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DEmocritos MOdeling Center for Research In aTOmistic Simulation INFM

HANDS-ON TUTORIAL ON THE QUANTUM-ESPRESSO PACKAGE

POST PROCESSING OF DATA:
- Density of states: DOS and PDOS
- Charge density and bonding charge
- STM image simulation

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Getting started

- Move to your own **scratch** directory:
  `cd /scratch/XXX/`
- Download this tutorial and the examples from:
  `http://[ESPRESSO-TUTORIAL-SITE]/tutorial_postproc.pdf`
  `http://[ESPRESSO-TUTORIAL-SITE]/examples_postproc.tgz`

- Untar the example file and enter in the resulting directory:
  `tar zxvf examples_postproc.tgz`
  `cd PostProcessing`
- Edit the `environment_variables` file:
  e.g., **`TMP_DIR=/scratch/XXX/tmp/`**
- Create the output directory as specified above:
  `mkdir /scratch/XXX/tmp/`

Exercise 1: DOS of bulk Ni

- Run the scf calculation for bulk Ni

```
run-ni.scf
```

- What happens? Why does the program stop? See the output file:

```
more ni.scf.out
```

- Add the required input

```
starting_magnetization(1)=0.0
```

… run again the simulation. Copy the output file:

```
cp ni.scf.out ni.scf.out-0magn
```

- Modify the starting magnetization in `run-ni.scf`

```
starting_magnetization(1)=0.7
```

… run again the simulation.

```
run-ni.scf
```

- Compare the total energies of the two simulations: do they differ? Why? What about the magnetization?

Exercise 1: DOS

- Edit the file **run-ni.nscf:**
  increase the number of bands to 8: **nbnd=8**
  and the set a denser k-point mesh: **12 12 12 0 0 0**
  Run the nscf calculation for bulk Ni: **run-ni.nscf**

- Have a look at the input file for the DOS calculation:

more run-ni.dos

```
&inputpp
    outdir='$TMP/DIR'
    prefix='ni'
    fildos='ni.dos'
    Emin=5.0, Emax=25.0, DeltaE=0.1
/
```

in eV!

… and run the DOS calculation:

run-ni.dos

Exercise 1: DOS

- Have a look at the output file containing the DOS: **ni.dos**

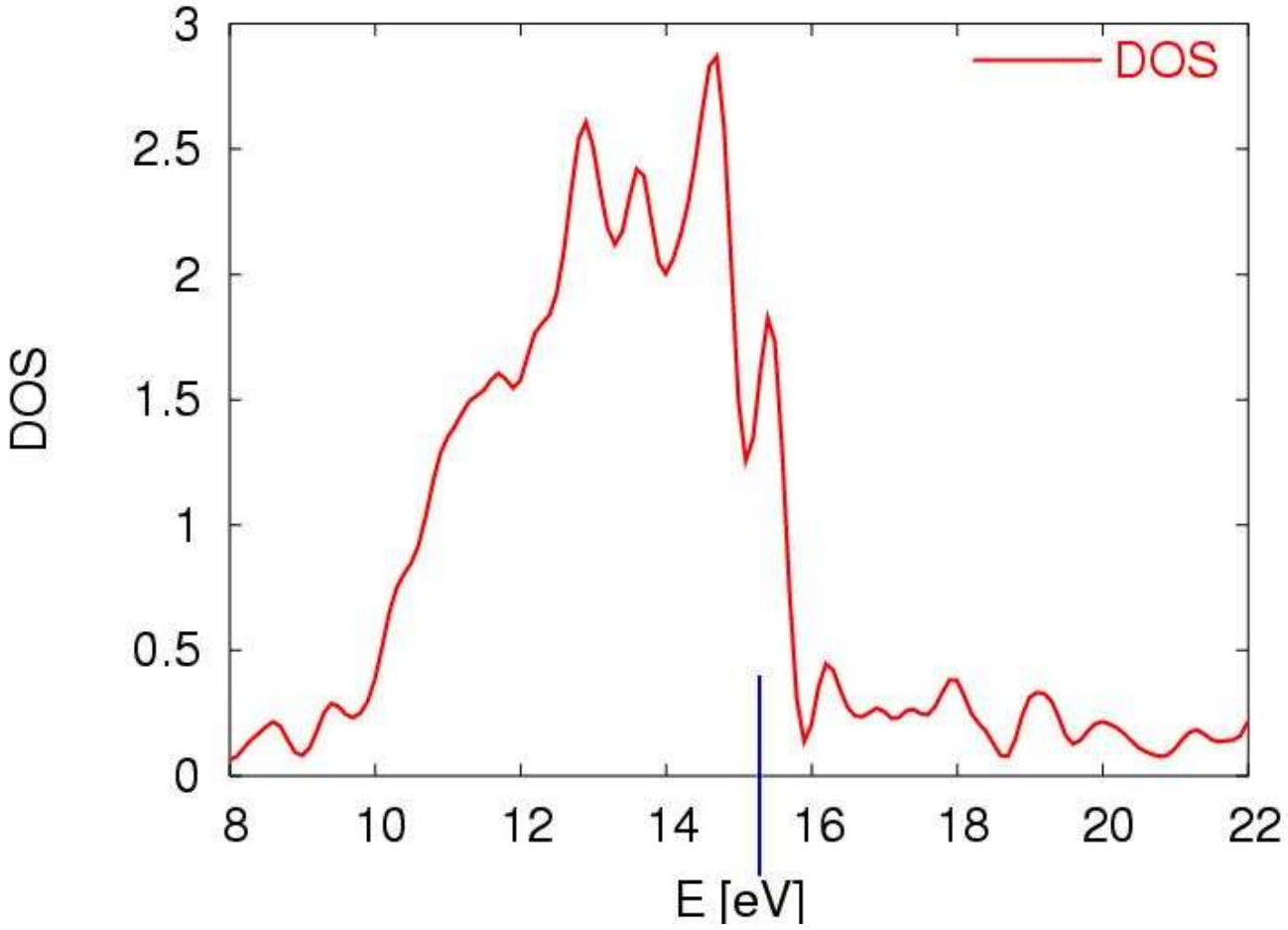
```
more ni.dos
```

```
#  E (eV)   dosup(E)     dosdw(E)   Int dos(E)
   5.000 -0.3790E-05 -0.2225E-05 -0.6015E-06
   5.100 -0.1772E-04 -0.1149E-04 -0.3523E-05
   5.200 -0.5902E-04 -0.4251E-04 -0.1368E-04
   5.300 -0.1373E-03 -0.1105E-03 -0.3846E-04
   5.400 -0.2211E-03 -0.1989E-03 -0.8046E-04
   5.500 -0.2479E-03 -0.2498E-03 -0.1302E-03
   5.600 -0.8376E-04 -0.1768E-03 -0.1563E-03
   5.700  0.1017E-02  0.4889E-03 -0.5688E-05
```

