

Wannier90 School, 25-27th March 2020 – Virtual Edition

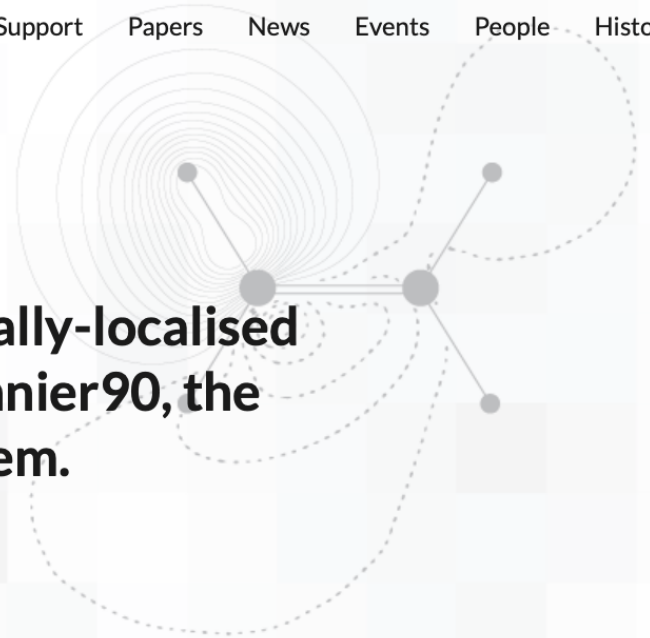
Wannier90: new features and future developments

Arash Mostofi

*The Thomas Young Centre for Theory and Simulation of Materials
Departments of Materials and Physics, Imperial College London*

Welcome! This is the home of maximally-localised Wannier functions (MLWFs) and Wannier90, the computer program that calculates them.

[FIND OUT MORE](#)



LATEST NEWS

Paper describing v3.0 of Wannier90 now published

January 23, 2020

We are very happy to announce that the paper describing v3.0 of the Wannier90 code, how it transitioned to a ... [Continue reading](#)

PLEASE CITE

Wannier90 as a community code: new features and applications, G. Pizzi et al., J. Phys. Cond. Matt. 32, 165902 (2020) [[ONLINE JOURNAL](#)]

in all publications resulting from your use of Wannier90.

Wannier Developers Group



Jonathan Yates
(Oxford)



Giovanni Pizzi
(EPFL)



Ivo Souza
(San Sebastian)



Nicola Marzari
(EPFL)



David Vanderbilt
(Rutgers)



Valerio Vitale
(Imperial)

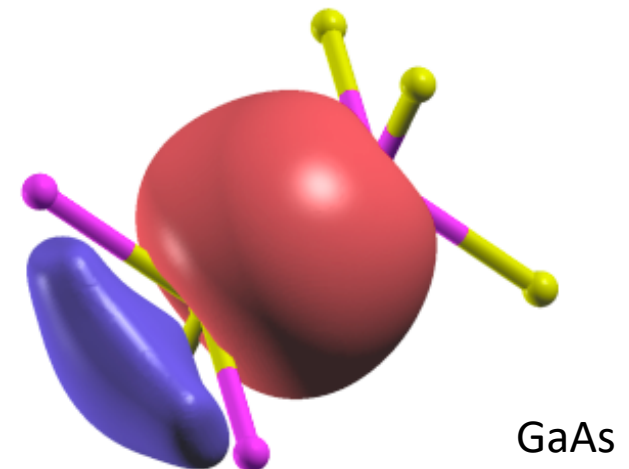
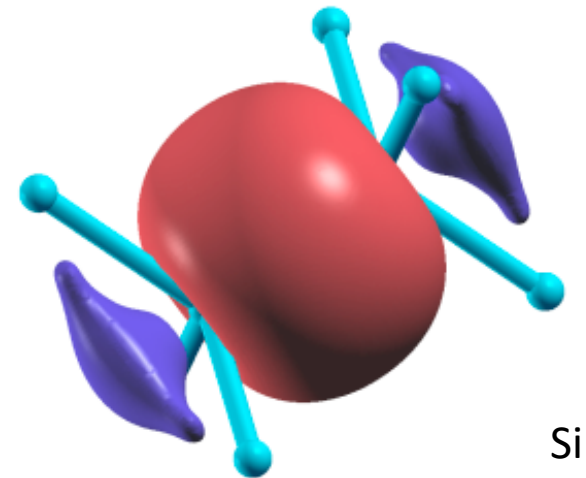


plus a global
community of 43
contributors and
counting...



