Introduction to Wannier90 and tutorial

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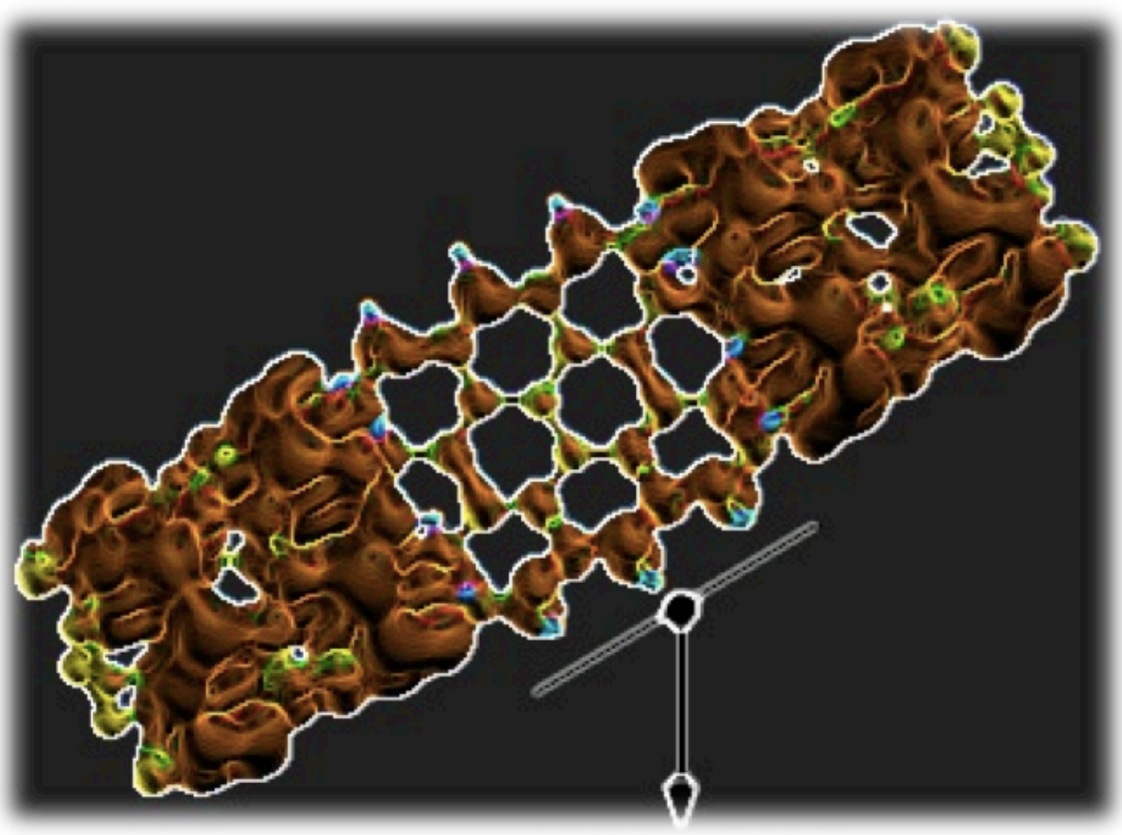
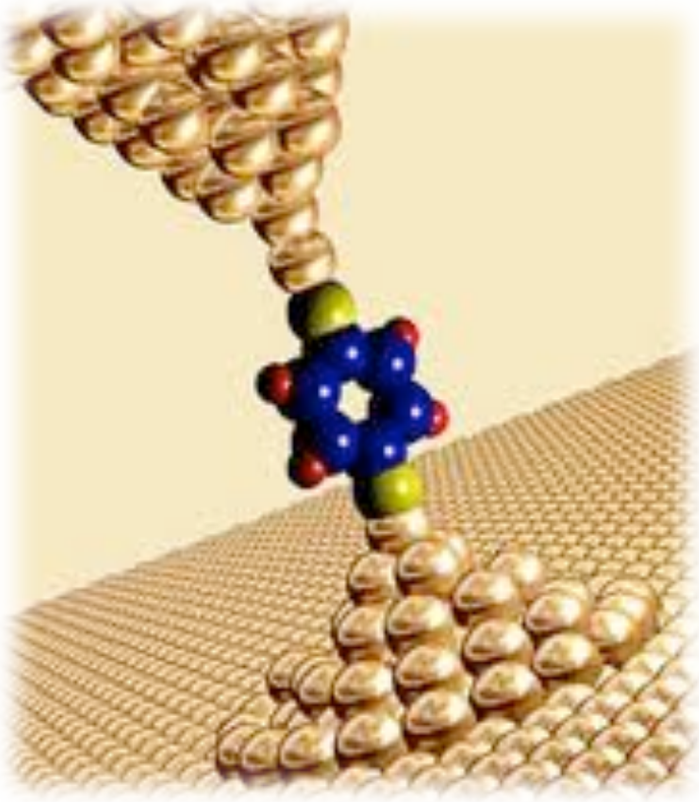
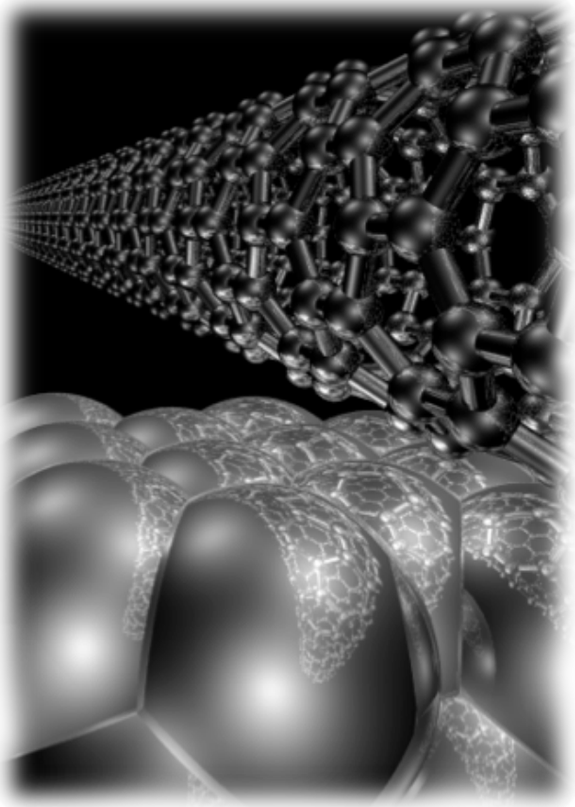
National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Switzerland

