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2522-1

Hands-on Tutorial on Electronic Structure Computations

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Transport with Wannier functions

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Transport with Wannier functions

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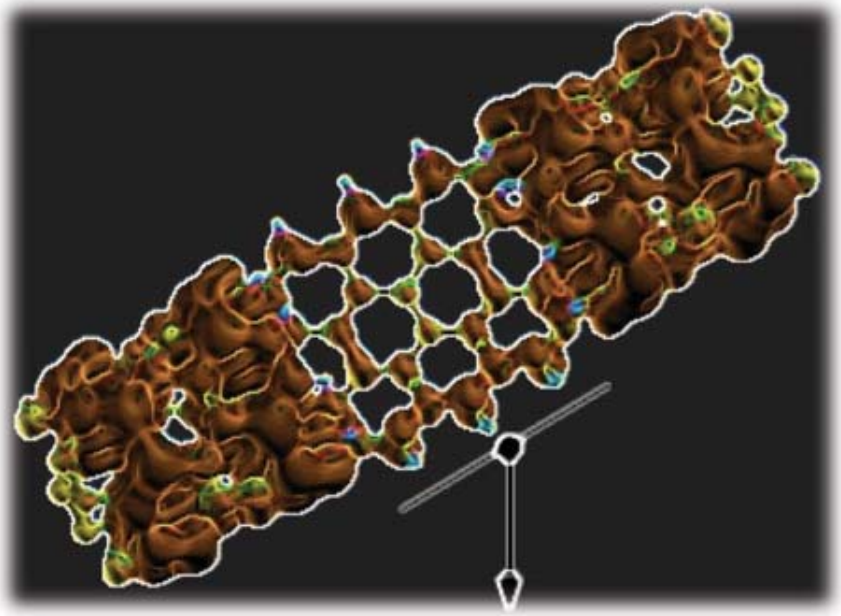
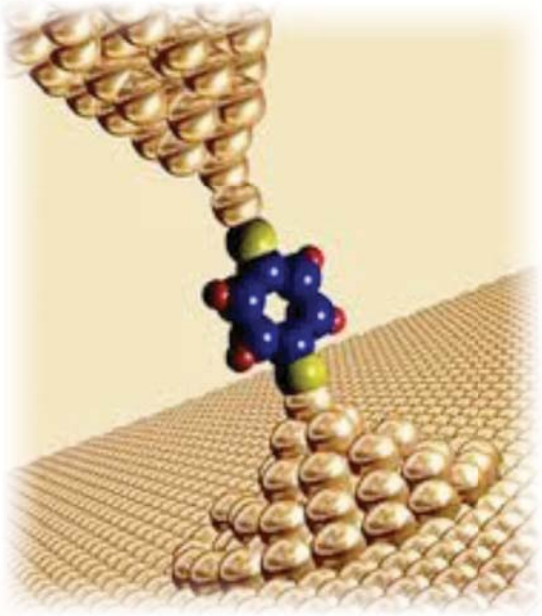
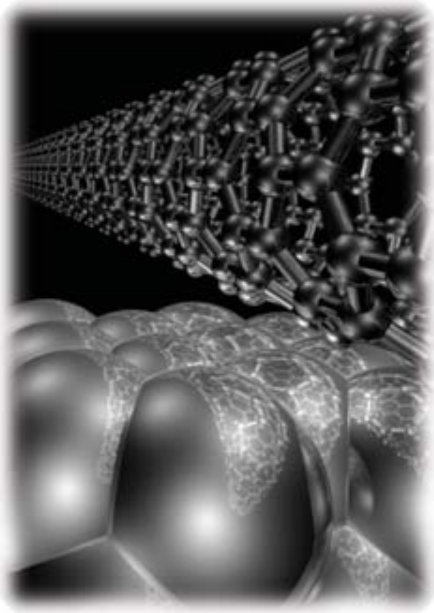
THEOS
THEORY AND SIMULATION OF MATERIALS

Hands-on Tutorial on Electronic Structure Computations

Trieste, Jan 15th, 2013







References

- Marzari, N., and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997)
- Souza, I., N. Marzari, and D. Vanderbilt, Phys. Rev. B 65, 035109 (2001)
- N. Marzari et al., Rev. Mod. Phys. 84, 1419–1475 (2012)
- R. M. Martin, Electronic Structure: Basic Theory and Practical Methods, Cambridge, 2004
- www.wannier.org
- S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge University Press, 1997

- **First part of the slides: courtesy of Prof. Nicola Marzari.**
  Can be found on the Wannier90 website: www.wannier.org under
  User Guide > NSF Summer School 2009 > N. Marzari Lecture Slides

PART III

Hands-on

www.wannier.org

WANNIER90

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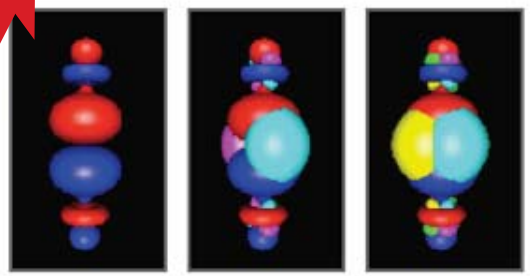
Welcome!

