ICTP/Psi-k/CECAM School on Electron-Phonon Physics from First Principles

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Maximally-localized Wannier functions

Giovanni Pizzi\textsuperscript{1}, Antimo Marrazzo\textsuperscript{1}, Valerio Vitale\textsuperscript{2}

\textsuperscript{1}Theory and Simulation of Materials, EPFL (Switzerland)
\textsuperscript{2}Cavendish Laboratory, Department of Physics, University of Cambridge (UK)

School on Electron-Phonon Physics from First Principles
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PART II

The Wannier90 code
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 13 January 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

in all publications resulting from your use of Wannier90.
# People involved

## WANNIER90 Authors

<table>
<thead>
<tr>
<th>Name</th>
<th>Role</th>
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<tbody>
<tr>
<td><strong>ARASH MOSTOFI</strong></td>
<td>Arash is Reader in Physics and Materials at Imperial College London. He is also a part of the Thomas Young Centre.</td>
</tr>
<tr>
<td><strong>YOUNG-SU LEE</strong></td>
<td>Young-Su is a Senior Research Scientist at the Korea Institute of Science and Technology (KIST), South Korea.</td>
</tr>
<tr>
<td><strong>NICOLA MARZARI</strong></td>
<td>Nicola holds the Chair of Theory and Simulation of Materials at EPFL.</td>
</tr>
<tr>
<td><strong>DAVID VANDERBILT</strong></td>
<td>David is Professor of Condensed Matter Theory at Rutgers University.</td>
</tr>
<tr>
<td><strong>JONATHAN YATES</strong></td>
<td>Jonathan is Associate Professor in Materials Modelling at the University of Oxford.</td>
</tr>
<tr>
<td><strong>GIOVANNI PIZZI</strong></td>
<td>Giovanni is a postdoctoral researcher at EPFL.</td>
</tr>
<tr>
<td><strong>IVO SOUZA</strong></td>
<td>Ivo is Research professor at the University of the Basque Country.</td>
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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 Andriopoulos, Nicholas D. M. Hine and Arash A. Mostofi (Imperial College) for the w90vsc code
- David Scubbe (MIT, USA): various bugs/fixes/improvements
- Gabriele Schlafer (ETH Zurich) for the k-energy 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 Greisch (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
- Stephan Tsirkin (Universidad del Pais Vasco, Spain): bug fixes in the berry module

...  

You can be a contributor as well!!
Advanced 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 $u_{nk}(r)$ 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

**Quantum Espresso way to plot the bands**

1. **BANDS-NSCF (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 of 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 (btw 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, ...

**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 XCrystal)
- 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](http://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
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

![Graphs showing DOS and QC for perfect and defected C chains.](image)
PART III

Wannier90 hands-on

A. Marraizzo and V. Vitale