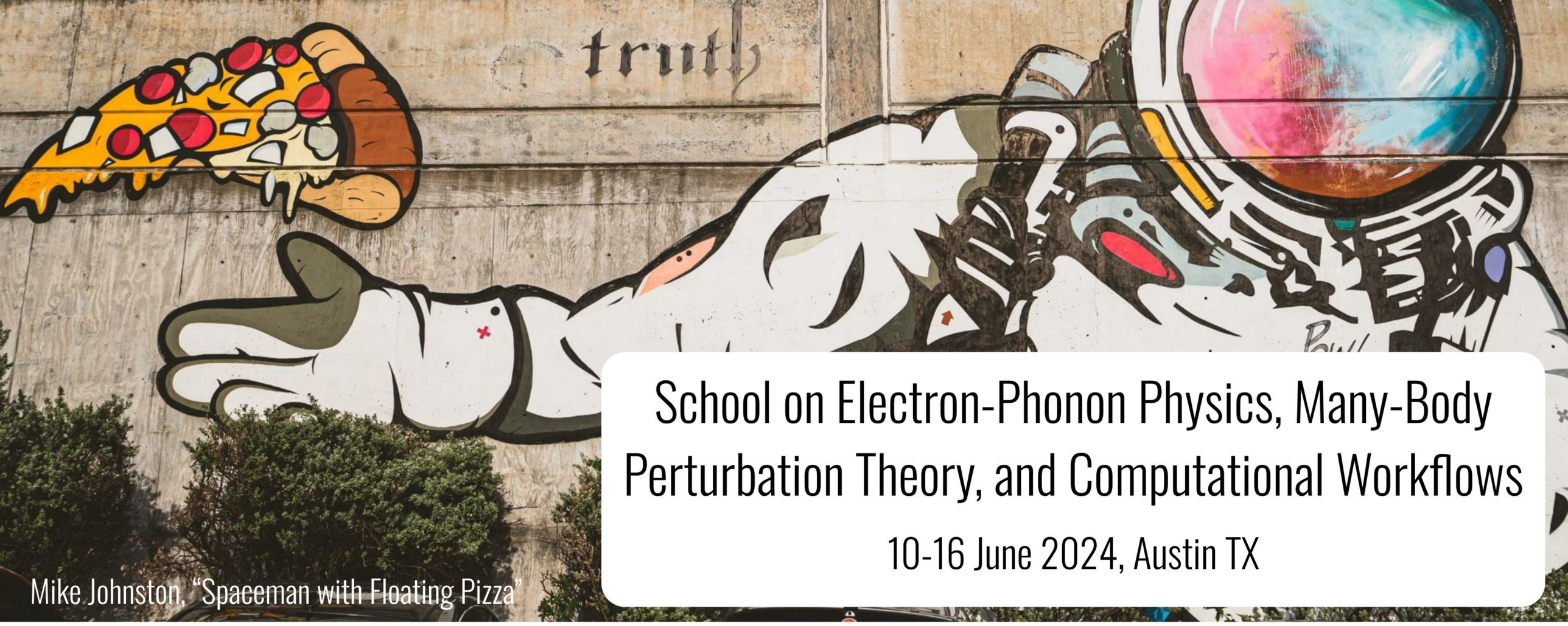

Mike Johnston, “Spaceman with Floating Pizza”

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

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Lecture Tue.1

The Wannier Function Software Ecosystem for Materials Simulations

Antimo Marrazzo

International School for Advanced Studies (SISSA), Trieste (Italy)

A quick recap from yesterday's lecture on Wannier functions

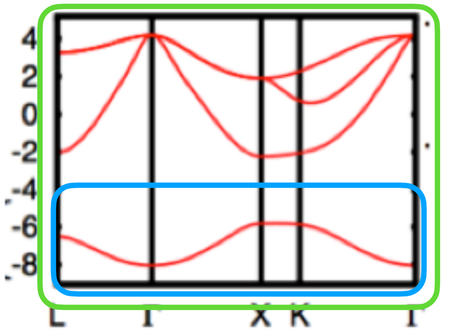
From Bloch to Wannier: gauge freedoms

Fourier transforming from reciprocal to real space

- One isolated band

$$|\mathbf{R}\rangle = \frac{V_{cell}}{(2\pi)^3}\int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} e^{\phi_{\mathbf{k}}} |\psi_{\mathbf{k}}\rangle$$

Arbitrary phase factors (for each k-point) are allowed



- Composite bands

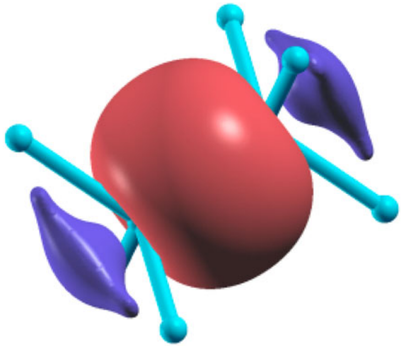
$$|\mathbf{R}j\rangle = \frac{V_{cell}}{(2\pi)^3}\int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{n=1}^{J} U_{\mathbf{k},nj} |\psi_{n\mathbf{k}}\rangle$$

Arbitrary unitary rotations (for each k-point) are allowed

Wannier functions: key properties

$$|\mathbf{R}j\rangle = \frac{V_{cell}}{(2\pi)^3}\int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{n=1}^{J} U_{\mathbf{k},nj}\,|\psi_{n\mathbf{k}}\rangle$$

- Orthogonal
- Span the same space of initial Bloch states
- (Supercell) periodic



N. Marzari et al, Rev. Mod. Phys. (2012)

How to choose U?

Many recipes available today, the most popular: **maximal localization**

Maximally-localized Wannier functions

We minimize the quadratic spread of the position operator of a manifold

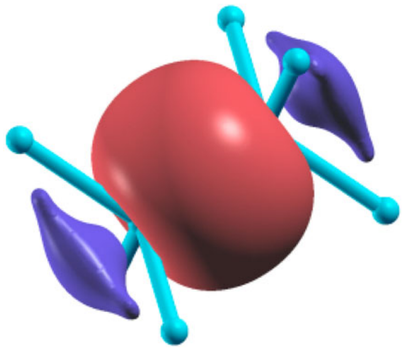
$$\Omega = \sum_{j=1}^{J} \left[\langle \mathbf{0}j \,|\, r^2 \,|\, \mathbf{0}j \rangle \; - \; |\langle \mathbf{0}j \,|\, \mathbf{r} \,|\, \mathbf{0}j \rangle|^2 \right]$$

through the optimization of the unitary matrices $U_{\mathbf{k},nj}$

$$|\mathbf{R}j\rangle = \frac{V_{cell}}{(2\pi)^3} \int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{n=1}^{J} U_{\mathbf{k},nj} \, |\psi_{n\mathbf{k}}\rangle$$

Iteratively refined towards maximal localization

From ab initio engines (e.g. Quantum ESPRESSO)



N. Marzari and D. Vanderbilt, PRB 56, 12847 (1997)

Project wisely and follow the gradient

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

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

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

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

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

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

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

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

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

minimize!

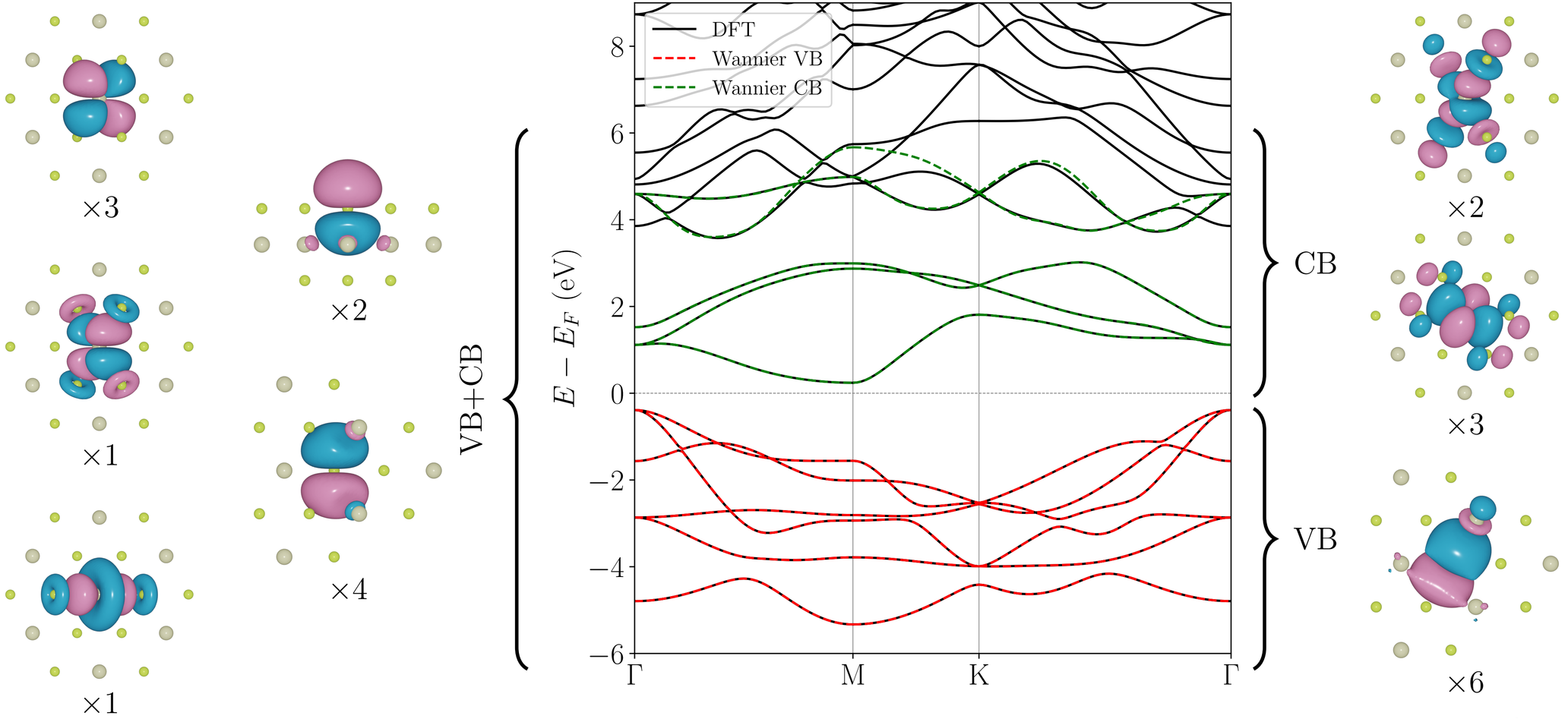
Follow the gradient and update the unitary matrices $U_{\mathbf{k}}$

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

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

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

From composite to entangled bands



A. Marrazzo et al., arXiv:2312.10769 (2023)

Extracting differentiable manifolds with optimal smoothness

Disentanglement

Disentanglement step

$$|\tilde{\psi}_{n\mathbf{k}}\rangle = \sum_{m=1}^{\mathcal{J}_{\mathbf{k}}} |\psi_{m\mathbf{k}}\rangle \, \tilde{V}_{\mathbf{k},mn}$$

Minimize Ω_I

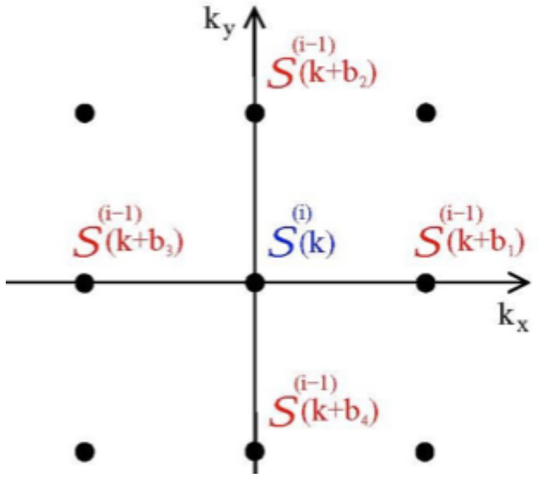
Maximal-localization step

Minimize $\tilde{\Omega}$

$$V_{\mathbf{k}} = \tilde{V}_{\mathbf{k}} U_{\mathbf{k}}$$

$$|\psi^{\mathrm{W}}_{j\mathbf{k}}\rangle = \sum_{n=1}^{\mathcal{J}_{\mathbf{k}}} |\psi_{n\mathbf{k}}\rangle \, V_{\mathbf{k},nj}$$

$$|\mathbf{R}j\rangle = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \, |\psi^{\mathrm{W}}_{j\mathbf{k}}\rangle$$



Minimize the degree of mismatch (a.k.a. spillage) between states and neighboring k-points

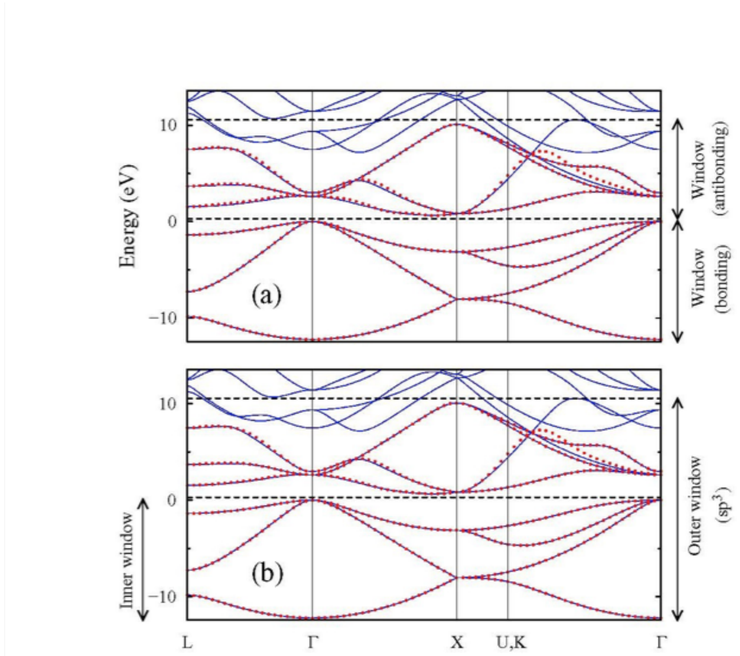
Max $\sum_{\mathbf{b}} \sum_{m=1}^{N} \left| \left\langle u^{(i)}_{n\mathbf{k}} \middle| u^{(i-1)}_{m,\mathbf{k}+\mathbf{b}} \right\rangle \right|^2$

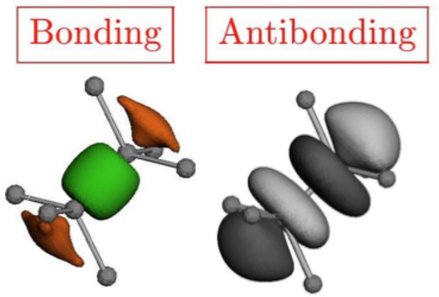
- 1st iteration: Choose trial subspace at each $\mathbf{k}$ (e.g. projected orbitals)
- i^{th} iteration: At each $\mathbf{k}$ pick the N highest eigenvectors of

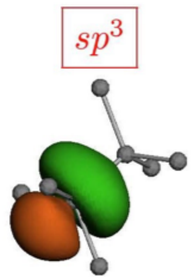
$$\left[\sum_{\mathbf{b}} \hat{P}^{(i-1)}_{\mathbf{k}+\mathbf{b}} \right] \left| u^{(i)}_{n\mathbf{k}} \right\rangle = \lambda^{(i)}_{n\mathbf{k}} \left| u^{(i)}_{n\mathbf{k}} \right\rangle$$

$\hat{P}^{(i-1)}_{\mathbf{k}+\mathbf{b}}$: Projector onto $\mathcal{S}^{(i-1)}(\mathbf{k}+\mathbf{b})$

- Repeat until self-consistency (when spaces $\mathcal{S}(\mathbf{k})$ stabilize)







I. Souza, N. Marzari and D. Vanderbilt, PRB 65, 035109 (2002)

Maximally-localized Wannier functions (MLWF) in a nutshell

Smooth gauge in reciprocal space ⟷ good localization in real space

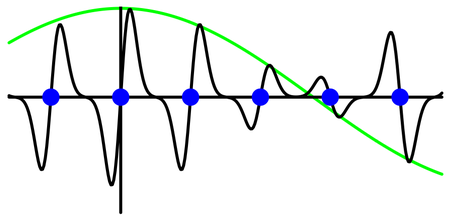
Electronic ground states from first-principles simulations (e.g. Quantum ESPRESSO) → Subspace-selection & unitary transformation of Bloch wave functions → MLWF in real space

$$|\mathbf{R}j\rangle = \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}\,|\psi^{\mathrm{W}}_{j\mathbf{k}}\rangle$$

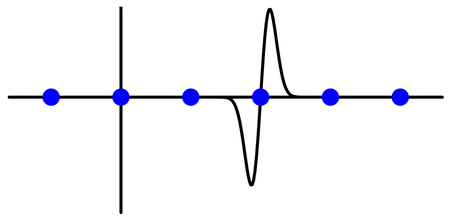
$$|\psi^{\mathrm{W}}_{j\mathbf{k}}\rangle = \sum_{n=1}^{\mathcal{J}_{\mathbf{k}}} |\psi_{n\mathbf{k}}\rangle\, V_{\mathbf{k},nj}\ ,$$

Choose $V_{\mathbf{k}}$ such that minimize $\Omega = \sum_{j=1}^{J}\Big[\langle\,\mathbf{0}j\,|\,r^2\,|\,\mathbf{0}j\,\rangle - |\langle\,\mathbf{0}j\,|\,\mathbf{r}\,|\,\mathbf{0}j\,\rangle|^2\Big]$

