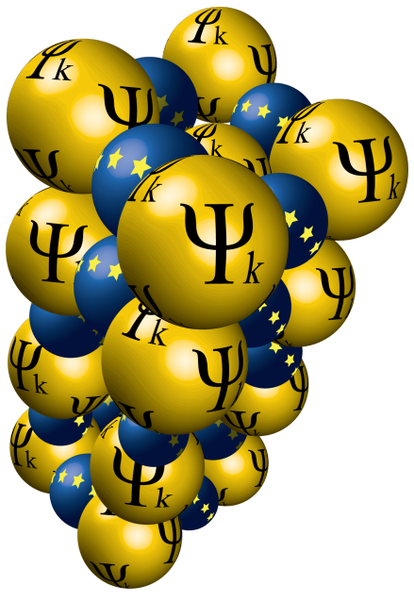
ICTP/Psi-k/CECAM School on

Electron-Phonon Physics from First Principles

Trieste, 19-23 March 2018



Centre Européen de Calcul Atomique et Moléculaire

Lecture Tue.2

Maximally-localized Wannier functions

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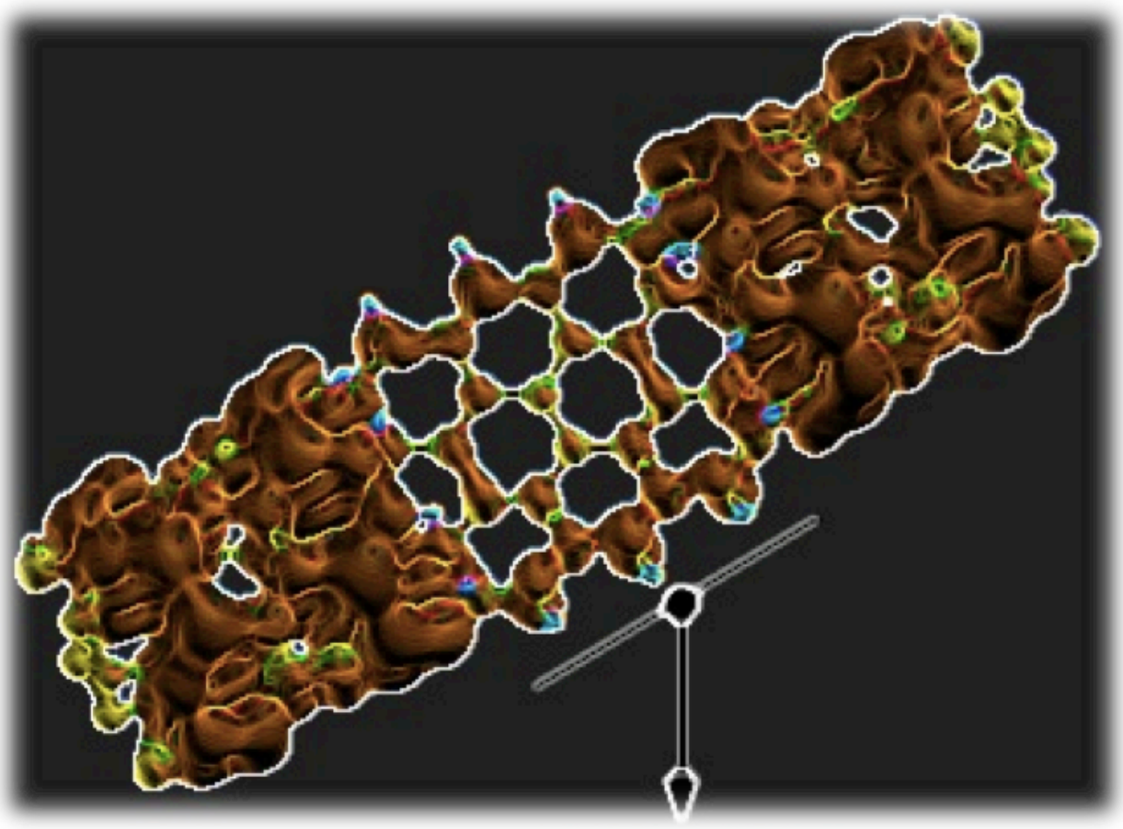
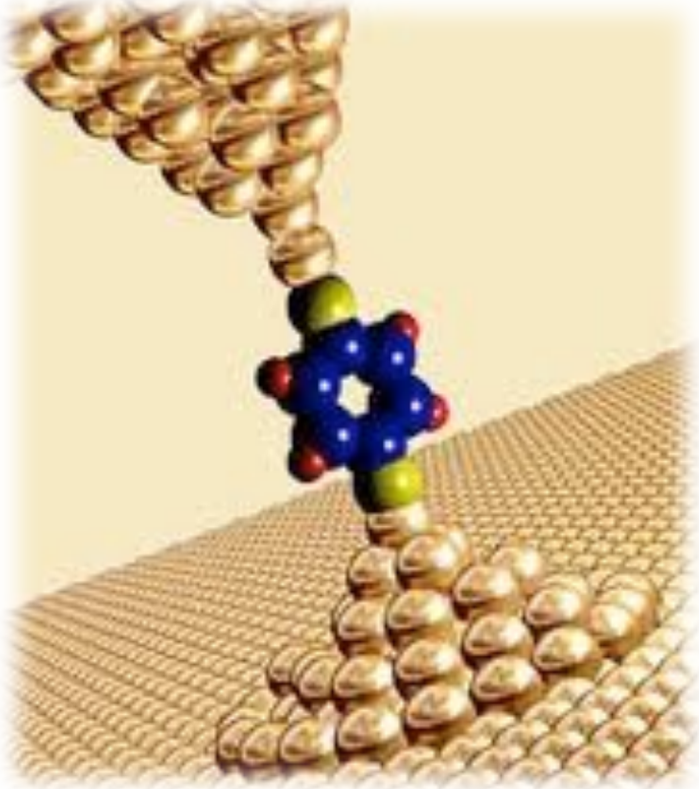
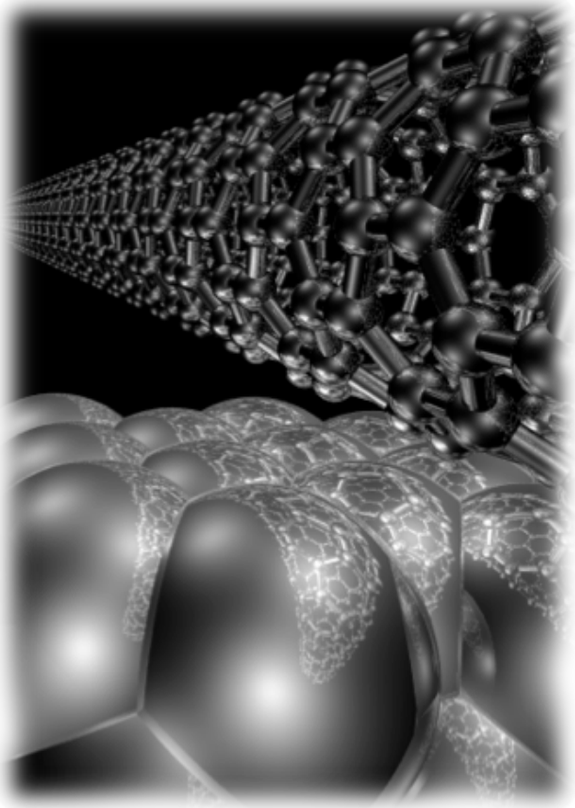
School on Electron-Phonon Physics from First Principles

