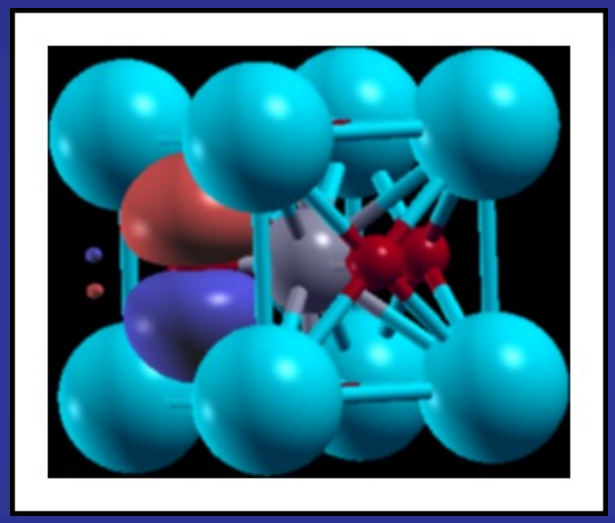
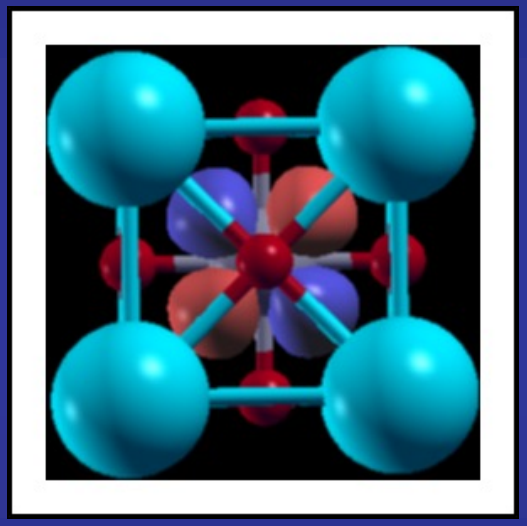
How to run WANNIER90 directly from SIESTA





Javier Junquera

UNIVERSIDAD DE CANTABRIA

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

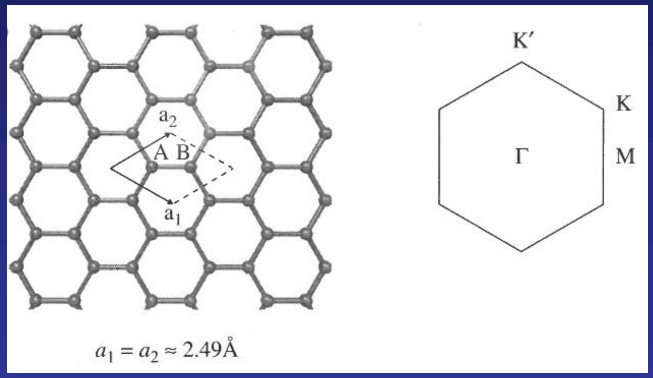
27th February 2019

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

Graphene structure

graphene.fdf

```
SystemName        graphene
#                 Graphene layer
#                 MeshCutoff: 600 Ry
#                 20 x 20 x 1 Monkhorst-Pack mesh

SystemLabel       graphene

LatticeConstant      1.47030 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
   1.500       -0.8660254038        0.000
   1.500        0.8660254038        0.000
   0.000        0.0000000000       20.000
%endblock LatticeVectors

AtomicCoordinatesFormat Fractional
%block AtomicCoordinatesAndAtomicSpecies
   0.3333333333   0.3333333333   0.000  1
   0.6666666667   0.6666666667   0.000  1
%endblock AtomicCoordinatesAndAtomicSpecies
```

