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Introduction to the hands-on tutorial: **Wannier interpolation of band structures**

Antimo Marrazzo¹,
Giovanni Pizzi² and Junfeng Qiao²

¹Physics Department, University of Trieste, Italy

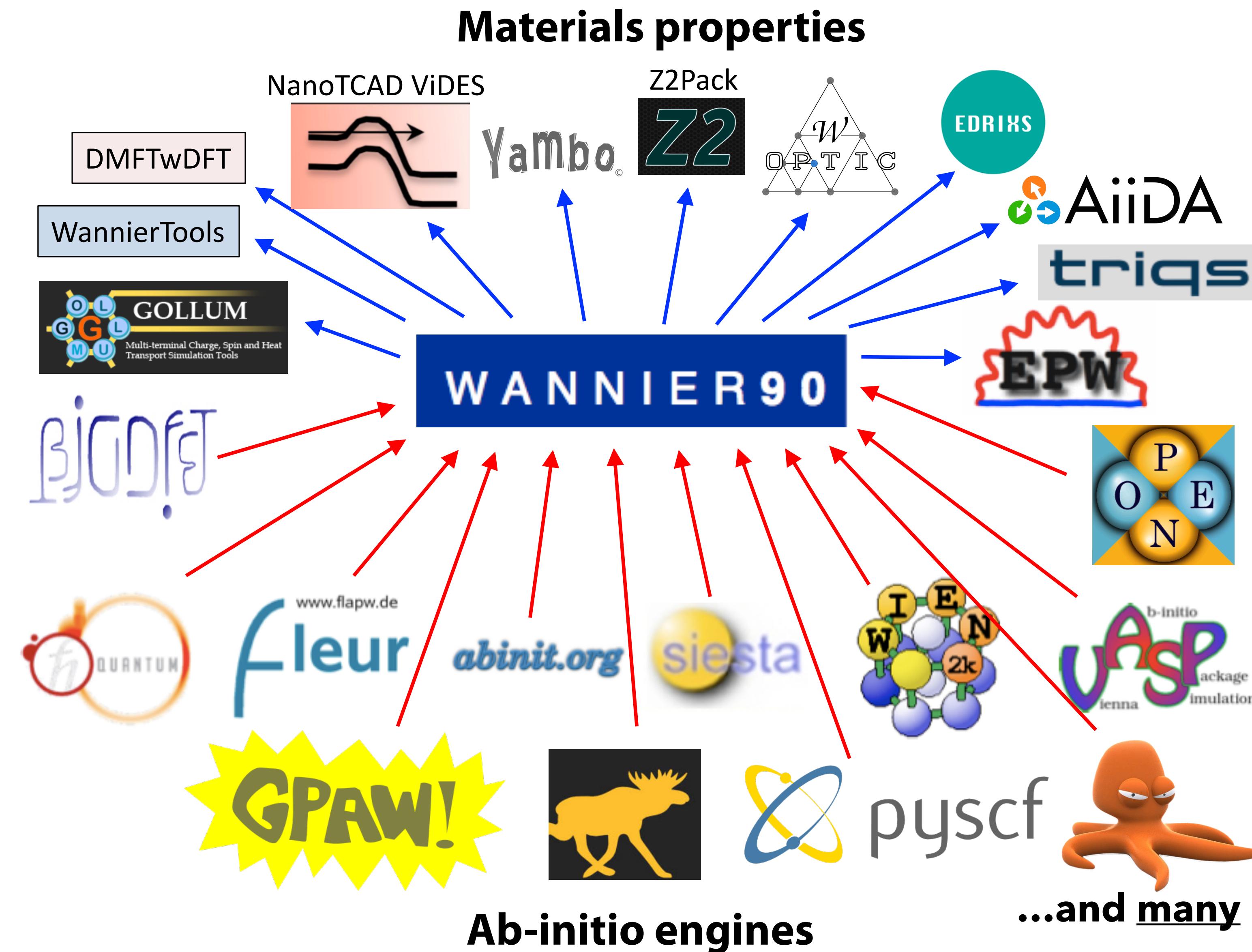
²Theory and Simulation of Materials (THEOS), EPFL, Switzerland

National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Switzerland

9 November 2022

Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response

Wannier90: The center of a software ecosystem

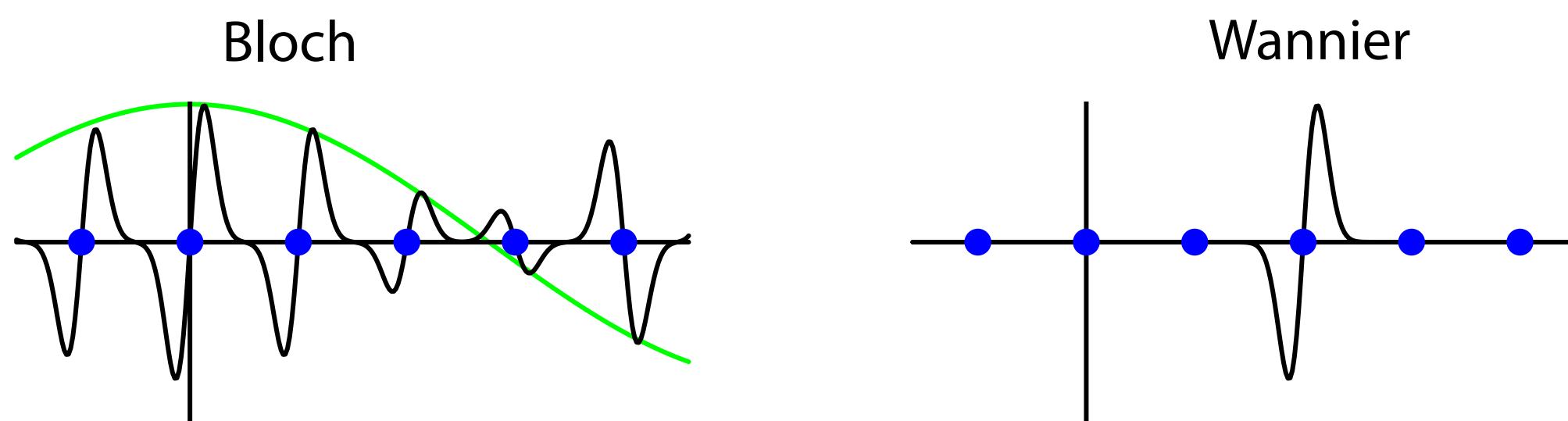


Maximally-localised Wannier functions (MLWF) in a nutshell

Electronic ground states
from first-principles simulations → Subspace-selection & unitary
(e.g. Quantum ESPRESSO) transformation of Bloch wave
functions → MLWF in real space

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

Choose $U_{mn\mathbf{k}}$ such that minimise $\Omega = \sum_{n=1}^J \left[\langle w_{n\mathbf{0}} | \mathbf{r} \cdot \mathbf{r} | w_{n\mathbf{0}} \rangle - |\langle w_{n\mathbf{0}} | \mathbf{r} | w_{n\mathbf{0}} \rangle|^2 \right].$



Maximally-localised Wannier functions (MLWF) in a nutshell

Gauge-invariant part of the spread functional

$$\Omega_I = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{b}} w_b \left(J - \sum_{mn} |M_{mn}^{(\mathbf{k}, \mathbf{b})}|^2 \right)$$

Gauge-dependent part of the spread functional

$$\begin{aligned} \tilde{\Omega} = & \frac{1}{N} \sum_{\mathbf{k}, \mathbf{b}} w_b \sum_{m \neq n} |M_{mn}^{(\mathbf{k}, \mathbf{b})}|^2 \\ & + \frac{1}{N} \sum_{\mathbf{k} \mathbf{b}} w_b \sum_n (-\text{Im} \ln M_{nn}^{(\mathbf{k}, \mathbf{b})} - \mathbf{b} \cdot \bar{\mathbf{r}}_n)^2. \end{aligned}$$

Follow the gradient and update the unitary
matrices $\mathbf{U}_{\mathbf{k}}$

minimise!

$$M_{mn}^{(0)(\mathbf{k}, \mathbf{b})} = \langle u_{m\mathbf{k}}^{(0)} | u_{n, \mathbf{k}+\mathbf{b}}^{(0)} \rangle$$

$$M^{(\mathbf{k}, \mathbf{b})} = U^{(\mathbf{k})\dagger} M^{(0)(\mathbf{k}, \mathbf{b})} U^{(\mathbf{k}+\mathbf{b})}$$

In principle the overlap matrices $M_{mn\mathbf{k}}$ are sufficient, in practice one needs (critical for disentanglement) to specify an **initial subspace** and an **initial gauge**.

$$|\phi_{n\mathbf{k}}\rangle = \sum_{m=1}^{J \text{ or } \mathcal{J}_{\mathbf{k}}} |\psi_{m\mathbf{k}}\rangle \langle \psi_{m\mathbf{k}}| g_n \rangle$$

↓

$$A_{mn\mathbf{k}} = \langle \psi_{m\mathbf{k}} | g_n \rangle$$

localised projection functions
(e.g. s, p, d, sp3, sp2, sp3d2)

$A_{mn\mathbf{k}}$ directly from SCDM
(not today)

$$S_{mn\mathbf{k}} = \langle \phi_{m\mathbf{k}} | \phi_{n\mathbf{k}} \rangle = (A_{\mathbf{k}}^\dagger A_{\mathbf{k}})_{mn},$$

$$|\tilde{\psi}_{n\mathbf{k}}\rangle = \sum_{m=1}^J |\phi_{m\mathbf{k}}\rangle S_{mn\mathbf{k}}^{-\frac{1}{2}}$$

$$= \sum_{m=1}^{J \text{ or } \mathcal{J}_{\mathbf{k}}} |\psi_{m\mathbf{k}}\rangle (A_{\mathbf{k}} S_{\mathbf{k}}^{-\frac{1}{2}})_{mn},$$

WANNIER90

Features Download Support Papers News Events People History

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

[FIND OUT MORE](#)

LATEST NEWS

Wannier 2022 Summer School (and Developers Meeting)
January 28, 2022
The “Wannier 2022 Summer School” will be held at ICTP (Trieste, Italy) from 16 to 20 May 2022 (and “Wannier 2022 ... [Continue reading](#)

Videos of the “Virtual Edition” Wannier90 School now online
April 1, 2020
The video recordings of the first “Virtual Edition” of the Wannier90 School are now all available in the Learn section ... [Continue reading](#)

School on Wannier90 v3.0: new features and applications, 25-27th March 2020 – Virtual Edition
March 13, 2020

PLEASE CITE

Wannier90 as a community code: new features and applications, G. Pizzi et al., J. Phys. Cond. Matt. 32, 165902 (2020) [[ONLINE JOURNAL](#), [OPEN ACCESS](#)] [[bibTeX](#)]
in all publications resulting from your use of Wannier90.

