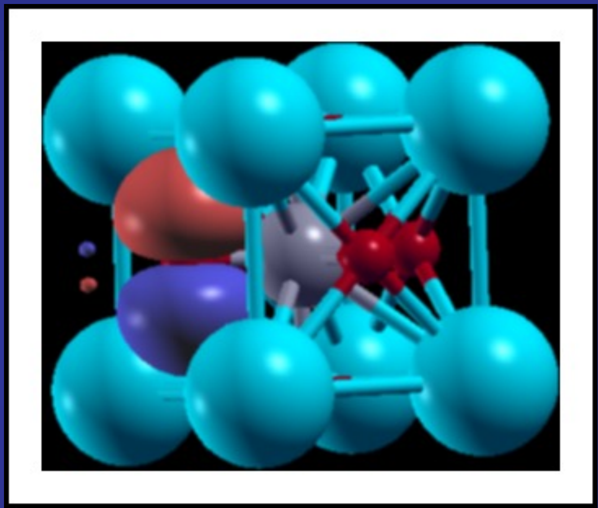
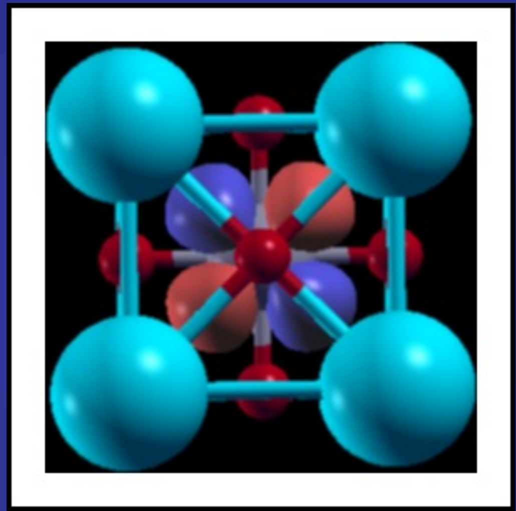
How to run WANNIER90 directly from SIESTA





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Important bibliography:

For a review on Maximally Localized Wannier functions:

REVIEWS OF MODERN PHYSICS, VOLUME 84, OCTOBER–DECEMBER 2012

Maximally localized Wannier functions: Theory and applications

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Important bibliography:

The user guide of the WANNIER90 code

wannier90: User Guide

Version 3.0

27th February 2019

Freely available from:
http://www.wannier.org

WANNIER90 code directly called from SIESTA

WANNIER90 code (version 3.0.0) has been compiled in library mode and called directly from SIESTA

That means that we can run all the functionalities of WANNIER90 directly from SIESTA

Advantages

- No need to prepare two different input files
- No need to run WANNIER90 in pre-processing mode
- We can use the basis set of SIESTA (numerical atomic orbitals) as the initial guess for the projections
- Wannierization of different manifolds can be done in the same run of SIESTA
- The unitary matrices connecting the Bloch and Wannier representations are available in SIESTA.

  New functionalities can follow (initial guesses for order-N simulations)
- Interface with other codes will be much easier:

  SCALE-UP (second-principles)

  DMFTwDFT (DMFT code by Aldo Romero's group)

WANNIER90 code directly called from SIESTA

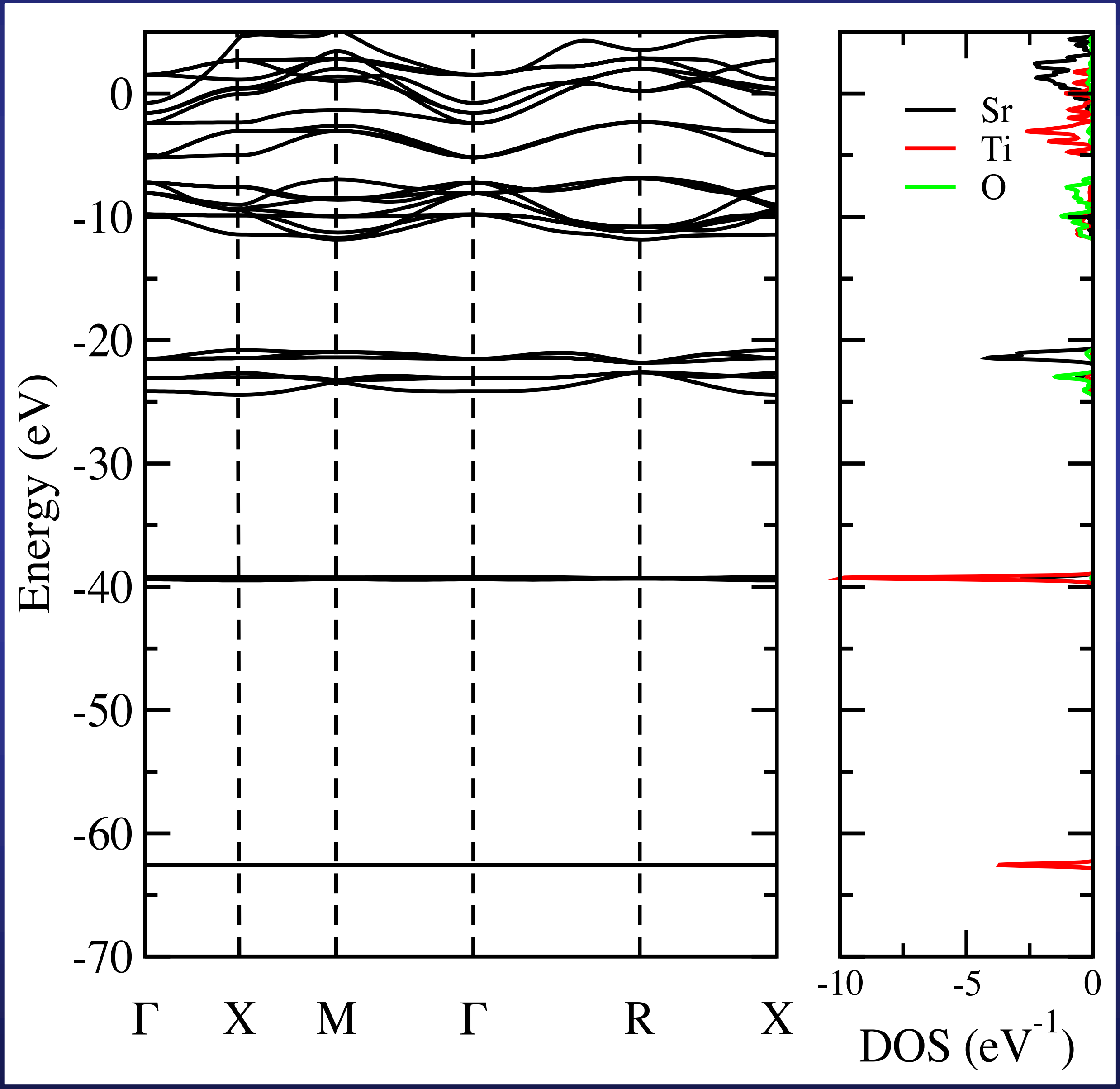
Practical examples:

Bulk $SrTiO_3$ in the cubic phase

Graphene

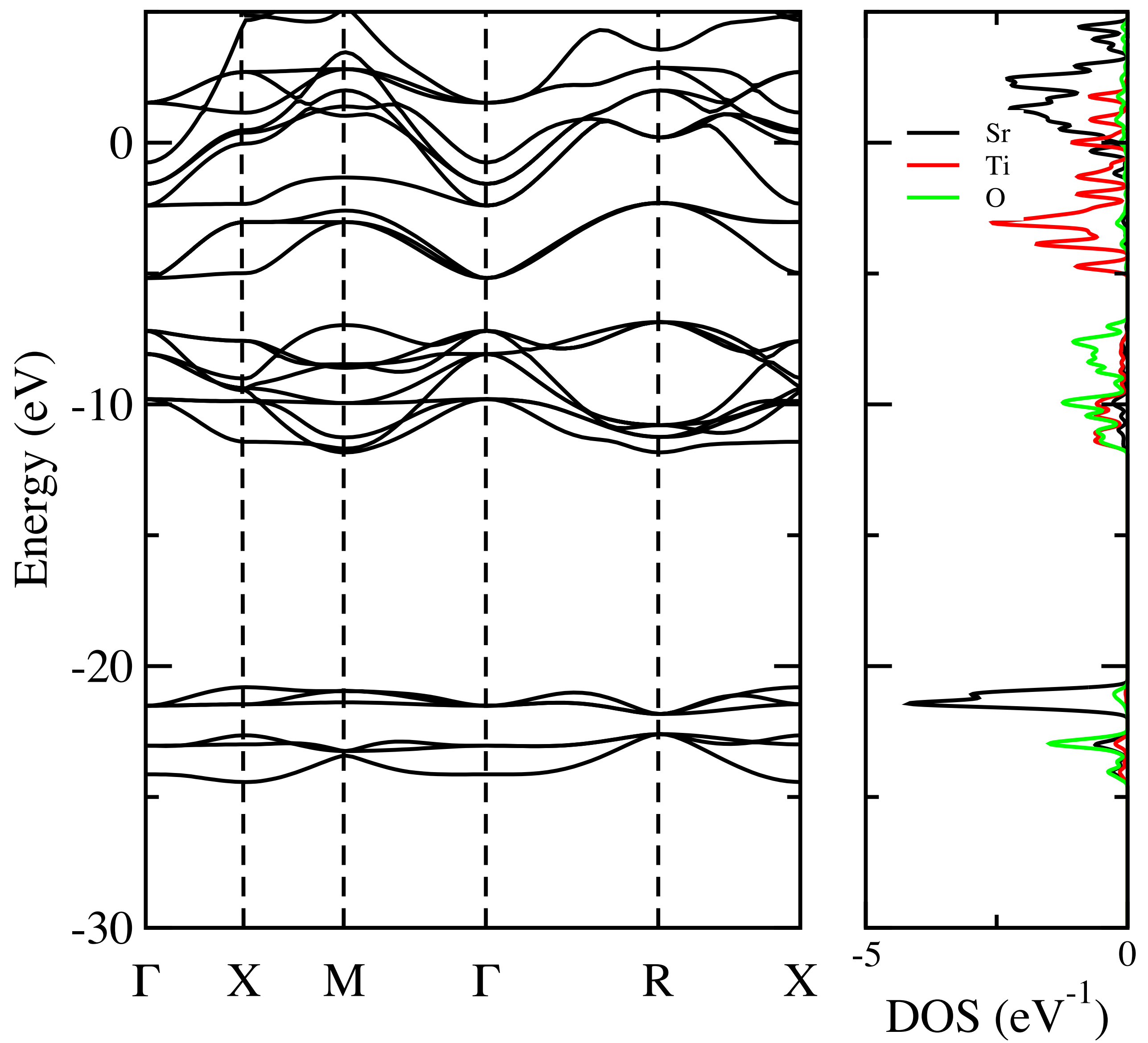
After running SIESTA and compute the PDOS, we can analyze the character of the different bands

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



We can analyze the character of the different bands

Which atoms contribute more to the bands at a particular energy window
Zoom around the top of the valence bands and bottom of conduction bands



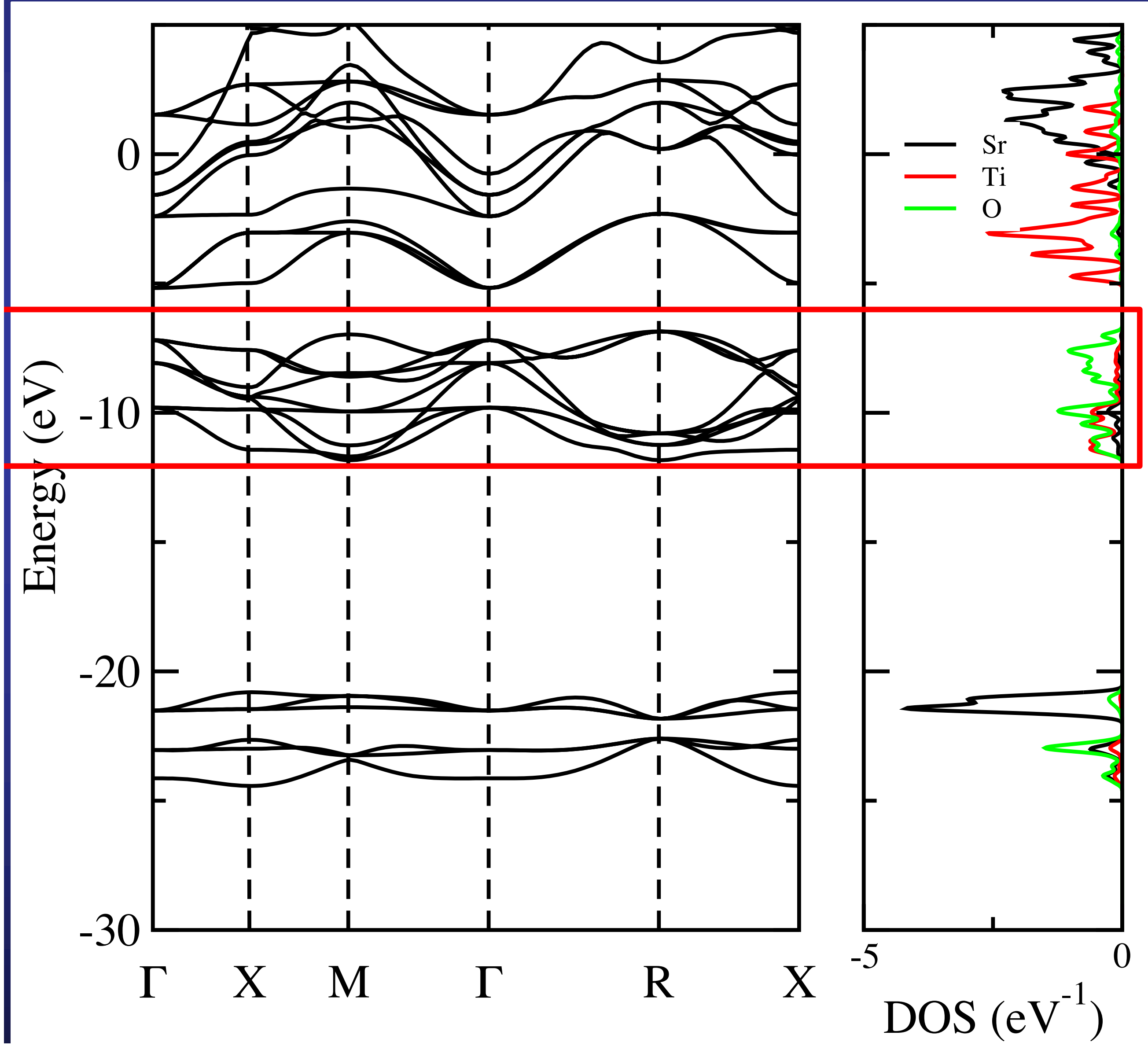
Bottom of conduction bands: mostly Ti t_{2g} character