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

15 JAN 2010

Wannier90 (v1.2) is now available for download here.

See here for our news archive.

Please cite

Wannier90: A Tool for Obtaining Maximally-Localised Wannier Functions
A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt and N. Marzari
Comput. Phys. Commun. **178**, 685 (2008) [ONLINE JOURNAL]

in all publications resulting from your use of Wannier90.

New release (v2.0)
to appear soon!

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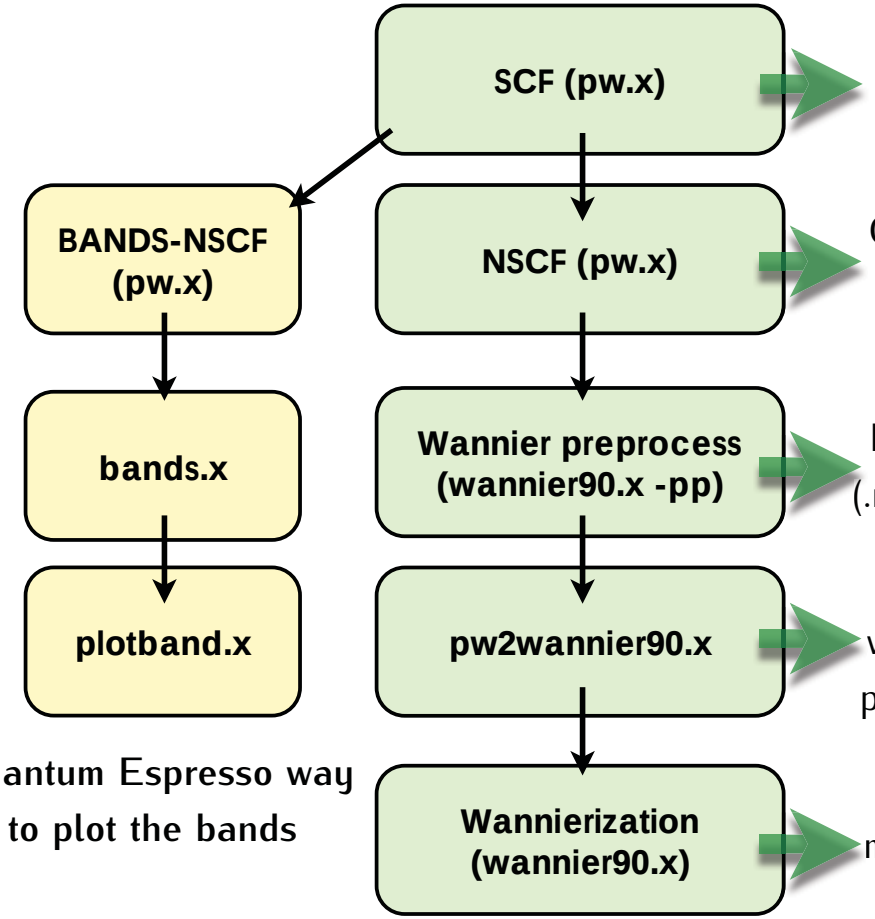
Wannier90 "input data"

- 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

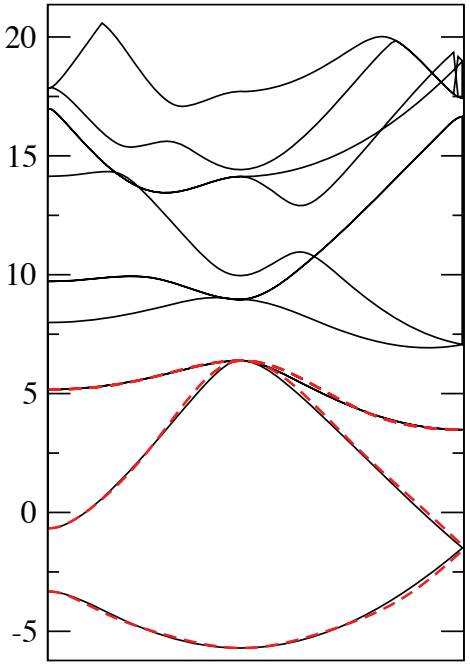
Reads the files produced by the previous step, minimizes the spread, calculates WF, calculates transport properties, ...