…

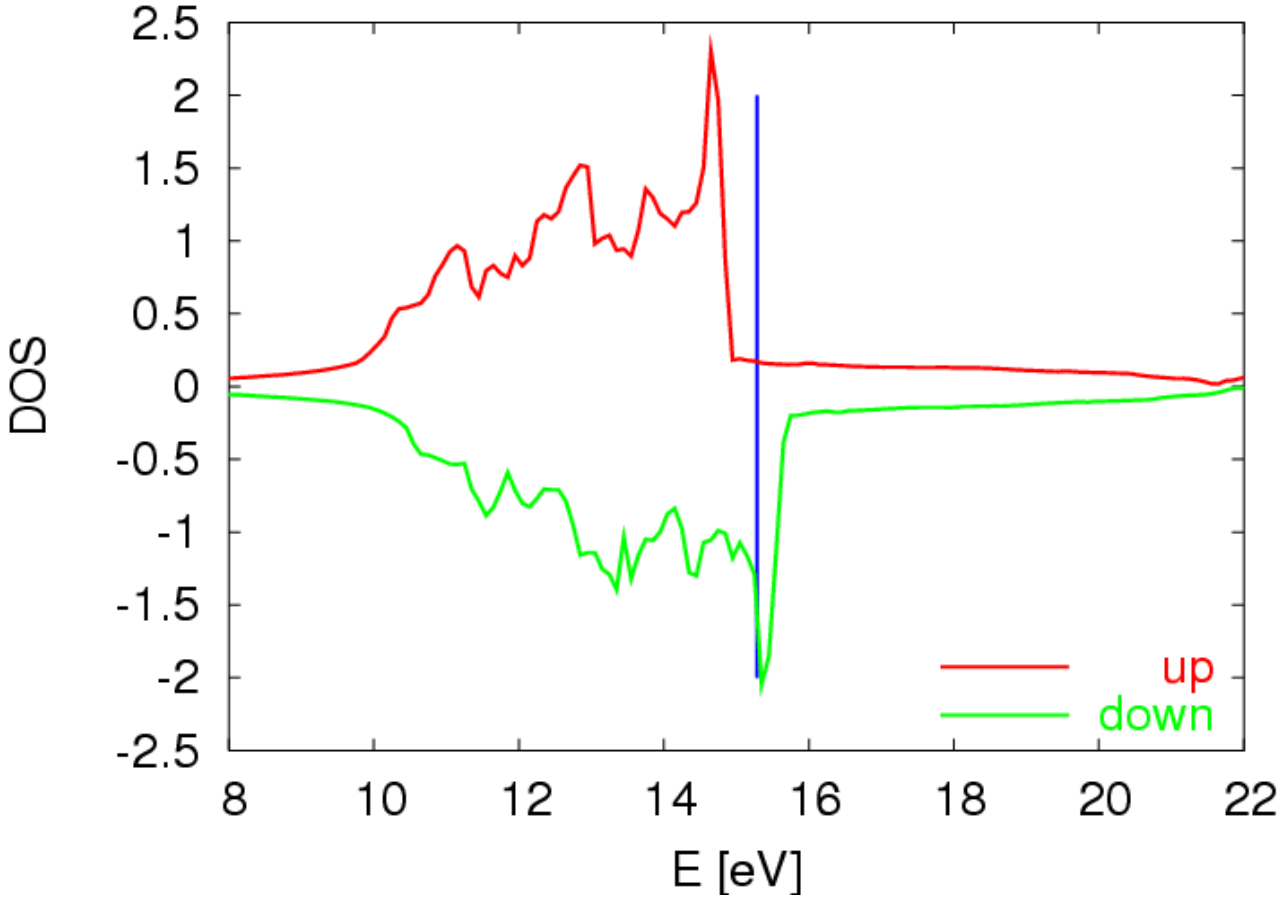
Exercise 1: DOS

- Plot the total density of states: **`gnuplot dos.gnu`**



Exercise 1: DOS

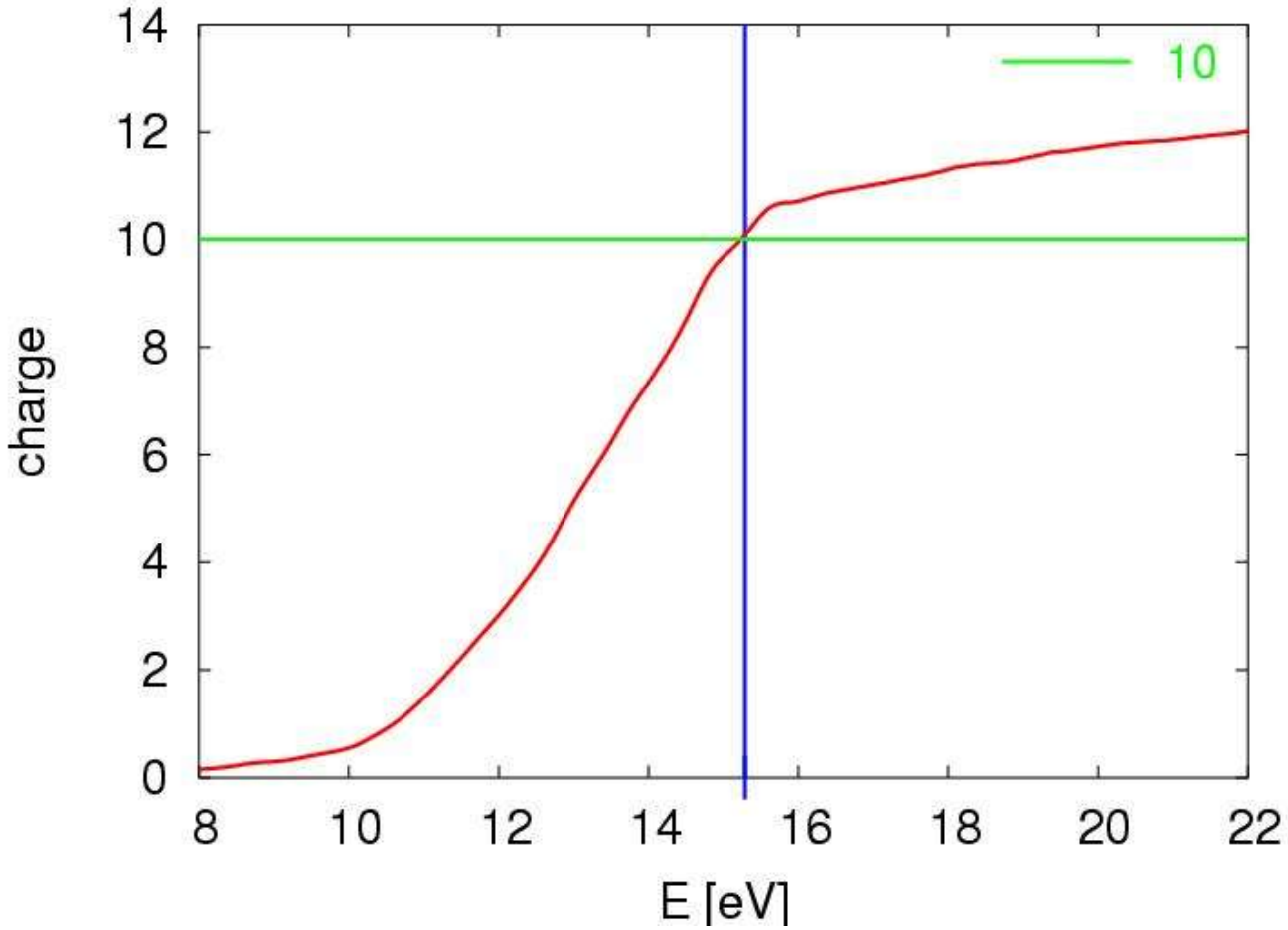
- Plot the total density of states: **`gnuplot dos.gnu`**
- Note difference between spin up and spin down components.



