The Wannier functions ecosystem: fundamentals & recent developments

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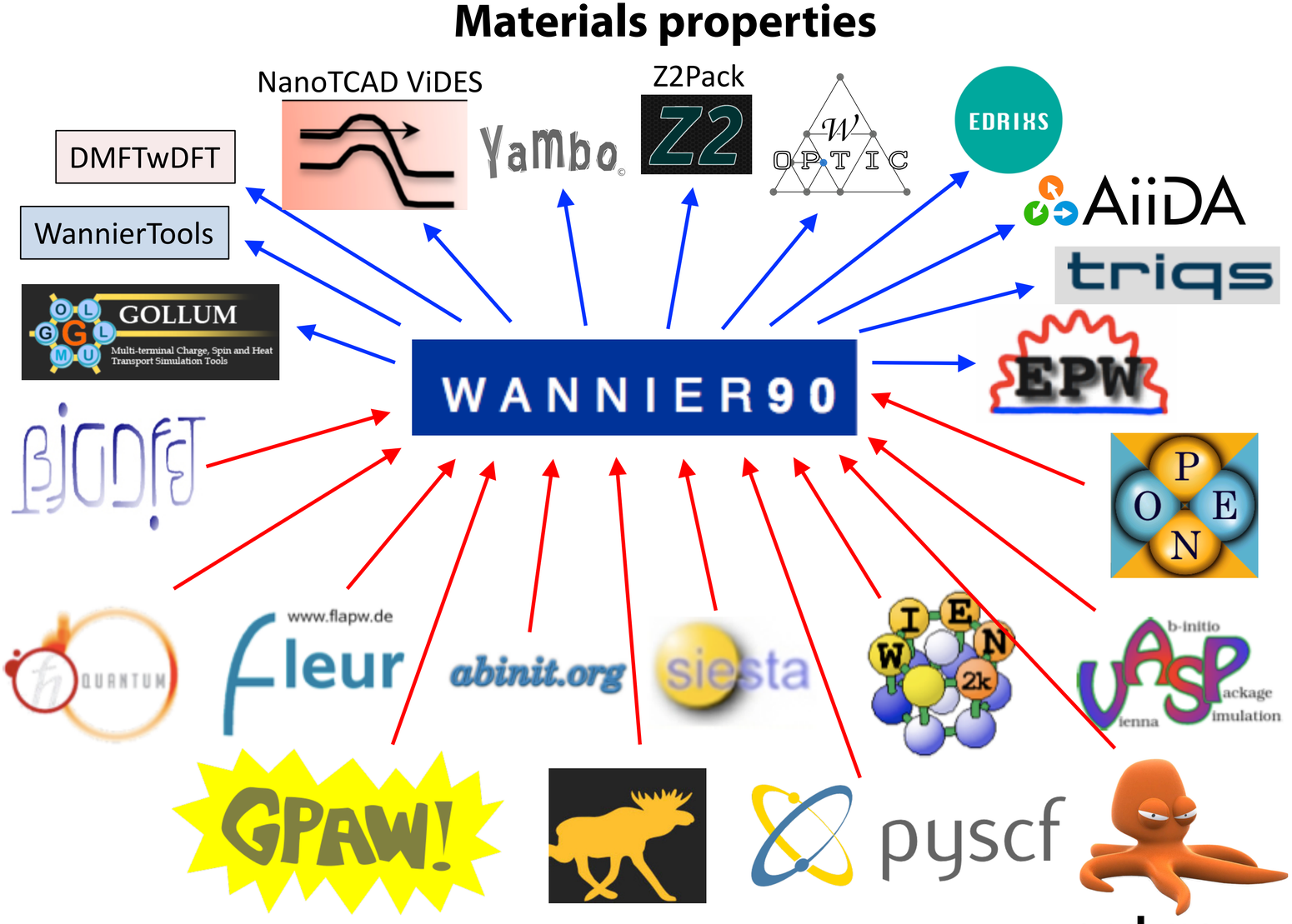
June 14th, 2022
School on Electron-Phonon Coupling from First Principles, Austin (USA)

Wannier90: The center of a software ecosystem



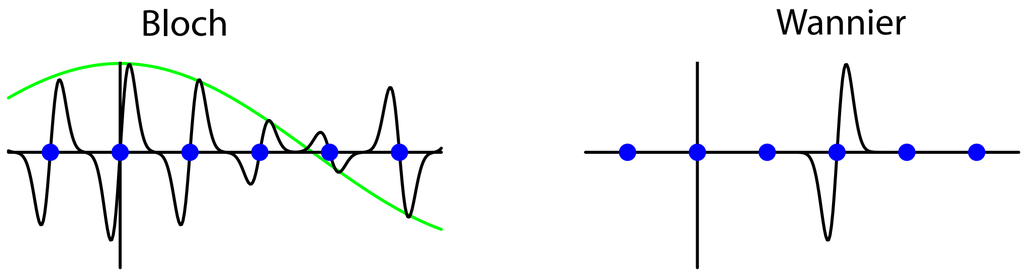
Adapted from Arash Mostofi, Wannier School 2021

Maximally-localised Wannier functions (MLWF) in a nutshell

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

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

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



N. Marzari and D. Vanderbilt, PRB 56, 12847 (1997)
I. Souza., N. Marzari, D. Vanderbilt, PRB 65, 035109 (2001)

Adapted from Wannier 2022 Summer School, by A. Mostofi

N. Marzari et al., Rev. Mod. Phys. 84, 4 (2012)
G. Pizzi et al, JPCM 32, 165902 (2022)

Maximally-localised Wannier functions (MLWF) in a nutshell

Gauge-invariant part of the spread functional

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

Gauge-dependent part of the spread functional

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

minimise!

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

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

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

In principle the overlap matrices $\underline{M_{mn\mathbf{k}}}$ 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)

$\underline{A_{mn\mathbf{k}}}$ directly from SCDM (more later)

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

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

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

N. Marzari et al., Rev. Mod. Phys. 84, 4 (2012)
G. Pizzi et al, JPCM 32, 165902 (2022)

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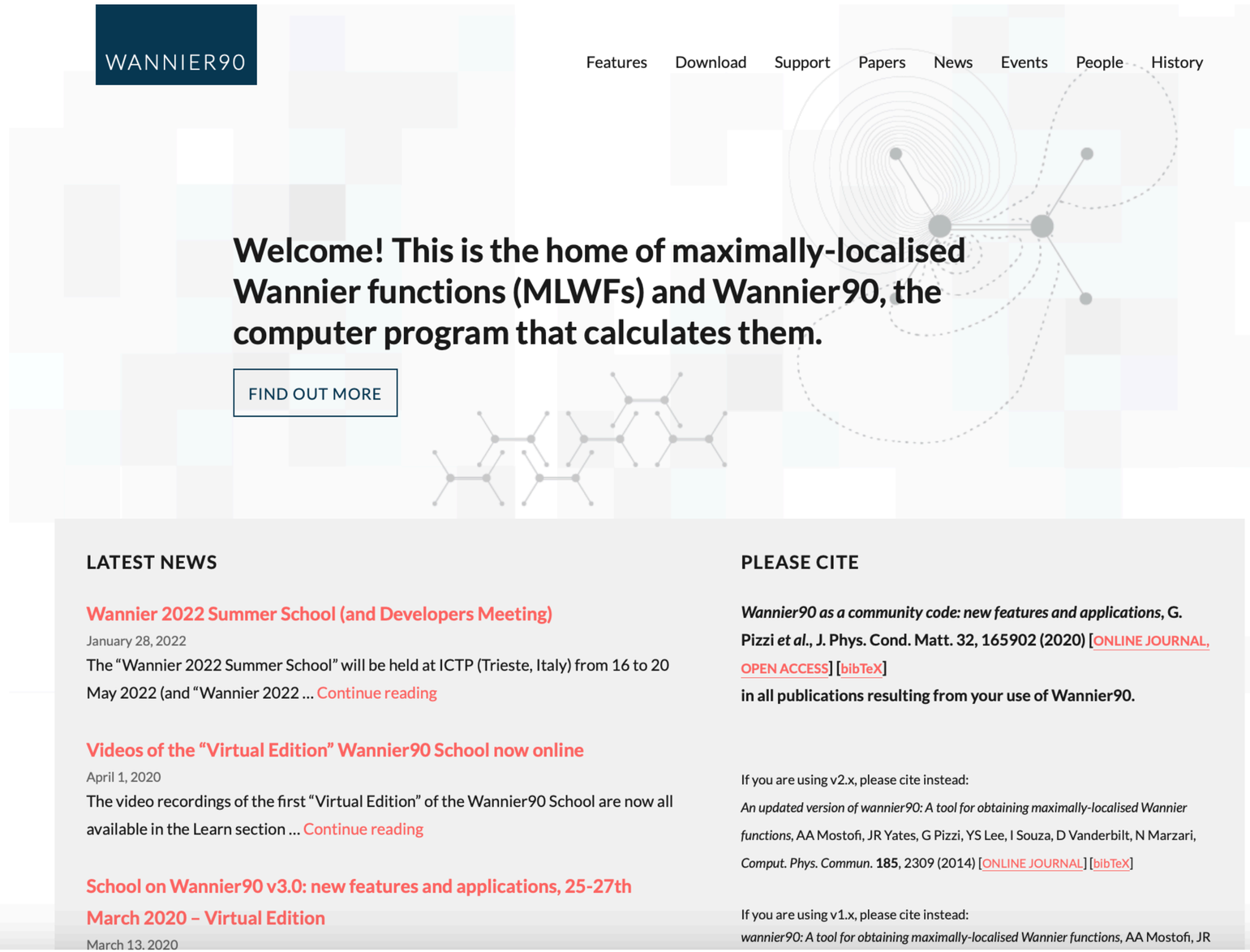

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Latest stable release (5 March 2020): Wannier90 (v3.1.0) [gzipped-tar]

Please note that:

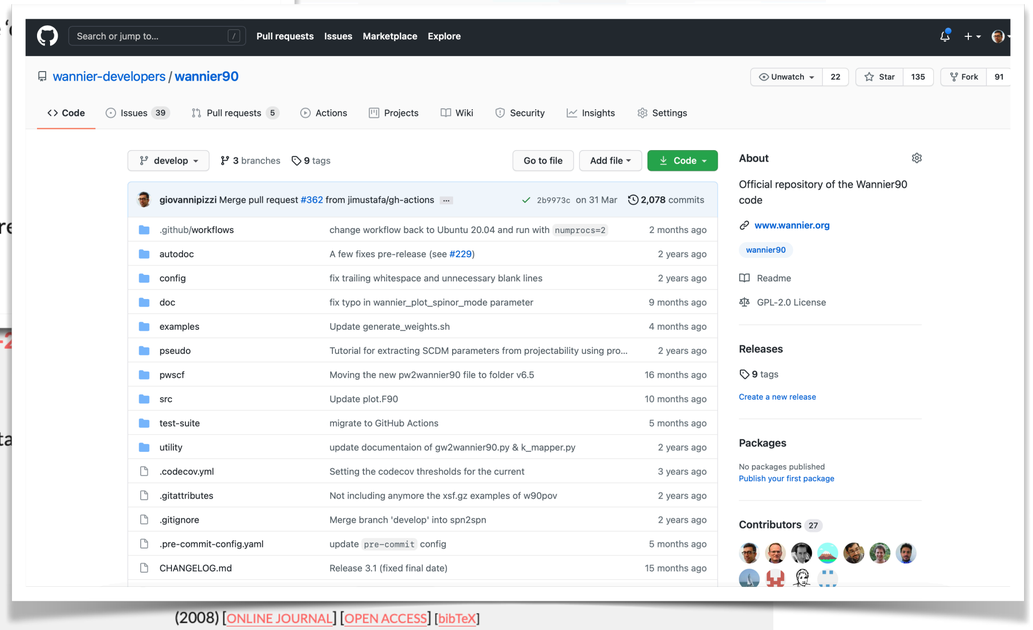
- Wannier90 is released under the GNU General Public License (v2)
- A summary of improvements may be found in CHANGE.log
- Installation instructions may be found in README.install
- The latest User Guide and Tutorial may be found here. They may also be found in the '
  current distribution.