Trieste, March 20th, 2018







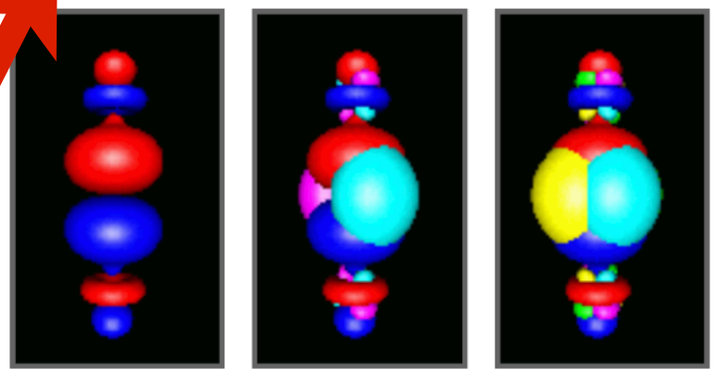
PART II

The Wannier90 code

www.wannier.org

WANNIER90

Home History Download User Guide Forum Papers Events Features People



Welcome!

This is the home of maximally-localised Wannier functions (MLWFs) and Wannier90, the computer program that calculates them. Wannier90 is released under the GNU General Public License.

Latest News

JANUARY 2017

Wannier90 (v2.1.0), released 13January-2017: [gzipped-tar]

SEPTEMBER 2016

A wannier90 coding week was held in San Sebastian during September 2016. 20 people attended to code in new features. A new release of Wannier90 will be available shortly. See the events page for more details.

See here for our news archive.

Please cite

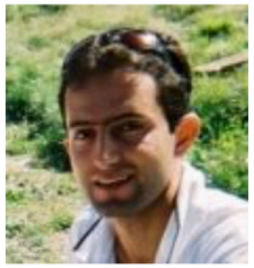
An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions
AA Mostofi, JR Yates, G Pizzi, YS Lee, I Souza, D Vanderbilt, N Marzari
Comput. Phys. Commun. **185**, 2309 (2014)|ONLINE JOURNAL]

in all publications resulting from your use of Wannier90.

UNIVERSITY OF OXFORD · Imperial College London · Universidad del País Vasco · Euskal Herriko Unibertsitatea · RUTGERS THE STATE UNIVERSITY OF NEW JERSEY · ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

