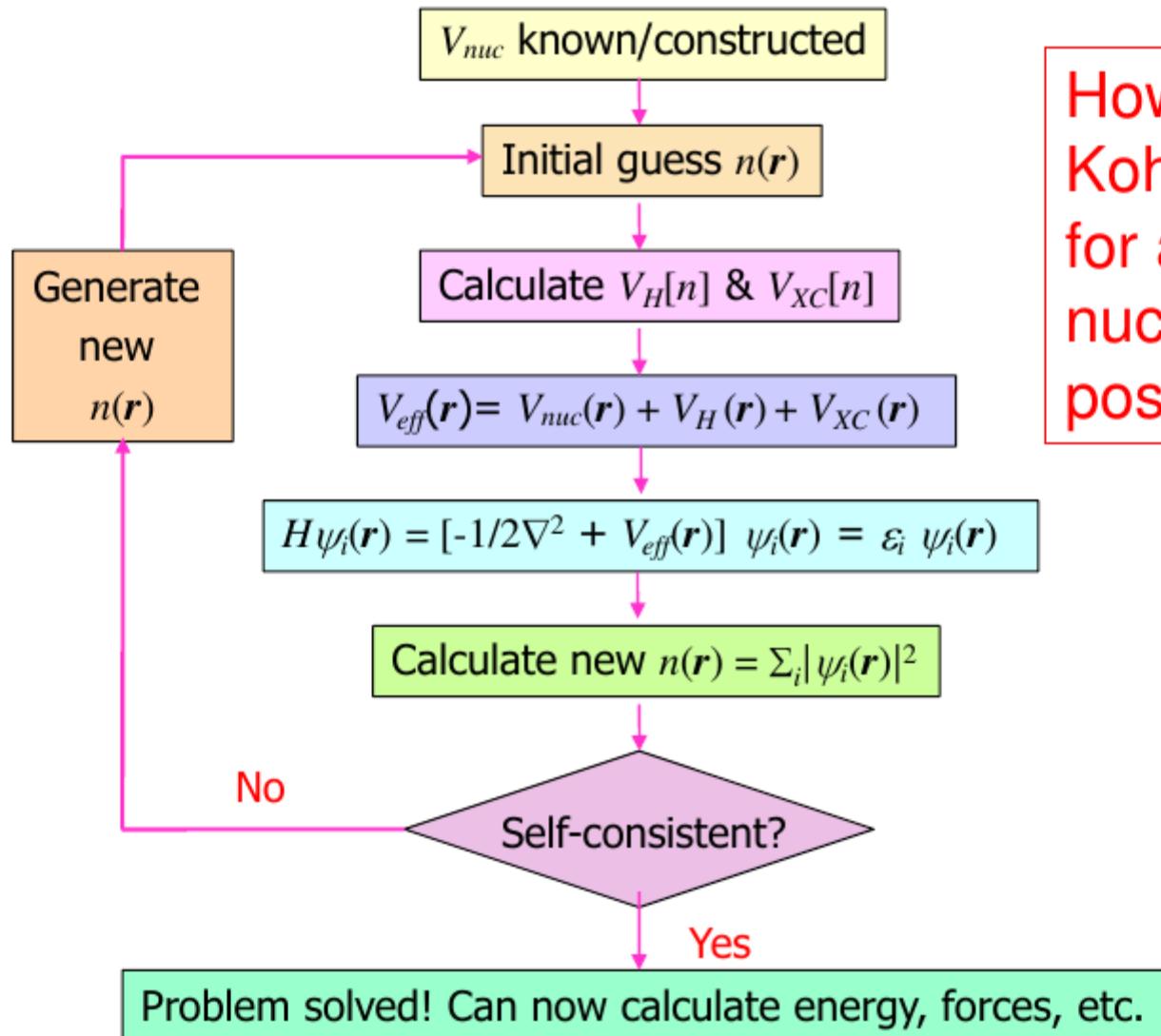
Code organization

• pw.x	main code
• pp.x	data analysis
• ph.x	phonons/electron-phonon coupling
• dos.x	density of states
• bands.x	plot band structure
• pwcond.x	transmittance
• cp.x	molecular dynamics

more tools available:

*x-ray spectra, optics ,EELS, superconductivity,
magnetic resonance (NMR) etc..*

Self-consistent Iterative Solution



How to solve the Kohn-Sham eqns. for a set of fixed nuclear (ionic) positions.

The input file for PWscf is structured in a number of **NAMELISTS** and **INPUT_CARDS**.

&NAMELIST1 ... /

&NAMELIST2 ... /

&NAMELIST3 ... /

INPUT_CARD1

....

....

INPUT_CARD2

....

....

NAMELISTS are a standard input construct in fortran90.

The use of **NAMELISTS** allows to specify the value of an input variable **only when it is needed** and to define **default values** for most variables that then need not be specified. Variable can be inserted **in any order**.

```
&NAMELIST
```

```
    needed_variable2=XX, needed_variable1=X,  
    character_variable1='a suitable string'
```

```
/
```

NAMELISTS are read in a specific order

NAMELISTS that are not required are ignored

INPUT_CARDS are specific of QuantumESPRESSO codes and are used to provide input data that are **always needed** and would be boring to specify with the `variable_name=variable_value` syntax used by NAMELIST.

INPUT_CARDS require data in specific order (which may depend on the situation and on the value of a **card_formatSpecifier**)

For instance:

```
INPUT_CARD    card_format_specifier
data(1,1)  data(1,2)  data(1,3)  ...
data(2,1)  data(2,2)  data(2,3)  ...
data(3,1)  data(3,2)  data(3,3)  ...
...  ...  ...
```

Logically independent **INPUT_CARDS** can be given in any order

There are **three mandatory** NAMELISTS in PWscf:

&CONTROL input variables that control the flux of the calculation and the amount of I/O on disk and on the screen.

&SYSTEM input variables that specify the system under study.

&ELECTRONS input variables that control the algorithms used to reach the self-consistent solution of KS equations for the electrons.

There are **three mandatory** INPUT_CARDS in PWscf

ATOMIC_SPECIES name, mass and pseudopotential used for each atomic species present in the system

ATOMIC_POSITIONS type and coordinates of each atom in the unit cell

K_POINTS coordinates and weights of the k-points used for BZ integration

Typical input file

```
&control
    prefix='silicon',
    pseudo_dir='./'
    outdir = './',
/
&system
    ibrav= 2,
    celldm(1) =10.2,
    nat= 2,
    ntyp= 1,
    ecutwfc = 12.0,
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.vbc.UPF
ATOMIC_POSITIONS {crystal}
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS automatic
2 2 2 0 0 0
```

