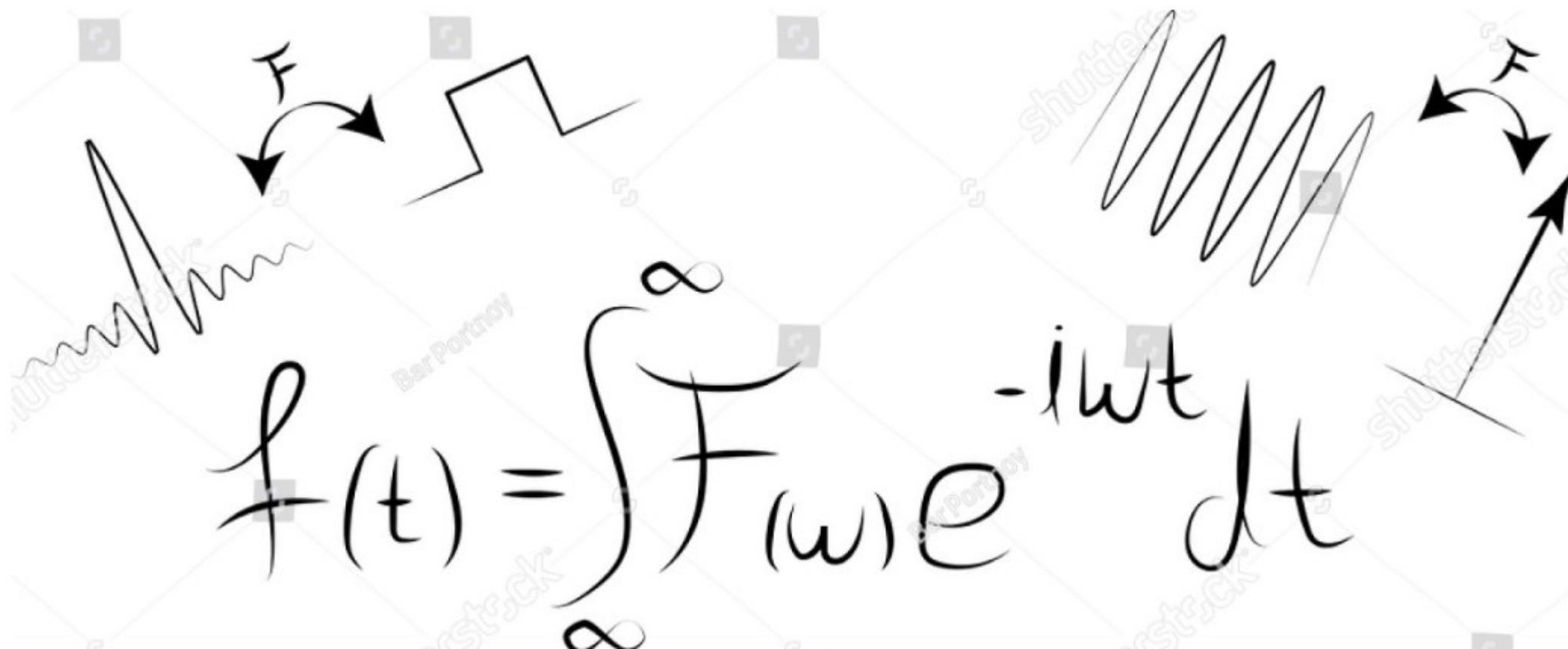


Approximations in DFT 2/2


$$f(t) = \int_{-\infty}^{\infty} F(\omega) e^{-i\omega t} d\omega$$

The Kohn-Sham problem

- Want to solve the Kohn-Sham equations:

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

H

- Note that **self-consistent solution** necessary, as H depends on solution:

$$\{\psi_i\} \rightarrow n(r) \rightarrow H$$

- Convention (most of the time, in this talk):

$$e = \hbar = m_e = 1$$

Kohn-Sham Equations in a Basis

- Can choose to expand wavefunctions in a **basis set**:

$$\psi_i(\mathbf{r}) = \sum_{\alpha=1}^{N_b} c_{i\alpha} f_{\alpha}(\mathbf{r})$$

- Now obtain a matrix equation:

$$\sum_{\beta} H_{\alpha\beta} c_{i\beta} = \epsilon_i c_{i\alpha}$$

Matrix element *Eigenvalue* *Eigenvector*

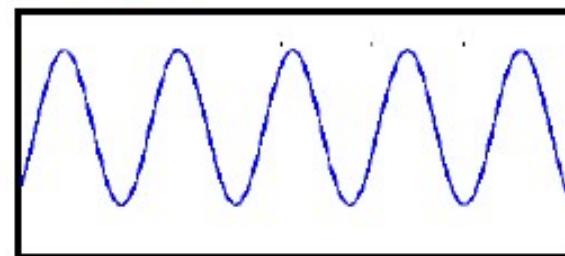
- Solving \Leftrightarrow Have to diagonalize a matrix of size $N_b \times N_b$

Size of basis

Some possible basis sets

- Various possible choices of basis:

- Plane waves $e^{iK \cdot r}$



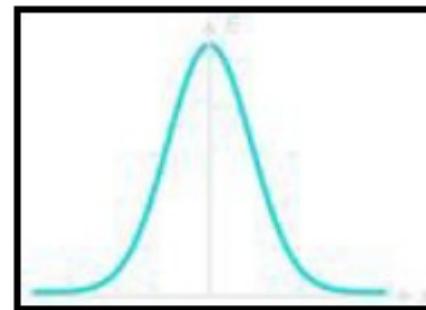
- Localized sets:

- e.g., Gaussians

- e.g., atomic orbitals
real-space grids

- Mixed basis

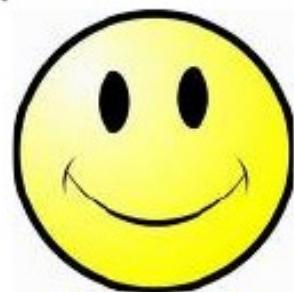
- Augmented basis



- Choose so that calculation is fast, accurate, convenient.
- Would like N_b to be small (within reason)?
- Would like form of $f_\alpha(\mathbf{r})$ to be simple?

Advantages of a Plane Wave Basis

- **Simple**: Easy to take derivatives, etc. \Rightarrow Coding is easy!
- **Orthonormal**: No overlap integrals.
- **Independent of atomic positions** \Rightarrow No “Pulay forces”; easy to calculate forces for structural relaxation & molecular dynamics.
- **Unbiased**: No assumption about where charge concentrated. (But \therefore also wasteful?)
- **Easy to control convergence** w.r.t. size of basis: only one parameter E_{cut} . (energy cut-off for planewaves)
- Can easily take advantage of FFT's : r-space \leftrightarrow k-space



Advantages of a Plane Wave Basis

Convenient use of FFTs:

$$\tilde{f}(k) = \sum_{n=0}^{N-1} f_n e^{-2\pi i kn/N}$$

Very practical to calculate convolutions, solve Poisson's equation, etc.

$$V(\mathbf{r}) = \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

$$\tilde{V}(\mathbf{G}) = 4\pi \frac{\tilde{n}(\mathbf{G})}{\mathbf{G}^2}$$

Disadvantages of a Plane Wave Basis

- Often need a **HUGE** number of plane waves to get an adequate expansion, i.e., N_b can be very large! ($\sim 10^5$ per atom)
(Will discuss...
solution = introduction of pseudopotentials.)
- The set of plane waves is discrete only if the system is periodic!
(Will discuss solution = introduction of artificial supercell or periodic approximat.)
- Sometimes (chemical) interpretation harder.