People involved

WANNIER90 AUTHORS



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WANNIER90 CONTRIBUTORS

- Matthew Shelley, PhD Student at Imperial College London
- Nicolas Poilvert, PhD Student at the Massachusetts Institute of Technology
- Daniel Aberg (LLNL, USA) for the POV-Ray routines
- Lampros Andrinopoulos, Nicholas D. M. Hine and Arash A. Mostofi (Imperial College) for the w90vdw code
- David Strubbe (MIT, USA): various bugfixes/improvements
- Gabriele Sclauzero (ETH Zurich) for the k-sphere disentanglement routines
- Rei Sakuma (Lund University, Sweden): Symmetry-adapted Wannier functions
- Yusuke Nomura (U. Tokyo, JP): Symmetry-adapted Wannier functions
- Takashi Koretsune (Riken, JP): Symmetry-adapted Wannier functions, non-collinear spin with ultrasoft in pw2wannier90
- Lorenzo Paulatto (UPMC Paris, FR): Improvements to the interpolation routines, non-collinear spin with ultrasoft in pw2wannier90
- Florian Thole (ETHZ, CH): non-collinear spin with ultrasoft in pw2wannier90
- Pablo Garcia Fernandez (Unican, ES): Matrix elements of the position operator
- Dominik Gresch (ETHZ, CH): FORD infrastructure for code documentation
- Samuel Ponce (Oxford University, UK): Test suite for Wannier90
- Marco Gibertini (EPFL, CH): Improvements to the interpolation routines
- Christian Stieger (ETHZ, CH): Routine to print the U matrices
- Stepan Tsirkin (Universidad del Pais Vasco, Spain): bug fixes in the berry module

...

You can be a contributor as well!!

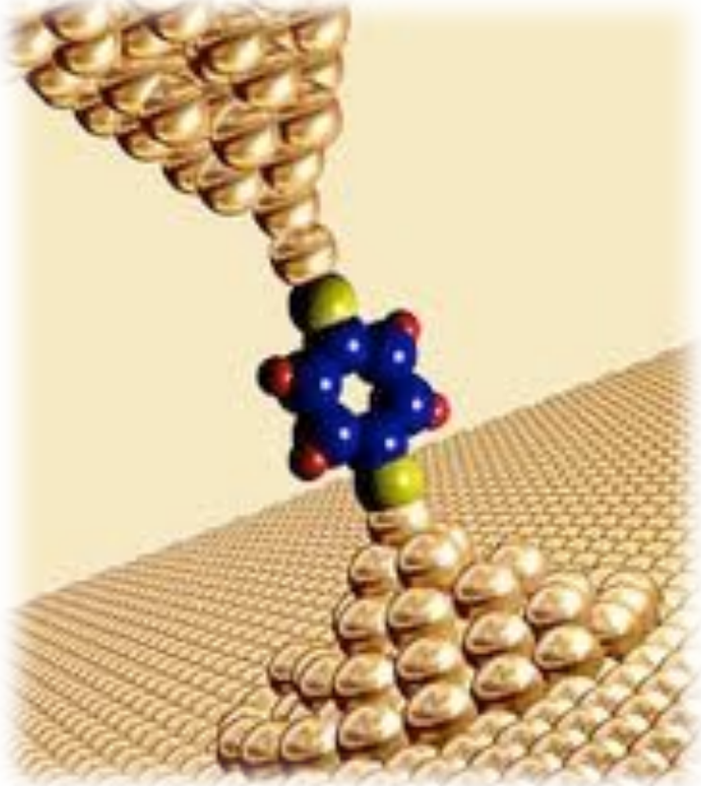
Avanced code features

Wannierization

- disentanglement in spheres
  (relevant k-points not easy to distinguish by energy window,
  but are close in space)
- Symmetry-adapted WFs (to enforce a given local symmetry)
- Support for spin-orbit coupling

Post-processing

- *Generic band interpolation* (and also analytical band derivatives)
- *Boltzmann transport* (electrical conductivity, Seebeck coefficient, ...)
- *Transport calculations* (quantum conductance)
- *Berry curvature, anomalous Hall conductivity and optical conductivity*
- *Orbital magnetisation*



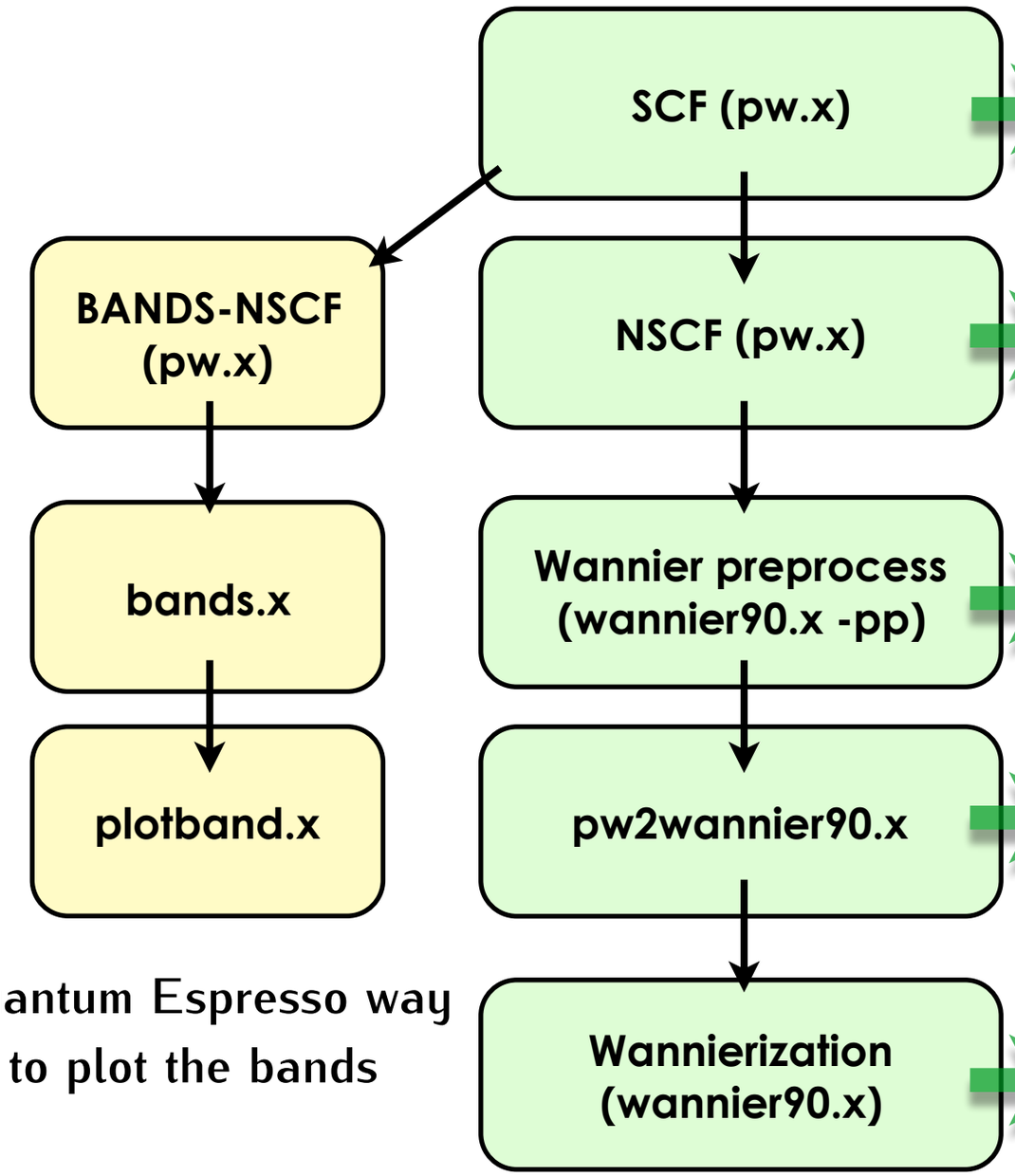
Wannier90 "input data"