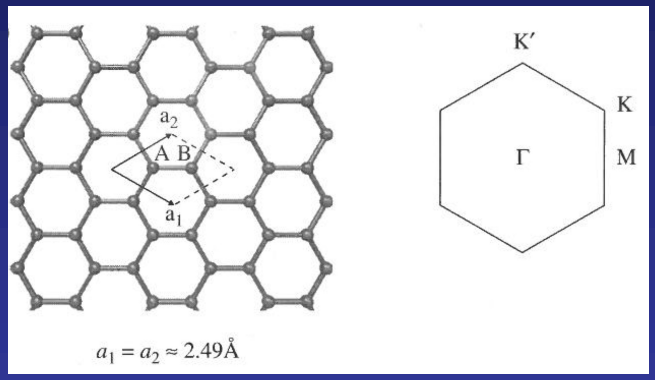


Here, the same lattice vectors,
but in Angstrom,
not in unit of the lattice constant.

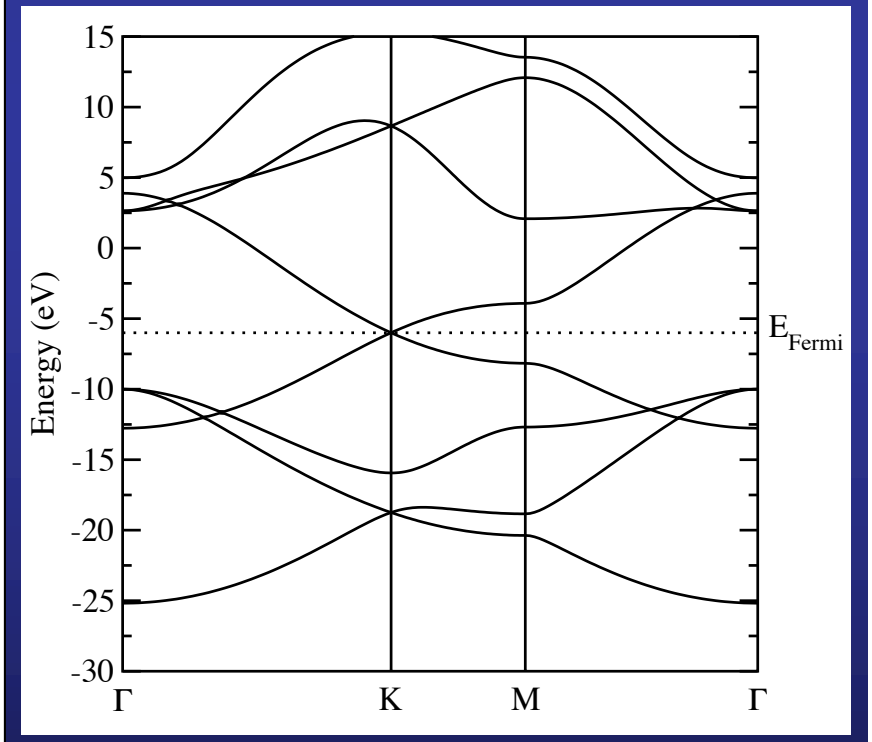
graphene.win

```
begin unit_cell_cart
Ang
2.20545 -1.27331715120714  0.000
2.20545  1.27331715120714  0.000
0.000    0.00000000000000 29.406000
end unit_cell_cart

begin atoms_frac
 C1       0.3333333333   0.3333333333   0.0000000000
 C2       0.6666666667   0.6666666667   0.0000000000
end atoms_frac
```

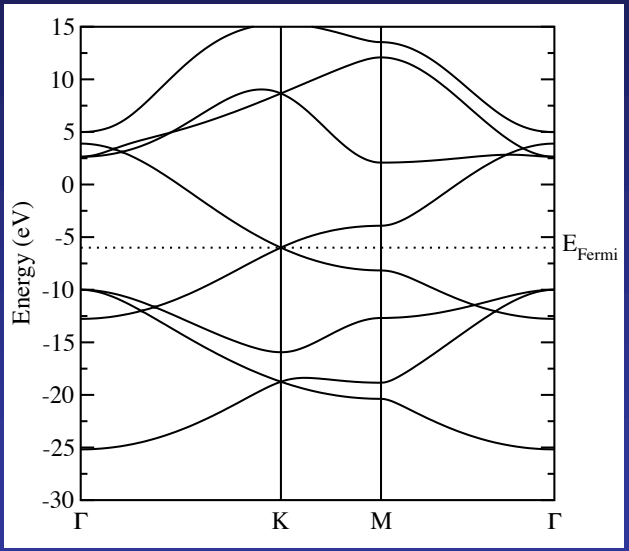
Graphene: plotting the band-structure in SIESTA




```
#
# 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
```