Bloch



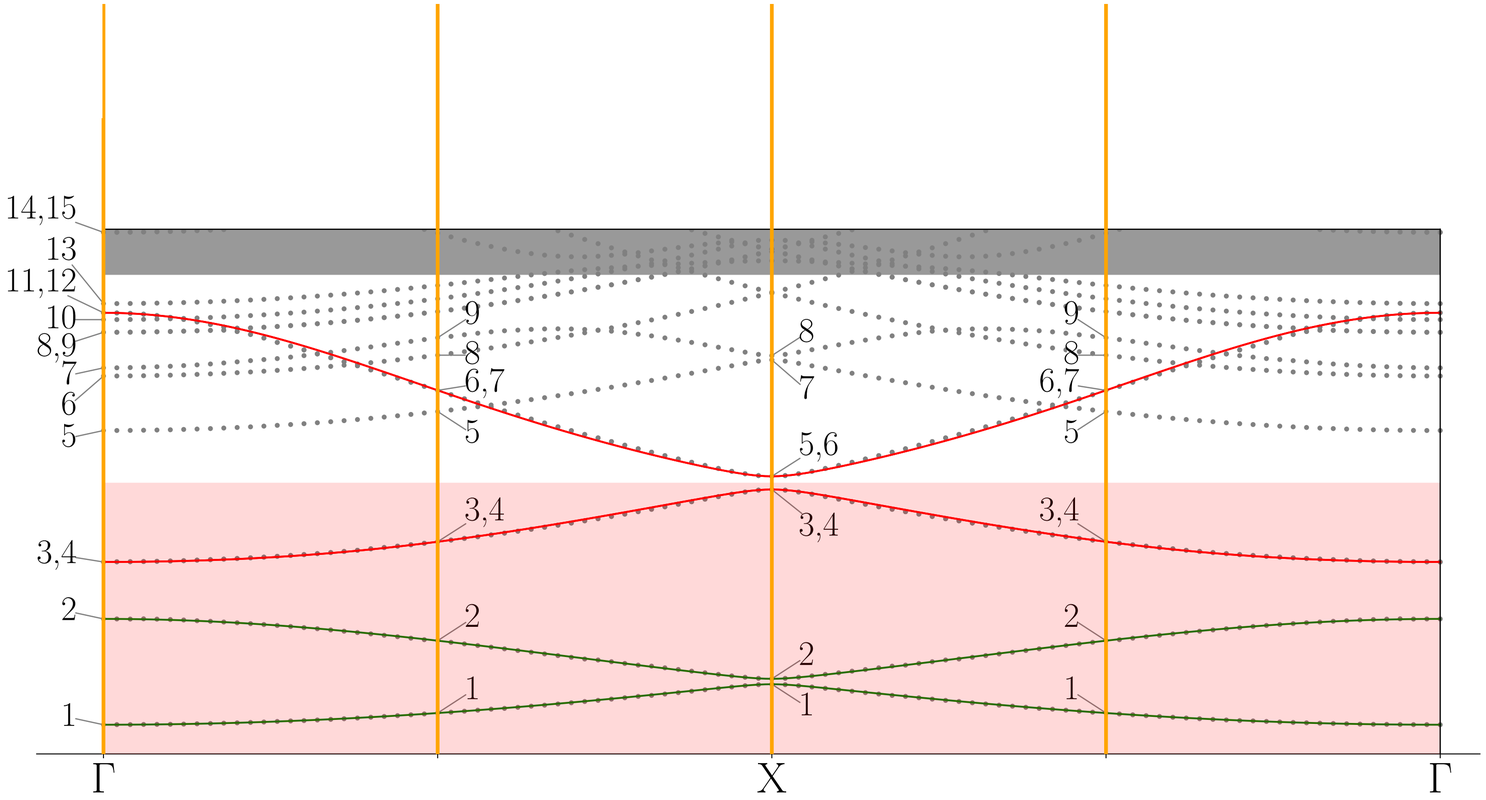
Wannier

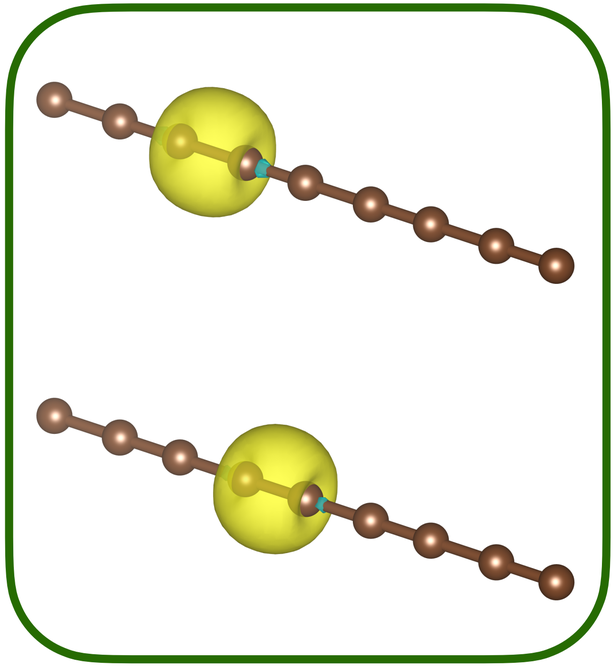


N. Marzari and D. Vanderbilt, PRB 56, 12847 (1997)
I. Souza., N. Marzari, D. Vanderbilt, PRB 65, 035109 (2001)

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

A toy example: carbon chains

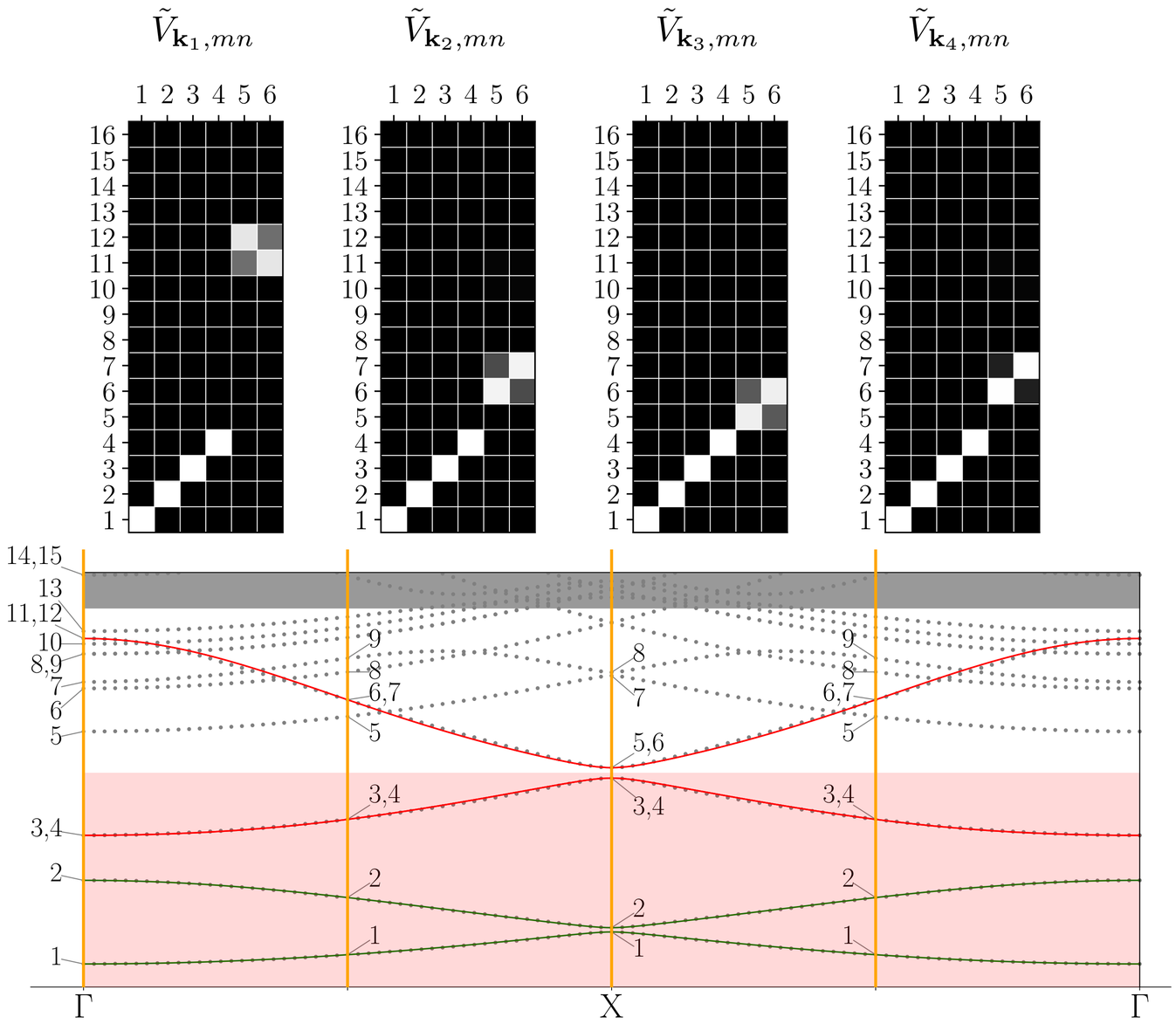


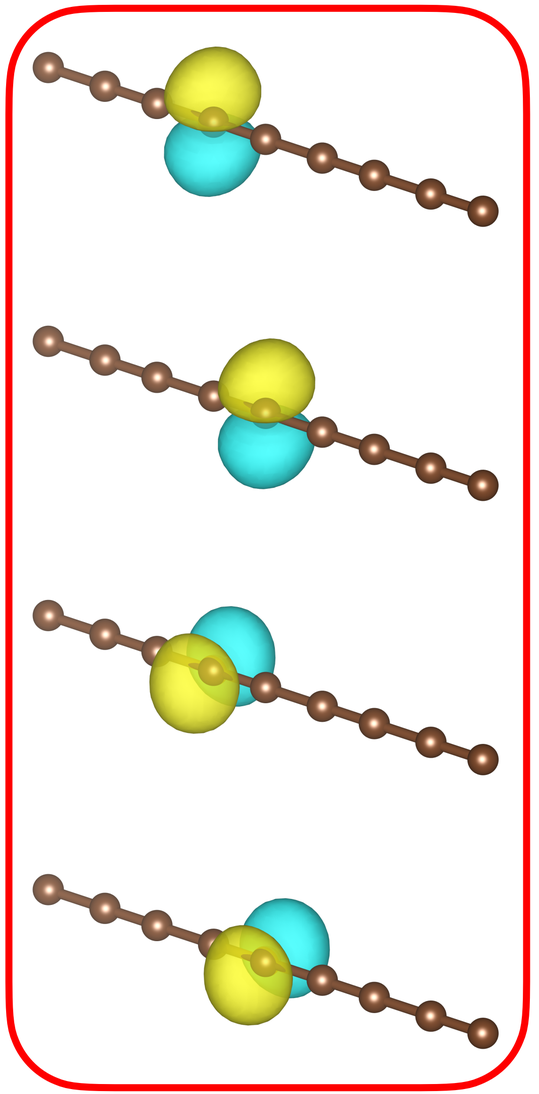


Courtesy of Giovanni Pizzi, PSI (Switzerland)

A. Marrazzo et al., arXiv:2312.10769 (2023)

A more challenging toy: disentanglement in carbon chains





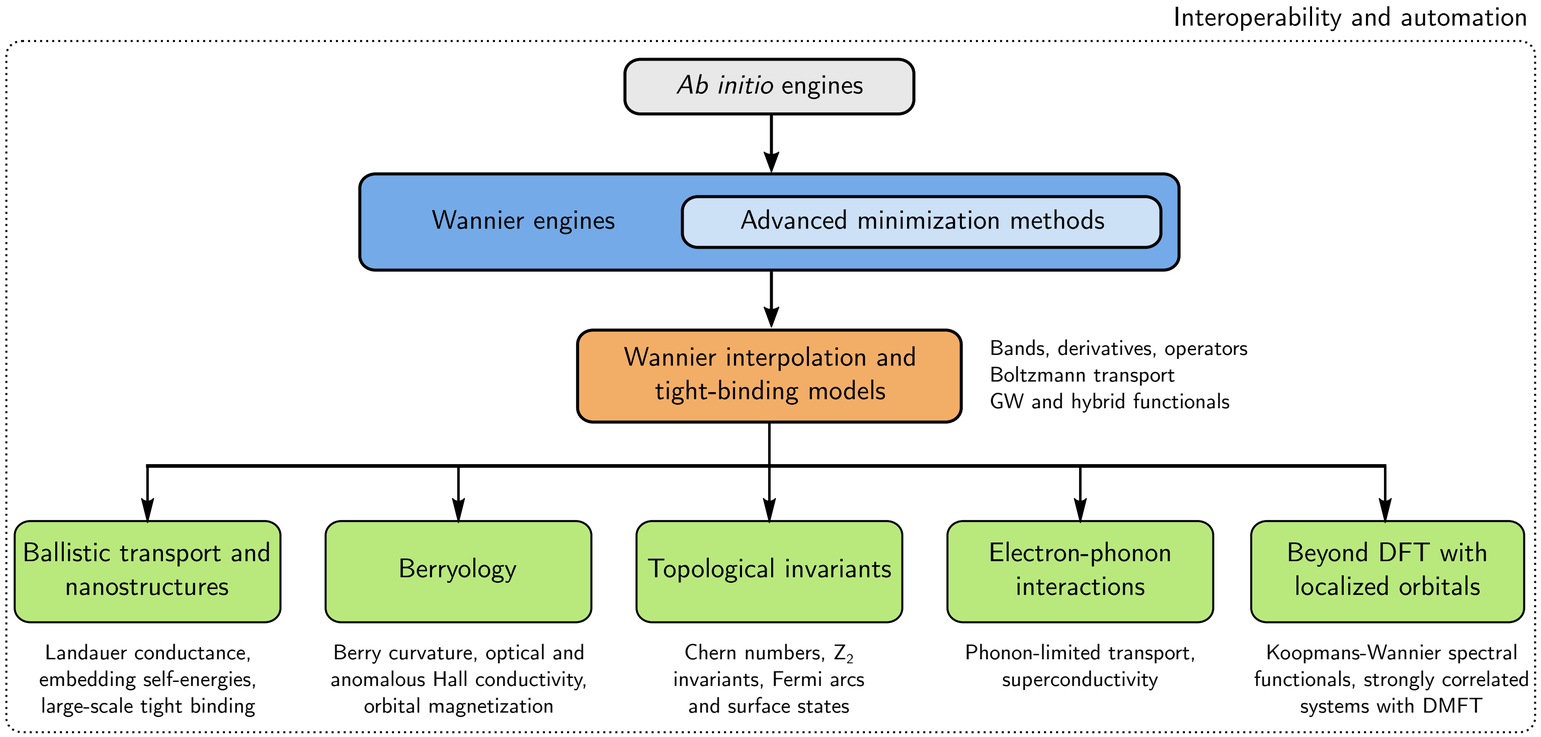
Courtesy of Giovanni Pizzi, PSI (Switzerland)

A. Marrazzo et al., arXiv:2312.10769 (2023)

Major applications of Wannier functions

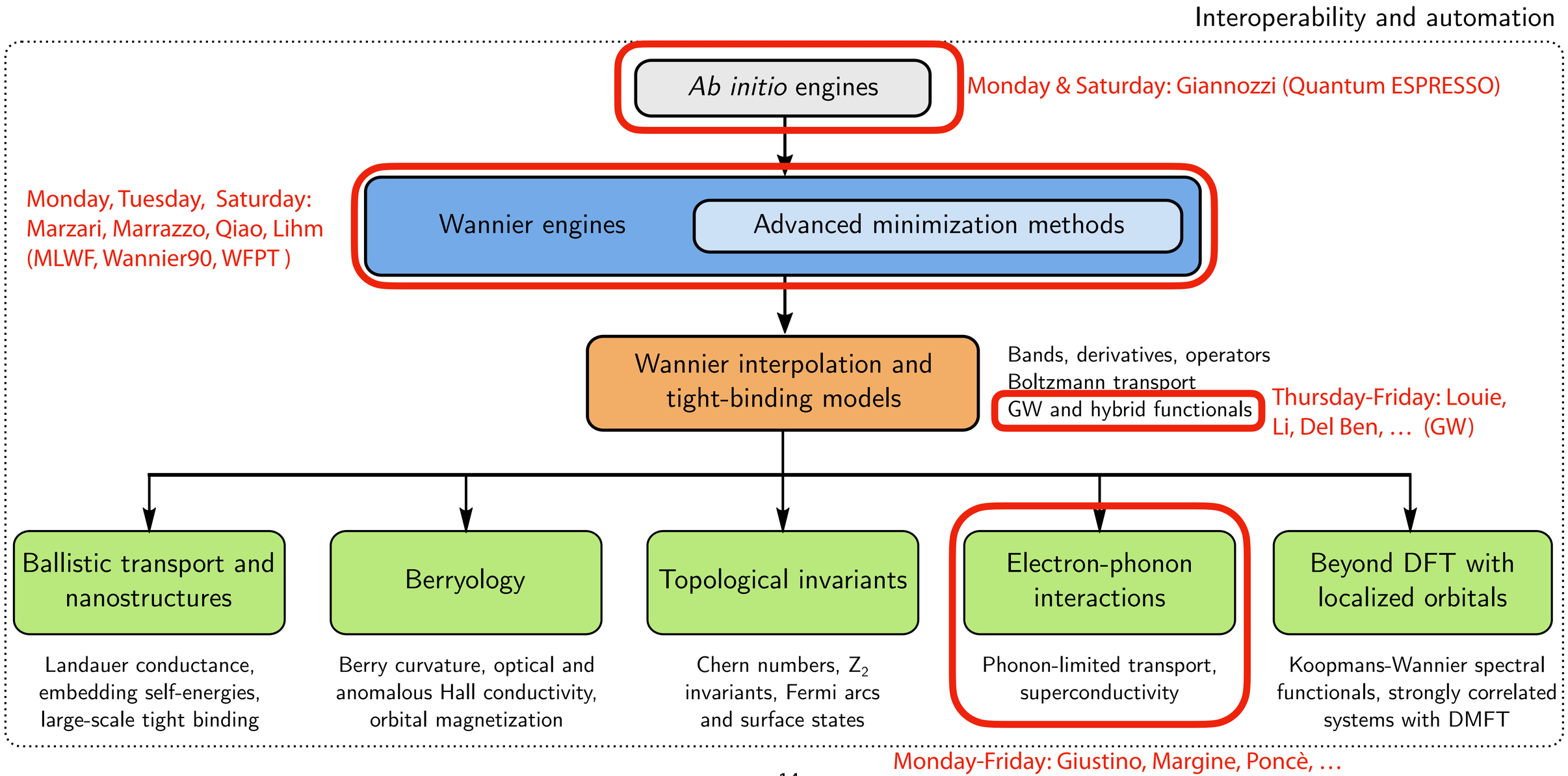
(0. Understand and characterize chemical bonding)