Top of valence bands: mostly O 2*p* character

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

Choose the Bloch states that will be used to compute the Wannier functions

In this particular example, we are interested in the wannierization of **three different manifolds**



Manifold number 1:

Top of valence bands: mostly O 2*p* character

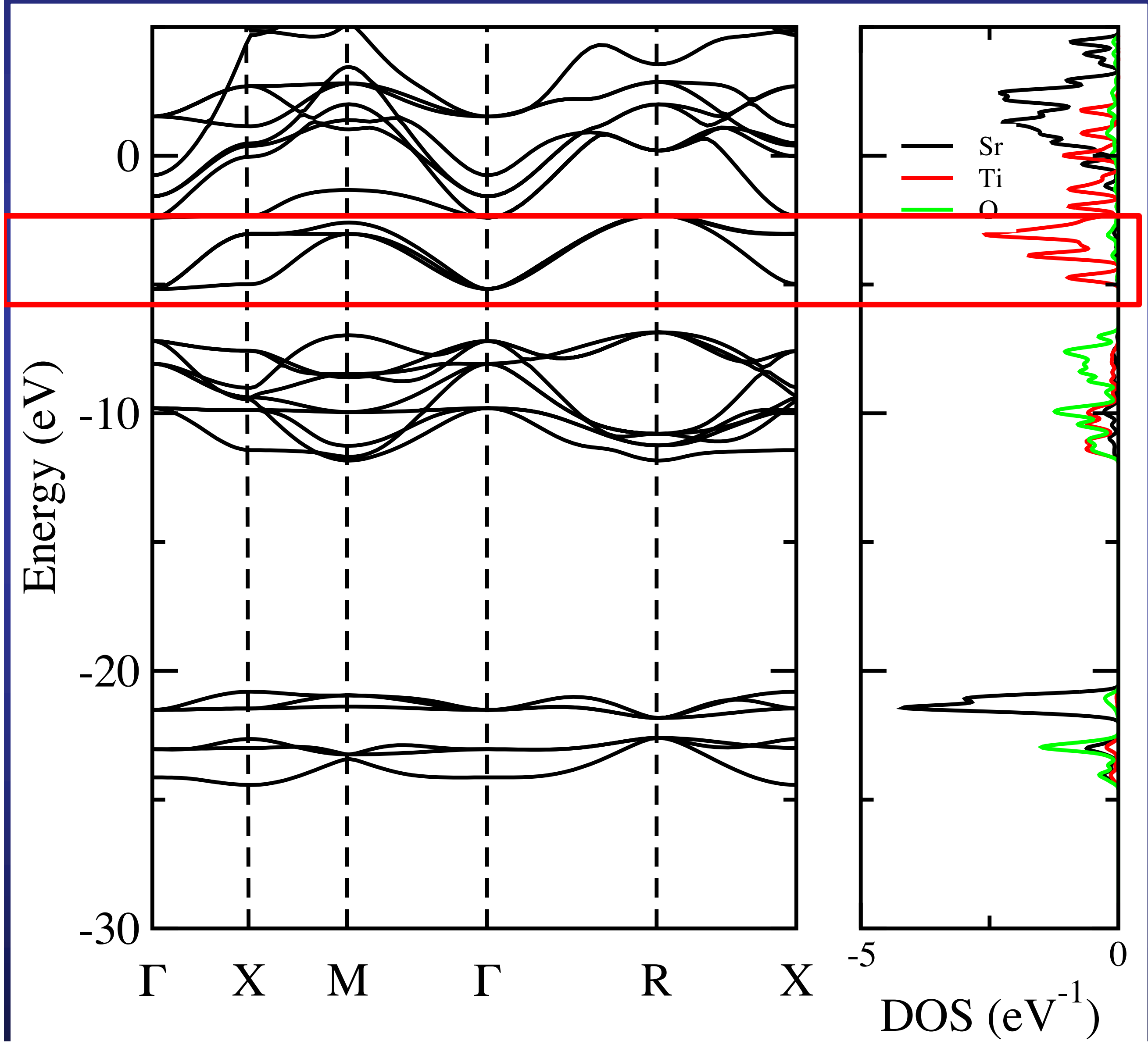
That means:

- 3 O *p* bands (p_x, p_y, p_z) × 3 O atoms

9 bands to wannierize

Choose the Bloch states that will be used to compute the Wannier functions

In this particular example, we are interested in the wannierization of
three different manifolds



Manifold number 2:

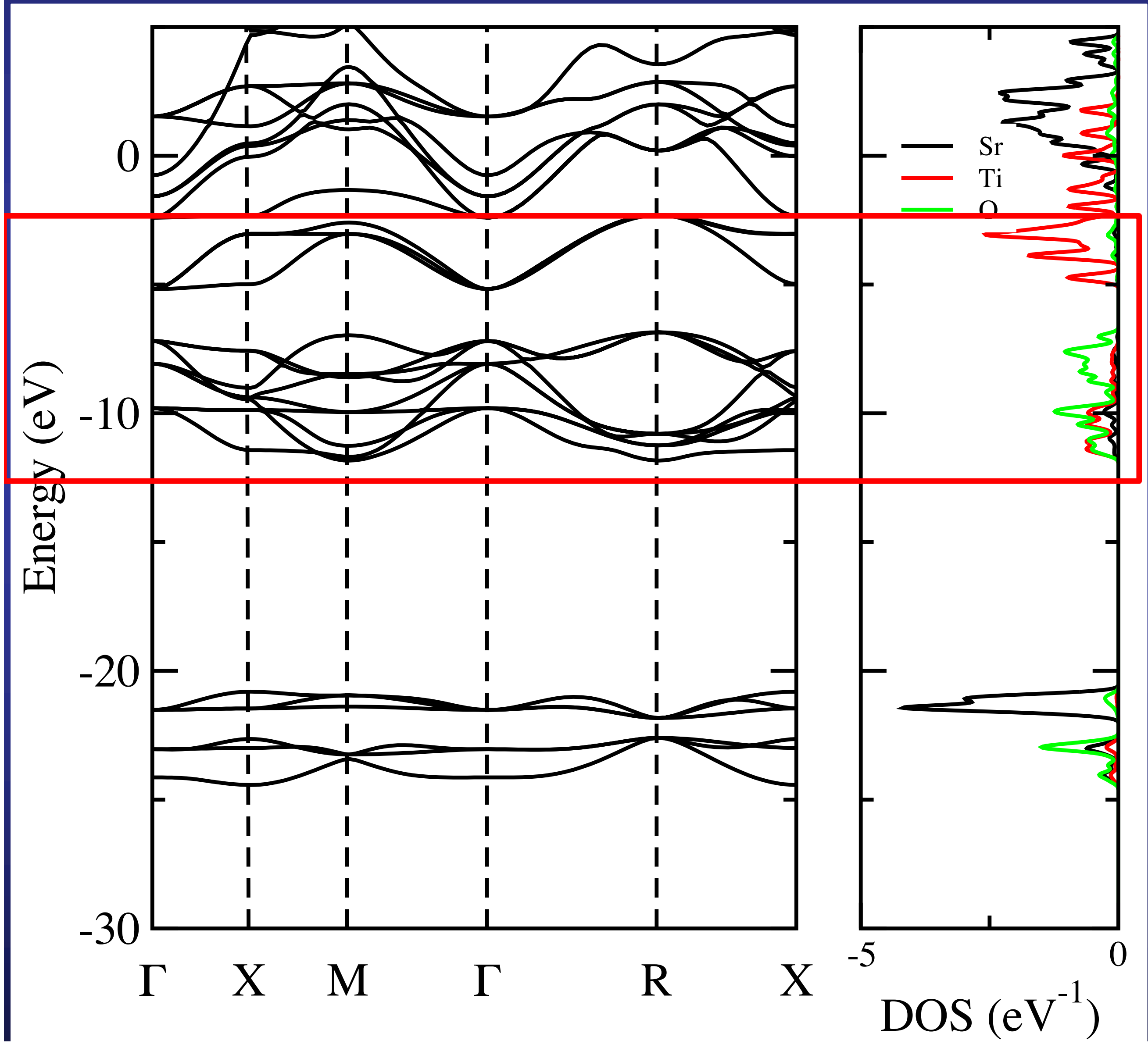
Bottom of conduction bands: mostly Ti t_{2g} character

That means:
-3 Ti t_{2g} bands (d_{xy}, d_{yz}, d_{xz})

3 bands to wannierize

Choose the Bloch states that will be used to compute the Wannier functions

In this particular example, we are interested in the wannierization of three different manifolds



Manifold number 3:

Bottom of conduction bands: mostly Ti t_{2g} character

Top of valence bands: mostly O 2p character

That means:

- **3 O p bands (p_x, p_y, p_z) × 3 O atoms**
- **3 Ti t_{2g} bands (d_{xy}, d_{yz}, d_{xz})**

12 bands to wannierize

SIESTA variables related with the wannierization

Number of manifolds to wannierize

```
%block WannierManifolds
  first
  second
  third
%endblock
```

As many lines in the block as manifolds will be wannierized

A nickname is given to each manifold

SIESTA variables related with the wannierization

Information for every manifold

As many WannierManifolds blocks as manifolds considered for wannierization

The nickname of every manifold is appended here to the keyword WannierManifold

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
  bands 12 20
  # Indices of the orbitals that will be used as localized trial orbitals
  #   (any number of lines allowed)
  trial-orbitals [36 37 38]
  trial-orbitals [49 50 51]
  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

SIESTA variables related with the wannierization

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
  bands 12 20
  # Indices of the orbitals that will be used as localized trial orbitals
  #   (any number of lines allowed)
  trial-orbitals [36 37 38]
  trial-orbitals [49 50 51]
  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

```
!
! For every k-point, the bands in Siesta are ordered from lowest to highest
! energy
! The character of the bands are known after computation of the PDOS.
! In order, for the case of SrTiO3:
! -----------------------------------------------------------------------
! Bands to be excluded
! -----------------------------------------------------------------------
! Band   1 (lowest band):  Ti-3s character
! Bands 2, 3, and 4:       Ti-3p character (px, py, and pz)
! Band   5:                Sr-4s character
! Bands 6, 7, and 8:       O-2s  character (1 band * 3 O atoms in the unit cell)
! Bands 9, 10, and 11:     Sr-4p character (px, py, and pz)
! -----------------------------------------------------------------------
! Bands to be wannierized
! -----------------------------------------------------------------------
! Bands 12-20:             O-2p  character (3 bands * 3 O atoms in the unit cell)
! Bands 21, 22, and 23:    Ti-t2g characer (dxy, dyz, dxz)
```

SIESTA variables related with the wannierization

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
  bands 12 20
  # Indices of the orbitals that will be used as localized trial orbitals
  #   (any number of lines allowed)
  trial-orbitals [36 37 38]
  trial-orbitals [49 50 51]
  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

SIESTA variables related with the wannierization

A good initial guess to project the bands of the top of the valence band are the O-2p orbitals

Take a look to the SystemLabel.ORB_INDX file

72   9000 = orbitals in unit cell and supercell. See end of file.