Wannier functions

- Localized, real-space picture of electronic structure
- Interpretation of chemical bonding
- Polarisation and orbital magnetisation
- Efficient Brillouin zone interpolation and integration
- Berry phase properties
- Electronic transport
- Constructing minimal basis-sets



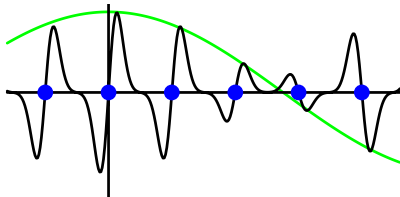
Maximally-localized Wannier functions

Electronic ground
state from *ab initio*
calculation

Unitary transform of
Bloch wavefunctions[†]

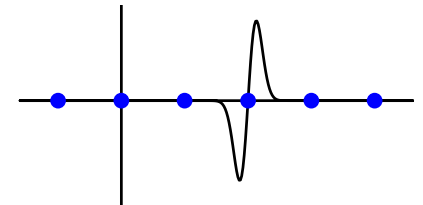
Maximally-localised
Wannier functions in
real-space

$$|\mathbf{R}n\rangle = \frac{V}{(2\pi)^3} \int_{\text{BZ}} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{m=1}^J U_{mn}^{(\mathbf{k})} |\psi_{m\mathbf{k}}\rangle$$