1. Reciprocal space **interpolation**
2. Quantum-geometry and topology (e.g., polarization, orbital magnetization, topological invariants)
3. Advanced electronic-structure methods (based on localized orbitals, e.g., DMFT)



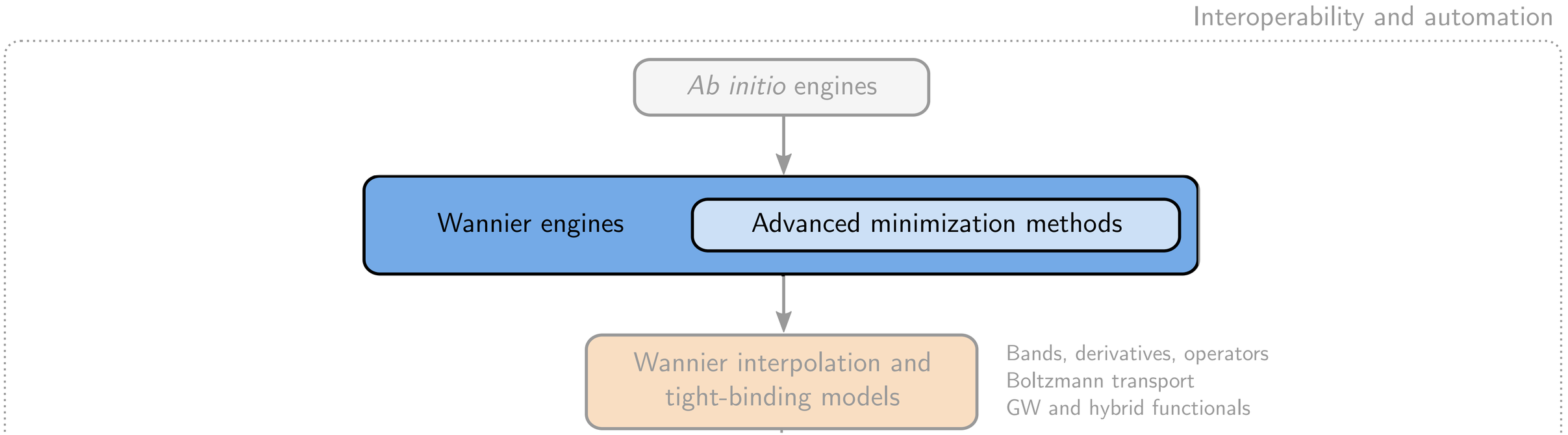
A. Marrazzo et al., arXiv:2312.10769 (2023)

What are Wannier functions doing here?



A. Marrazzo et al., arXiv:2312.10769 (2023)

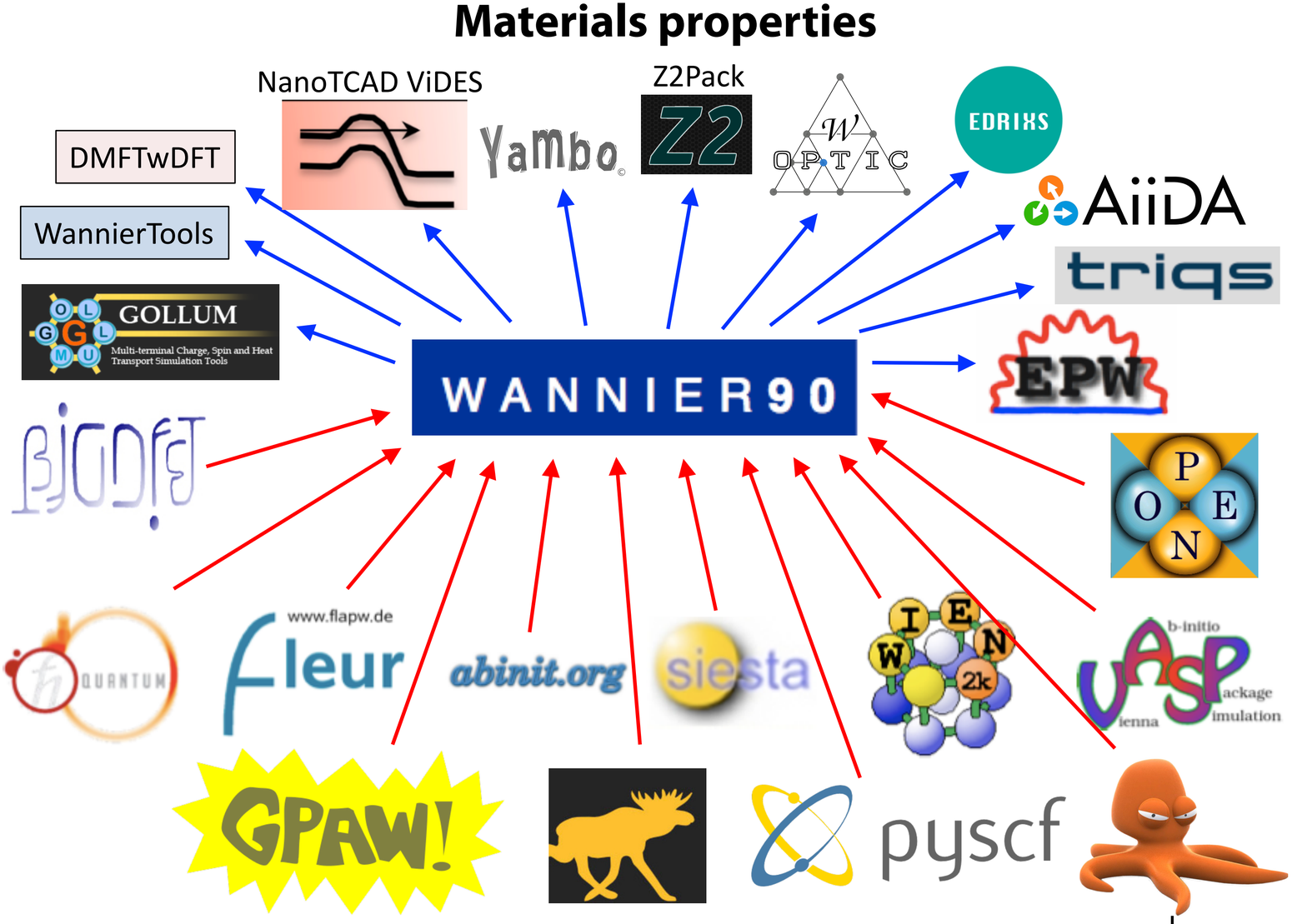
Wannier engines



- Wannier engines: codes to obtain localized Wannier functions and related properties
- The most popular is **Wannier90**, but other engines are available such as ASE and Wannier.jl (in Julia)

A. Marrazzo et al., arXiv:2312.10769 (2023)

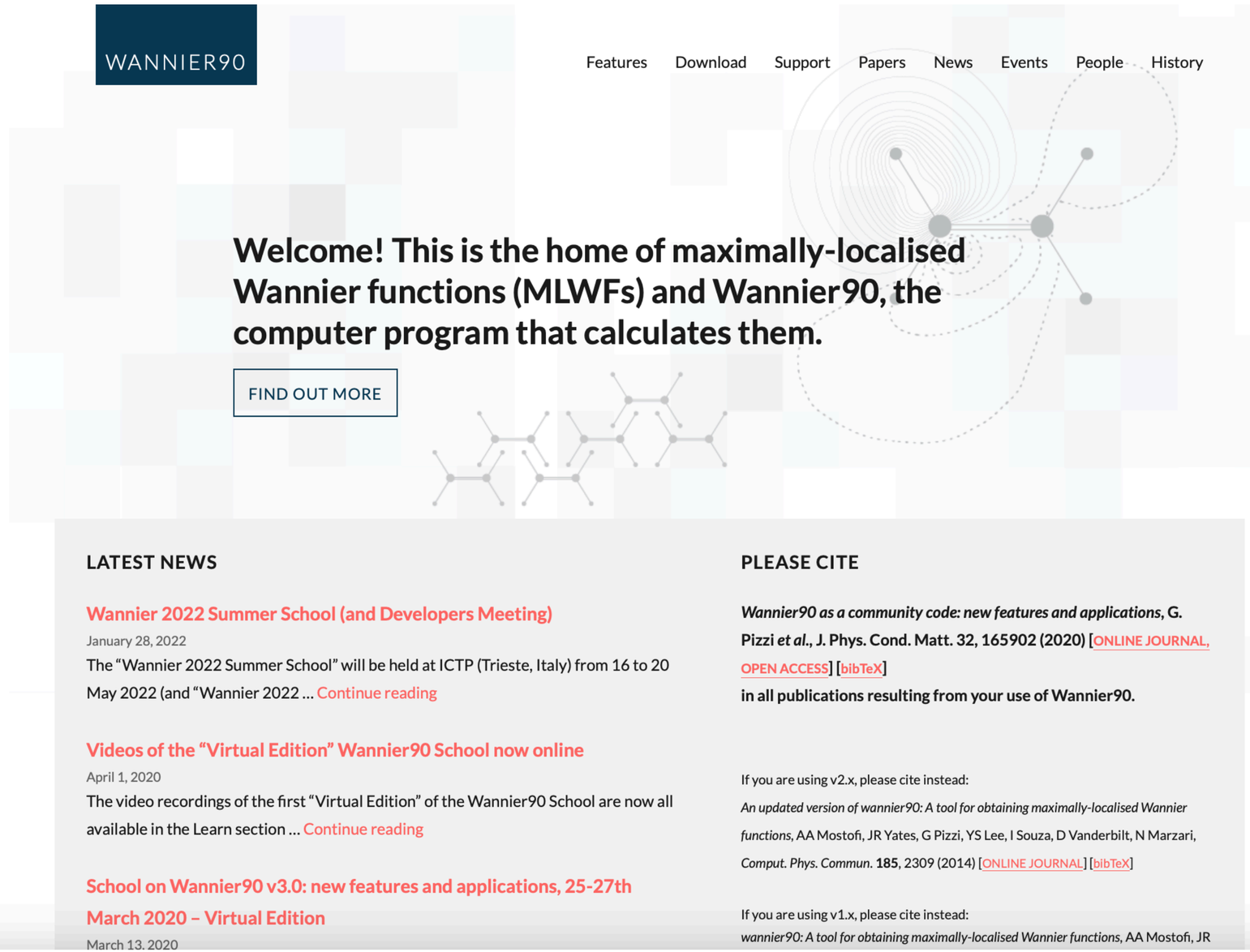
Wannier90: The center of a software ecosystem



…and <u>many</u> more other packages!

Adapted from Arash Mostofi, Wannier School 2021

www.wannier.org



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Download

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

Please note that:

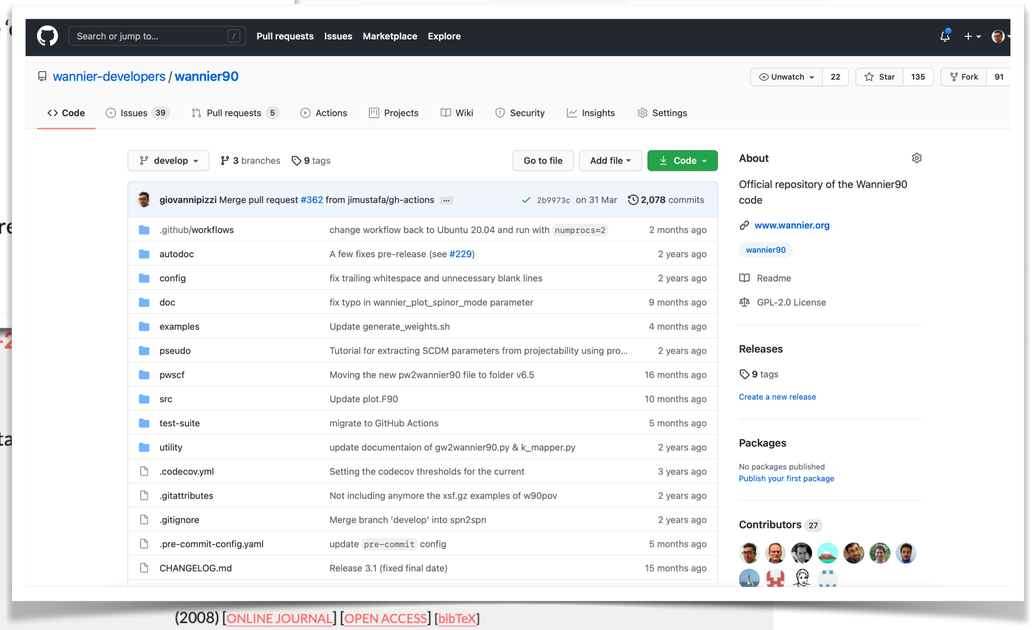
- Wannier90 is released under the GNU General Public License (v2)
- A summary of improvements may be found in CHANGE.log
- Installation instructions may be found in README.install
- The latest User Guide and Tutorial may be found here. They may also be found in the '
  current distribution.

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.*

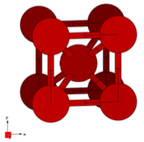

Figure 21: Unit cell of Iron crystal plotted with the XCrySDen program.

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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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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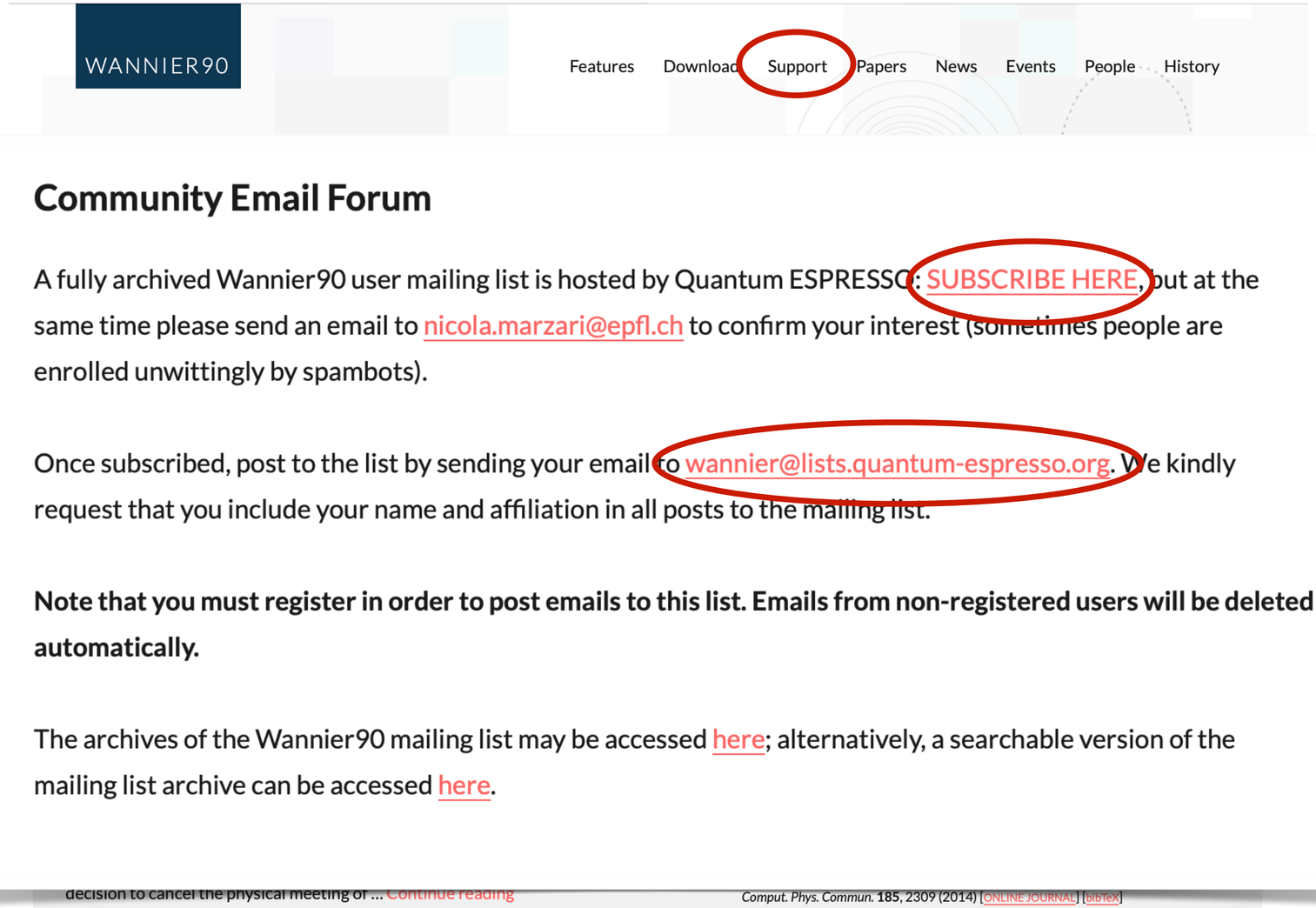