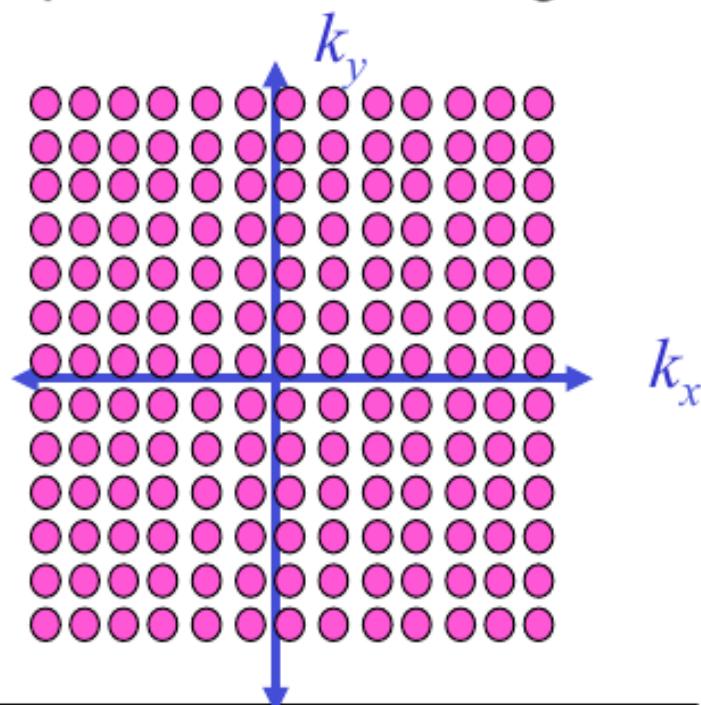
Plane Waves & Periodic Systems

- So, 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.

Periodic Systems & Bloch's Theorem

- For a periodic system, recall Bloch's Theorem:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

- $u_{\mathbf{k}}(\mathbf{r})$ has the periodicity of the system, i.e.,

$$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}), \quad \text{where } \mathbf{R} = \text{lattice vector}$$

- As for all lattice-periodic functions, only certain plane waves will appear in the Fourier expansion of $u_{\mathbf{k}}(\mathbf{r})$:

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

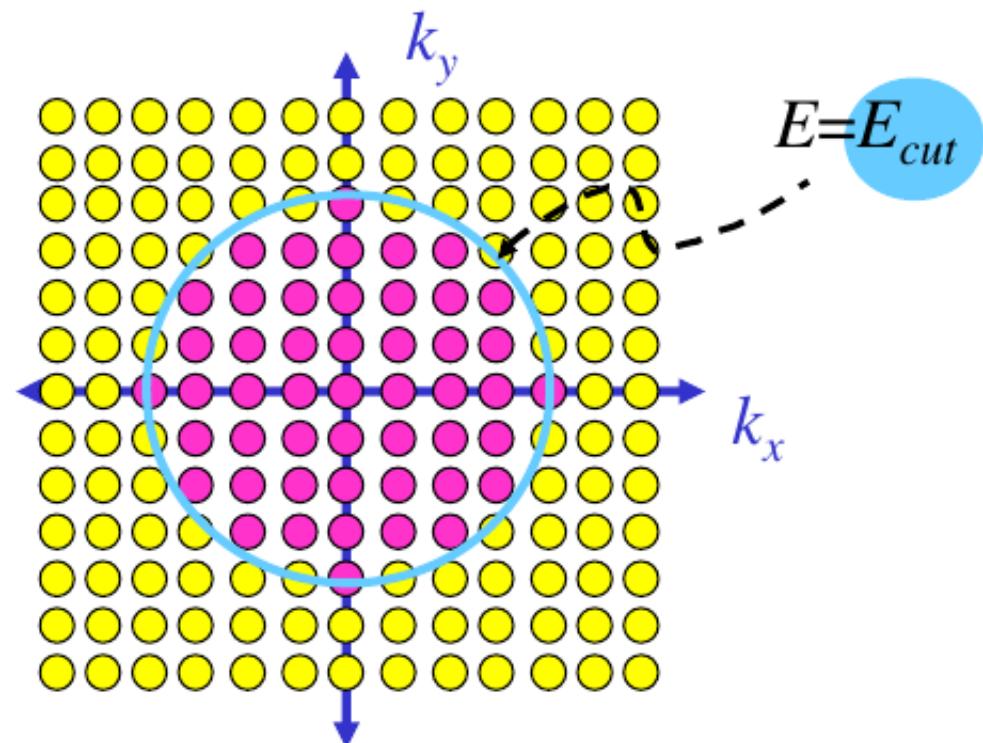
where \mathbf{G} = reciprocal lattice vector

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:

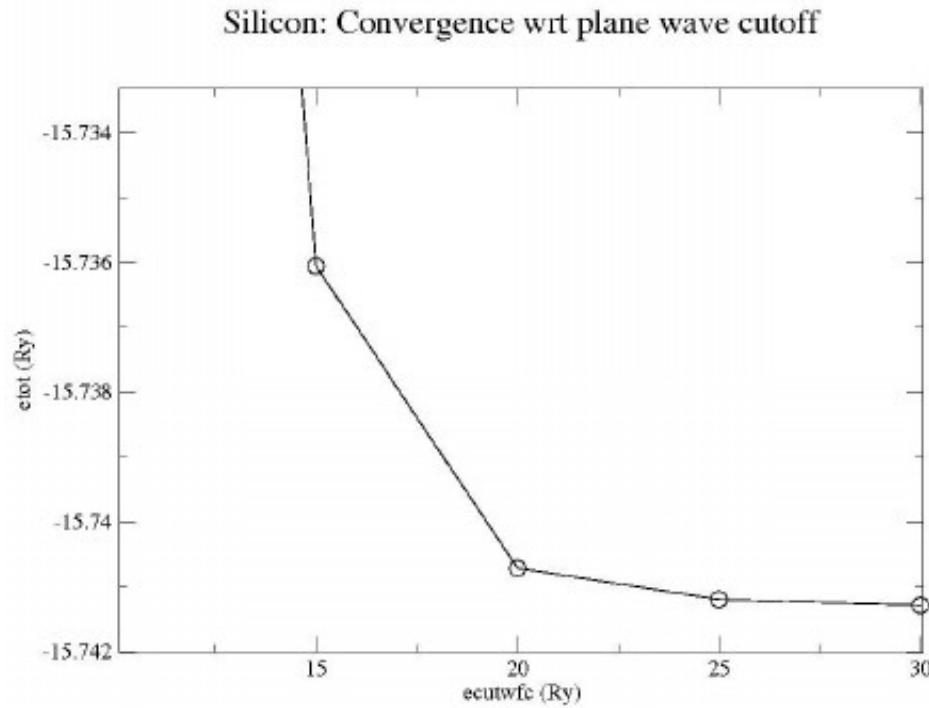
$$\frac{\hbar^2 |k + \mathbf{G}|^2}{2m} \leq E_{cut}$$

Input parameter **ecutwfc**



Checking Convergence wrt ecutwfc

- Must always check.
- Monotonic (variational).



Periodic Systems & Bloch's Theorem

- For a periodic system, recall Bloch's Theorem:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

- $u_{\mathbf{k}}(\mathbf{r})$ has the periodicity of the system, i.e.,

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

where \mathbf{G} = reciprocal lattice vector

Types of k-point meshes

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

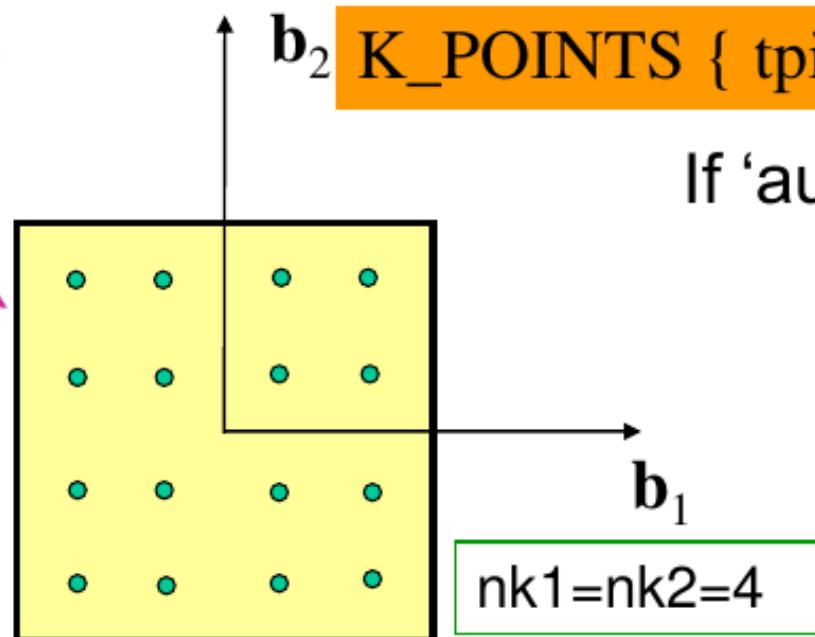
Points designed to give quick convergence for particular crystal structures.

- **Monkhorst-Pack:**

Equally spaced mesh in reciprocal space.