If you are using v2.x, please cite instead:
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](#)] [[bibTeX](#)]

If you are using v1.x, please cite instead:
wannier90: A tool for obtaining maximally-localised Wannier functions, AA Mostofi, JR

WANNIER90

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Download

Latest stable release (5 March 2020): Wannier90 (v3.1.0) [[gzipped-tar](#)]

Please note that:

- Wannier90 is released under the [GNU General Public License \(v2\)](#)
- A summary of improvements may be found in [CHANGE.log](#)
- Installation instructions may be found in [README.install](#)
- The latest User Guide and Tutorial may be found [here](#). They may also be found in the current distribution.

<https://github.com/wannier-developers/wannier90>

For developers (GitHub)

The development of Wannier90 is managed on the [Wannier developers GitHub site](#) where on-going developments, and [how to contribute to Wannier90](#).

School on Wannier90 v3.0: new features and applications, 25-26 March 2020 – Virtual Edition

March 13, 2020
Due to ongoing concerns related to the coronavirus pandemic, we have taken the decision to cancel the physical meeting of ... [Continue reading](#)

Wannier90 (v3.1.0) released

March 5, 2020
Wannier90 (v3.1.0) has been released today!

ALL NEWS

The screenshot shows the GitHub repository for Wannier90. It includes a list of recent commits, a sidebar with repository statistics like 22 unwatched, 135 stars, and 91 forks, and sections for About, Releases, Packages, and Contributors.

Commit	Description	Date
giovannipizzi Merge pull request #362 from jimustafa/gh-actions ...	change workflow back to Ubuntu 20.04 and run with numprocs=2	2 months ago
.github/workflows	A few fixes pre-release (see #229)	2 years ago
autodoc	fix trailing whitespace and unnecessary blank lines	2 years ago
config	fix typo in wannier_plot_spinor_mode parameter	9 months ago
doc	Update generate_weights.sh	4 months ago
examples	Tutorial for extracting SCDM parameters from projectability using pro...	2 years ago
pseudo	Moving the new pw2wannier90 file to folder v6.5	16 months ago
pwscf	Update plot.F90	10 months ago
src	migrate to GitHub Actions	5 months ago
test-suite	update documentaion of gw2wannier90.py & k_mapper.py	2 years ago
utility	Setting the codecov thresholds for the current	3 years ago
.codecov.yml	Not including anymore the xsf.gz examples of w90pov	2 years ago
.gitattributes	Merge branch 'develop' into spn2spn	2 years ago
.gitignore	update pre-commit config	5 months ago
.pre-commit-config.yaml	Release 3.1 (fixed final date)	15 months ago
CHANGELOG.md		

(2008) [ONLINE JOURNAL] [OPEN ACCESS] [bibTeX]

The screenshot shows the Wannier90 website with a red circle highlighting the "Support" menu item in the top navigation bar. The "Support" page contains sections for User Guide, Tutorial, and Source Code Documentation, along with links to PDF files and video recordings of a virtual edition.

Support

User Guide, Tutorial and Source Code Documentation

The Wannier90 user guide and tutorial are both available in the 'doc' directory of the [current distribution](#). They are also available for direct download here:

- User guide v3.1.0: [\[PDF\]](#)
- Tutorial v3.1.0: [\[PDF\]](#)
- Tutorial solutions v3.1.0: [\[PDF\]](#)

Videos of the “Virtual Edition” Wannier90 School
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School on Wannier90 v3.0: new features and applications
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ALL NEWS

If `bands_plot = true`, then the code will calculate the band structure, through Wannier interpolation, along the path in k-space defined by `bands_kpath` using `bands_num_points` along the first section of the path and write out an output file in a format specified by `bands_plot_format`. The default value is `false`.

2.9.11 kpoint_path

Defines the path in k-space along which to calculate the bandstructure. Each line gives the start and end point (with labels) for a section of the path. Values are in fractional coordinates with respect to the primitive reciprocal lattice vectors.

```
begin kpoint_path
    G 0.0 0.0 0.0 L 0.0 0.0 1.0
    L 0.0 0.0 1.0 N 0.0 1.0 1.0
    :
end kpoint_path
```

There is no default

2.9.12 integer :: bands_num_points

wannier90: A tool for obtaining maximally-localised Wannier functions, AA Mostofi, JR Yates, YS Lee, I Souza, D Vanderbilt, N Marzari, *Comput. Phys. Commun.* **178**, 685 (2008) [[ONLINE JOURNAL](#)] [[OPEN ACCESS](#)] [[bibTeX](#)]

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- Tutorial solutions v3.1.0: [\[PDF\]](#)

8: Iron — Spin-polarized WFs, DOS, projected WFs versus MLWFs

• Outline: Generate both maximally-localized and projected Wannier functions for ferromagnetic bcc Fe. Calculate the total and orbital-projected density of states by Wannier interpolation.

Figure 21: Unit cell of Iron crystal plotted with the XCRYSDEN program.

Final State			
WF centre and spread	1	(0.709852, 0.000108, 0.000131)	1.08935224
WF centre and spread	2	(0.000131, 0.000053, -0.709852)	1.08935218
WF centre and spread	3	(-0.709852, -0.000108, -0.000131)	1.08935221
WF centre and spread	4	(0.000108, -0.709852, -0.000053)	1.08935218
WF centre and spread	5	(-0.000131, -0.000053, 0.709852)	1.08935226
WF centre and spread	6	(0.000000, 0.000000, 0.000000)	0.43234428
WF centre and spread	7	(-0.000000, 0.000000, 0.000000)	0.43234429
WF centre and spread	8	(-0.000108, 0.709852, 0.000053)	1.08935225
WF centre and spread	9	(0.000000, 0.000000, -0.000000)	0.43234428
Sum of centres and spreads		(0.000000, -0.000000, -0.000000)	7.83314616
Spreads (Ang ⁻²)	Omega I	= 5.948424630	
=====	Omega D	= 0.017027691	
	Omega OD	= 1.867693841	
Final Spread (Ang ⁻²)	Omega Total	= 7.833146162	

If you are using v1.x, please refer to the [wannier90: A tool for obtaining maximally-localized Wannier functions](#) paper by Yates, YS Lee, I Souza, D Vanderbilt, and J. P. Perdew (2008) [[ONLINE JOURNAL](#)] [[PDF](#)].

and for spin-down MLWFs is

ALL NEWS

The screenshot shows the official website for Wannier90. At the top, there is a dark blue header bar with the text "WANNIER90". Below this is a light gray navigation bar with several links: "Features", "Download", "Support" (which is circled in red), "Papers", "News", "Events", "People", and "History". The main content area has a white background. It features a section titled "Community Email Forum". Inside this section, there is text about a mailing list, with a link to subscribe highlighted by a red oval. Another red oval highlights the email address for posting. A note below specifies that registration is required to post. Further down, it mentions the availability of mailing list archives. At the bottom of the page, there is a news summary about a decision to cancel a meeting, a link to the journal article, and a news item about the release of version 3.1.0.

WANNIER90

Features Download Support Papers News Events People History

Community Email Forum

A fully archived Wannier90 user mailing list is hosted by Quantum ESPRESSO: [SUBSCRIBE HERE](#), but at the same time please send an email to nicola.marzari@epfl.ch to confirm your interest (sometimes people are enrolled unwittingly by spambots).

Once subscribed, post to the list by sending your email to wannier@lists.quantum-espresso.org. We kindly request that you include your name and affiliation in all posts to the mailing list.

Note that you must register in order to post emails to this list. Emails from non-registered users will be deleted automatically.