- Needs the overlap matrices $M_{mn}^{(k,k+b)}$ between neighboring *k* points, and the $A_{mn}(k)$ projection matrices
- Other possible inputs:
  - the **list of eigenvalues** at each *k*-point (for interpolation)
  - the $\mathbf{u_{nk}}(\boldsymbol{r})$ in real space (for plotting the WFs)
- This input can be obtained from various programs; there exists interfaces for a set of ab-initio codes
  - We will use **Quantum Espresso**
  - **Reminder**: *pw.x* documentation in

    http://www.quantum-espresso.org/wp-content/uploads/Doc/INPUT_PW.html

    (you can find the link in the PDF with the exercises)

How to run a Wannier90 calculation



Calculates the ground state density using a given K_POINTS mesh

Calculates the wavefunctions u_{nk} on a **complete** k-mesh (not necessarily the same of above!)

Reads the Wannier90 input file and prepares a file (.nnkp) with the information for the interface program

Interface program (btw QE and W90): reads the wavefunctions of the NSCF step, the .nnkp file and produces the .mmn, .amn, .eig, ... files for Wannier90

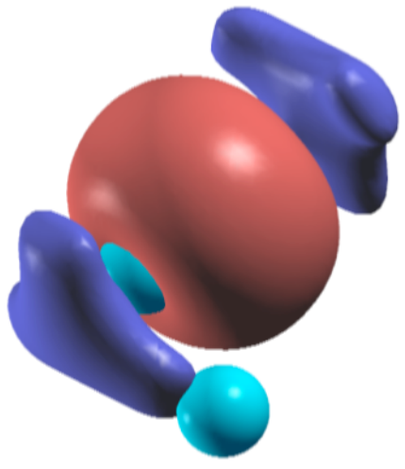
Reads the files produced by the previous step, minimizes the spread, calculates WF, calculates transport properties, ...