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

$$\Omega = \sum_n [\langle r^2 \rangle_n - \langle \mathbf{r} \rangle_n^2]$$

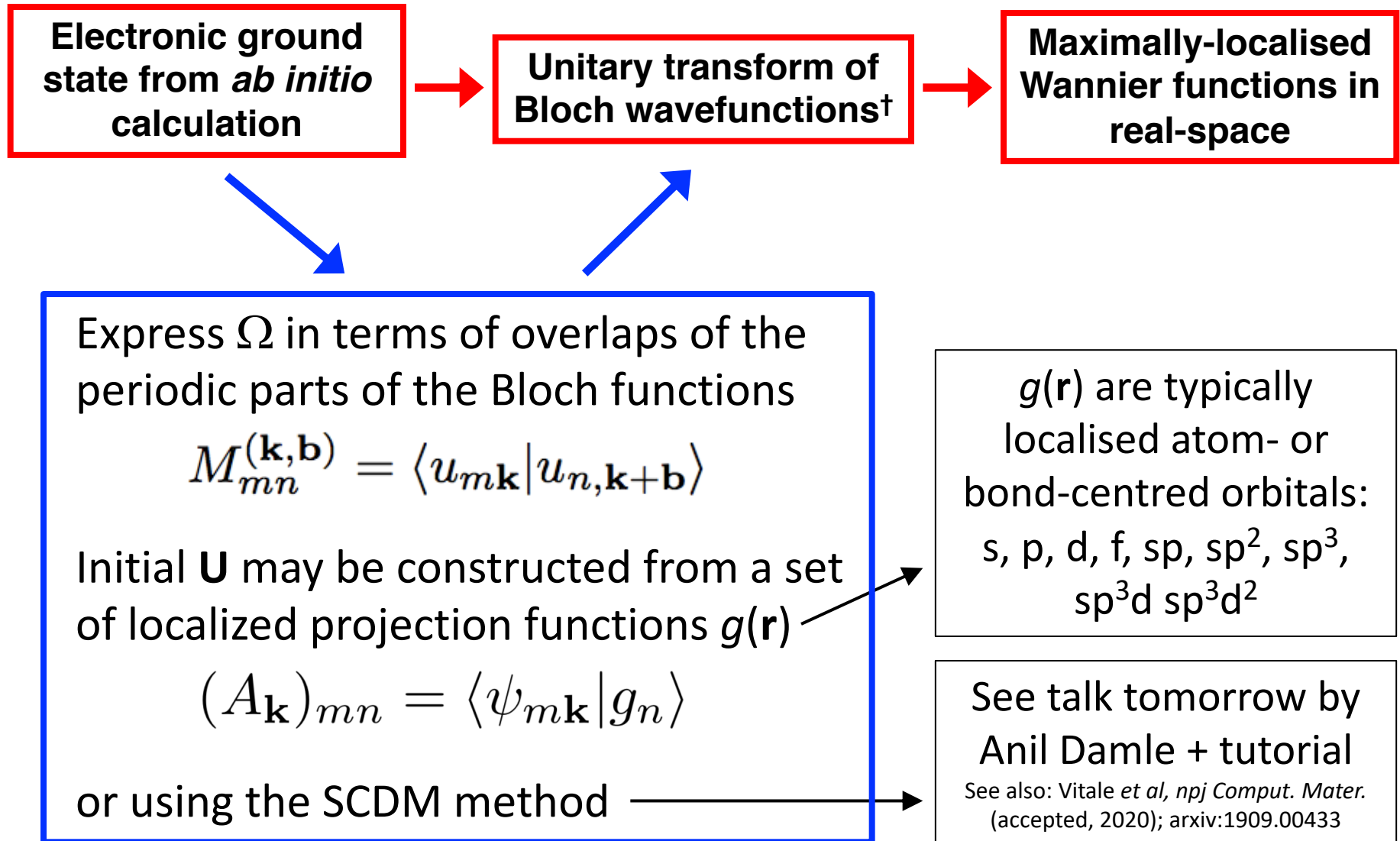


Marzari et al, Rev Mod Phys **84**, 1419 (2012)

Minimize spread functional Ω wrt
arbitrary unitary transformations $U^{(\mathbf{k})}$

[†]N. Marzari and D. Vanderbilt, *Phys. Rev. B* **56**, 12847 (1997)

