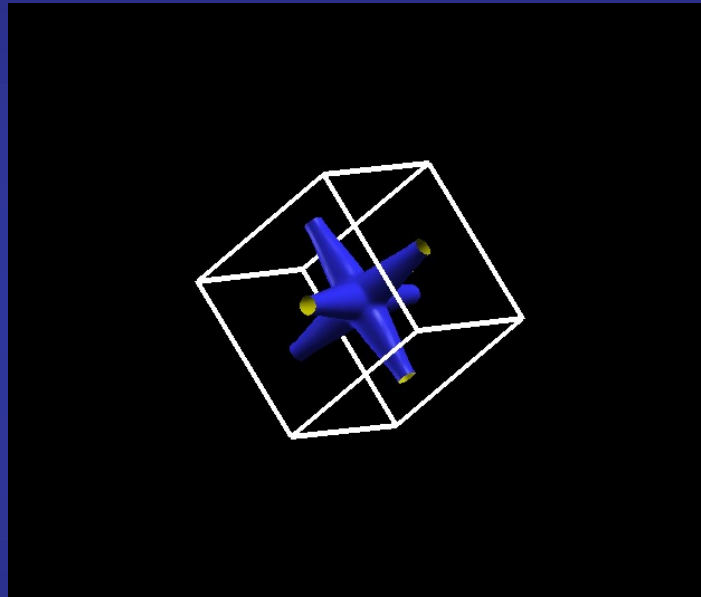


How to plot the Fermi surface using SIESTA and WANNIER90



Javier Junquera

We are going to plot the Fermi surface of electron-doped bulk SrTiO₃

To charge slightly the bulk unit cell of SrTiO₃, 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