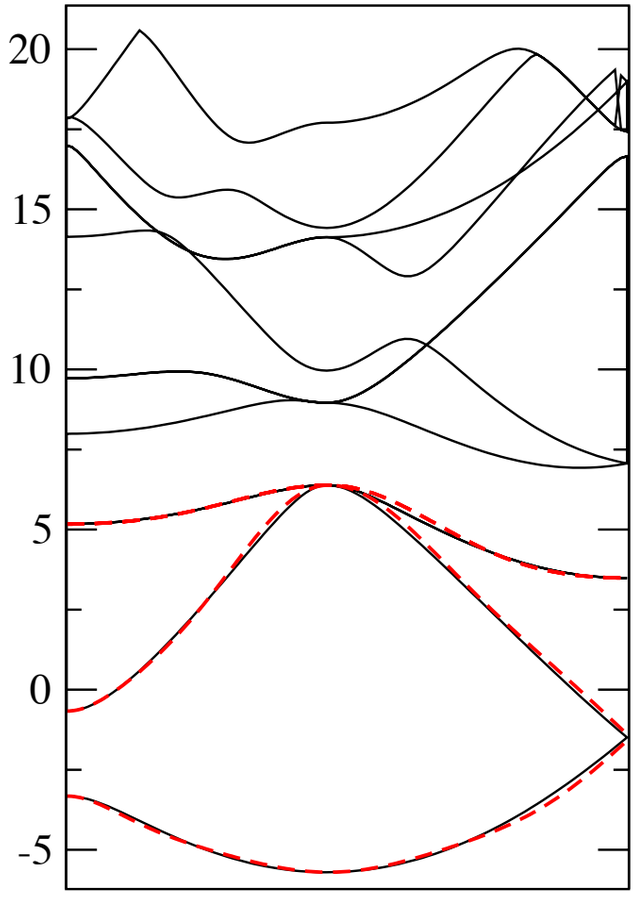
Quantum Espresso way to plot the bands

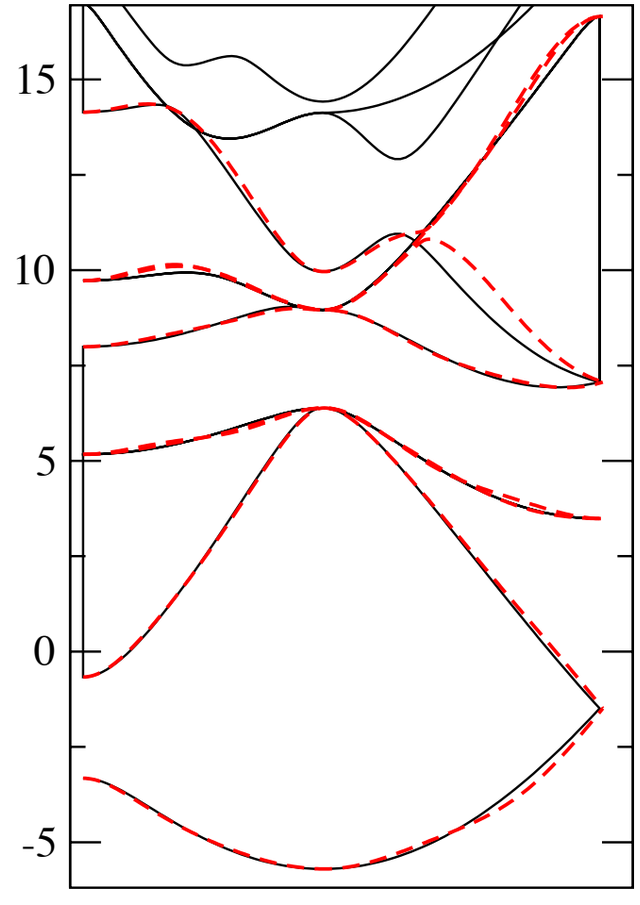
Note: DON'T MIX the yellow and green path! Otherwise the content of the 'output' folder of Quantum Espresso is overwritten and you will get some error.
First follow one path (e.g. the yellow one), and when you get to the bottom box, start again from NSCF

Exercises 1 and 2: Silicon

- Calculate Wannier functions for Silicon (VB only, and VB+CB)
- Check the results
- Plot the real-space WFs (using **XCrysDen**)
- Plot the ab-initio and the interpolated band structure (using **xmgrace** or **gnuplot**)







How to run and input file

- The Wannier90 input file must have a .win extension (e.g.: **ex1.win**)
- To run the code, pass the *basename* (i.e., the name without the .win extension) as a command line parameter to wannier90.x:

  wannier90.x -pp ex1 **(for the pre-process step)**

  wannier90.x ex1 **(for the Wannierization step)**
- Input file format: very simple, there are *no* namelists but only:
  - Variables (order is not important; not case sensitive)

    num_wann = 4
    mp_grid : 6 6 6
  - Blocks

    begin atoms_frac
    Si -0.25 0.75 -0.25
    Si 0.00 0.00 0.00
    end atoms_frac
- Default units for lengths are **angstrom** (bohr are also accepted), for energies are **eV**

Example of input file (ex1)

```
num_bands        =  XXX
num_wann         =  XXX
num_iter         =  100

! restart              =  plot
wannier_plot           =  true
wannier_plot_supercell =  3

bands_plot     =  true
begin kpoint_path
L 0.5  0.5 0.5 G 0.0  0.0 0.0
G 0.0  0.0 0.0 X 0.5  0.0 0.5
end kpoint_path

begin projections
f=-0.125,-0.125, 0.375:s
f= 0.375,-0.125,-0.125:s
f=-0.125, 0.375,-0.125:s
f=-0.125,-0.125,-0.125:s
end projections
```

```
mp_grid  =  XXX XXX XXX
begin kpoints
XXX
XXX
XXX
end kpoints

begin atoms_frac
Si -0.25  0.75  -0.25
Si  0.00  0.00   0.00
end atoms_frac

begin unit_cell_cart
bohr
-5.10    0.00    5.10
 0.00    5.10    5.10
-5.10    5.10    0.00
end unit_cell_cart
```

Practical information

- You can find the PDF with the instructions online, or inside **/home/nfs3/smr3191/tutorials/wannier90/wannier-tutorial.pdf**