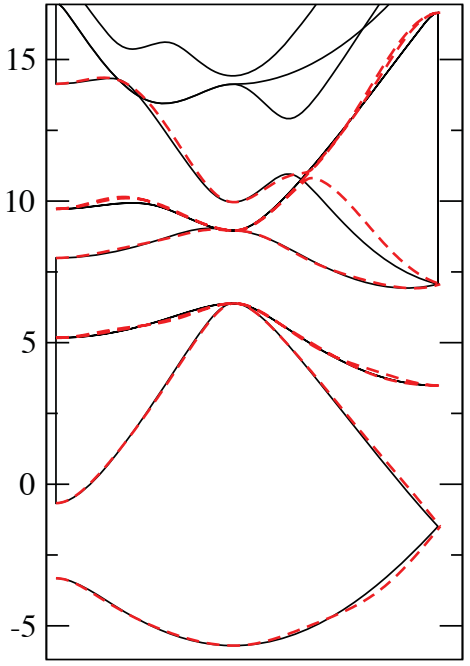
Quantum Espresso way to plot the bands

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

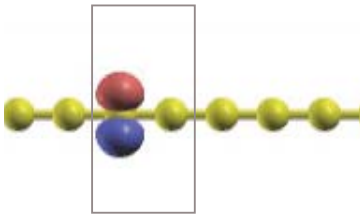
- Calculate Wannier functions for Silicon (VB only, and VB+CB)
- Check the results
- Plot the real-space WFs (using **XCrysDen**)
- Plot the ab-initio and the interpolated band structure (using **xmgrace** or **gnuplot**)

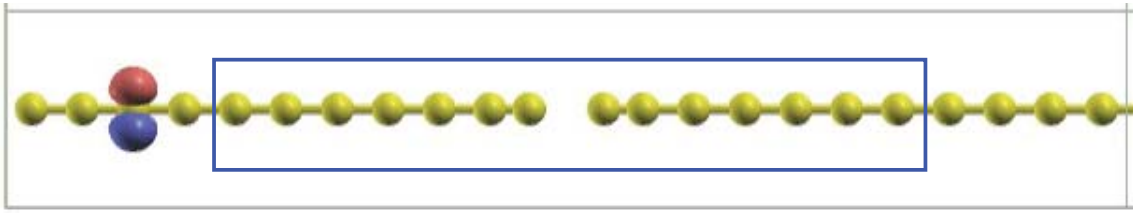




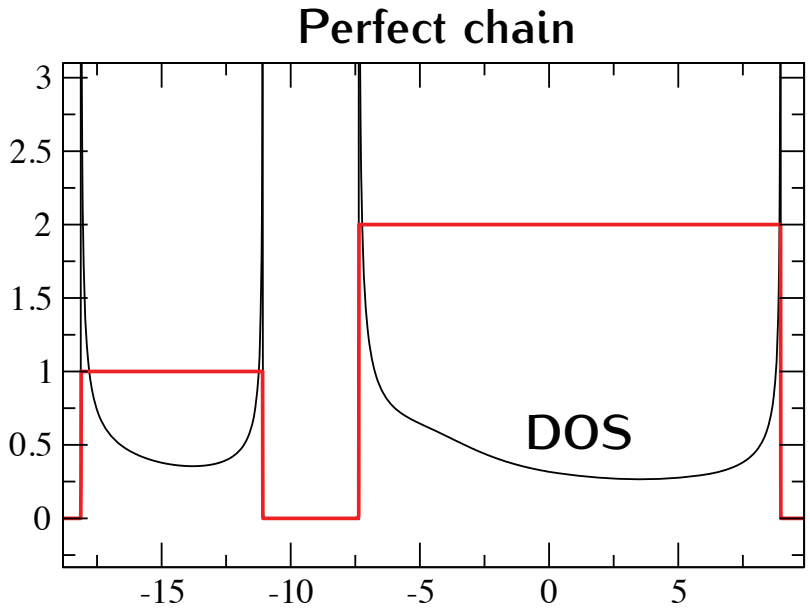
Exercises 3 and 4: C chain

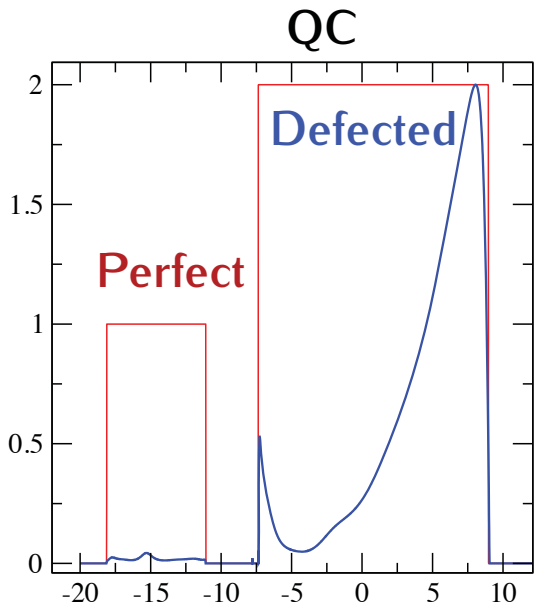
- Calculate the band structure, DOS and the Quantum Conductance (QC) of a periodic C chain