The archives of the Wannier90 mailing list may be accessed [here](#); alternatively, a searchable version of the mailing list archive can be accessed [here](#).

decision to cancel the physical meeting or ... [Continue reading](#)

Comput. Phys. Commun. **185**, 2309 (2014) [[ONLINE JOURNAL](#)] [[bibTeX](#)]

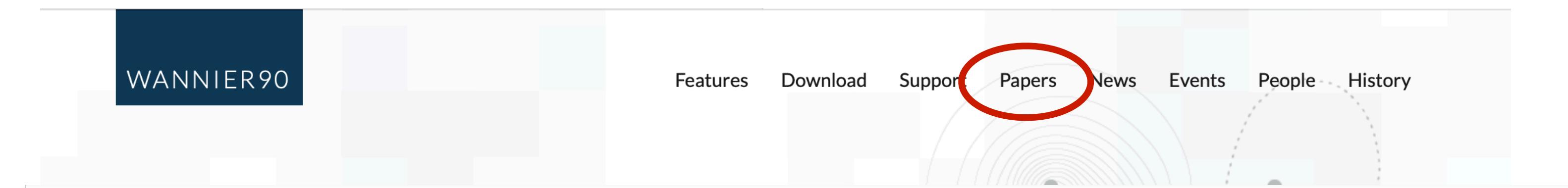
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[ALL NEWS](#)



In publications arising from the use of Wannier90 please cite

Wannier90 as a community code: new features and applications

G. Pizzi, V. Vitale, R. Arita, S. Blügel, F. Freimuth, G. Géranton, M. Gibertini, D. Gresch, C. Johnson, T. Koretsune, J. Ibañez-Azpiroz, H. Lee, J. M. Lihm, D. Marchand, A. Marrazzo, Y. Mokrousov, J. I. Mustafa, Y. Nohara, Y. Nomura, L. Paulatto, S. Poncé, T. Ponweiser, J. Qiao, F. Thöle, S. S. Tsirkin, M. Wierzbowska, N. Marzari, D. Vanderbilt, I. Souza, A. A. Mostofi, and J. R. Yates, *J. Phys. Cond. Matt.* **32**, 165902 (2020) [[ONLINE JOURNAL](#), [OPEN ACCESS](#)]

Please cite this new paper if you use a recent
version of Wannier90
(bibtex available on the homepage)

MARCH 2020 – VIRTUAL EDITION

March 13, 2020

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A community effort!

People

Wannier Developers Group



Arash Mostofi
Professor of Theory and
Simulation of Materials –
Imperial College London



Jonathan Yates
Associate Professor of
Materials Modelling –
University of Oxford



Giovanni Pizzi
Senior Scientist – EPFL



Valerio Vitale
Postdoctoral Research
Associate – University of
Cambridge and Imperial
College London



Nicola Marzari
Chair of Theory and
Simulation of Materials –
EPFL



Ivo Souza
Research Professor –
University of the Basque
Country



David Vanderbilt
Professor of Condensed Matter
Theory – Rutgers University

Wannier90 is a community development effort and would not be possible without the involvement and effort of a large number of contributors. A [full list of authors and contributors](#) is maintained on our [GitHub site](#).

Many more people involved
in the past years:
**Wannier90 transitioned
to a community code**

*By citing the new paper, you acknowledge
the important work of all these coauthors!*

OPEN ACCESS
IOP Publishing

Journal of Physics: Condensed Matter

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

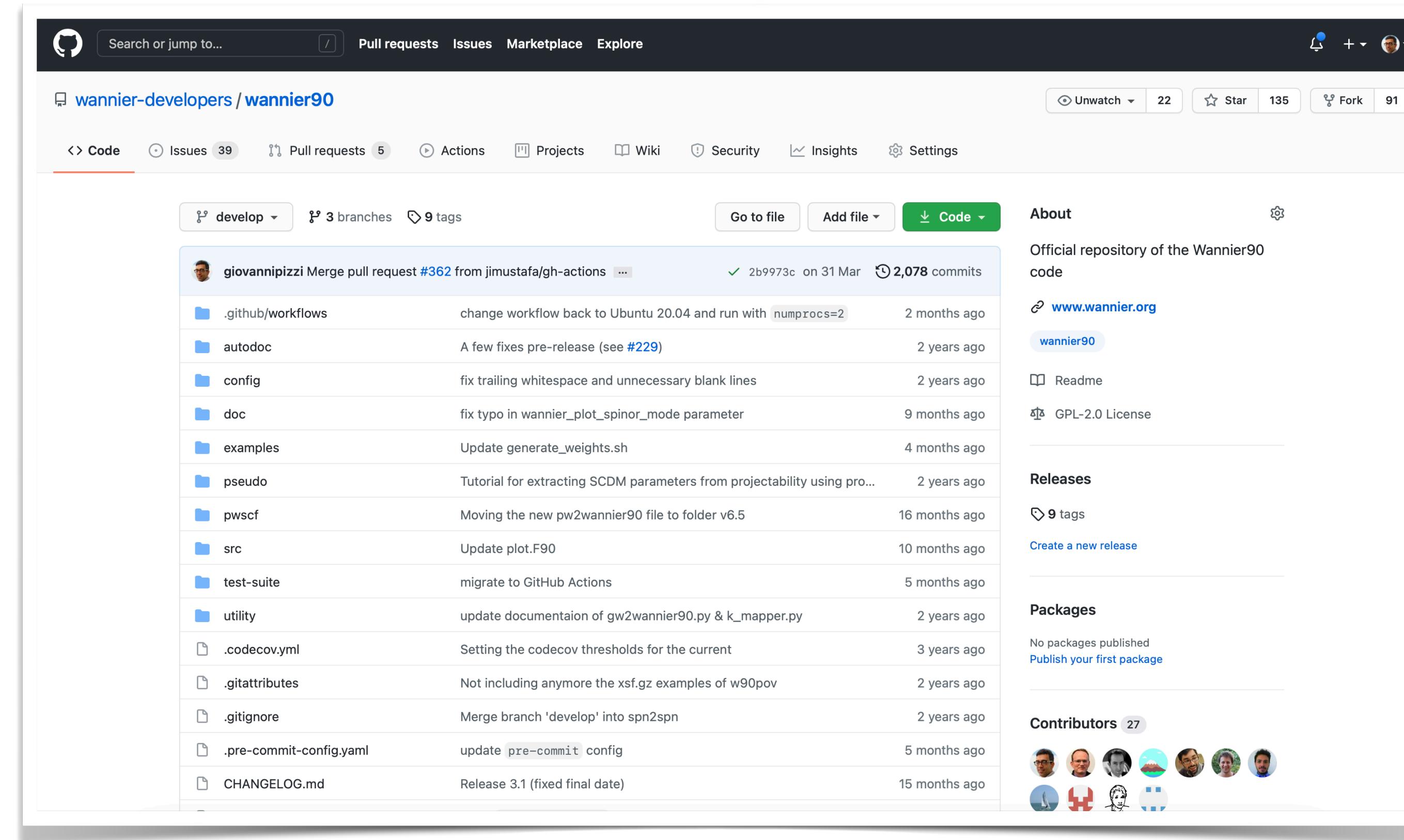
<https://doi.org/10.1088/1361-648X/ab51ff>

Wannier90 as a community code: new features and applications

Giovanni Pizzi^{1,29,30}, Valerio Vitale^{2,3,29}, Ryotaro Arita^{4,5}, Stefan Blügel⁶, Frank Freimuth⁶, Guillaume Géranton⁶, Marco Gibertini^{1,7}, Dominik Gresch⁸, Charles Johnson⁹, Takashi Koretsune^{10,11}, Julen Ibañez-Azpiroz¹², Hyungjun Lee^{13,14}, Jae-Mo Lihm¹⁵, Daniel Marchand¹⁶, Antimo Marrazzo¹, Yuriy Mokrousov^{6,17}, Jamal I Mustafa¹⁸, Yoshiro Nohara¹⁹, 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}.

W90 as a community-driven code

<https://github.com/wannier-developers/wannier90>



You can be a contributor too!

**Create pull requests with documentation improvement,
bug fixes, and new features: they are very welcome!**

Code (old and new) features

Calculation of Maximally-Localised Wannier Functions

- Wannier localisation scheme of Marzari and Vanderbilt [[REF](#)]
- Disentanglement scheme of Souza, Marzari and Vanderbilt [[REF](#)] for entangled bands (e.g. metals, conduction states)
- Optimised algorithm for Gamma-point calculations [[REF](#)]
- Symmetry-adapted Wannier functions [[REF](#)]
- Wannier functions without the need to define initial projections (via the SCDM method) [[REF1](#), [REF2](#)]
- Projection-only Wannier functions (without disentanglement and/or Wannierisation)
- Hamiltonian and position operators represented in the real-space Wannier function basis (eg, for use in tight-binding calculations)
- Spinor Wannier functions
- Export of Wannier functions for plotting as xsf (XCrySDen), cube format, and ray-tracing using POV-Ray
- Calculation of van der Waals energies [[REF1](#)], [[REF2](#)]
- Disentanglement within selected regions of k-space

Wannier90 exploits the real-space localisation of WFs to obtain many spectral and Fermi-surface properties at high-resolution in the Brillouin zone (so-called Wannier interpolation). Many of these properties can take advantage of multicore processors and compute clusters using MPI.