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

1st BZ



K_POINTS { tpiba | automatic | crystal | gamma }

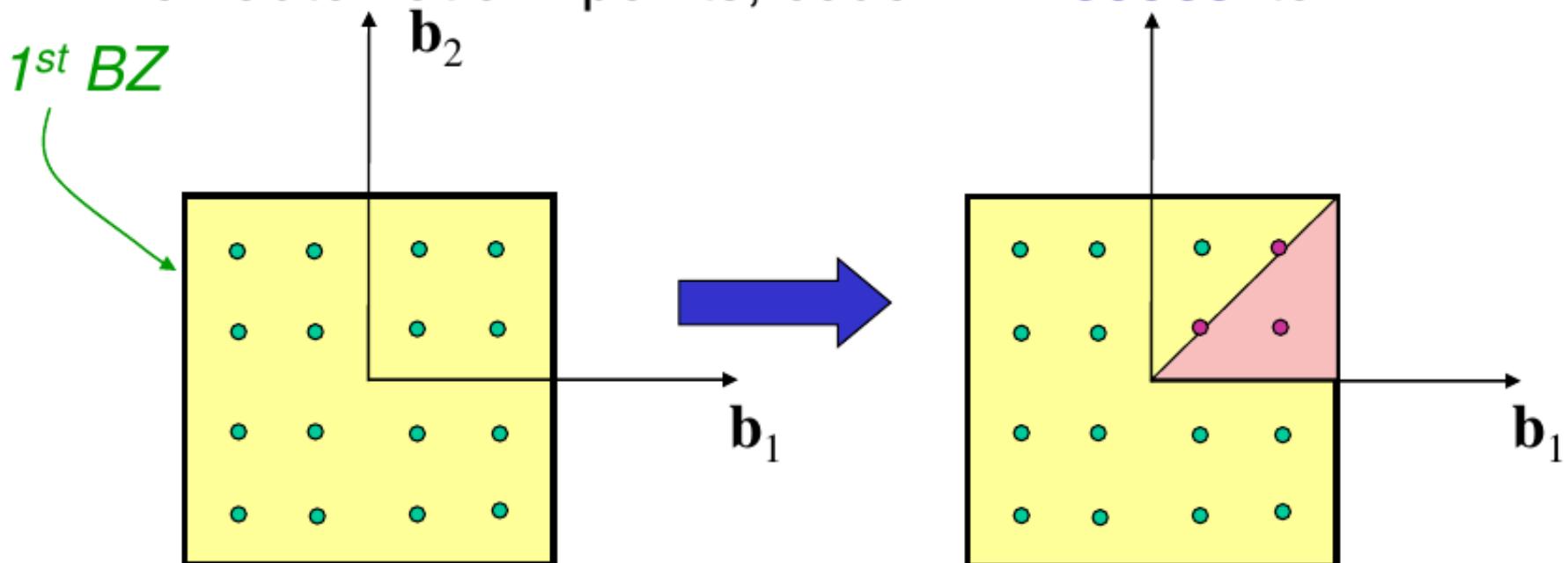
If 'automatic', use M-P mesh:

$nk_1, nk_2, nk_3, k_1, k_2, k_3$

shift

Irreducible Brillouin Zone

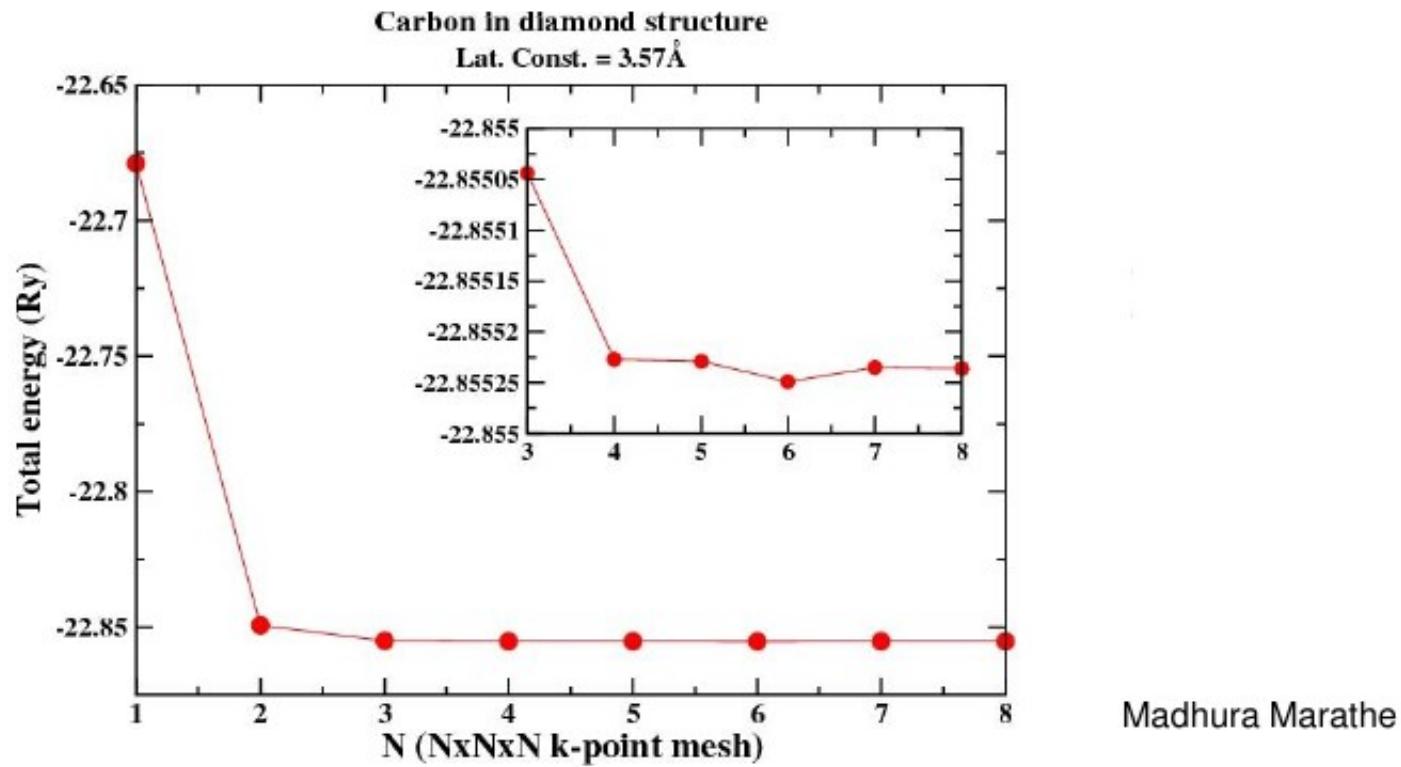
- **IBZ** depends on symmetries of system.
- Can save computational time by using appropriately weighted **k-points from IBZ** alone.
- For ‘automatic’ k-points, code will ‘reduce’ to IBZ.