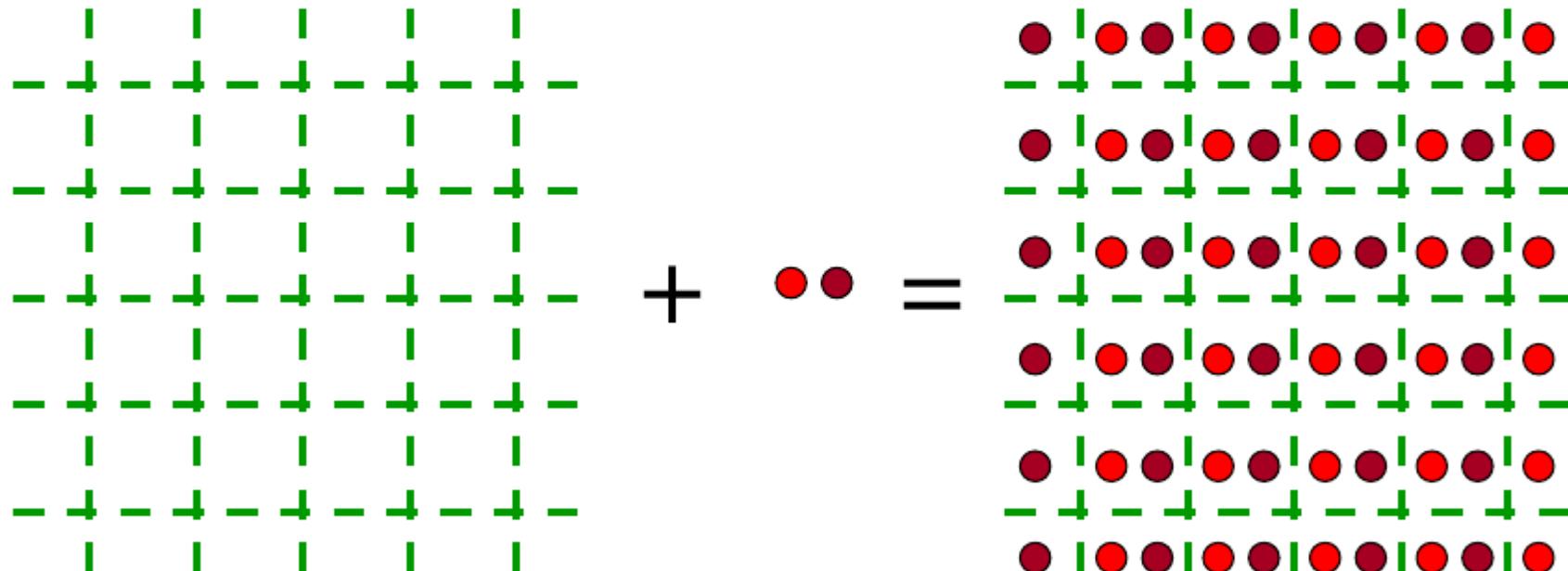
Step 0: Defining the (periodic) system



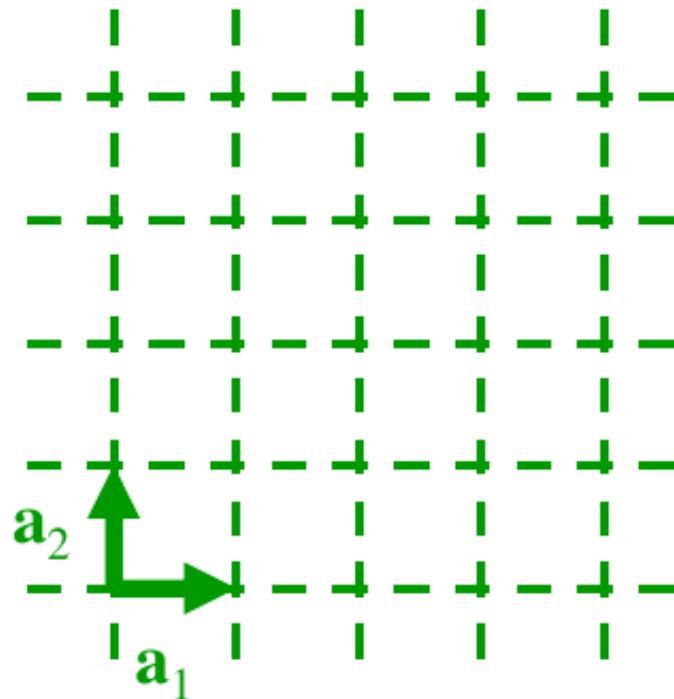
Namelist '**SYSTEM**'

How to Specify the System

- All periodic systems can be specified by a Bravais Lattice and an atomic basis.



How to Specify the Bravais Lattice / Unit Cell



Input parameter **ibrav**

- Gives the type of **Bravais lattice** (SC, BCC, Hex, etc.)

Input parameters {**celldm(i)** }

- Give the lengths [& directions, if necessary] of the lattice vectors **a₁**, **a₂**, **a₃**

- Note that one can choose a non-primitive unit cell (e.g., 4 atom SC cell for FCC structure).

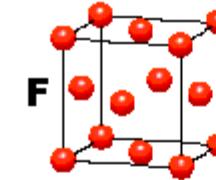
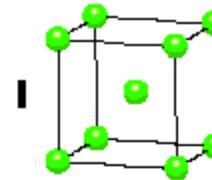
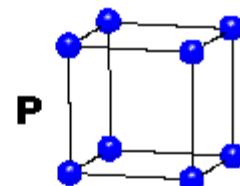
Bravais Lattices: `ibrav` flag

https://en.wikipedia.org/wiki/Bravais_lattice

`ibrav = 1, 3, 2`

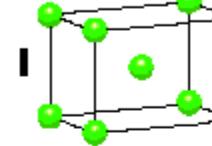
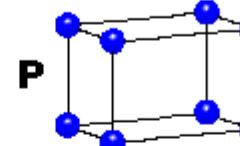
CUBIC

$a = b = c$
 $\alpha = \beta = \gamma = 90^\circ$



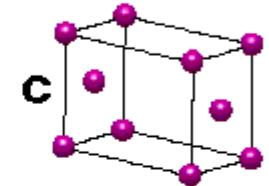
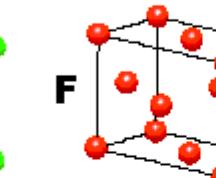
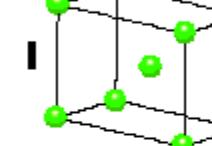
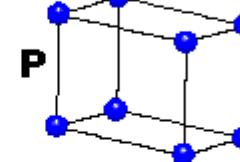
TETRAGONAL

$a = b \neq c$
 $\alpha = \beta = \gamma = 90^\circ$



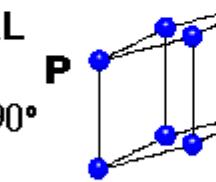
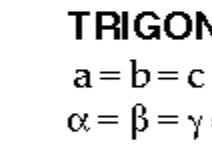
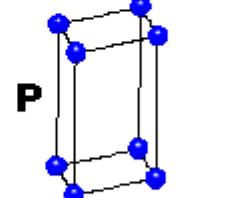
ORTHORHOMBIC

$a \neq b \neq c$
 $\alpha = \beta = \gamma = 90^\circ$



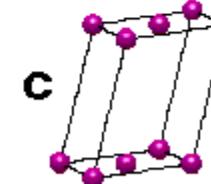
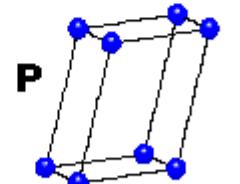
HEXAGONAL

$a = b \neq c$
 $\alpha = \beta = 90^\circ$
 $\gamma = 120^\circ$



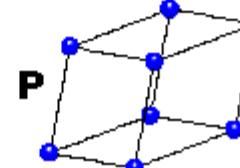
MONOCLINIC

$a \neq b \neq c$
 $\alpha = \gamma = 90^\circ$
 $\beta \neq 120^\circ$



TRICLINIC

$a \neq b \neq c$
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$



4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

+

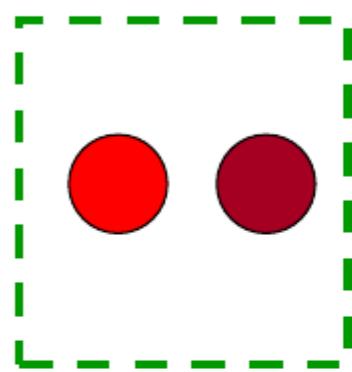
7 Crystal Classes

→ 14 Bravais Lattices

`ibrav = 12, -12, 13`

`ibrav = 14`

Atoms Within Unit Cell – How many, where?



