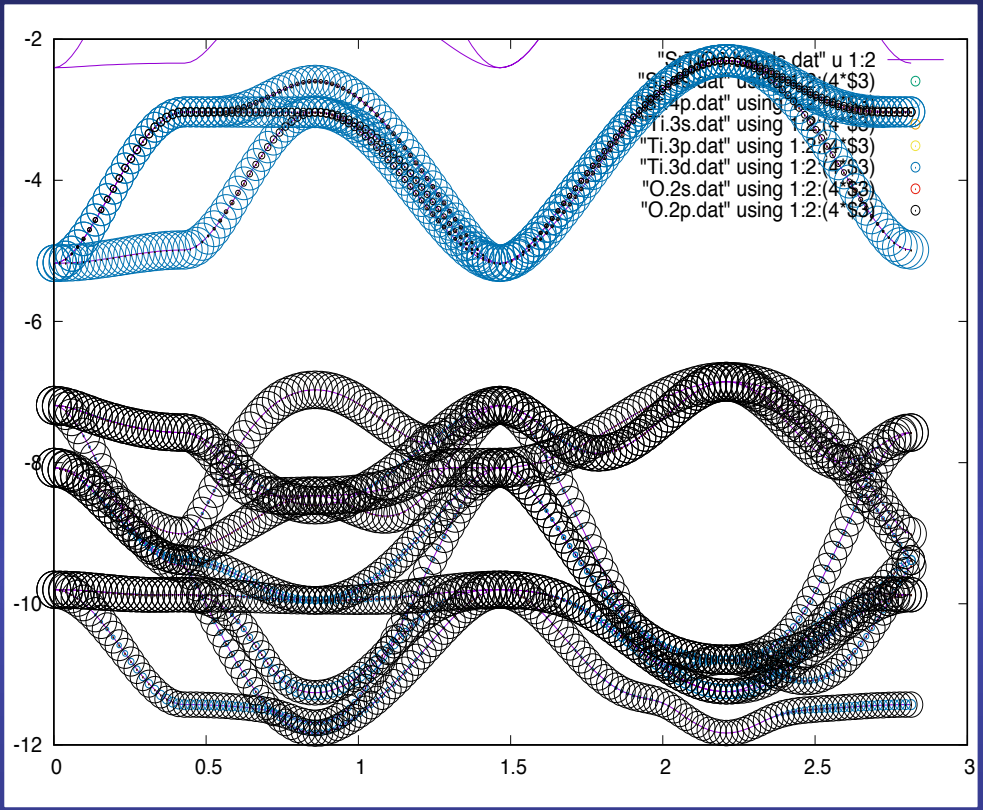
# How to plot fat bands with SIESTA





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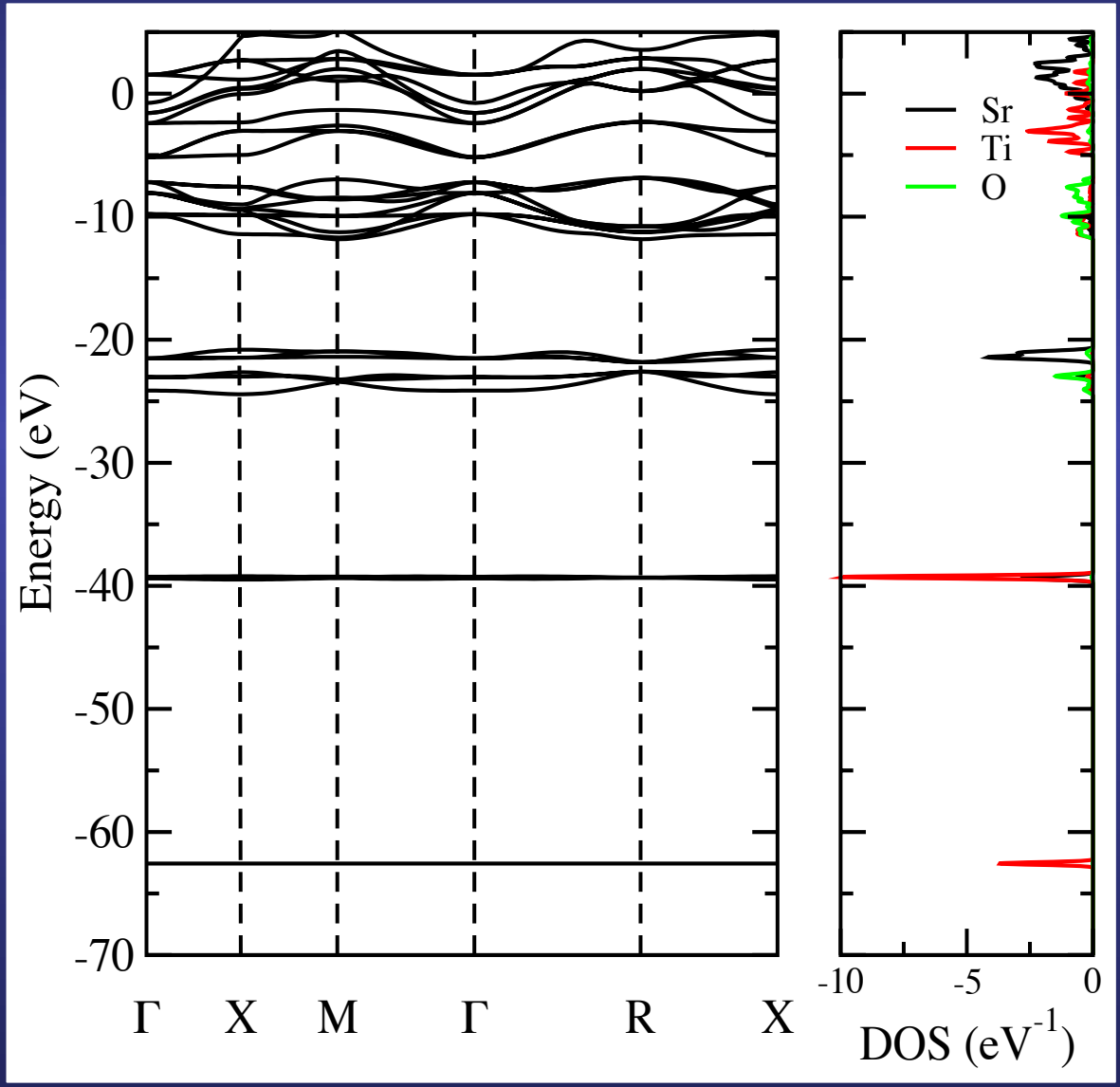