June 14th, 2021







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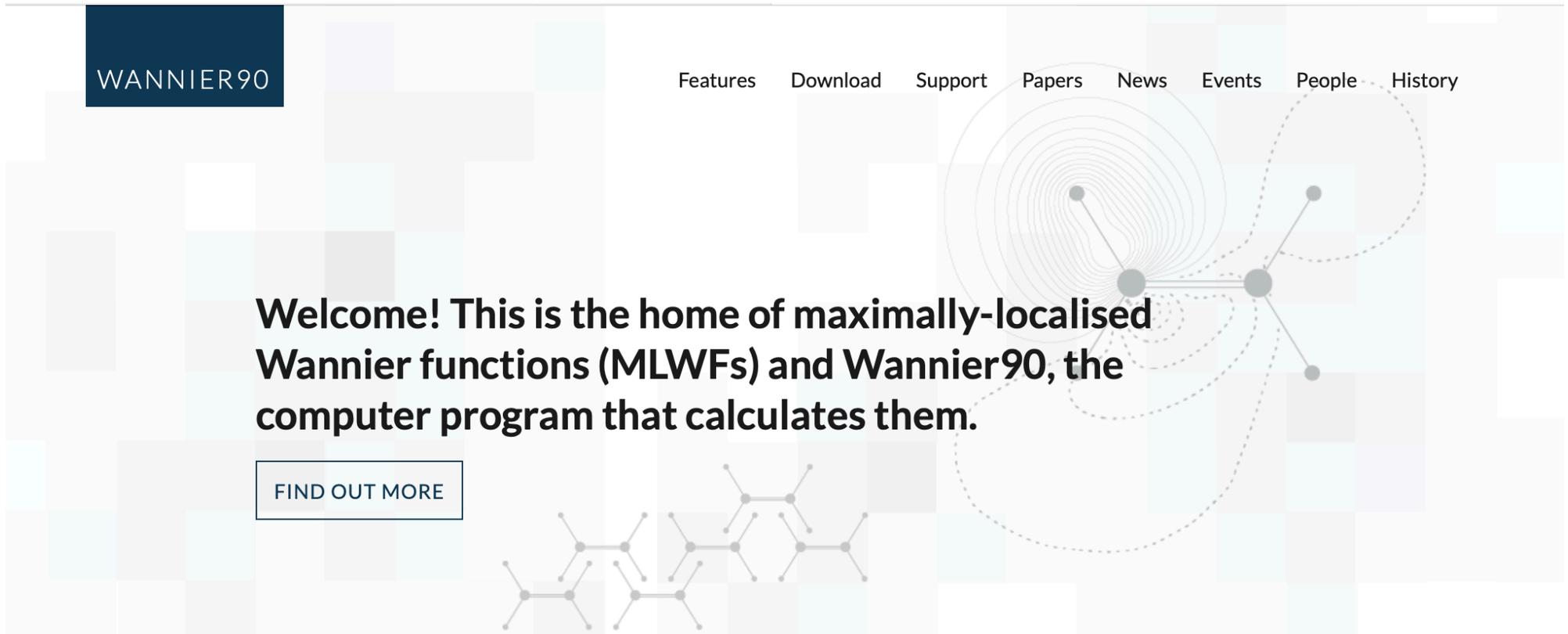

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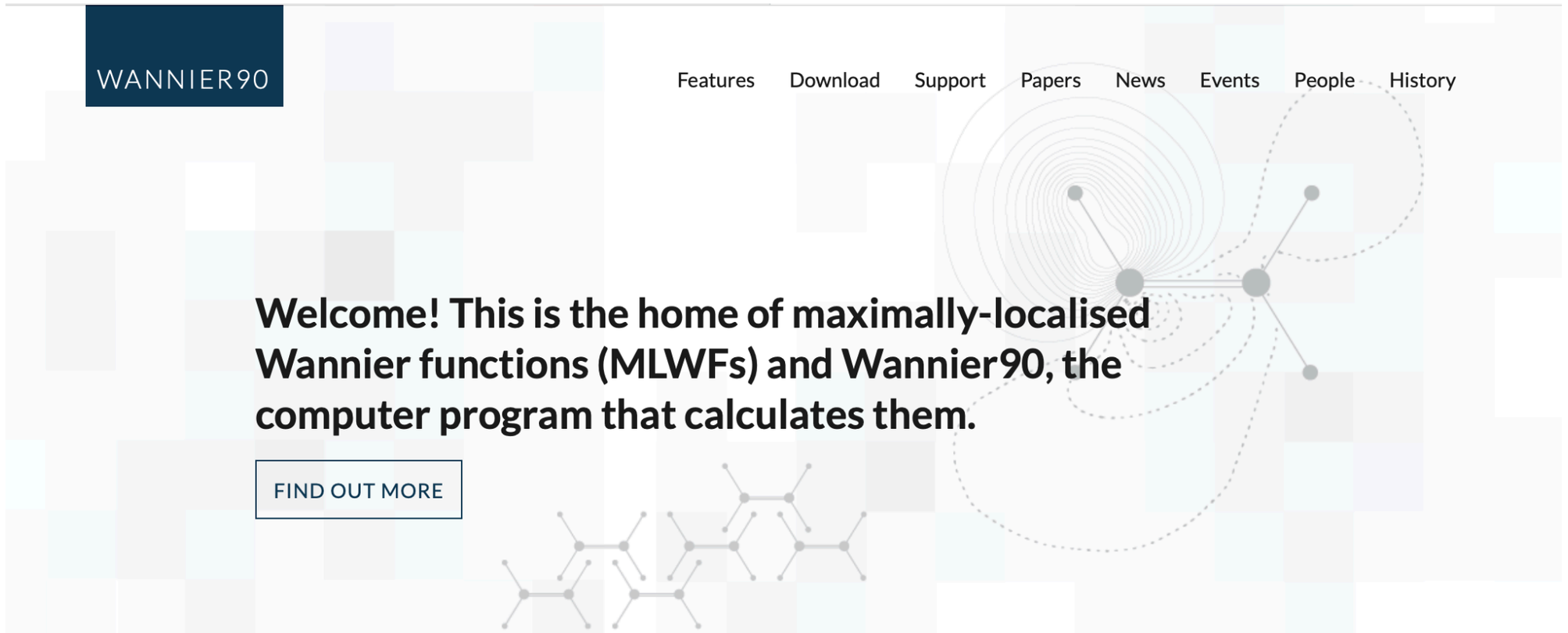

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Please note that:

- 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 'doc' directory of the current distribution.

For developers (GitHub)

The development of Wannier90 is managed on the Wannier developers GitHub site where you will find details of on-going developments, and how to contribute to Wannier90.