Input parameter **nat**

- Number of atoms in the unit cell

Input parameter **ntyp**

- Number of types of atoms

FIELD ATOMIC_POSITIONS

- Initial positions of atoms (may vary when “**relax**” done).
- Can choose to give in units of lattice vectors (“**crystal**”) or in Cartesian units (“**alat**” or “**bohr**” or “**angstrom**”)

Typical input file

```
&control
    prefix='silicon',
    pseudo_dir='./'
    outdir = './',
/
&system
    ibrav= 2,
    celldm(1) =10.2,
    nat= 2,
    ntyp= 1,
    ecutwfc = 12.0,
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.vbc.UPF
ATOMIC_POSITIONS {crystal}
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS automatic
2 2 2 0 0 0
```

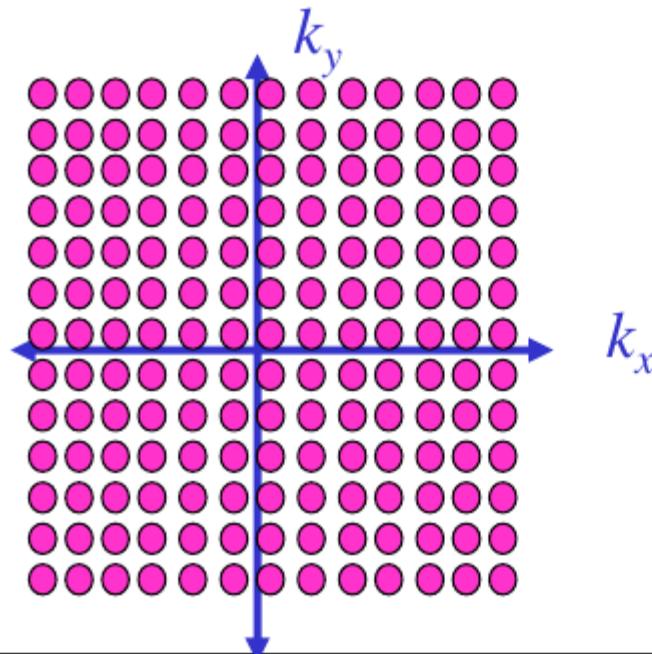
Plane Waves & Periodic Systems

- For a periodic system:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{G}} c_{\mathbf{k},\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G}) \cdot \mathbf{r}}$$

where \mathbf{G} = reciprocal lattice vector

- The **plane waves** that appear in this expansion can be represented as a grid in k-space:



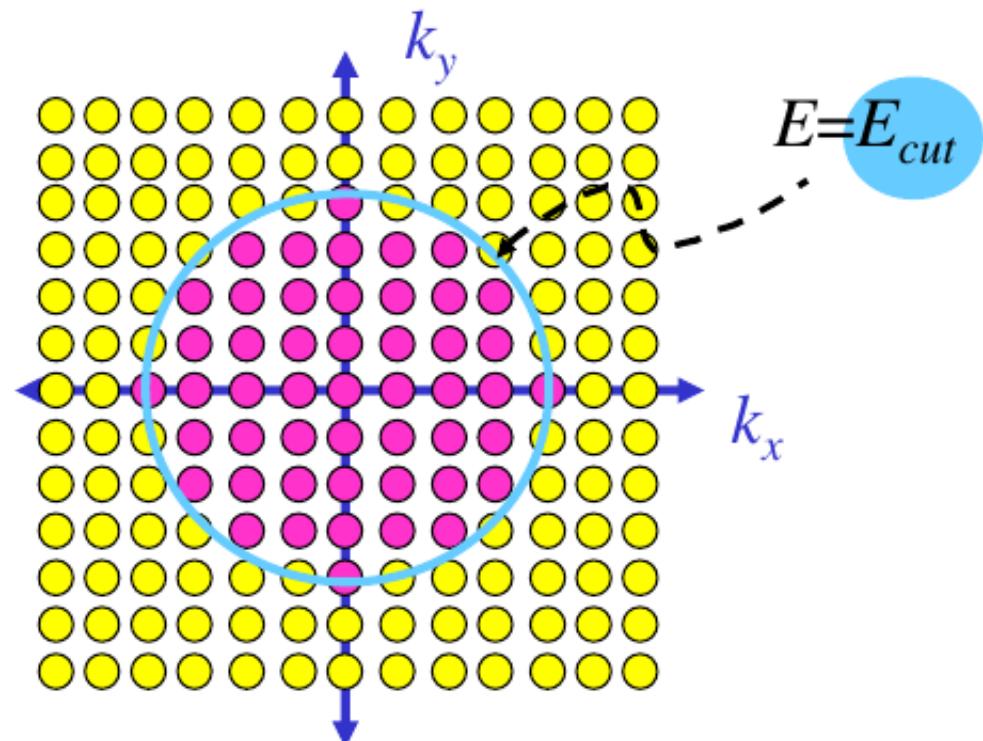
- Only true for periodic systems that grid is discrete.
- In principle, still need infinite number of plane waves.

Truncating the Plane Wave Expansion

- In practice, the contribution from higher Fourier components (large $|k+G|$) is small.
- So truncate the expansion at some value of $|k+G|$.
- Traditional to express this cut-off in energy units:

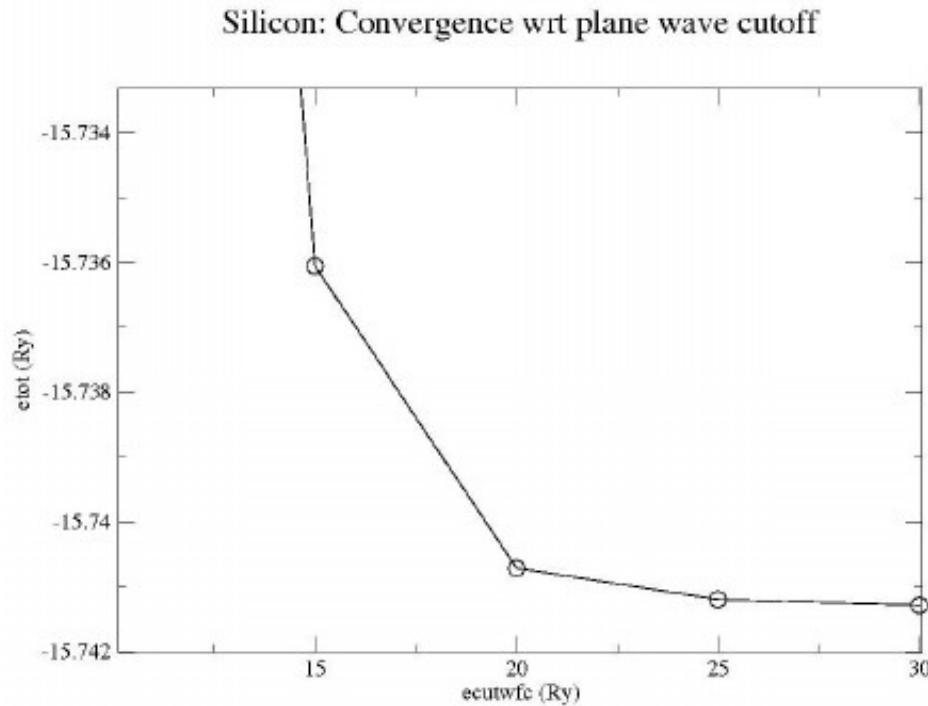
$$\frac{\hbar^2 |k + \mathbf{G}|^2}{2m} \leq E_{cut}$$

Input parameter **ecutwfc**



Checking Convergence wrt ecutwfc

- Must always check.
- Monotonic (variational).



Typical input file

```
&control
    prefix='silicon',
    pseudo_dir='./'
    outdir = './',
/
&system
    ibrav= 2,
    celldm(1) =10.2,
    nat= 2,
    ntyp= 1,
    ecutwfc = 12.0,
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.vbc.UPF
ATOMIC_POSITIONS {crystal}
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS automatic
2 2 2 0 0 0
```

Pseudopotentials for Quantum Espresso - 1

- Go to <http://www.quantum-espresso.org>; Click on “PSEUDO”



The screenshot shows the Quantum Espresso homepage. At the top right, there is a horizontal navigation bar with several menu items: HOME :: PROJECT :: WHAT CAN QE DO :: DOWNLOAD :: LEARN :: **PSEUDO** :: TOOLS :: QE WIKI :: CONTACTS :: QUOTE :: LOGOS ::. The "PSEUDO" menu item is highlighted with a red oval circle around it.

13 July 2010 A bugfix release, v.4.2.1, of the Quantum ESPRESSO distribution is available for download.

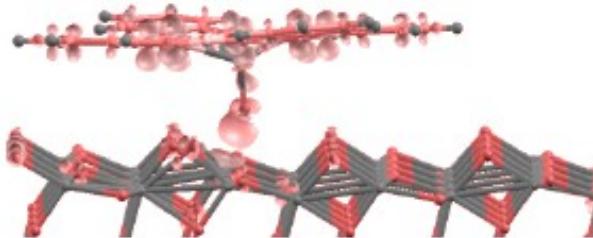
10 May 2010 A new version, v.4.2, of the Quantum ESPRESSO distribution is available for download.

12 April 2010 The final bugfix release, v.4.1.3, of a Quantum ESPRESSO distribution is available for download. This supersedes all previous 4.1.x releases.

20 July 2009 The new release of the Quantum ESPRESSO distribution is available for download (version 4.1)

21 April 2009 The final bugfix release, v.4.0.5, of the Quantum ESPRESSO distribution, is available for download. This supersedes all previous 4.0.x releases.

Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft).



What I cannot compute, I do not understand [adapted from Richard P. Feynman]

Pseudopotentials for Quantum Espresso - 2

- Click on element for which pseudopotential wanted.

The screenshot shows the Quantum Espresso Pseudopotentials website. At the top left is the logo 'QUANTUM ESPRESSO'. Below it is a navigation bar with links: HOME :: PROJECT :: WHAT CAN QE DO :: DOWNLOAD :: LEARN :: **PSEUDO** :: TOOLS :: QE WIKI :: CONTACTS :: QUOTE :: LOGOS ::. A sidebar on the left has links for 'About' and 'Notes'. The main content is a periodic table of elements. The oxygen atom (O) is circled in yellow. The table includes elements from Hydrogen (H) to Rutherfordium (Rf), and Lanthanoids (La) and Actinoids (Ac). The table is color-coded with red for most elements and grey for transition metals and some others. At the bottom of the table, there is a link 'Download the full archive (~30MB)'.

1 H	2 He
3 Li	4 Be
5 Na	12 Mg
19 K	20 Ca
37 Rb	38 Sr
55 Cs	56 Ba
87 Fr	88 Ra
57-70 Lu	71 Hf
103 Lr	104 Rf
105 Db	106 Bg
107 Bh	108 Hs
109 Mt	
37 La	58 Ce
90 Th	59 Pr
91 Pa	60 Nd
92 U	61 Pm
93 Np	62 Sm
94 Pu	63 Eu
95 Am	64 Gd
96 Cm	65 Tb
97 Bk	66 Dy
98 Cf	67 Ho
99 Es	68 Er
100 Fm	69 Tm
101 Md	70 Yb

Download the full archive (~30MB)

Pseudopotentials for Quantum-ESPRESSO

Name: Oxygen
Symbol: O
Atomic number: 8
Atomic configuration: [He] 2s2 2p4
Atomic mass: 15.9994 (3)

Available pseudopotentials:

[O.blyp-mt.UPF](#) ([details](#))

Becke-Lee-Yang-Parr (BLYP) exch-corr
Martins-Troullier

[O.pbe-rrkjus.UPF](#) ([details](#))

Perdew-Burke-Ernzerhof (PBE) exch-corr
Rabe Rappe Kaxiras Joannopoulos (ultrasoft)

[O.pbe-van_bm.UPF](#) ([details](#))

Perdew-Burke-Ernzerhof (PBE) exch-corr
Vanderbilt ultrasoft
author: bm

[O.pz-mt.UPF](#) ([details](#))

Perdew-Zunger (LDA) exch-corr
Martins-Troullier

[O.pz-rrkjus.UPF](#) ([details](#))

Perdew-Zunger (LDA) exch-corr
Rabe Rappe Kaxiras Joannopoulos (ultrasoft)

[O.blyp-van_ak.UPF](#) ([details](#))

Becke-Lee-Yang-Parr (BLYP) exch-corr
Vanderbilt ultrasoft
author: ak

Pseudopotential's name
gives information about :

- type of exchange-correlation functional
- type of pseudopotential
- e.g.:

[O.pbe-rrkjus.UPF](#) ([details](#))

Perdew-Burke-Ernzerhof (PBE) exch-corr
Rabe Rappe Kaxiras Joannopoulos (ultrasoft)

We will use only Norm-conserving pseudo types: mt, vbc, hgh

Element & V_{ion} for Quantum-ESPRESSO

- Should have same exchange-correlation functional for all pseudopotentials.

input

```
mixing_alpha = 0.8, mixing_beta  
mixing_beta = 0.7, conv_thr = 1.0  
/  
ATOMIC_SPECIES  
Fe 55.85 Fe pzfnd-rrkjus.UPF  
Co 58.93 Co pbe-nd-rrkjus.UPF  
ATOMIC_POSITIONS {crystal}  
Fe 0.00 0.00 0.00
```

oops!