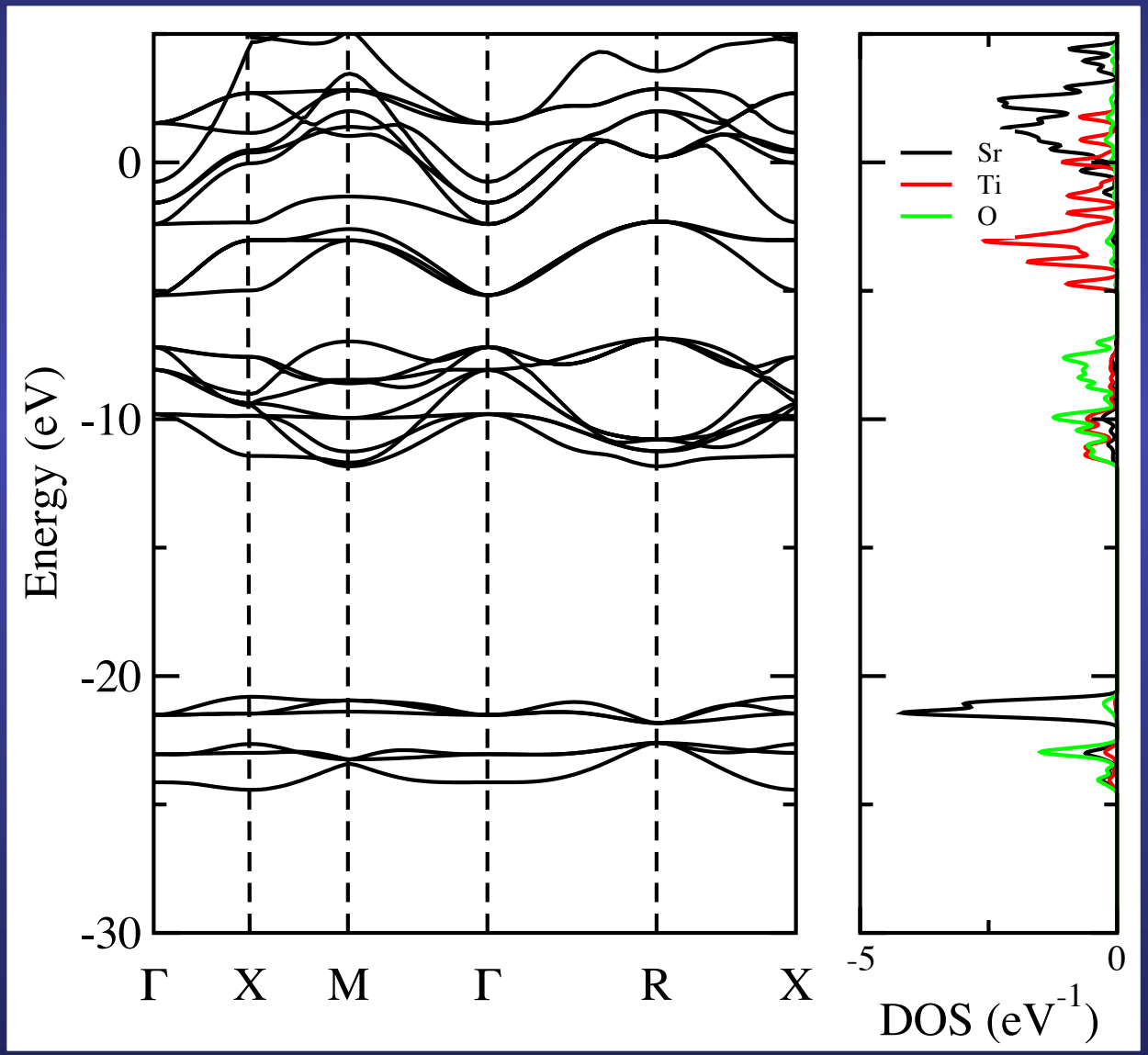
# After running SIESTA and compute the PDOS, we can analyze the character of the different bands