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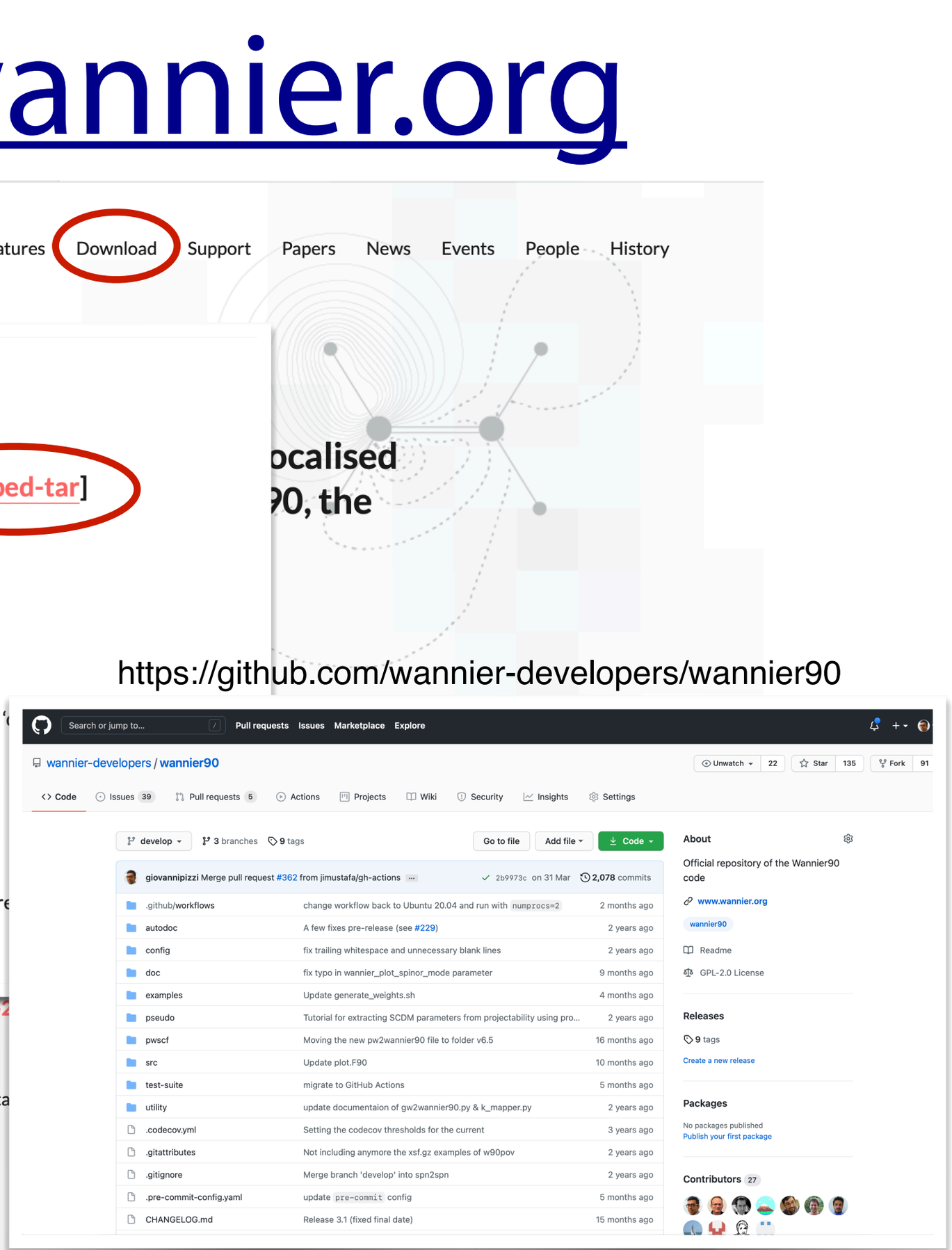

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- User guide v3.1.0: [PDF]
- Tutorial v3.1.0: [PDF]
- Tutorial solutions v3.1.0: [PDF]

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
```

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