output

```
Max angular momentum in pseudopotentials  
from readpp : error # 2  
inconsistent DFT read  
stopping ..■
```

Typical input file

```
&control
    prefix='silicon',
    pseudo_dir='./'
    outdir = './',
/
&system
    ibrav= 2,
    celldm(1) =10.2,
    nat= 2,
    ntyp= 1,
    ecutwfc = 12.0,
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.vbc.UPF
ATOMIC_POSITIONS {crystal}
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS automatic
2 2 2 0 0 0
```

Types of k-point meshes

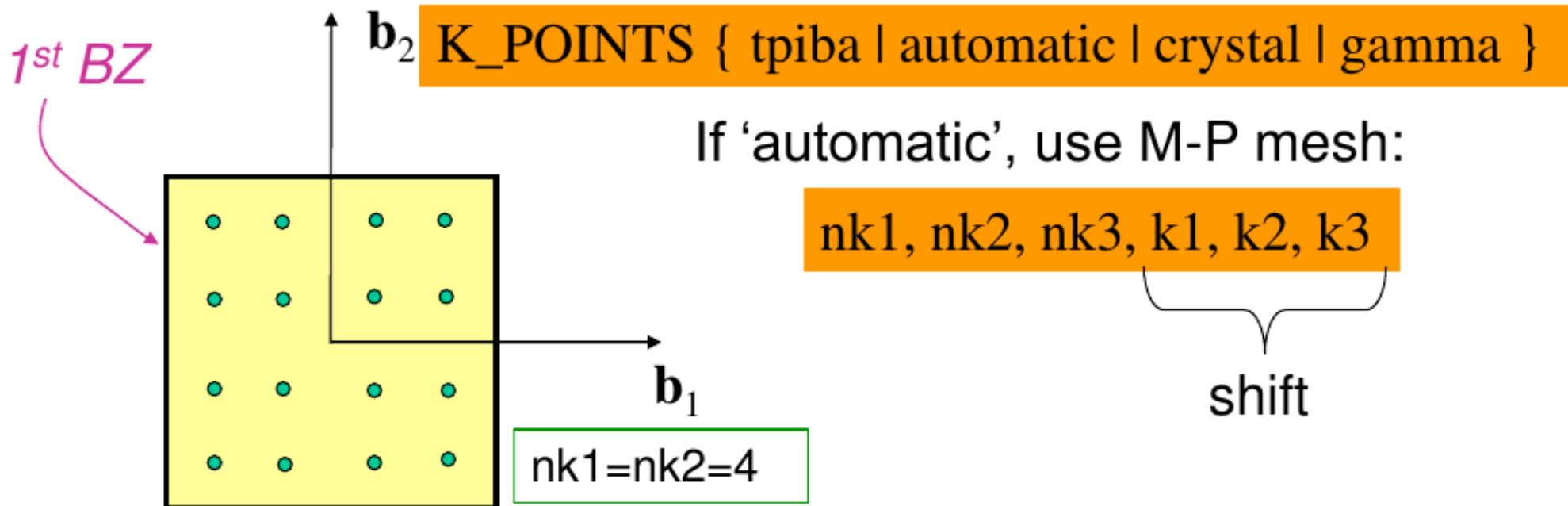
- **Special Points:** [Chadi & Cohen]

Points designed to give quick convergence for particular crystal structures.

- **Monkhorst-Pack:**

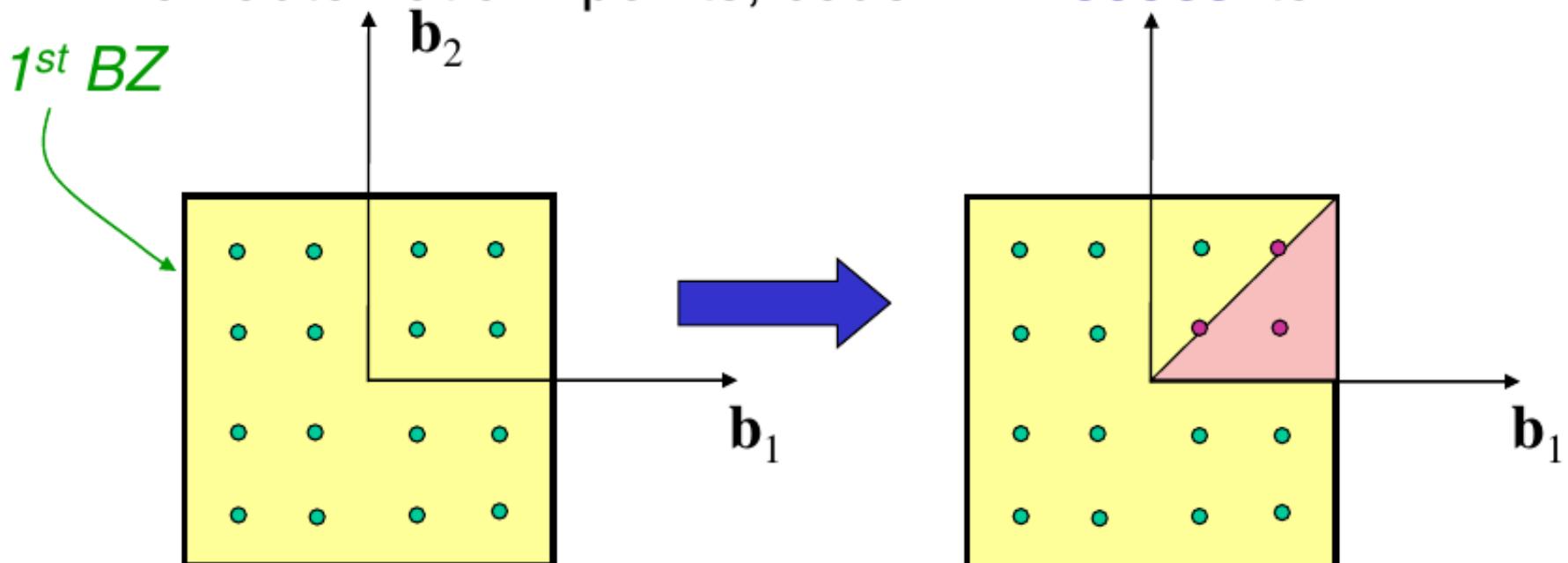
Equally spaced mesh in reciprocal space.