Code (old and new) features

Density of States

- Band structures
- Density of states (using fixed or adaptive smearing [[REF](#)])
- Wannier projected DOS and bandstructure
- Total spin moment
- Fermi surfaces (via bxsf file)
- GW bands interpolation (via an interface to the Yambo code)

Berry phase properties including:

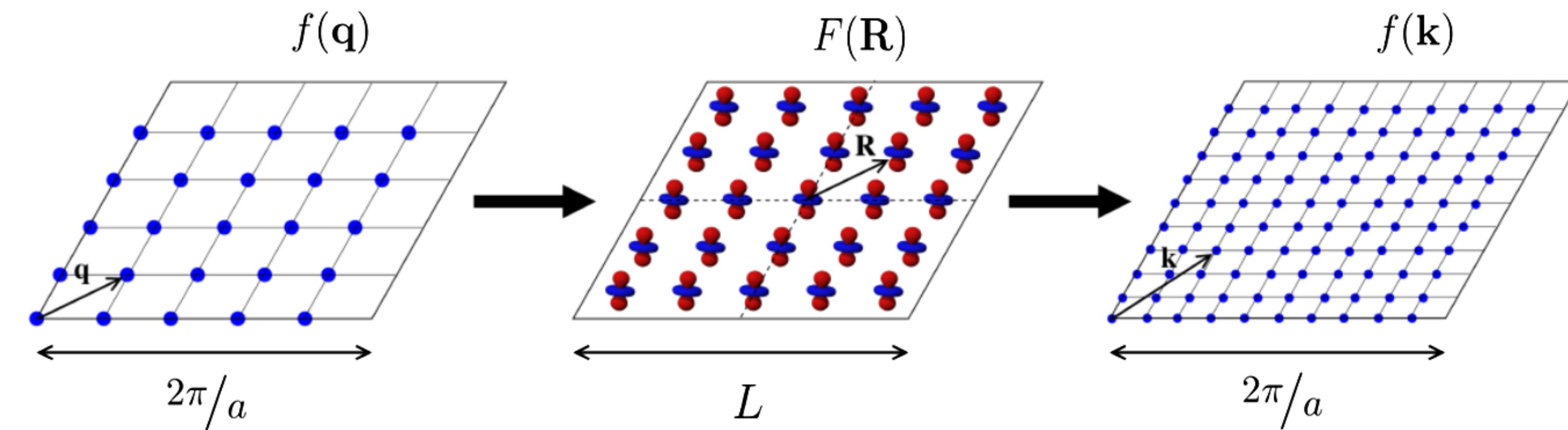
- Berry curvature [[REF](#)]
- Anomalous Hall conductivity [[REF](#)]
- Orbital magnetisation [[REF](#)]
- Shift currents [[REF](#)]
- Gyrotropic effects [[REF](#)]

Transport

- Ballistic (Landauer-Buttiker) transport [[REF1](#)], [[REF2](#)], [[REF3](#)])
- Boltzmann transport (BoltzWann) [[REF](#)]
 - Boltzmann transport equation in the relaxation time approximation
 - Electrical conductivity
 - Seebeck coefficients
 - Electronic contribution to the thermal conductivity
 - Spin Hall conductivity [[REF](#)]

Improved Wannier interpolation by minimal-distance replica selection

Wannier interpolation: similar to Fourier interpolation, which uses discrete Fourier transforms to reconstruct faithfully continuous signals from a discrete sampling, provided that the signal has a finite bandwidth and that the sampling rate is at least twice the bandwidth (Nyquist–Shannon condition).



$$\tilde{H}_{mn\mathbf{R}} = \langle w_{m\mathbf{0}} | H | w_{n\mathbf{R}} \rangle = \frac{1}{N} \sum_{j=1}^N e^{-i\mathbf{k}_j \cdot \mathbf{R}} H_{mn\mathbf{k}_j}$$

$$H_{mn\mathbf{k}} = \sum_{\mathbf{R}'} e^{i\mathbf{k} \cdot \mathbf{R}'} \tilde{H}_{mn\mathbf{R}'}$$

exponential decay w.r.t. $|\mathbf{R}|$

The interpolated band structure at an arbitrary \mathbf{k} -point can be obtained by diagonalising $H_{mn\mathbf{k}}$, and many other quantities can be interpolated using the same approach!

Improved Wannier interpolation by minimal-distance replica selection

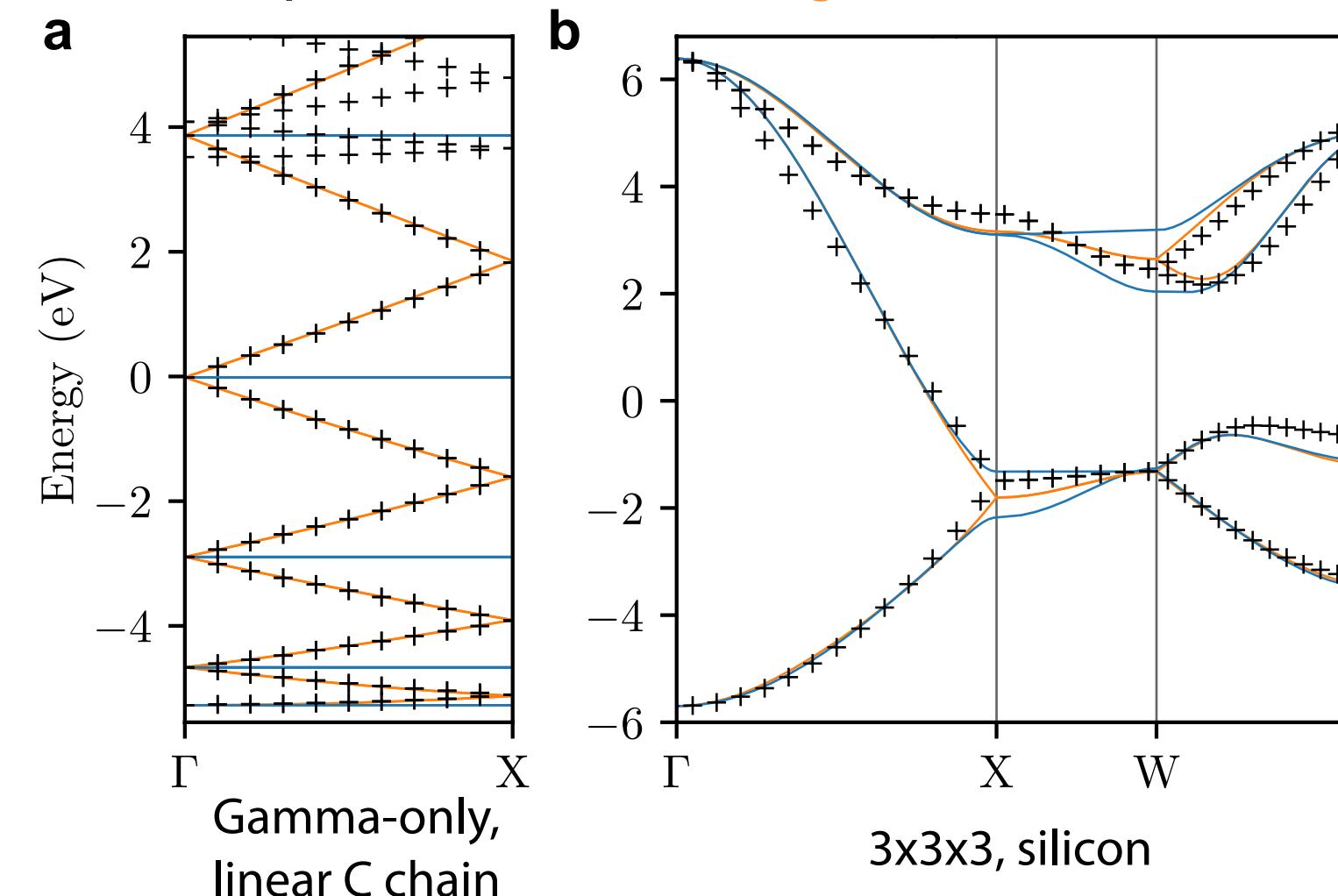
The diagram illustrates the Wigner-Seitz supercell (orange boundary) containing a green parallelogram representing the Brillouin zone. A point \mathbf{r}_m is shown within the zone. Three Wannier functions are depicted: $w_{n\mathbf{R}}(\mathbf{r})$ (blue), $w_{m\mathbf{0}}(\mathbf{r})$ (orange), and $w_{n\mathbf{R}+\mathbf{T}}(\mathbf{r})$ (blue). Vectors \mathbf{a}_1 and \mathbf{a}_2 define the parallelogram. The equation shows the transition from a sum over all \mathbf{R}' to a sum over vectors \mathbf{T} that minimize the distance between \mathbf{r}_m and the points $(\mathbf{r}_n + \mathbf{R} + \mathbf{T})$.

$$H_{mn\mathbf{k}} = \sum_{\mathbf{R}'} e^{i\mathbf{k}\cdot\mathbf{R}'} \tilde{H}_{mn\mathbf{R}'}$$

$$H_{mn\mathbf{k}} = \sum_{\mathbf{R}} \frac{1}{N_{mn\mathbf{R}}} \sum_{j=1}^{N_{mn\mathbf{R}}} e^{i\mathbf{k}\cdot(\mathbf{R} + \mathbf{T}_{mn\mathbf{R}}^{(j)})} \tilde{H}_{mn\mathbf{R}}$$

$\{\mathbf{T}_{mn\mathbf{R}}^{(j)}\}$ vectors \mathbf{T} that minimise the distance $|\mathbf{r}_m - (\mathbf{r}_n + \mathbf{R} + \mathbf{T})|$

Blue: old implementation, orange: current default in Wannier90 (v3.x)