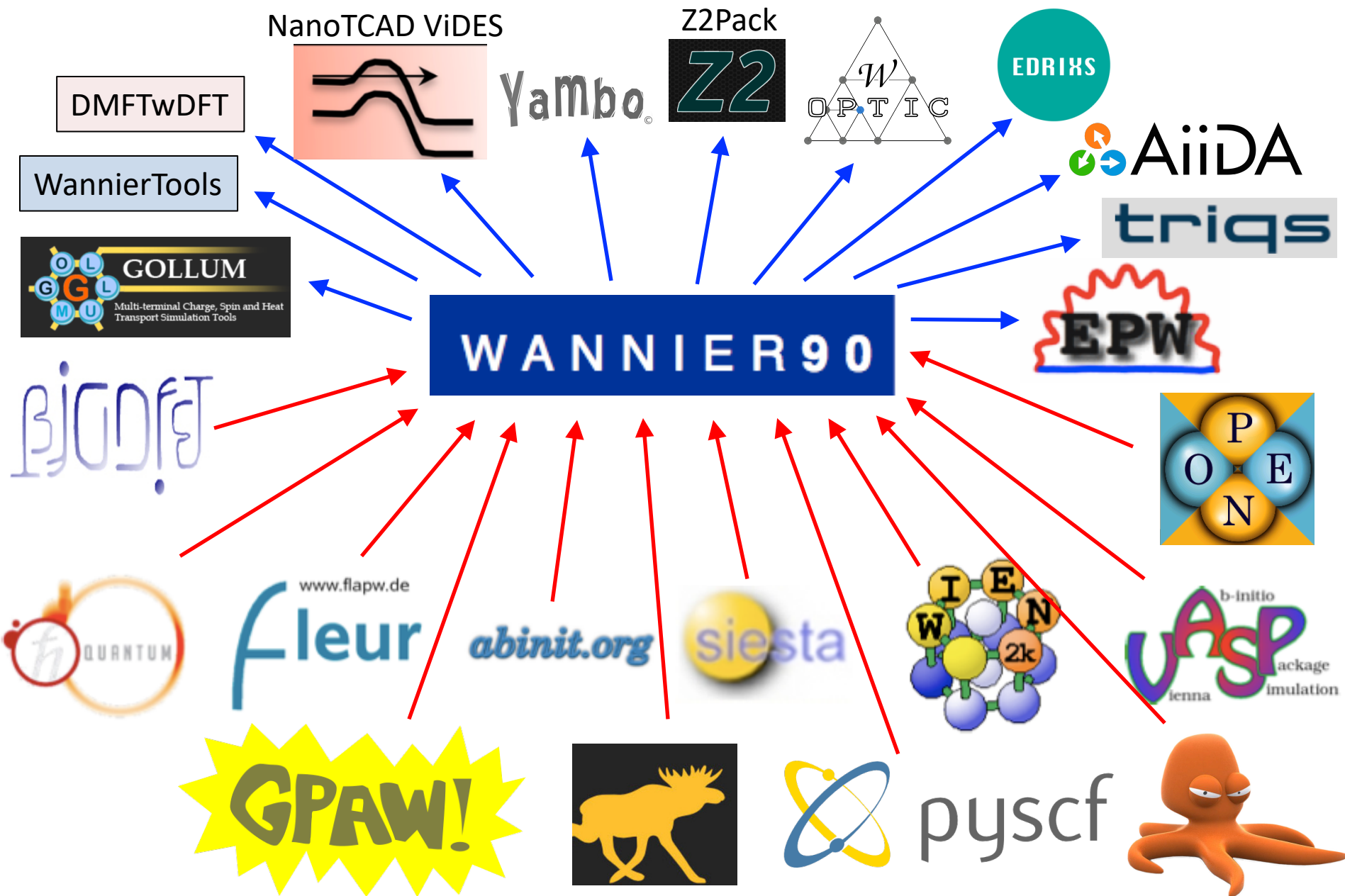
Maximally-localized Wannier functions



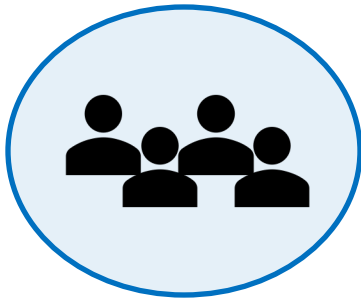
Wannier90: design philosophy

- Modular
- Written in modern Fortran
- Documented and commented
- Open source (GPLv2)
- Version control repository, integrated automatic testing
- Easy to add new functionality
- Easy to interface to generic electronic structure code
 - only require matrix elements
 - information about basis set and FFT grid not required

