

Quantum-ESPRESSO

PWSCF: first steps

What can I learn in this lecture ?

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How to run PWscf (pw.x) in self-consistent mode for Silicon

How to get the band structure of Silicon along the main symmetry directions

How to draw charge density map of Silicon in a given plane

How to deal with metals (Aluminum)

How to deal with spin polarized systems (Nickel)

What are the basic convergence parameters to have under control

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How to run PWscf (pw.x) in self-consistent mode for Silicon

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How to deal with metals (Aluminum, Copper)

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What are the basic convergence parameters to have under control

Download example file `examples_pwscf_ex.tgz` and unpack it.

This will create a sub-directory named `examples_pwscf_ex` containing several files.

Move to `examples_pwscf_ex` and check its content

```
prompt> cd examples_pwscf_ex
```

```
prompt> ls
```

al.g.12	al.m-p.12	al.m-v.12	al.scf.in	run_si_eos	si.pp_rho
al.g.16	al.m-p.16	al.m-v.16	bands.in	si.etot_vs_ecut	si.scf.in
al.g.6	al.m-p.6	al.m-v.6	k-point-path	si.etot_vs_nks	
al.g.8	al.m-p.8	al.m-v.8	ni.scf.in	si.plotrho.in	

Self-consistent calculation for Silicon in the diamond structure

Edit input file `si.scf.in`

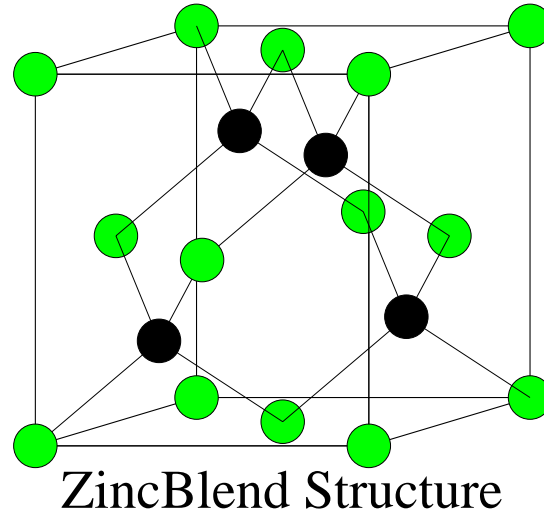
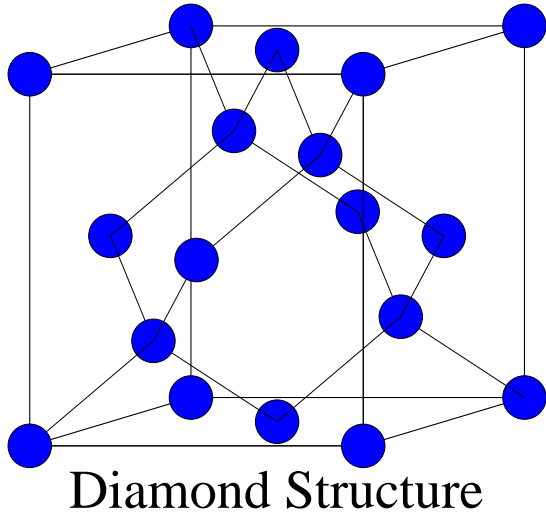
Notice that it is an scf calculation (default value)

Write the appropriate values for `outdir` and `pseudo_dir`

```
outdir = 'temporary directory for large files'  
        example: /scratch/"my_name"/espresso  
pseudo_dir = 'directory where pp-files are kept'  
        example: "espresso_dir"/pseudo
```

Check that these directories exist, have read/write permission and that `pseudo_dir` contains pseudopotential file `Si.vbc.UPF` for Silicon

How the crystal structure is defined ?



check in the input file

How the Bravais lattice is selected ?

How many and which parameters are needed to completely define Bravais lattice geometry ?

How many atoms in the unit cell ?

How many different atomic species ?

Which ones ?

Where the atoms are located in the unit cell ?

