From Plane Waves... 

... to Wannier.

Hands-on Shanghai, July 2013
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

in all publications resulting from your use of Wannier90.
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

in all publications resulting from your use of Wannier90.
www.wannier.org

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

in all publications resulting from your use of Wannier90.

New release (v2.0) to appear soon!
People involved

**WANNIER90 AUTHORS**

**ARASH MOSTOFI**
Arash is Senior Lecturer in Physics and Materials at Imperial College London. He is also a part of the Thomas Young Centre.

**JONATHAN YATES**
Jonathan is a Lecturer in Materials at the University of Oxford.

**YOUNG-SU LEE**
Young-Su is a Senior Research Scientist at the Korea Institute of Science and Technology (KIST), South Korea.

**WANNIER77 AUTHORS**

**NICOLA MARZARI**
Nicola holds the Chair of Theory and Simulation of Materials at EPFL

**IVO SOUZA**
Ivo is Research professor at the University of the Basque Country.

**DAVID VANDERBILT**
David is Professor of Condensed Matter Theory at Rutgers University.
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 $u_{nk}(r)$ 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
  
  (you can find the link in the PDF with the exercises)
How to run a Wannier90 calculation

1. SCF (pw.x)
   Calculates the ground state density using a given K_POINTS mesh

2. NSCF (pw.x)
   Calculates the wavefunctions \( u_{nk} \) on a complete k-mesh (not necessarily the same as above!)

3. Wannier preprocess (wannier90.x -pp)
   Reads the Wannier90 input file and prepares a file (.nnkp) with the information for the interface program

4. pw2wannier90.x
   Interface program (between QE and W90): reads the wavefunctions of the NSCF step, the .nnkp file and produces the .mmn, .amn, .eig, ... files for Wannier90

5. Wannierization (wannier90.x)
   Reads the files produced by the previous step, minimizes the spread, calculates WF, calculates transport properties, ...
How to run a Wannier90 calculation

- **BANDS-NSCF (pw.x)**
  - **bands.x**
  - **plotband.x**

Quantum Espresso way to plot the bands

- **SCF (pw.x)**
  - Calculates the ground state density using a given K_POINTS mesh

- **NSCF (pw.x)**
  - Calculates the wavefunctions $u_{nk}$ on a complete k-mesh (not necessarily the same as above!)

- **Wannier preprocess (wannier90.x -pp)**
  - 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

- **pw2wannier90.x**

- **Wannierization (wannier90.x)**
  - Reads the files produced by the previous step, minimizes the spread, calculates WF, calculates transport properties, ...
How to run a Wannier90 calculation

Diagram:

1. BANDS-NSCF (pw.x)
   - bands.x
   - plotband.x

2. SCF (pw.x)
   - NSCF (pw.x)
   - Wannier preprocess (wannier90.x -pp)
   - pw2wannier90.x
   - Wannierization (wannier90.x)

3. Calculates the ground state density using a given K_POINTS mesh
4. Calculates the wavefunctions \( u_{nk} \) on a complete k-mesh (not necessarily the same as above!)
5. Reads the Wannier90 input file and prepares a file (.nnkp) with the information for the interface program
6. 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
7. Reads the files produced by the previous step, minimizes the spread, calculates WF, calculates transport properties, ...

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

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

! 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

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
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
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
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
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 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 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

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
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
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
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
```
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
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
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
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