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.

ocalised
90, the

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



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

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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]

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
```

$$\begin{array}{llllllll} G & 0.0 & 0.0 & 0.0 & L & 0.0 & 0.0 & 1.0 \\ L & 0.0 & 0.0 & 1.0 & N & 0.0 & 1.0 & 1.0 \\ \vdots & & & & & & & \end{array}$$

```
end kpoint_path
```

There is no default

2.9.12 integer :: bands_num_points

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April 1, 2020

The video recordings of the first "Virtual Edition" of t
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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, projec

- Outline: *Generate both maximally-localized and projecte*
  bcc Fe. Calculate the total and orbital-projected density
- Directory: `examples/example8/`
- Input Files
  - `iron.scf` *The* PWSCF *input file for the spin-polariz*
  - `iron.nscf` *The* PWSCF *input file to obtain Bloch st*
  - `iron_{up,down}.pw2wan` *Input files for* `pw2wannier`
  - `iron_{up,down}.win` *Input files for* `wannier90` *and*
- Note that in a spin-polarized calculation the spin-up and
  arately. (The more general case of spinor WFs will be tr

1. Run PWSCF to obtain the ferromagnetic ground state of
   `pw.x < iron.scf > scf.out`
2. Run PWSCF to obtain the Bloch states on a uniform k-p
   `pw.x < iron.nscf > nscf.out`

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.*

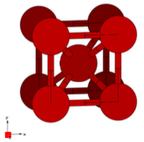

Figure 21: Unit cell of Iron crystal plotted with the XCrySDen program.

1-5 *Converged values for the total spread functional and its components for both spin channels are shown in Tab. 5.* The final state for spin-up MLWFs is