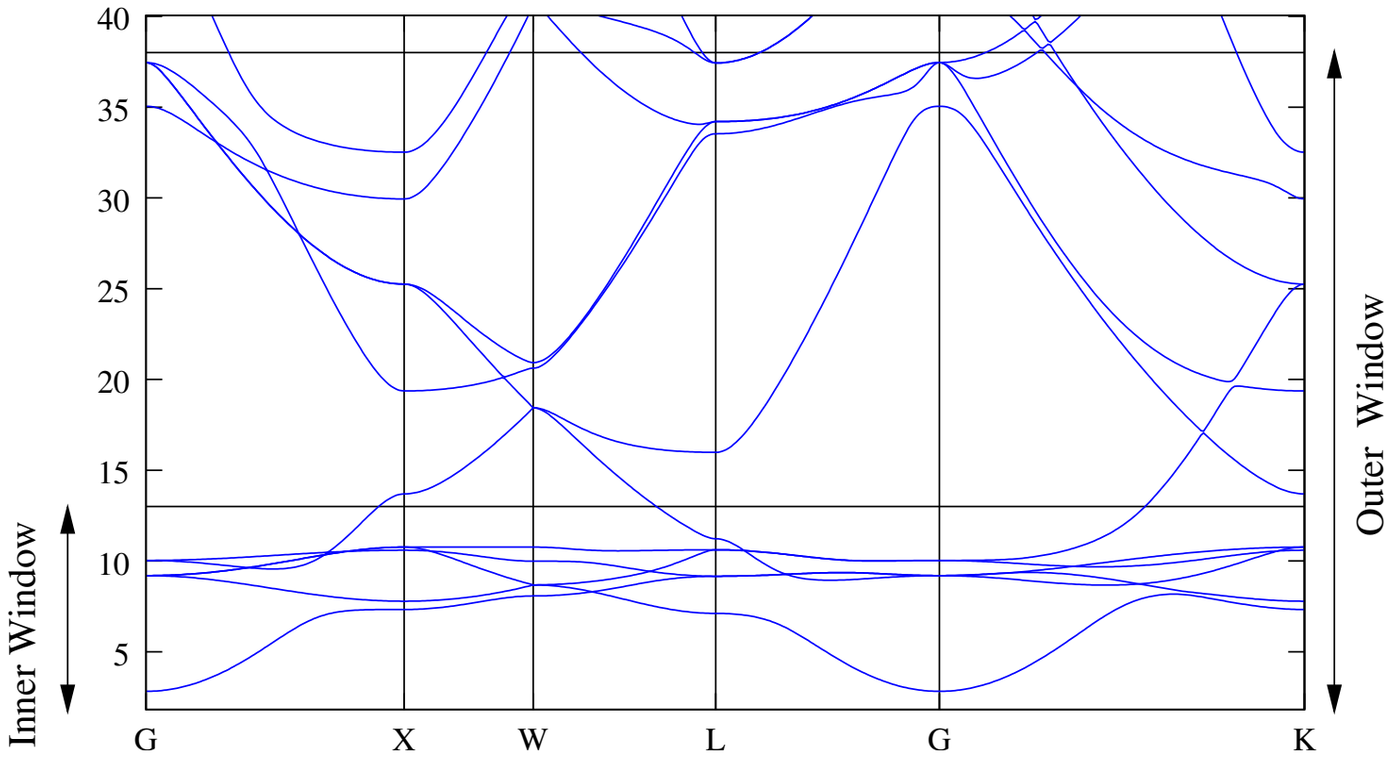
- Before starting the tutorials, copy the whole folder above on the local scratch of your computer:

```
cp -r /home/nfs3/smr3191/tutorials/wannier90/w90-tutorial-files/ /scratch/w90-tutorial-files/
```

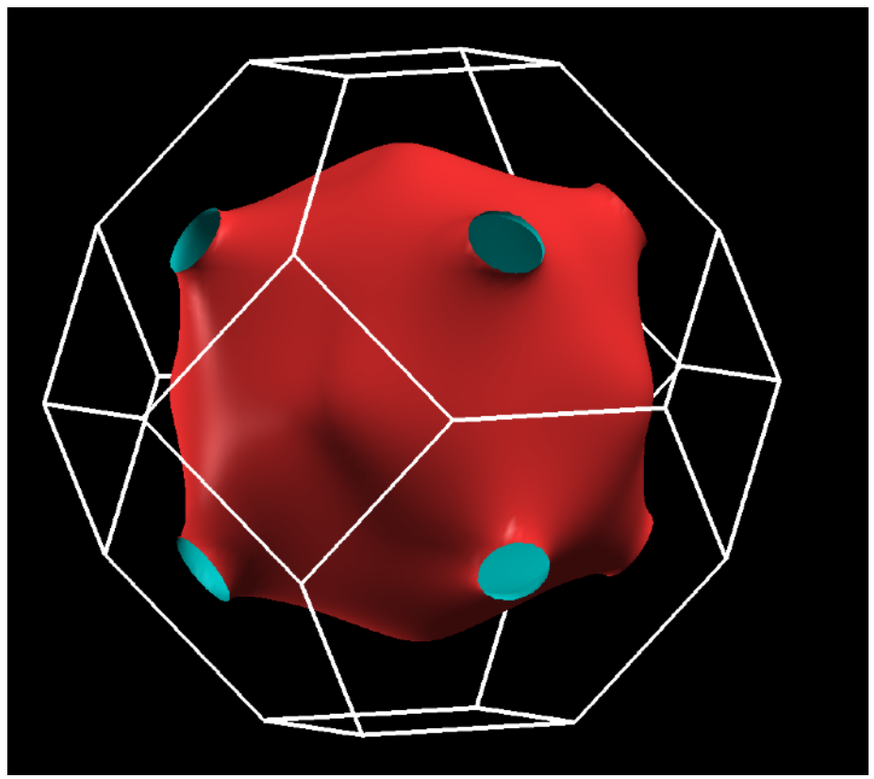
- To get help (from tomorrow on...): www.wannier.org
  - User guide, tutorials
  - Read the source code!
  - Wannier90 mailing list