Wannier90: interfaces



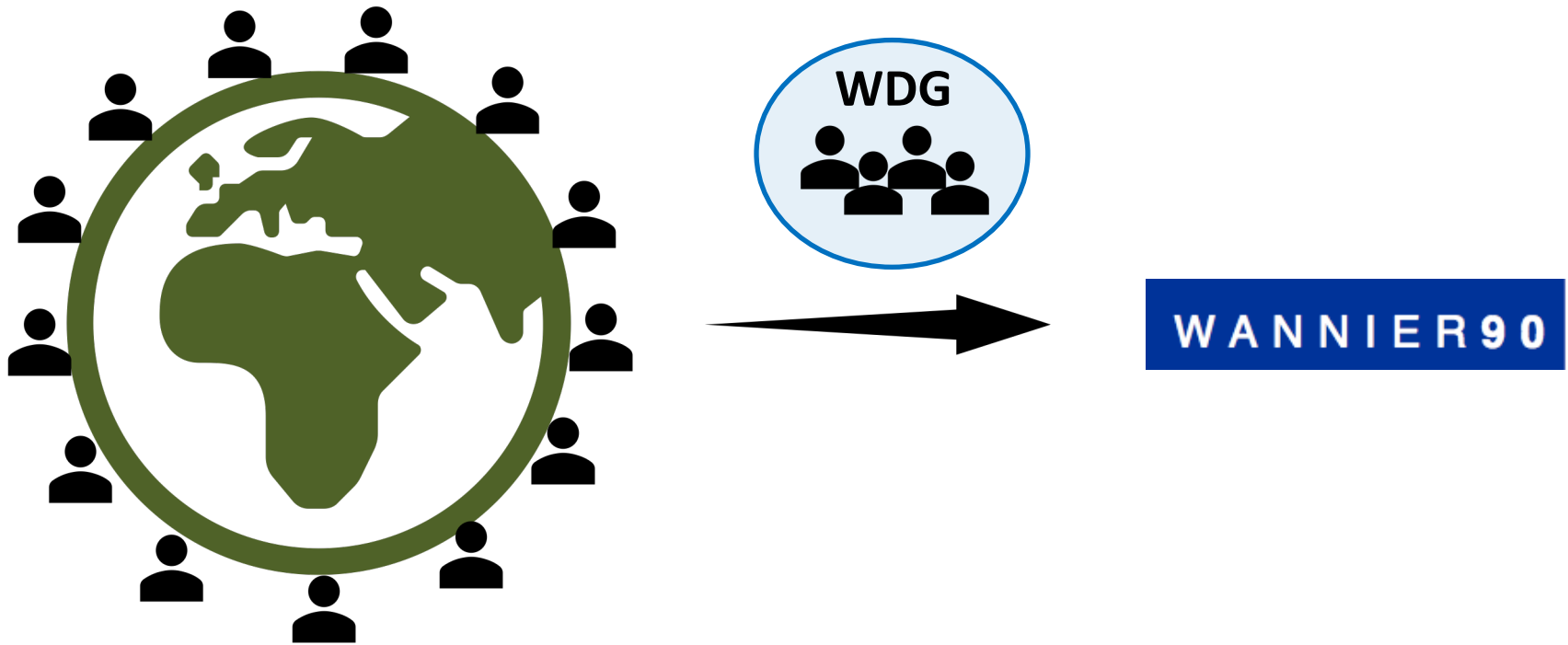
Community-driven development model



Wannier
Developers Group
(WDG)



Community-driven development model



Global community of
Wannier contributors

www.github.com/wannier-developers/wannier90

Wannier90 as a community code: new features and applications

Giovanni Pizzi^{1,29}, Valerio Vitale^{2,3,29}, Ryotaro Arita^{4,5},
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Yusuke Nomura⁴, Lorenzo Paulatto²⁰, Samuel Poncé²¹,
Thomas Ponweiser²², Junfeng Qiao²³, Florian Thöle²⁴,
Stepan S Tsirkin^{12,25}, Małgorzata Wierzbowska²⁶, Nicola Marzari^{1,29},
David Vanderbilt^{27,29}, Ivo Souza^{12,28,29}, Arash A Mostofi^{3,29}
and Jonathan R Yates^{21,29}

J. Phys.: Condens. Matter **32** (2020) 165902 (25pp)

31 contributors and developers on most recent paper

Wannier90 v3.x distribution

- v3.0 released 27th February 2019
- v3.1 released 5th March 2020
- `wannier90.tar` – 173 MB distribution
 - test suite: 85 MB
 - examples and pseudopotentials: 40 MB
 - documentation: 33 MB
 - source code: only 1.6 MB (uncompressed)
- 40,000 lines `!!including comments`

Wannier90 v3.x

- `wannier90.x`
 - serial or parallel (MPI) executable
 - spread minimization, MLWF visualisation, band interpolation, Fermi surface plotting, real-space Hamiltonian, quantum transport
- `postw90.x`
 - serial or parallel (MPI) executable
 - all other properties
- Requirements
 - Fortran 95 compiler
 - LAPACK and BLAS libraries
 - MPI libraries (for parallel executables)
 - Build with GNU `make`

Wannier90 v3.x: developer features

- `git` version control on GitHub; ‘fork and pull-request’ model
- Suite of tests using a modified version of `testcode`
 - Code coverage of tests is measured with `codecov`
 - Nightly automated build & test on a `buildbot` test farm
- Continuous integration with `Travis CI`
 - Upon any commit, the test suite is run in serial and parallel
 - Any failure is reported back and pull request is blocked
- Documented coding style guide; `git` pre-commit hooks with `fprettify`
- Improved command-line interface options, eg, `-d` ‘dry-run’ mode