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

Input parameter nosym

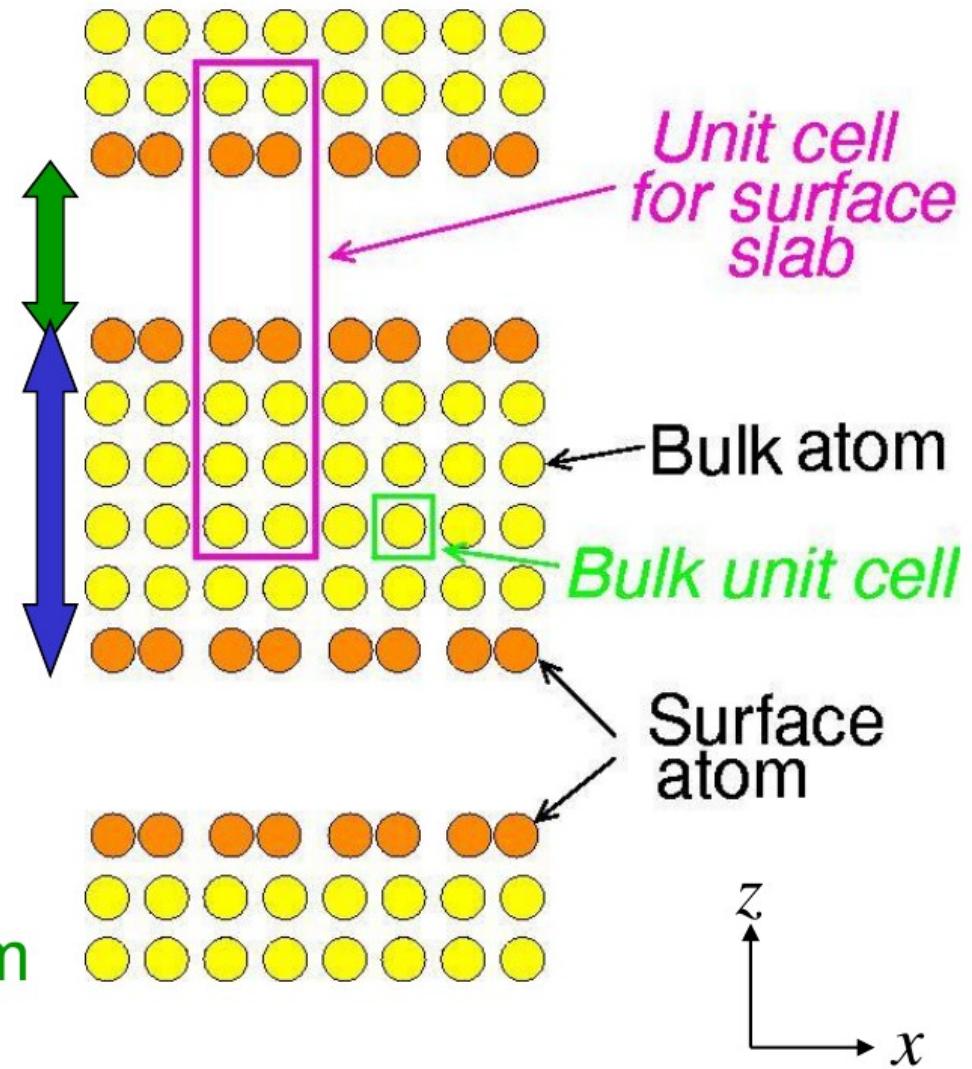
Convergence wrt BZ sampling



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).

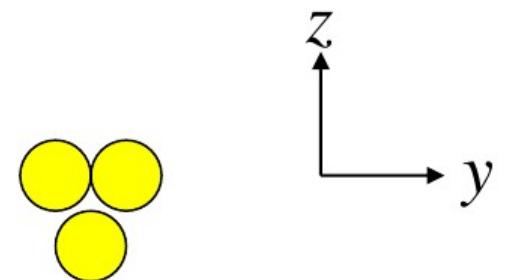
What if the system is not periodic?

- Example 1: Want to study properties of a system with a **surface**.
- Presence of surface \Rightarrow No periodicity along z .
- Use a **supercell**: **artificial periodicity along z** by repeating slabs separated by **vacuum**.
- Have to check convergence w.r.t. **slab thickness & vacuum thickness**.



What if the system is not periodic?

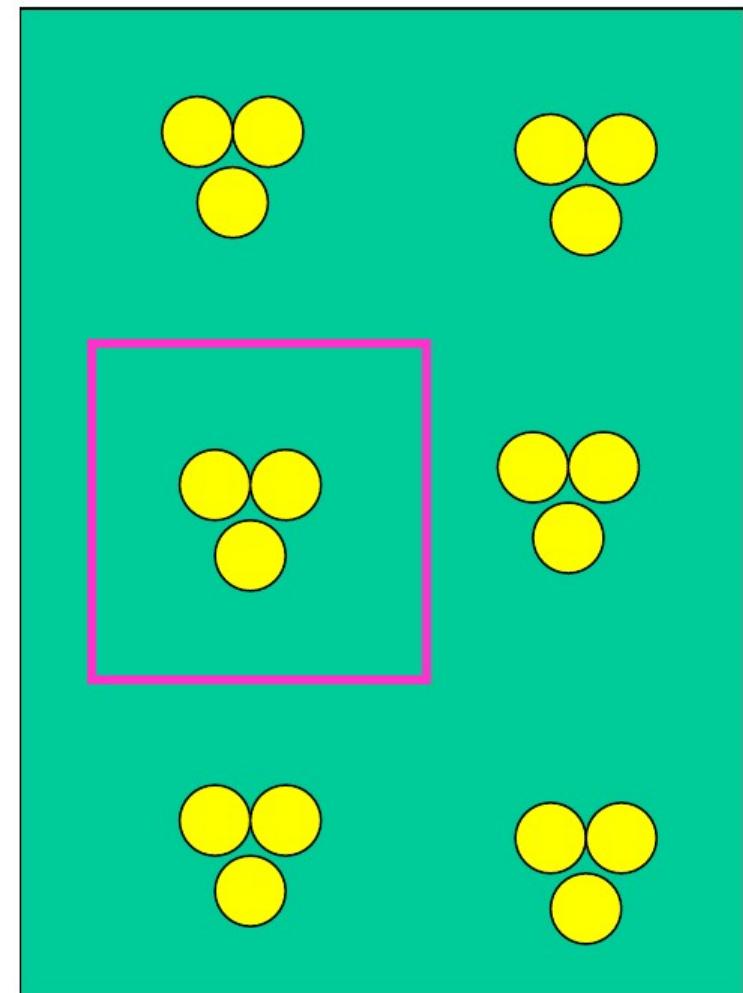
- Example 2: Want to study properties of a nanowire.



- Example 3: Want to study properties of a cluster

What if the system is not periodic?

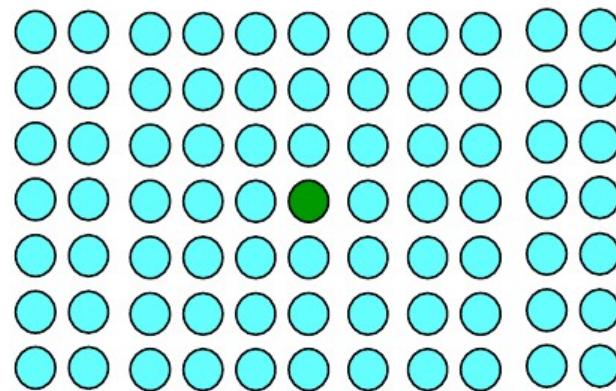
- Example 2: Want to study properties of a nanowire \Rightarrow introduce **artificial periodicity along y & z** .
- Example 3: Want to study properties of a cluster \Rightarrow introduce **artificial periodicity along x , y & z** .



y
 z

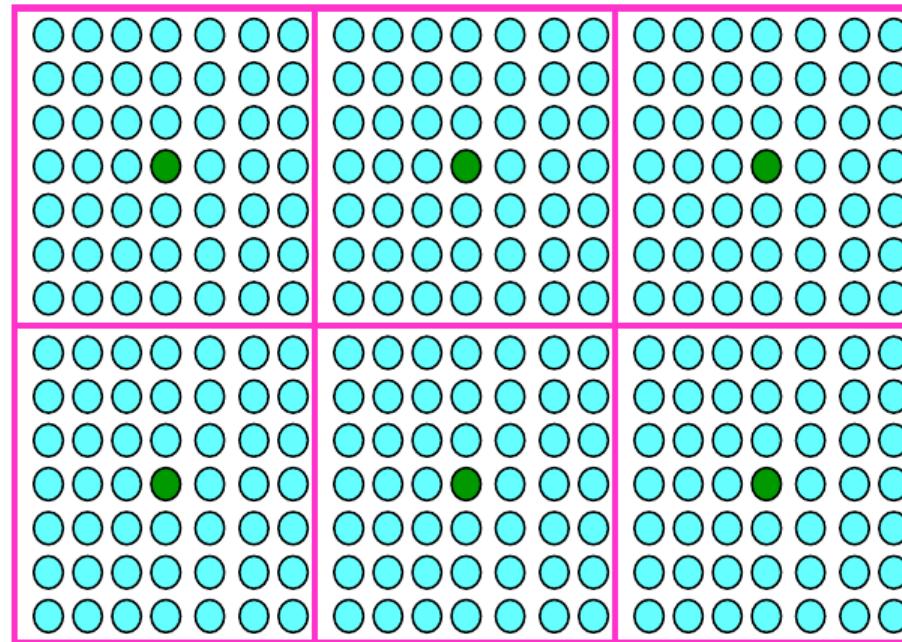
What if the system is not periodic?

