PROGRESS REPORT: Visualizing Silicon's QE output to XSF

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GENERAL METHOD FOR VISUALIZING QE OUTPUT TO XSF

- Generate an XSF file using the PW tools
- Visualize xsf in VESTA
- Examine xsf format - lattice constant, lattice vectors, translation vector, atomic coordinates
- Compare with the pw.x input file
- Modify atomic positions in pw.x to create 2D structure, generate xsf file and visualize in vesta

Generating an XSF file using the PW tools

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ vi Si.scf.in
```

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat Si.scf.in
&CONTROL
prefix = 'silicon',
outdir = './tmp/'
pseudo_dir = '/home/meyn/q-e-qe-7.1/pseudo/'
verbosity = 'high'
/

&SYSTEM
ibrav = 2,
celldm(1) = 10.26,
nat = 2,
ntyp = 1,
ecutwfc = 30
nbnd = 8
/

&ELECTRONS
mixing_beta = 0.6
/


ATOMIC_SPECIES
Si 28.0855 Si.pz-vbc.UPF

ATOMIC_POSITIONS (alat)
Si 0.00 0.00 0.00 0 0 0
Si 0.25 0.25 0.25 0 0 0

K_POINTS (automatic)
6 6 6 0 0 0
```

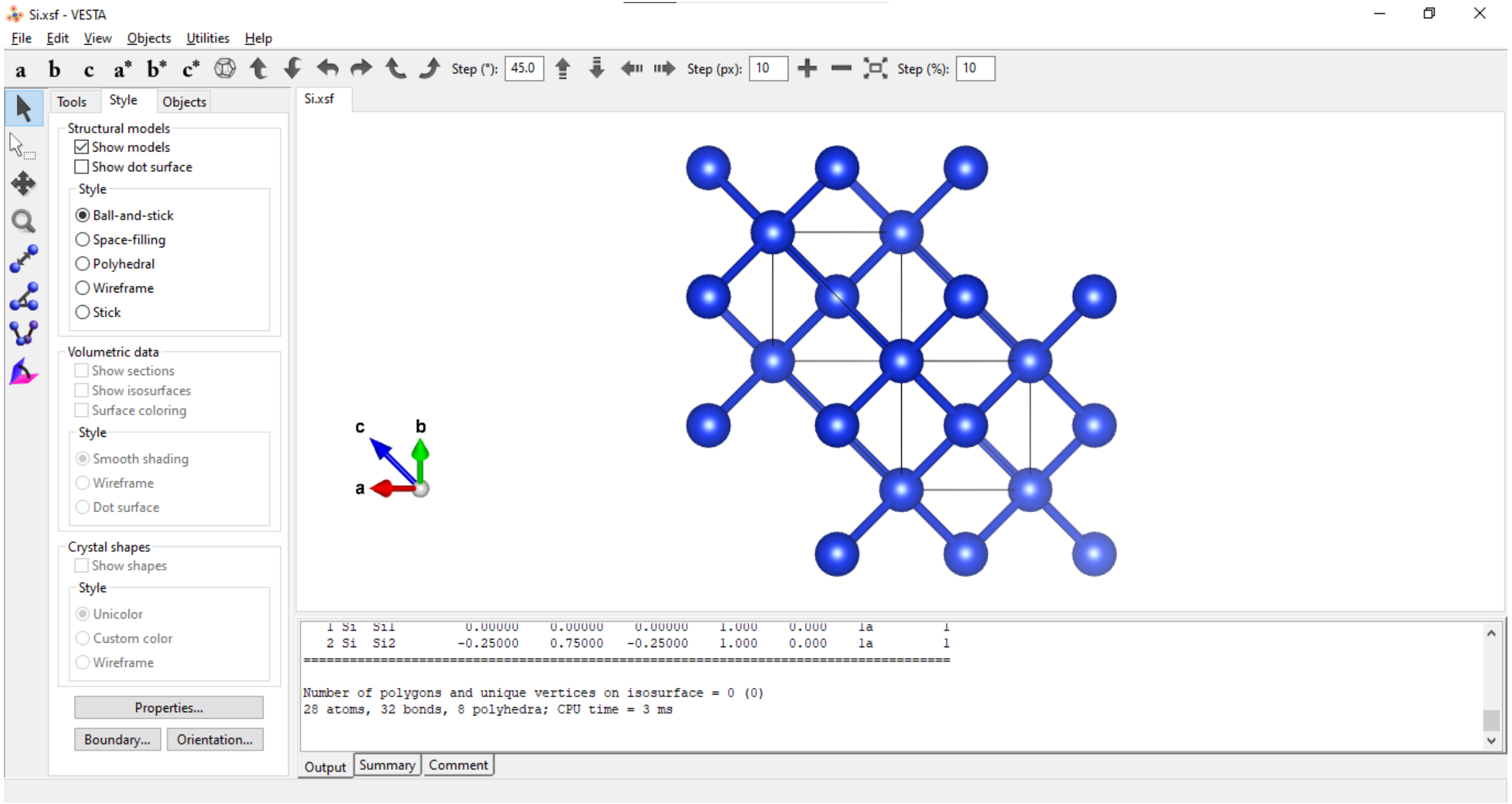
```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ pw.x < Si.scf.in > Si.scf.out
```