```
 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
 ---------------------------------------------------------------------------
```

and for spin-down MLWFs is

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Comput. Phys. Commun. **185**

If you are using v1.x, please
wannier90: A tool for obtaini
Yates, YS Lee, I Souza, D Va
(2008) [ONLINE JOURNAL] [C

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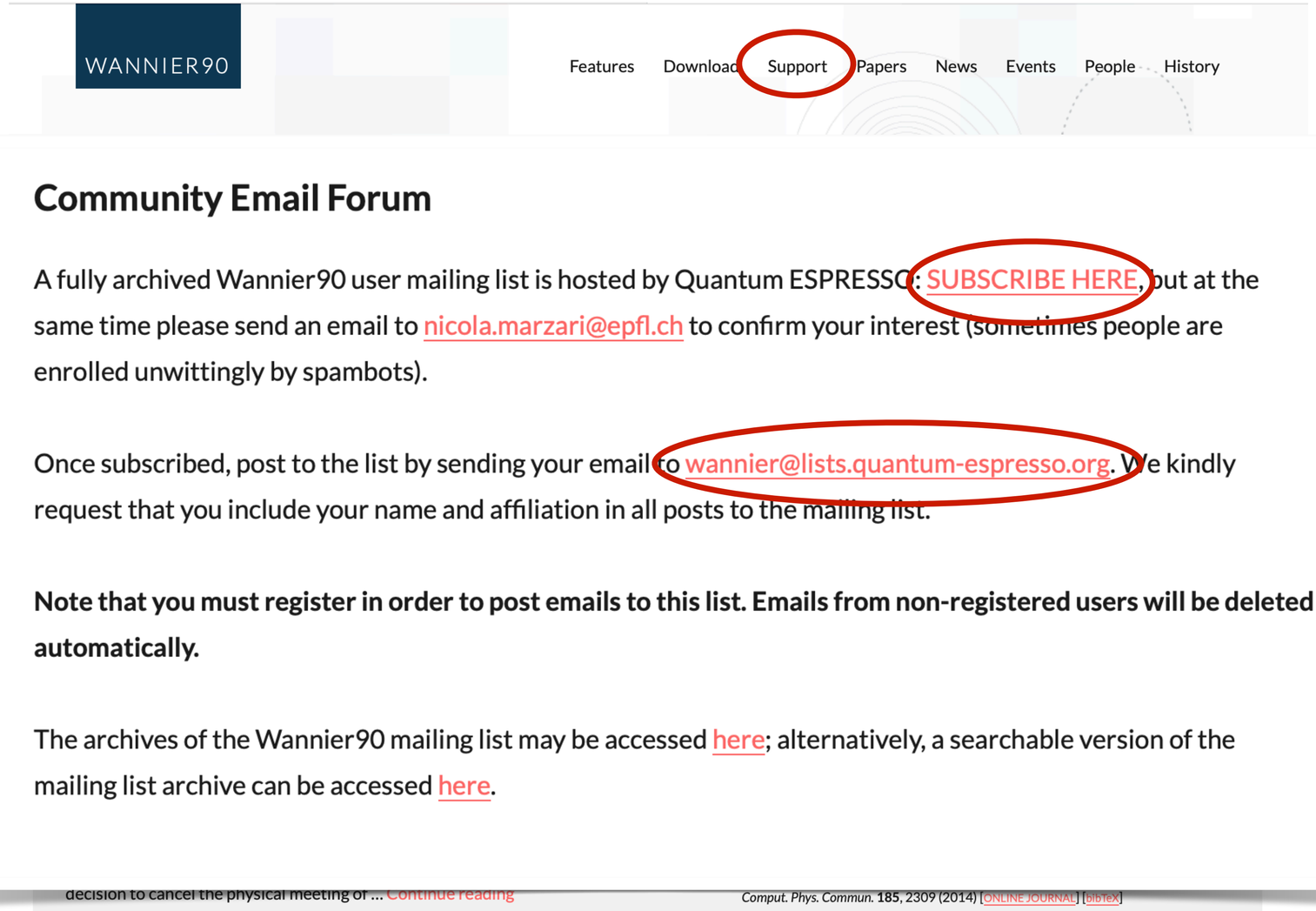

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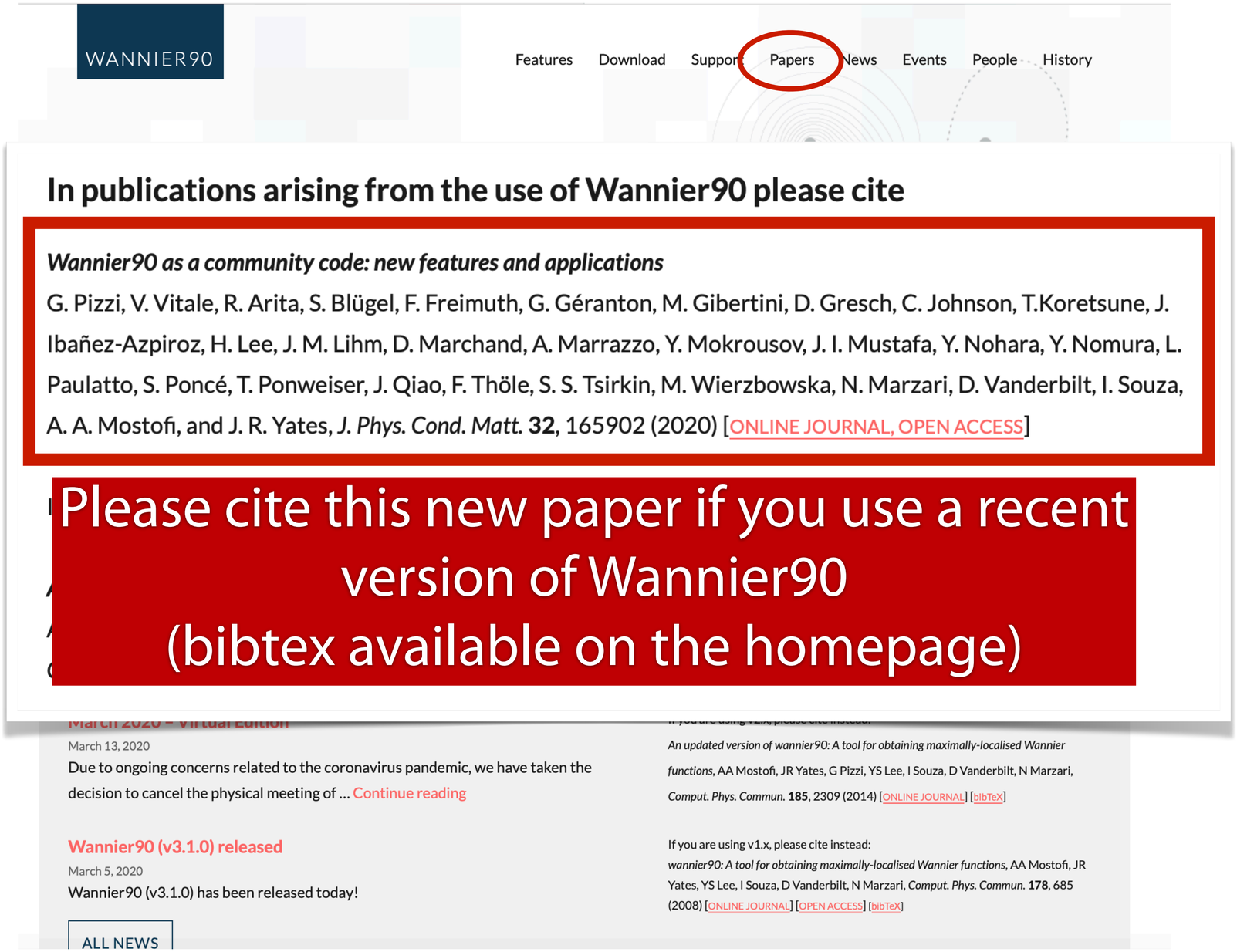


A community effort!

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**

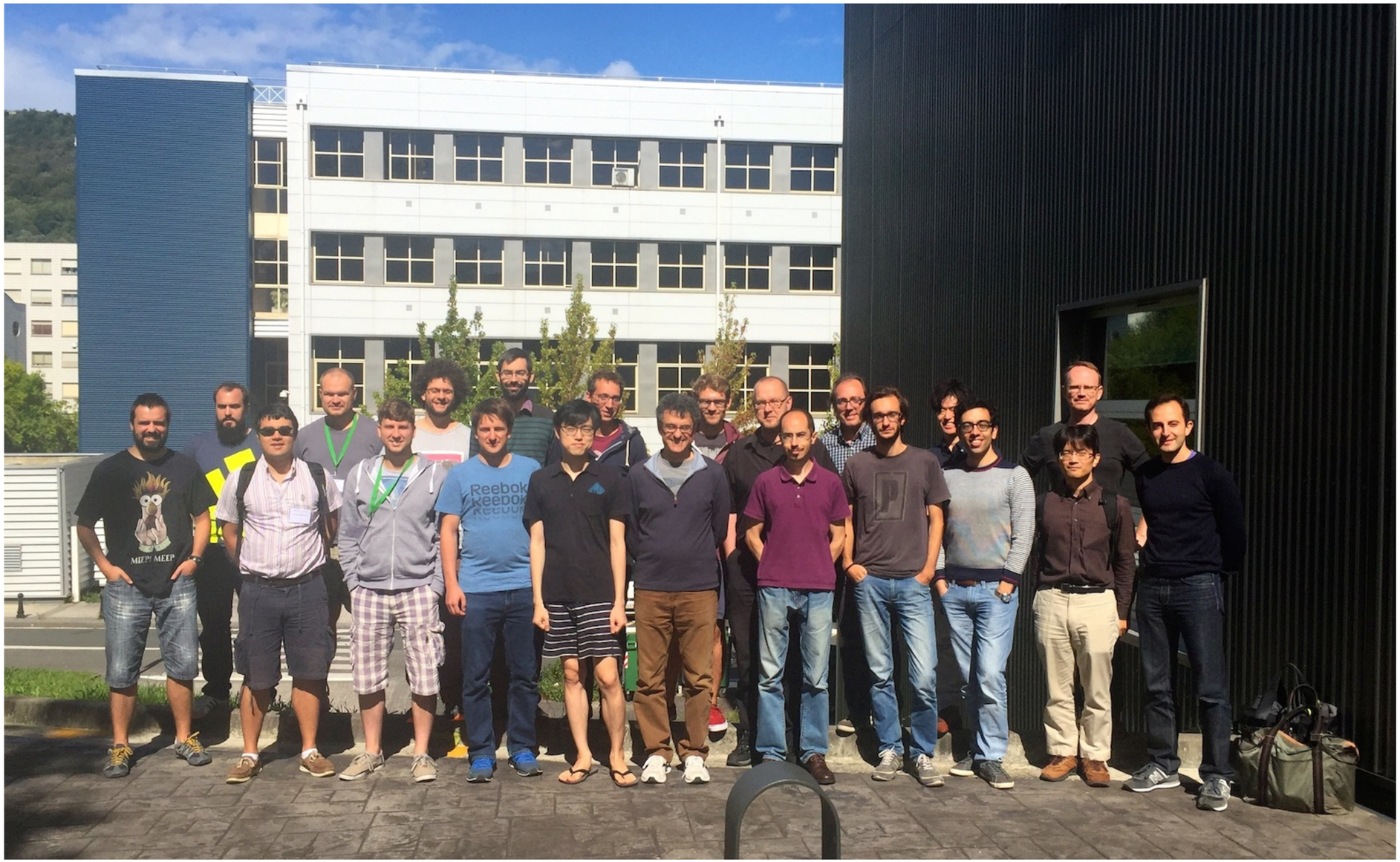
By citing the new paper, you acknowledge
the important work of all these coauthors!

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 Blügel[6], Frank Freimuth[6], Guillaume Géranton[6], Marco Gibertini[1,7], Dominik Gresch[8], Charles Johnson[9], Takashi Koretsune[10,11], Julen Ibañez-Azpiroz[12], Hyungjun Lee[13,14], Jae-Mo Lihm[15], Daniel Marchand[16], Antimo Marrazzo[1], Yuriy Mokrousov[6,17], Jamal I Mustafa[18], Yoshiro Nohara[19], Yusuke Nomura[4], Lorenzo Paulatto[20], Samuel Poncé[21], Thomas Ponweiser[22], Junfeng Qiao[23], Florian Thöle[24], Stepan S Tsirkin[12,25], Małgorzata Wierzbowska[26], Nicola Marzari[1,29], David Vanderbilt[27,29], Ivo Souza[12,28,29], Arash A Mostofi[3,29] and Jonathan R Yates[21,29]

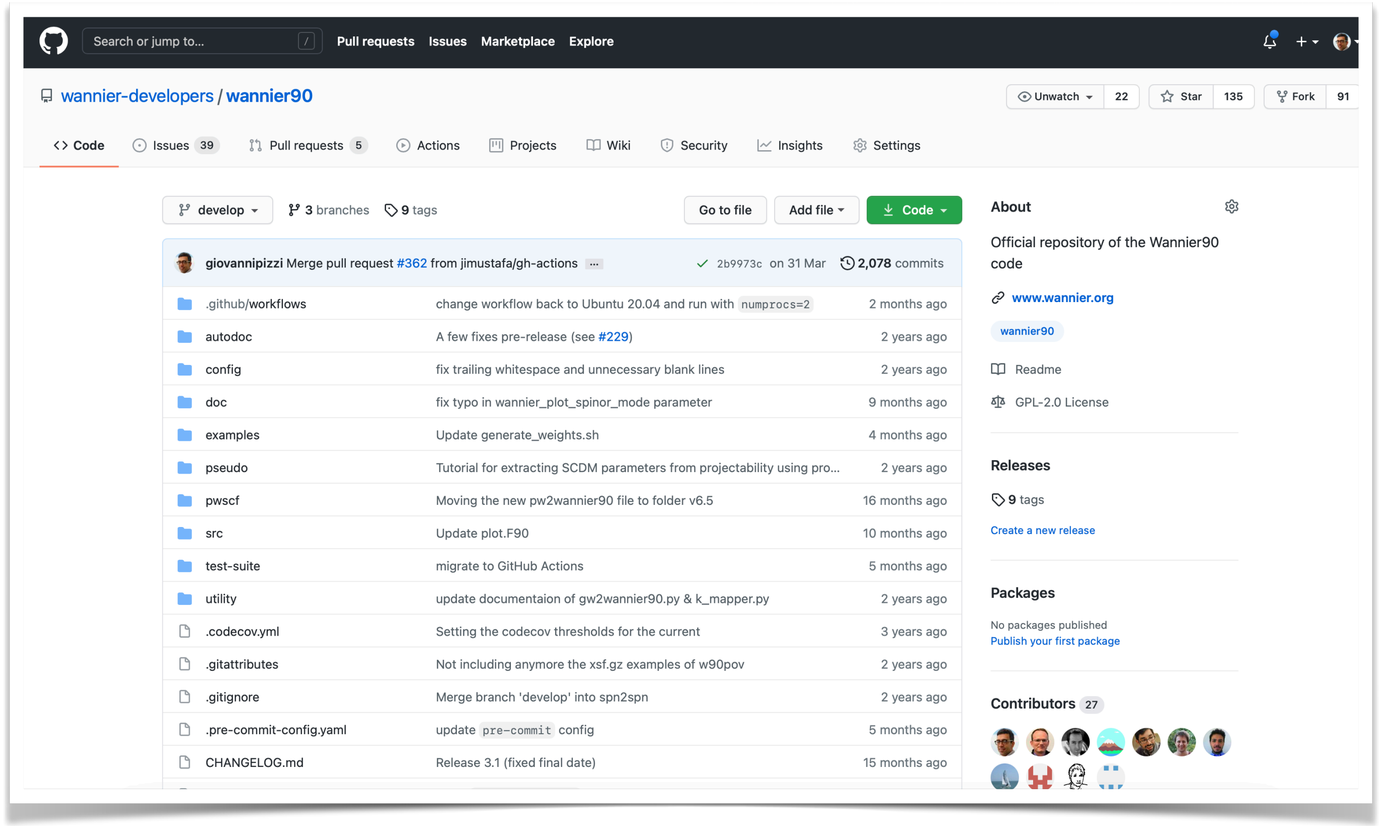
San Sebastian 2016: Wannier Coding Week



Wannier90 goes on GitHub!

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:

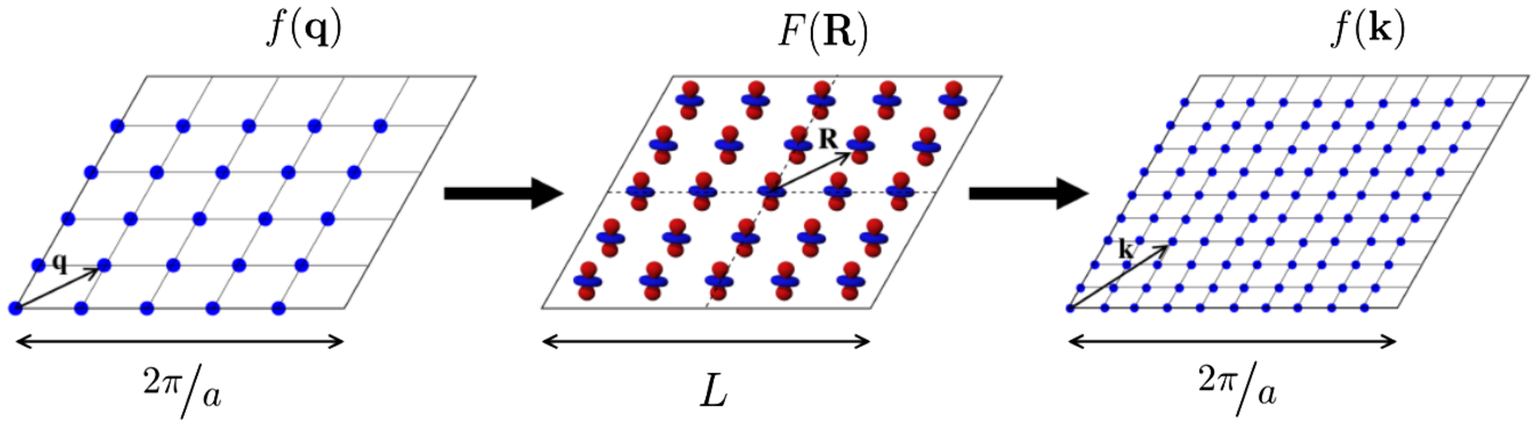
- Berry curvature [REF]
- Anomalous Hall conductivity [REF]
- Orbital magnetisation [REF]
- Shift currents [REF]
- Gyrotropic effects [REF]

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).



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

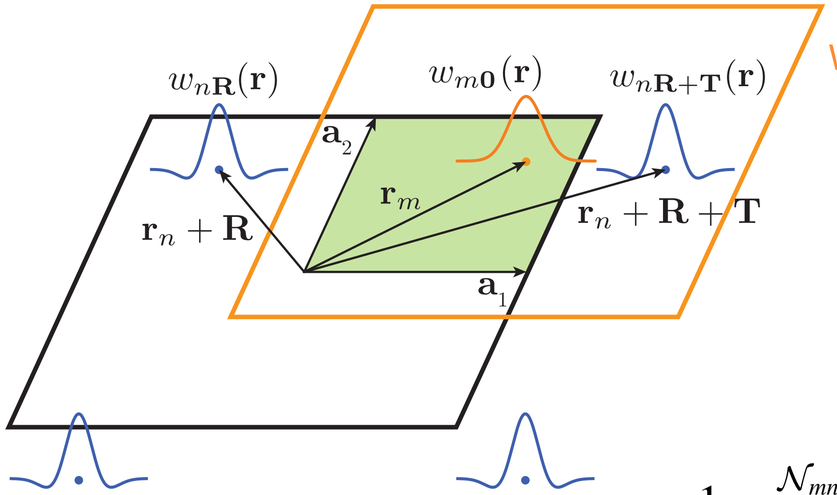
$$H_{mn\mathbf{k}} = \sum_{\mathbf{R}'} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}'} \widetilde{H}_{mn\mathbf{R}'}$$

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

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

N. Marzari et al., Rev. Mod. Phys. 84, 4 (2012)
G. Pizzi et al, JPCM 32, 165902 (2020)

Improved Wannier interpolation by minimal-distance replica selection

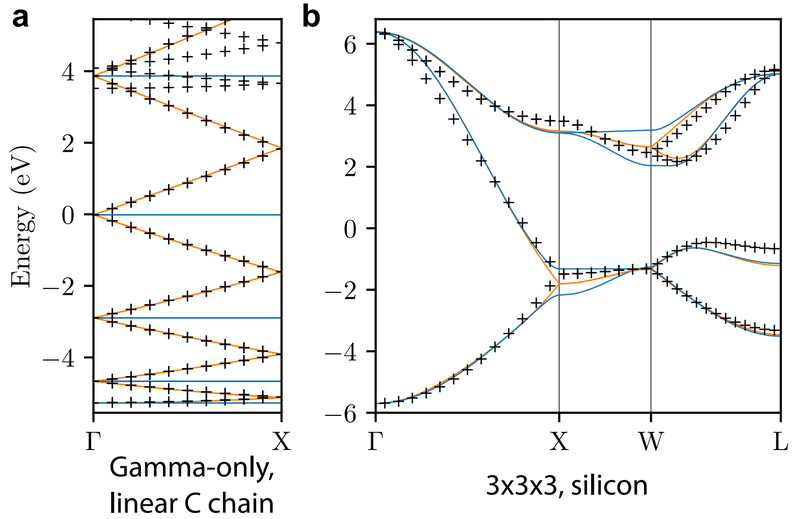


Wigner-Seitz supercell

$$H_{mn\mathbf{k}} = \sum_{\mathbf{R}'} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}'} \widetilde{H}_{mn\mathbf{R}'} \longrightarrow H_{mn\mathbf{k}} = \sum_{\mathbf{R}} \frac{1}{\mathcal{N}_{mn\mathbf{R}}} \sum_{j=1}^{\mathcal{N}_{mn\mathbf{R}}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{R}+\mathbf{T}^{(j)}_{mn\mathbf{R}})} \widetilde{H}_{mn\mathbf{R}}$$

$\left\{\mathbf{T}^{(j)}_{mn\mathbf{R}}\right\}$ vectors 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)



Gamma-only, linear C chain

3x3x3, silicon

Clear example: gamma-only $H_{mn\mathbf{k}} = \frac{\widetilde{H}_{mn\mathbf{0}}}{\mathcal{N}_{mn\mathbf{0}}} \sum_{j=1}^{\mathcal{N}_{mn\mathbf{0}}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{T}^{(j)}_{mn\mathbf{0}}}$