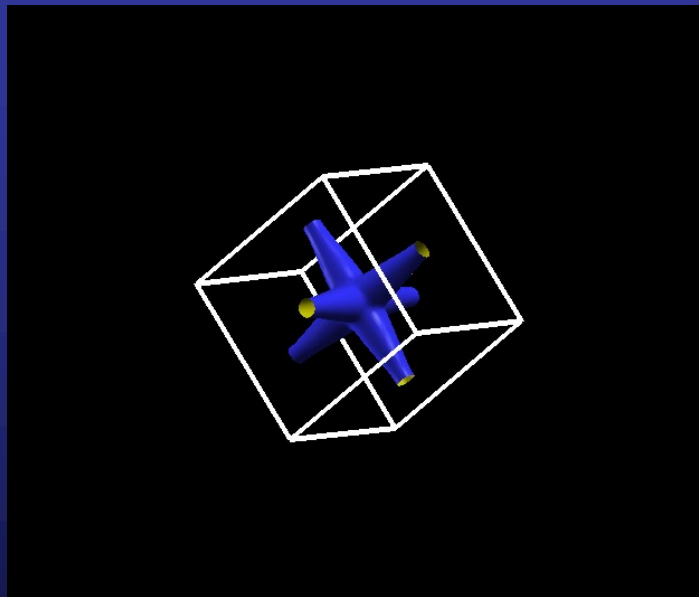
How to plot the Fermi surface

WANNIER90 has produced a file called seedname.bxsf

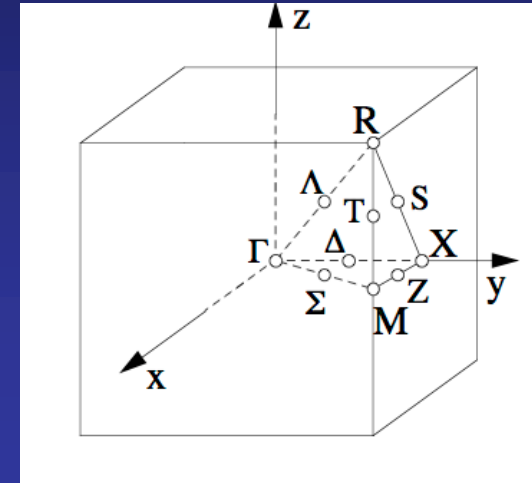
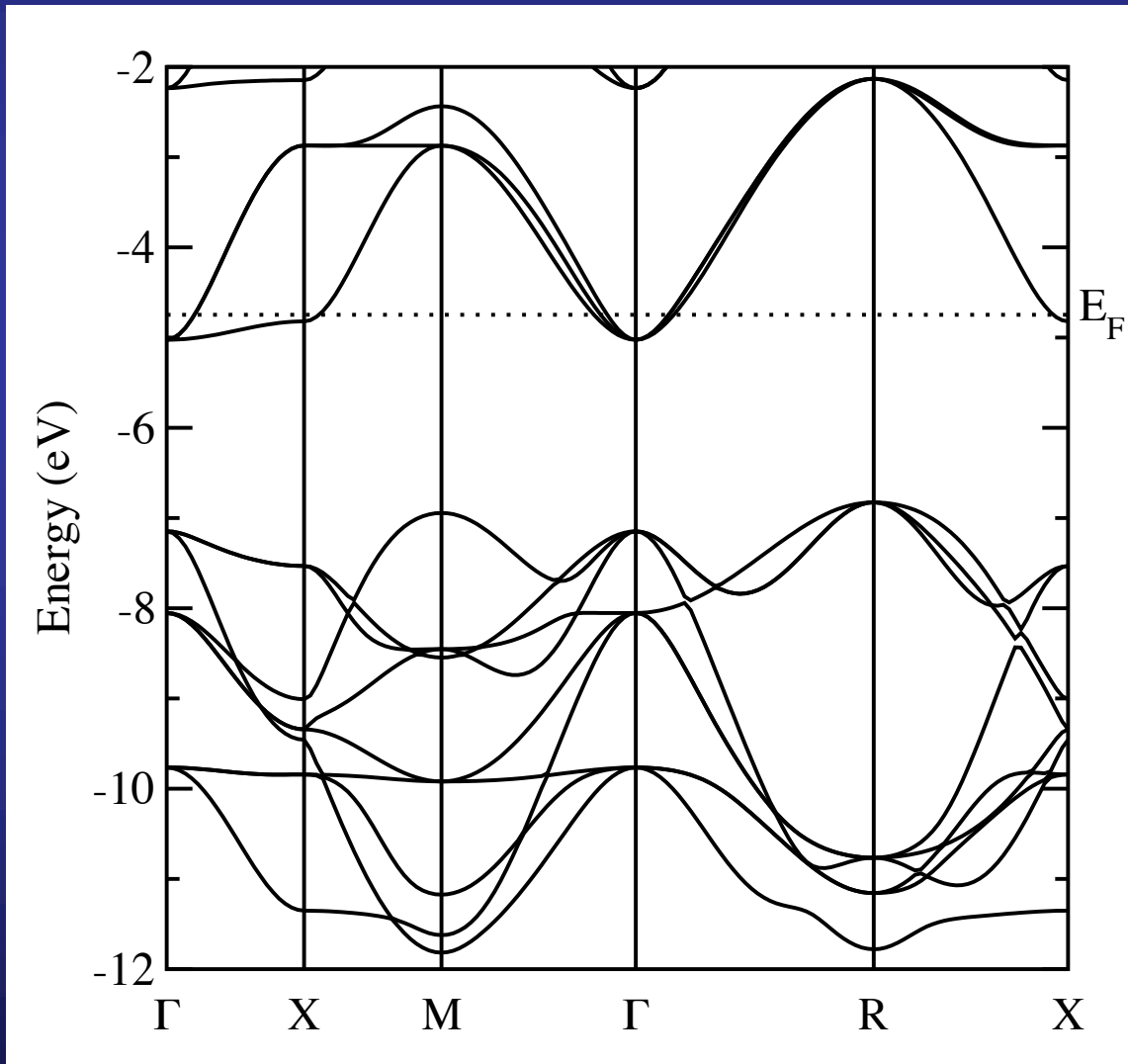
```
$ xcrysden --bxsf SrTiO3.bxsf
```

Specify the Fermi energy in the dialog box
(it will take directly the Fermi energy computed in
siesta)
and type OK

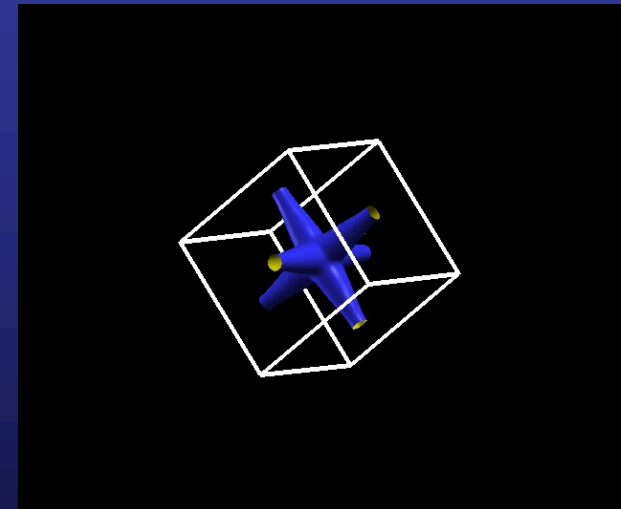
Select the bands that cross the Fermi energy
(they cross an horizontal dashed line in the BARGraph).
In this example, they are the bands 10, 11, and 12