io	ia	is	spec	iao	n	l	m	z	p	sym	rc	isc			iuo
1	1	1	Sr	1	4	0	0	1	F	s	6.602	0	0	0	1
2	1	1	Sr	2	5	0	0	1	F	s	7.116	0	0	0	2
3	1	1	Sr	3	5	0	0	2	F	s	5.542	0	0	0	3
4	1	1	Sr	4	4	1	-1	1	F	py	6.769	0	0	0	4
5	1	1	Sr	5	4	1	0	1	F	pz	6.769	0	0	0	5
6	1	1	Sr	6	4	1	1	1	F	px	6.769	0	0	0	6
7	1	1	Sr	7	5	1	-1	1	F	py	4.004	0	0	0	7
8	1	1	Sr	8	5	1	0	1	F	pz	4.004	0	0	0	8
9	1	1	Sr	9	5	1	1	1	F	px	4.004	0	0	0	9
10	1	1	Sr	10	4	2	-2	1	F	dxy	6.602	0	0	0	10
11	1	1	Sr	11	4	2	-1	1	F	dyz	6.602	0	0	0	11
12	1	1	Sr	12	4	2	0	1	F	dz2	6.602	0	0	0	12
13	1	1	Sr	13	4	2	1	1	F	dxz	6.602	0	0	0	13
14	1	1	Sr	14	4	2	2	1	F	dx2-y2	6.602	0	0	0	14
15	2	2	Ti	1	3	0	0	1	F	s	5.806	0	0	0	15
16	2	2	Ti	2	4	0	0	1	F	s	6.104	0	0	0	16
17	2	2	Ti	3	4	0	0	2	F	s	5.124	0	0	0	17
18	2	2	Ti	4	3	1	-1	1	F	py	5.806	0	0	0	18
19	2	2	Ti	5	3	1	0	1	F	pz	5.806	0	0	0	19
20	2	2	Ti	6	3	1	1	1	F	px	5.806	0	0	0	20
21	2	2	Ti	7	4	1	-1	1	F	py	3.108	0	0	0	21
22	2	2	Ti	8	4	1	0	1	F	pz	3.108	0	0	0	22
23	2	2	Ti	9	4	1	1	1	F	px	3.108	0	0	0	23
24	2	2	Ti	10	3	2	-2	1	F	dxy	5.953	0	0	0	24
25	2	2	Ti	11	3	2	-1	1	F	dyz	5.953	0	0	0	25
26	2	2	Ti	12	3	2	0	1	F	dz2	5.953	0	0	0	26
27	2	2	Ti	13	3	2	1	1	F	dxz	5.953	0	0	0	27
28	2	2	Ti	14	3	2	2	1	F	dx2-y2	5.953	0	0	0	28
29	2	2	Ti	15	3	2	-2	2	F	dxy	4.754	0	0	0	29
30	2	2	Ti	16	3	2	-1	2	F	dyz	4.754	0	0	0	30
31	2	2	Ti	17	3	2	0	2	F	dz2	4.754	0	0	0	31
32	2	2	Ti	18	3	2	1	2	F	dxz	4.754	0	0	0	32
33	2	2	Ti	19	3	2	2	2	F	dx2-y2	4.754	0	0	0	33
34	3	3	O	1	2	0	0	1	F	s	4.931	0	0	0	34
35	3	3	O	2	2	0	0	2	F	s	3.653	0	0	0	35
36	3	3	O	3	2	1	-1	1	F	py	5.056	0	0	0	36
37	3	3	O	4	2	1	0	1	F	pz	5.056	0	0	0	37
38	3	3	O	5	2	1	1	1	F	px	5.056	0	0	0	38
39	3	3	O	6	2	1	-1	2	F	py	3.937	0	0	0	39
40	3	3	O	7	2	1	0	2	F	pz	3.937	0	0	0	40
41	3	3	O	8	2	1	1	2	F	px	3.937	0	0	0	41
42	3	3	O	9	3	2	-2	1	F	dxy	2.774	0	0	0	42
43	3	3	O	10	3	2	-1	1	F	dyz	2.774	0	0	0	43
44	3	3	O	11	3	2	0	1	F	dz2	2.774	0	0	0	44
45	3	3	O	12	3	2	1	1	F	dxz	2.774	0	0	0	45
46	3	3	O	13	3	2	2	1	F	dx2-y2	2.774	0	0	0	46
47	4	3	O	1	2	0	0	1	F	s	4.931	0	0	0	47
48	4	3	O	2	2	0	0	2	F	s	3.653	0	0	0	48
49	4	3	O	3	2	1	-1	1	F	py	5.056	0	0	0	49
50	4	3	O	4	2	1	0	1	F	pz	5.056	0	0	0	50
51	4	3	O	5	2	1	1	1	F	px	5.056	0	0	0	51
52	4	3	O	6	2	1	-1	2	F	py	3.937	0	0	0	52
53	4	3	O	7	2	1	0	2	F	pz	3.937	0	0	0	53
54	4	3	O	8	2	1	1	2	F	px	3.937	0	0	0	54
55	4	3	O	9	3	2	-2	1	F	dxy	2.774	0	0	0	55
56	4	3	O	10	3	2	-1	1	F	dyz	2.774	0	0	0	56
57	4	3	O	11	3	2	0	1	F	dz2	2.774	0	0	0	57
58	4	3	O	12	3	2	1	1	F	dxz	2.774	0	0	0	58
59	4	3	O	13	3	2	2	1	F	dx2-y2	2.774	0	0	0	59
60	5	3	O	1	2	0	0	1	F	s	4.931	0	0	0	60
61	5	3	O	2	2	0	0	2	F	s	3.653	0	0	0	61
62	5	3	O	3	2	1	-1	1	F	py	5.056	0	0	0	62
63	5	3	O	4	2	1	0	1	F	pz	5.056	0	0	0	63
64	5	3	O	5	2	1	1	1	F	px	5.056	0	0	0	64
65	5	3	O	6	2	1	-1	2	F	py	3.937	0	0	0	65
66	5	3	O	7	2	1	0	2	F	pz	3.937	0	0	0	66
67	5	3	O	8	2	1	1	2	F	px	3.937	0	0	0	67
68	5	3	O	9	3	2	-2	1	F	dxy	2.774	0	0	0	68
69	5	3	O	10	3	2	-1	1	F	dyz	2.774	0	0	0	69
70	5	3	O	11	3	2	0	1	F	dz2	2.774	0	0	0	70
71	5	3	O	12	3	2	1	1	F	dxz	2.774	0	0	0	71
72	5	3	O	13	3	2	2	1	F	dx2-y2	2.774	0	0	0	72

p-orbitals of the first O atom

p-orbitals of the second O atom

p-orbitals of the third O atom

SIESTA variables related with the wannierization

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
  bands 12 20
  # Indices of the orbitals that will be used as localized trial orbitals
  #   (any number of lines allowed)
  trial-orbitals [36 37 38]
  trial-orbitals [49 50 51]
  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

Number of iterations for the minimization of the localization functional

If zero, then the procedure is the same as a Löwdin orthonormalization

The resulting Wannier functions will keep the symmetry of the projection function, but it will not be maximally localized

SIESTA variables related with the wannierization

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
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  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

Instruction to plot the Wannier functions

The integer refers to the size of the supercell for plotting the Wannier functions

SIESTA variables related with the wannierization

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
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  trial-orbitals [49 50 51]
  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

Flag to determine whether the Fermi Surface is computed or not

SIESTA variables related with the wannierization

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
  bands 12 20
  # Indices of the orbitals that will be used as localized trial orbitals
  #   (any number of lines allowed)
  trial-orbitals [36 37 38]
  trial-orbitals [49 50 51]
  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

Flag to determine whether the Hamiltonian in real space in a basis of Wannier functions is written

SystemLabel.manifold.X_hr.dat

X is the nickname of the manifold

SIESTA variables related with the wannierization

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
  bands 12 20
  # Indices of the orbitals that will be used as localized trial orbitals
  #   (any number of lines allowed)
  trial-orbitals [36 37 38]
  trial-orbitals [49 50 51]
  trial-orbitals [62 63 64]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
%endblock
```

Flag to determine whether the lattice vectors, Hamiltonian in real space and position operator in a basis of Wannier functions are written

SystemLabel.manifold.X_tb.dat

X is the nickname of the manifold

SIESTA variables related with the wannierization