Better interpolation and degeneracies, especially for very coarse grids

G. Pizzi et al, JPCM 32, 165902 (2020)

Symmetry-adapted Wannier functions

- **MLWF**: maximally-localised Wannier functions
- **SAWF**: symmetry-adapted Wannier functions

  -> additional constraints on the unitary matrices $U_{\mathbf{k}}$ during the spread minimisation

  (R. Sakuma, PRB 87, 235109 (2013))

represents how the Bloch states are transformed by the symmetry operation g

$$U_{\mathbf{k}} D_{\mathbf{k}}(g_{\mathbf{k}}) = \widetilde{d}_{\mathbf{k}}(g_{\mathbf{k}}) U_{\mathbf{k}}, \quad g_{\mathbf{k}} \in G_{\mathbf{k}}$$

is the matrix representation of the symmetry operation g

- **SLWF**: selectively-localised Wannier functions

  -> selective localisation of a subset of the Wannier functions

  (R. Wang et al, PRB 90 165125 (2014))
- **SLWF+C**: " with constrained centres

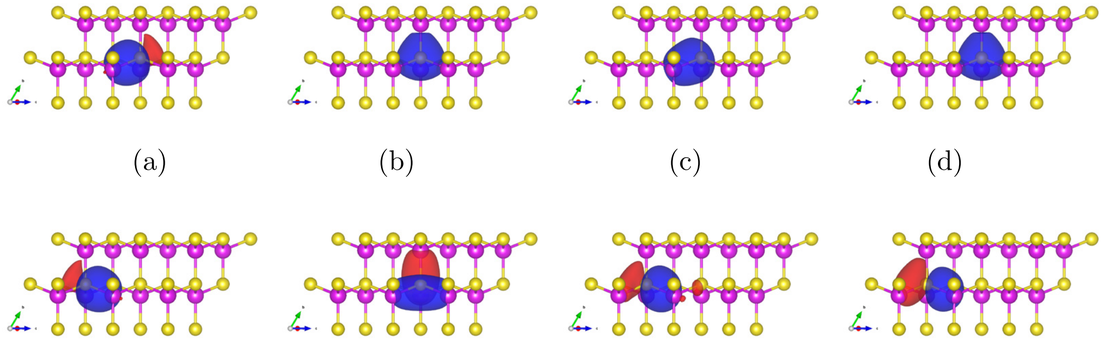
  -> penalty term on the deviation from the predefined centres

$$\Omega'_{\lambda} = \sum_{n=1}^{J'<J} [\langle w_{n\mathbf{0}} | r^2 | w_{n\mathbf{0}} \rangle - |\langle w_{n\mathbf{0}} | \mathbf{r} | w_{n\mathbf{0}} \rangle|^2 + \lambda (\bar{\mathbf{r}}_n - \mathbf{x}_n)^2]$$

Symmetry-adapted Wannier functions

- **MLWF**: maximally-localized Wannier function
- **SAWF**: symmetry-adapted Wannier functions
- **SLWF**: selectively-localized Wannier functions
- **SLWF+C**: " with constrained centres

GaAs, 4 valence states



(a) (b) (c) (d)

(e) (f) (g) (h)

Method		$\bar{\mathbf{r}}$ [Å]	$\langle r^2\rangle - \bar{r}^2$ [Å^2]		$\bar{\mathbf{r}}$ [Å]	$\langle r^2\rangle - \bar{r}^2$ [Å^2]	Ω [Å^2]
MLWF	(a)	(–0.857,0.857,0.857)	1.78	(e)	(0.857,–0.857,0.857)	1.78	7.12
SAWF	(b)	(–1.413,1.413,1.413)	1.64	(f)	(–1.413,1.413,1.413)	2.83	10.14
SLWF	(c)	(–0.89, 0.89, 0.89)	1.42	(g)	(0.89,–0.89,0.92)	2.14	9.8
SLWF+C	(d)	(–1.413,1.413,1.413)	1.63	(h)	(1.23,–1.23,1.08)	2.72	7.87

G. Pizzi et al,
JPCM 32, 165902 (2020)

Hunting for projections

- Usually, code **needs user to specify initial projections** (guesses for the minimisation procedure)
- This needs a lot of chemical understanding and experience. Biggest challenges for new users, and very hard to automate
- Recently: **SCDM** method (selected columns of the density matrix) [1,2] proposed, aiming at automatically finding Wannier functions

Some recent emails from the Wannier90 mailing list:

Dear Experts,
How can I define the correct projection of particular material? […]

Dear Sir,
I need to know the correct projection of Graphene for a converged wannier calculation. […]

Dear Wannier Community,
[...]
My question is how do I define three projections for the half-filled p states of the two As atoms?

[1] Damle, A., Lin, L. & Ying, L. Compressed representation of Kohn–Sham orbitals via selected columns of the density matrix. *Journal of Chemical Theory and Computation* 11, 1463–1469 (2015).
[2] Damle, A. & Lin, L. Disentanglement via entanglement: A unified method for Wannier localization. *Multiscale Modeling & Simulation* 16, 1392–1410 (2018).

Overview of the SCDM method

Number of occupied ("valence") states