```
end kpoint_path
```

There is no default

2.9.12 integer :: bands_num_points

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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.*
- Directory: `examples/example8/`
- Input Files
  - `iron.scf` *The* PWSCF *input file for the spin-polarized ground state calculation*
  - `iron.nscf` *The* PWSCF *input file to obtain Bloch states on a uniform grid*
  - `iron_{up,down}.pw2wan` *Input files for* `pw2wannier90`
  - `iron_{up,down}.win` *Input files for* `wannier90` *and* `postw90`
- Note that in a spin-polarized calculation the spin-up and spin-down MLWFs are computed separately. (The more general case of spinor WFs will be treated in Example 17.)

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

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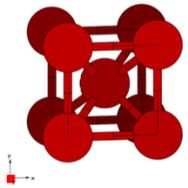

Figure 21: Unit cell of Iron crystal plotted with the XCrySDen program.

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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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.

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People involved: 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!

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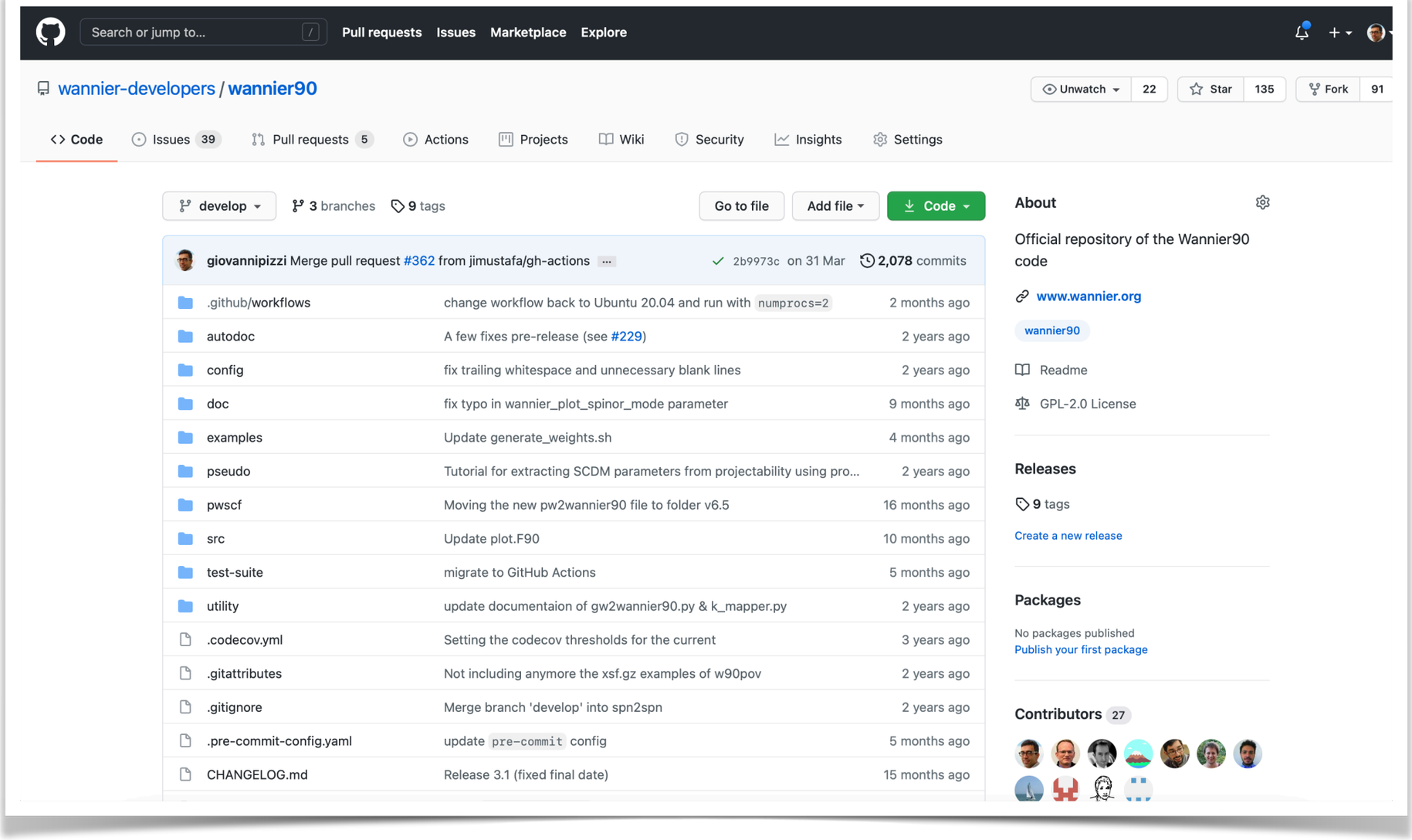
J. Phys.: Condens. Matter **32** (2020) 165902 (25pp)
https://doi.org/10.1088/1361-648X/ab51ff

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]

People involved: a community effort!

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)

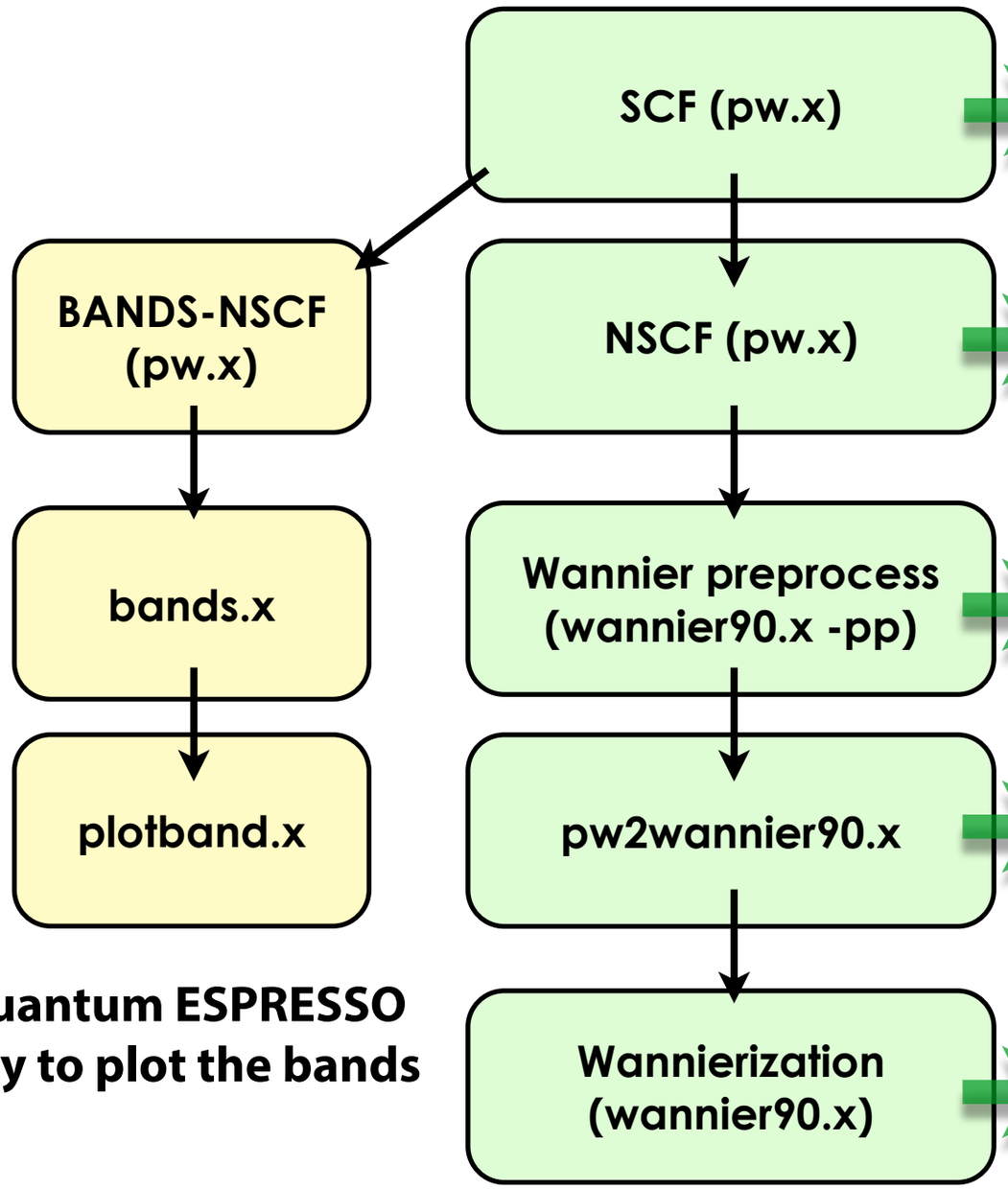
Berry phase properties including:

- 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]

How to run a Wannier90 calculation



Calculates the ground state density using a given (converged) K_POINTS mesh (in the irreducible wedge)

Calculates the wavefunctions u_{nk} on a **complete** k-mesh (not reduced by symmetry, and not necessarily the same of above!)

Reads the Wannier90 input file and prepares a file (.nnkp) with the information for the interface program

Interface program (btw QE and W90): reads the wavefunctions of the NSCF step, the .nnkp file and produces the .mmn, .amn, .eig, ... files for Wannier90

Reads the files produced by the previous step, minimizes the spread, calculates WF, calculates transport properties, ...

Quantum ESPRESSO way to plot the bands

Note: DON'T MIX the yellow and green path! Otherwise the content of the 'output' folder of Quantum ESPRESSO is overwritten and you will get some error.
First follow one path (e.g. the yellow one), and when you get to the bottom box, start again from NSCF

PART II

Wannier90 hands-on

Giovanni Pizzi, Junfeng Qiao

Tutorial exercises

- **If you never used Wannier90:**
  - *Exercise 1 and 2*: Silicon valence band and valence+conduction band; continue with 3 if you have time
- **If you have minimal experience of Wannier90:**
  - *Exercise 3*: Lead: band structure (metal), Fermi surface
- **If you are an experienced user of Wannier90 (optional, or "do at home" for new users):**
  - *Exercise 4*: Automatic choice of projections with the SCDM method, [1,2] and protocol to choose automatically all parameters [3] (for lead)
  - Exercise 5: Wannier functions for $BaTiO_3$

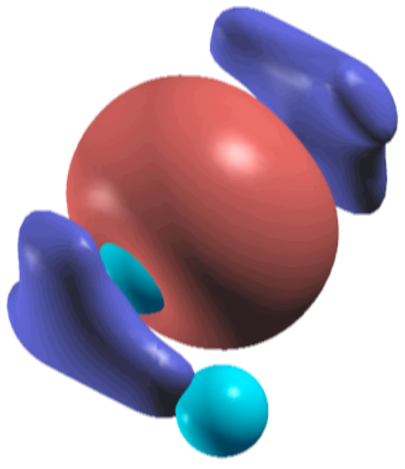
[1] Damle, A., Lin, L. & Ying, L. J. Compressed representation of Kohn–Sham orbitals via selected columns of the density matrix. J. Chem. Theory & Comp. 11, 1463–1469 (2015).

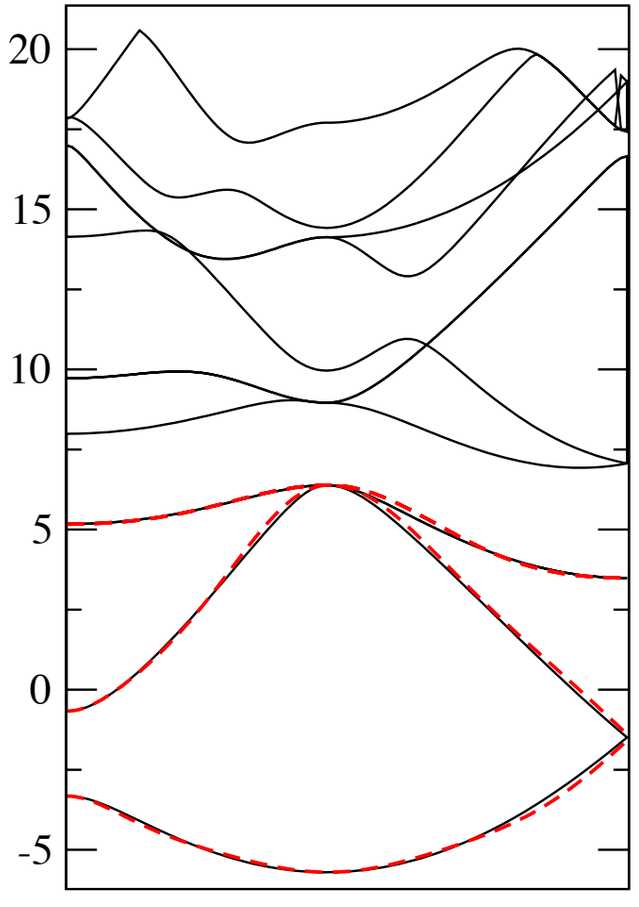
[2] Damle, A. & Lin, L. Disentanglement via entanglement: A unified method for Wannier localization. Mult. Scale. Model. & Simul. 16, 1392–1410 (2018).

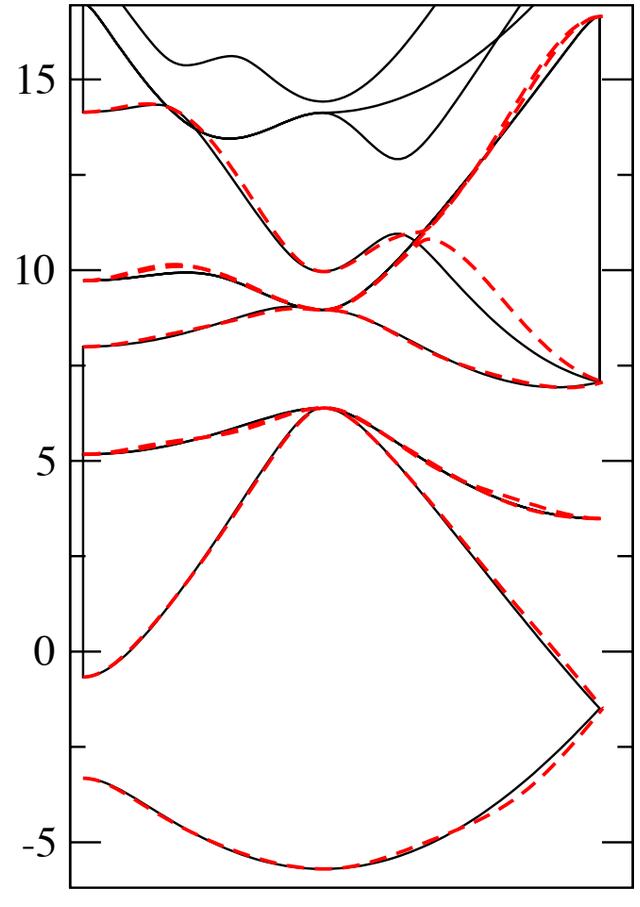
[3] Vitale, V., Pizzi, G., Marrazzo, A. et al. Automated high-throughput Wannierisation. npj Comput Mater 6, 66 (2020). https://doi.org/10.1038/s41524-020-0312-y

Exercises 1 and 2: Silicon

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







The Quantum ESPRESSO input file

NAMELISTS

