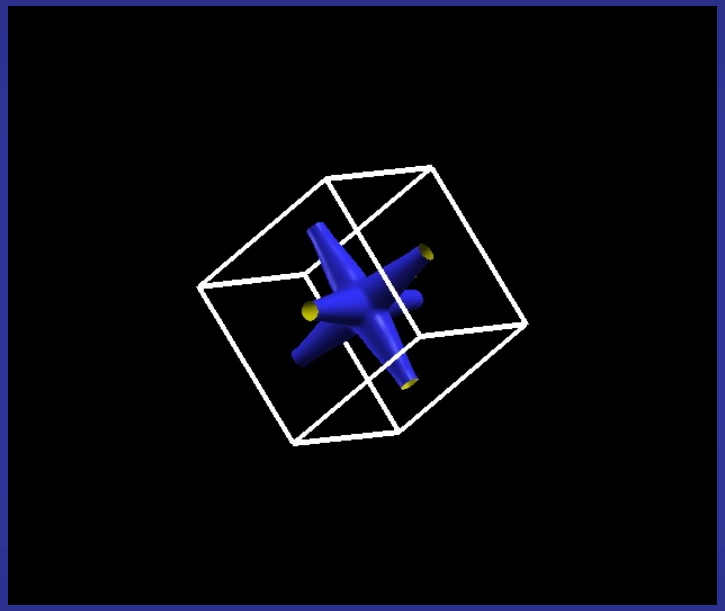
How to plot the Fermi surface using SIESTA and WANNIER90



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We are going to plot the Fermi surface of electron-doped bulk $SrTiO_3$

To charge slightly the bulk unit cell of $SrTiO_3$, introduce the following line in the input file

NetCharge -0.10

Then, follow step by step all the process described in the exercise about the Wannier functions

Flowchart to compute Maximally Localized Wannier functions from the input provided by SIESTA

1. Prepare compatible input files for SIESTA and WANNIER90

2. Run WANNIER90 in pre-processing format

3. Run SIESTA and generate the required files to feed WANNIER90

4. Change the extension to the SystemLabel.eigW file

5. Run WANNIER90 to minimize the localization functional, plot the Wanniers, interpolate bands, etc as a post-processing tool

Flowchart to compute Maximally Localized Wannier functions from the input provided by SIESTA

1. Prepare compatible input files for SIESTA and WANNIER90

2. Run WANNIER90 in pre-processing format

```
$ wannier90.x -pp SrTiO3
```

This generates a seedname.nnkp file that is digested by SIESTA

Flowchart to compute the Maximally Localized Wannier functions from the input provided by siesta

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```
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3. Run SIESTA and generate the required files to feed WANNIER90

```
$ siesta < SrTiO3.fdf > SrTiO3.out
```

Succesful output of SIESTA

```
siesta2wannier90: Reading the SrTiO3.nnkp file

read_nnkp: Checking info from the SrTiO3.nnkp file
read_nnkp: Reading data about real lattice
read_nnkp:      - Real lattice is ok
read_nnkp: Reading data about reciprocal lattice
read_nnkp:      - Reciprocal lattice is ok
read_nnkp: Reading data about k-points
read_nnkp: Reading data about projection centers
read_nnkp: Reading data about k-point neighbours
read_nnkp: Reading data about excluded bands

noccbands: Total number of electrons    40
noccbands: Number of occupied bands    20
number_bands_wannier: Number of bands for wannierization
number_bands_wannier: before excluding bands              =    23    0

Number of bands for wannierization after excluding bands:   12    0
Bands to be wannierized:
   12   13   14   15   16   17   18   19   20   21   22   23

compute_pw_matrix: Computing the matrix elements of a plane wave

mmn: Overlap matrices between periodic part of wavefunctions
mmn: written in SrTiO3.mmn file


amn: Overlap matrices between trial projection functions and wavefunctions
amn: written in SrTiO3.amn file

eig: Eigenvalues of the Hamiltonian
eig: written in SrTiO3.eigW file

siesta2wannier90: All the information dumped in the corresponding files
siesta2wannier90: End of the interface between Siesta and Wannier90
```