density matrix (DM): $P = \sum_{i=1}^{N} |\psi_i\rangle \langle\psi_i|$

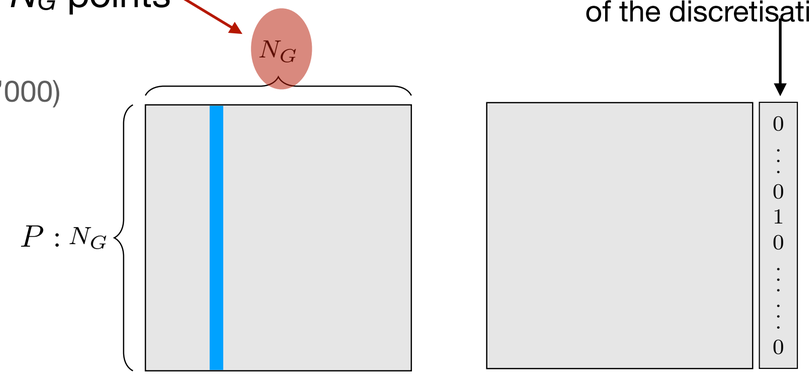
It is a projector (on the valence subspace):

$$P = P^2,\ P = P^*$$

Discretisation on a real-space grid with with N_G points

(N~10-100, N_G~100'000-1'000'000)

- Columns of P ("**CDM**"):



Wavefunction localized only on i-*th* point of the discretisation grid (a "delta")

Therefore, the *j*-th column of the DM is the *projection of this very localized function on the valence eigenspace*

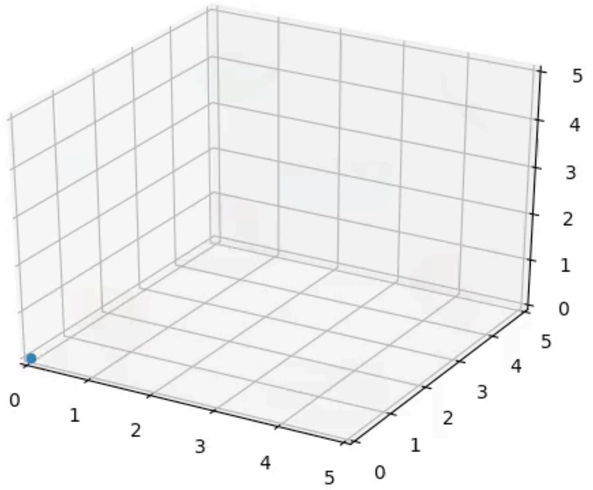
These projections (the columns) are localized! (but are not orthogonal)

Reason: "nearsightedness" of the density matrix

- J. Des Cloizeaux, Phys. Rev. 135, A685 (1964)
- E. Prodan and W. Kohn, Nearsightedness of electronic matter, PNAS 102, 11635 (2005).
- M. Benzi, P. Boito, and N. Razouk. Decay properties of spectral projectors with applications to electronic structure. SIAM Rev., 55, 3 (2013).
- A. Marrazzo and R. Resta, Local theory of the insulating state, Phys. Rev. Lett. 122, 16602 (2019)

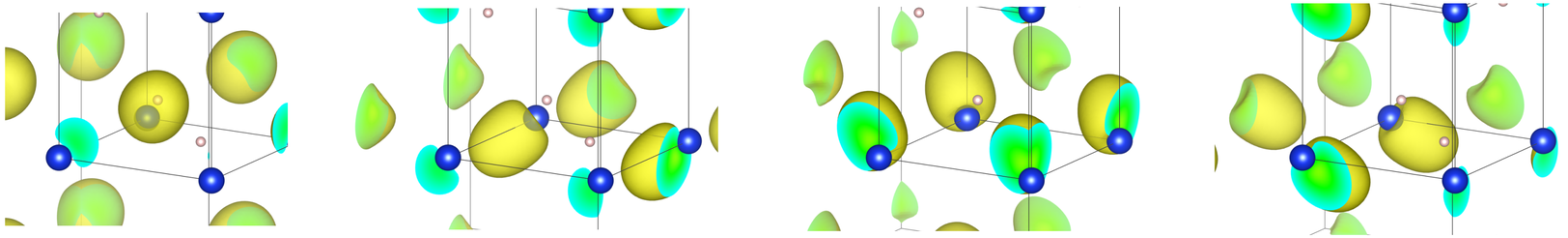
SCDM - columns of the density matrix

Silane, Γ-only



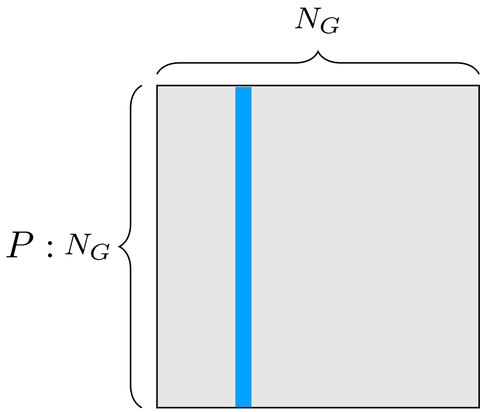
- *Isosurface* of square modulus at 1/10 of the maximum
- *Transparency* to indicate the norm (transparent: zero norm; opaque: max norm)
- *Dot*: real-space position associated with the DM column

For comparison: The four MLWF



SCDM - using N CDMs to span the valence subspace

1. Columns are localised



2. Therefore: any N linearly-independent columns yield a *localized* basis for the span of valence states (because P is a projector on the valence subspace)

However: if I pick N random columns (that are NOT orthogonal), I might get "very overlapping" (almost linearly-dependent) columns.

How can we select the "most representative" columns?
(intuitively: *the ones with less overlap*)

SCDM - using N CDMs to span the valence subspace

Main idea: use the QRCP algorithm (QR decomposition with column-pivoting)
(implemented in LAPACK: *ZGEQP3*)

$$P\Pi = QR$$

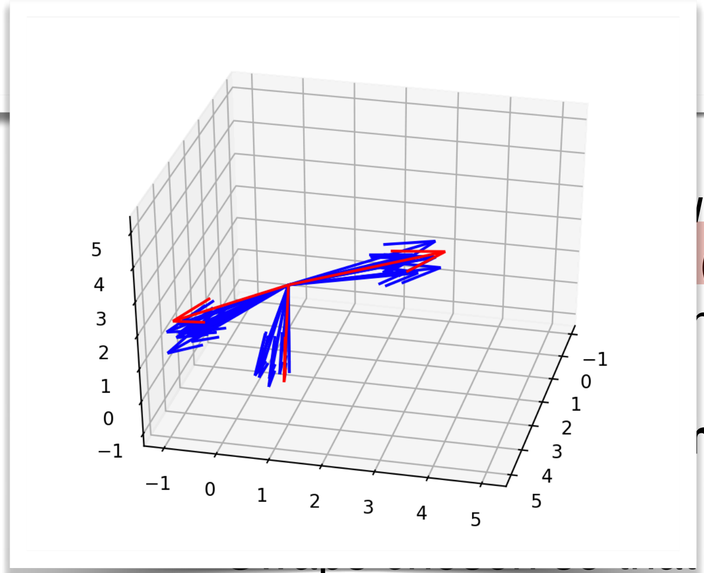
- *P*: density matrix (*input*)
- Π: permutation matrix (**swaps columns**)
- *Q*: orthogonal/unitary matrix (***columns* are orthogonal**: Q*Q=I)
- *R*: **upper-triangular matrix**

- Swaps chosen so that **diagonal elements of *R* are decreasing**: $|R_{11}| > |R_{22}| > \ldots$

SCDM - using N CDMs to span the valence subspace

Main idea: use the QRCP algorithm (QR decomposition with column-pivoting)

ZGEQP3)



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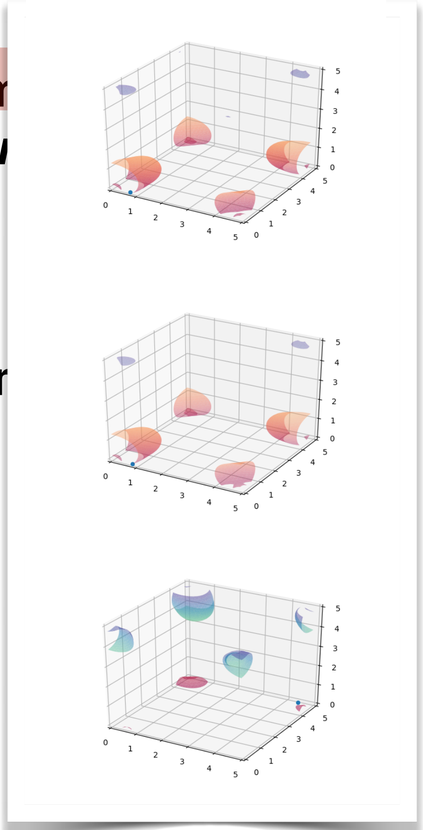


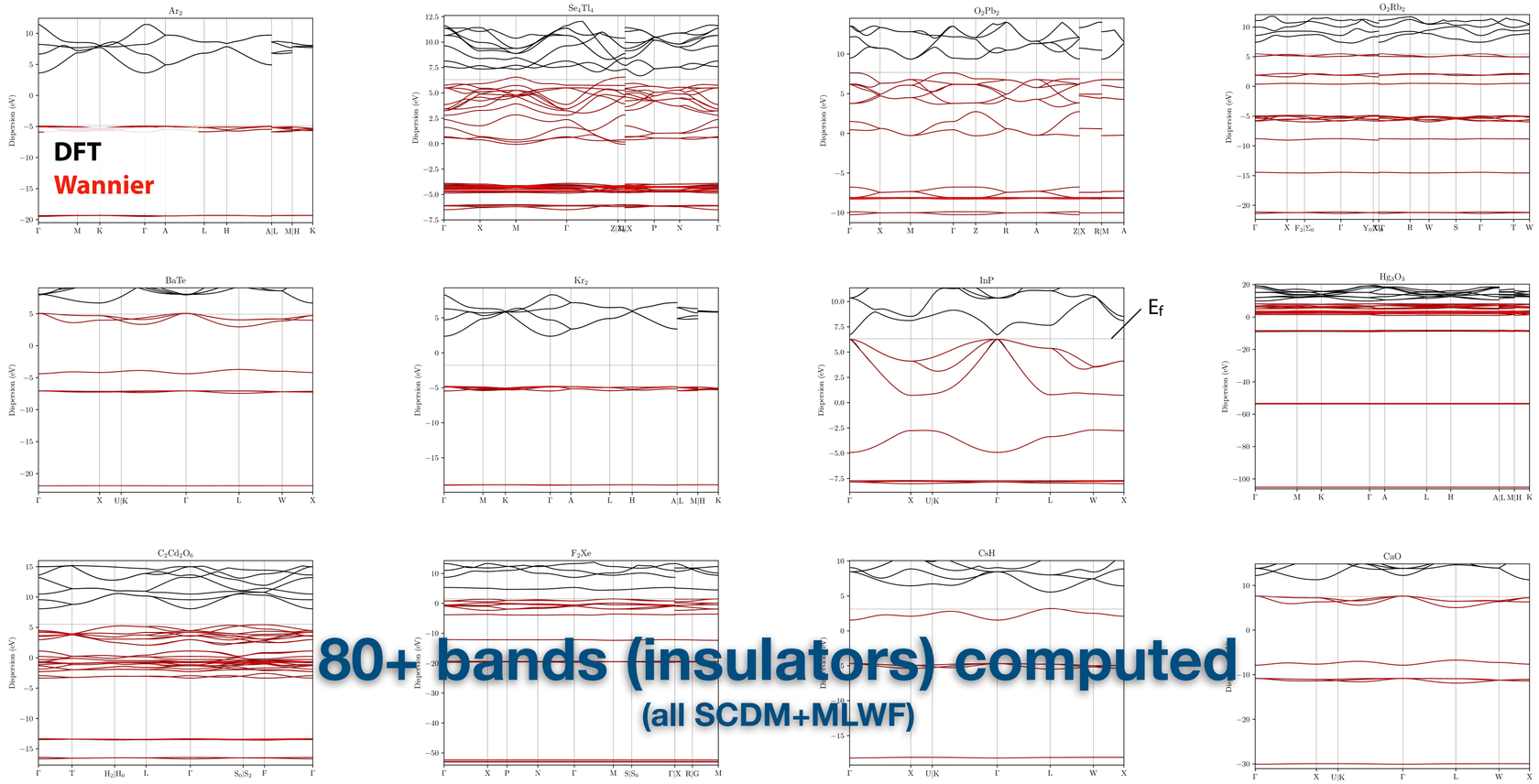
The rule for swaps finds the most representative ("most orthogonal") columns: SCDM

A final orthonormalisation (Löwdin) completes the algorithm

The method can be extended to the case of k-points

SCDM - results for insulators

Results from our high-throughput validation
using AiiDA



80+ bands (insulators) computed
(all SCDM+MLWF)

V. Vitale, G. Pizzi, A. Marrazzo et al., Automated high-throughput Wannierisation,
npj Computational Materials 6, 66 (2020)