Clear example:
gamma-only

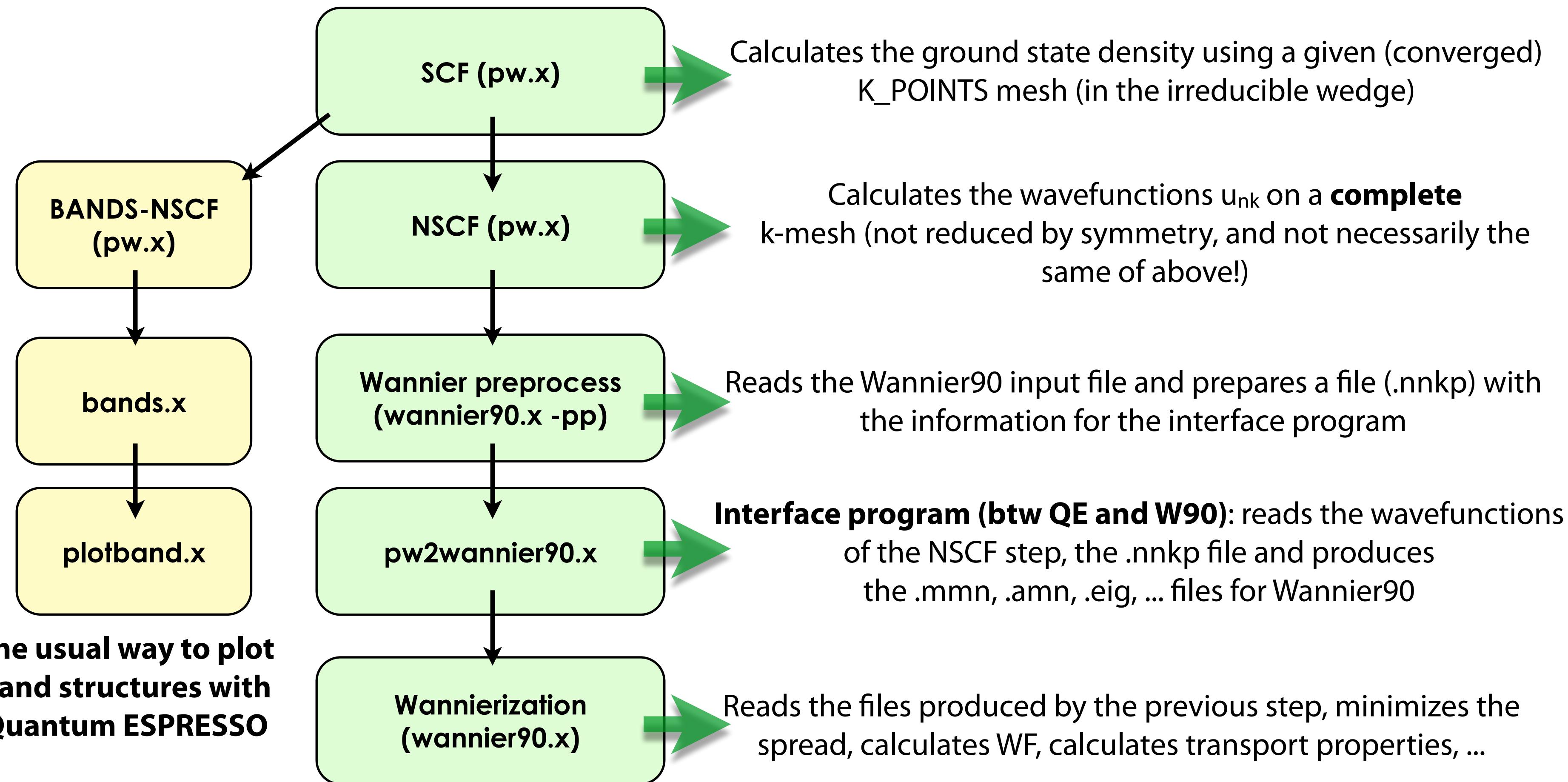
$$H_{mn\mathbf{k}} = \frac{\tilde{H}_{mn\mathbf{0}}}{N_{mn\mathbf{0}}} \sum_{j=1}^{N_{mn\mathbf{0}}} e^{i\mathbf{k}\cdot\mathbf{T}_{mn\mathbf{0}}^{(j)}}$$

Better interpolation and degeneracies,
especially for very coarse grids

Wannier90 “input data”

- W90 needs the overlap matrices $M_{mn}^{(k,k+b)}$ between neighboring k points, and the $A_{mn}(k)$ projection matrices
- Other possible (and common) inputs:
 - the **list of Hamiltonian eigenvalues** $E_n(k)$ at each k -point (for interpolation)
 - the $u_{nk}(r)$ in real space (for plotting the WFs)
 - Other (optional) matrices: spin components, uHu and ulu , and more.
- This input can be obtained from various programs; there exists interfaces for a set of ab-initio codes
 - We will use **Quantum ESPRESSO (QE)**
 - **Reminder:** $pw.x$ documentation in
https://www.quantum-espresso.org/Doc/INPUT_PW.html
(you can find the link in the PDF with the exercises)

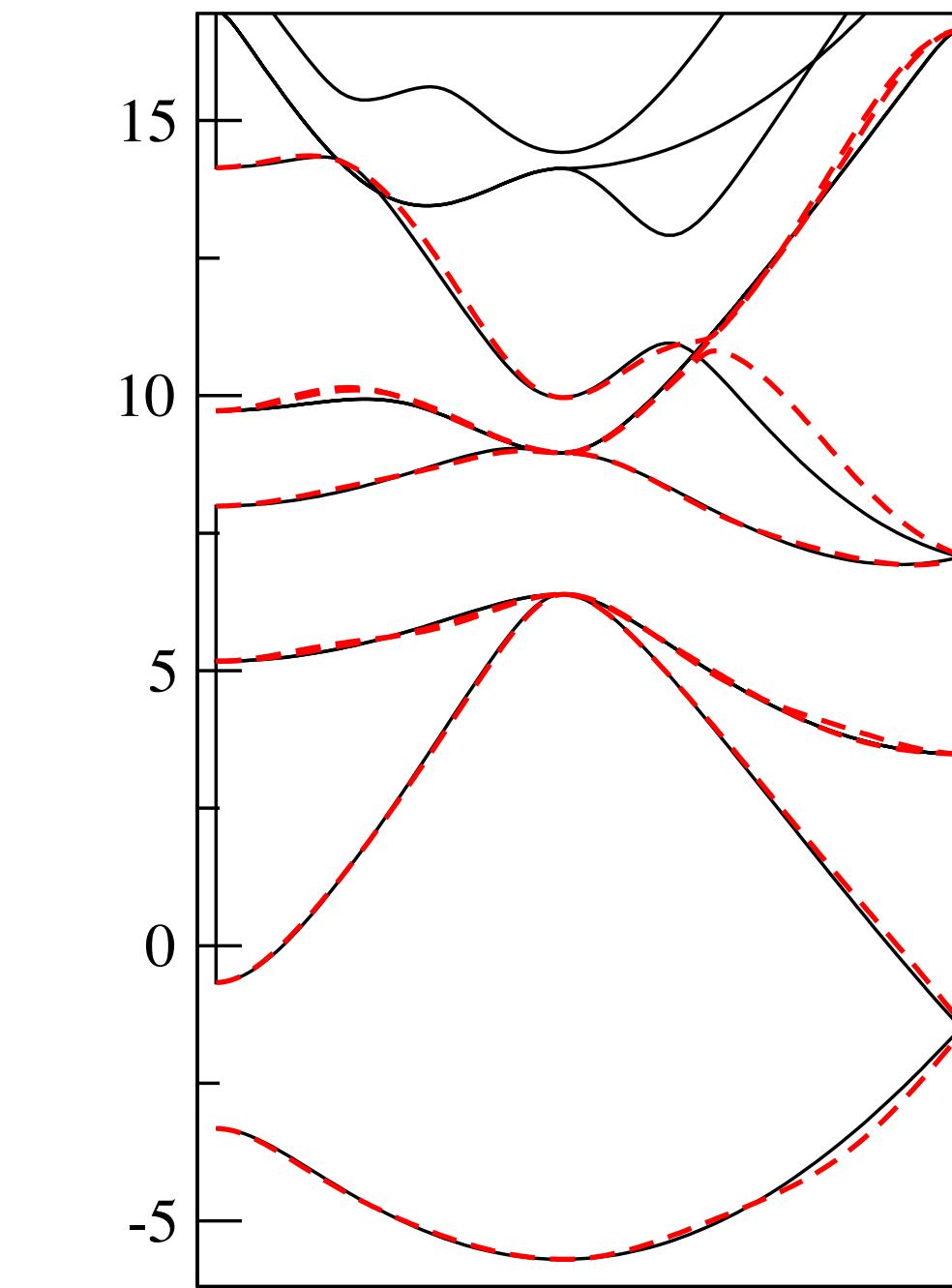
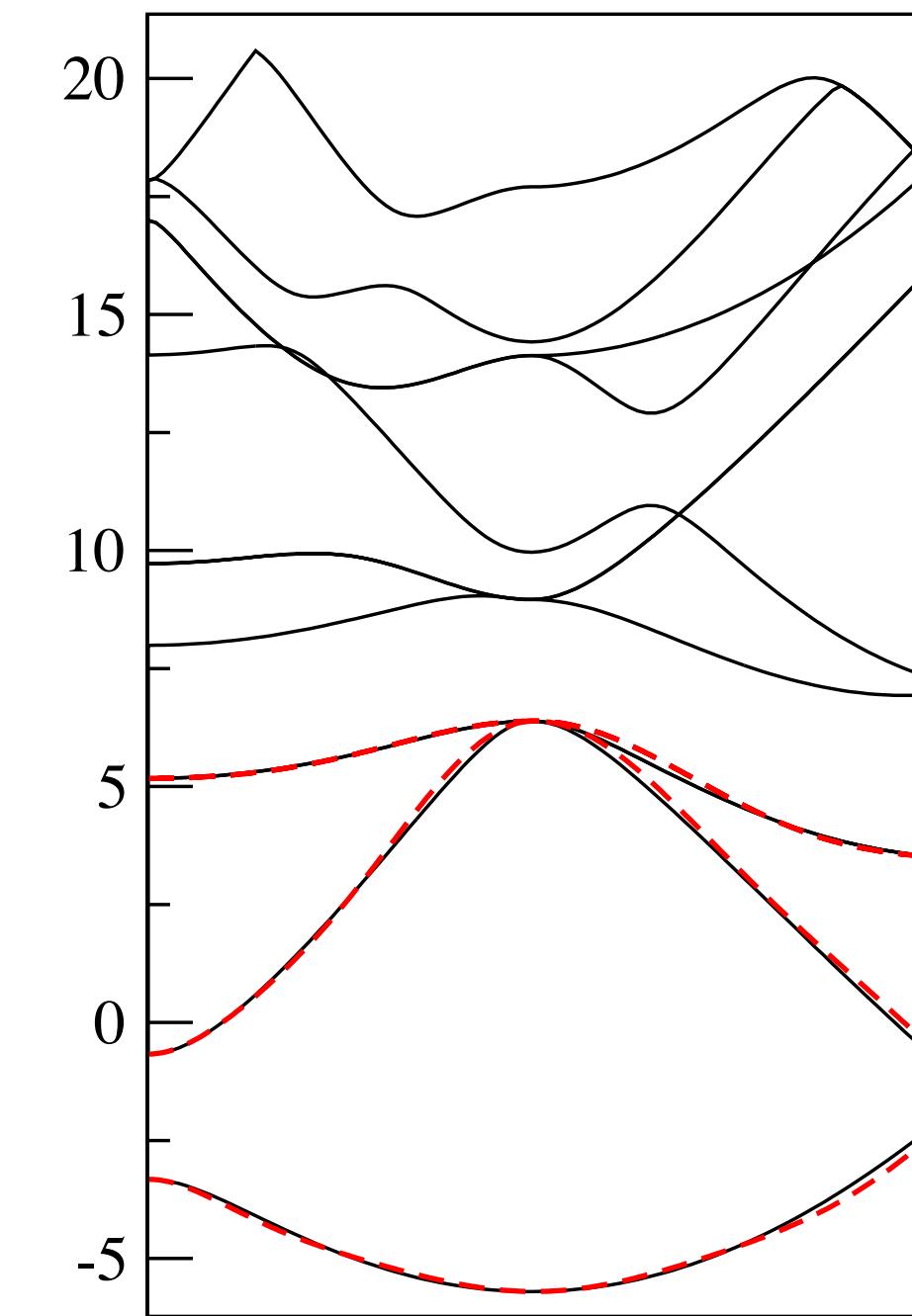
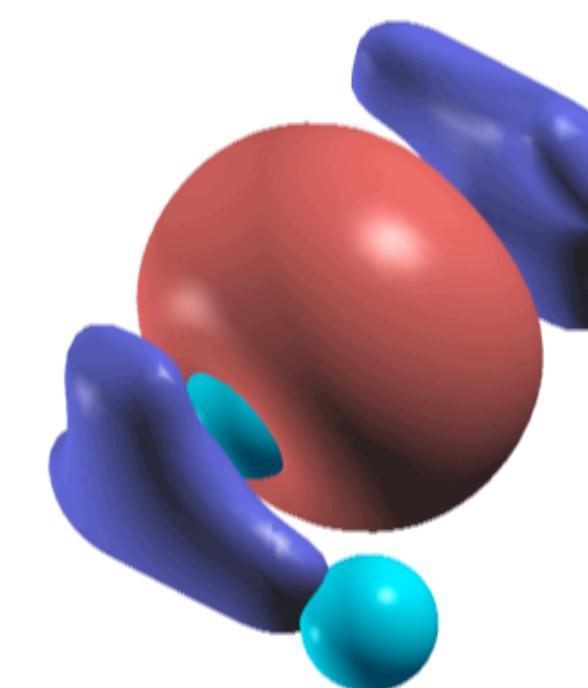
How to run a Wannier90 calculation