Brillouin zone sampling

BZ sampling is performed using 2 Chadi-Cohen special points for the fcc lattice.

For an introduction to special points techniques see for instance A. Baldereschi, *Phys. Rev. B* **7**, 5212 (1973).

D.J. Chadi e M.L. Cohen, *Phys. Rev. B* **8**, 5747 (1973).

H.J. Monkhorst e J.D. Pack, *Phys. Rev. B* **13**, 5188 (1976).

check in the input file how k-points are provided manually

k-points are given (default) in cartesian coordinates
in unit of $2\pi/\text{celldm}(1)$

k-point weights need not add-up to 1,
they are later normalized

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

Bands at high-symmetry points in silicon:

Copy file `si.scf.in` to `si.nscf.in`

Edit file `si.nscf.in` and set it for a non-self-consistent band calculation in three high symmetry points:

$\Gamma = (0,0,0)$, $X=(1,0,0)\frac{2\pi}{a}$ and $L=(1/2,1/2,1/2)\frac{2\pi}{a}$

```
define calculation='bands' in CONTROL namelist
```

```
define nbnd=8 (4 valence + 4 conduction) in SYSTEM namelist
```

```
define the three k-points in the K_POINTS card
```

```
K_POINTS
```

```
3
```

```
0.0 0.0 0.0    1
```

```
1.0 0.0 0.0    2  WEIGHTS ARE MEANINGLESS IN NSCF CALCS
```

```
0.5 0.5 0.5    3
```

DO NOT MODIFY `outdir` or `prefix`,

DO NOT REMOVE files from scratch area

Bands at high-symmetry points in silicon:

run pw.x code

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

look at the output

how many iteration have been performed ?

which potential is used in the diagonalization ?

which wfcs are used as initial guess ?

is the charge density and/or the total energy computed ?

Band structure calculation for silicon:

Copy file `si.nscf.in` to `si.bands.in`

Edit file `si.bands.in` and modify the k-point list so as to perform a path in the BZ along Λ , Δ and Σ directions as defined by in file `k-point-path`
run `pw.x` code

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

Now collect band results for plotting:

edit file `bands.in` in order to define the proper value for `outdir` and then
run `bands.x`

```
prompt> espresso_dir/bin/bands.x < bands.in > bands.out
```

verify the content of file `bands.out` and `bands.dat`, notice the value of the valence band maximum at Γ and then run `plotband.x` interactively