Exercise 3: band structure and Fermi surface of copper

- Interpolate the band structure of copper



- Show the Fermi surface of copper



Optional exercise 4: band interpolation using GW

- Interpolate the band structure of silicon including G_0W_0 corrections

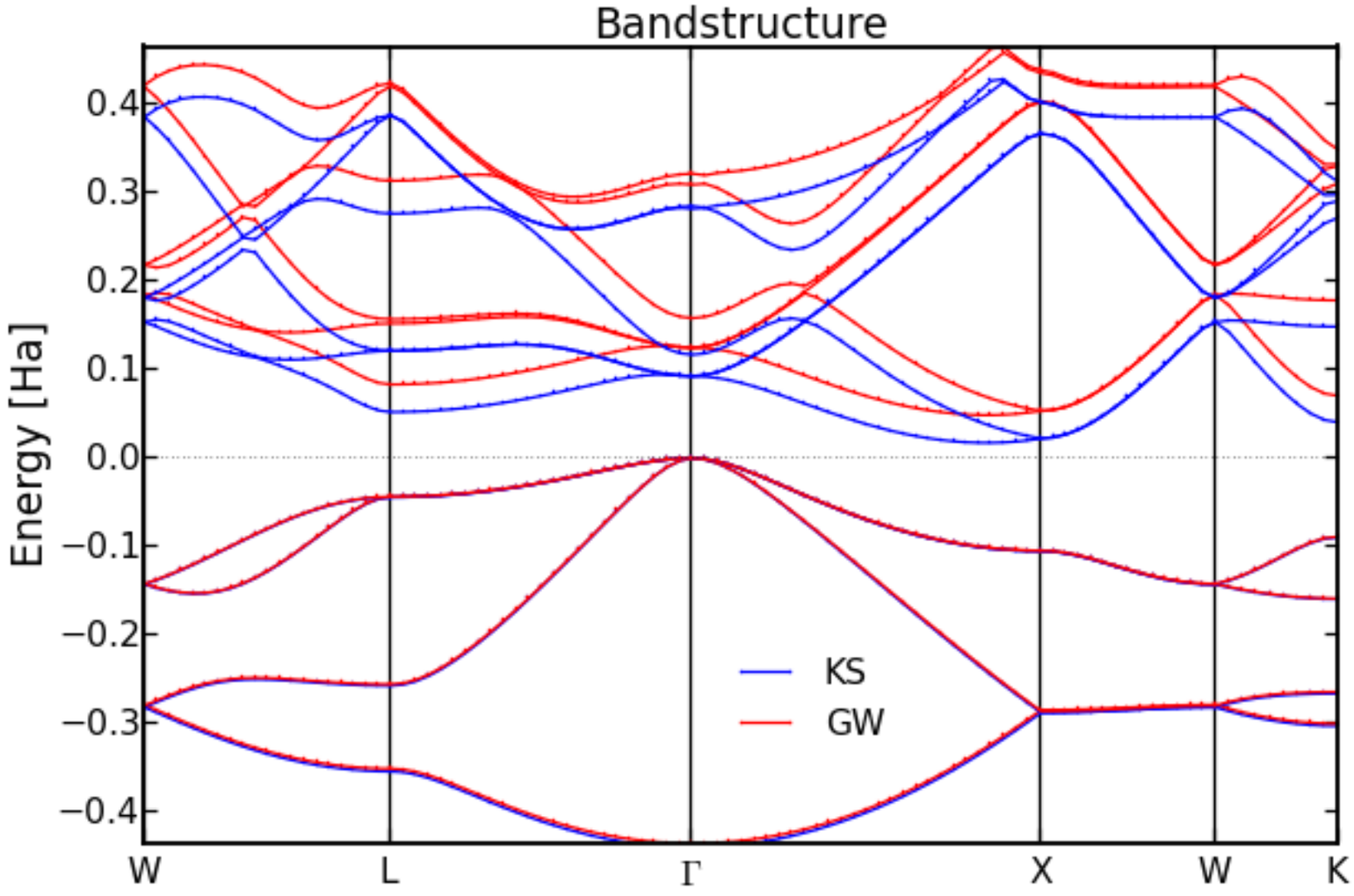
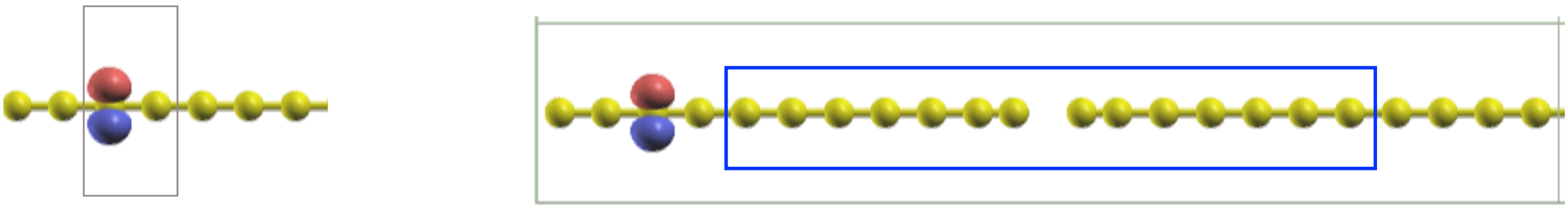