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: valence band only (Ex. 1), and valence band+conduction band
- Check the results
- Plot the real-space WFs (using **XCrysDen** or **VESTA**)
 - You will need to run these codes on your computers
- Plot the ab-initio and the interpolated band structure (using **xmGrace** or **gnuplot**)



The Quantum ESPRESSO input file

NAMELISTS

```
&control
  calculation = 'scf'
  restart_mode = 'from_scratch'
  prefix       = 'si'
  pseudo_dir   = 'pseudo/'
  outdir       = 'out/'

/&system
  ibrav      = 0
  nat        = 2
  ntyp       = 1
  ecutwfc    = 25.0
  ecutrho    = 200.0

/&electrons
  conv_thr   = 1.0d-10

/ATOMIC_SPECIES
Si 28. Si.pbe-n-van.UPF
/ATOMIC_POSITIONS crystal
Si -0.25 0.75 -0.25
Si 0.00 0.00 0.00
/K_POINTS automatic
10 10 10 0 0 0
/CELL_PARAMETERS bohr
-5.1 0.0 5.1
0.0 5.1 5.1
-5.1 5.1 0.0
```

→ Type of calculation, location of pseudopotentials and of output files, ...

→ System description (number of atoms and of species, energy cutoffs, ...)

→ Thresholds for charge-density calculations

→ Definition of species ("atom types"), with mass and pseudopotential files

→ Definition of atomic positions

→ Definition of k-points grid (10x10x10 here, no shift = including Gamma)

→ Definition of the cell (FCC here)

The Quantum ESPRESSO input generator

<https://www.materialscloud.org/work/tools/qeinputgenerator>

Quantum ESPRESSO input generator and structure visualizer

- ▶ [About the Quantum ESPRESSO input generator and structure visualizer](#)
- ▶ [Instructions](#)
- ▶ [Acknowledgements](#)

Upload your structure

Upload a crystal structure: no file selected

Select here the file format:

Select here the pseudopotential library:

Select here the magnetism/smearing:

Select here the k-points distance (1/Å)

(and smearing (eV) in case of fractional occupations):

Refine cell (using spglib):

By continuing, you agree with the [terms of use](#) of this service.

The Quantum ESPRESSO input generator

<https://www.materialscloud.org/work/tools/qeinputgenerator>

If you use the results of this tool in a publication, please cite the following works:

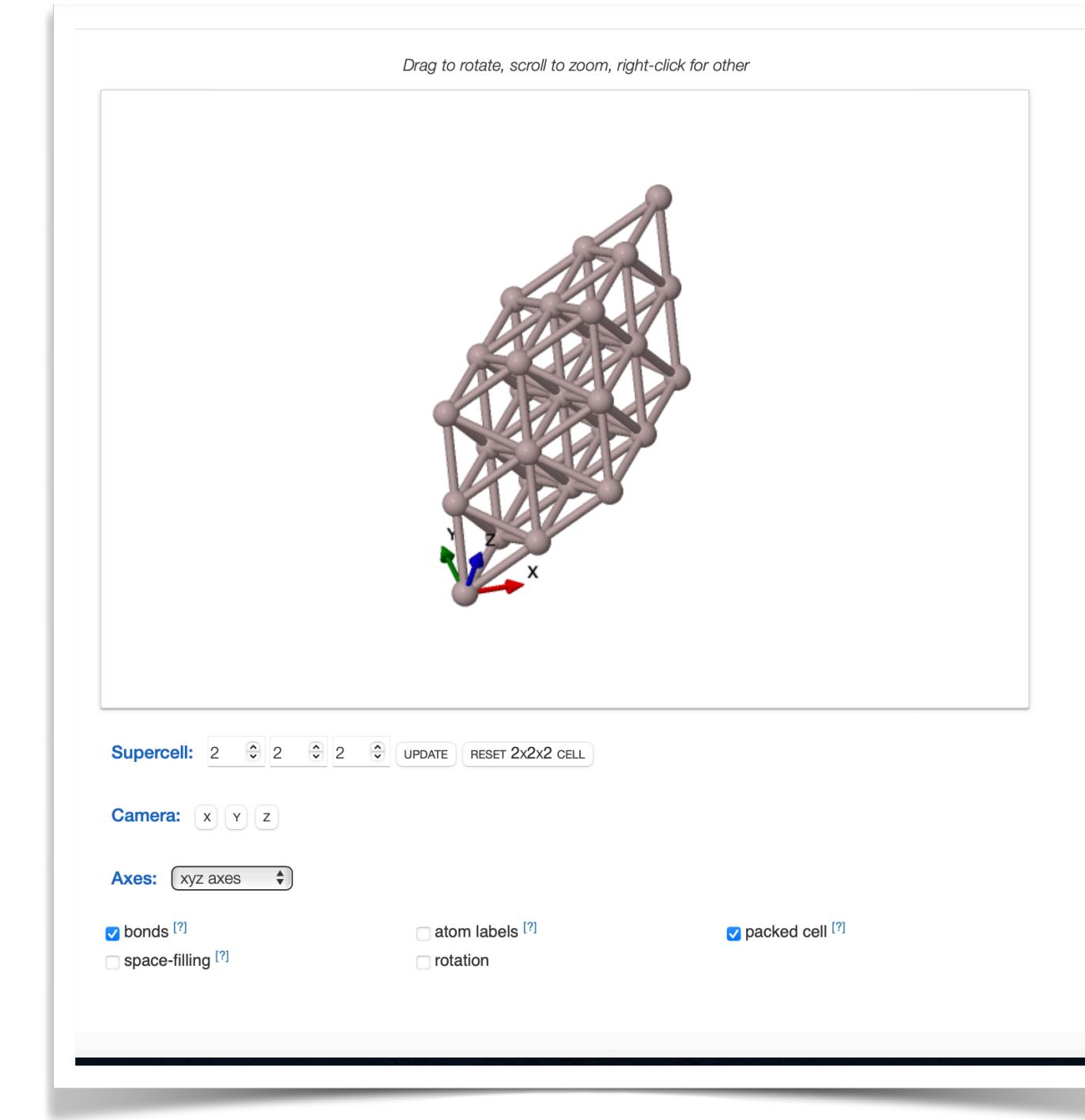
- SSSP (for the pseudopotential library)
G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet and N. Marzari, *npj Computational Materials* **4**, 72 (2018).
WEB: <http://materialscloud.org/sssp>.
- Pseudopotentials:
 - Al.pbesol-n-kjpaw_psl.1.0.0.UPF,
from [Pslibrary 1.0.0](#): A. Dal Corso, *Comput. Mater. Sci.* **95**, 337 (2014).
DOI: [10.1016/j.commatsci.2014.07.043](https://doi.org/10.1016/j.commatsci.2014.07.043), WEB: <http://www.quantum-espresso.org/pseudopotentials>, LICENSE: GNU General Public License (version 2 or later).