Wannier90 v3.x: user features

- MLWF for isolated and entangled bands
 - Symmetry-adapted WFs
 - SCDM method
 - Selective localization
 - Constrained centres
 - Preconditioning
 - Parallelisation of core modules
 - Spinor WFs
- Visualisation of MLWFS
 - `xsf`, `cube` and `povray`
 - Spinor WFs
- Wannier interpolation in the BZ
 - Bandstructures
 - Fermi surface
 - Berry phase properties
- Efficient Γ -point-only algorithms
- Quantum and Boltzmann transport
- DoS (fixed/adaptive smearing)
- Berry phase properties
 - Berry curvature
 - anomalous Hall conductivity
 - spin Hall conductivity
 - shift current
 - gyrotropic effects
 - orbital magnetisation
- van der Waals energies from MLWFs
- GW bands interpolation (via Yambo)
- AiiDA plugin (workflow management)
- Many interfaces (eg, EPW)
- Checkpointing and restarts
- Extensive tutorial and solution book

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Wannier90 School: Virtual Edition

Enabled by:

- Zoom videoconferencing (zoom.us)



- Quantum Mobile Virtual Machine
(www.materialscloud.org/work/quantum-mobile)



Wannier90 School: Virtual Edition

UK Time	Central EU Time	New York Time	Tokyo Time	Content	Speaker/Tutors
Wed 25 Mar, 09:00	Wed 25 Mar, 10:00	Wed 25 Mar, 05:00	Wed 25 Mar, 18:00	Talk: Introduction to new features in Wannier90	Arash Mostofi
Wed 25 Mar, 10:00	Wed 25 Mar, 11:00	Wed 25 Mar, 06:00	Wed 25 Mar, 19:00	Talk: Berry Phases and topological properties	QuanSheng Wu
Wed 25 Mar, 11:00	Wed 25 Mar, 12:00	Wed 25 Mar, 07:00	Wed 25 Mar, 20:00	Tutorial (setup of Quantum Mobile)	Antimo Marrazzo, Giovanni Pizzi
Wed 25 Mar, 12:00	Wed 25 Mar, 13:00	Wed 25 Mar, 08:00	Wed 25 Mar, 21:00	BREAK	
Wed 25 Mar, 13:00	Wed 25 Mar, 14:00	Wed 25 Mar, 09:00	Wed 25 Mar, 22:00	Tutorial: Berry Phases and topological properties	Ivo Souza, QuanSheng Wu
Wed 25 Mar, 14:00	Wed 25 Mar, 15:00	Wed 25 Mar, 10:00	Wed 25 Mar, 23:00	Tutorial: Berry Phases and topological properties	Ivo Souza, QuanSheng Wu
Wed 25 Mar, 15:00	Wed 25 Mar, 16:00	Wed 25 Mar, 11:00	Thu 26 Mar, 00:00	BREAK	
Wed 25 Mar, 16:00	Wed 25 Mar, 17:00	Wed 25 Mar, 12:00	Thu 26 Mar, 01:00	Tutorial: Berry Phases and topological properties	Ivo Souza, QuanSheng Wu
Wed 25 Mar, 17:00	Wed 25 Mar, 18:00	Wed 25 Mar, 13:00	Thu 26 Mar, 02:00	Tutorial: Berry Phases and topological properties	Ivo Souza, QuanSheng Wu
Thu 26 Mar, 08:00	Thu 26 Mar, 09:00	Thu 26 Mar, 04:00	Thu 26 Mar, 17:00	Talk: Symmetry-adapted Wannier functions	Yusuke Nomura
Thu 26 Mar, 09:00	Thu 26 Mar, 10:00	Thu 26 Mar, 05:00	Thu 26 Mar, 18:00	Tutorial: Symmetry-adapted Wannier functions	Yusuke Nomura, Valerio Vitale
Thu 26 Mar, 10:00	Thu 26 Mar, 11:00	Thu 26 Mar, 06:00	Thu 26 Mar, 19:00	Tutorial: Symmetry-adapted Wannier functions	Yusuke Nomura, Valerio Vitale