```
&control
    calculation     =  'scf'
    restart_mode    =  'from_scratch'
    prefix          =  'si'
    pseudo_dir      =  'pseudo/'
    outdir          =  'out/'
/
&system
    ibrav           =   0
    nat             =   2
    ntyp            =   1
    ecutwfc         =  25.0
    ecutrho         = 200.0
/
&electrons
    conv_thr        =   1.0d-10
/
ATOMIC_SPECIES
Si  28.  Si.pbe-n-van.UPF
ATOMIC_POSITIONS crystal
Si  -0.25   0.75   -0.25
Si   0.00   0.00    0.00
K_POINTS automatic
10 10 10 0 0 0
CELL_PARAMETERS bohr
-5.1    0.0    5.1
 0.0    5.1    5.1
-5.1    5.1    0.0
```

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

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

Thresholds for charge-density calculations

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

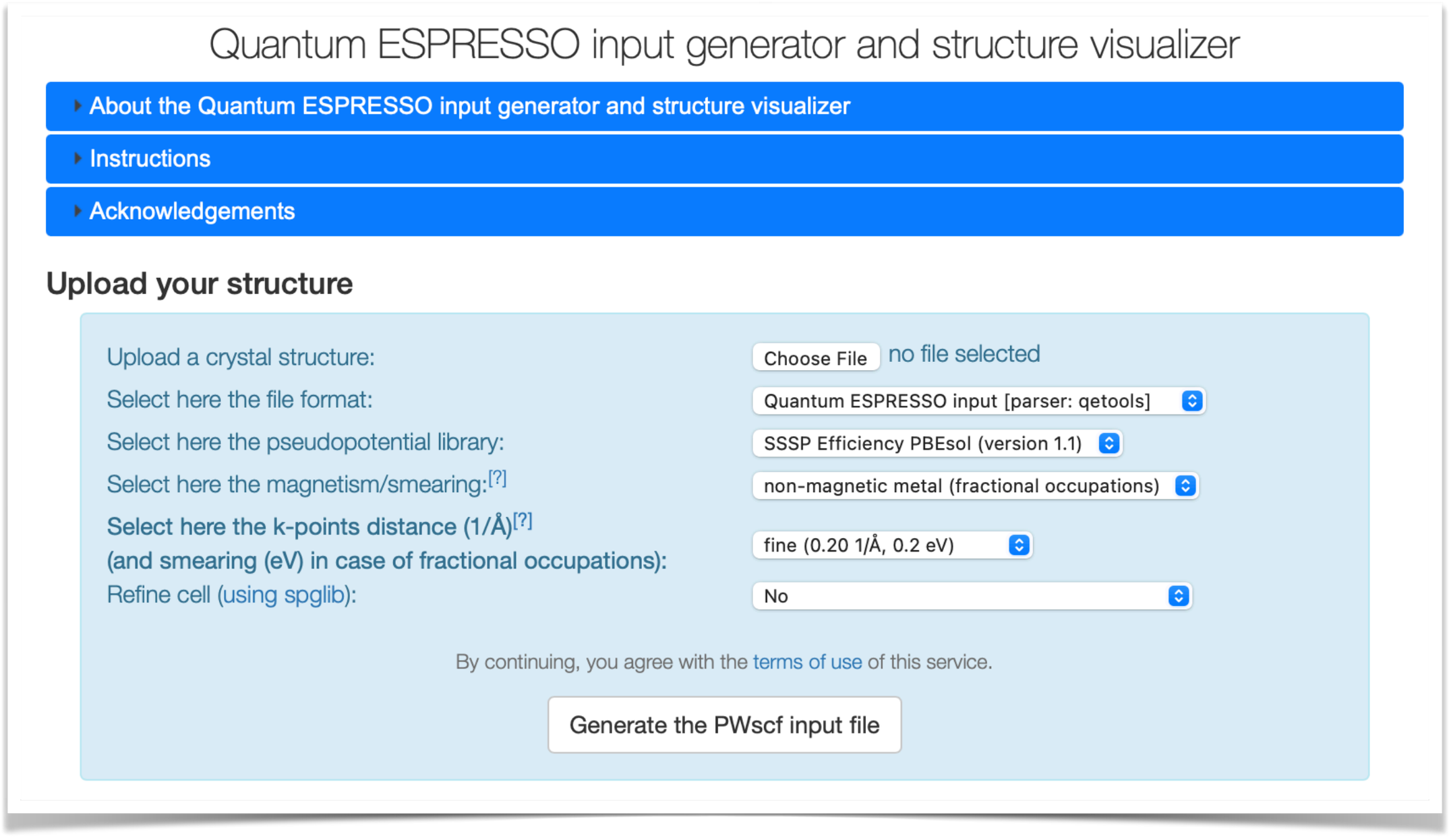
Definition of atomic positions

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

Definition of the cell (FCC here)

The Quantum ESPRESSO input generator

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



The Quantum ESPRESSO input generator

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

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

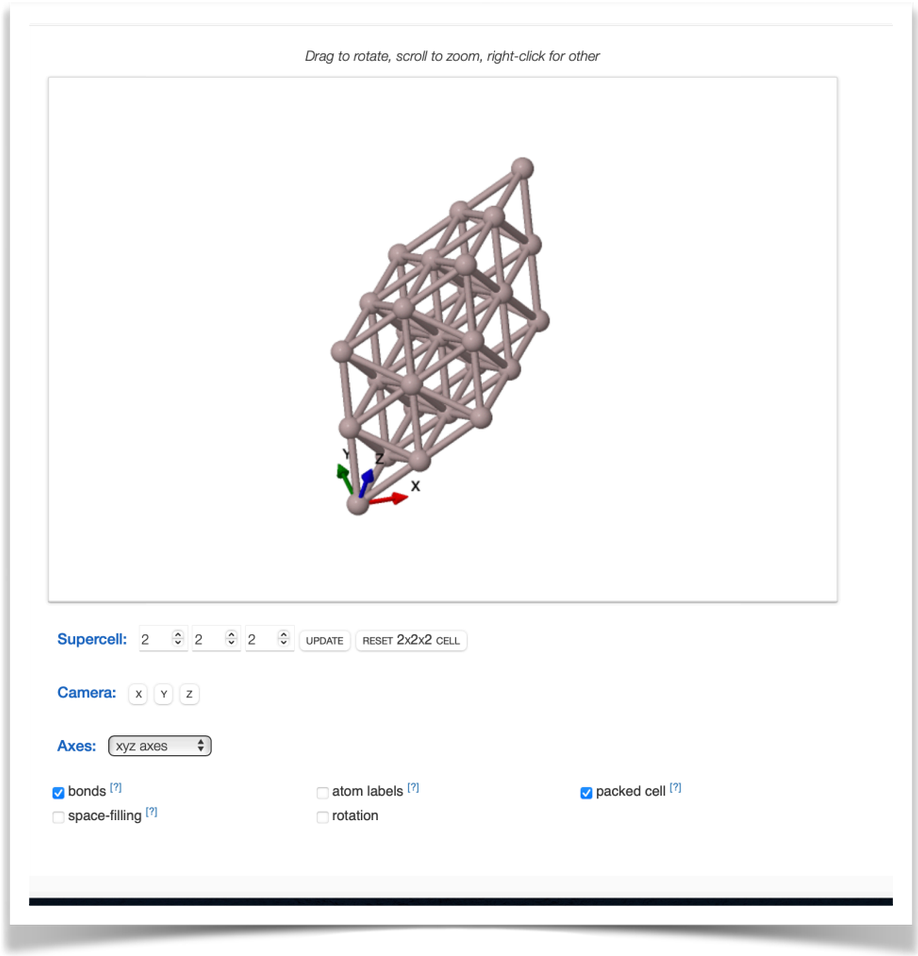
- SSSP (for the pseudopotential library)
  G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet and N. Marzari, npj Computational Materials **4**, 72 (2018).
  WEB: http://materialscloud.org/sssp.
- Pseudopotentials:
  - Al.pbesol-n-kjpaw_psl.1.0.0.UPF,
    from Pslibrary 1.0.0: A. Dal Corso, *Comput.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

Download zip of input file and pseudopotentials | **Change parameters** | **Choose a different structure**

Quantum ESPRESSO PWscf input

Copy to clipboard