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```

3. Run SIESTA and generate the required files to feed WANNIER90

```
$ siesta < SrTiO3.fdf > SrTiO3.out
```

4. Change the extension to the SystemLabel.eigW file

```
$ mv SrTiO3.eigW SrTiO3.eig
overwrite SrTiO3.eig? (y/n [n]) y
```

Flowchart to compute the Maximally Localized Wannier functions from the input provided by siesta

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$ mv SrTiO3.eigW SrTiO3.eig
overwrite SrTiO3.eig? (y/n [n]) y
```

5. Edit the output file of SIESTA, and check the value of the Fermi energy. Introduce this value in the input file of WANNIER90

Search the value of the Fermi Energy

In the output file of SIESTA

```
siesta:  Final energy (eV):
siesta:  Band Struct.  =    -874.801969
siesta:  Kinetic       =    1854.126943
siesta:  Hartree       =     819.875433
siesta:  Edftu         =       0.000000
siesta:  Eso           =       0.000000
siesta:  Ext. field    =       0.000000
siesta:  Exch.-corr.   =    -600.147252
siesta:  Ion-electron  =   -3582.103253
siesta:  Ion-ion       =   -2231.630020
siesta:  Ekinion       =       0.000000
siesta:  Total         =   -3739.878148
siesta:  Fermi         =      -4.747334
```

In the input file of WANNIER90, add the following lines

```
fermi_energy   = -4.747334  ! The value of the Fermi energy (-4.747334 eV)
                            ! was obtained from the initial first-principles
                            ! simulations with Siesta
fermi_surface_plot = true   ! This makes Wannier90 to generate the
                            ! Fermi surface for SrTiO3
```

Flowchart to compute the Maximally Localized Wannier functions from the input provided by siesta

1. Prepare compatible input files for SIESTA and WANNIER90

2. Run WANNIER90 in pre-processing format

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3. Run SIESTA and generate the required files to feed WANNIER90

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$ siesta < SrTiO3.fdf > SrTiO3.out
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4. Change the extension to the SystemLabel.eigW file

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$ mv SrTiO3.eigW SrTiO3.eig
overwrite SrTiO3.eig? (y/n [n]) y
```

5. Edit the output file of SIESTA, and check the value of the Fermi energy. Introduce this value in the input file of WANNIER90

6. Run WANNIER90 to minimize the localization functional, plot the Wanniers, interpolate bands, and compute the Fermi surface as a post-processing tool

```
$ wannier90.x SrTiO3
```

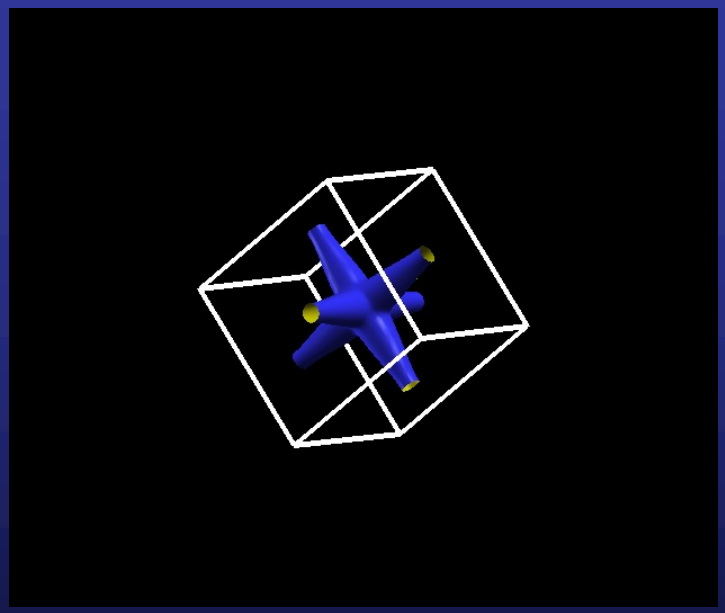
How to plot the Fermi surface

WANNIER90 has produced a file called seedname.bxsf

```
$ xcrysden --bxsf SrTiO3.bxsf
```

Specify the Fermi energy in the dialog box and type OK

Select the bands that cross the Fermi energy
(they cross an horizontal dashed line in the BARGraph).
In this example, they are the bands 10, 11, and 12