May be centred on origin ['non-shifted'] or not ['shifted']



Irreducible Brillouin Zone

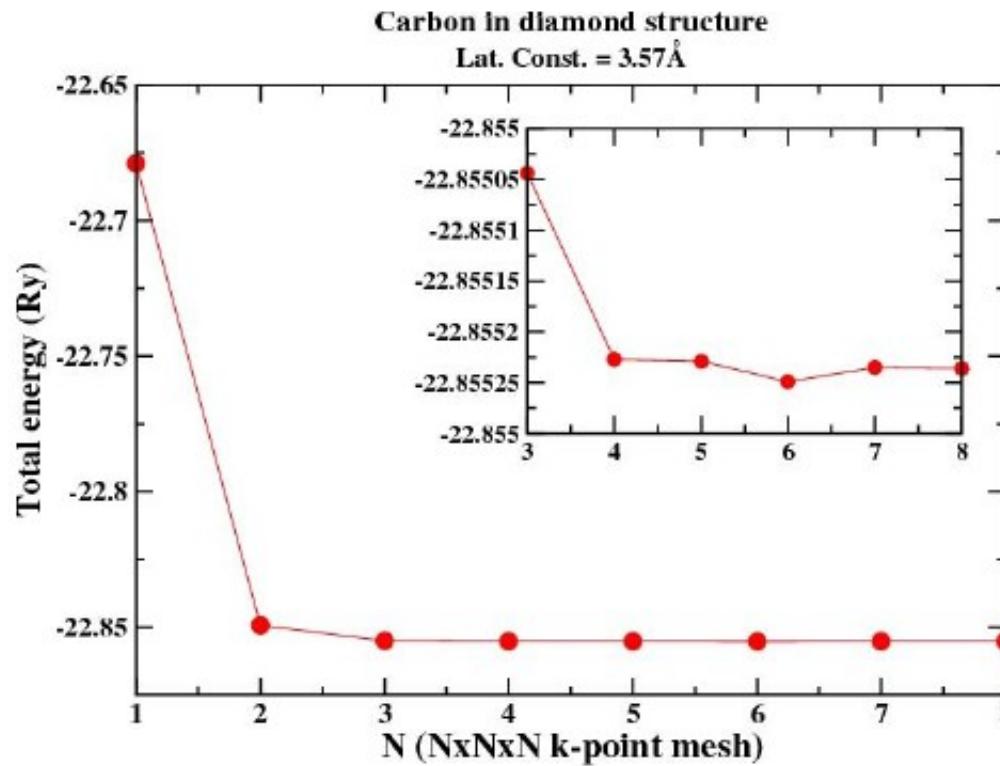
- **IBZ** depends on symmetries of system.
- Can save computational time by using appropriately weighted **k-points from IBZ** alone.
- For ‘automatic’ k-points, code will ‘reduce’ to IBZ.



- May not want to maintain symmetries in relaxation/MD.

Input parameter nosym

Convergence wrt BZ sampling



Madhura Marathe

Note: Differences in energy usually converge faster than absolute value of total energy because of error cancellation (if supercells & k-points are identical or commensurate).

Typical input file

```
&control
    prefix='silicon',
    pseudo_dir='./'
    outdir = './',
/
&system
    ibrav= 2,
    celldm(1) =10.2,
    nat= 2,
    ntyp= 1,
    ecutwfc = 12.0,
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.vbc.UPF
ATOMIC_POSITIONS {crystal}
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS automatic
2 2 2 0 0 0
```

First calculation: Self-consistent calculation for Silicon in the diamond structure

Tutorial files: on Dropbox

didatticaSdM (1)/EsercitazioneDFT_2017-2018/DFT-2017-2018/

Copy to your local machine:

```
user% cd
```

```
user% cp -r [....]/DFT-2017-2018 .
```

```
user% ls DFT-2017-2018
```

```
Codes Docs ENVIRONMENT_VARIABLES Pseudo Si_bulk
```

```
user% cd DFT-2017-2018/Si_bulk
```

```
user% ls
```

```
0_alat 0_cutoff 0_kpoints 1_scf 2_bandstructure Reference
```

```
user% cd 0_alat
```

```
user% pw.x < si.scf.in > si.scf.out & (run in background)
```

```
user% tail si.scf.out
```

Look the output file: check electrons, convergence, etc...

Run pw.x code, self consistent calculation

```
User% pw.x < si.scf.in > si.scf.out
```

Look at outdir and contents

```
User% ls ./tmp/Si.save
```

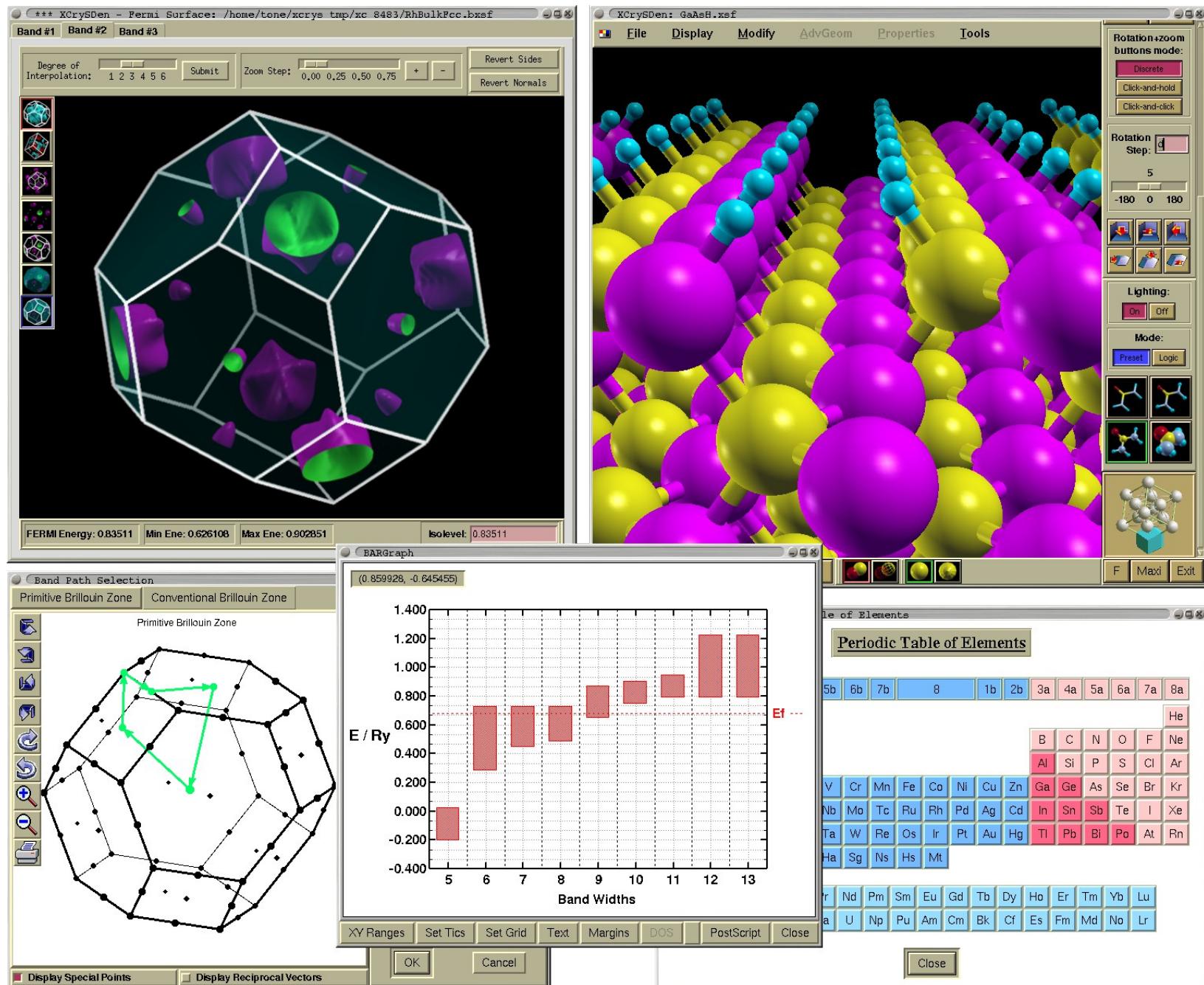
Examine output file and look how convergence proceeds

```
User% grep -e "total energy" -e "scf" si.scf.out
```

```
total energy          =      -15.84398090 Ry
estimated scf accuracy <       0.05984738 Ry
total energy          =      -15.84707445 Ry
estimated scf accuracy <       0.00205519 Ry
total energy          =      -15.84735326 Ry
estimated scf accuracy <       0.00005253 Ry
total energy          =      -15.84736503 Ry
estimated scf accuracy <       0.00000177 Ry
total energy          =      -15.84736536 Ry
estimated scf accuracy <       0.00000005 Ry
!
total energy          =      -15.84736537 Ry
estimated scf accuracy <       1.7E-10 Ry
```