- Plot the integrated charge

Exercise 1: DOS

- Plot the integrated charge



Exercise 1: DOS

- More input variables:

```
&inputpp
    outdir='$TMP/DIR'
    prefix='ni'
    ngauss= 0,1,-1,99
    degauss= xx
    fildos='ni.dos'
    Emin=5.0, Emax=25.0, DeltaE=0.1
/
```

in Ry!

in eV!

Exercise 2: PDOS of bulk Ni

- Have a look at the input file for the PDOS calculation:

```
more run-pdos.in
```

```
&inputpp
    outdir='$TMP_DIR/'
    prefix='ni'
    io_choice='both'
    Emin=5.0, Emax=25.0, DeltaE=0.1
    ngauss=1, degauss=0.02
/
```

… and run the PDOS calculation (`projwfc.x`):

```
run-ni.pdos
```

Exercise 2: PDOS

- Have a look at the output file ni.pdos.out:
  more ni.pdos.out

```
… … … …

Lowdin Charges:

     Atom #   1: total charge =   9.881 …
                 spin up      =   5.239 …
                 spin down    =   4.6426 …
                 polarization =   0.5965 …
     Spilling Parameter:   0.0118
```

Exercise 2: PDOS

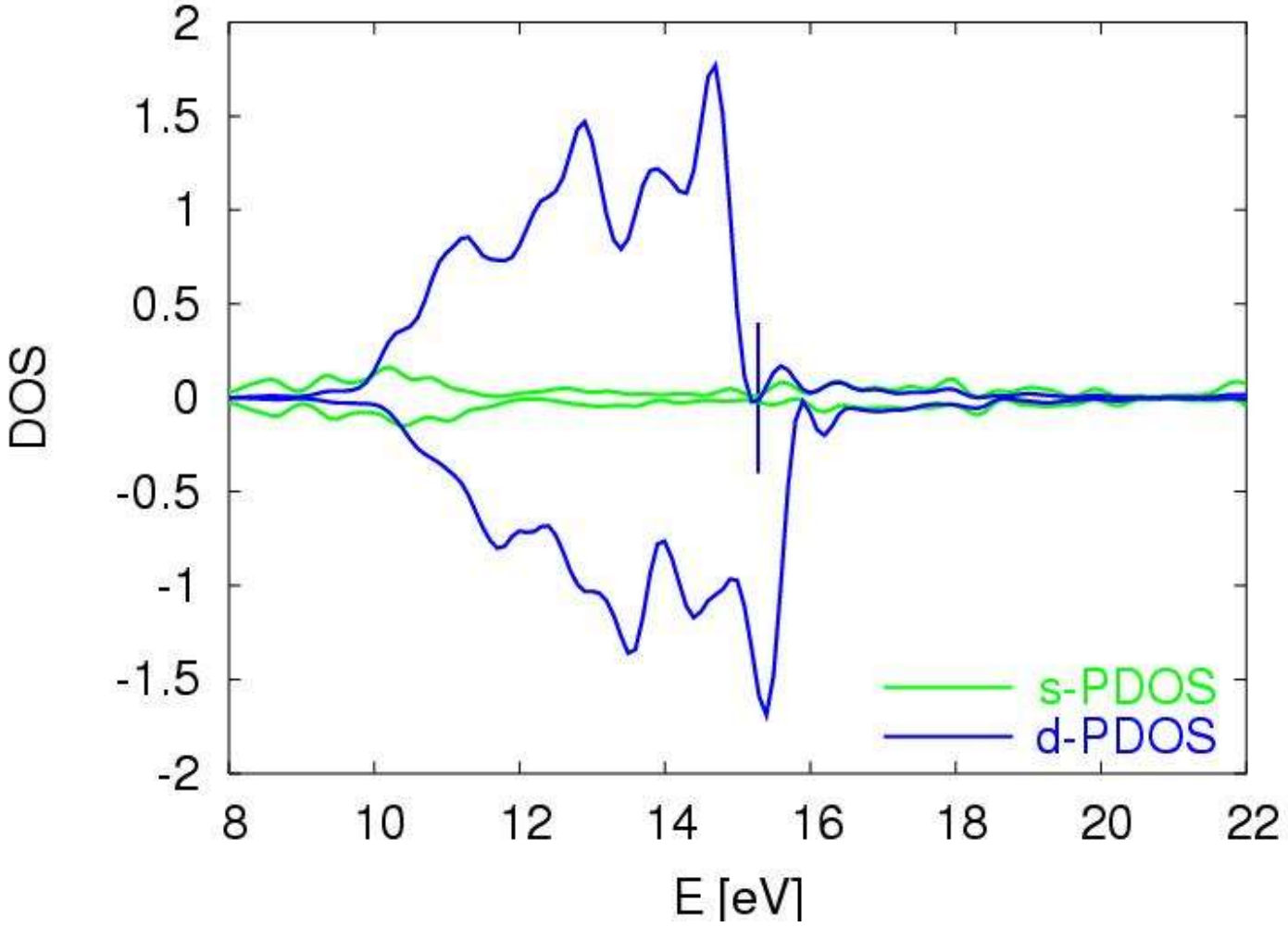
• Have a look at the output files containing the s and d components of the PDOS:

```
more ni.pdos_atm#1(Ni)_wfc#1(s)
more ni.pdos_atm#1(Ni)_wfc#2(d)
```

```
# E (eV)  ldosup(E)  ldosdw(E) pdosup(E)  pdosdw(E)
  5.000 -0.378E-05 -0.222E-05 -0.378E-05 -0.222E-05
  5.100 -0.177E-04 -0.115E-04 -0.177E-04 -0.115E-04
  5.200 -0.589E-04 -0.425E-04 -0.589E-04 -0.425E-04
  5.300 -0.137E-03 -0.110E-03 -0.137E-03 -0.110E-03
  5.400 -0.221E-03 -0.199E-03 -0.221E-03 -0.199E-03
  5.500 -0.247E-03 -0.249E-03 -0.247E-03 -0.249E-03
  5.600 -0.831E-04 -0.176E-03 -0.831E-04 -0.176E-03
  5.700  0.102E-02  0.489E-03  0.102E-02  0.489E-03
  5.800  0.491E-02  0.331E-02  0.491E-02  0.331E-02
  5.900  0.126E-01  0.996E-02  0.126E-01  0.996E-02
```