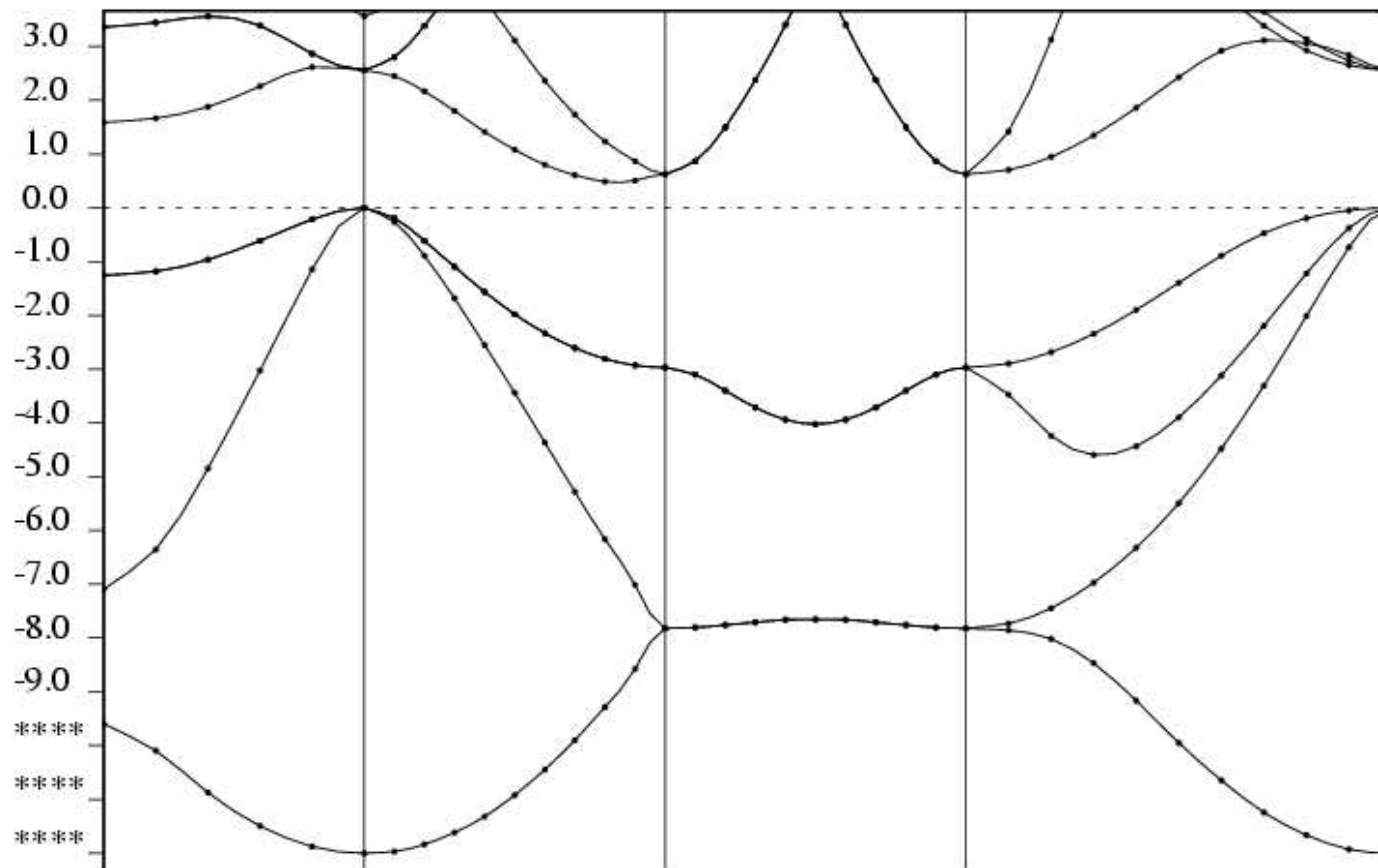
```
prompt> espresso_dir/bin/plotband.x
```

Band structure calculation for silicon:

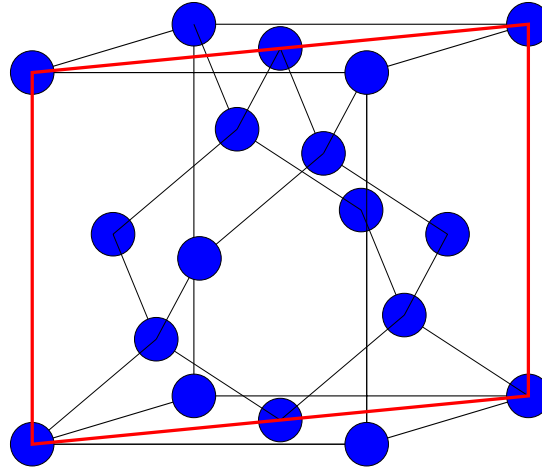
```
prompt> espresso_dir/bin/plotband.x
input file > bands.dat
Reading      8 bands at    36 k-points
Range: -5.6680 16.4950eV  Emin, Emax > -6.0 10.0
high-symmetry point:  0.5000 0.5000 0.5000
high-symmetry point:  0.0000 0.0000 0.0000
high-symmetry point:  0.0000 0.0000 1.0000
high-symmetry point:  0.0000 1.0000 1.0000
high-symmetry point:  0.0000 0.0000 0.0000
output file (xmgr) > si.bands.xmgr
bands in xmgr format written to file si.bands.xmgr
output file (ps) > si.bands.ps
Efermi > 6.337
deltaE, reference E (for tics) 1.0, 6.337
bands in PostScript format written to file si.bands.ps
```