WANNIER90

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 of ... Continue reading

Wannier90 (v3.1.0) released

March 5, 2020

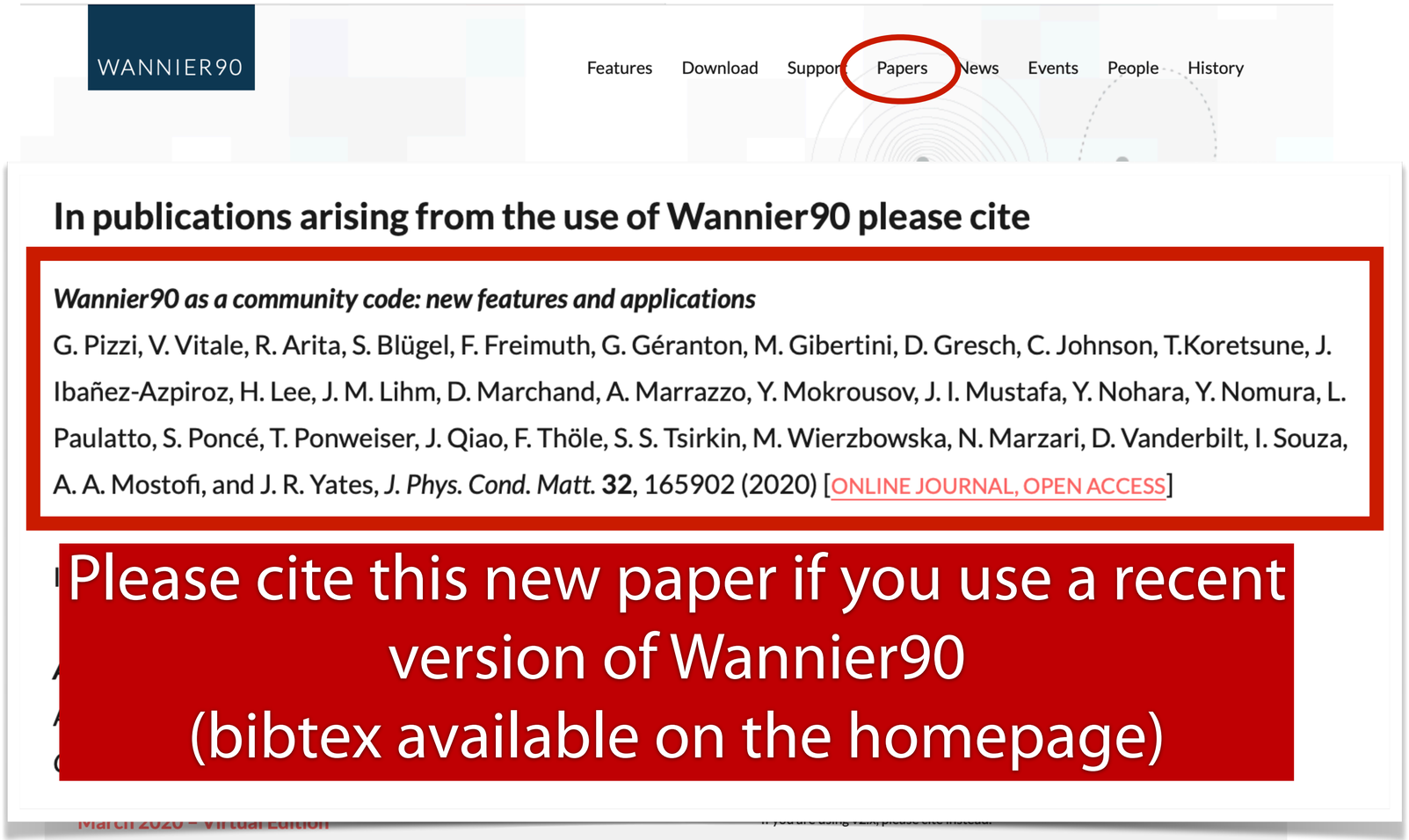
Wannier90 (v3.1.0) has been released today!

ALL NEWS

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 Yates, YS Lee, I Souza, D Vanderbilt, N Marzari, *Comput. Phys. Commun.* **178**, 685 (2008) [ONLINE JOURNAL] [OPEN ACCESS] [bibTeX]

www.wannier.org



A community effort!

People

Wannier Developers Group

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

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Associate Professor of Materials Modelling – University of Oxford

Giovanni Pizzi
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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.

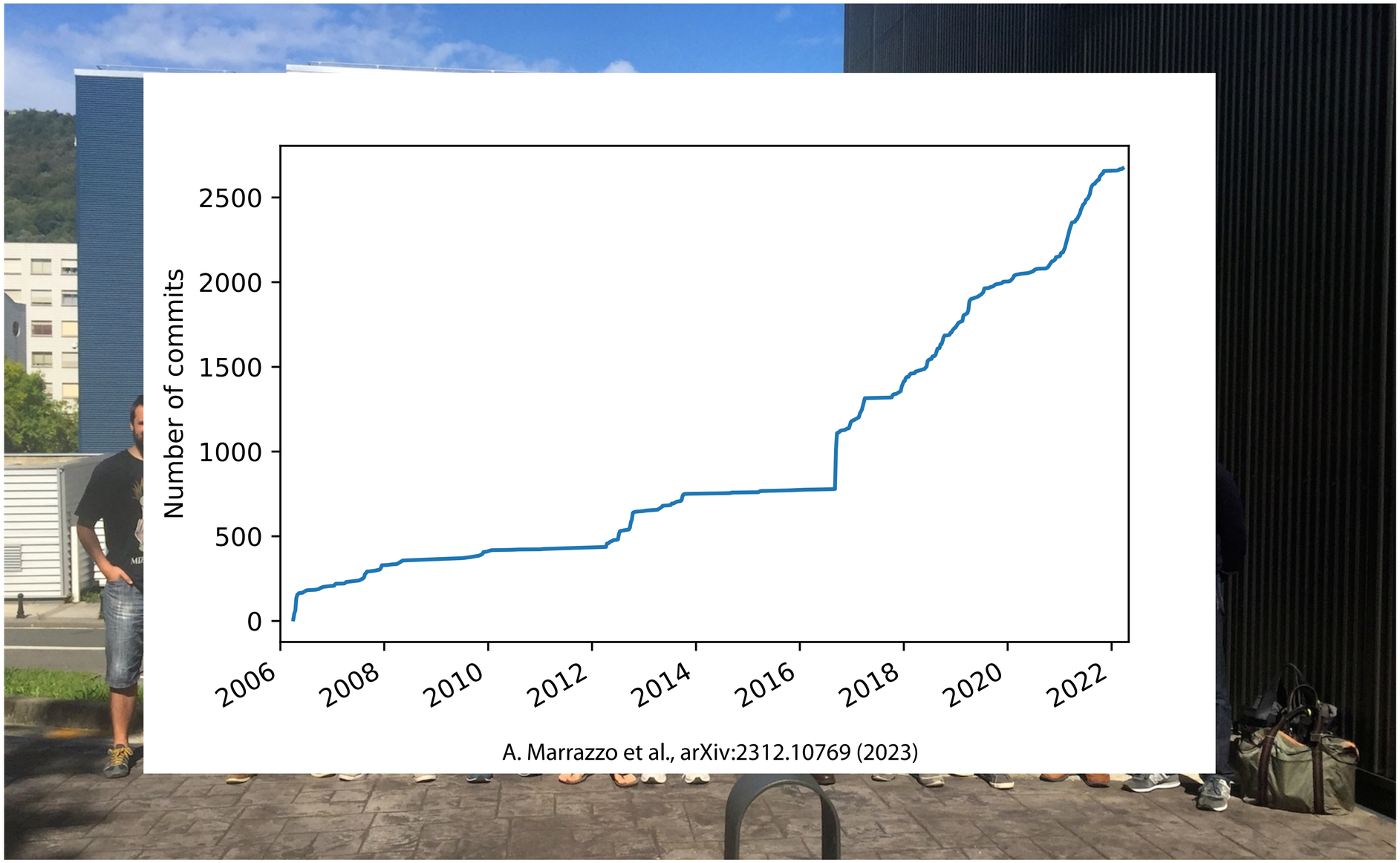
Many more people involved
in the past years:
**Wannier90 transitioned
to a community code**

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]

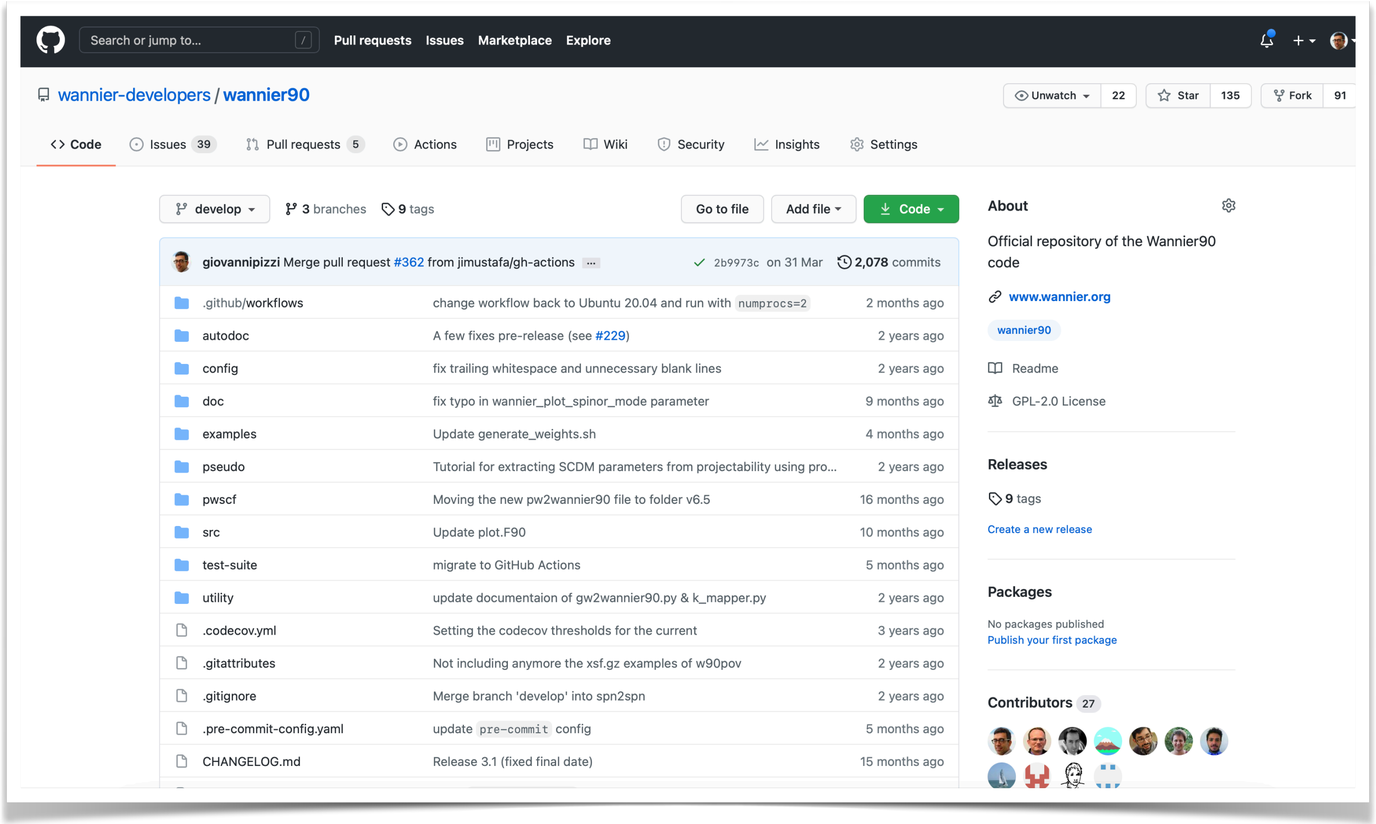
San Sebastian 2016: Wannier Coding Week



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 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 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)

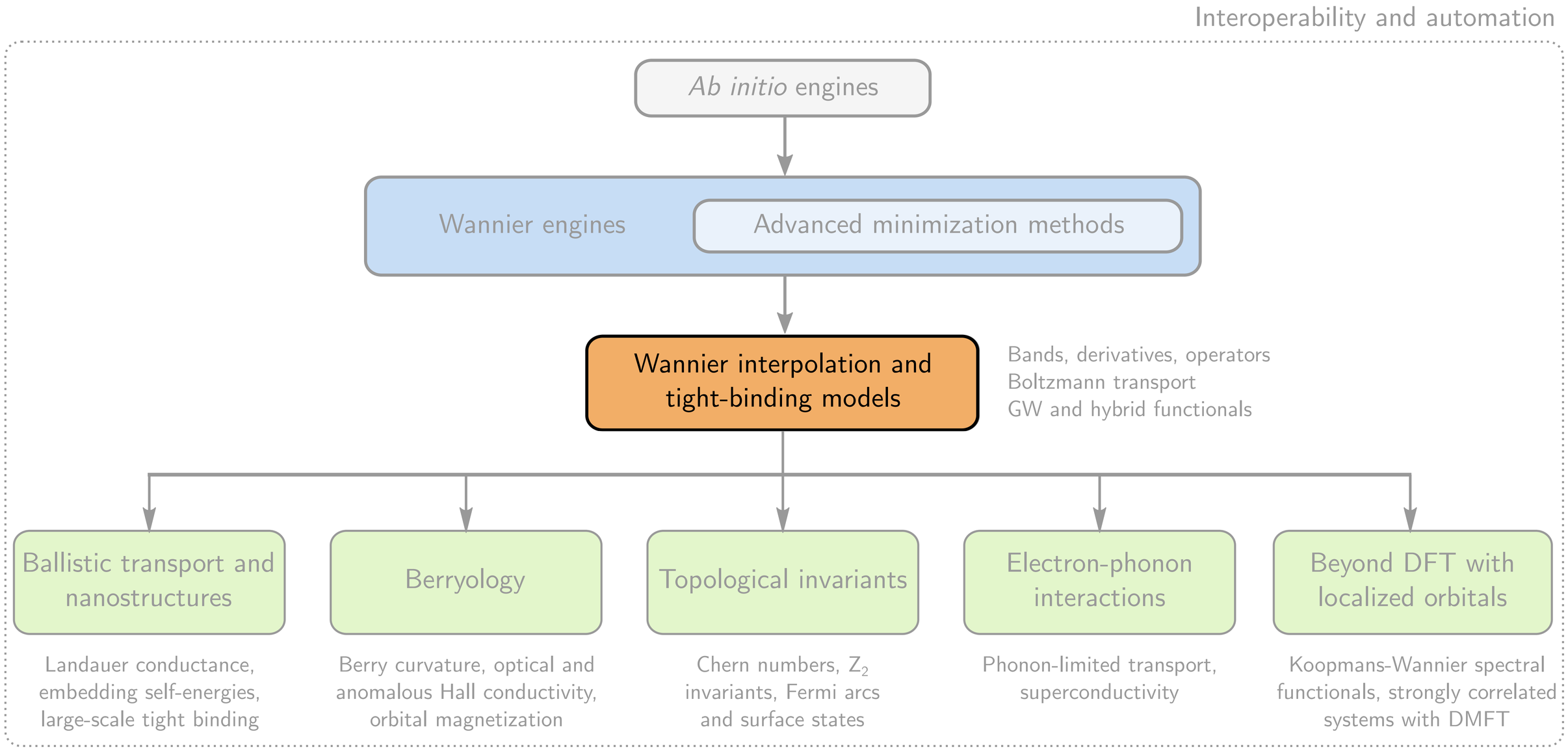
Berry phase properties including:

- 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]

Wannier interpolation

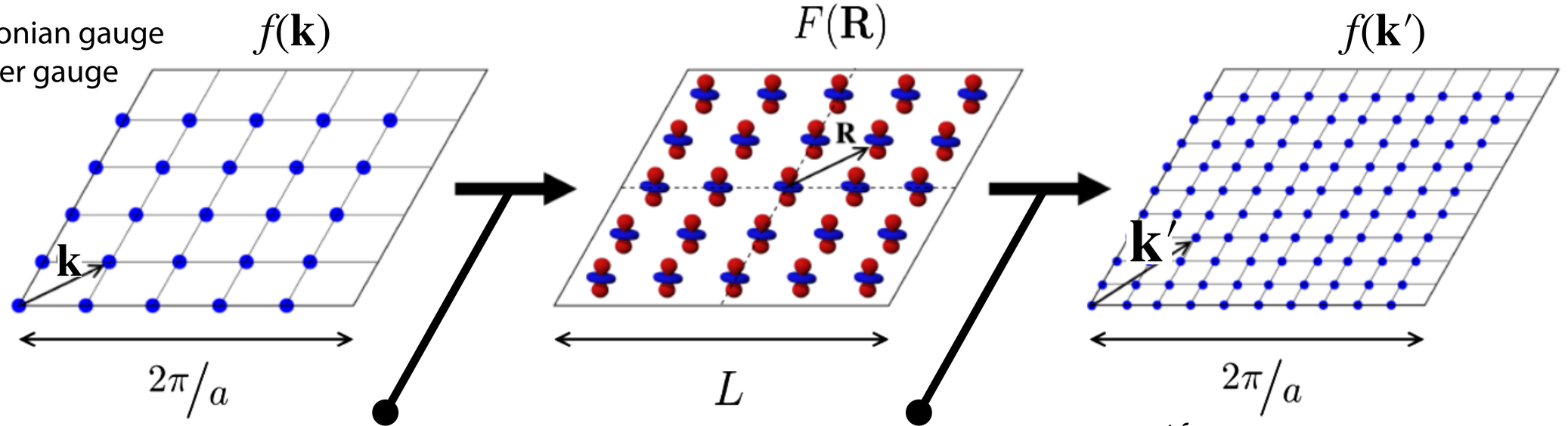


A. Marrazzo et al., arXiv:2312.10769 (2023)

Wannier interpolation

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).

(H): Hamiltonian gauge
(W): Wannier gauge



$$H^{\mathrm{W}}_{ij}(\mathbf{R}) = \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{n=1}^{\mathcal{J}_{\mathbf{k}}} V^{*}_{\mathbf{k},ni}\varepsilon_{n\mathbf{k}}V_{\mathbf{k},nj}$$

$$H^{\mathrm{W}}_{\mathbf{k}',ij} = \sum_{\mathbf{R}}^{\mathrm{WS}} \frac{1}{\mathcal{N}_{\mathbf{R},ij}} \sum_{l=1}^{\mathcal{N}_{\mathbf{R},ij}} e^{i\mathbf{k}'\cdot(\mathbf{R}+\mathbf{T}^{l}_{\mathbf{R},ij})} H^{\mathrm{W}}_{ij}(\mathbf{R})$$

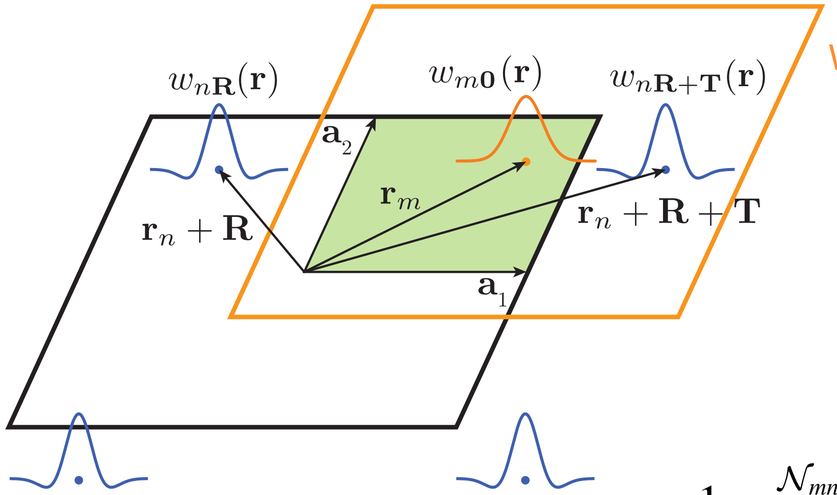
Exponential decay in real space inherited from Wannier functions!