Specification of the number of bands to Wannierize



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)

graphene.fdf

```
# Variables related with the Wannierization of the manifold
Siesta2Wannier90.WriteMmn       .true.
Siesta2Wannier90.WriteAmn       .true.
Siesta2Wannier90.WriteEig       .true.
Siesta2Wannier90.WriteUnk       .true.

Siesta2Wannier90.NumberOfBands   8
```

graphene.win

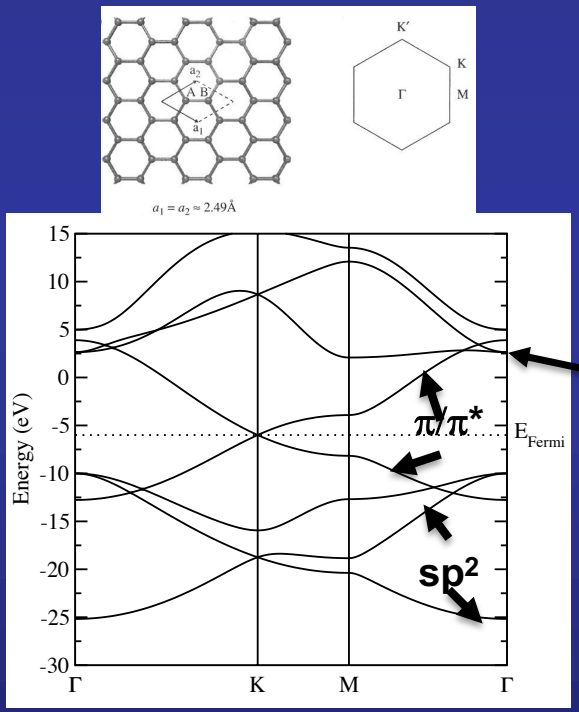
```
num_bands      =  8          ! Number of bands in the first-principles calculation
                             !   used to form the overlap matrices
                             !   seedname.mmn file
                             !   Default: num_bands = num_wann
num_wann       =  5          ! Number of Wannier functions to be found
                             !   There must be as many projectors in the
                             !   projections bloch as num_wann functions here.
                             !   If num_wann < num_bands, then the disentaglement
                             !   procedure is activated
```

Entangled bands

In many applications, the bands of interest are not isolated.

The desired bands lie within a limited energy range, but overlap and hybridize with other bands that extend further out in energy

Graphene



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

At this point, the π bands are crossed by other unwanted bands

Which states to choose to form J WFs, particularly in those regions of $\vec{k}$ space where the bands of interest are hybridized with other unwanted bands?

Entangled bands

The problem of computing well localized WFs starting from entangled bands is broken down into two distint steps

Subspace selection

For a given $\vec{k}$ point, a prescription is needed for constructing J states from a linear combination of the states of the larger manifold

If the J -dimensional Bloch manifold is constructed so it varies smoothly as a function of $\vec{k}$

Gauge selection

Once a suitable J -dimensional manifold has been identified at each $\vec{k}$, apply the same procedure than for isolated manifolds to generate localized WFs spannig that manifold