[Download zip of input file and pseudopotentials](#) [Change parameters](#) [Choose a different structure](#)

Quantum ESPRESSO PWscf input

[Copy to clipboard](#)

```
&CONTROL
  calculation = 'scf'
  etot_conv_thr =  1.000000000d-05
  forc_conv_thr =  1.000000000d-04
 outdir = './out/'
  prefix = 'aiida'
  pseudo_dir = './pseudo/'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  degauss =  1.4699723600d-02
  ecutrho =  2.400000000d+02
  ecutwfc =  3.000000000d+01
  ibrav = 0
  nat = 1
  nosym = .false.
  ntyp = 1
  occupations = 'smearing'
  smearing = 'cold'
/
&ELECTRONS
  conv_thr =  2.000000000d-10
  electron_maxstep = 80
  mixing_beta =  4.000000000d-01
/
ATOMIC_SPECIES
Al    26.981538 Al.pbesol-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS crystal
Al      0.000000000      0.000000000      0.000000000
K_POINTS automatic
14 14 14 0 0 0
CELL_PARAMETERS angstrom
  2.020000000      2.020000000      0.000000000
  2.020000000      0.000000000      2.020000000
  0.000000000      2.020000000      2.020000000
```



- Return optimal parameters and pseudopotentials from SSSP [1,2]
- Copy-paste and download options
- Also works as a structure visualiser!

[1] <https://www.materialscloud.org/sssp>

[2] G. Prandini*, A. Marrazzo* *et al.*, *npj Comp. Mat.* **4**, 72 (2018)

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:** lengths are **angstrom** (bohr are also accepted), 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
```

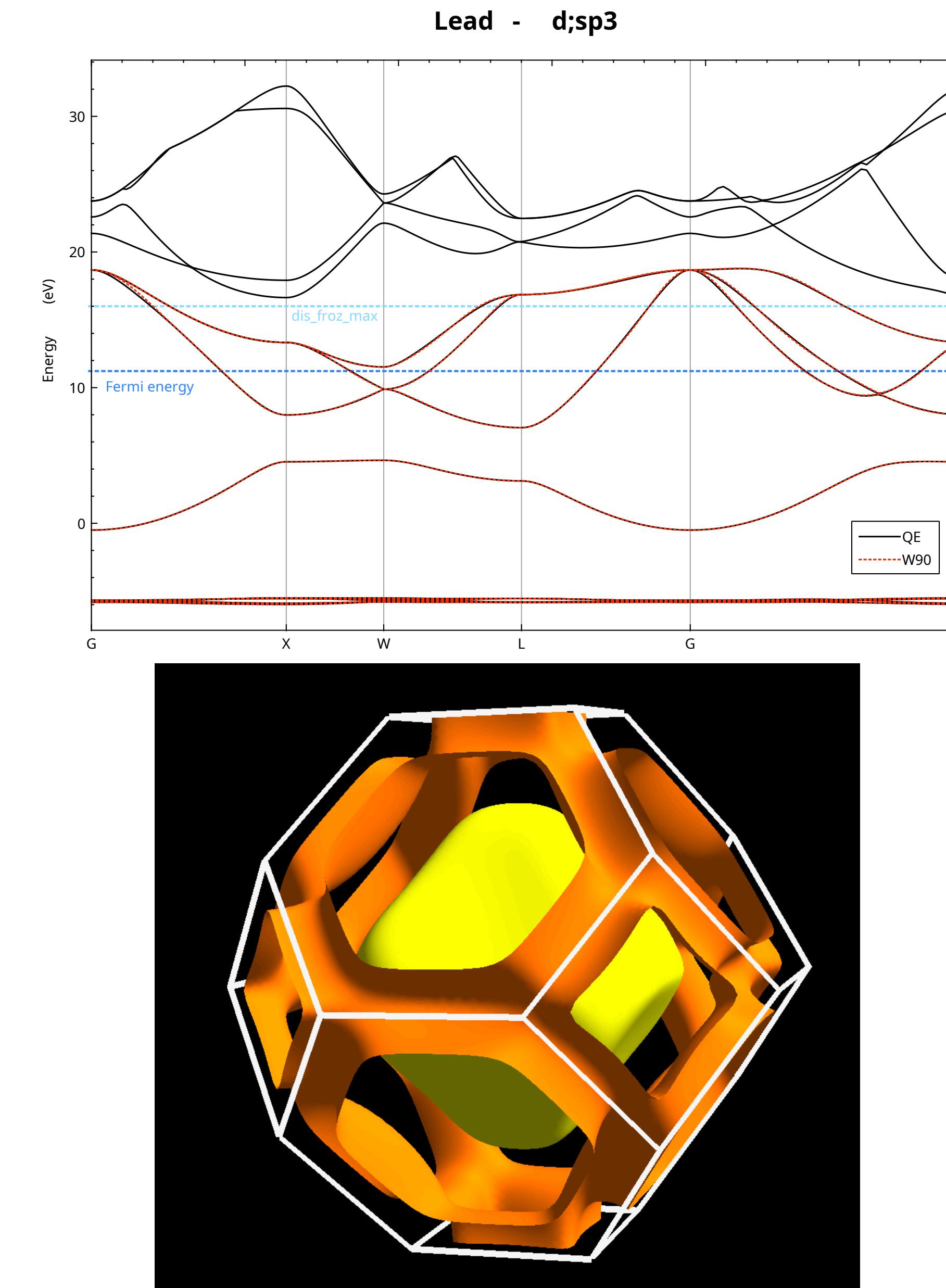
```
mp_grid = XXX XXX XXX
begin kpoints
XXX
XXX
XXX
end kpoints