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

$$\left[\mathcal{U}^{\dagger}_{\mathbf{k}'} H^{\mathrm{W}}_{\mathbf{k}'} \mathcal{U}_{\mathbf{k}'}\right]_{mn} = \delta_{mn}\varepsilon^{\mathrm{H}}_{n\mathbf{k}'}$$

N. Marzari et al., Rev. Mod. Phys. 84, 4 (2012); G. Pizzi et al, JPCM 32, 165902 (2020); A. Marrazzo et al., arXiv:2312.10769 (2023)

Improved Wannier interpolation by minimal-distance replica selection

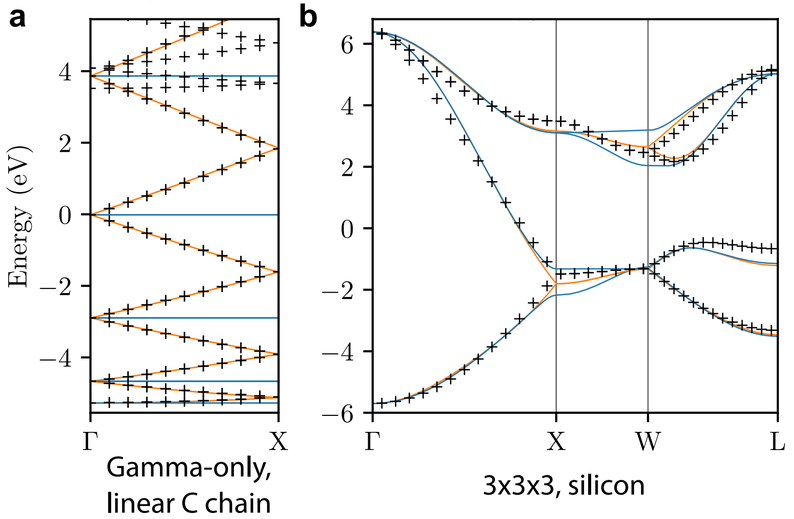


Wigner-Seitz supercell

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

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

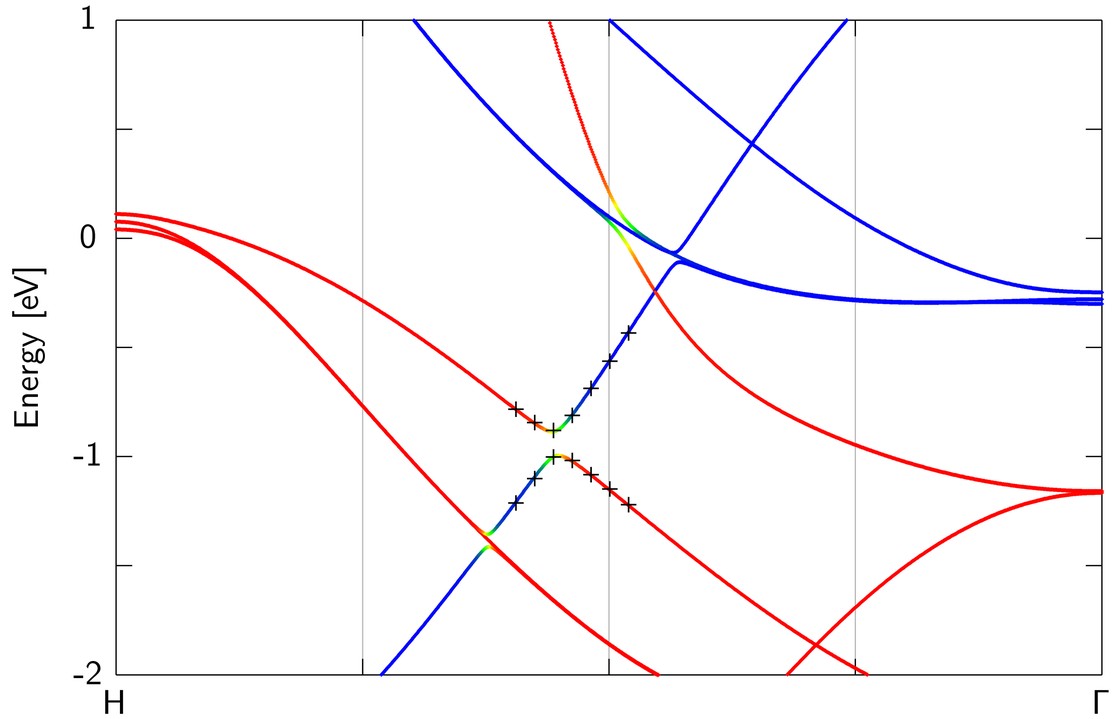
3x3x3, silicon

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)

Wannier interpolation beyond band structures



Color is the expectation value of the spin S_z
BCC Iron

Wannier representation

$$X^{\mathrm{W}}_{ij}(\mathbf{R}) = \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{m.n=1}^{\mathcal{J}_{\mathbf{k}}} V^{*}_{\mathbf{k},mi}\langle\psi_{m\mathbf{k}}|\hat{X}|\psi_{n\mathbf{k}}\rangle V_{\mathbf{k},nj}$$

Fourier transform
(mind the minimal-distance replica method)

$$\longrightarrow X^{\mathrm{W}}_{\mathbf{k}',ij} = \sum_{\mathbf{R}} e^{i\mathbf{k}'\cdot\mathbf{R}} X^{\mathrm{W}}_{ij}(\mathbf{R}) = \langle\psi^{\mathrm{W}}_{i\mathbf{k}'}|\hat{X}|\psi^{\mathrm{W}}_{j\mathbf{k}'}\rangle$$

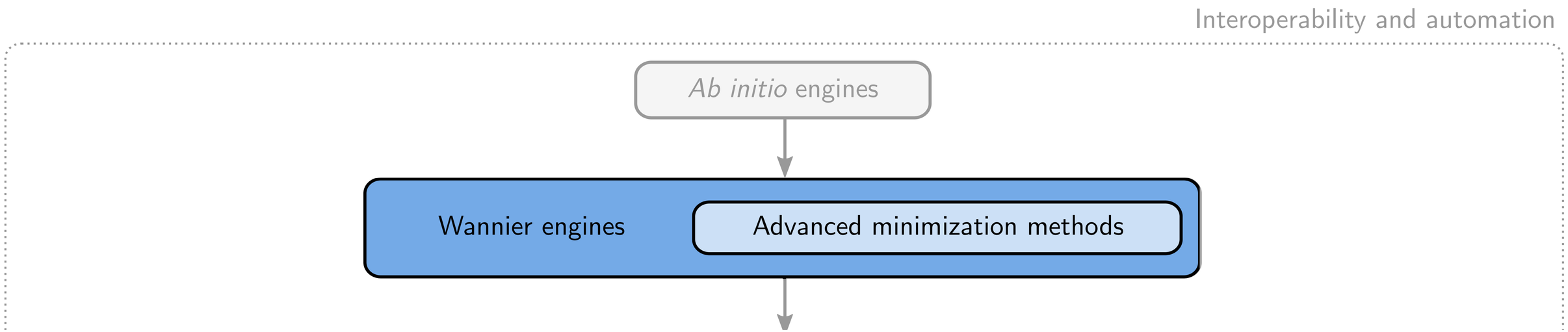
Diagonalize
(from Wannier to Hamiltonian gauge)

$$\longrightarrow X^{\mathrm{H}}_{\mathbf{k}',mn} = \left(\mathcal{U}^{\dagger}_{\mathbf{k}'} X^{\mathrm{W}}_{\mathbf{k}'} \mathcal{U}_{\mathbf{k}'}\right)_{mn} = \langle\psi^{\mathrm{H}}_{m\mathbf{k}'}|\hat{X}|\psi^{\mathrm{H}}_{n\mathbf{k}'}\rangle$$

J. Yates et al, Phys. Rev. B 75, 195121 (2007)

A. Marrazzo et al., arXiv:2312.10769 (2023)

Gauge freedoms



➡No minimization: "projection-only" WFs

➡Change the minimization functional

- MLWF: maximally-localized Wannier functions
- SAWF: symmetry-adapted Wannier functions
- SLWF: selectively-localized Wannier functions
- SLWF+C: " with constrained centres
- POWFs: partly occupied Wannier functions (Thygesen, 2005)
- Generalized spread functionals (Gygi et al, 2003):
  - mixed Wannier-Bloch (Giustino and Pasquarello, 2006)
  - dually localized (Mahler et al, 2022)
- …

➡Change starting point and/or algorithm

- Atomic or hybrid orbitals
- Automation strategies (e.g., optimized projection functions by Mustafa et al., 2015)
- Selected columns of the density matrix (SCDM, Damle et al., 2015)
- Continuos Bloch gauges (parallel transport, Cancès et al., 2017)
- Projectability disentanglement & manifold remixing (Saturday lecture by J. Qiao)
- …

A. Marrazzo et al., arXiv:2312.10769 (2023)

Symmetry-adapted Wannier functions

- **MLWF**: maximally-localized 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-localized Wannier functions

  -> selective localization of a subset of the Wannier functions

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

  -> *penalty term on the deviation from the predefined centers*

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

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
- (More sophisticated and accurate methods will be discussed by Junfeng Qiao in his lecture and tutorial on Saturday)

Some typical 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): $P = \sum_{i=1}^{N} |\psi_i\rangle \langle\psi_i|$

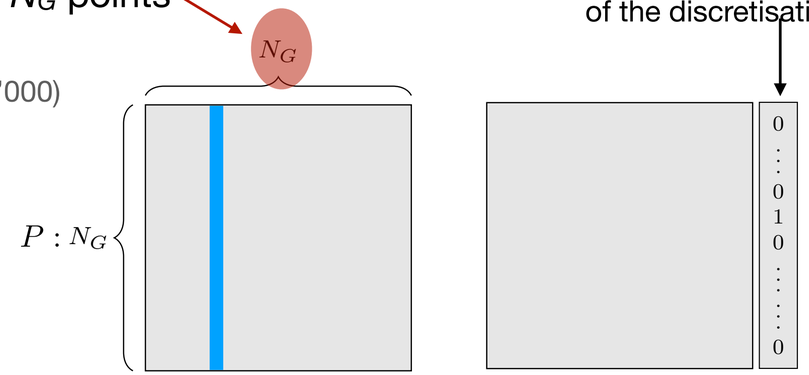
It is a projector (on the valence subspace):

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

Discretization 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*

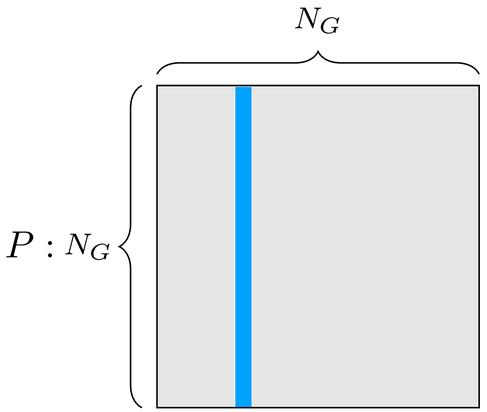
These projections (the columns) are localized! (but are not orthogonal)

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 - 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**

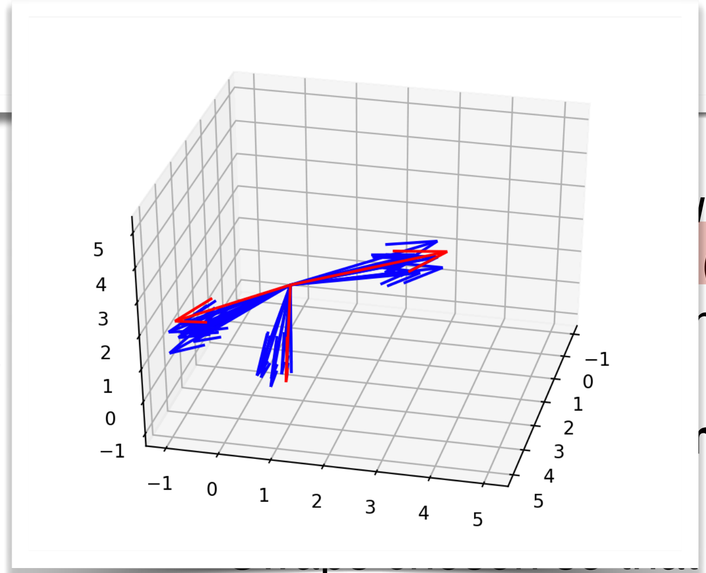
- Swaps chosen so that **diagonal elements of *R* are decreasing**: $|R_{11}| > |R_{22}| > \ldots$

SCDM - using *N* CDMs to span the valence subspace

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

ZGEQP3)

$$P\Pi = QR$$



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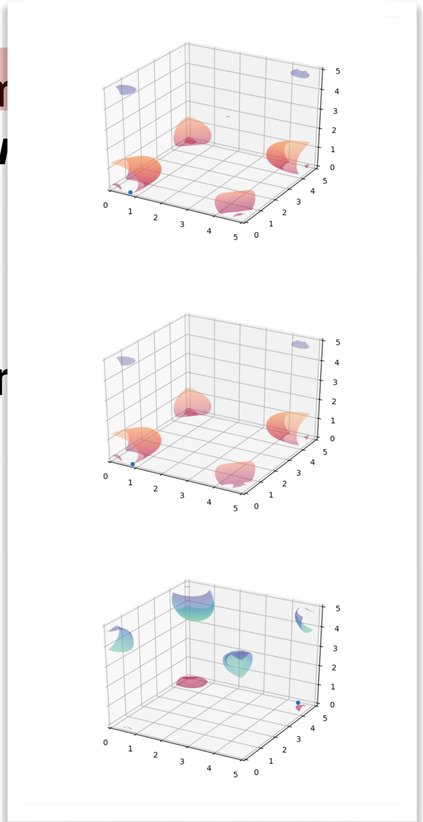
are decreasing: $|R_{11}| > |R_{22}| > \ldots$



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

A final orthonormalization (Löwdin) completes the algorithm

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

SCDM - entangled bands

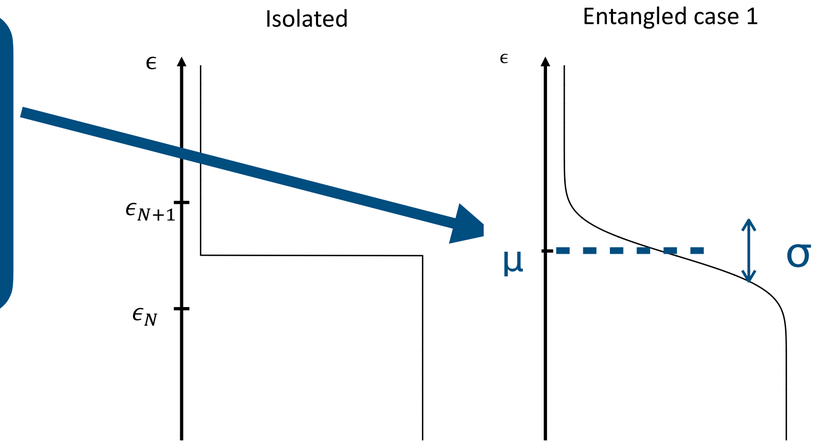
- We consider (formally) all eigenstates, and give a weight in the *quasi-density-matrix P*

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

- *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)

Projectabilities

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

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)

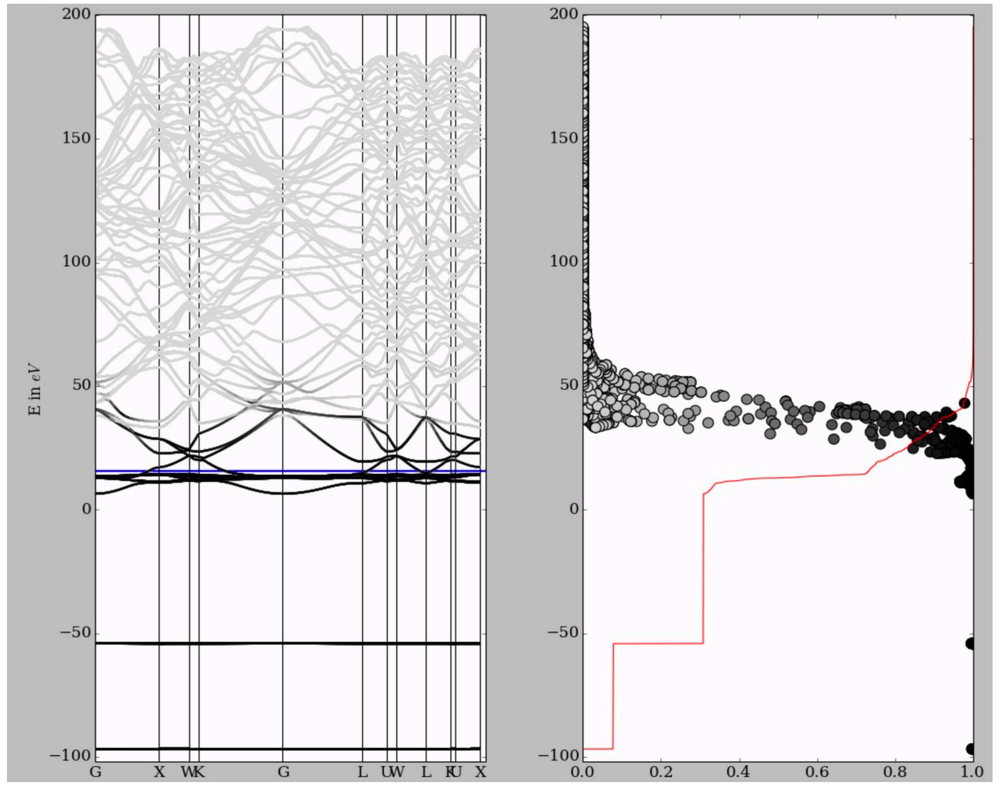


Image: courtesy of Daniel Marchand, EPFL

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

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:

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

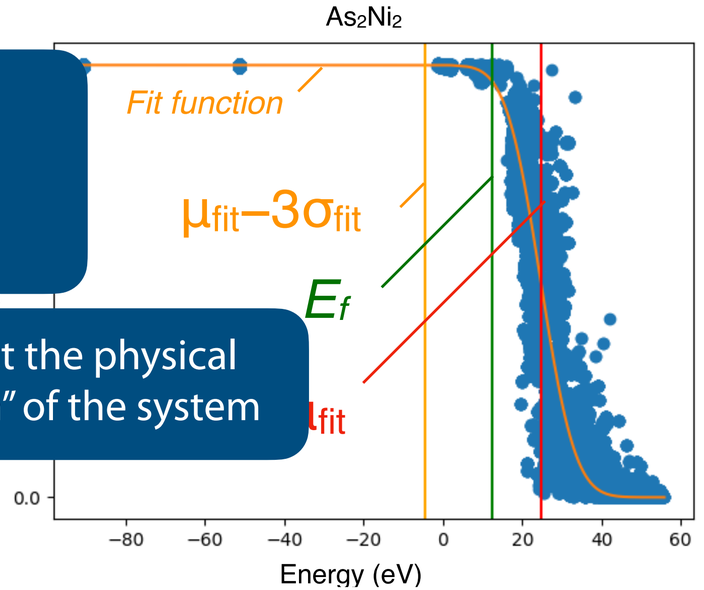
μ: when projectability≲0.9, weight≲10^{-3}

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

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

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

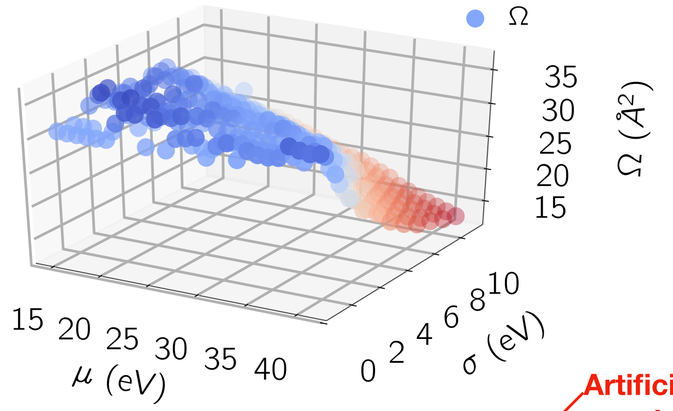
$$\mu = \mu_{\text{fit}} - 3\sigma_{\text{fit}}; \qquad \sigma = \sigma_{\text{fit}}$$



Parameter choice validation: tungsten (W)

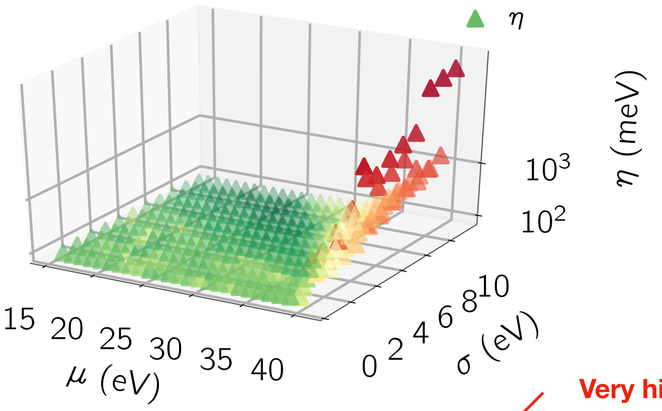
Spread

as a function of μ and σ



Bands distance w.r.t direct DFT diagonalization

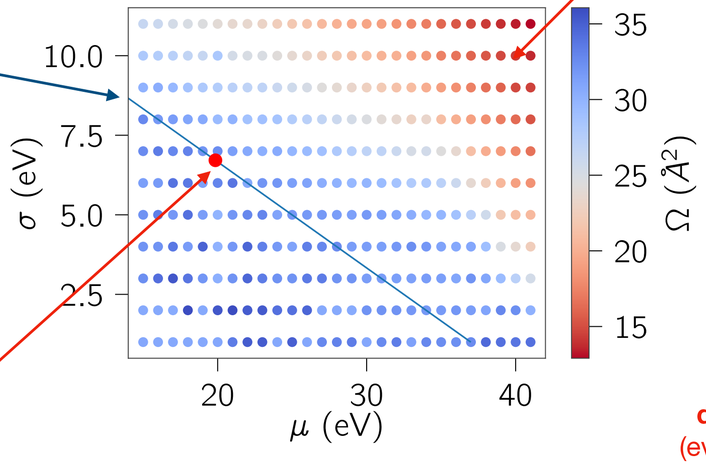
as a function of μ and σ



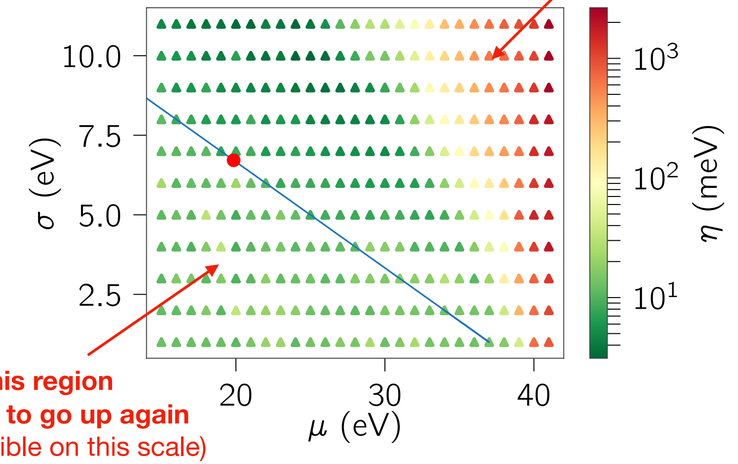
Artificially low total spread

Very high bands distance

μ = μfit – 3σ



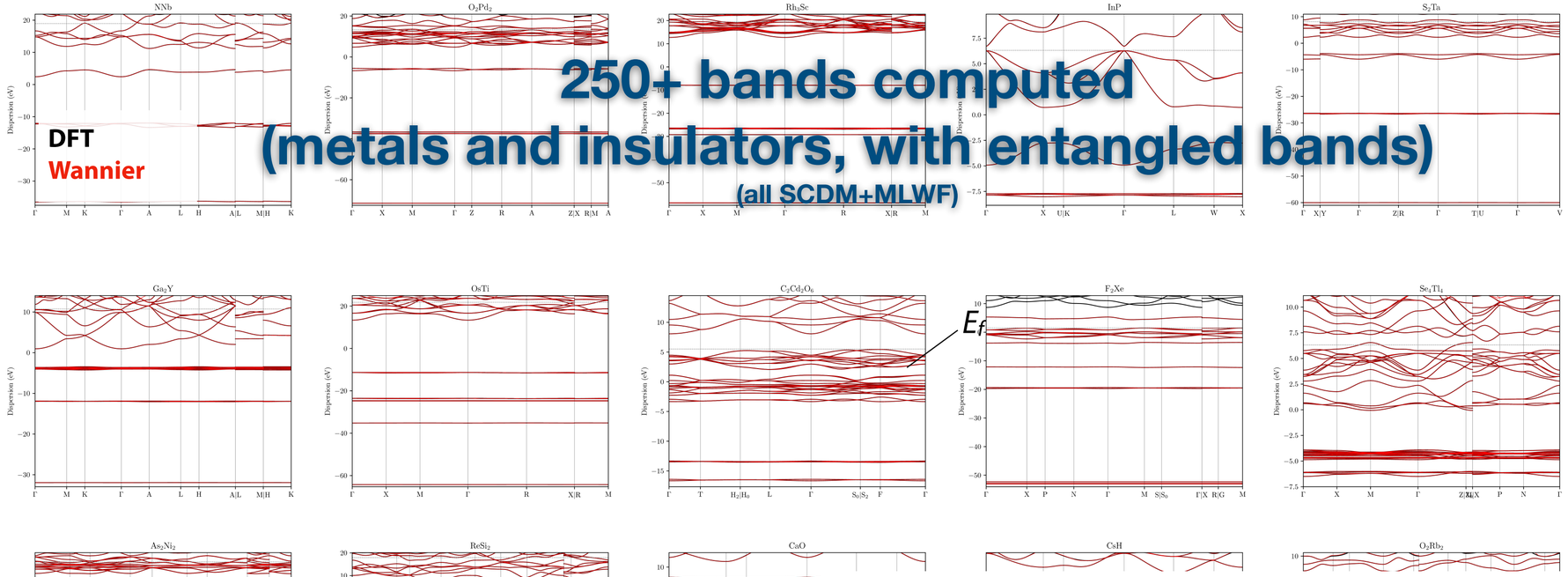
Our protocol:
μ = μfit – 3σfit



Also in this region distance starts to go up again
(even if not so visible on this scale)

V. Vitale, G. Pizzi, A. Marrazzo et al., npj Computational Materials 6, 66 (2020)

Automated high-throughput Wannierization



- 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)

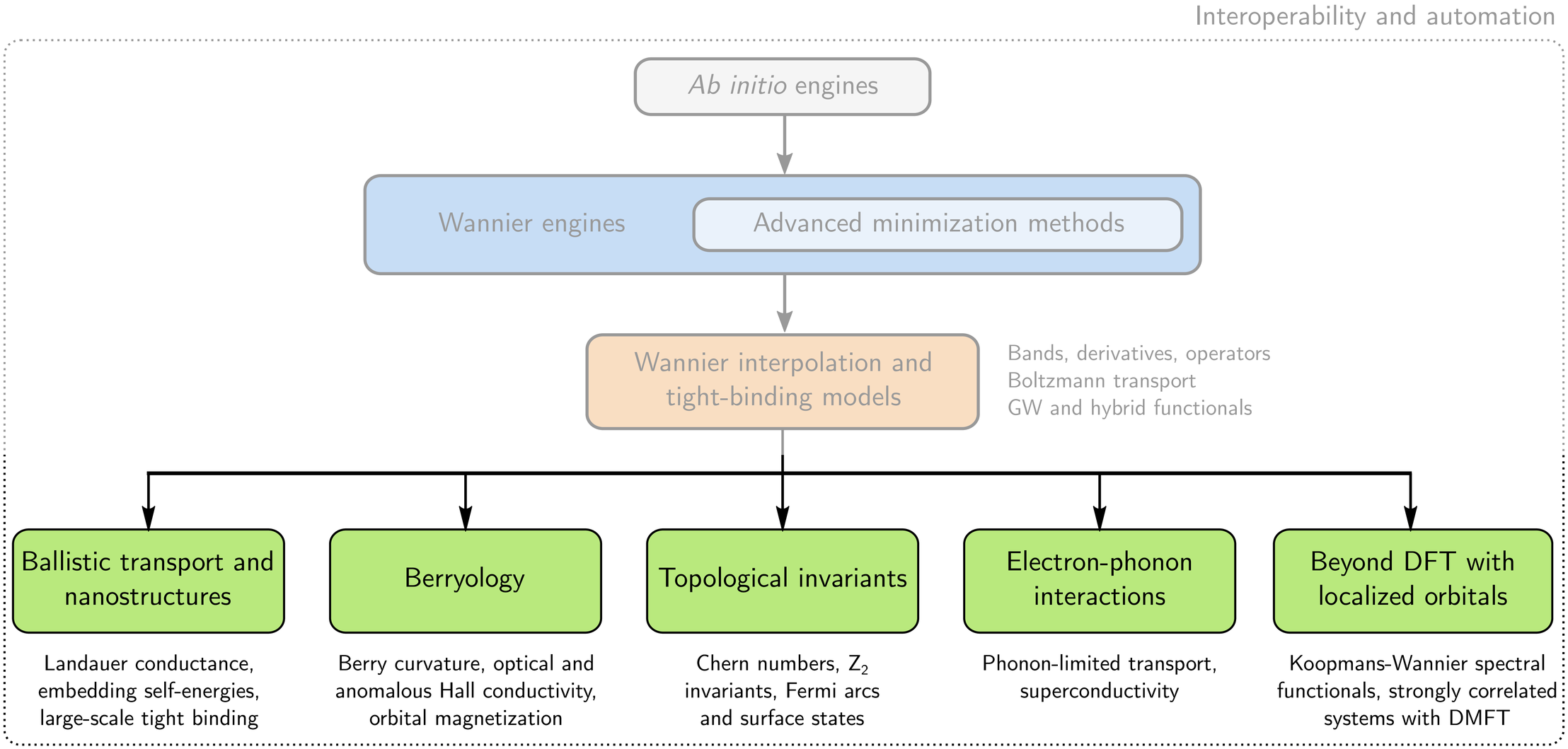
- All workflows available; see tutorial:

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

- **We will not use AiiDA today**; in Exercise 4, you will run all steps "by hand" - but check out the AiiDA tutorials if you are interested

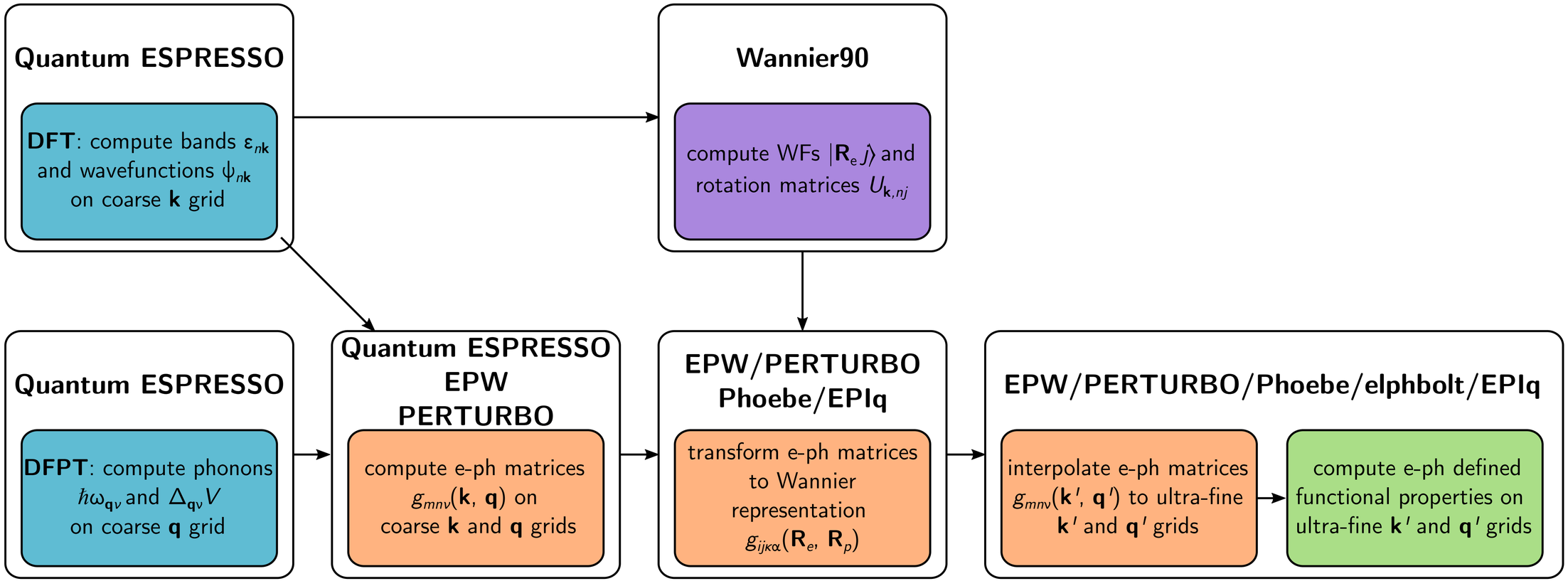
V. Vitale, G. Pizzi, A. Marrazzo et al., npj Computational Materials 6, 66 (2020)

A bird's-eye view on the ecosystem



A. Marrazzo et al., arXiv:2312.10769 (2023)

Electron-phonon coupling



Wannier interpolation of electron-phonon coupling matrix elements
(See lectures by Giustino, Margine, Poncè, Lafuente, etc.)