Exercise 2: PDOS

- Plot the *s* and *d* components of the DOS: **`gnuplot dos.gnu`**



Exercise 3: Charge density of Si

- Run the scf calculation for bulk Si:
  run-si.scf

- Modify the input file for the post processing **run-si.pp** for calculating the total charge density. First modify the **inputpp** namelist:

```
&inputpp
    prefix  = 'si'
    outdir  = '/tmp/',
    filplot = 'si.charge'
    plot_num= XXX
/
```

… see espresso/Docs/INPUT_PP for the value of **plot_num** corresponding to the charge density.

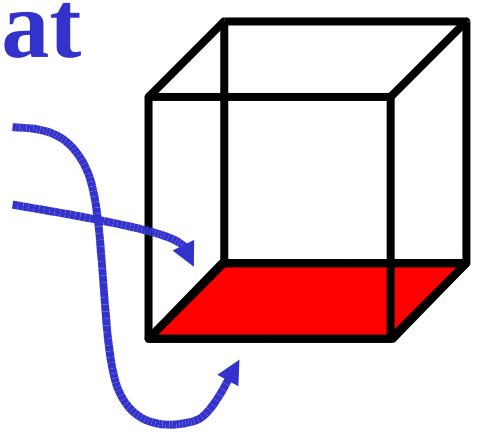
Exercise 3: Charge density of Si

• Then modify the **plot** namelist to convert data in a format compatible with the selected visualization packages (plotrho, gnuplot, XCrysDen... Now use plotrho):

```
vi run-si.pp
&plot
   nfile=1
   filepp(1)='si.charge'
   iflag=XXX
   output_format=XXX
   e1(1)=1.0, e1(2)=0.0, e1(3)=0.0,
   e2(1)=0.0, e2(2)=1.0, e2(3)=0.0,
   x0(1)=0.0, x0(2)=0.0, x0(3)=0.0,
   nx=40, ny=40
   fileout='si.charge001.dat'
/
```

2D plot

plotrho format



001 plane

• Run the calculation: **run-si.pp**

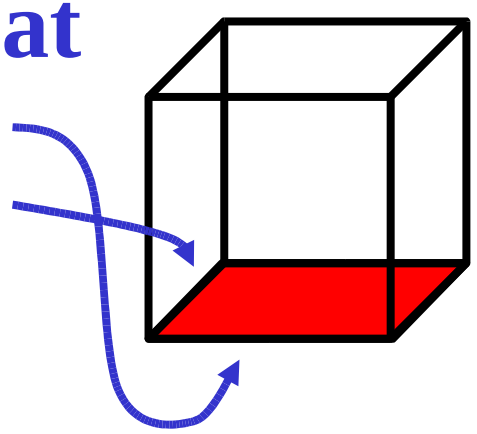
Exercise 3: Charge density of Si

• Then modify the **plot** namelist to convert data in a format compatible with the selected visualization packages (plotrho, gnuplot, XCrysDen... Now use **plotrho**):

```
vi run-si.pp
&plot
   nfile=1
   filepp(1)='si.charge'
   iflag=2
   output_format=2
   e1(1)=1.0, e1(2)=0.0, e1(3)=0.0,
   e2(1)=0.0, e2(2)=1.0, e2(3)=0.0,
   x0(1)=0.0, x0(2)=0.0, x0(3)=0.0,
   nx=40, ny=40
   fileout='si.charge001.dat'
/
```

2D plot

plotrho format

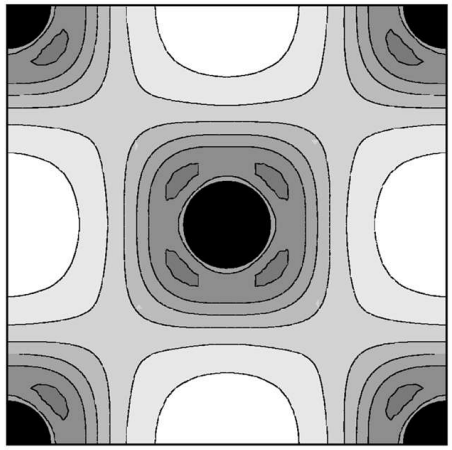


001 plane

• Run the calculation: **run-si.pp**

Exercise 3: Charge density of Si

- Visualize the charge on the (001) plane by using the program **plotrho.x** (included in espresso):