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
```

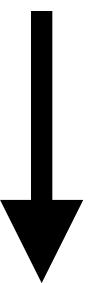
Exercise 3: band structure and Fermi surface of lead

- Interpolate the band structure of lead
- Show the Fermi surface of lead
 - Requires a very dense grid of points in the BZ!
 $\sim 50^3 = 125000$
 - Wannier interpolation essential to compute it efficiently



Wannier interpolation for beyond-DFT methods

Wannier interpolation is particularly useful to calculate **band structure with beyond-DFT methods**, such as **hybrid functionals** (HSE), **Koopmans-compliant functional** and **many-body perturbation theory** (MBPT GW)



- Only in **plain DFT** the potential is actually a functional of the sole charge density, so **the Hamiltonian can be easily diagonalised at any arbitrary k-point**: regular band structure calculation with LDA or PBE.
- **Otherwise, the k-point needs to be part of the grid** used to compute the total energy (hybrids) or the self energy (MBPT). Hence, **dense band structures** can be computed in practice **only through interpolation methods**, such as Wannier interpolation.

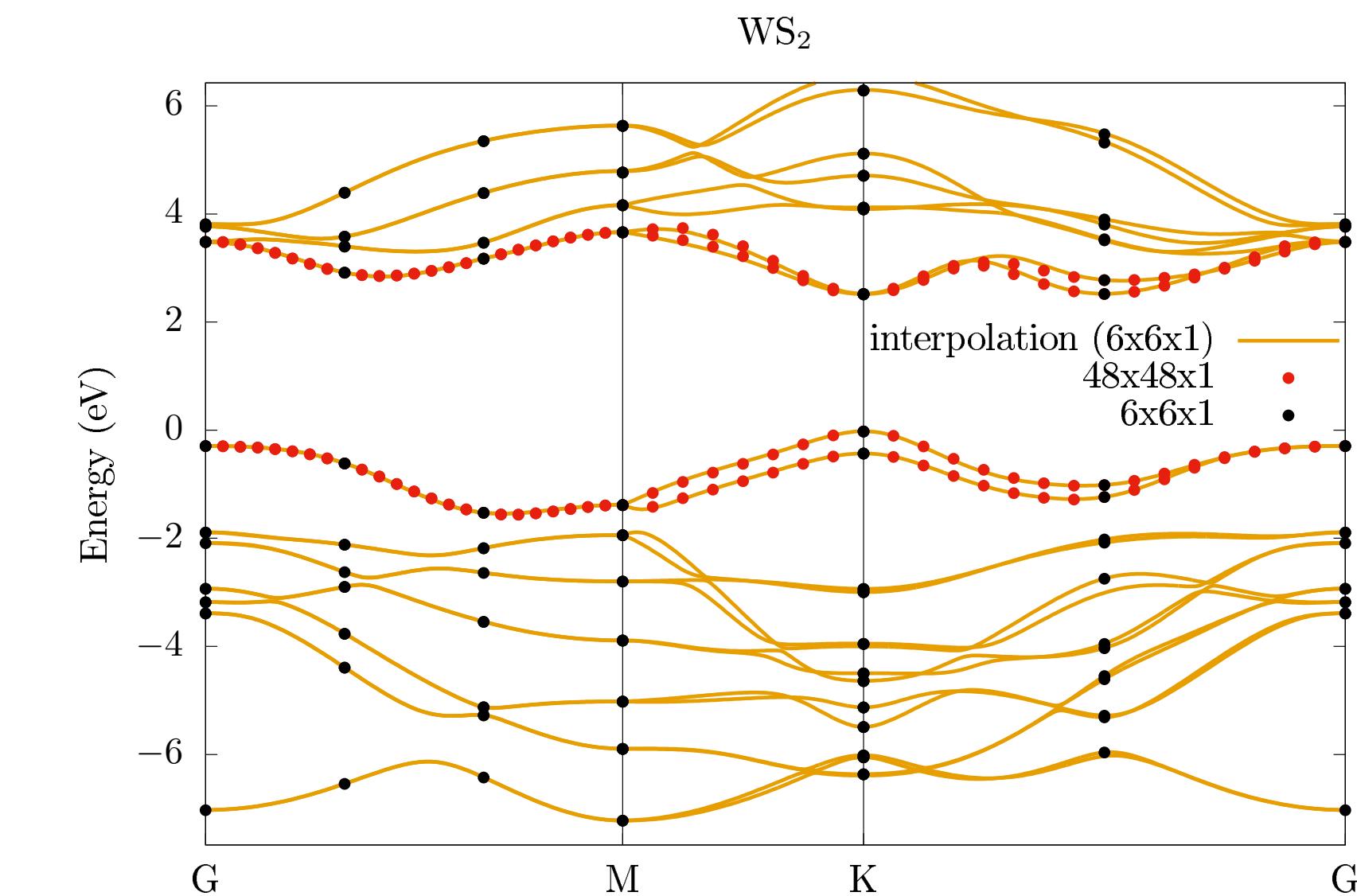
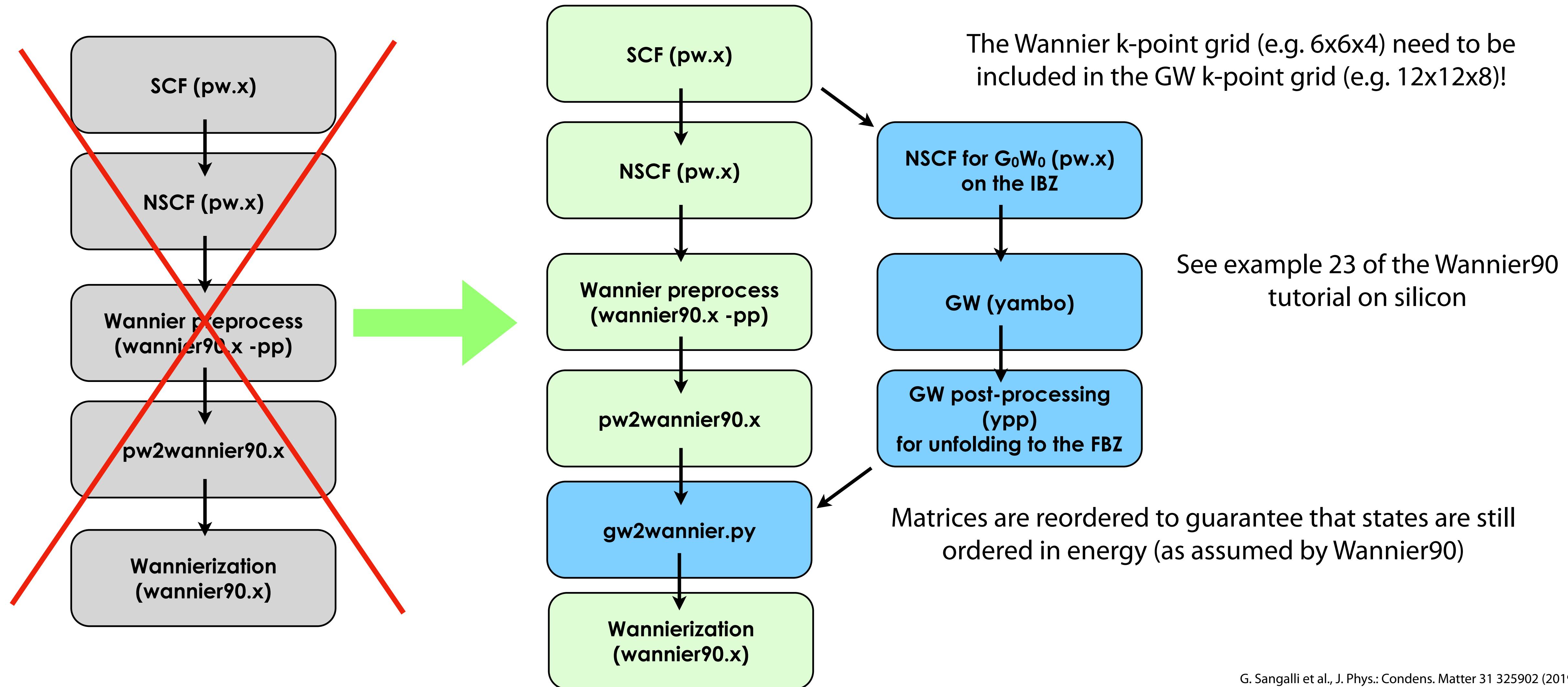


FIG. 6: (Color online). G_0W_0 band structure of monolayer WS_2 including spin-orbit coupling and using $48 \times 48 \times 1$ k -points grid for the self-energy. The orange lines represent Wannier-interpolated bands obtained from 7 QP energies corresponding to a $6 \times 6 \times 1$ grid (black dots), while the red dots shows the QP energies of the full $48 \times 48 \times 1$ grid.

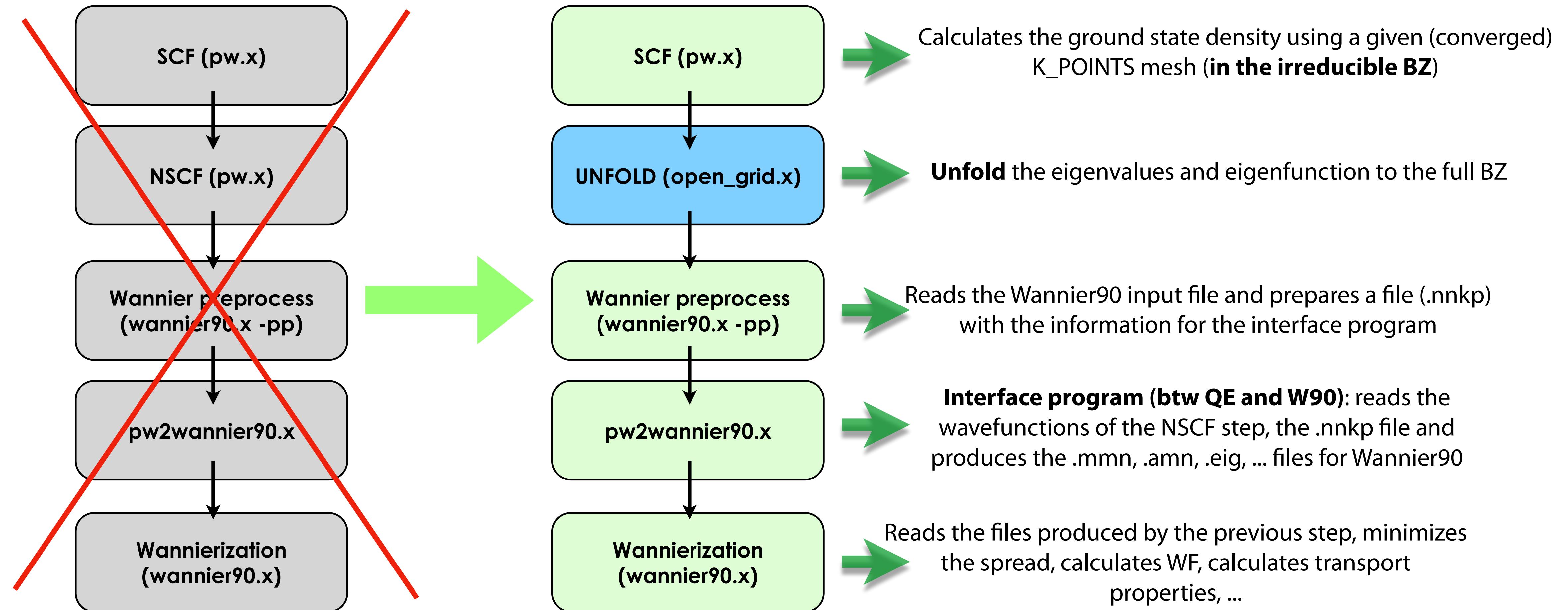
Wannier interpolation for G_0W_0 with QE & YAMBO

G_0W_0 is done on the IBZ, on a (possibly denser) k-point grid, quasi-particle corrections on the (possibly less dense) Wannier grid and unfolded to the full BZ.



Wannier interpolation for hybrid-functionals with QE

No NSCF with hybrids, but unfolding from the IBZ to the FBZ with open_grid.x



Example at https://gitlab.com/QEF/q-e/-/tree/master/PP/examples/W90_open_grid_example

Getting help

- **Today:** ask me and Junfeng :-)
- **From tomorrow on:** www.wannier.org
 - User guide, tutorials (with solutions)
 - Register to the Wannier90 mailing list
 - Actually read the source code!