A. Marrazzo et al., arXiv:2312.10769 (2023)

Berryology

Berry phases and related quantities are central to the description of the electronic properties of materials, some examples:

Polarization

$$\mathbf{P}_{\rm el} = -e \sum_n^{\rm occ} \int_{\rm BZ} \frac{d^3k}{(2\pi)^3}\, \mathbf{A}_{\mathbf{k},nn}$$

$$\mathbf{A}_{\mathbf{k},mn} = i\langle u_{m\mathbf{k}} | \boldsymbol{\nabla}_{\mathbf{k}} u_{n\mathbf{k}} \rangle$$

Optical conductivity

$$\sigma_{ab}(\omega) = \frac{ie^2}{\hbar} \sum_{m,n} \int_{\rm BZ} \frac{d^3k}{(2\pi)^3}\, (f_{m\mathbf{k}} - f_{n\mathbf{k}}) \times$$

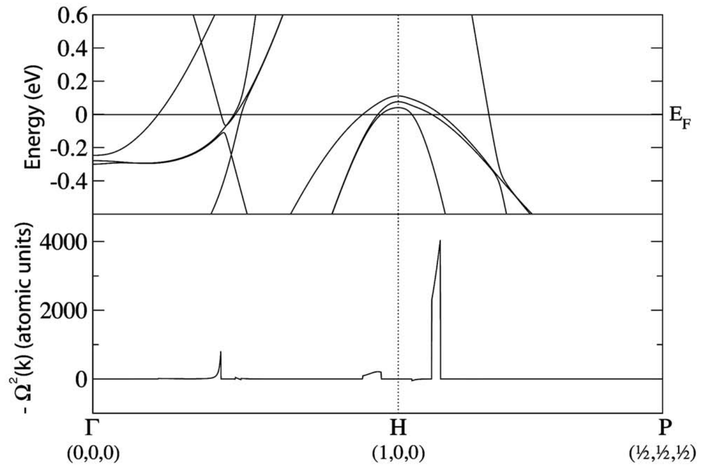
$$\times \frac{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}} - \hbar(\omega + i0^+)} A^a_{\mathbf{k},nm} A^b_{\mathbf{k},mn}$$

Anomalous Hall conductivity

$$\sigma_{yx} = \frac{e^2}{\hbar} \int_{\rm BZ} \frac{d^3k}{(2\pi)^3} \sum_n f_{n\mathbf{k}} \Omega^z_{n\mathbf{k}}$$

$$\boldsymbol{\Omega}_{n\mathbf{k}} = \boldsymbol{\nabla}_{\mathbf{k}} \times \mathbf{A}_{\mathbf{k},nn} = -{\rm Im}\, \langle \boldsymbol{\nabla}_{\mathbf{k}} u_{n\mathbf{k}} | \times | \boldsymbol{\nabla}_{\mathbf{k}} u_{n\mathbf{k}} \rangle$$

They can be efficiently calculated by representing the Hamiltonian, the position operator (and possibly other operators) on a basis of exponentially localized Wannier functions



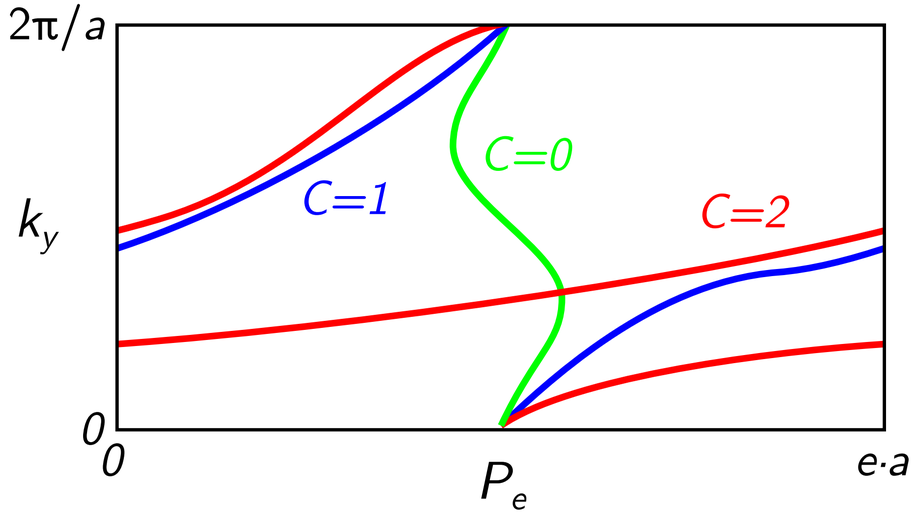
X. Wang et al, PRB 74, 195118 (2006)

Wannier interpolation is key to integrate spiky Berry curvatures due to avoided crossings.
Dedicated codes for these properties: postw90, WannierBerri

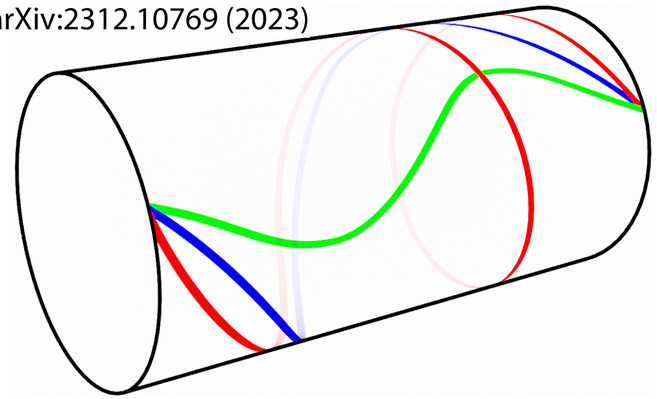
A. Marrazzo et al., arXiv:2312.10769 (2023)

Topological invariants

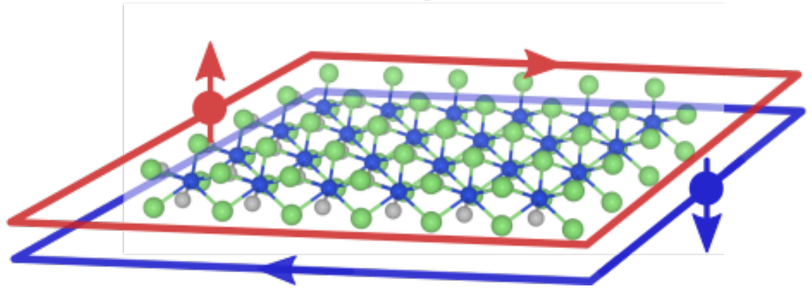
2D Brillouin zone



A. Marrazzo et al., arXiv:2312.10769 (2023)



Topological insulators do not admit a Wannier representation (that do not break any protecting symmetry of the topological phase): they cannot be mapped to their atomic limit without closing the gap



Hybrid/Hermaphrodite Wannier functions (Sgiarovello et al., 2001): Wannier along one direction, Bloch along the others

$$|h_{k_1 ln}\rangle = \frac{1}{N_2}\sum_{k_2} e^{-i2\pi k_2 l}\,|\psi_{n\mathbf{k}}\rangle$$

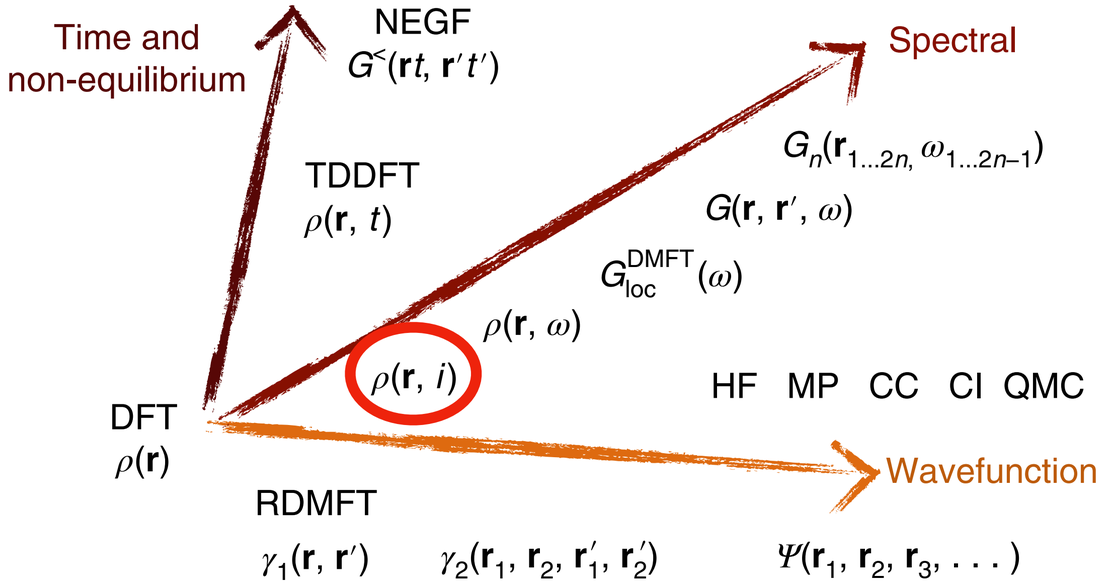
$$x_{2,k_1 ln} = \langle h_{k_1 ln}|\hat{x}_2|h_{k_1 ln}\rangle$$

The sum of the Wannier centers is the electronic polarization (Berry phase)

Topological invariants can be expressed by tracking the evolution of the hybrid/hermaphrodite Wannier centers (Soluyanov and Vanderbilt, see e.g. Vanderbilt's book *Berry phases in electronic structure theory*)

Spectral functionals from Wannier functions

Spectral properties with a functional theory based on localized orbitals
(As opposed to diagrammatic many-body approaches, such as GW)



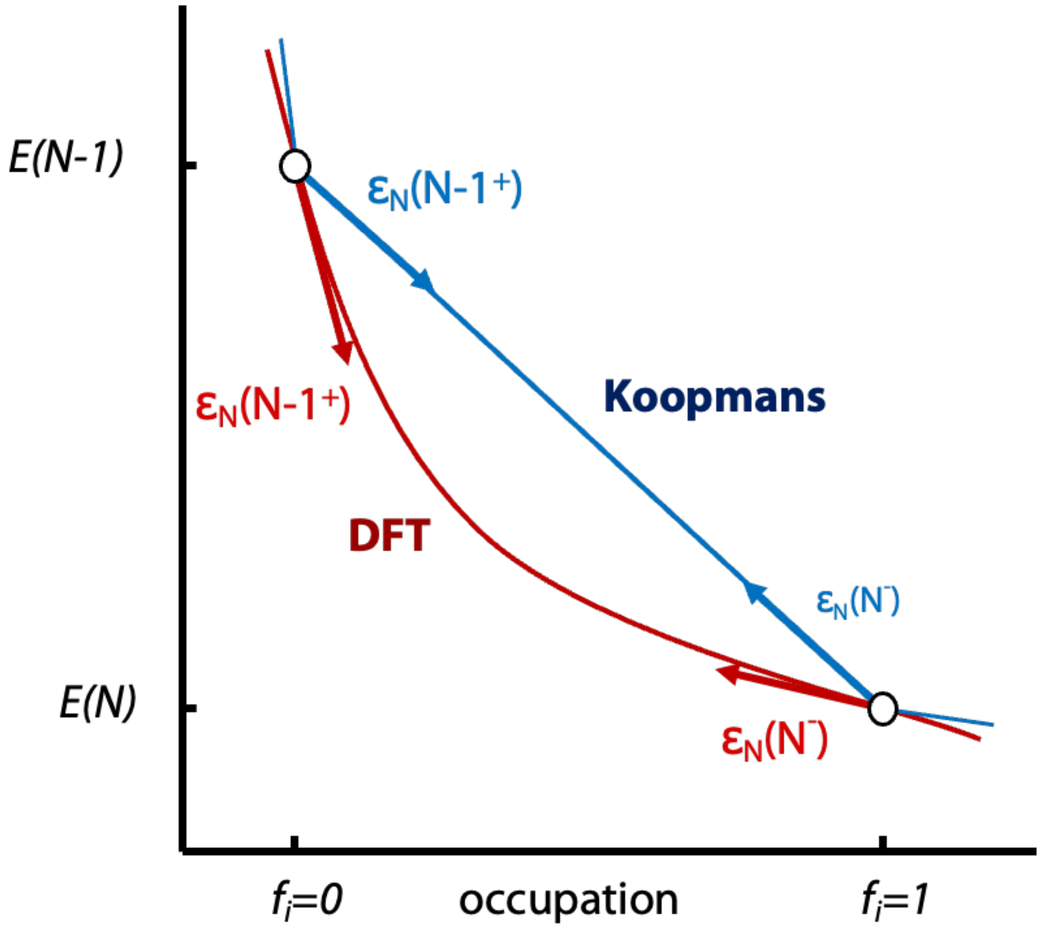
N. Marzari, A. Ferretti, and C. Wolverton Nature Materials 20, 736 (2021)

We need to go **beyond DFT**: a functional of the local, static density can only give the total energy

➡A functional of the **local spectral density** ρ(**r**,ω) can provide also charged excitations

➡In a quasi-particle picture, $\rho(\boldsymbol{r},\omega) \rightarrow \rho(\boldsymbol{r},i)$: **orbital-density-dependent functionals**

Koopmans-compliant spectral functionals



We impose **piece-wise linearity**:
All orbitals energies are independent from their own occupations

$$\varepsilon_i = \frac{dE}{df_i} = \langle \phi_i | \hat{H} | \phi_i \rangle$$

$$\varepsilon_i = E_i^{N\pm1} - E^N$$

I. Dabo et al. arXiv.0910.2637 (2009); I. Dabo et al. PRB 82, 115121 (2010)

Linearization + screening

- **Linearization** (first, at frozen orbital)

  I. Dabo *et al.* PRB **82**, 115121 (2010); Borghi et *al.* PRB **90**, 075135 (2014)

$$E^{\mathrm{KI}} = E^{\mathrm{DFT}} + \sum_i \left[- \int_0^{f_i} ds \, \langle \phi_i | H^{\mathrm{DFT}}(s) | \phi_i \rangle + f_i \int_0^1 ds \, \langle \phi_i | H^{\mathrm{DFT}}(s) | \phi_i \rangle \right]$$

- **Screening** and **relaxation** effects

  I. Dabo *et al.* PRB **82**, 115121 (2010); N. Colonna *et al.* JCTC **14**, 2549 (2018)

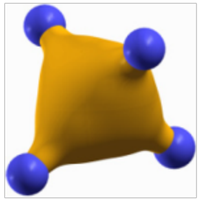
$$E^{\mathrm{KI}} = E^{\mathrm{DFT}} + \sum_i \alpha_i \left[- \int_0^{f_i} ds \, \langle \phi_i | H^{\mathrm{DFT}}(s) | \phi_i \rangle + f_i \int_0^1 ds \, \langle \phi_i | H^{\mathrm{DFT}}(s) | \phi_i \rangle \right]$$

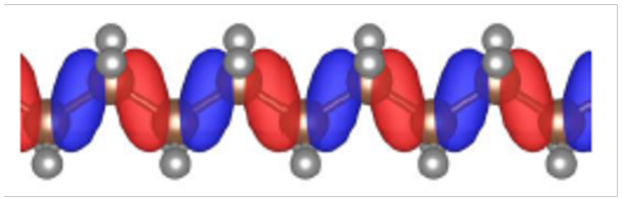
$$\alpha_i = \frac{\langle n_i | \epsilon^{-1} f_{\mathrm{Hxc}} | n_i \rangle}{\langle n_i | f_{\mathrm{Hxc}} | n_i \rangle}$$

A theory not invariant under unitary transformations: Wannier functions in disguise

$$E_{\mathrm{gs}}^{\mathrm{KC}} = \min_{\{\phi_i\}} \left\{ E^{\mathrm{KC}}[\rho, \{\rho_i\}] - \sum_{ij} \Lambda_{ji}(\langle \phi_i | \phi_j \rangle - \delta_{ij}) \right\}$$

CANONICAL

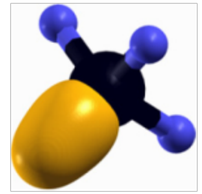


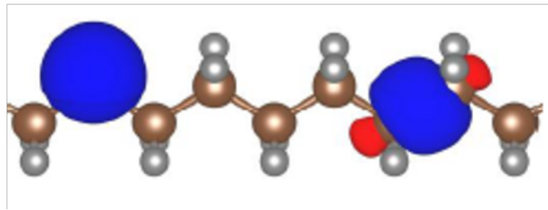


$$\lambda_m = \sum_{ij} U_{mj} \Lambda_{ji} U_{im}^{\dagger}$$

$$|\psi_m\rangle = \sum_{i} |\phi_i\rangle U_{im}^{\dagger}$$

VARIATIONAL





Maximally-localized Wannier functions can be used as a proxy for variational orbitals

N.L. Nguyen et al, Phys. Rev. X 8, 021051 (2018)

Non-collinear Koopmans-Wannier functionals

$$\Pi_i^{\mathrm{rKI}} = -\left\{E^{\mathrm{DFT}}[\rho, \mathbf{m}] - E^{\mathrm{DFT}}[\rho^{f_i=0}, \mathbf{m}^{f_i=0}]\right\} + f_i\left\{E^{\mathrm{DFT}}[\rho^{f_i=1}, \mathbf{m}^{f_i=1}] - E^{\mathrm{DFT}}[\rho^{f_i=0}, \mathbf{m}^{f_i=0}]\right\}$$

$$\Pi_i^{(2)\mathrm{rKI}} = \frac{1}{2} f_i(1-f_i)\frac{d^2 E^{\mathrm{DFT}}}{df_i^2}\Big|_{\bar{f}}$$

2nd order expansion

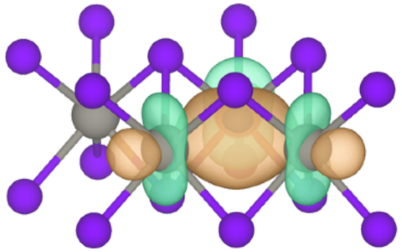
$$\mathcal{V}_i^{KI(2)}(\mathbf{r}) = -\frac{1}{2}\int d\mathbf{r} d\mathbf{r}' \boldsymbol{n}_i(\mathbf{r}) \mathbb{F}_{Hxc}(\mathbf{r}, \mathbf{r}') \boldsymbol{n}_i(\mathbf{r}') \sigma_0 + (1-f_i)\sum \int d\mathbf{r}' \left[\mathbb{F}_{Hxc}(\mathbf{r}, \mathbf{r}') \boldsymbol{n}_i(\mathbf{r}')\right]_\alpha \sigma_\alpha$$

Wannier function charge density

Wannier function spin density

$$\left(n_\rho(\mathbf{r}), n_{m_x}(\mathbf{r}), n_{m_y}(\mathbf{r}), n_{m_z}(\mathbf{r})\right)$$

$$\Delta H_{ij}^{\mathrm{KI}(2)}(\mathbf{R}) = -\frac{1}{2}\Delta_{\mathbf{0j}}^{\mathrm{KI}(2)}\delta_{\mathbf{R},\mathbf{0}}\delta_{i,j} + \Delta H_{ij,\mathbf{r}}^{\mathrm{KI}(2)}(\mathbf{R})$$



One-shot correction on top of DFT
Orbitals are maximally-localized Wannier functions