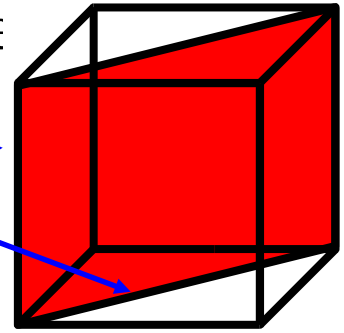
```
 run-si.plot
input file > si.charge001.dat
output file > si.charge001.ps
Logarithmic scale (y/n)? > n
min, max, # of levels > 0.01 0.08 8
 gv si.charge001.ps
```

Exercise 3: Charge density of Si

Calculate and plot the charge density of Si on the (110) plane:

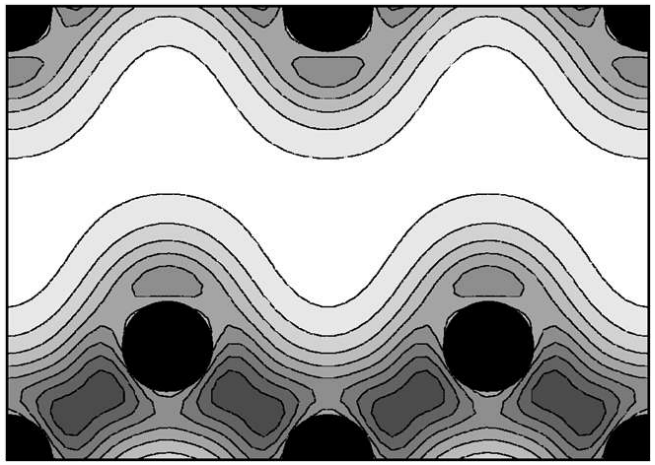
- cp **run-si.pp to run-si.pp110**
- Modify the input file so that to define the (110) plane

```
e1(1)=?, e1(2)=?, e1(3)=?,
e2(1)=?, e2(2)=?, e2(3)=?,
  …
 fileout='si.charge110.dat'
```



- Run the **pp.x** calculation: **run-si.pp110**

Run the **plotrho.x** program and visualize the result: **run-si.plot**



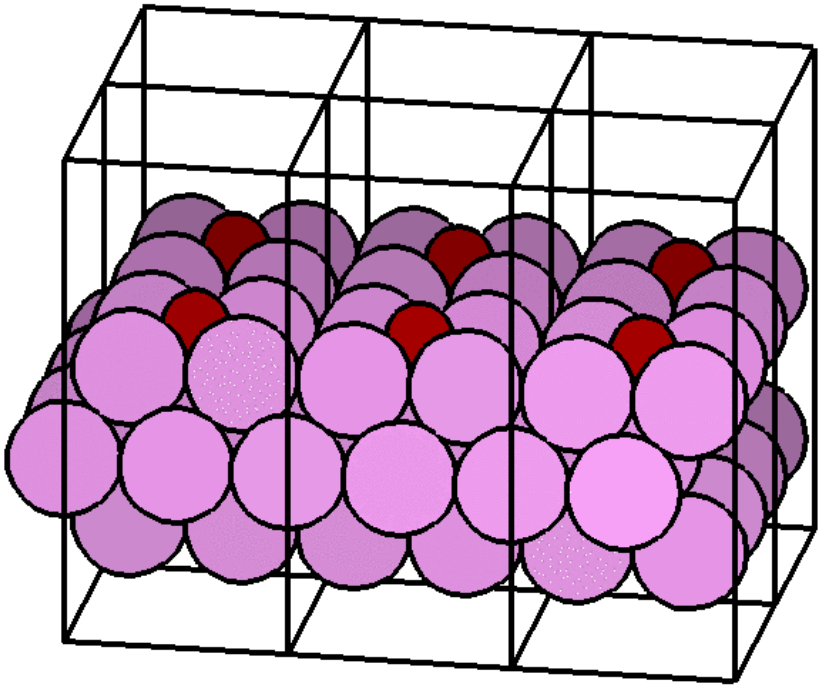
Exercise 4: Bonding charge density

Bonding charge density of an O atom on the Al (001) surface

- Run the following script: **`run-Al-O-OAl-scf-pp &`**

It follows the step seen in Ex 3 to calculate the charge densities of:

1) an O atom adsorbed on an Al(001) slab,
2) an Al(001) slab,
3) an O atom.



- Compare the atomic coordinates of the O atom in the file **`O.scf.out`** with those in **`OAl.scf.out`**. What do you notice? Why are they so?

Exercise 4: Bonding charge density

• Use the program chdens.x to subtract the charge densities of the Al (001) slab and of the O atom from the that one of the complete system O/Al(001): (file: **run-OAl.chdiff**)

```
&input
   nfile=3
   filepp(1)='???', weight(1)=???
   filepp(2)='???', weight(2)=???
   filepp(3)='???', weight(3)=???
   iflag=?? 3D
   output_format=?? XCrySDen
   fileout='OAl.chdensDIFF.xsf'
/
```

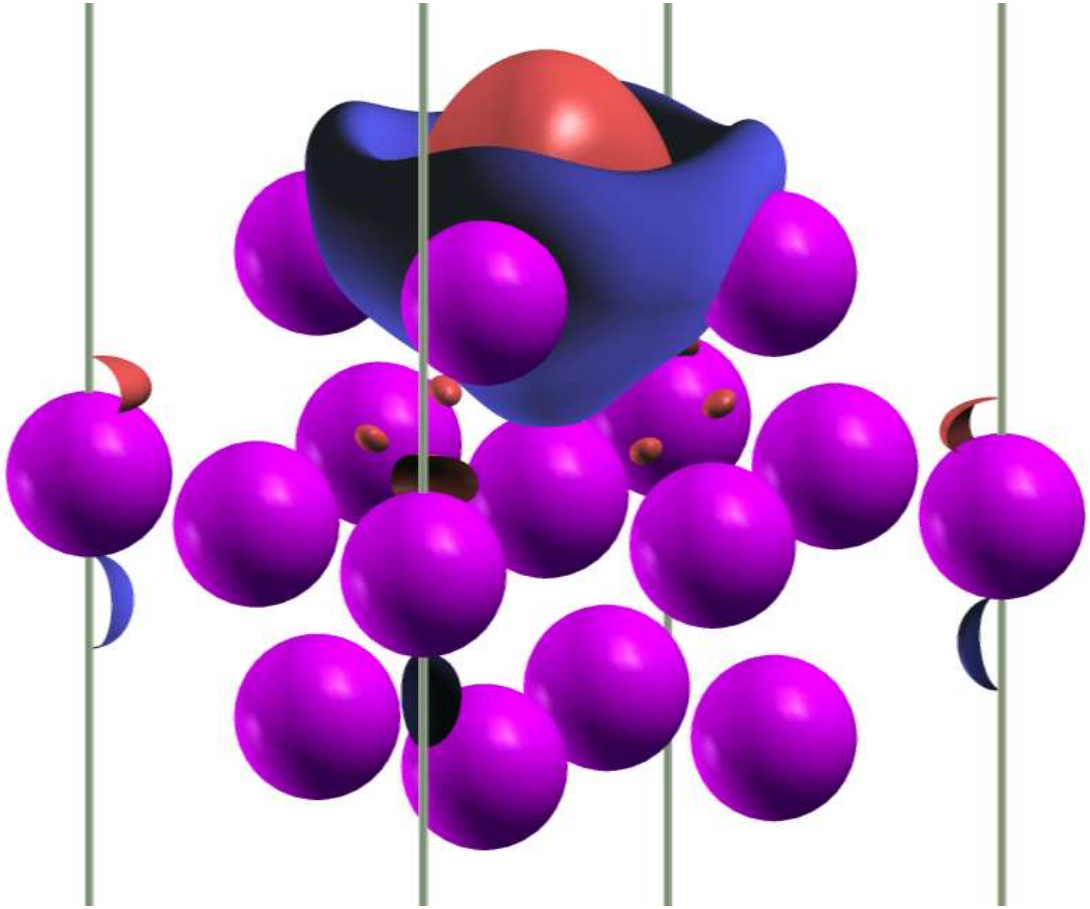
The first file is the one for the O/Al(001) system