Then the corresponding WFs are well localized

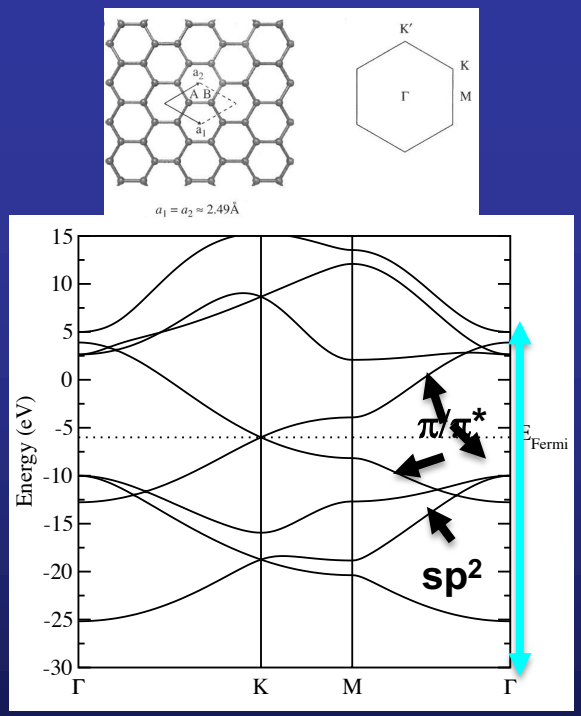
Entangled bands

The problem of computing well localized WFs starting from entangled bands is broken down into two distint steps

Subspace selection

For a given $\vec{k}$ point, a prescription is needed for constructing J states from a linear combination of the states of the larger manifold

Graphene



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

For all the $\vec{k}$ points, we should construct five Bloch-like functions, since we are interested in five Wanniers

We start with a larger set of Bloch bands, $\mathcal{J}_{\vec{k}}$, lying:

- **Within a given energy window (the outer window)**
- **Within a specified range of bands**

$$\mathcal{J}_{\vec{k}} \geq J$$

In our example, the energy window contains 8 bands at some $\vec{k}$ points, while we are interested in five Wanniers

Entangled bands: subspace selection via projection

Starting point:
A set of J localized trial wave functions $g_n(\vec{r})$

Project each of them onto the space spanned by the chosen eigenstates at each $\vec{k}$

$$|\phi_{n\vec{k}}\rangle = \sum_{m=1}^{\mathcal{J}_{\vec{k}}} |\psi_{m\vec{k}}\rangle\langle\psi_{m\vec{k}}|g_n\rangle$$

The same as before, but the overlap matrix $\left(A_{\vec{k}}\right)_{mn} = \langle\psi_{m\vec{k}}|g_n\rangle$ is rectangular

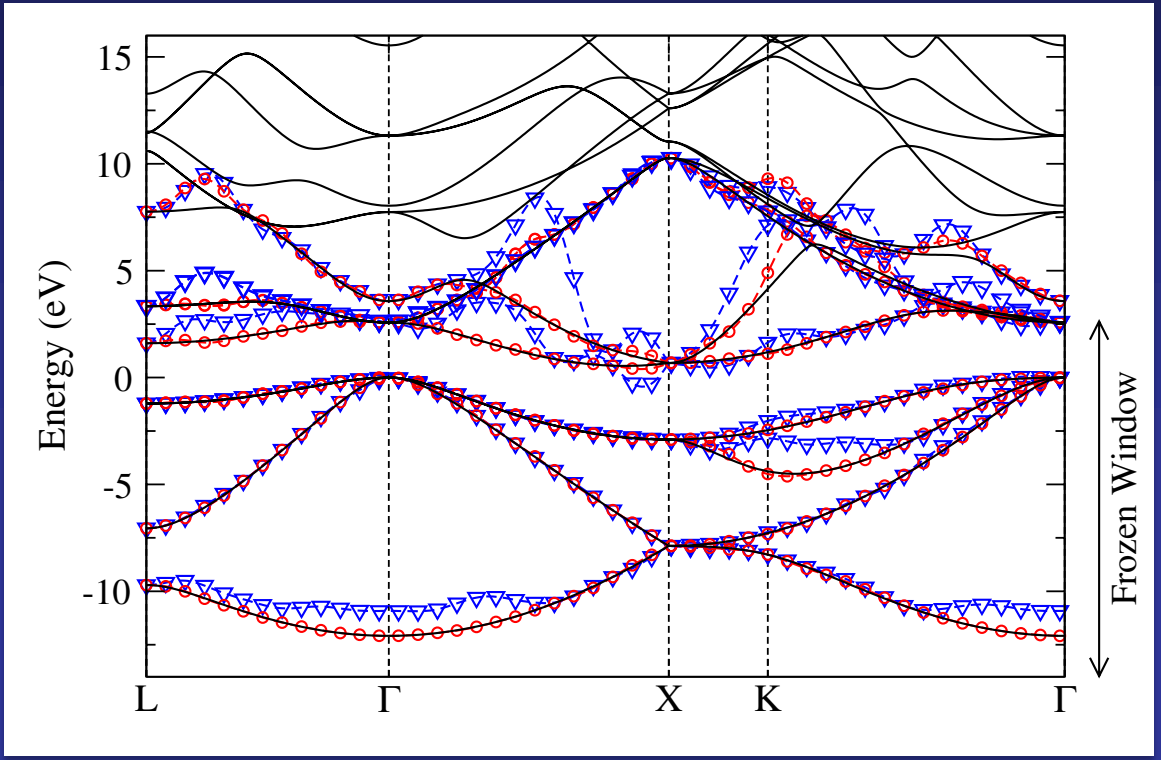
We then orthonomarlize the resulting J orbitals to produce
a set of J smoothly varying Bloch-like functions