```
Wannier.k [4 4 4]
```

Number of k-points used in the Wannierization

Succesful output of SIESTA

```
switch_local_projection: Populating the relevant matrices for
switch_local_projection: calling WANNIER90 directly from SIESTA
switch_local_projection: band manifold = first

compute_pw_matrix: Computing the matrix elements of a plane wave

mmn: Overlap matrices between periodic part of wavefunctions
mmn: written in w90_in_siesta.manifold.first.mmn file

amn: Overlap matrices between trial projection functions and wavefunctions
amn: written in w90_in_siesta.manifold.first.amn file

eig: Eigenvalues of the Hamiltonian
eig: written in w90_in_siesta.manifold.first.eigW file

compute_matrices: All the information dumped in the corresponding files
compute_matrices: End of the interface between Siesta and Wannier90
... Calling wannier90 for this manifold
... See file w90_in_siesta.manifold.first.wout for information
```

Succesful output of SIESTA

```
*------------------------------- WANNIERISE ---------------------------------*
 +--------------------------------------------------------------------+<-- CONV
 | Iter  Delta Spread     RMS Gradient      Spread (Ang^2)      Time  |<-- CONV
 +--------------------------------------------------------------------+<-- CONV

 ------------------------------------------------------------------------------
 Initial State
  WF centre and spread    1  ( -0.000000,  1.937000,  1.937000 )     1.28449725
  WF centre and spread    2  ( -0.000000,  1.937000,  1.937000 )     1.28449725
  WF centre and spread    3  (  0.000000,  1.937000,  1.937000 )     1.17470279
  WF centre and spread    4  (  1.937000, -0.000000,  1.937000 )     1.17470279
  WF centre and spread    5  (  1.937000,  0.000000,  1.937000 )     1.28449725
  WF centre and spread    6  (  1.937000, -0.000000,  1.937000 )     1.28449725
  WF centre and spread    7  (  1.937000,  1.937000,  0.000000 )     1.28449726
  WF centre and spread    8  (  1.937000,  1.937000,  0.000000 )     1.17470278
  WF centre and spread    9  (  1.937000,  1.937000,  0.000000 )     1.28449726
  Sum of centres and spreads ( 11.622000, 11.622000, 11.622000 )    11.23109189

      0     0.112E+02      0.0000000000       11.2310918853       0.00  <-- CONV
        O_D=      0.0000000 O_OD=      0.1485757 O_TOT=     11.2310919 <-- SPRD
 ------------------------------------------------------------------------------
 Final State
  WF centre and spread    1  ( -0.000000,  1.937000,  1.937000 )     1.28449725
  WF centre and spread    2  ( -0.000000,  1.937000,  1.937000 )     1.28449725
  WF centre and spread    3  (  0.000000,  1.937000,  1.937000 )     1.17470279
  WF centre and spread    4  (  1.937000, -0.000000,  1.937000 )     1.17470279
  WF centre and spread    5  (  1.937000,  0.000000,  1.937000 )     1.28449725
  WF centre and spread    6  (  1.937000, -0.000000,  1.937000 )     1.28449725
  WF centre and spread    7  (  1.937000,  1.937000,  0.000000 )     1.28449726
  WF centre and spread    8  (  1.937000,  1.937000,  0.000000 )     1.17470278
  WF centre and spread    9  (  1.937000,  1.937000,  0.000000 )     1.28449726
  Sum of centres and spreads ( 11.622000, 11.622000, 11.622000 )    11.23109189

         Spreads (Ang^2)       Omega I      =     11.082516189
        ================       Omega D      =      0.000000000
                               Omega OD     =      0.148575697
    Final Spread (Ang^2)       Omega Total  =     11.231091885
 ------------------------------------------------------------------------------
 Time for wannierise              0.002 (sec)
```

The output is exactly the same as the WANNIER90 code

9 WF centered on the three O
The spread of the Wannier functions (in Å) is three and six fold degenerated

How to plot the Wannier functions

First of all, SIESTA has to write the periodic part of the Bloch functions in a 3D grid. The number of points in the grid along the three lattice vectors are given by

seedname.fdf file
(input of SIESTA)

```
Wannier.Manifolds.Unk   .true.

Siesta2Wannier90.UnkGrid1        30
Siesta2Wannier90.UnkGrid2        30
Siesta2Wannier90.UnkGrid3        30
```

This produces many files with the name UNKXXXXX.Y where

- XXXXX is the number of the k-point, from 1 to the number of points included in seedname.win file
- Y refers to the spin compoment (1 or 2)

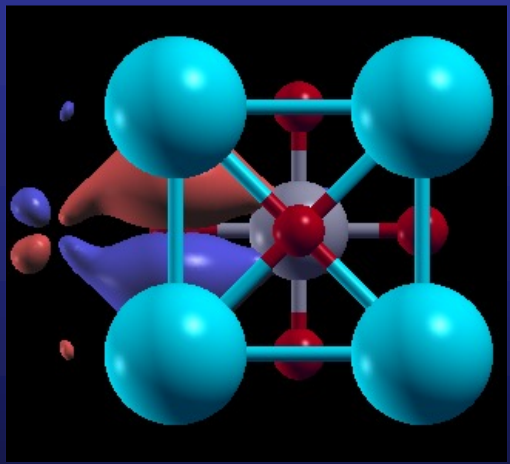
How to plot the Wannier functions

WANNIER90 produces files with the name:
SystemLabel.manifold.X_0000Y.xsf that can be directly plotted with XCRYSDEN

Once XCrySDen starts, click on
File → Open structure (Select your xsf file)
Tools → Data Grid

Click on OK
Then, select:
Degree of triCubic Spline: 3
Click on Render+/- isovalue
Select the desired isovalue (in this example 0.1)
Submit

SrTiO3.manifold.first_00001.xsf



WANNIER90 code directly called from SIESTA

Practical examples:

Bulk $SrTiO_3$ in the cubic phase

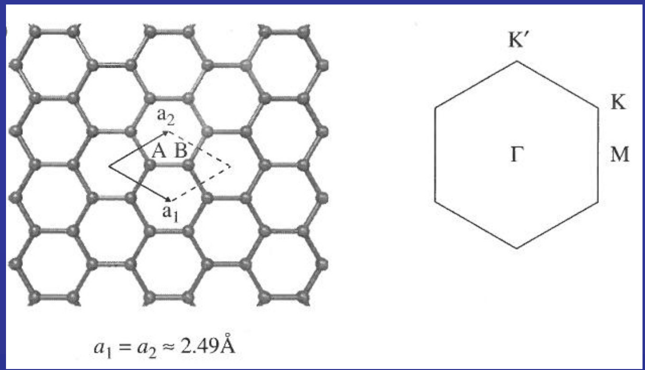
Graphene

Graphene, including bond centered Hydrogen ghost atoms

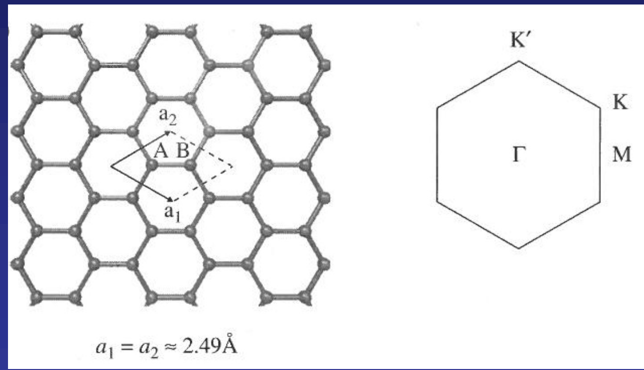
```
SystemName          graphene
#                   Graphene layer
#                   Ghost atoms included at the center of the bonds
#                   MeshCutoff: 600 Ry
#                   20 x 20 x 1 Monkhorst-Pack mesh