How to plot the interpolated band structure obtained from the subspace spanned by the Wannier function

Seedname.win file
(input of WANNIER90)

```
begin kpoint_path                                  ! Defines the path in k-space along
G 0.000  0.000 0.000 X 0.500  0.000 0.000          ! which to calculate the
X 0.500  0.000 0.000 M 0.500  0.500 0.000          ! bandstructure. Each line gives the
M 0.500  0.500 0.000 G 0.000  0.000 0.000          ! start and end point (with labels)
G 0.000  0.000 0.000 R 0.500  0.500 0.500          ! for a section of the path.
R 0.500  0.500 0.500 X 0.500  0.000 0.000          ! Values are in fractional
end kpoint_path                                    ! coordinates with respect to the
                                                   ! primitive reciprocal lattice
                                                   ! vectors.
bands_plot =T
```

```
$ wannier90.x SrTiO3
```

This will produce three files that can be directly plotted by gnuplot

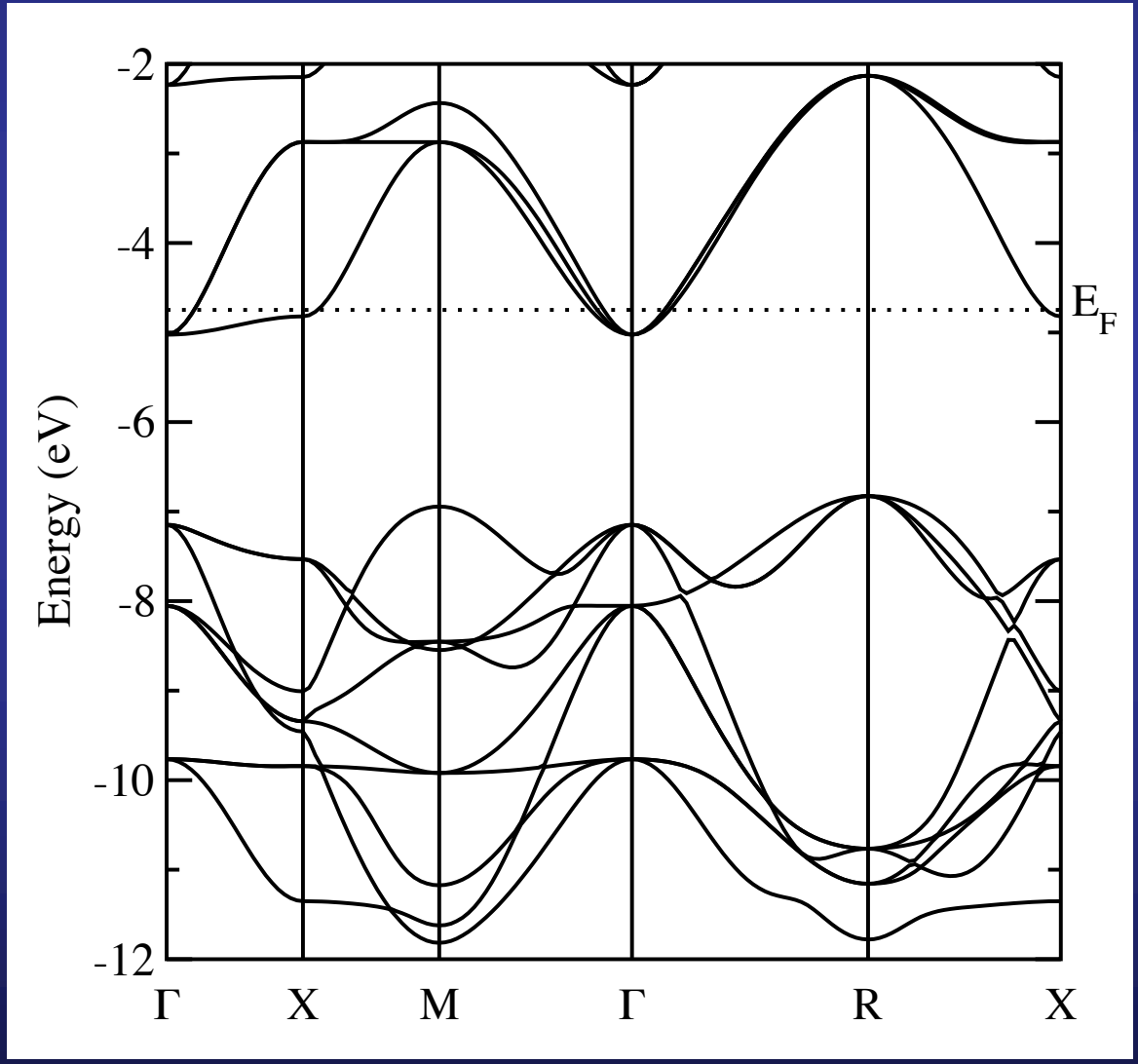
SrTiO3_band.gnu
SrTiO3_band.kpt
SrTiO3_band.dat