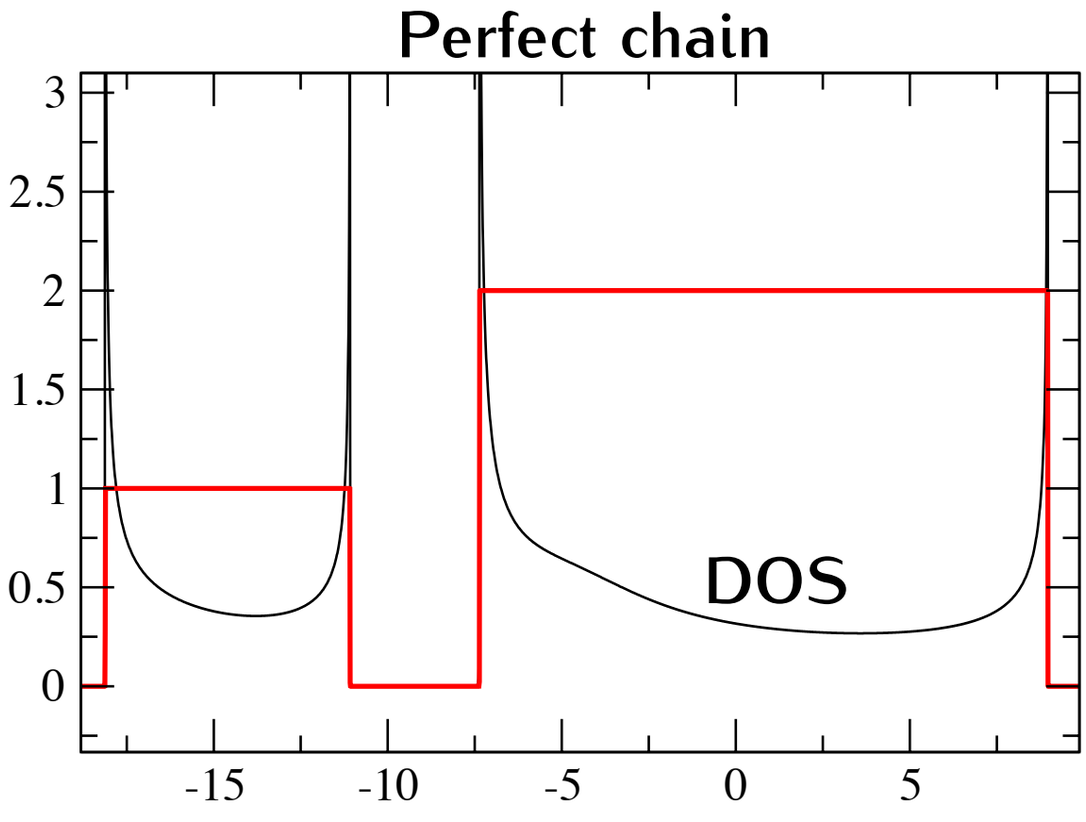
Image from exciting-code.org

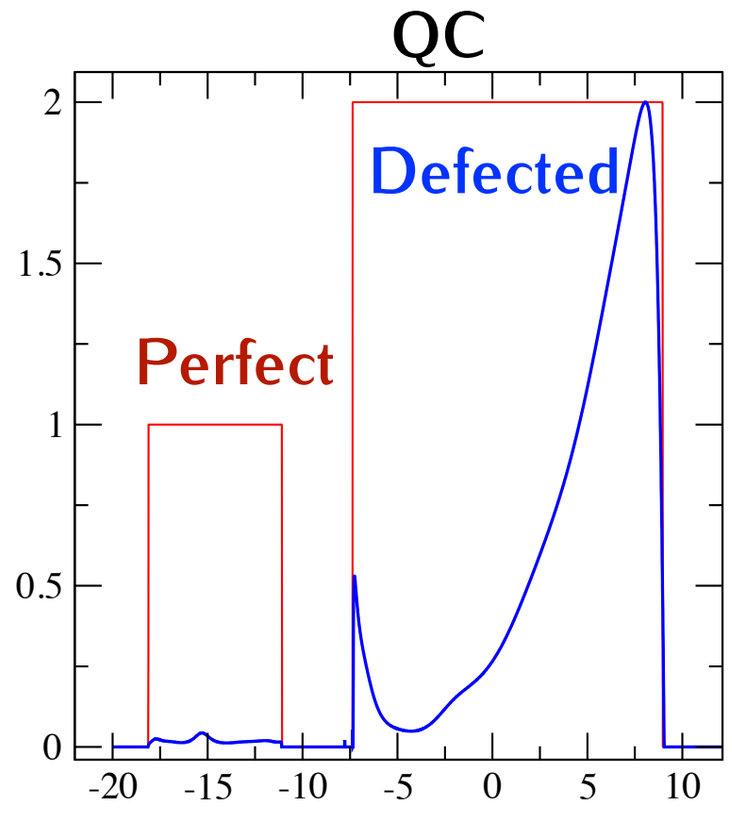
Optional exercises 5 and 6: C chain

- Calculate the band structure, DOS and the Quantum Conductance (QC) of a periodic C chain



- Calculate the DOS and QC of a defected C chain





PART III

Wannier90 hands-on

A. Marrazzo and V. Vitale