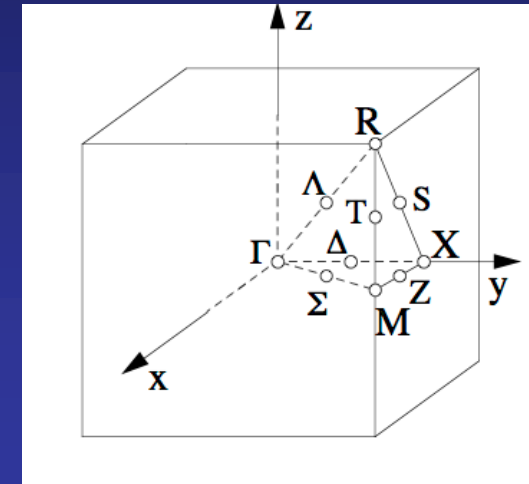
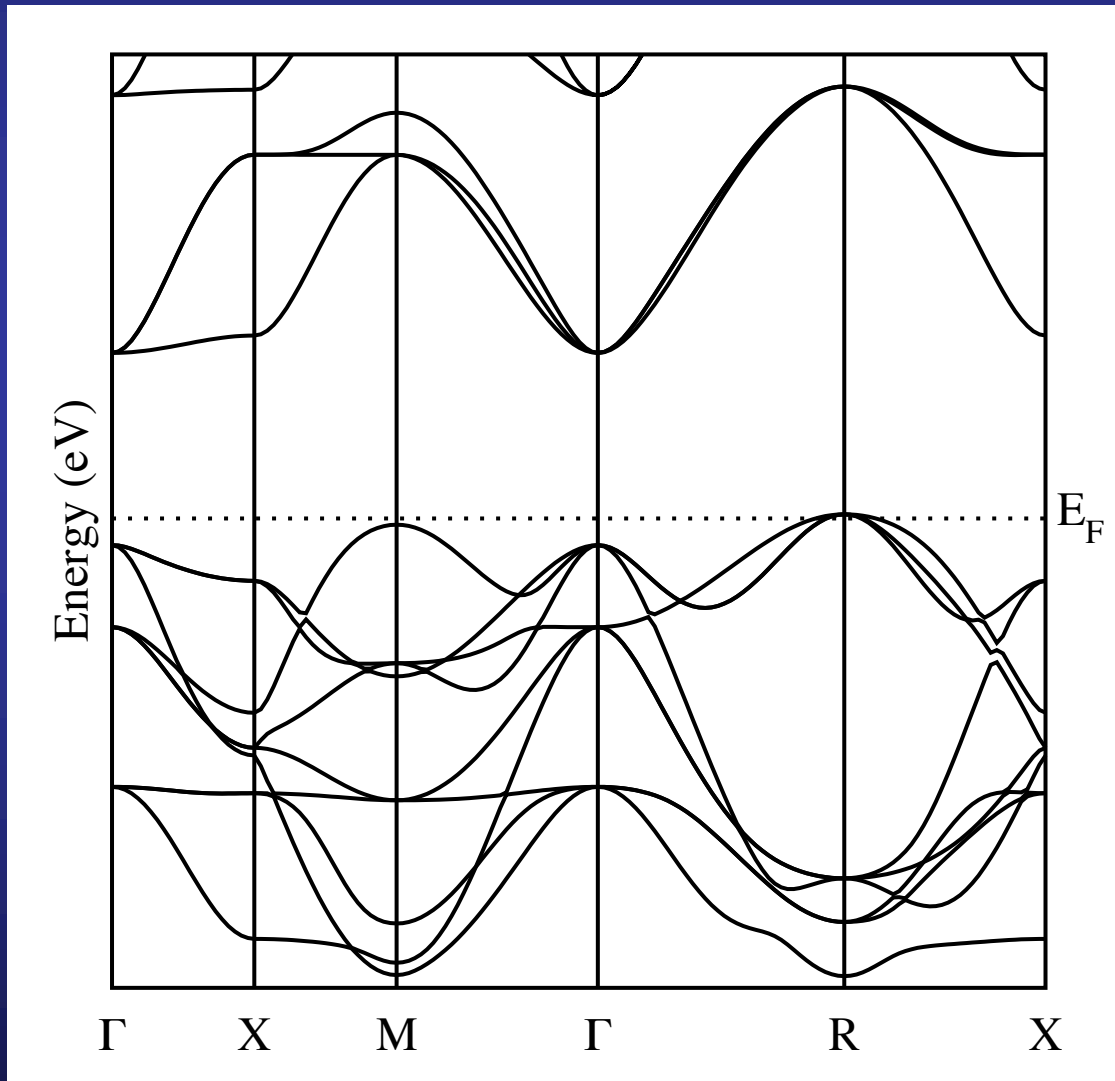
Fermi surface of electron doped SrTiO₃



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



Repeat the exercise for a hole-doped system



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