Thu 26 Mar, 11:00	Thu 26 Mar, 12:00	Thu 26 Mar, 07:00	Thu 26 Mar, 20:00	BREAK	
Thu 26 Mar, 12:00	Thu 26 Mar, 13:00	Thu 26 Mar, 08:00	Thu 26 Mar, 21:00	Talk: Automated Wannier functions (SCDM)	Anil Damle
Thu 26 Mar, 13:00	Thu 26 Mar, 14:00	Thu 26 Mar, 09:00	Thu 26 Mar, 22:00	Talk: AiiDA: automated Wannierisation workflows	Giovanni Pizzi
Thu 26 Mar, 14:00	Thu 26 Mar, 15:00	Thu 26 Mar, 10:00	Thu 26 Mar, 23:00	Tutorial: SCDM	Anil Damle, Antimo Marrazzo, Giovanni Pizzi
Thu 26 Mar, 15:00	Thu 26 Mar, 16:00	Thu 26 Mar, 11:00	Fri 27 Mar, 00:00	Tutorial: SCDM (30 min) + AiiDA (30 min)	Anil Damle, Antimo Marrazzo, Giovanni Pizzi, Junfeng Qiao
Thu 26 Mar, 16:00	Thu 26 Mar, 17:00	Thu 26 Mar, 12:00	Fri 27 Mar, 01:00	BREAK	
Thu 26 Mar, 17:00	Thu 26 Mar, 18:00	Thu 26 Mar, 13:00	Fri 27 Mar, 02:00	Tutorial: AiiDA	Antimo Marrazzo, Giovanni Pizzi, Junfeng Qiao
Thu 26 Mar, 18:00	Thu 26 Mar, 19:00	Thu 26 Mar, 14:00	Fri 27 Mar, 03:00	Tutorial: AiiDA	Antimo Marrazzo, Giovanni Pizzi, Junfeng Qiao
Fri 27 Mar, 13:00	Fri 27 Mar, 14:00	Fri 27 Mar, 09:00	Fri 27 Mar, 22:00	Talk: el-ph coupling and the EPW code	Roxana Margine
Fri 27 Mar, 14:00	Fri 27 Mar, 15:00	Fri 27 Mar, 10:00	Fri 27 Mar, 23:00	Tutorial: EPW	Roxana Margine, Samuel Poncé
Fri 27 Mar, 15:00	Fri 27 Mar, 16:00	Fri 27 Mar, 11:00	Sat 28 Mar, 00:00	Tutorial: EPW	Roxana Margine, Samuel Poncé
Fri 27 Mar, 16:00	Fri 27 Mar, 17:00	Fri 27 Mar, 12:00	Sat 28 Mar, 01:00	BREAK	
Fri 27 Mar, 17:00	Fri 27 Mar, 18:00	Fri 27 Mar, 13:00	Sat 28 Mar, 02:00	Tutorial: EPW	Roxana Margine, Samuel Poncé
Fri 27 Mar, 18:00	Fri 27 Mar, 19:00	Fri 27 Mar, 14:00	Sat 28 Mar, 03:00	Tutorial: EPW	Roxana Margine, Samuel Poncé
Fri 27 Mar, 19:00	Fri 27 Mar, 20:00	Fri 27 Mar, 15:00	Sat 28 Mar, 04:00	Closing remarks + feedback	

Future directions: library mode



Future directions: library mode



Wannier90 also has a library mode, but basic functionality only. Schematically:

```
program my_code()  
  call calculate_electronic_structure(...)  
  call wannier_setup(...)  
  call calculate_things_w90_needs(...)  
  call wannier_run(...)  
  call calculate_things_from_w90_results(...)  
end program
```

Future directions: library mode

- Major effort about to start to improve library mode
 - 2 years manpower from UKRI (EPSRC) via UK CCP9 network
- Challenges and next steps
 - Collect “user stories”
 - Prototype required
parallelism behaviour
 - Safe yet unobtrusive error
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Future directions: library mode

- Major effort about to start to improve library mode
 - 2 years manpower from UKRI (EPSRC) via UK CCP9 network
- Challenges and next steps
 - Collect “user stories”
 - Prototype required parallelism behaviour
 - Safe yet unobtrusive error handling
 - Restructure Wannier90 as a wrapper for its own library