$$|\tilde{\psi}_{n\vec{k}}\rangle = \sum_{m=1}^{J} |\phi_{m\vec{k}}\rangle \left(S_{\vec{k}}^{-1/2}\right)_{mn}$$

$$\left(S_{\vec{k}}\right)_{mn} = \langle\phi_{m\vec{k}}|\phi_{n\vec{k}}\rangle_V = \left(A_{\vec{k}}^{\dagger}A_{\vec{k}}\right)_{mn}$$

Same procedure as with the disentangled bands, but with rectangular $A_{\vec{k}}$ matrix

Example: band structure of Si

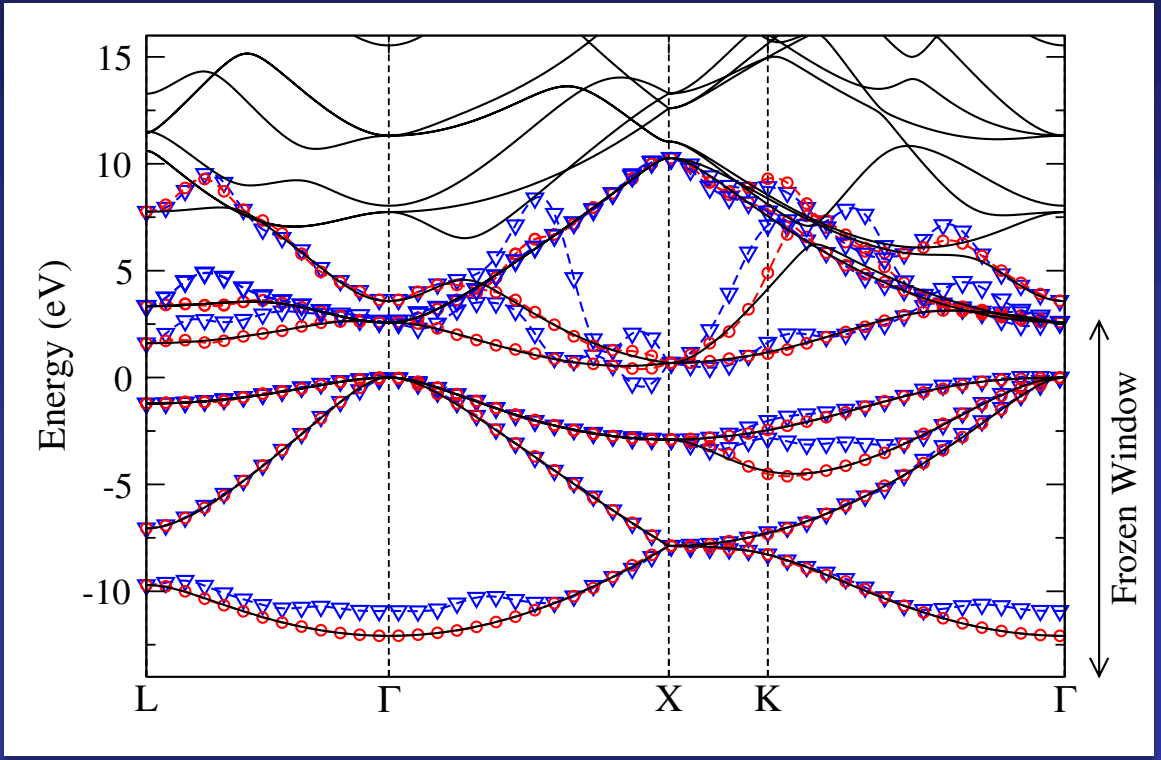


N. Marzari *et al.*
Rev. Mod. Phys.
84, 1419 (2012)

- We are interested in eigth Wanniers
- We choose as localized trial wave functions eigth atomic like sp^3 hybrids
- The outer energy window coincide with the entire energy axis shown (i.e. We take many more Bloch functions than Wanniers