**Which atoms contribute more to the bands at a particular energy window**



# Fat bands: plot both band eigenvalues and information about orbital projections on same foot




Bottom of conduction bands: mostly Ti character

Top of valence bands: mostly O character

We can project on particular atomic orbitals within an atom to further define the character.

# A couple of utility programs must be compiled to run this exercise

```
$ cd <your_siesta_directory>/Util/COOP
$ make OBJDIR=Obj
```

```
$ cd <your_siesta_directory>/Util/Bands
$ make OBJDIR=Obj
```

Replace Obj by the directory where you have compiled siesta
(the path should start at the same level than the Obj or Src directories)

# New variables in SIESTA to plot the fat bands

```
COOP.Write                .true.     # Instructs the program to generate
                                     # SystemLabel.fullBZ.WFSX
                                     # (packed wavefunction file)
                                     # and SystemLabel.HSX (H, S and X ij file),
                                     # to be processed by Util/COOP/mprop and
                                     # Util/COOP/fat and
                                     # to generate COOP/COHP curves,
                                     # (projected) densities of states,
                                     # fat bands, etc.
WFS.Write.For.Bands       .true.     # Instructs the program to compute and
                                     # write the wave functions associated to the
                                     # bands specified
                                     # (by a BandLines or a BandPoints block)
                                     # to the file SystemLabel.bands.WFSX.
WFS.band.min              1          #Specifies the lowest band index of the
                                     # wave-functions to be written to the file
                                     # (in this context) SystemLabel.fullBZ.WFSX
                                     # for each k-point
                                     # (all k-points in the BZ sampling
                                     # are affected).
WFS.band.max              23         # Same as before, but for the
                                     #highest band index


BandLinesScale       pi/a
%block BandLines
1   0.0   0.0   0.0   \Gamma              # Begin at \Gamma
22  1.0   0.0   0.0   X                  # 22 points from \Gamma to X
22  1.0   1.0   0.0   M                  # 22 points from X to M
33  0.0   0.0   0.0   \Gamma              # 33 points from M to \Gamma
39  1.0   1.0   1.0   R                  # 39 points from \Gamma to R
33  1.0   0.0   0.0   X                  # 33 points from R to X
%endblock BandLines
```