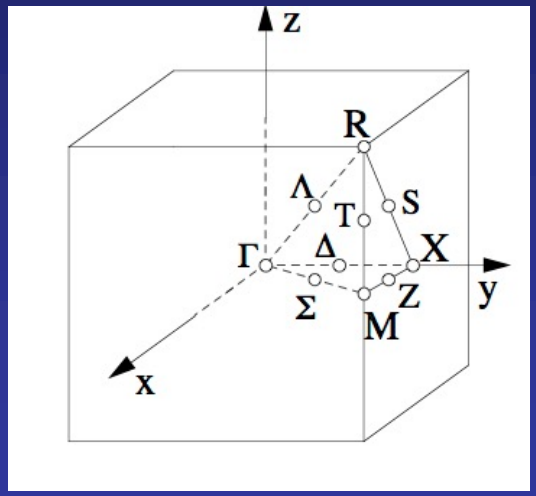
(in the last version of gnuplot, it is very likely that you have to edit SrTiO3_band.gnu and change the first line to

set style data dots

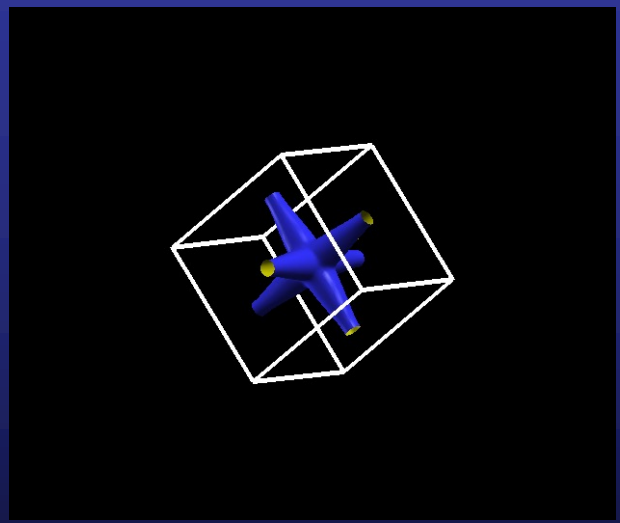
How to plot the interpolated band structure obtained from the subspace spanned by the Wannier function

```
$ gnuplot
$ load “SrTiO3_band.gnu”
```