A. Marrazzo and N. Colonna, arXiv:2402.14575 (2024) - in press on Physical Review Research

Non-collinear Koopmans-Wannier functionals

Non-collinear Koopmans potential $\mathcal{V}_i^{KI(2)}(\mathbf{r}) = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\boldsymbol{n}_i(\mathbf{r})\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}')\boldsymbol{n}_i(\mathbf{r}')\sigma_0 + (1-f_i)\sum\int d\mathbf{r}'\left[\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}')\boldsymbol{n}_i(\mathbf{r}')\right]_\alpha\sigma_\alpha$

charge-charge interaction

charge-spin interaction

Wannier function charge density

Wannier function spin density

$$\left(n_\rho(\mathbf{r}), n_{m_x}(\mathbf{r}), n_{m_y}(\mathbf{r}), n_{m_z}(\mathbf{r})\right)\cdot\begin{pmatrix}\mathbb{F}_{Hxc}^{\rho,\rho} & \mathbb{F}_{xc}^{\rho,m_x} & \mathbb{F}_{xc}^{\rho,m_y} & \mathbb{F}_{xc}^{\rho,m_z}\\ \mathbb{F}_{xc}^{m_x,\rho} & \mathbb{F}_{xc}^{m_x,m_x} & \mathbb{F}_{xc}^{m_x,m_y} & \mathbb{F}_{xc}^{m_x,m_z}\\ \mathbb{F}_{xc}^{m_y,\rho} & \mathbb{F}_{xc}^{m_y,m_x} & \mathbb{F}_{xc}^{m_y,m_y} & \mathbb{F}_{xc}^{m_y,m_z}\\ \mathbb{F}_{xc}^{m_z,\rho} & \mathbb{F}_{xc}^{m_z,m_x} & \mathbb{F}_{xc}^{m_z,m_y} & \mathbb{F}_{xc}^{m_z,m_z}\end{pmatrix}\cdot\begin{pmatrix}n_\rho(\mathbf{r})\\ n_{m_x}(\mathbf{r})\\ n_{m_y}(\mathbf{r})\\ n_{m_z}(\mathbf{r})\end{pmatrix}$$

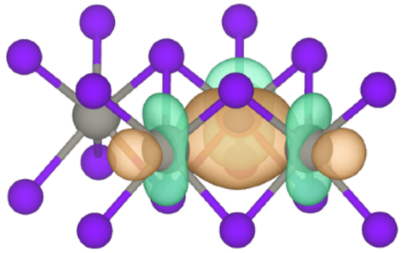
spin-spin interaction

screened interaction

un-screened interaction

interacting response function

$$\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}') = \mathbf{F}_{Hxc}(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}''\mathbf{F}_{Hxc}(\mathbf{r},\mathbf{r}'')\int d\mathbf{r}'''\boldsymbol{\chi}(\mathbf{r}'',\mathbf{r}''')\mathbf{F}_{Hxc}(\mathbf{r}''',\mathbf{r}')$$



charge-charge

charge-spin

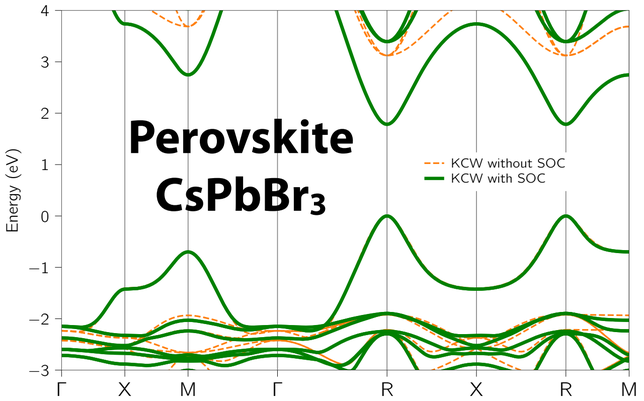
$$\begin{pmatrix}\chi^{\rho,\rho} & \chi^{\rho,m_x} & \chi^{\rho,m_y} & \chi^{\rho,m_z}\\ \chi^{m_x,\rho} & \chi^{m_x,m_x} & \chi^{m_x,m_y} & \chi^{m_x,m_z}\\ \chi^{m_y,\rho} & \chi^{m_y,m_x} & \chi^{m_y,m_y} & \chi^{m_y,m_z}\\ \chi^{m_z,\rho} & \chi^{m_z,m_x} & \chi^{m_z,m_y} & \chi^{m_z,m_z}\end{pmatrix}\cdot\begin{pmatrix}F_{Hxc}^{\rho,\rho} & F_{xc}^{\rho,m_x} & F_{xc}^{\rho,m_y} & F_{xc}^{\rho,m_z}\\ F_{xc}^{m_x,\rho} & F_{xc}^{m_x,m_x} & F_{xc}^{m_x,m_y} & F_{xc}^{m_x,m_z}\\ F_{xc}^{m_y,\rho} & F_{xc}^{m_y,m_x} & F_{xc}^{m_y,m_y} & F_{xc}^{m_y,m_z}\\ F_{xc}^{m_z,\rho} & F_{xc}^{m_z,m_x} & F_{xc}^{m_z,m_y} & F_{xc}^{m_z,m_z}\end{pmatrix}$$

spin-spin

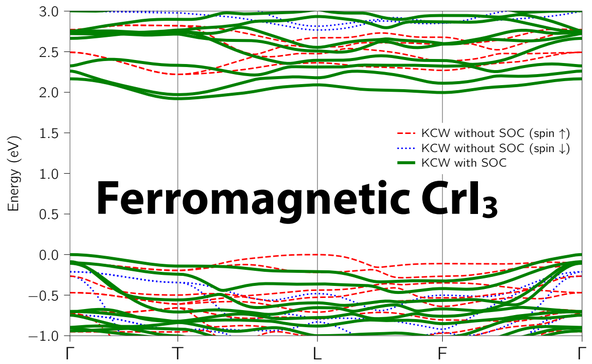
Spin-dependent interactions and **screening** effects that are missing in standard diagrammatic approaches based on the random phase approximation.

A. Marrazzo and N. Colonna, arXiv:2402.14575 (2024) - in press on Physical Review Research

Non-collinear Koopmans-Wannier functionals



While including orbital- and spin-dependent interactions in many-body perturbation theory (e.g., GW) requires self-screening or vertex corrections, they emerge naturally in Koopmans functionals



	Method	Band gap (eV)
without SOC	LDA	1.40
	HSE	2.09
	G_0W_0	2.56 [35]
	$QSGW\tilde{W}$	3.15 [35]
	KCW	3.12
with SOC	LDA	0.18
	HSE	0.78
	G_0W_0	0.94 [35]
	$QSGW\tilde{W} + \Delta_{\mathrm{SOC}}^{G_0W_0}$	1.53 [35]
	KCW	1.78
	Exp $+\Delta E_T$	1.85 [35, 96]

Accuracy in presence of spin-orbit coupling (SOC) comparable to state-of-the-art diagrammatic approaches, at low computational cost and complexity

	Method	Band gap (eV)
without SOC	LDA	0.89
	HSE	1.85
	G_0W_0	2.07 [101]
	$QSGW80$	2.23 [102]
	$QSGW$	3.11 [101]
	KCW	2.22
with SOC	LDA	0.63
	HSE	1.45
	G_0W_0	1.99 [101]
	$QSGW80$	1.68 [102]
	$QSGW$	2.64 [101],3.0 [98, 99]
	$QSGW\tilde{W}$	2.5 [98], 2.2 [99]
	KCW	1.92
	Exp [100]$+E_b$ (1 eV)	2.2

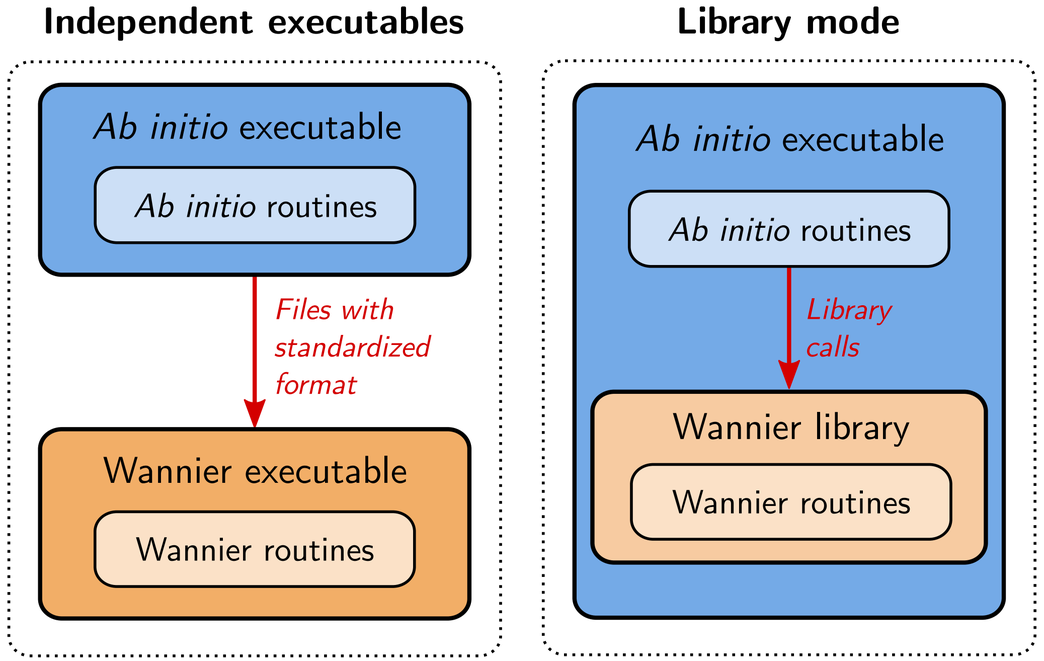
Soon available in Quantum ESPRESSO

A. Marrazzo and N. Colonna, arXiv:2402.14575 (2024) - in press on Physical Review Research

Towards Wannier90 4.0

Major restructuring of the code (lead by J. Jackson and colleagues at STFC, Daresbury, UK):

- a library interface to Wannier90 functionality that is capable of being invoked by an external calling program in a parallel (MPI) environment, with significant changes to the structure of the code since the last release (v3.1.0).
- Towards a unified python interface and I/O for Wannier90



The library mode will include all functionalities,
the "standalone" mode will be a wrapper calling the library.

A. Marrazzo et al., arXiv:2312.10769 (2023)

For newcomers and experts alike

The Wannier Function Software Ecosystem for Materials Simulations

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A. Marrazzo et al., arXiv:2312.10769 (2023)
Updated version 2 on arXiv soon, under revision at Rev. Mod. Phys.

Contents

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®

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

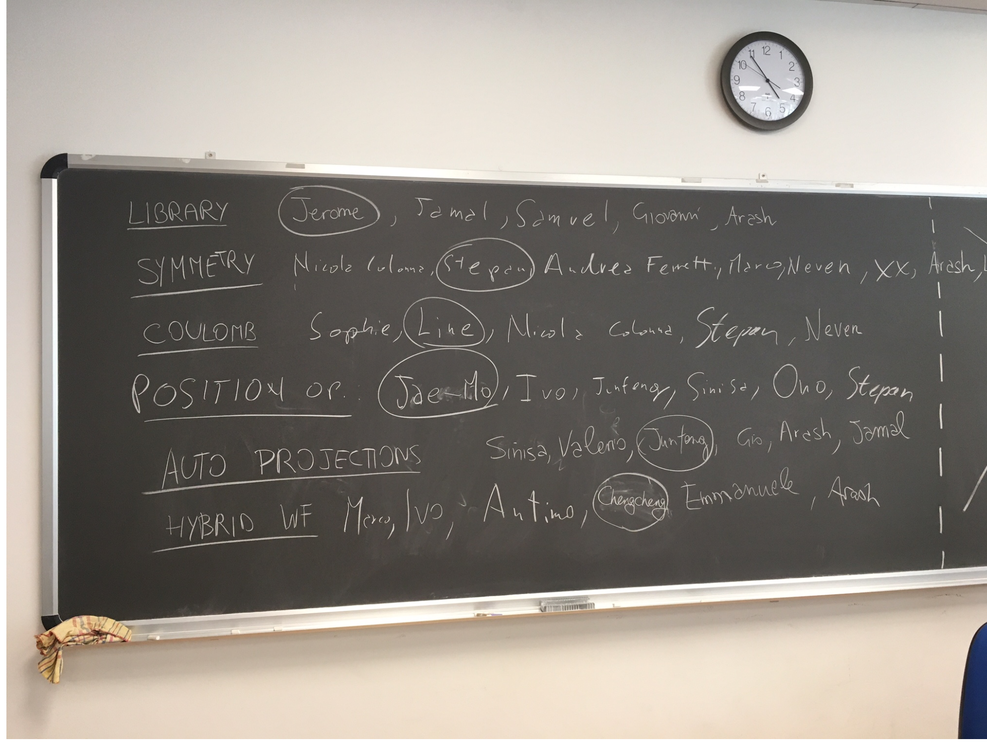
Trieste 2022: Wannier Developers Meeting

The first developer meeting for 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!

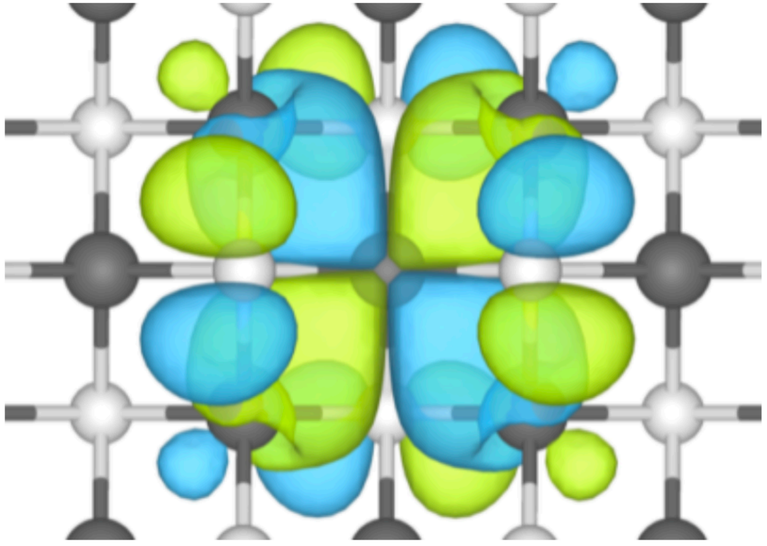


The Wannier 2022 Developers Meeting gathers the community that sustains various software packages built around the concept of maximally-localised Wannier functions (MLWF), strengthening interactions between the developers and promoting a synergetic research and software ecosystem.

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

A couple of talks have been cited as references in papers!

Wannier Developer Meeting 2023



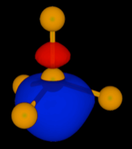
Location

Daresbury Laboratory,
Keckwick Lane,
Warrington WA4 4AD, UK

Wannier 2024 Developer Meeting (PSI, Switzerland)

https://wannier.org/events/

Wannier Software Ecosystem Registry



Wannier Software Ecosystem Registry

[View on GitHub/register your code]

Total number of codes: 53

Codes

If you think that a code is missing in this registry, you can simply add it by opening a GitHub pull request, following the instructions that you find in the README file of the repository.

Codes are sorted alphabetically by their ID.

ABINIT

Ab initio engines | Beyond-DFT with localized orbitals

ABINIT is a software suite to calculate the optical, mechanical, vibrational, and other observable properties of materials. Starting from the quantum equations of density functional theory, you can build up to advanced applications with perturbation theories based on DFT, and many-body Green's functions (GW and DMFT).

Show details

EPW

Electron-phonon coupling | Transport

EPW is an open-source community code for ab initio calculations of electron-phonon interactions using Density-Functional Perturbation Theory and Maximally Localized Wannier Functions.

Show details

https://wannier-developers.github.io/wannier-ecosystem-registry/

My take on Wannier trends for 2024

1. Initial projections are not a problem anymore: more applications are unlocked

   Wannierization is fully automated and comes with AiiDA workflows for Quantum ESPRESSO, YAMBO (G_0W_0) and Wannier90

   - Selected columns of the density-matrix (SCDM, Damle & Lin (2018), Vitale et al (2020))
   - Projectability disentanglement & manifold remixing (Saturday lecture by J. Qiao)
   - Automated G_0W_0-Wannier calculations (M. Bonacci et al., npj Computational Materials 9, 74 (2023))

2. Trading localization for symmetries is OK for a number of applications

   Less localized but more symmetric and possibly atom-centered Wannier functions: still not fully automated though

3. Wannier90 as a pure Wannierization engine & Fortran library:
   reference implementation and wide collection of well-established algorithms

   - Growing number of packages of the Wannier ecosystem dedicated to specific materials properties
   - Methods development might be done on Julia or other implementations, before a W90 release
   - Codes in the ecosystem will (slowly) shift from using W90 as standalone to internal calls to the library

22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Trieste (Italy), January 8-10, 2025

Organizers: Ion Errea (University of the Basque Country), Antimo Marrazzo (SISSA), Shobhana Narasimhan (JNCASR, Bangalore, India), Gian-Marco Rignanese (Université Catholique de Louvain)

- Great line-up of invited speakers
  - Leeor Kronik, Weizman Institute (Israel)
  - Nisanth Nair, IIT Kanpur (India)
  - Tommaso Chiarotti, EPFL (Switzerland)
  - Maria Chatzieleftheriou, Ecole polytechnique (France)
  - Gianluca Stefanucci, University of Rome Tor Vergata (Italy)
  - Gábor Csányi, University of Cambridge (UK)
  - Vikram Gavini, University of Michigan (USA)
  - Mariana Rossi, Max Planck Hamburg (Germany)
  - Raffaello Bianco, University of Modena e Reggio Emilia (Italy)
  - Roxane Margine, Binghamton University (USA)
  - Maria Clelia Righi, University of Bologna (Italy)
  - Claudio Zeni, Microsoft Research AI4Science (UK)
  - QuanSheng Wu, IOP CAS (China)
  - Giulia Galli, University of Chicago (USA)
  - Giuseppe Carleo, EPFL (Switzerland)
  - Federica Agostini, University Paris-Saclay (France)
  - Nicola Colonna, PSI (Switzerland)
  - Massimiliano Stengel, ICREA (Spain)
- Some contributed abstracts will be upgraded to invited talks
- Applications will open relatively soon, monitor Psi-k mailing list and ICTP website over the summer

PhD and postdoc positions available

Ab initio Research GrOup (ARGO) at SISSA,
Trieste (Italy)

- 2 postdoc positions (2 years, possible renewals)
- 2 PhD positions with industry and startups

Design and discovery of novel materials, magnetism and spin-orbit coupling physics, development of machine-learning methods for electronic structure simulations, topological materials, Wannier functions and much more…

Drop me an email if interested!

Thank you!