• Run the calculation: **run-chdens.diff**

Exercise 4: Bonding charge density

- Visualizing the output file with XCrysDen:

```
xcrysden --xsf OAl.chdensDIFF.xsf
```



Hint: see the isosurfaces by selecting: **tools - datagrid - ok - isovalue=0.003 - render+/-isovalue - submit**

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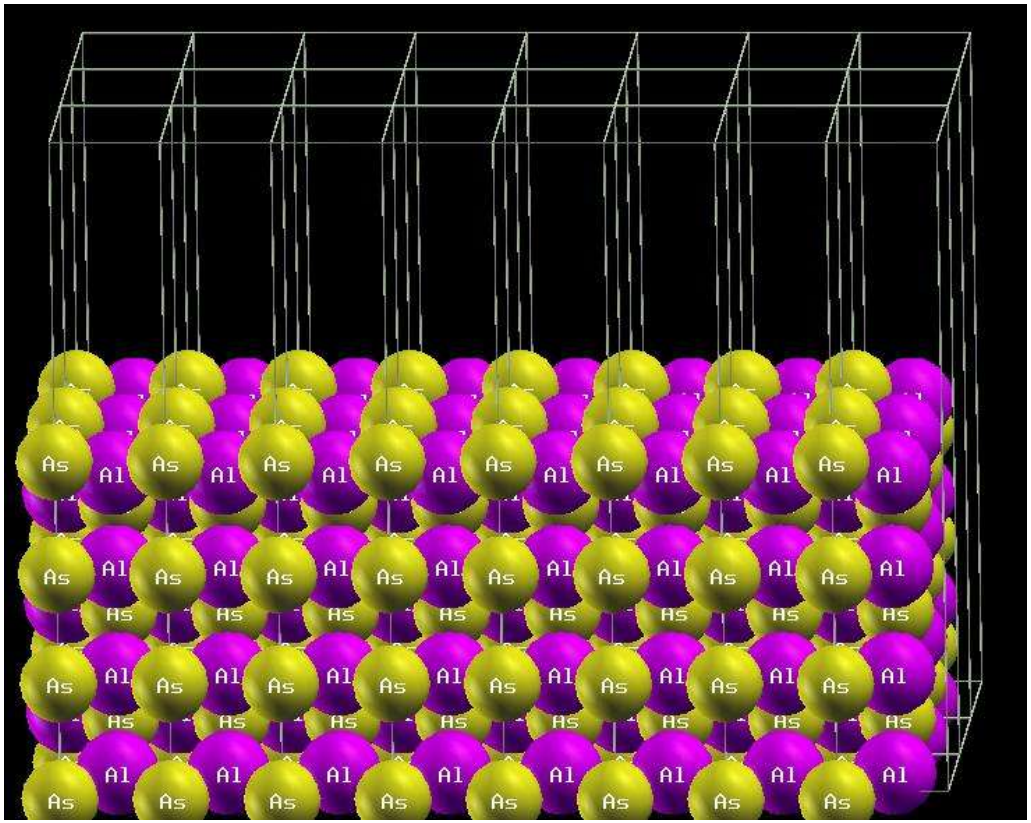
Exercise 5: STM simulation

Simulating the STM image of the AlAs (110) surface



- Run the scf calculation for the AlAs (110) surface
  `run-AlAs.scf`
- Run the non scf calculation for the AlAs (110) surface:
  `run-AlAs.nscf`

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Exercise 5: STM simulation

- Set up the input file for the post processing; **`inputpp`** namelist (see **`run-AlAs.stm`**):

```
&inputpp
    prefix  = 'AlAs110'
    outdir='$TMP_DIR/',
    filplot = 'AlAs-1.0'
    sample_bias=-0.0735d0,
    stm_wfc_matching=.false.,
    plot_num= XXX
/
```