- Example 4: Want to study a system with a defect, e.g., a **vacancy** or **impurity**:



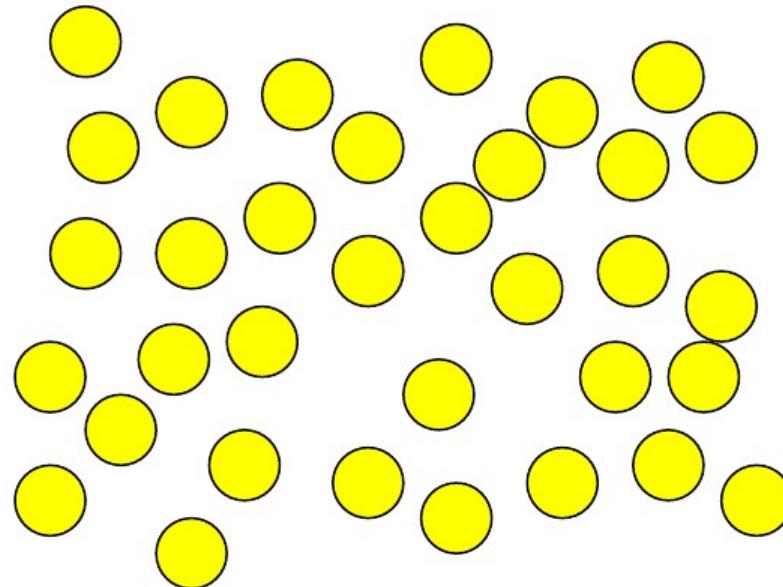
What if the system is not periodic?

- Example 4: Want to study a system with a defect, e.g., a **vacancy** or **impurity**:



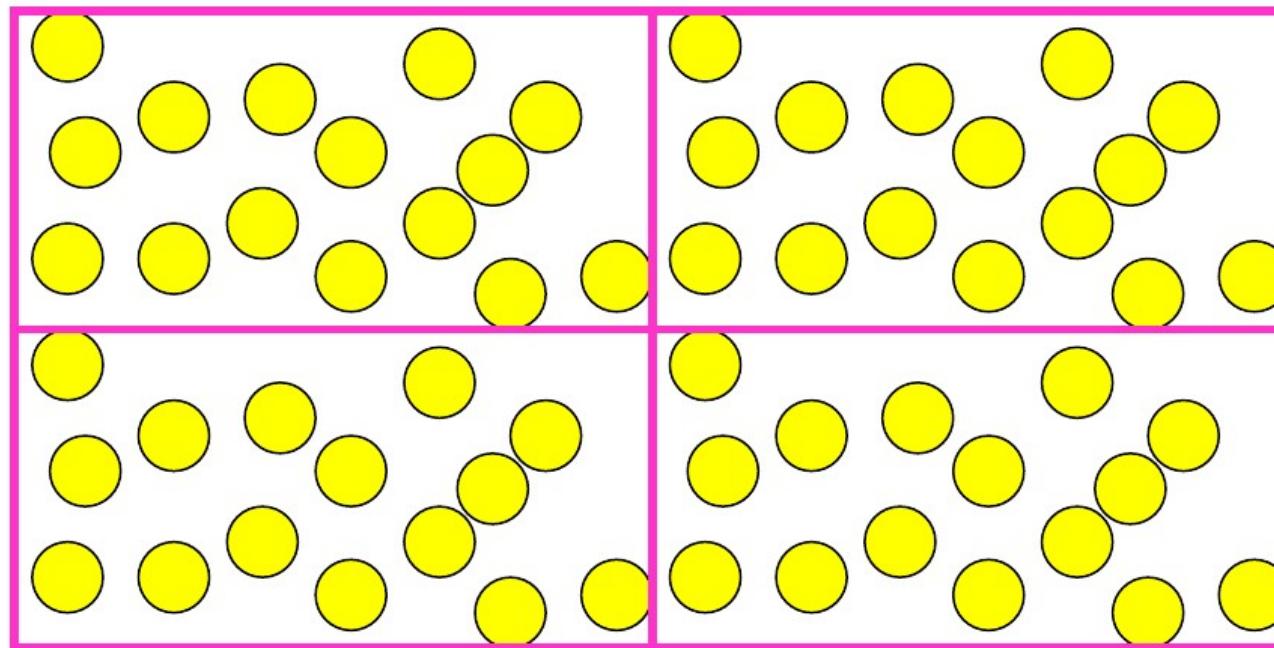
What if the system is not periodic?

- Example 5: Want to study an amorphous or quasicrystalline system.



What if the system is not periodic?

- Example 5: Want to study an amorphous or quasicrystalline system: approximate by a periodic system (with large **unit cell**).