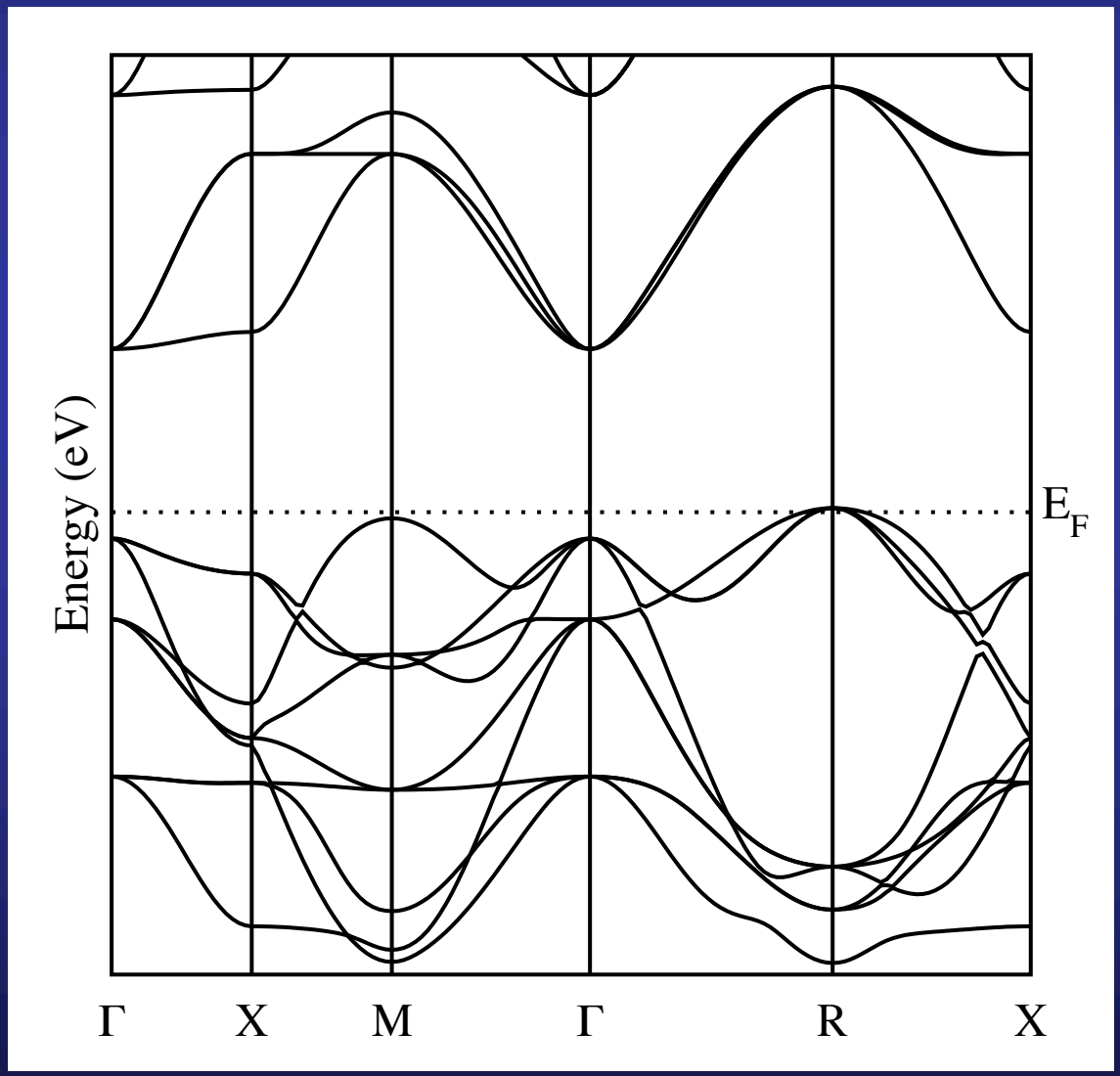


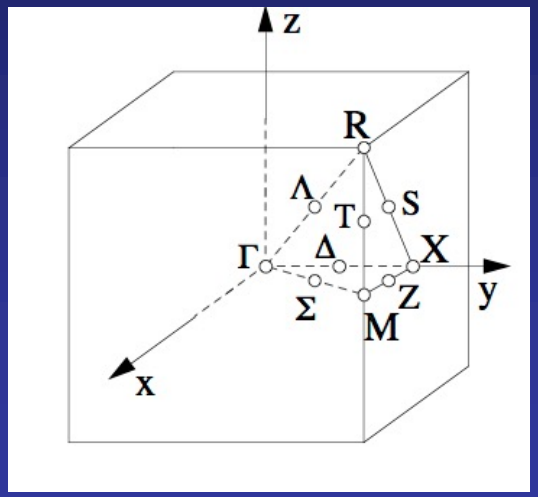
The part of the conduction band that is occupied is along the ΓX line, as reflected by the Fermi surface



Repeat the exercise for a hole-doped system

NetCharge +0.10





The part of the valence band that is desoccupied is at the R point, as reflected by the Fermi surface