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ pwi2xsf.sh Si.scf.in
```

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ ls
Si.scf.in         si_bands.dat          si_bands.gnuplot.3    si_bands_scf.in   si_relax.out
Si.scf.out        si_bands.dat.gnu      si_bands.gnuplot.4.1  si_bands_scf.out  si_scf_dos.in
fort.5            si_bands.dat.rap      si_bands.gnuplot.4.2  si_dos.dat        si_scf_dos.out
input.in          si_bands.gnuplot.1.1  si_bands.in           si_dos.in         silicon.in
output.out        si_bands.gnuplot.1.3  si_bands.out          si_dos.out        silicon.out
pw.x.xsf          si_bands.gnuplot.2.1  si_bands.ps           si_nscf_dos.in    tmp
pwi2xsf.xsf       si_bands.gnuplot.2.4  si_bands_pp.in        si_nscf_dos.out   wannier90.werr
pwi2xsf.xsf_out   si_bands.gnuplot.2.5  si_bands_pp.out       si_relax.in
```

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ mv pwi2xsf.xsf_out Si.xsf
```

Visualizing the XSF file in VESTA



Si.xsf - VESTA

File Edit View Objects Utilities Help

a b c a* b* c* Step (°): 45.0 Step (px): 10 Step (%): 10

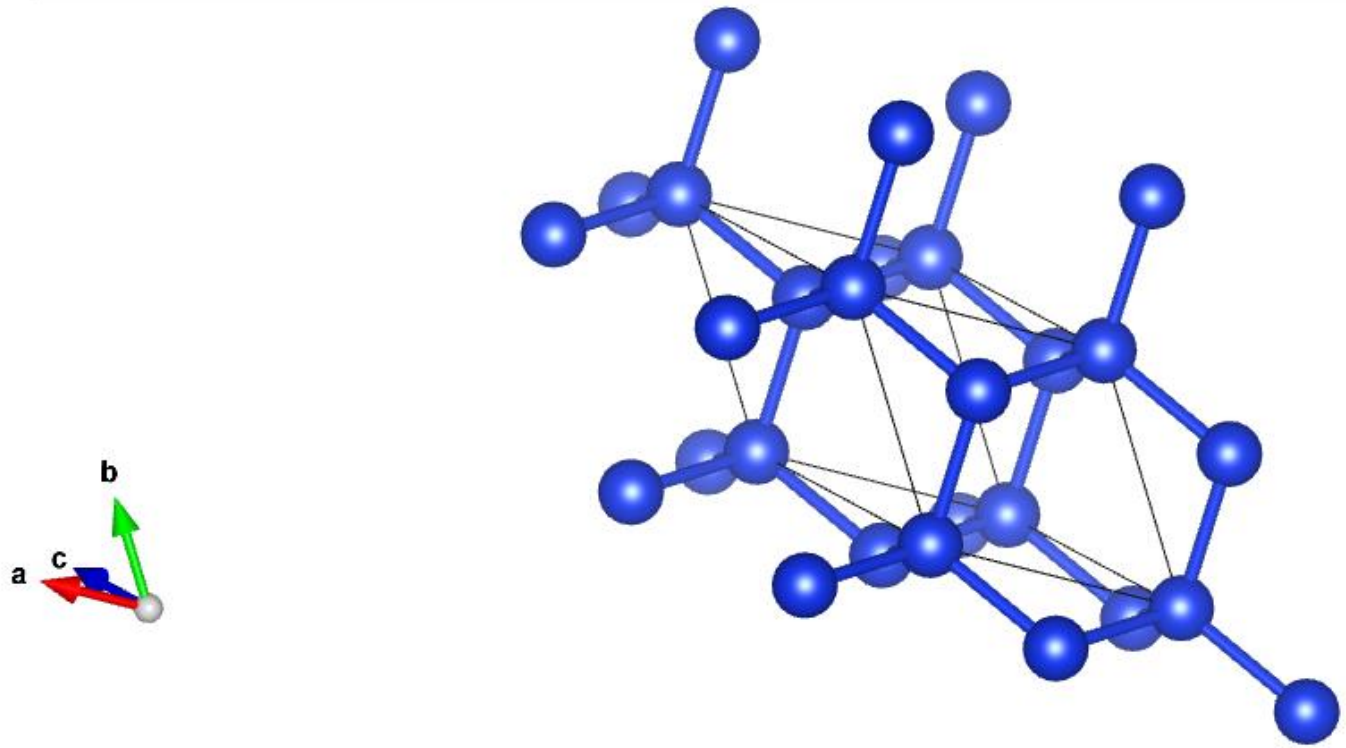
Tools Style Objects

V	Title
☑	XCrySDen XSF file
☑	Atoms
☑	Bonds
☑	Polyhedra

Toggle data: < 1/1 >

Site	r (Å)	C	L	S
Si	1.18			
Si1	1.18			
Si2	1.18			

Si.xsf



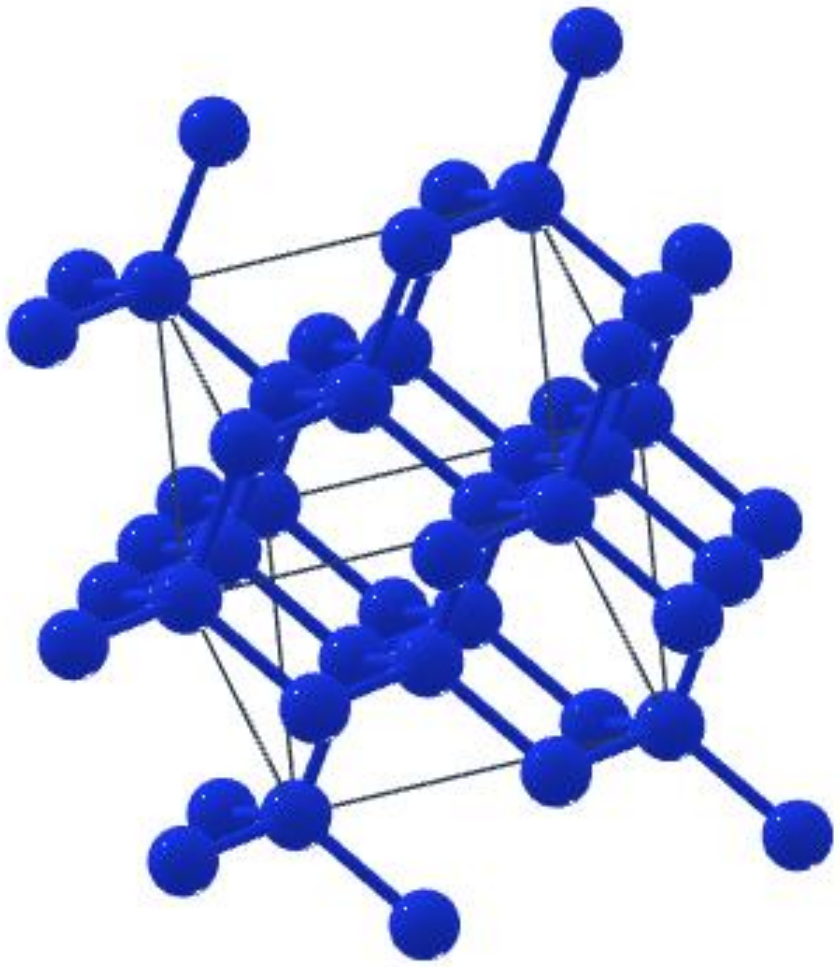

```
   a        b        c       alpha    beta     gamma
 3.83914  3.83914  3.83914  60.0000  60.0000  60.0000