The total energy is the sum of the following terms:

Using XCrySDen to verify input/output



Using Xcrysden to verify input/output

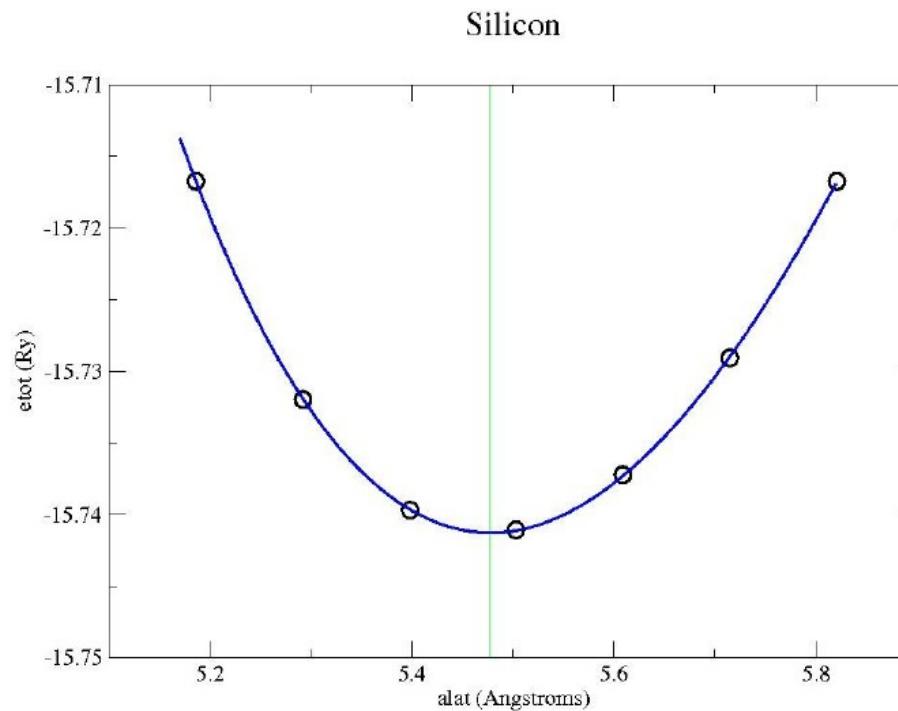
- Visualization of structures from PW.X **input** file:
 - `xcrysden --pwi input.file`
- Visualization of structures from PW.X **output** file:
 - `xcrysden --pwo output.file`

What can we do with the total energy?

Structure optimization, phonons,
compressibility, phase transitions, binding
energy, etc...

Second calculation: Optimal lattice parameter for Silicon

- Perhaps the most important output quantity is the TOTAL ENERGY
- Can use, e.g., to optimize structure
- e.g., for a cubic crystal, where the structure can be specified by a single parameter (side of cube):



Calculate the total energy for all values of a_0 (celldm) listed in the E_vs_cell.dat file

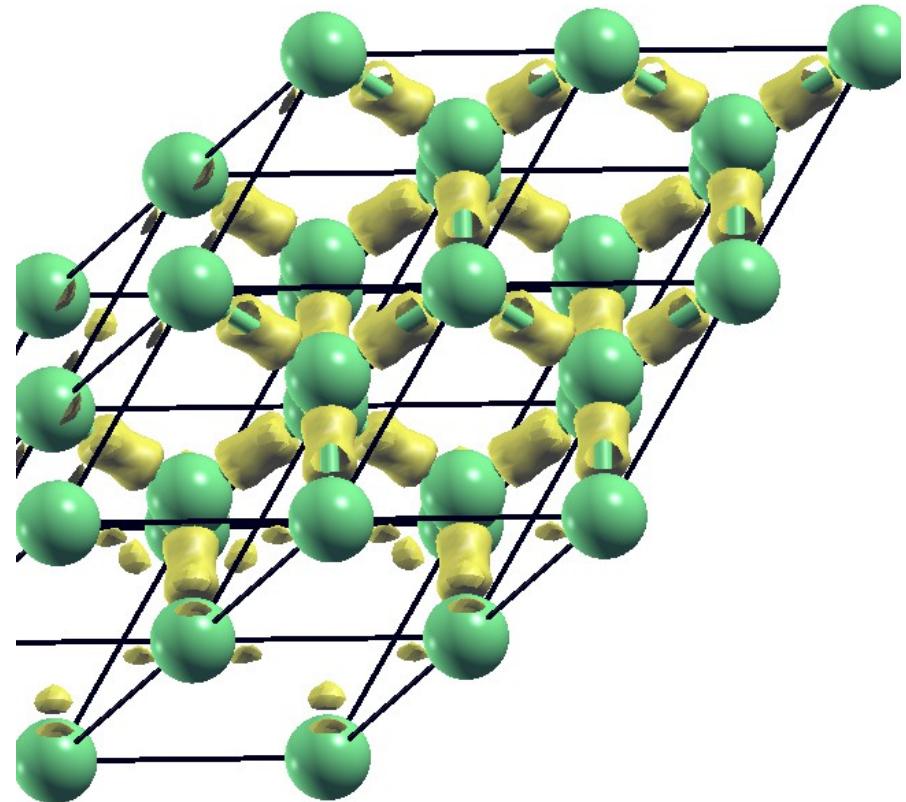
`user% pw.x < si.scf.in > si.scf.out_10.10`

Plot the data to estimate the minimum a_0 , and use the gnuplot "DoFit.gnu" file to fit the data to the Murnaghan equation of state

Third calculation: data analysis

Charge density

```
&inputpp
  prefix = 'silicon'
  outdir='./'
  filplot = 'sicharge'
  plot_num= 0
/
&plot
  iflag = 3
  output_format = 5
  fileout = 'si.rho.xsf'
/
```



User% cd 1_scf

User% pw.x < si.scf.in > si.scf.out

Run post processing tool pp.x

user% pp.x < charge.in > charge.out

Visualize with Xcrysden

user% xcrysden --xsf charge.xsf

```

&control
  calculation='bands',
  prefix='silicon',
  pseudo_dir='./'
 outdir = './',
/
&system
  ibrav= 2,
  celldm(1) =10.21,
  nat= 2,
  ntyp= 1,
  ecutwfc = 20.0,
  nbnd=10
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.vbc.UPF
ATOMIC_POSITIONS {crystal}
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS {crystal_b}
6
0.000 0.500 0.000 8 ! L
0.000 0.000 0.000 8 ! Gamma
0.500 0.500 0.000 8 ! X
0.500 1.000 0.500 4 ! X2
0.375 0.750 0.375 8 ! K
0.000 0.000 0.000 1 ! Gamma

```

New
calculation
type

Number
of bands

←

k-points list in
crystal or
cartesian (tpiba) units
6 lines
k1 k2 k3 npts

Fourth calculation: Silicon band structure

User% cd 2_bandstructure

User% pw.x < si.scf-manual.in > si.scf.out

User%

pw.x < si.bands-manual.in > si.bands.out

You can also instead use the script

User% ./run_bands

Bands plot

Eigenvalues are written at the end of the **si.bands.out** file

Use the simple code

.../.../Codes/plot_pwbands.f90

to reorder the data in a plottable format.