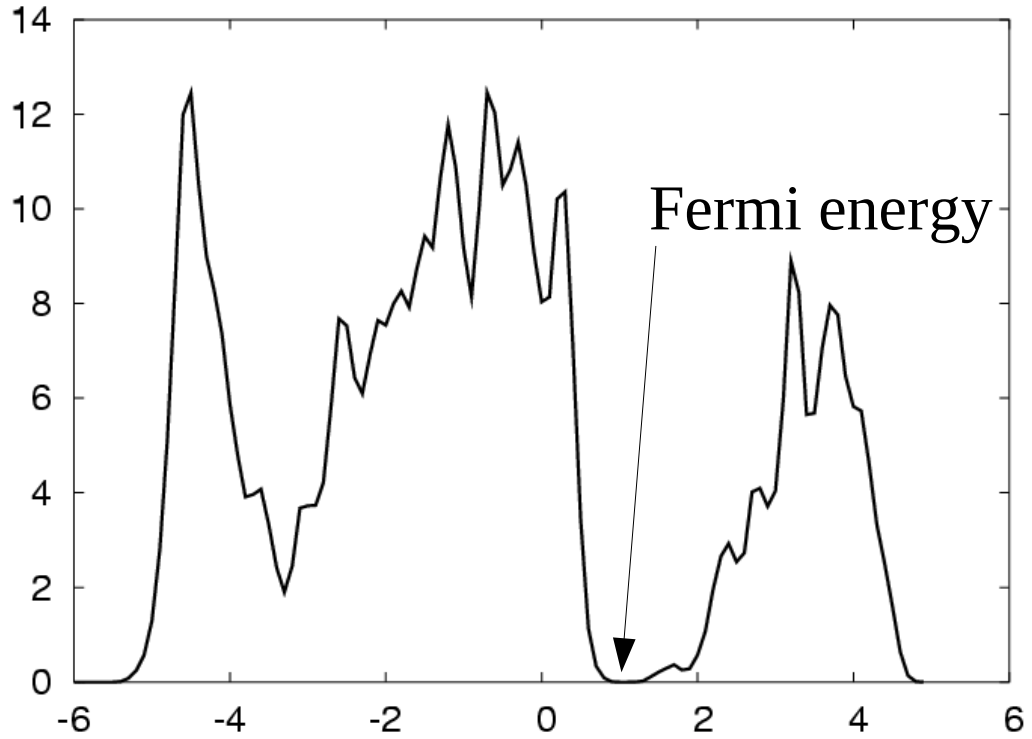
in Ry!

… see O-sesame/pwdocs/INPUT_PP

- How to choose the **`sample_bias`**?

Exercise 5: STM simulation

- How to choose the **`sample_bias`**? What is the DOS?



- Exercise: image empty states

Exercise 5: STM simulation

- Set **`plot`** namelist to produce a 3D file comptatible with the XCrySDen package:

```
vi run-AlAs.stm
...
&plot
  nfile=1
  filepp(1)='AlAs-1.0'
  weight(1)=1.0
  iflag=3
  output_format=5
  fileout='AlAs110-1.0.xsf'
/
```

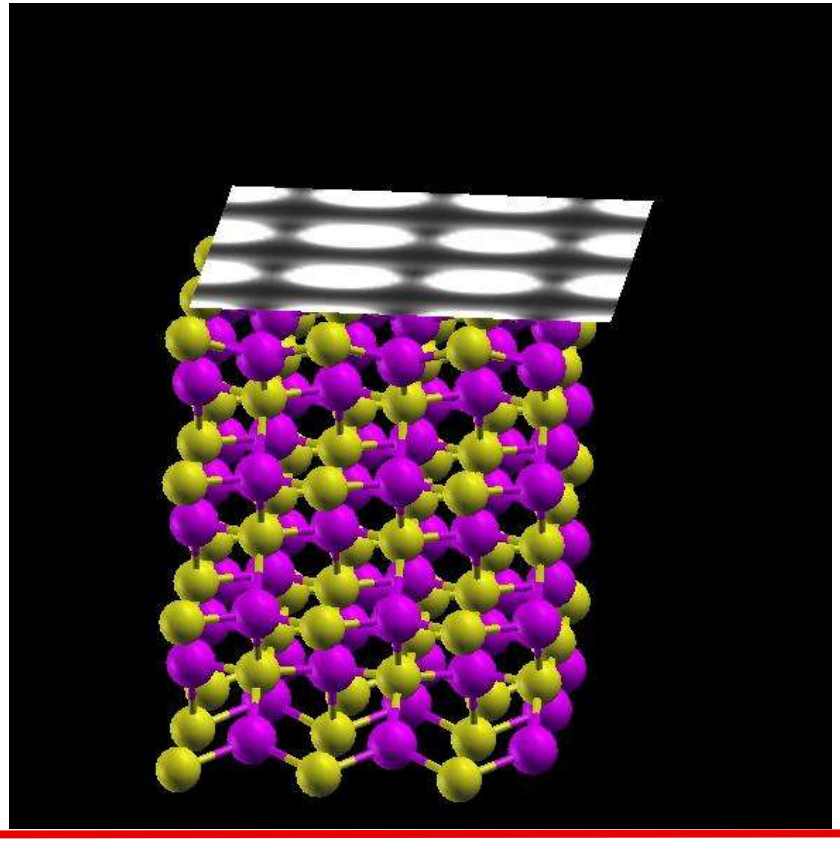
3D plot

XCrysDen format

Exercise 5: STM simulation

- Run the post-processing simulation:
  `run-AlAs.stm`

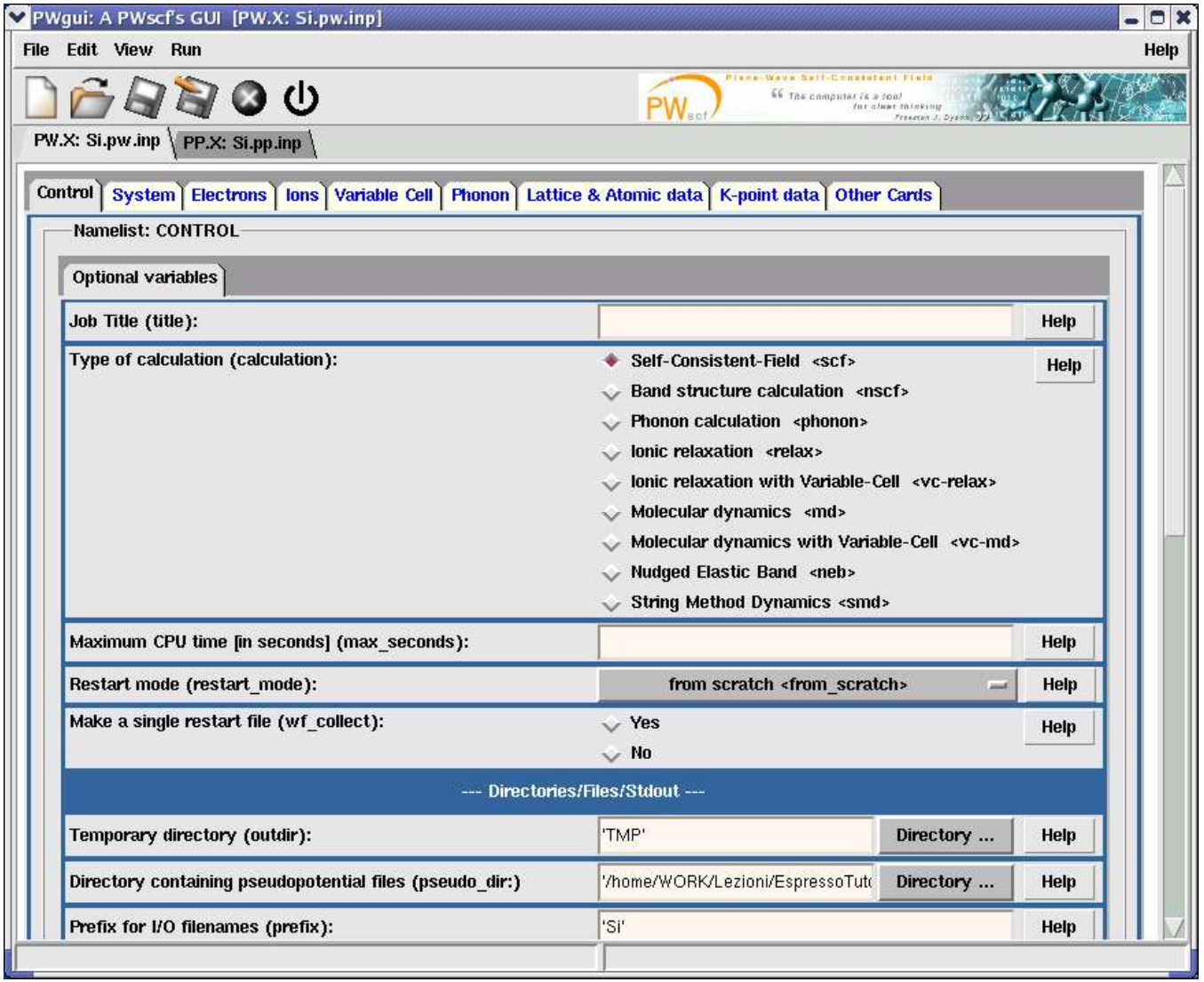
- Visualize the output file with the XCrysDen package:
  `xcrysden –xsf AlAs110-1.0.xsf`