Unit-cell volume = 40.011557 Å^3

Structure parameters
```

Output Summary Comment

From Materials Project



Lattice (Primitive)

a	3.85 Å
b	3.85 Å
c	3.85 Å
α	60.00 °
β	60.00 °
γ	60.00 °
Volume	40.33 Å^3

Creating and Visualizing Silicon’s 2D Structure using Si bulk Structure

Generating an XSF file using the PW tools

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ vi Si.scf.modified.in
```

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ cat Si.scf.modified.in
&CONTROL
prefix = 'silicon',
outdir = './tmp/'
pseudo_dir = '/home/meyn/q-e-qe-7.1/pseudo/'
verbosity = 'high'
/

&SYSTEM
ibrav = 2,
celldm(1) = 10.26,
nat = 2,
ntyp = 1,
ecutwfc = 30
nbnd = 8
/

&ELECTRONS
mixing_beta = 0.6
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ATOMIC_SPECIES
Si 28.0855 Si.pz-vbc.UPF

ATOMIC_POSITIONS (alat)
Si 0.00 0.00 0 0
Si 0.25 0.25 0 0

K_POINTS (automatic)
6 6 6 0 0 0
```
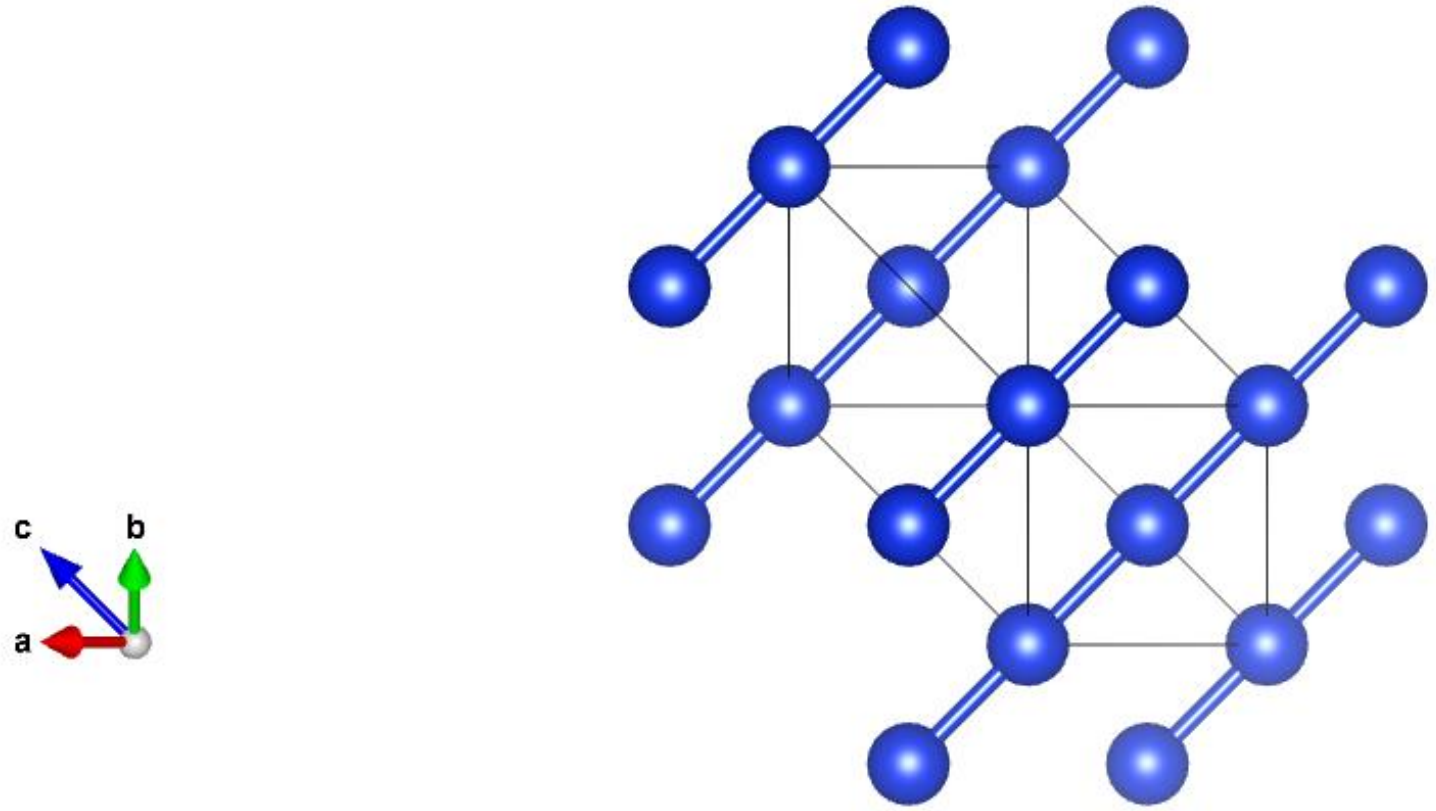

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ pw.x < Si.scf.modified.in > Si.scf.modified.out
--------------------------------------------------------------------------
MPI_ABORT was invoked on rank 0 in communicator MPI_COMM_WORLD
with errorcode 1.

NOTE: invoking MPI_ABORT causes Open MPI to kill all MPI processes.
You may or may not see output from other processes, depending on
exactly when Open MPI kills them.
```