SystemLabel         graphene

NumberOfAtoms           5          # Number of atoms in the unit cell
                                   # We include here:
                                   # - The two carbon atoms of the motif
                                   # - Three Hydrogen ghost atoms at the center
                                   #   of the bonds between first-neighbors
                                   # Only the atomic orbitals of the atoms
                                   #   will be included in the simulation,
                                   #   while the atomic nuclei will not be
                                   #   considered
NumberOfSpecies         2          # Number of different atomic species in the
                                   #   simulation.
                                   # We include here:
                                   # - C (with an atomic number of 6)
                                   # - pseudo-Hydrogen atom
                                   #   (with an atomic number of -1)
%block ChemicalSpeciesLabel        # Chemical species label as indicated above
  1   6  C
  2  -1  Ghost-H
%endblock ChemicalSpeciesLabel
```

Graphene: atomic structure in SIESTA

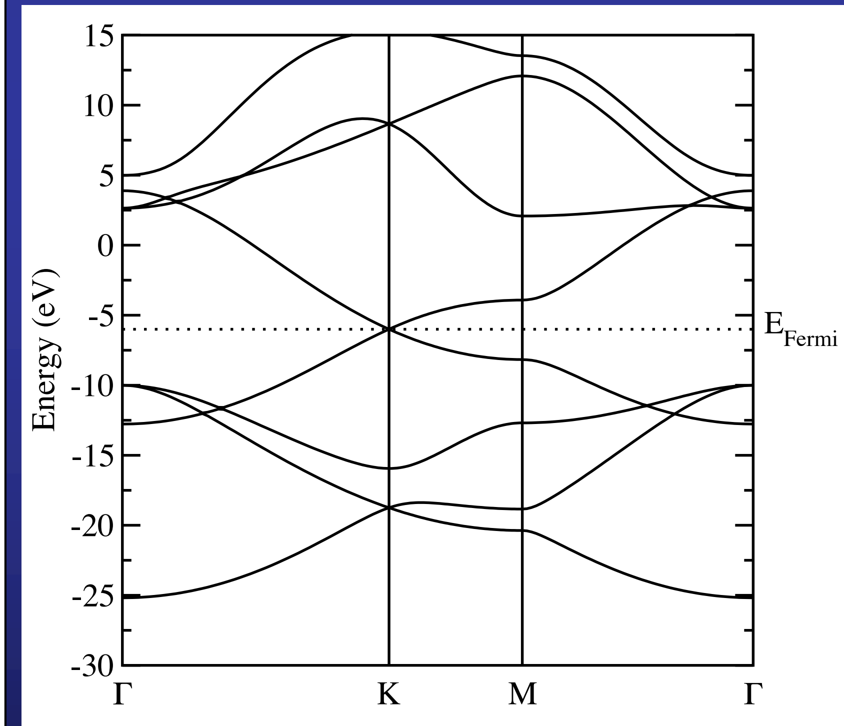
```
#
# Atomic structure: lattice vectors and atomic coordinates
#

LatticeConstant      1.46700 Ang # Nearest-neighbor distance, d
                                 # The primitive translation vectors
                                 #   will be given by
                                 #   a_{1} = (3/2 d, - sqrt(3)/2 d, 0)
                                 #   a_{2} = (3/2 d, + sqrt(3)/2 d, 0)
                                 #   Here the z-component of the vectors
                                 #   is large enough to avoid interactions
                                 #   between periodic replicas of the slab

%block LatticeVectors
   1.500000000      -0.8660254038       0.0000000000
   1.500000000       0.8660254038       0.0000000000
   0.000000000       0.0000000000      20.0000000000
%endblock LatticeVectors

AtomicCoordinatesFormat Fractional
%block AtomicCoordinatesAndAtomicSpecies
   0.3333333333   0.3333333333   0.0000000000  1
   0.6666666667   0.6666666667   0.0000000000  1
   0.5000000000   0.5000000000   0.0000000000  2
   0.5000000000   0.0000000000   0.0000000000  2
   0.0000000000   0.5000000000   0.0000000000  2
%endblock AtomicCoordinatesAndAtomicSpecies

%block kgrid_Monkhorst_Pack
  20    0    0   0.0
   0   20    0   0.0
   0    0    1   0.0
%endblock Kgrid_Monkhorst_Pack
```



Graphene: plotting the band-structure in SIESTA

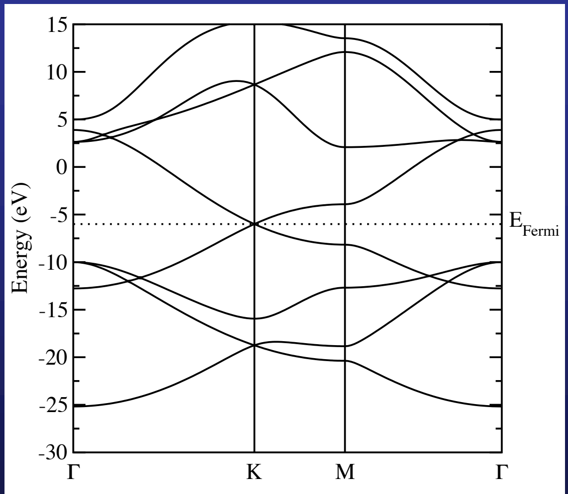



```
#
# Plotting the band structure
#

BandLinesScale      ReciprocalLatticeVectors
%block BandLines
1    0.0        0.0         0.0    \Gamma      # Begin at \Gamma
50   0.33333    0.666667    0.0    K           # 50 points from \Gamma to K
50   0.5        0.5         0.0    M           # 50 points from K to M
50   0.0        0.0         0.0    \Gamma      # 50 points from M to \Gamma
%endblock BandLines

#
# Plotting the Projected Density Of States
#

%block ProjectedDensityOfStates
  -70.00  5.00  0.150 3000  eV
%endblock ProjectedDensityOfStates