```
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   1.0000000000d-05
  forc_conv_thr =   1.0000000000d-04
  outdir = './out/'
  prefix = 'aiida'
  pseudo_dir = './pseudo/'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  degauss =   1.4699723600d-02
  ecutrho =   2.4000000000d+02
  ecutwfc =   3.0000000000d+01
  ibrav = 0
  nat = 1
  nosym = .false.
  ntyp = 1
  occupations = 'smearing'
  smearing = 'cold'
/
&ELECTRONS
  conv_thr =   2.0000000000d-10
  electron_maxstep = 80
  mixing_beta =   4.0000000000d-01
/
ATOMIC_SPECIES
Al     26.981538 Al.pbesol-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS crystal
Al           0.0000000000       0.0000000000       0.0000000000
K_POINTS automatic
14 14 14 0 0 0
CELL_PARAMETERS angstrom
      2.0200000000       2.0200000000       0.0000000000
      2.0200000000       0.0000000000       2.0200000000
      0.0000000000       2.0200000000       2.0200000000
```



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

[1] https://www.materialscloud.org/sssp
[2] G. Prandini *et al.*, npj Comp. Mat. 4, 72 (2018)

How to run and input file

- The Wannier90 input file must have a .win extension (e.g.: **ex1.win**)
- To run the code, pass the *basename* (i.e., the name without the .win extension) as a command line parameter to wannier90.x:

  wannier90.x -pp ex1 (for the pre-process step)

  wannier90.x ex1 (for the Wannierization step)

- Input file format: very simple, there are *no* namelists but only:
  - Variables (order is not important; not case sensitive)

    num_wann = 4
    mp_grid : 6 6 6

  - Blocks

    begin atoms_frac
    Si -0.25 0.75 -0.25
    Si 0.00 0.00 0.00
    end atoms_frac

- Default units: lengths are **angstrom** (bohr are also accepted), energies are **eV**

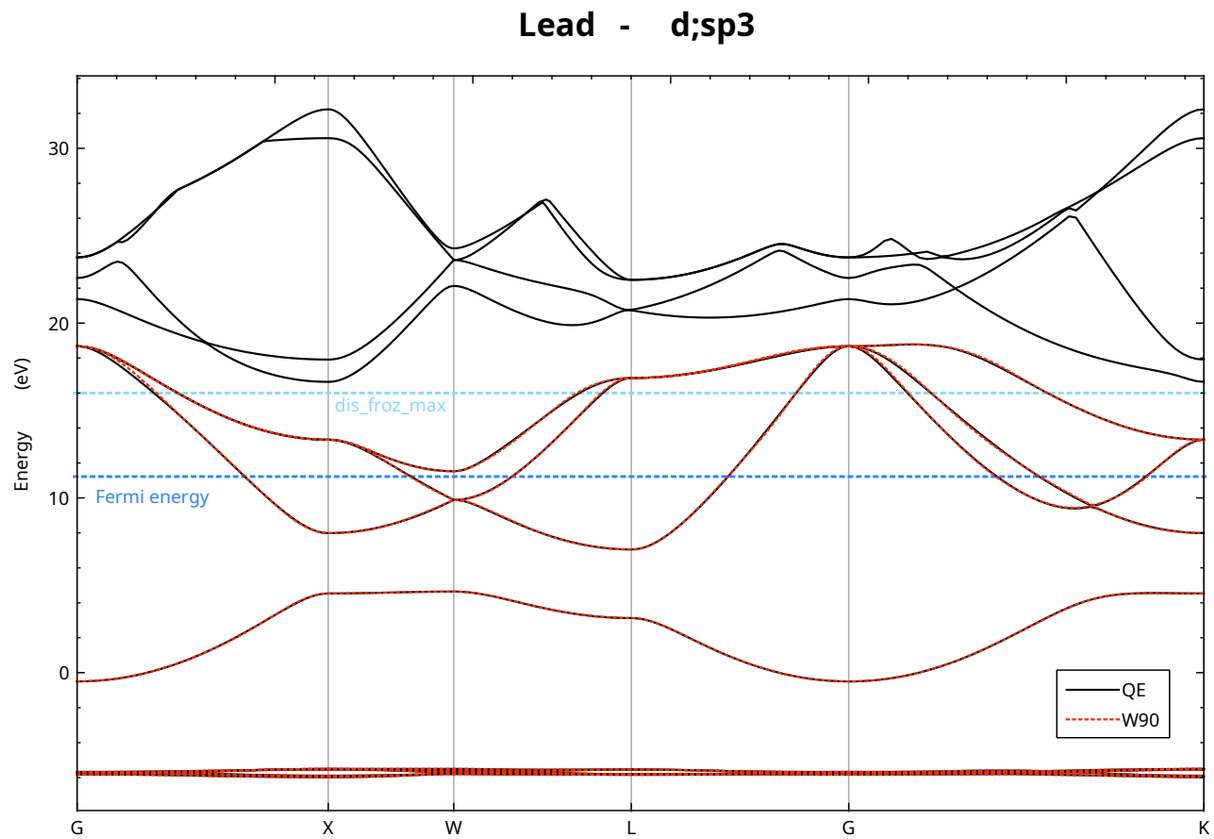
Example of input file (ex1)