- The disentangle bands shown as blue triangles

The overall agreement, in general, is good
Significant deviations found wherever higher unoccupied bands and unwanted states possessing some significant sp^3 character are admixed with the projected manifold

Example: band structure of Si



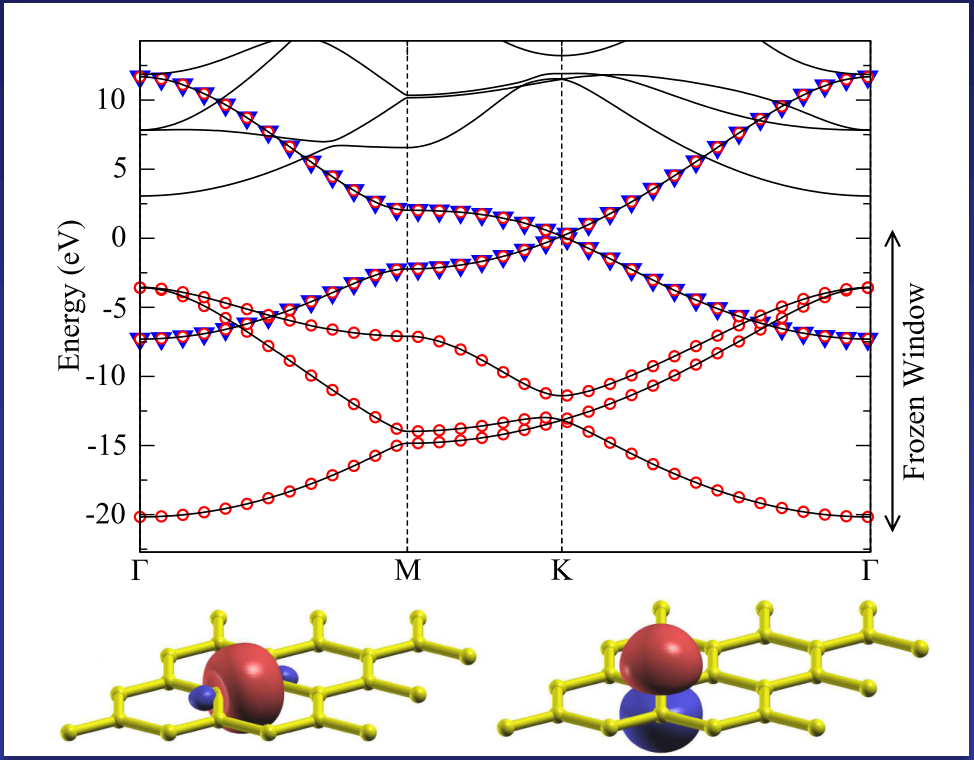
N. Marzari *et al.*
Rev. Mod. Phys.
84, 1419 (2012)

This behavior can be avoided by forcing certain Bloch states to be preserved identically in the projected manifold;
We refer to those as belonging to a frozen "inner" window
The placement and range of this window will depend on the problem at hand.