SCDM - entangled bands

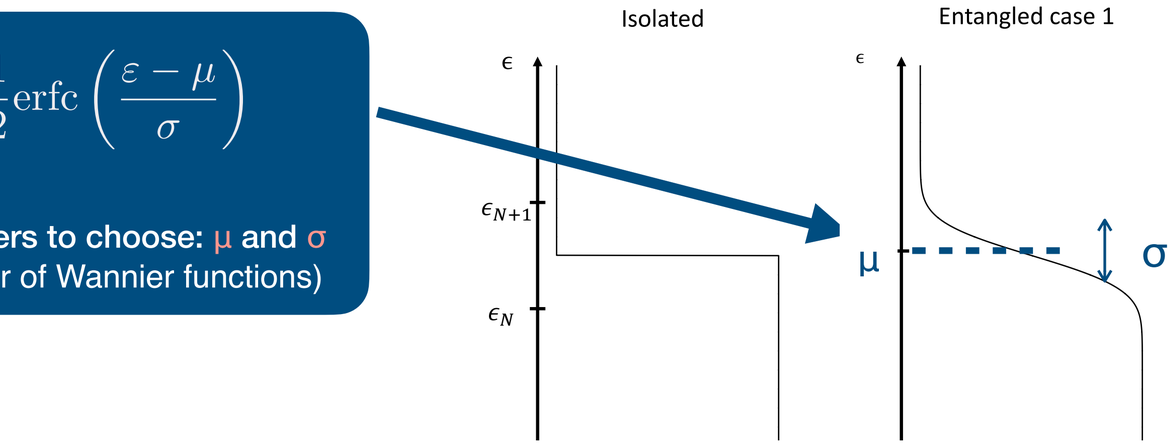
- We consider (formally) all eigenstates, and give a weight in the quasi-density-matrix P

$$P = \sum_i |\psi_i\rangle f(\varepsilon_i) \langle\psi_i| = f(H)$$

- *f:* smooth function of energy, selecting relevant states. If *f* is smooth: *P*(**r**,**r**') decays rapidly [2]
- We select the most N_w representative columns; procedure is analogous to isolated case

$$f(\varepsilon) = \frac{1}{2}\mathrm{erfc}\left(\frac{\varepsilon - \mu}{\sigma}\right)$$

Arbitrary parameters to choose: μ and σ
(and *N*, the number of Wannier functions)

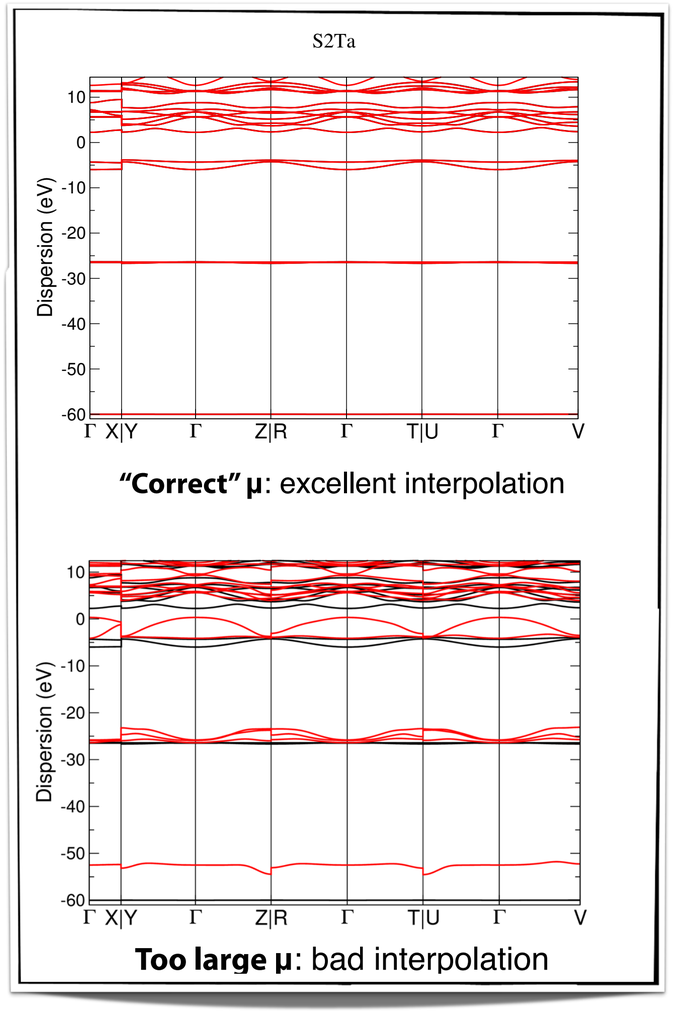


[2] A. Damle, L. Lin, Disentanglement via entanglement: A unified method for Wannier localization, arXiv:1703.06958 (2017)

SCDM - choice of parameters for entangled bands

- The SCDM method does not suggest how to choose the ***μ*** *and* ***σ*** *parameters* (and *neither the number* ***N*** *of Wannier functions*)
- The choice cannot be arbitrary: “bad” values generate bad interpolations
- **μ too small**: not enough information on high-energy bands: QRCP will pick top states randomly
- **μ too large**: high-energy states (that we are not interested into) might have a large weight and QRCP might prefer to select them: interpolation tends to have higher energy than the actual bands

How to choose these parameters (automatically)?



Important ingredient: projectability

$$p(|\psi_{n,\mathbf{k}}\rangle) = \sum_i |\langle o_i|\psi_{n,\mathbf{k}}\rangle|^2$$

atomic orbitals o_i described in the pseudopotential

- For each band (n,k), it is the **projection** of that state on all the pseudo-atomic orbitals described in the pseudopotential file
- Easy to obtain from Quantum ESPRESSO's projwfc.x

Copper

Orbitals: s,p,d (no nodes) + s,p (1 node)

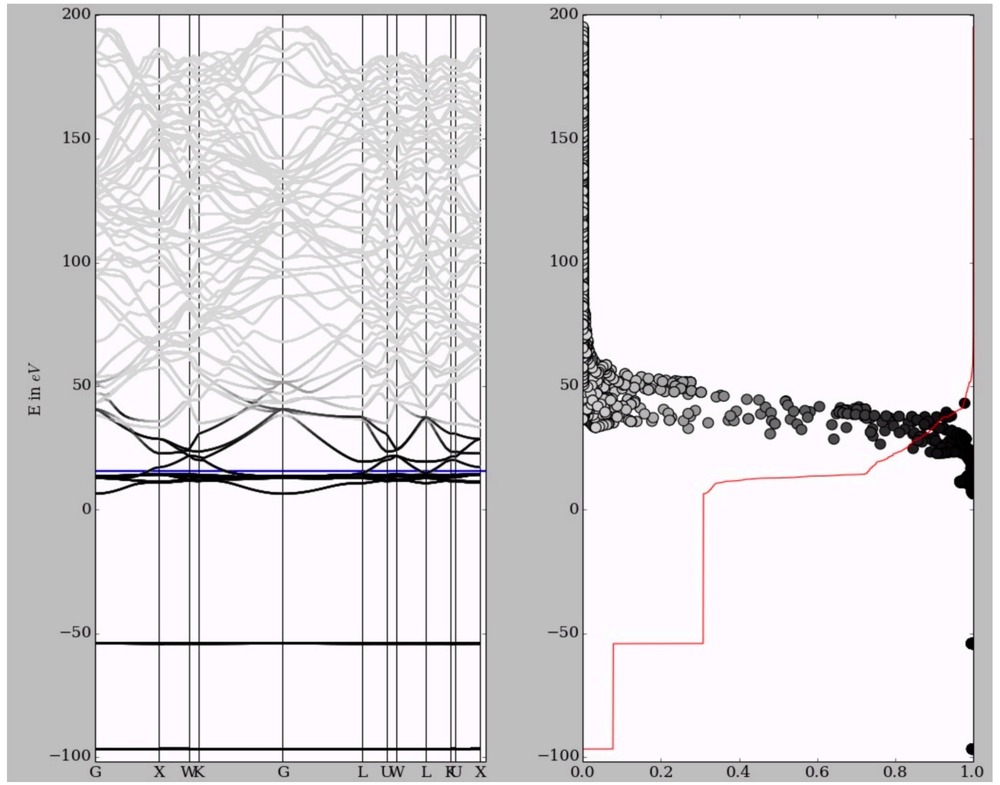


Image: courtesy of Daniel Marchand, EPFL

$$p(|\psi_{n,\mathbf{k}}\rangle) = \sum_i |\langle o_i|\psi_{n,\mathbf{k}}\rangle|^2$$

Can we automate the choice of N, μ and σ?

- We aim at getting a good band interpolation for the low-lying bands
- 1: choose **N as the number of atomic orbitals for which we have information in the pseudopotential file** (see also Agapito et al., PRB 88, 165127 (2013))
- 2: compute the "projectability" of each state as the projection of each state on the subspace of the atomic orbitals o_i described in the pseudopotential:

$$p(|\psi_{n,\mathbf{k}}\rangle) = \sum_i |\langle o_i|\psi_{n,\mathbf{k}}\rangle|^2$$

μ: when projectability≲0.9, weight≲10^{-3}

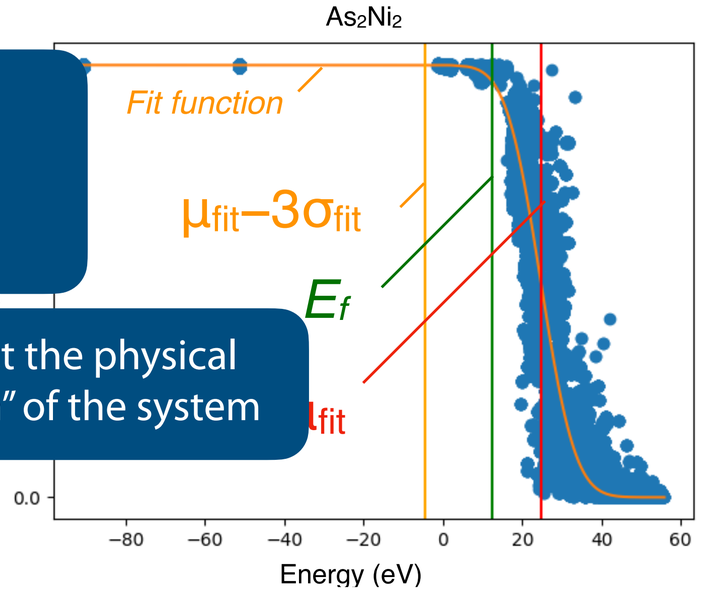
need to exponentially **suppress high-energy states** to affect SCDM choice

$$\left(\frac{\cdot}{2}\right)\left(\frac{\cdot}{\sigma_{\mathrm{fit}}}\right)$$

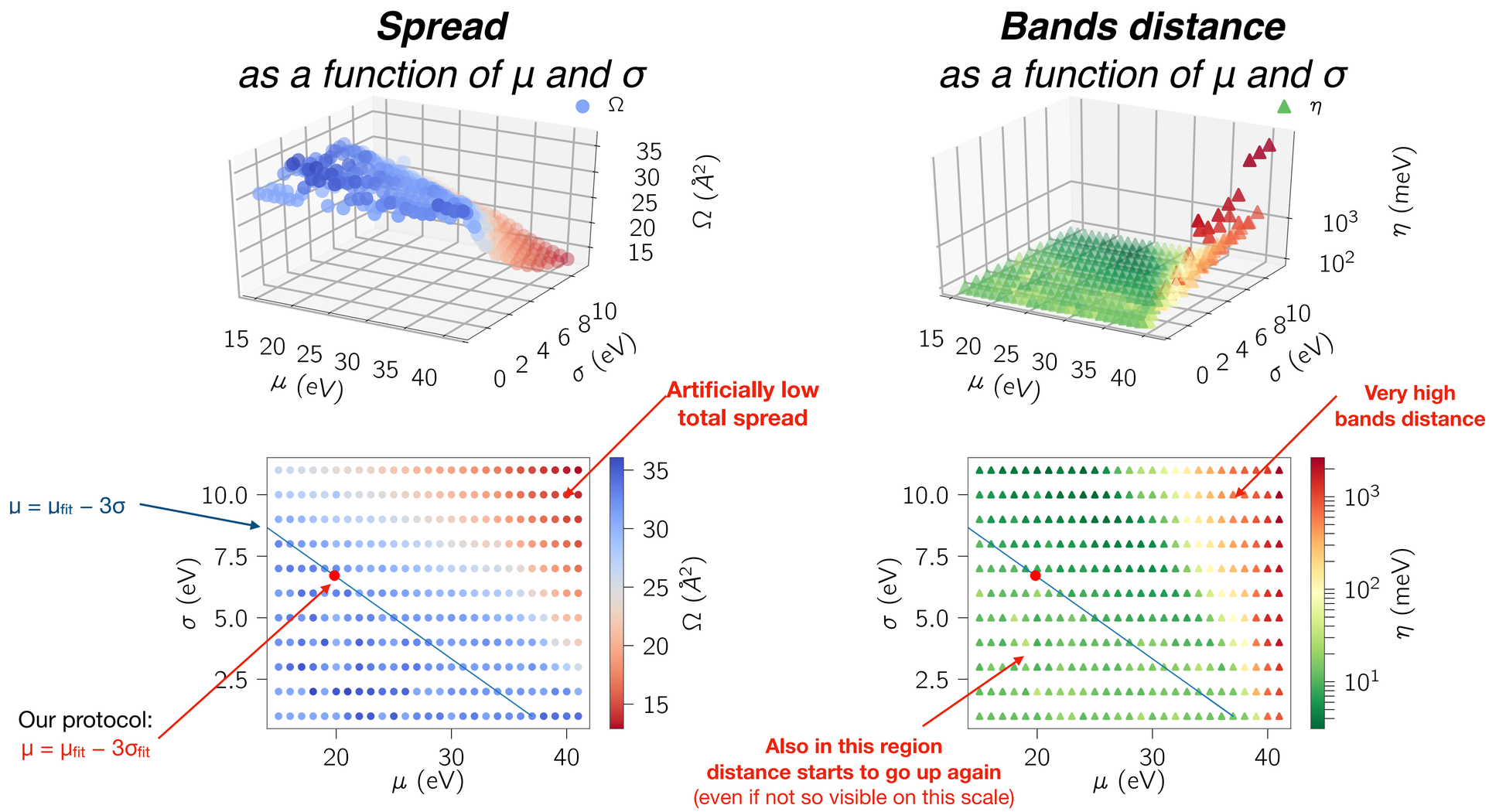
- **4: choose the parameters μ and σ a**

σ: we select the physical "band width" of the system

$$\mu = \mu_{\mathrm{fit}} - 3\sigma_{\mathrm{fit}}; \qquad \sigma = \sigma_{\mathrm{fit}}$$

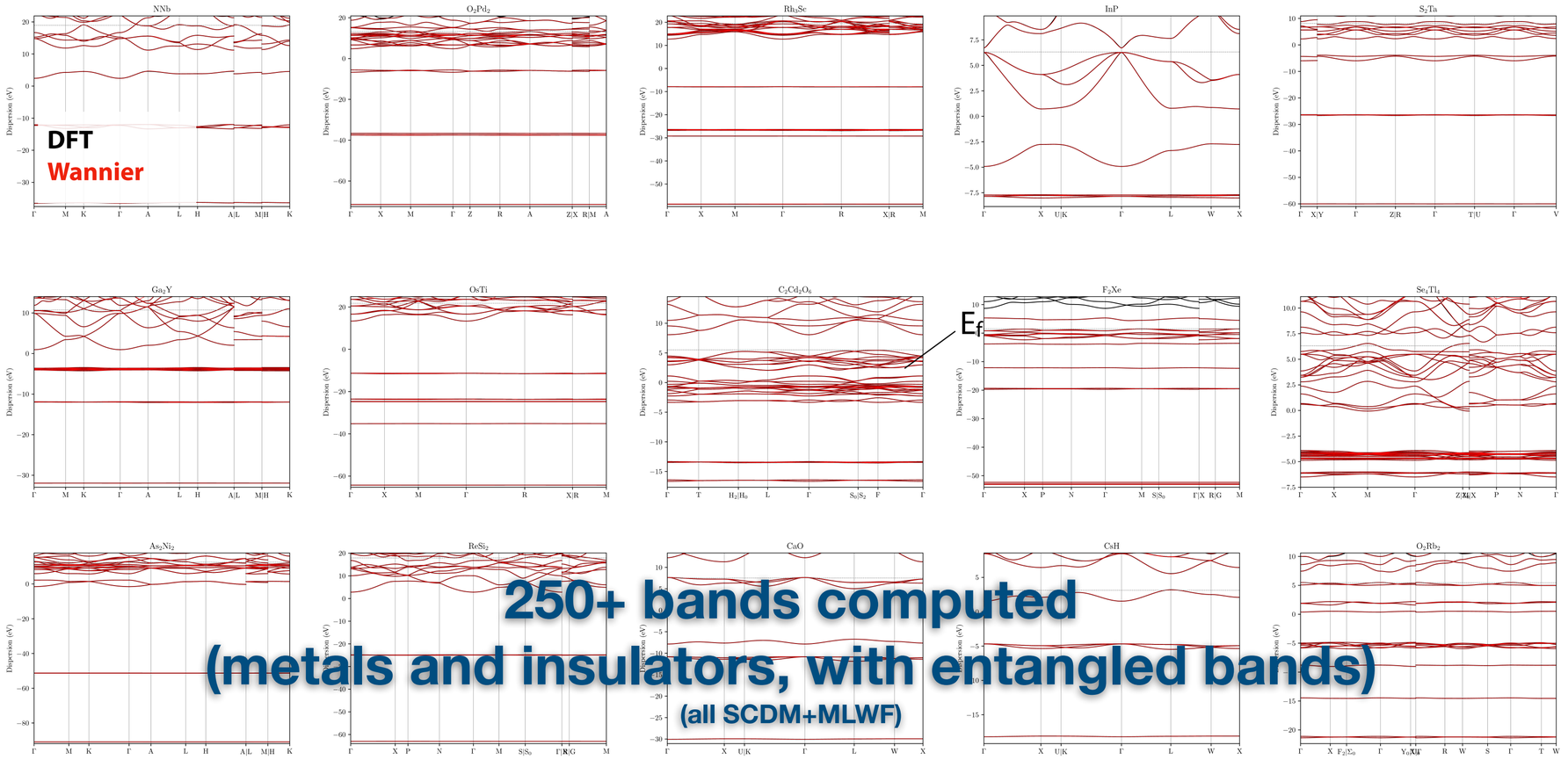


Parameter choice validation: tungsten (W)



SCDM - results for entangled bands