```
num_bands      =  XXX
num_wann       =  XXX
num_iter       =  100

! restart            =  plot
wannier_plot         =  true
wannier_plot_supercell =  3

bands_plot     =  true
begin kpoint_path
L 0.5  0.5 0.5 G 0.0  0.0 0.0
G 0.0  0.0 0.0 X 0.5  0.0 0.5
end kpoint_path

begin projections
f=-0.125,-0.125, 0.375:s
f= 0.375,-0.125,-0.125:s
f=-0.125, 0.375,-0.125:s
f=-0.125,-0.125,-0.125:s
end projections
```

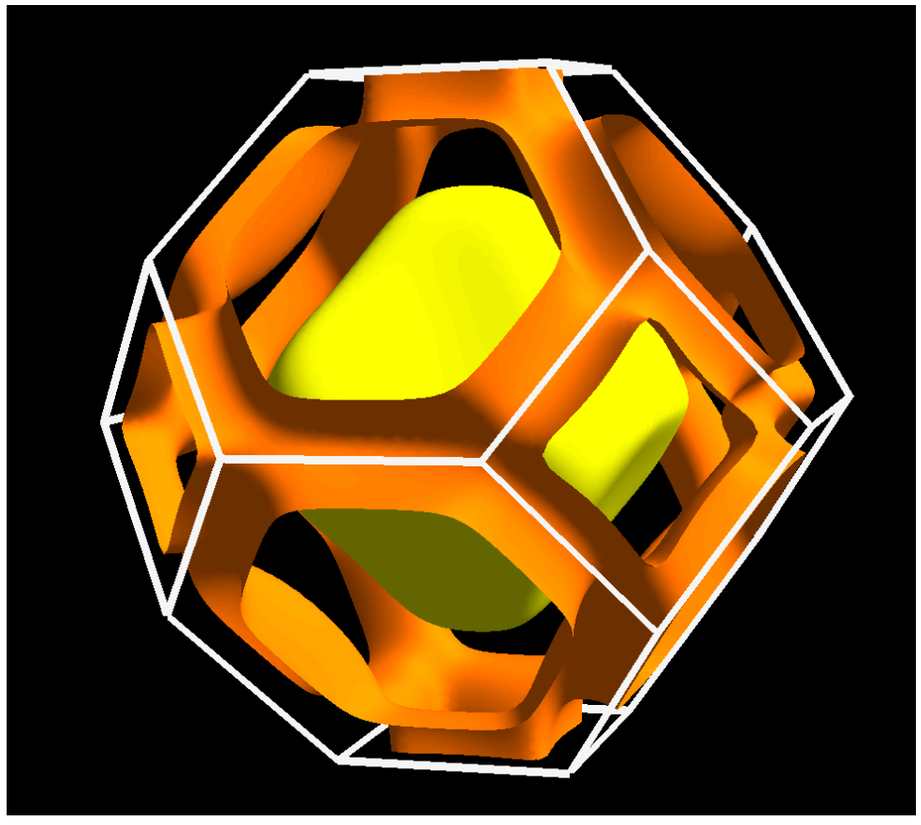
```
mp_grid  =  XXX XXX XXX
begin kpoints
XXX
XXX
XXX
end kpoints