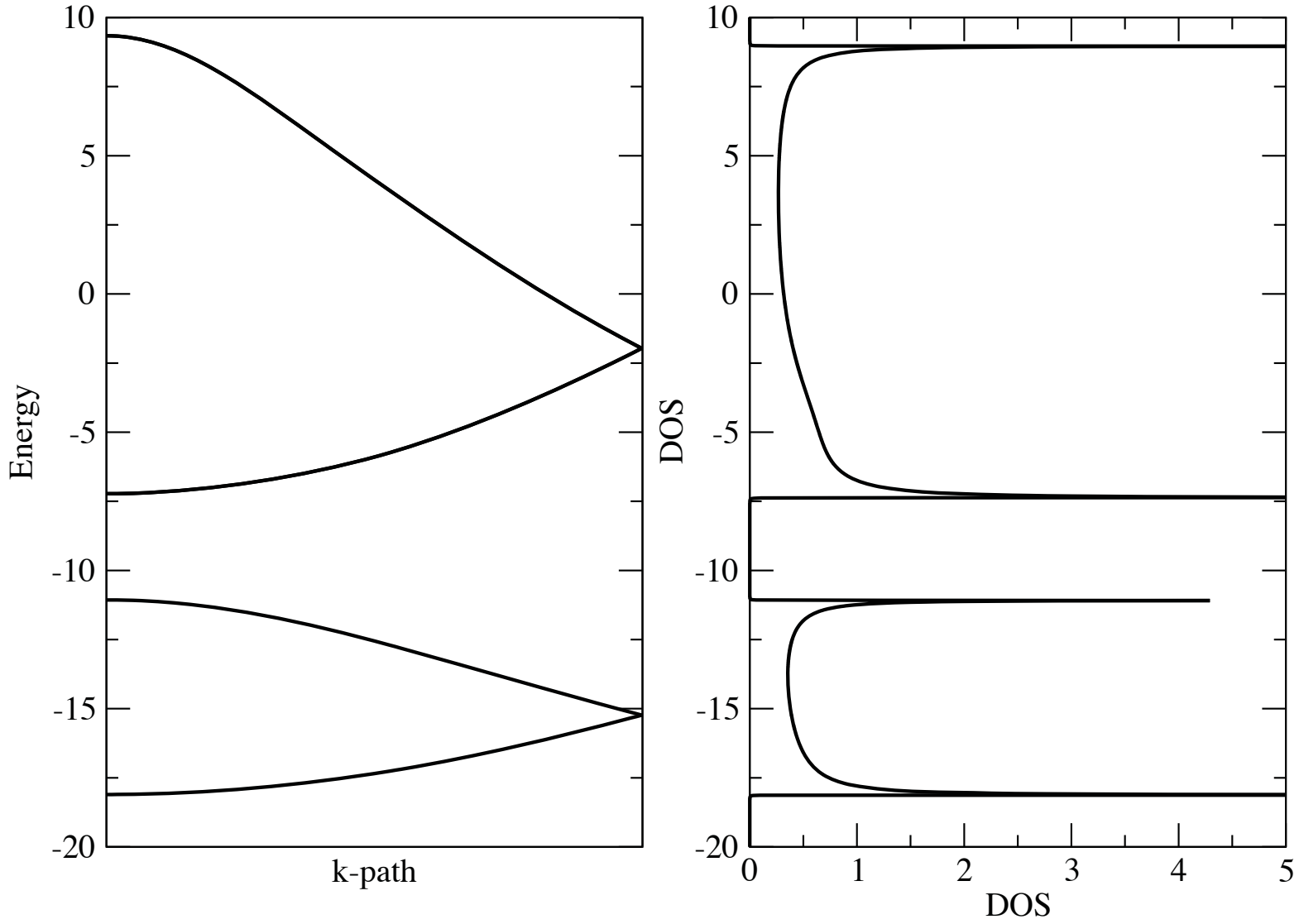


- Calculate the DOS and QC of a defected C chain





Van Hove singularities in 1D



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 inside **/afs/ictp.it/public/shared/smr2522/WANNIER_TUTORIAL/**
- Before starting the tutorials, copy the whole folder above on the local scratch of your computer:

```
cp -r /afs/ictp.it/public/shared/smr2522/WANNIER_TUTORIAL/ /scratch/WANNIER_TUTORIAL
```

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