Band structure calculation for silicon:

```
prompt> ghostview si.bands.ps
```



Charge density plot for silicon in the $[1-10]$ plane:



Edit file `si.pp_rho.in` to properly define `outdir` and then run the postprocessing code (`pp.x`) to extract the charge density (`plotnum=0`)

```
prompt> espresso_dir/bin/pp.x < si.pp_rho.in
```

```
prompt> espresso_dir/bin/pp.x < si.pp_rho.in
```

```
Program POST-PROC v.3.1 starts ...
```

```
Today is 26May2006 at 20:17:44
```

```
nbndx   =      8  nbnd    =      8  natomwfc =      8  npwx    =     200  
nelec   =   8.00  nkb     =      8  ngl      =     43
```

```
Calling punch_plot, plot_num = 0
```

```
Writing data to file sicharge
```

```
Reading header from file sicharge
```

```
Reading data from file sicharge
```

```
Writing data to be plotted to file si.rho.dat
```

```
Min, Max, imaginary charge:      0.002838      0.093121      0.000000
```

```
Plot Type: 2D contour           Output format: plotrho.x
```


Charge density plot for silicon in the [1-10] plane:

run `plotrho.x` produce the plot

```
prompt> espresso_dir/bin/plotrho.x
```

```
input file > si.rho.dat
```

```
r0      :    0.0000    0.0000    0.0000
```

```
tau1    :    1.0000    1.0000    0.0000
```

```
tau2    :    0.0000    0.0000    1.0000
```

```
read     2 atomic positions
```

```
output file > si.rho.ps
```

```
Read  56 * 40  grid
```

```
Logarithmic scale (y/n)? > n
```

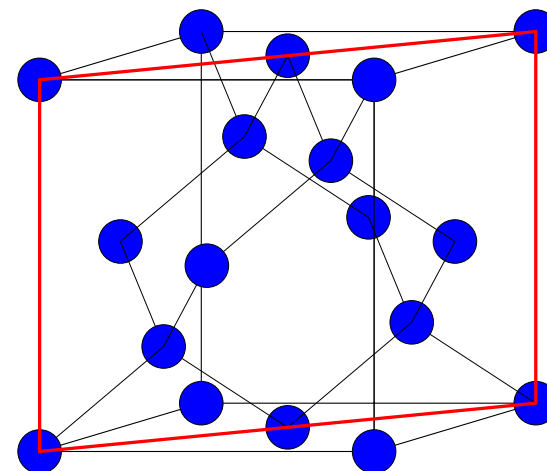
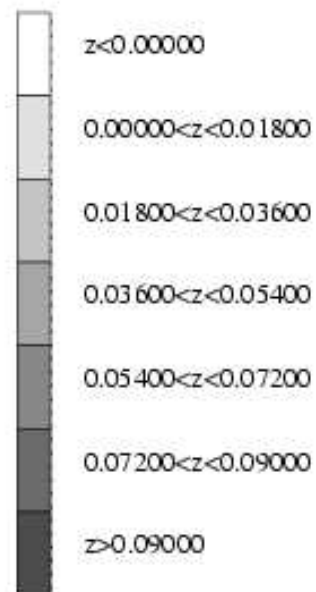
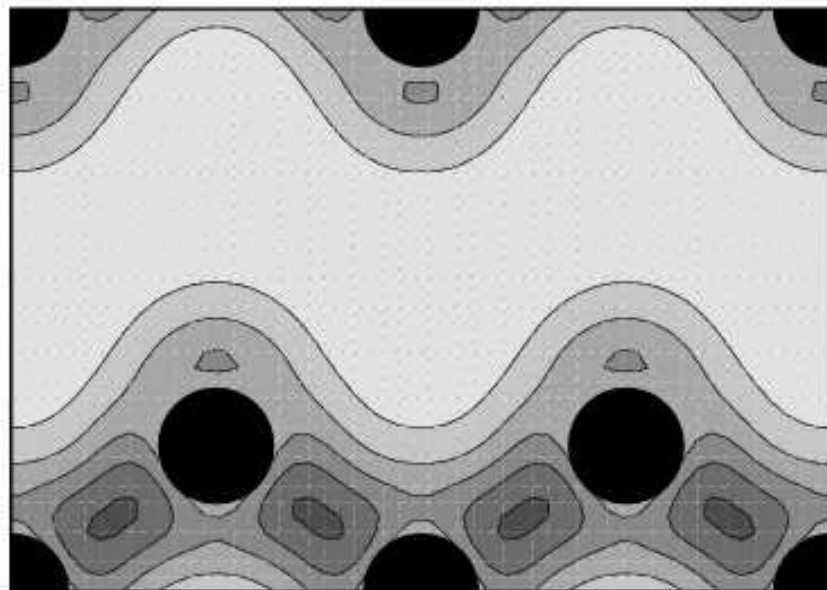
```
Bounds:      0.002839      0.093110
```

```
min, max, # of levels > 0 0.09 6
```