I. Souza *et al.* Phys. Rev. B 65, 035109 (2001)

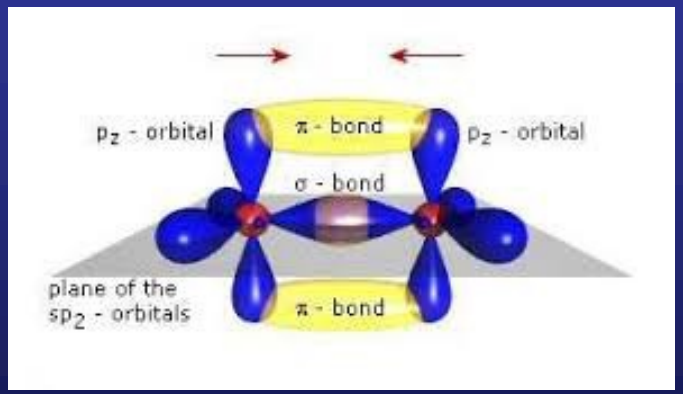
Circles: the results obtained by forcing the entire valence manifold to be preserved, leading to a set of eight projected bands that reproduce exactly the four valence bands, and follow quite closely the four low-lying conduction bands

Example: band structure graphene



N. Marzari *et al.*
Rev. Mod. Phys.
84, 1419 (2012)

Projection on p_z orbitals of C and on three sp^2-like orbitals

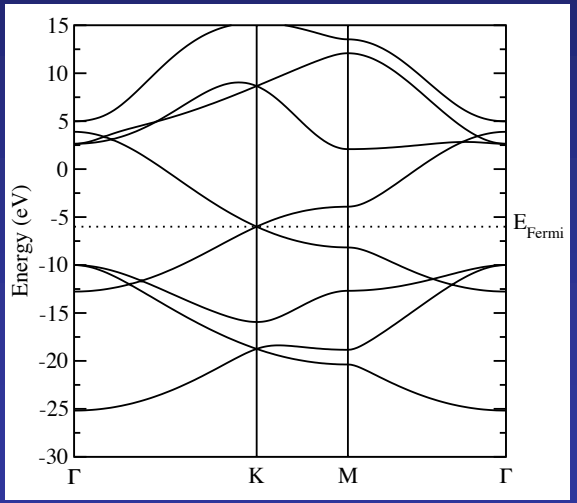


Why sp^2-like orbitals?

Because the valence bands can be considered as bonding combinations of sp^2 hybrids

There will be a maximum of charge shared in a symmetric way at the center of the bond

The disentanglement procedure



Frozen energy window

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)

```
dis_win_min      -30.0    ! Bottom of the outer energy window
dis_win_max        5.0    ! Top of the outer energy window
dis_froz_min     -30.0    ! Bottom of the inner (frozen) energy window
dis_froz_max      -7.5    ! Top of the inner (frozen) energy window
```

The projection functions

We are interested in obtaining 5 Wannier functions
so
We need five inital projections

Wannier90 allows to introduce:

- Three hydrogenoid functions with sp^2 symmetry of one of the C
- The two p_z functions, centered on each C

graphene.win

```
begin projections      ! The projections block defines a set of
C1:sp2;pz              !  localised functions used to generate an
C2:pz                  !  initial guess for the unitary transformations.
end projections
```