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**

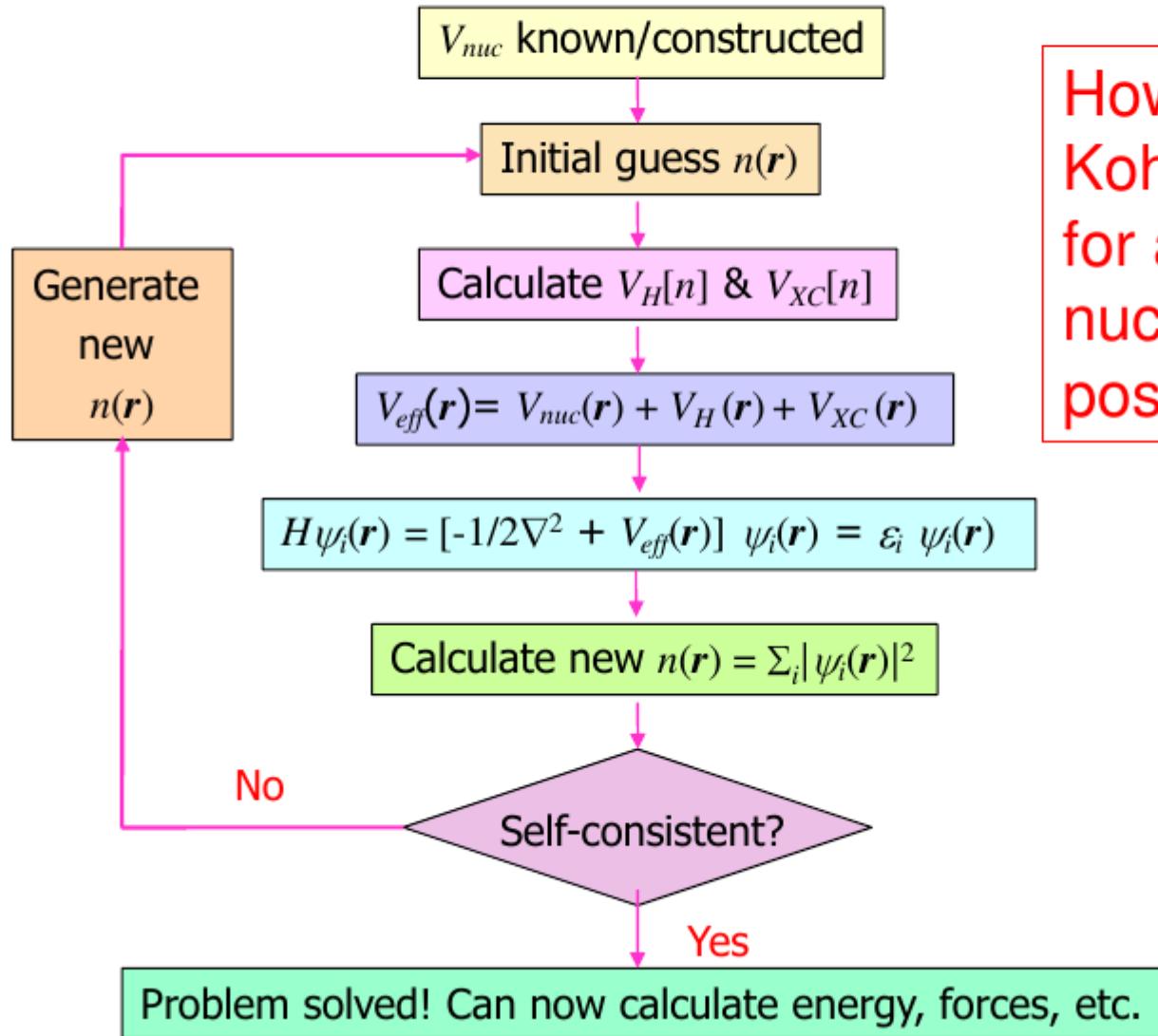
Code organization

• 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), Raman, 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
```

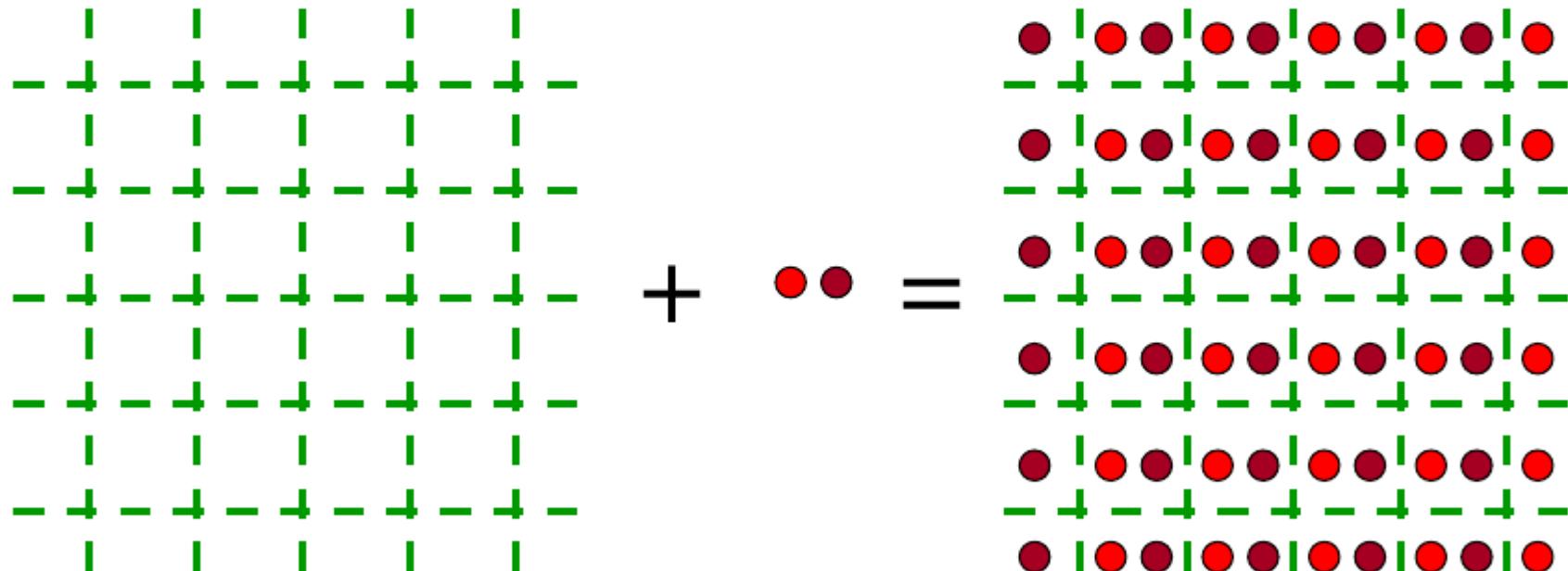
Step 0: Defining the (periodic) system



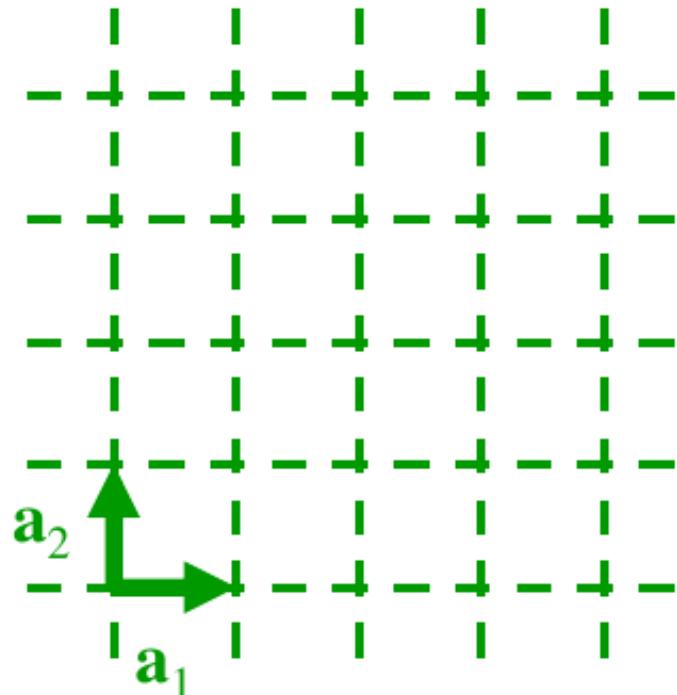
Namelist '**SYSTEM**'

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 \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3

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

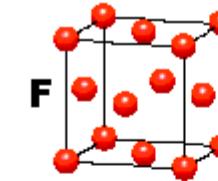
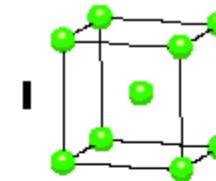
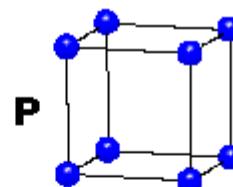
Bravais Lattices: ibrav flag

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

ibrav = 1, 3, 2

CUBIC

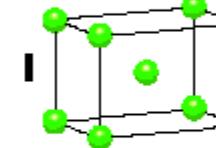
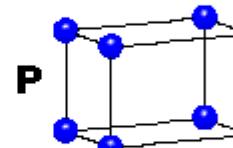
$a = b = c$
 $\alpha = \beta = \gamma = 90^\circ$



ibrav = 6, 7

TETRAGONAL

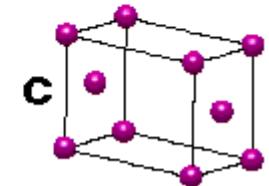
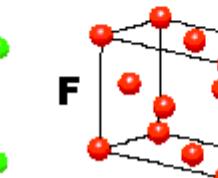
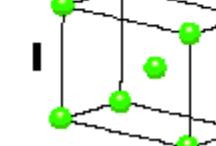
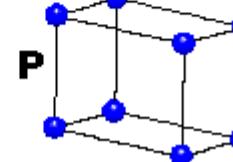
$a = b \neq c$
 $\alpha = \beta = \gamma = 90^\circ$



ibrav = 8, 9, 10, 11

ORTHORHOMBIC

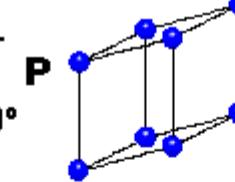
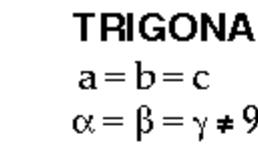
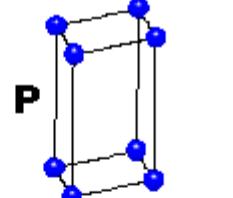
$a \neq b \neq c$
 $\alpha = \beta = \gamma = 90^\circ$



ibrav = 4, 5, -5

HEXAGONAL

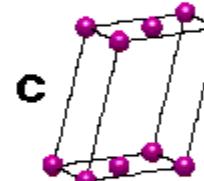
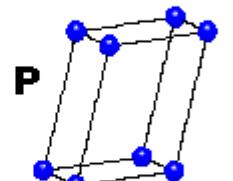
$a = b \neq c$
 $\alpha = \beta = 90^\circ$
 $\gamma = 120^\circ$



ibrav = 12, -12, 13

MONOCLINIC

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



ibrav = 14

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

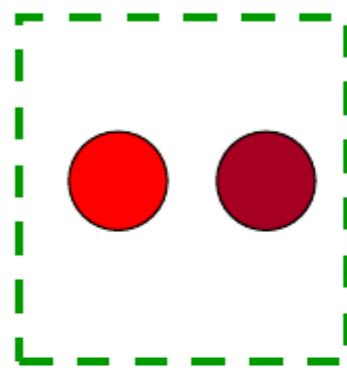
C = Side-Centred

+

7 Crystal Classes

→ 14 Bravais Lattices

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
```