Charge density plot for silicon in the $[1-10]$ plane:

```
prompt> ghostview si.rho.ps
```

si.rho.dat



Convergence w.r.t. kinetic energy cutoff:

Clean `outdir`;

Change value of `ecutwfc` in `si.scf.in` input file to 16, 20, 24 Ry ;

Run `pw.x` again and again and complete the data in `si_etot_vs_ecut` ;

Plot the data in `si_etot_vs_ecut` and notice the monotonic convergence.

Convergence w.r.t to cutoff is a property of the `pseudopotential`

Convergence w.r.t. k-points:

Clean outdir;

Edit `si.scf.in` and set back `ecutwfc` to 12 Ryd ;

Change k-points using automatic grid with `nk=2,4,6`

```
K_POINTS automatic
```

```
2 2 2 1 1 1
```

Run `pw.x` and complete entries in file `si_etot_vs_nks` ;

Convergence is not necessarily monotonic ;

There is no variational principle w.r.t. k-points number

A metallic example: Aluminum

Clean `outdir`;

Edit file `al.scf.in` and define `outdir` and `pseudo_dir`;

Notice the use of variables `occupations`, `smearing`, `degauss`;

Run `pw.x`

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

Notice in output file that `nbnd` is automatically set to a value larger than $\text{nelec}/2$ and that `Efermi` is computed.

Convergence with respect to degauss/smearing ...

Edit file `al.scf.in` and vary variables `smearing`

[gaussian (g), marzari-vanderbilt (m-v), methfessel-paxton (m-p)]

and `degauss` [0.06, 0.07, 0.08, 0.09, 0.10]

in order to complete entries of `al.g.6`, `al.m-v.6`, `al.m-p.6` files

Plot the content of `al.g.6`, `al.g.8`, `al.g.12`, `al.g.16`, and similarly for m-v and m-p

Notice that for metals convergence is **SLOW**

It can be improved by using m-v or m-p.

A magnetic example: Nickel

Clean `outdir`;

Edit file `ni.scf.in` and define `outdir` and `pseudo_dir`;

Notice use of variables `nspin` and `starting_magnetization`.

Notice that this is a `metallic` calculation.

Nickel pseudopotential is US-PP: `ecutrho > 4×ecutwfc`

Run `pw.x`

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

Notice that the number of k-points is doubled w.r.t non-magnetic case

Notice different number of calls and timing of `cft3` and `cft3s` routines.

Why it is convenient to introduce a different cutoff for `wfcs` and `rho` ?

Equation of State: Silicon

edit `run_si_eos` and define variables `espresso_dir`, `pseudo_dir` and `outdir`.

```
prompt> sh run_si_eos
```

Notice how file `si.etot_vs_alat` is created at the end of script file

Plot content of `si.etot_vs_alat`

```
prompt> gnuplot  
gnuplot> plot "si.etot_vs_alat" w l
```


HOMEWORK

Modify the script and change cutoff, k-points and so on.

Verify that Energy_vs_alat curves are shifted down rather uniformly with increasing cutoff and are not strongly dependent on k-points.

Structural properties and energy differences converge faster than total energies.

Compute the equation of state of Ni.

THE END