%PDOS.kgrid_Monkhorst_Pack
   60  0  0  0.5
    0 60  0  0.5
    0  0  2  0.5
%end PDOS.kgrid_Monkhorst_Pack
```



WANNIER90 code directly available from SIESTA

```
%block WannierManifold.first
  # Indices of the initial and final band of the manifold
  bands 1    8
  # Indices of the orbitals that will be used as localized trial orbitals
  #   (any number of lines allowed)
  trial-orbitals [9 10 11 3 7]
  # Number of iterations for the minimization of \Omega
  spreading.nitt 0
  wannier_plot 3
  fermi_surface_plot true
  write_hr true
  write_tb true
  # Bottom and top of the outer energy window for band disentanglement (in eV)
  window        -30.0    5.0   eV
  # Bottom and top of the inner energy window for band disentanglement (in eV)
  window.frozen -30.0   -7.5   eV
%endblock
```



We have eight bands in the outer energy window

We are interested in project over the wannierization over the three sp^2 orbitals and the π/π^* manifold (five Wannier functions in total)

WANNIER90 code directly available from SIESTA

```
%block WannierManifold.first
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  window.frozen -30.0   -7.5   eV
%endblock
```
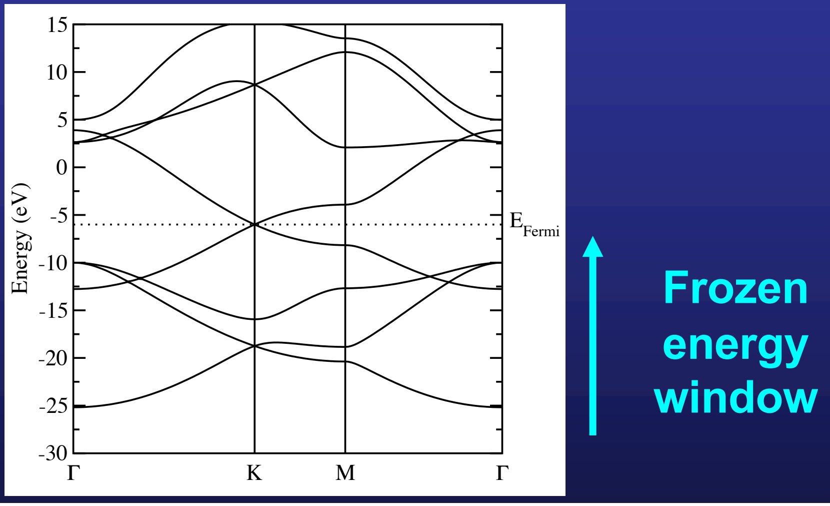



Some Bloch states are forced to be preserved identically in the projected manifold; those are referred to as belonging to a frozen "inner" window

We are interested in project over the wannierization over the three sp^2 orbitals and the π / π^* manifold (five Wannier functions in total)

Output of a succesful run

```
*------------------------------- WANNIERISE ---------------------------------*
 +--------------------------------------------------------------------+<-- CONV
 | Iter  Delta Spread     RMS Gradient      Spread (Ang^2)      Time  |<-- CONV
 +--------------------------------------------------------------------+<-- CONV

 ------------------------------------------------------------------------------
 Initial State
  WF centre and spread    1  (  2.200500,  0.000000,  0.000000 )     0.71294917
  WF centre and spread    2  (  1.100250, -0.635230,  0.000000 )     0.71294809
  WF centre and spread    3  (  1.100250,  0.635230,  0.000000 )     0.71294809
  WF centre and spread    4  (  1.467000, -0.000000,  0.000000 )     0.81286407
  WF centre and spread    5  (  2.933999, -0.000000,  0.000000 )     0.81286543
  Sum of centres and spreads (  8.801998, -0.000000,  0.000000 )     3.76457484

      0     0.376E+01     0.0000000000        3.7645712185       0.04  <-- CONV
        O_D=      0.0016044 O_OD=      0.7962785 O_TOT=      3.7645712 <-- SPRD
 ------------------------------------------------------------------------------
 Final State
  WF centre and spread    1  (  2.200500,  0.000000,  0.000000 )     0.71294917
  WF centre and spread    2  (  1.100250, -0.635230,  0.000000 )     0.71294809
  WF centre and spread    3  (  1.100250,  0.635230,  0.000000 )     0.71294809
  WF centre and spread    4  (  1.467000, -0.000000,  0.000000 )     0.81286407
  WF centre and spread    5  (  2.933999, -0.000000,  0.000000 )     0.81286543
  Sum of centres and spreads (  8.801998, -0.000000,  0.000000 )     3.76457484

         Spreads (Ang^2)       Omega I      =     2.966688302
        ================       Omega D      =     0.001604421
                               Omega OD     =     0.796278495
    Final Spread (Ang^2)       Omega Total  =     3.764571218
 ------------------------------------------------------------------------------
 Time for wannierise              0.004 (sec)
```

Three sp_2 type-Wanniers

The π/π^* manifold

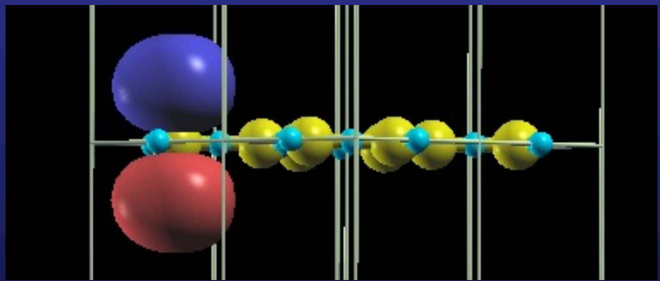
How to plot the Wannier functions

WANNIER90 produces files with the name:
SystemLabel.manifold.X_0000Y.xsf that can be directly plotted with XCRYSDEN

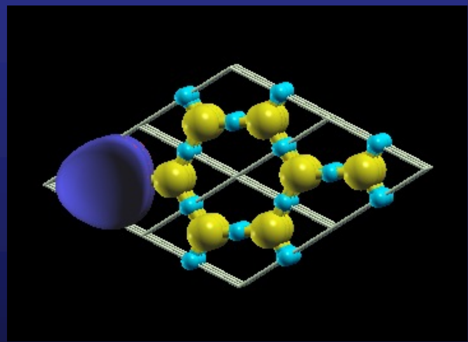
Once XCrySDen starts, click on
File → Open structure (Select your xsf file)
Modify → Number of units drawn 2 (along x) 2 (along y) 1 (along z)
Tools → Data Grid

Click on OK
Then, select:
Degree of triCubic Spline: 3
Click on Render+/- isovalue
Select the desired isovalue (in this example 0.1)
Submit
graphene.manifold.first_00004.xsf

Lateral view



Top view



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FONDO EUROPEO DE
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MINISTERIO DE ECONOMÍA, INDUSTRIA Y COMPETITIVIDAD
AGENCIA ESTATAL DE INVESTIGACIÓN