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ pwi2xsf.sh Si.scf.modified.in
 CRYSTAL
 PRIMVEC
  -2.7146790801     0.0000000000     2.7146790801
   0.0000000000     2.7146790801     2.7146790801
  -2.7146790801     2.7146790801     0.0000000000
 CONVVEC
   5.4293581601     0.0000000000     0.0000000000
   0.0000000000     5.4293581601     0.0000000000
   0.0000000000     0.0000000000     5.4293581601
 PRIMCOORD
           2           1
SI      0.0000000000   0.0000000000   0.0000000000
SI      1.3573395400   1.3573395400   0.0000000000
```

```
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ ls
CRASH                Si_modified.xsf   si_bands.dat.rap      si_bands.gnuplot.4.1  si_bands_scf.in   si_relax.in
Si.scf.in            input.in          si_bands.gnuplot.1.1  si_bands.gnuplot.4.2  si_bands_scf.out  si_relax.out
Si.scf.modified.in   input_tmp.in      si_bands.gnuplot.1.3  si_bands.in           si_dos.dat        si_scf_dos.in
Si.scf.modified.out  output.out        si_bands.gnuplot.2.1  si_bands.out          si_dos.in         si_scf_dos.out
Si.scf.out           pwi2xsf.xsf_out   si_bands.gnuplot.2.4  si_bands.ps           si_dos.out        silicon.in
Si.xsf               si_bands.dat      si_bands.gnuplot.2.5  si_bands_pp.in        si_nscf_dos.in    silicon.out
Si_2D.xsf            si_bands.dat.gnu  si_bands.gnuplot.3    si_bands_pp.out       si_nscf_dos.out   tmp
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ mv pwi2xsf.xsf_out Si_2D.xsf
meyn@LAPTOP-C0A2DPIS:~/q-e-qe-7.1/test_calculation$ ls
CRASH                Si_modified.xsf   si_bands.gnuplot.1.1  si_bands.gnuplot.4.2  si_bands_scf.out  si_relax.out
Si.scf.in            input.in          si_bands.gnuplot.1.3  si_bands.in           si_dos.dat        si_scf_dos.in
Si.scf.modified.in   input_tmp.in      si_bands.gnuplot.2.1  si_bands.out          si_dos.in         si_scf_dos.out
Si.scf.modified.out  output.out        si_bands.gnuplot.2.4  si_bands.ps           si_dos.out        silicon.in
Si.scf.out           si_bands.dat      si_bands.gnuplot.2.5  si_bands_pp.in        si_nscf_dos.in    silicon.out
Si.xsf               si_bands.dat.gnu  si_bands.gnuplot.3    si_bands_pp.out       si_nscf_dos.out   tmp
Si_2D.xsf            si_bands.dat.rap  si_bands.gnuplot.4.1  si_bands_scf.in       si_relax.in
```

Visualizing the XSF file in VESTA

Si_2D.xsf




```
   1 Si  Si1          0.00000     0.00000     0.00000     1.000     0.000     1a          1
   2 Si  Si2         -0.50000     0.50000     0.00000     1.000     0.000     1a          1
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
22 atoms, 16 bonds, 0 polyhedra; CPU time = 1 ms
```

References

- https://pranabdas.github.io/espresso/hands-on/scf
- https://manpages.ubuntu.com/manpages/xenial/man1/pwi2xsf.1.html