These ranges can also be specified with

WFS.Energy.Max

WFS.Energy.Min

# New variables in SIESTA to plot the fat bands

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

**This will produce files with the extensions**
**SystemLabel.HSX**
**SystemLabel.bands.WFSX**
**SystemLabel.WFSX**

**The unformatted WFSX files contain the information of the k-points for which wavefunctions coefficients are written, and the energies and coefficients of each wavefunction which was specified in the input file.**

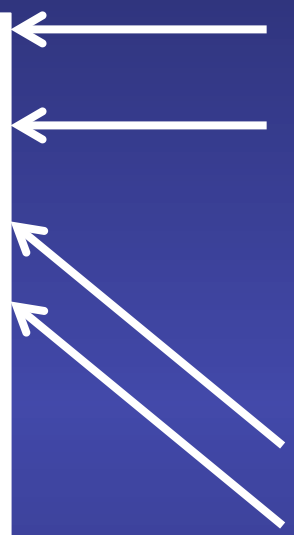
**It also contains information on the atomic species and the orbitals for postprocessing purposes.**

**The unformatted HSX file contains the information about the overlap matrices as well as other data required to generate bands and density of states**

# Prepare an input file required by the auxiliary utility code that produces the fat bands

SystemLabel.mpr

```
SrTiO3
DOS
fatbands_Sr_4s
Sr_4s
fatbands_Sr_4p
Sr_4p
fatbands_Ti_3s
Ti_3s
fatbands_Ti_3p
Ti_3p
fatbands_Ti_3d
Ti_3d
fatbands_O_2s
O_2s
fatbands_O_2p
O_2p
```



System Label

We need to compute the projected density of states for the creation of fat bands plots

Name of the output file where…

…the eigenvalues and the projection weight for this orbital set will be stored

The orbital sets are included as: Atomic symbol_shell

# Run the utility code to fat bands

```
$ cp SrTiO3.bands.WFSX SrTiO3.WFSX
$ <your_path_to_siesta_directory>/Util/COOP/fat SrTiO3
```

```
Reading wf file: SrTiO3.WFSX
 Minimum/Maximum number of wfs per k-point:    23   23
Min_eigval, max_eigval on WFS file:     -62.5675     -2.3030
Min_eigval, max_eigval in band set :     -62.5675     -2.3030
Band set used: (min, max):   1  23
 SrTiO3.HSX nnao, no_s, nspin, nh:          72       15552           1       93728
 Size of set_mask:           72
 Size of set_mask:           72
 Size of set_mask:           72
 Size of set_mask:           72
 Size of set_mask:           72
 Size of set_mask:           72
 Size of set_mask:           72
 Total number of curves processed:            7
Writing files: SrTiO3.stt ...
Fatband coeffs set:    fatbands_Sr_4s  Base orbitals and interactions:      1          719
Fatband coeffs set:    fatbands_Sr_4p  Base orbitals and interactions:      3         2166
Fatband coeffs set:    fatbands_Ti_3s  Base orbitals and interactions:      1          499
Fatband coeffs set:    fatbands_Ti_3p  Base orbitals and interactions:      3         1306
Fatband coeffs set:    fatbands_Ti_3d  Base orbitals and interactions:     10         4170
Fatband coeffs set:    fatbands_O_2s  Base orbitals and interactions:      6         2156
Fatband coeffs set:    fatbands_O_2p  Base orbitals and interactions:     18         7130
```

Output of a successful run

```
-rw-r--r--  1 javier  staff     9209  5 may 17:55 SrTiO3.info
-rw-r--r--  1 javier  staff    86009  5 may 17:55 SrTiO3.fatbands_Sr_4s.EIGFAT
-rw-r--r--  1 javier  staff    86009  5 may 17:55 SrTiO3.fatbands_Ti_3s.EIGFAT
-rw-r--r--  1 javier  staff    86009  5 may 17:55 SrTiO3.fatbands_Ti_3p.EIGFAT
-rw-r--r--  1 javier  staff    86009  5 may 17:55 SrTiO3.fatbands_Sr_4p.EIGFAT
-rw-r--r--  1 javier  staff    86009  5 may 17:55 SrTiO3.fatbands_Ti_3d.EIGFAT
-rw-r--r--  1 javier  staff    86009  5 may 17:55 SrTiO3.fatbands_O_2s.EIGFAT
-rw-r--r--  1 javier  staff    86009  5 may 17:55 SrTiO3.fatbands_O_2p.EIGFAT
```