See inside the code for the required input.

User% cp si.bands.out bands.dat

User% vi bands.dat

User% .../.../Codes/plot_pwbands.x

User% gnuplot

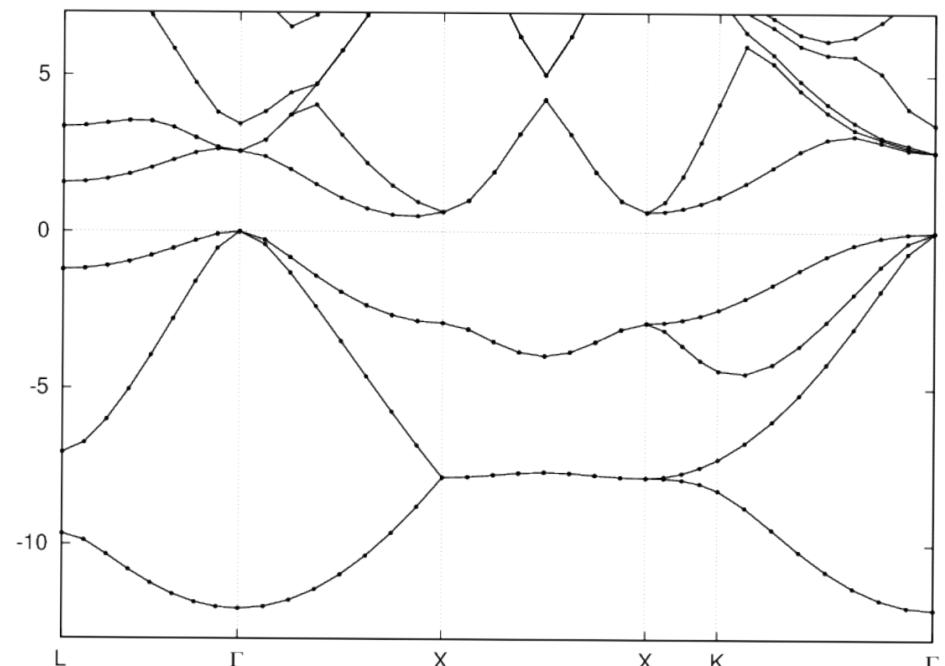
Gnuplot> plot "plot.dat" u 1:2 w lp

See also the file

Reference/plot_bands_Si.gnu

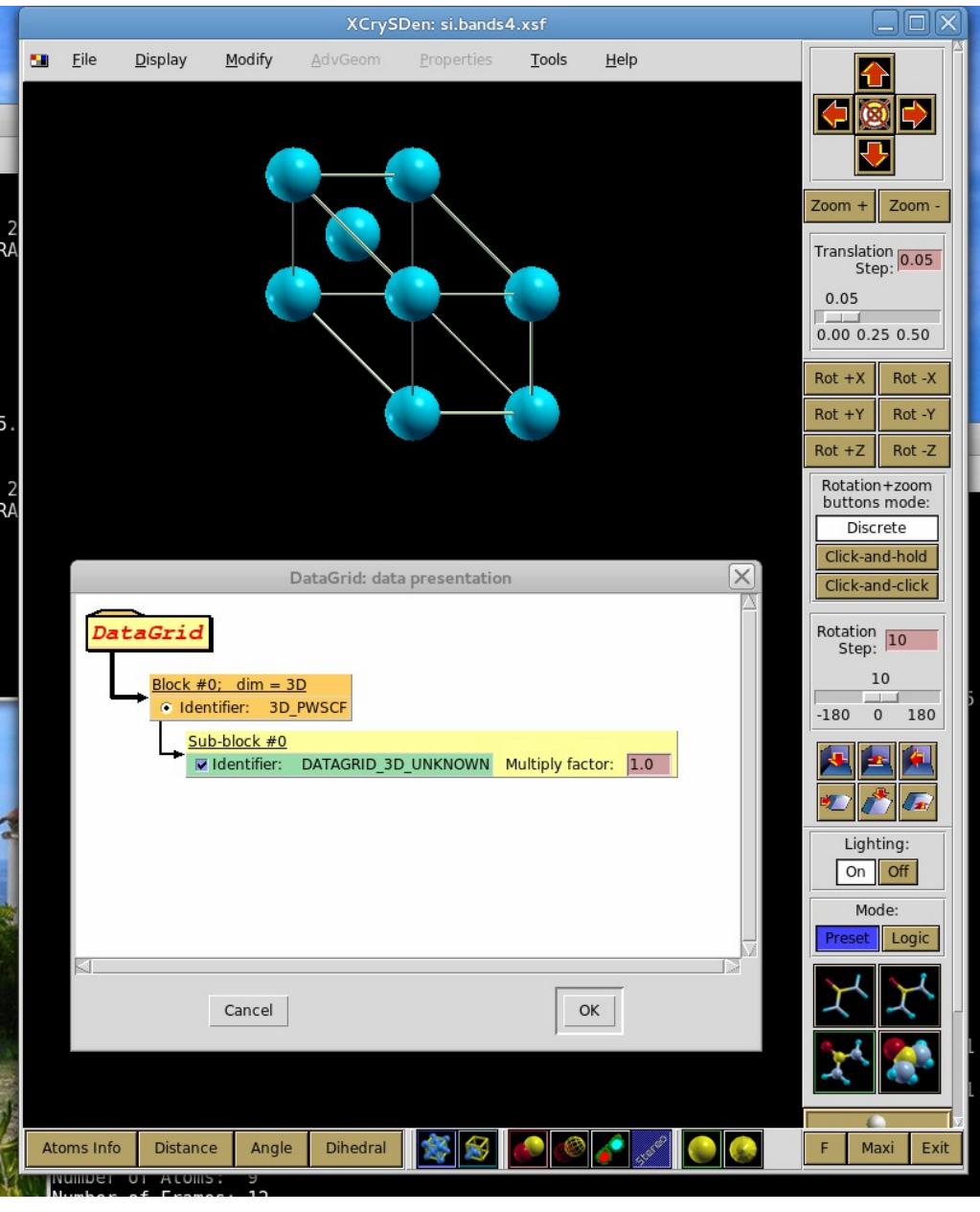
You can instead use the **run_bands** script, but you should first understand what it does.

(correct the format)



Data Visualization with XCrySDen

Tools → Data grid



Set Isolevel