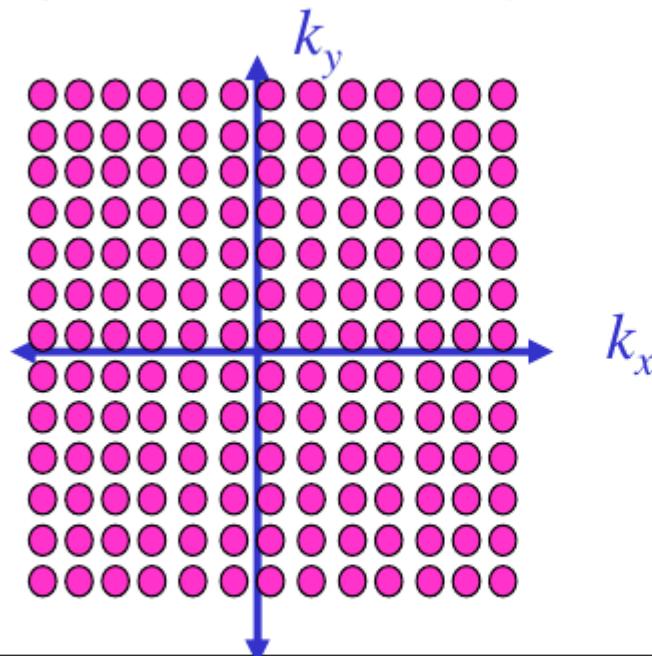
Plane Waves & Periodic Systems

- 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:



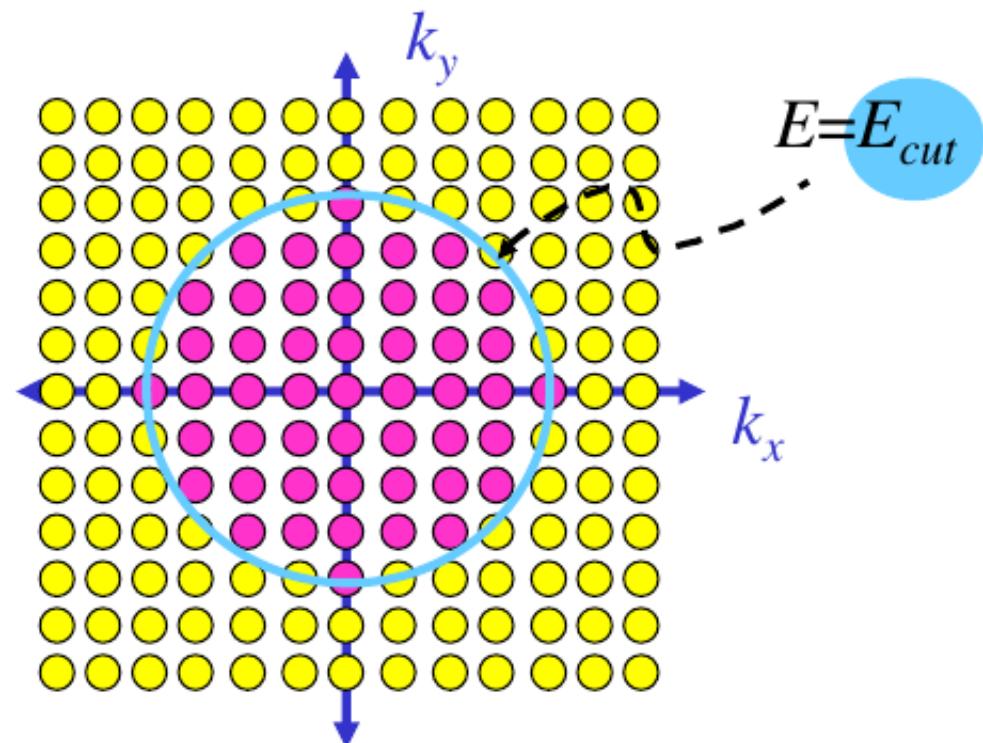
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- So truncate the expansion at some value of $|k+G|$.
- Traditional to express this cut-off in energy units:

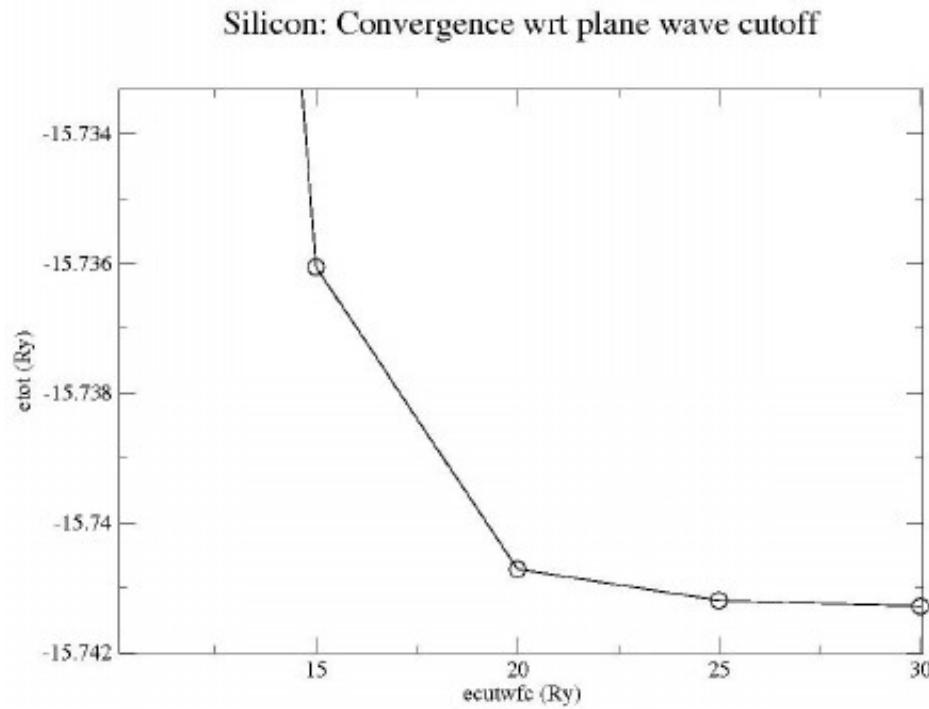
$$\frac{\hbar^2 |k + \mathbf{G}|^2}{2m} \leq E_{cut}$$

Input parameter **ecutwfc**



Checking Convergence wrt ecutwfc

- Must always check.
- Monotonic (variational).



Typical input file

```
&control
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    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" item is highlighted with a red oval. On the left side, there is a sidebar with a circular logo and a list of recent releases:

- 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.

In the center, there is a large red banner with white text: "13 July 2010 A bugfix release, v.4.2.1, of the Quantum ESPRESSO distribution is available for download." Below the banner, there is a brief description of what Quantum Espresso is: "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).". To the right of the text, there is a 3D visualization of a crystal lattice structure with red spheres representing atoms. At the bottom, there is a quote: "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.

Quantum Espresso

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PSEUDOPOTENTIALS

Updated: Sat, 14 Aug 2010 21:10:03 CEST

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

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
```

Install QE on your PC

- **LINUX**
 - LinuxMint or Ubuntu
use “**synaptic**” to install “quantum-espresso” and “xcrysden”
or type
`sudo apt-get install quantum-espresso`
`sudo apt-get install xcrysden`
- **MacOSX**
 - Use MacPorts, open the terminal and type
`sudo port install quantum-espresso`
see here: <https://ports.macports.org/port/quantum-espresso/>
- **WINDOWS**
 - download “putty” we will provide a server with QE and Octopus installed
<https://www.putty.org/>
 - Install the Quantum Mobile virtual machine
<https://quantum-mobile.readthedocs.io/en/latest/>

**We will provide two laptops
with QE, Xcrysden and Octopus installed**

First calculation:

Self-consistent calculation for Silicon in the diamond structure

Espace de Travail: /media/MateriApps

First tutorial: /media/MateriApps/tutorial/examples_pwscf_ex.tgz

Unpack files: tar zxvf tutorial/examples_pwscf_ex.tgz

Look the input file:

```
cd examples_pwscf_ex/  
emacs si.scf.in
```

Run calculations!!

```
pw.x < si.scf.in > output_scf
```

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

run pw.x code

```
prompt> espresso_dir/bin/pw.x < si.scf.in > si.scf.out
```

look at outdir and its content

```
prompt> ls /scratch/my_name/espresso
```

```
silicon.save    silicon.wfc
```

examine output file and look how convergence proceeds

```
prompt> grep -e 'total energy' -e estimate si.scf.out
```

```
total energy          = -15.78885161 ryd
```

```
estimated scf accuracy < 0.06378063 ryd
```

```
total energy          = -15.79407709 ryd
```

```
estimated scf accuracy < 0.00231243 ryd
```

```
total energy          = -15.79448017 ryd
```

```
estimated scf accuracy < 0.00006733 ryd
```