Output files produced

# Process the EIGFAT files produced in the previous run to generate files that can be read by a ploter

For this, we will use the eigfat2plot files, included in the Util/Bands directory

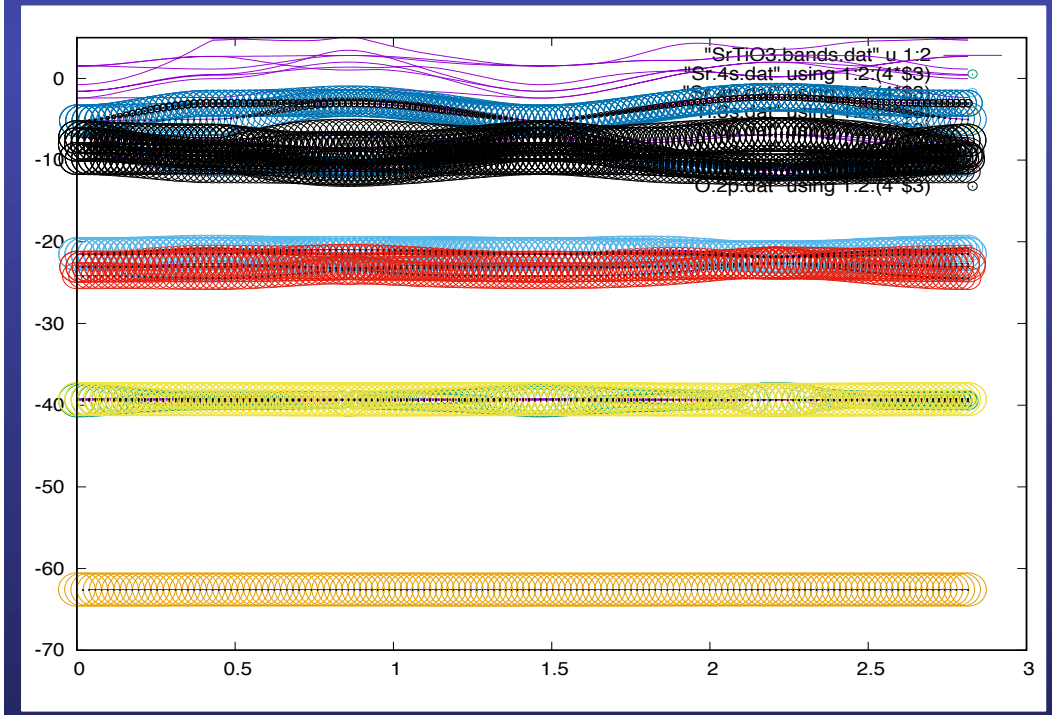
```
$ <your_path_to_siesta_directory>/Util/Bands/eigfat2plot SrTiO3.fatbands_Sr_4s.EIGFAT > Sr.4s.dat
$ <your_path_to_siesta_directory>/Util/Bands/eigfat2plot SrTiO3.fatbands_Sr_4p.EIGFAT > Sr.4p.dat
$ <your_path_to_siesta_directory>/Util/Bands/eigfat2plot SrTiO3.fatbands_Ti_3s.EIGFAT > Ti.3s.dat
$ <your_path_to_siesta_directory>/Util/Bands/eigfat2plot SrTiO3.fatbands_Ti_3p.EIGFAT > Ti.3p.dat
$ <your_path_to_siesta_directory>/Util/Bands/eigfat2plot SrTiO3.fatbands_Ti_3d.EIGFAT > Ti.3d.dat
$ <your_path_to_siesta_directory>/Util/Bands/eigfat2plot SrTiO3.fatbands_O_2s.EIGFAT > O.2s.dat
$ <your_path_to_siesta_directory>/Util/Bands/eigfat2plot SrTiO3.fatbands_O_2p.EIGFAT > O.2p.dat
```

Produce the file to plot the band structure

```
<your_path_to_siesta_dir>/Util/Bands/new.gnubands SrTiO3.bands > SrTiO3.bands.dat
```