Results from our high-throughput validation
using AiiDA



250+ bands computed
(metals and insulators, with entangled bands)
(all SCDM+MLWF)

V. Vitale, G. Pizzi, A. Marrazzo et al., Automated high-throughput Wannierisation,
npj Computational Materials 6, 66 (2020)

SCDM - results for entangled bands

- To assess quality of Wannierisation and interpolation: we define a **bands distance** (between DFT bands and interpolated bands)

$$\eta = \sqrt{\sum_{n\mathbf{k}} \left(\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} - \varepsilon_{n\mathbf{k}}^{\mathrm{Wan}}\right)^2},$$

Average bands distance

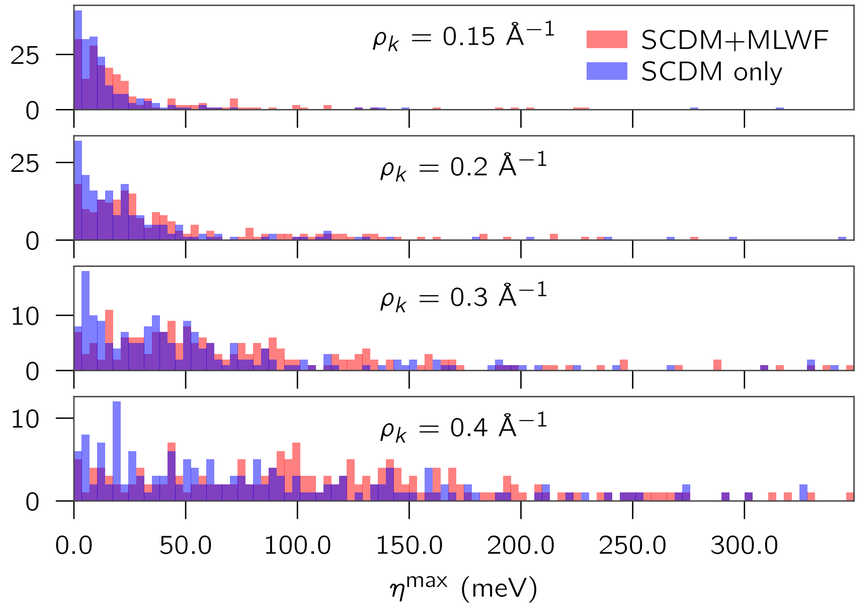
$$\eta^{\max} = \max_{n\mathbf{k}} \left(\left|\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} - \varepsilon_{n\mathbf{k}}^{\mathrm{Wan}}\right|\right)$$

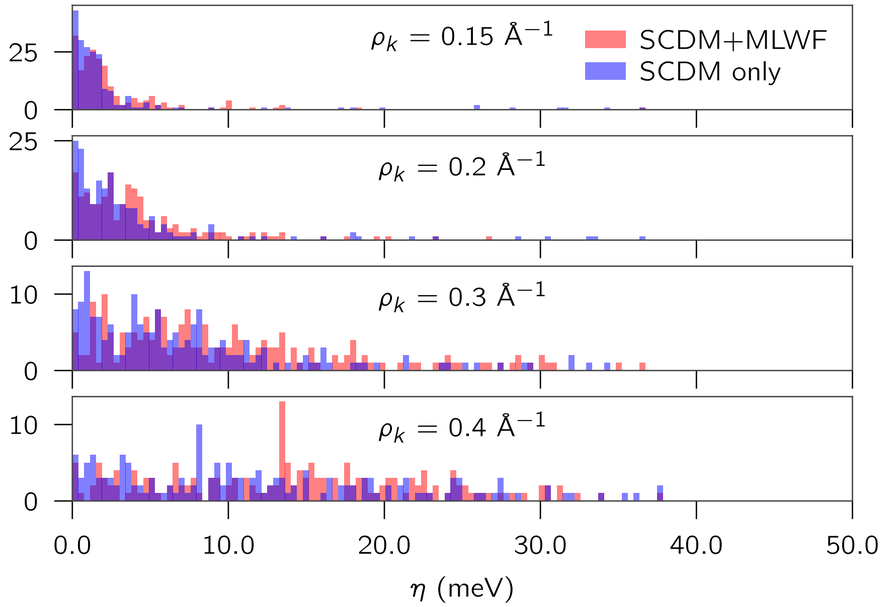
Max bands distance

- Moreover, we want to assess the importance of the **density of k-points** in the NSCF/Wannierisation step

  We will use a linear density ρ_k in Å^{-1}

SCDM - results for entangled bands





- Good results require a density of at least 0.2 Å^{-1} or more dense
- **For insulators**, SCDM-only already provides very good results; MLWF improves them
- In general, very small band distances (i.e. very good interpolation)

V. Vitale, G. Pizzi, A. Marrazzo et al., Automated high-throughput Wannierisation,
npj Computational Materials 6, 66 (2020)

Automating it all with AiiDA

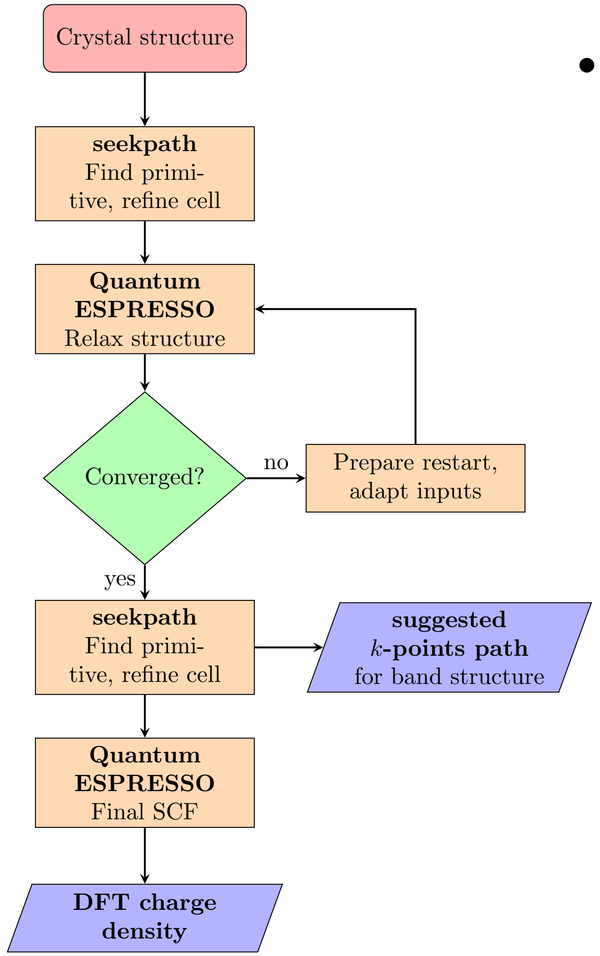
- Many steps; all automated with AiiDA (www.aiida.net)

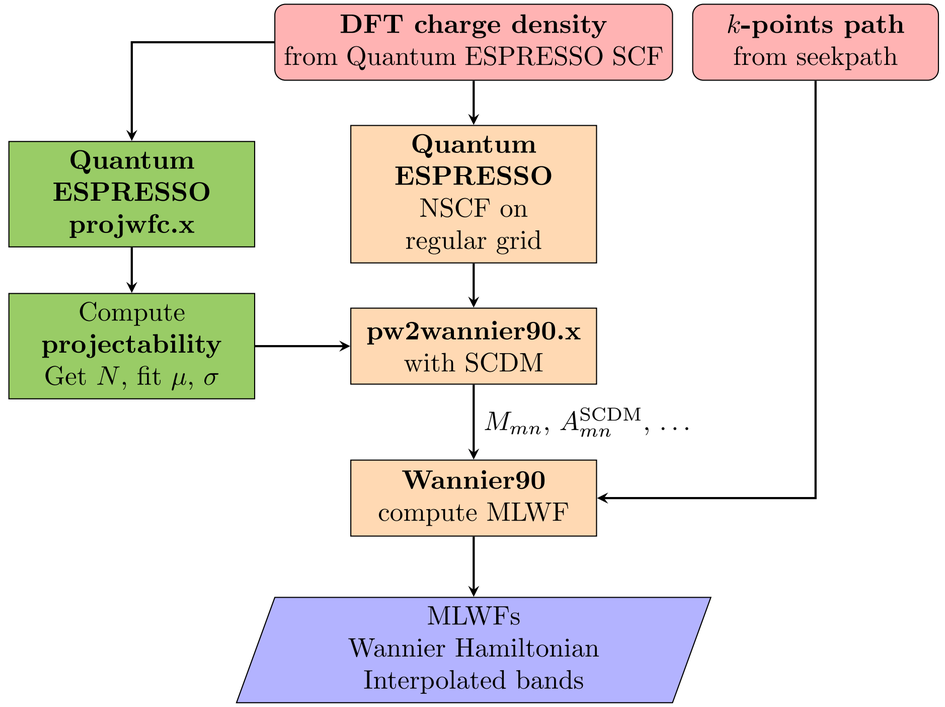
  S.P. Huber et al., Scientific Data 7, 300 (2020)
  M. Uhrin et al., Comp. Mat. Sci. 187 (2021)
  G. Pizzi et al. Comp. Mat. Sci. 111, 218-230 (2016)

- All workflows available; see tutorial:

  https://aiida-tutorials.readthedocs.io/en/latest/pages/2020_Oxford/

- **We will not see AiiDA today**; in Exercise 4, you will run all steps "by hand" - but feel free to check the tutorial if you are curious





The present, the future

Trieste 2022: Wannier Summer School

solid_dmft

A versatile python wrapper to perform DFT + DMFT calculations utilizing the TRIQS software library.

WANNIER90

Z2Pack

PythTB

EPW

WANNIER BERRi

AiiDA

Wannier Tools®

Beyond Wannier90: the Wannier ecosystem

Trieste 2022: Wannier Summer School

This 5-day school consists of lectures and hands-on sessions on a wide range of electronic-structure methods based on Wannier functions. The event targets graduate students, early-career scientists and experienced users.

- Maximally-localized Wannier functions (Wannier90)
- Advanced Wannier functions methods: symmetry-adapted, SCDM, transport (Wannier90)
- Partly occupied Wannier functions (ASE)
- Tight-binding models (PythTB)
- Topological properties (Z2pack & WannierTools)
- Berry-phase properties (WannierBerri)
- Automated wannierisation (AiiDA)
- Electron-phonon coupling (EPW)
- Dynamical mean-field theory (TRIQS)

Speaker:

R. ARITA, Tokyo University and RIKEN, Japan
S. BECK, Flatiron Institute, USA
F. GIUSTINO, UT Austin, USA
L. LIN, UC Berkeley, USA
N. MARZARI, EPFL, Switzerland