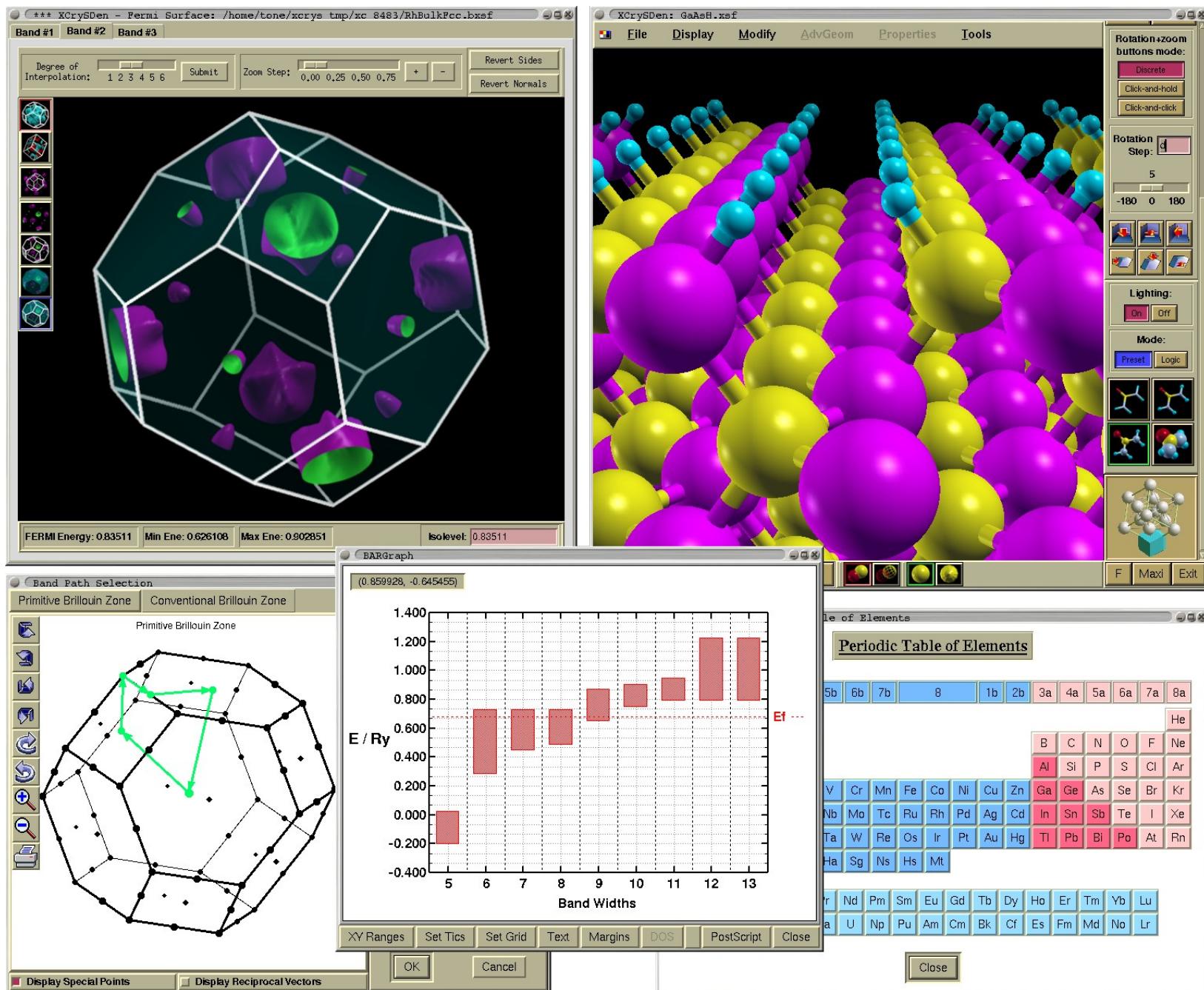
```
total energy          = -15.79449452 ryd
```

```
estimated scf accuracy < 0.00000619 ryd
```

```
! total energy          = -15.79449556 ryd
```

```
estimated scf accuracy < 0.00000006 ryd
```

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**

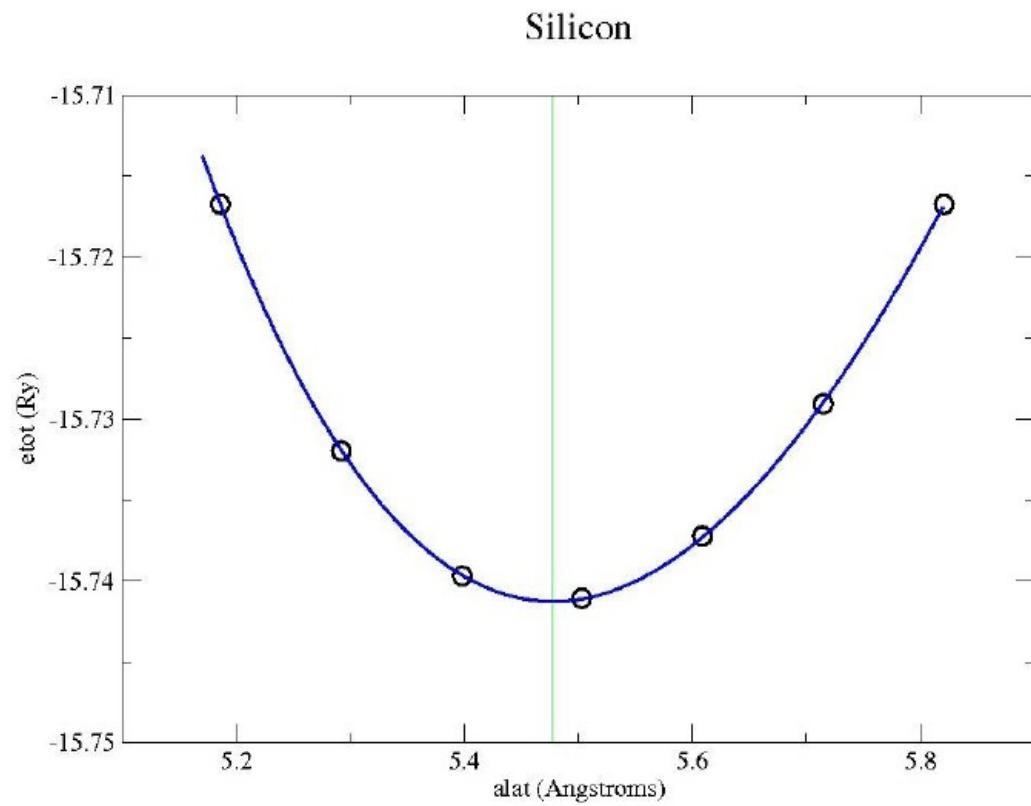
What can we do with the total energy?

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):



Third calculation: Silicon band structure

```
&control
  calculation='nscf', ← New calculation type
  prefix='silicon',
  pseudo_dir='./'
  outdir = './',
/
&system
  ibrav= 2,
  celldm(1) =10.2,
  nat= 2,
  ntyp= 1,
  ecutwfc = 12.0,
  nbnd=8 ← Number of bands
/
&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 tbipa ← k-points list in tbipa units
(k-points list in the k-point-path file)
```

Bands plot

```
&bands
  prefix = 'silicon'
  outdir= './'
  filband = 'bands.dat'
/

```

bands.in file

Run bands.x

```
bands.x < bands.in > output_scf
```

Plot with gnuplot

```
gnuplot
gnuplot> plot 'bands.dat.gnu' u 1:2 w l
```

4th calculation: data analysis

Charge density

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

Wave-functions

```
&inputpp
  prefix = 'silicon'
  outdir='./'
  filplot = 'sicharge'
  plot_num= 7
  kpoint=1
  kband=4
  lsign=.true.
/
&plot
  iflag = 3
  output_format = 5
  fileout = 'si.bands4.xsf'
/
```

Run pp.x

```
pp.x < si.pp_rho.in > output_pp
```

Visualize with Xcrysden

```
xcrysden --xsf si.rho.xsf
```

Data Visualization with XCrySDen

Tools → Data grid

Set Isolevel