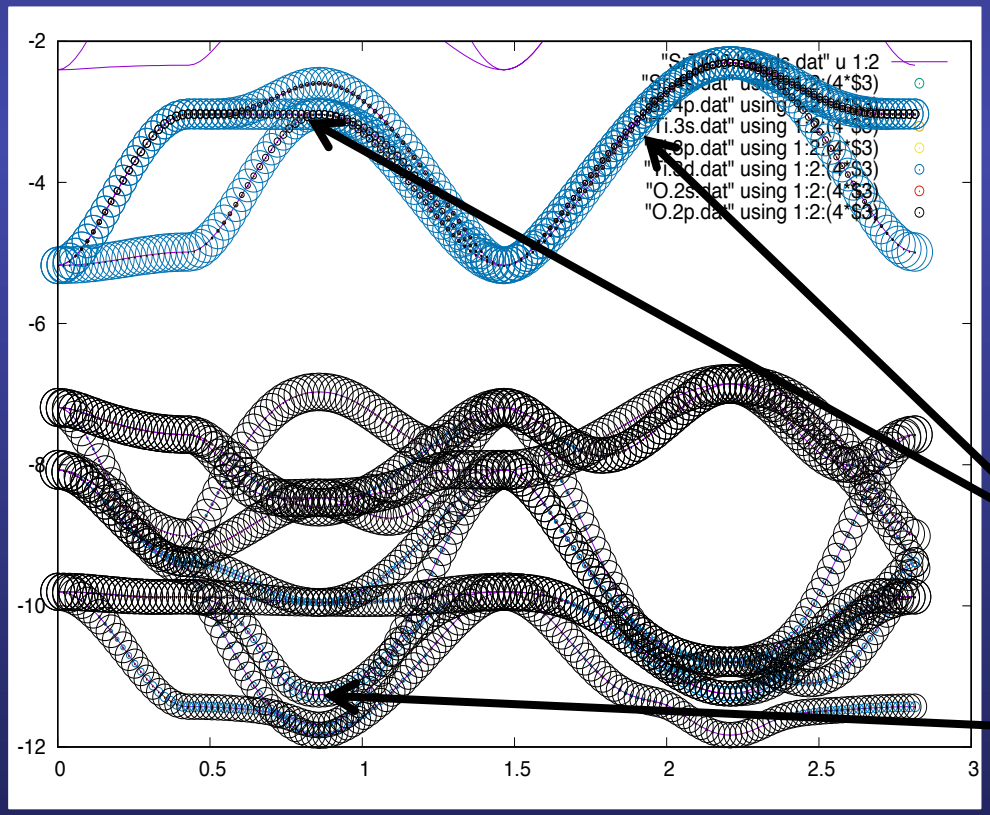
# Plot the band structure with gnuplot

```
$ gnuplot
gnuplot> set yrange [-70:5]
gnuplot> plot "SrTiO3.bands.dat" u 1:2 w l,
"Sr.4s.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Sr.4p.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Ti.3s.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Ti.3p.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Ti.3d.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"O.2s.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"O.2p.dat" using 1:2:(4*$3) with points pt 6 ps variable
gnuplot> set terminal postscript color
Terminal type set to 'postscript'
Options are 'landscape enhanced defaultplex \
   leveldefault color colortext \
   dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 14  fontscale 1.0 '
gnuplot> set output "all.ps"
```



# Focusing on the top of the valence band and the bottom of the conduction bands

```
gnuplot> set yrange [-12:-2]
gnuplot> plot "SrTiO3.bands.dat" u 1:2 w l,
"Sr.4s.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Sr.4p.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Ti.3s.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Ti.3p.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"Ti.3d.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"O.2s.dat" using 1:2:(4*$3) with points pt 6 ps variable,
"O.2p.dat" using 1:2:(4*$3) with points pt 6 ps variable
gnuplot> set terminal postscript color
Terminal type set to 'postscript'
Options are 'landscape enhanced defaultplex \
   leveldefault color colortext \
   dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 14  fontscale 1.0 '
gnuplot> set output "val-con.ps"
```




**Clear hybridization of Ti $t_{2g}$ and O 2$p$ orbitals**

**Small contributions of the O 2$p$ on the bottom of the conduction band**

**Small contributions of the Ti 3$d$ on top of the valence band**