A. MOSTOFI, Imperial College London, UK
Y. NOMURA, Keio University, Japan
S. PONCÉ, EPL, Belgium
J. QIAO, EPFL, Switzerland
R. RESTA, CNR-IOM, Italy
I. SOUZA, CFM and UPV, Spain
K. THYGESEN, DTU, Denmark
D. VANDERBILT, Rutgers University, USA
M. VERGNIORY, DIPC, Spain
V. VITALE, Imperial College London, UK
Q. WU, IOPCAS, China
J. YATES, Oxford University, UK

All lectures have been **recorded** and are available at https://indico.ictp.it/event/9789/ or https://youtu.be/T8r_3vzWCUM

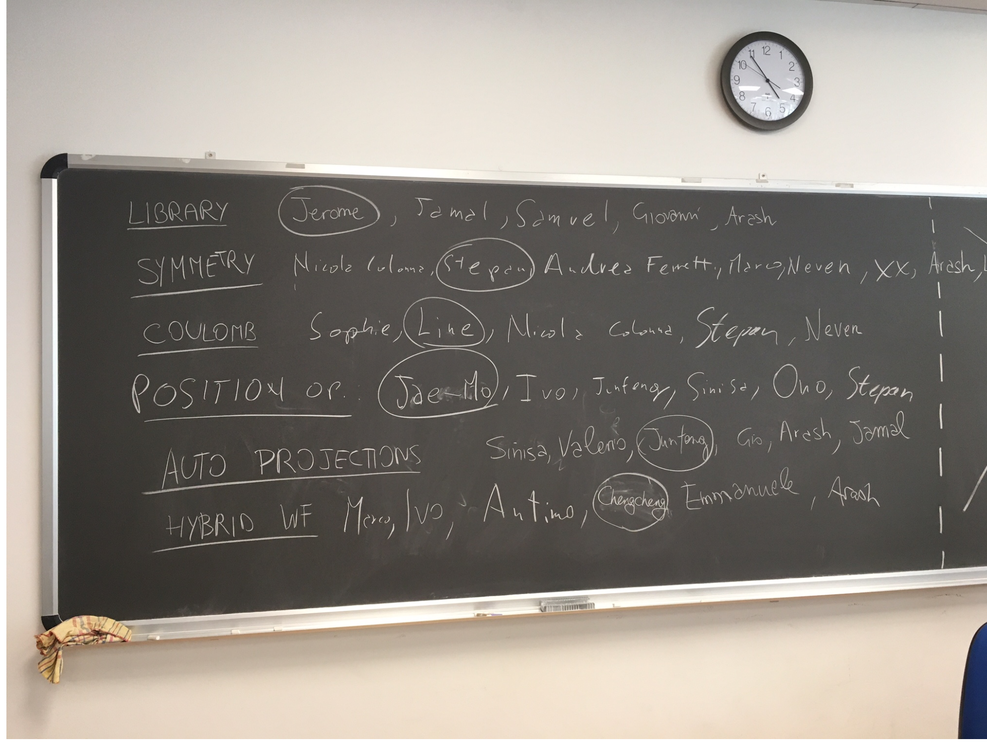
Trieste 2022: Wannier Developers Meeting

Beyond Wannier90: the Wannier ecosystem

Wannier 2022 Developers Meeting

23 - 27 May 2022
An ICTP Hybrid Meeting
Trieste, Italy

Talks and discussions on Wannier functions theory, electron-phonon coupling, magnetic interactions, quantum computing, and much more!



The Wannier 2022 Developers Meeting gathers the community that sustains various software packages built around the concept of maximally-localised Wannier functions (MLWF), strengthening interactions between the developers and promoting a synergetic research and software ecosystem.

Talks have been **recorded** and are available at https://indico.ictp.it/event/9851/ or https://youtu.be/rl2gt2a1RVM

Beyond Wannier90: the Wannier ecosystem

The Wannier ecosystem

We are spontaneously going towards a decentralised software ecosystem (as opposed to a monolithic Wannier code), hence:

- Some (small) duplication of efforts (multiple implementations)
- What you want to compute might be already implemented…but not in Wannier90! **Check existing packages** of the Wannier ecosystem
- Not all implementation are equals, newer implementations can be much faster (e.g. TBmodels VS PythTB, WannierBerri VS postw90)
- Bio**diversity** in software is good
- Some packages might stop being maintained (e.g. the authors goes to industry), but the ecosystem always survives

Future directions

Novel functionalities - soon available

- **Symmetries:** the projection (A_{mn}) and overlap (M_{mn}) matrices can be computed on the irreducible wedge in the Brillouin zone (as opposed to the full BZ). Existing implementation by (Takashi Koretsune) in Fortran & Python is complete.
- **Band parallelisation** in pw2wannier90.x (two existing implementations).
- **Major restructuring of the code.** The library mode is being extensively developed to include all functionalities, the "standalone" mode will be a wrapper calling the library.
- Towards a unified python interface for Wannier90
- …

My take on Wannier trends

1. **We will trade localisation for symmetries** (less localized but more symmetric and atom-centred Wannier functions)
2. **Initial projections will not be a problem anymore** (SCDM already available and being improved, Qiao-Marzari-Pizzi projectability disentanglement in the future)
3. We will use Wannier90 more and more as **library,** to be called from external codes of the Wannier ecosystem dedicated to calculate specific properties

We shall not cease from exploration, and the end of all our exploring will be to arrive where we started and know the place for the first time.
(T.S. Eliot)