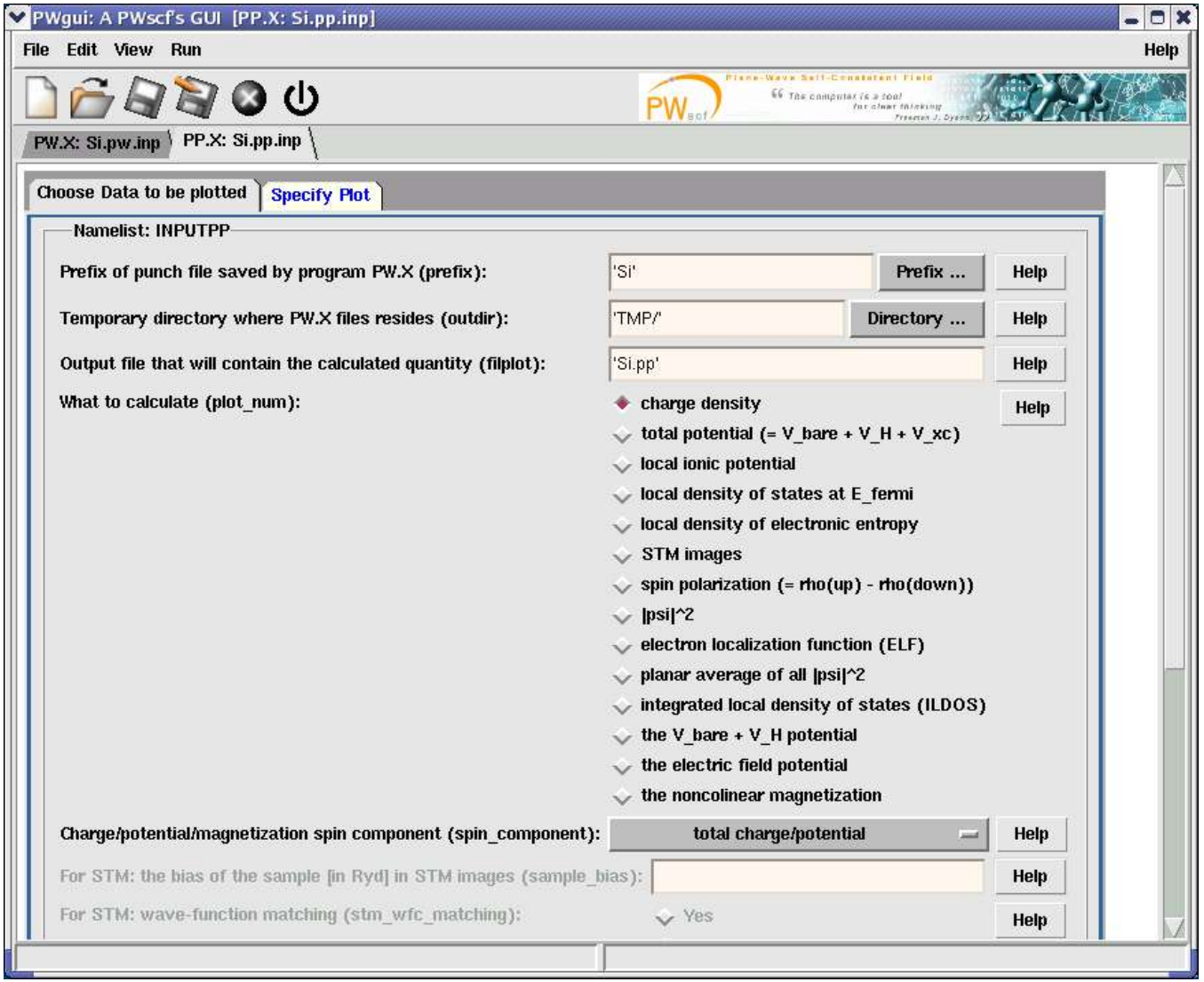
Exercise 6: Si charge (using PWgui)

- from SCF calculation of Si bulk to visualization of its charge density with **`xcrysden`**. Use **`pwgui`** to construct appropriate input files and run the necessary calculations:
  - SCF calculation: use **`pw.x`** program
  - post-processing: use **`pp.x`** program (select the "charge-density", and transform the charge-density to XSF format, suitable for xcrysden)
  - visualize the calculated charge density stored in *file*.xsf with **`xcrysden`**

Input for **pw.x**: SCF calculation



Input for **pp.x**: extract the charge density



Input for **pp.x**: generate file for XCrySDen