How to run the wannierization

Run WANNIER90 in preprocessing mode to generate the .nnkp file

$wannier90.x –pp graphene.win

Run SIESTA to generate the .mmn, the .amn and the .eigW files

$siesta < graphene.fdf |tee graphene.out

Change the extension of the .eigW file

$mv graphene.eigW graphene.eig

Run again WANNIER90 to perform the wannierization

$wannier90.x graphene.win

Output of a succesful run of WANNIER90

```
Final State
 WF centre and spread    1  (  1.102724,  0.636660, -0.000000 )     0.72756529
 WF centre and spread    2  (  1.102724, -0.636660,  0.000000 )     0.72756529
 WF centre and spread    3  (  2.205452,  0.000000, -0.000000 )     0.72754515
 WF centre and spread    4  (  1.470301,  0.000001,  0.000000 )     0.82576316
 WF centre and spread    5  (  2.940600, -0.000001, -0.000000 )     0.82564525
 Sum of centres and spreads (  8.821801, -0.000001, -0.000000 )     3.83408414
```

Three sp_2 type-Wannier

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:

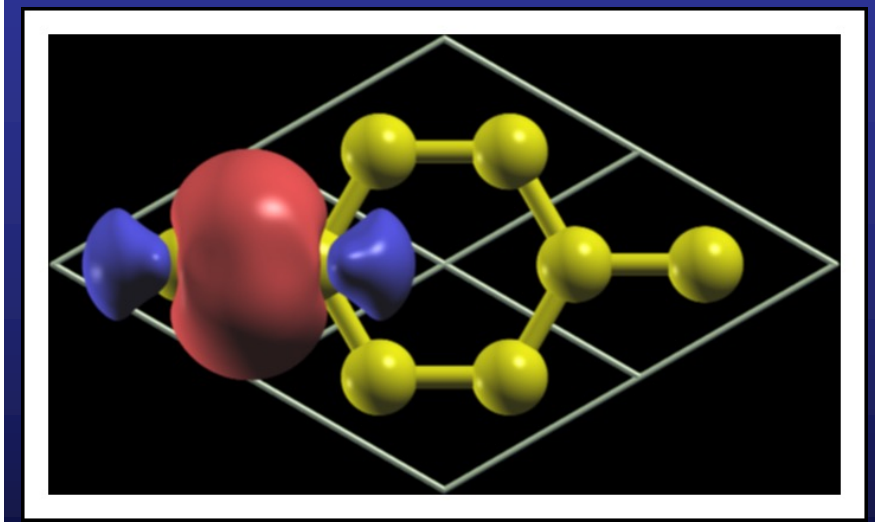
Degree of triCubic Spline: 3

Click on Render+/- isovalue

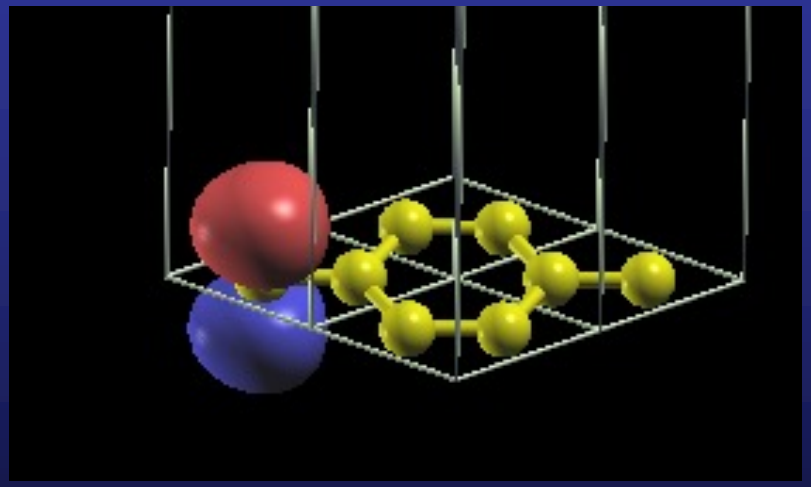
Select the desired isovalue (in this example 0.1)

Submit

graphene.manifold.1_00003.xsf



graphene.manifold.1_00004.xsf



Funding

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