begin atoms_frac
Si -0.25  0.75  -0.25
Si  0.00  0.00   0.00
end atoms_frac

begin unit_cell_cart
bohr
-5.10   0.00   5.10
 0.00   5.10   5.10
-5.10   5.10   0.00
end unit_cell_cart
```

Exercise 3: band structure and Fermi surface of lead

- Interpolate the band structure of lead

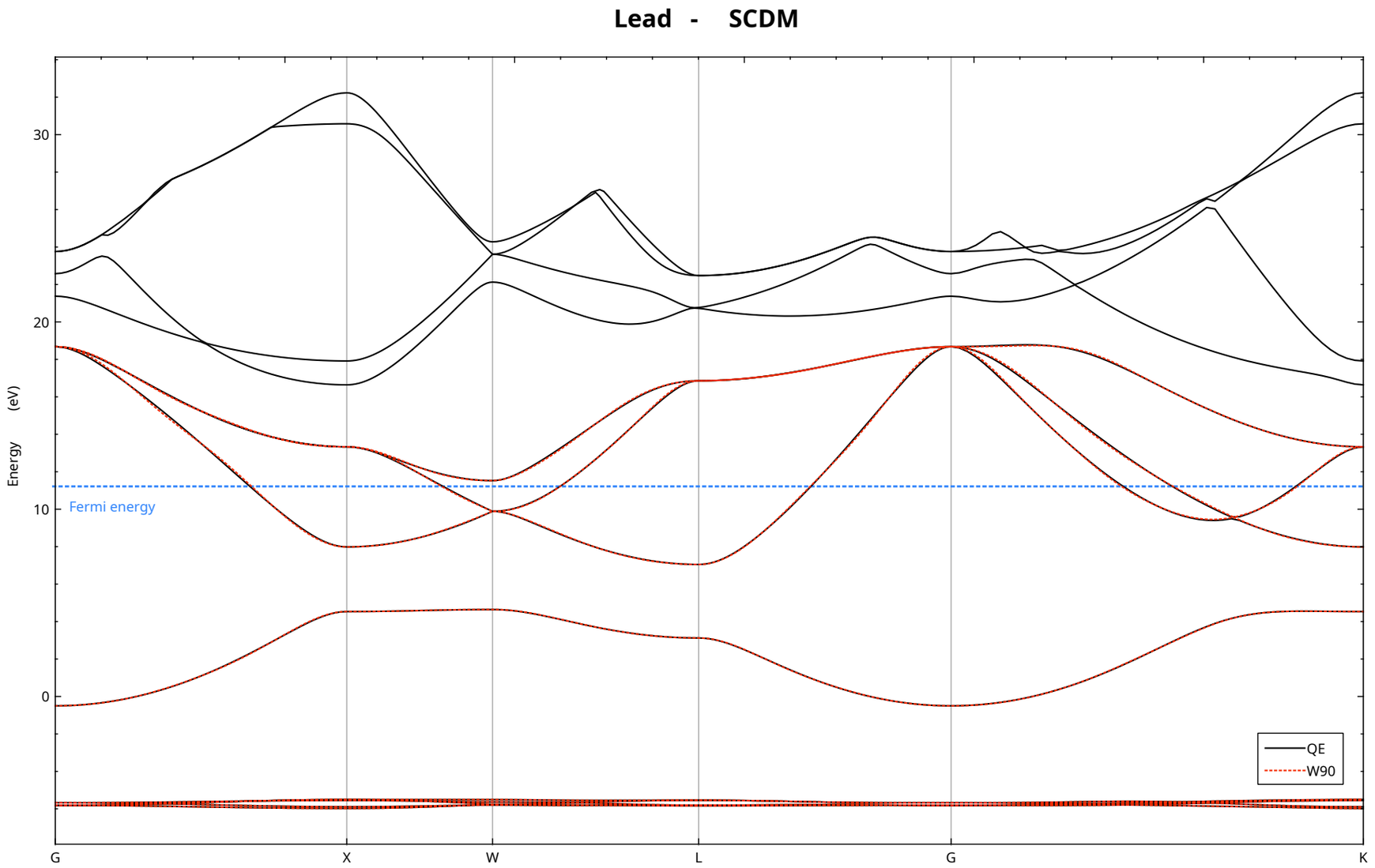


- Show the Fermi surface of lead
  - Requires a very dense grid of points in the BZ! ~50^3=125000
  - Wannier interpolation essential to compute it efficiently



Exercise 4: automatic projections with SCDM

- Obtain the Wannier functions and the band structure of lead **without having to explicitly specify the projections!**



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):

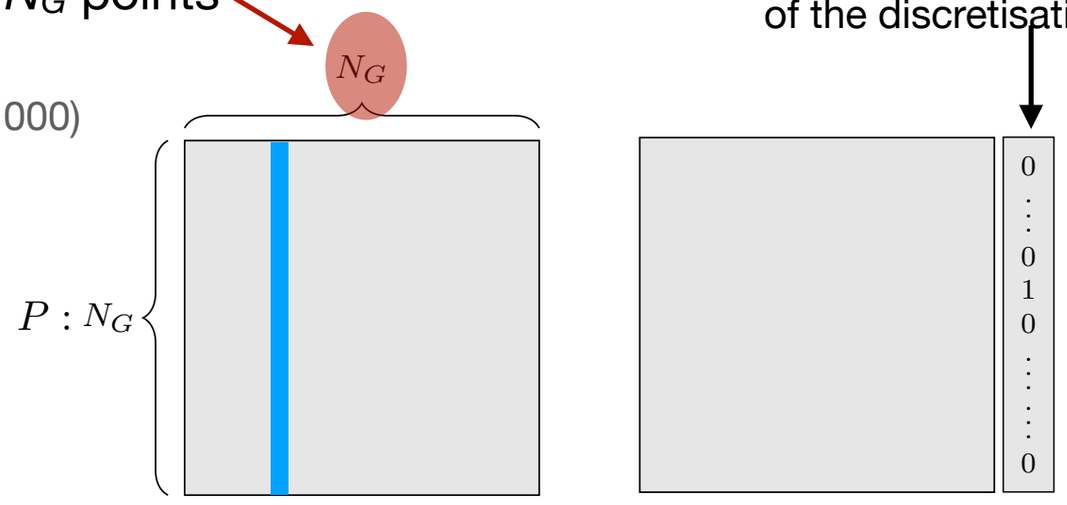
$$P = P^2,\ P = P^*$$

Discretisation on a real-space grid with with N_G points

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

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

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



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

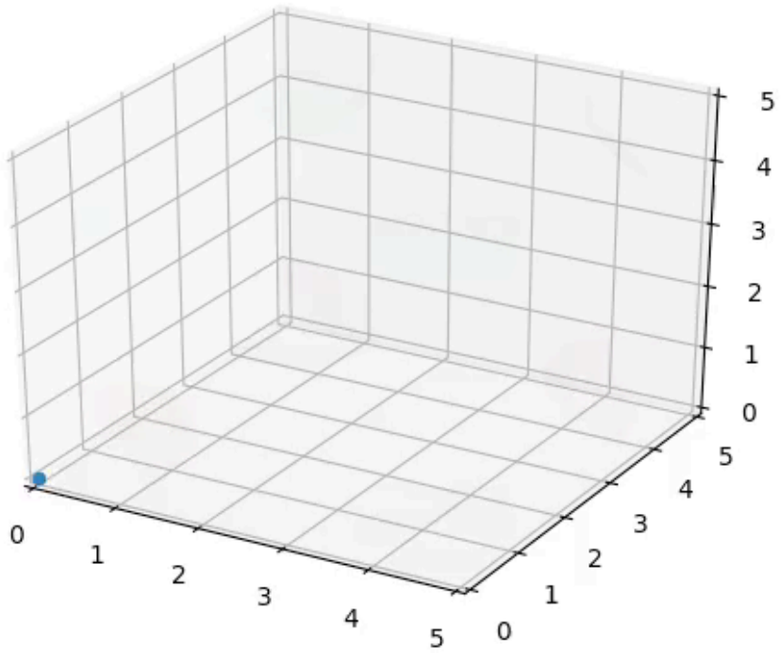
These projections (the columns) are localized! (but are not orthogonal)

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).

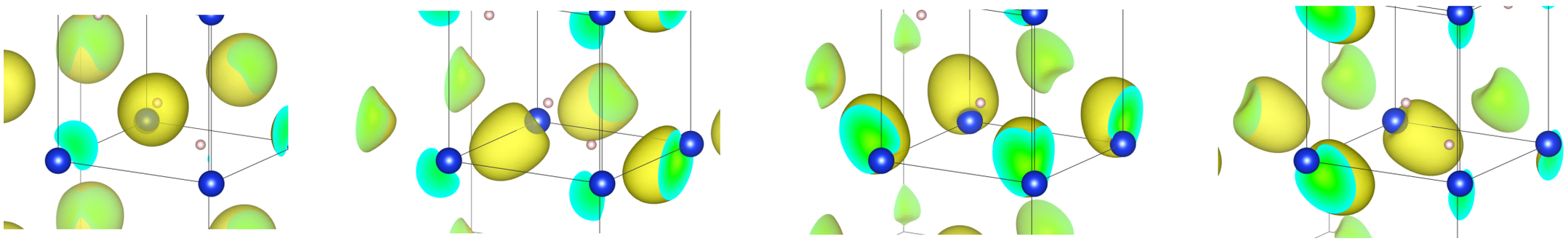
SCDM - columns of the density matrix

Silane, Γ-only



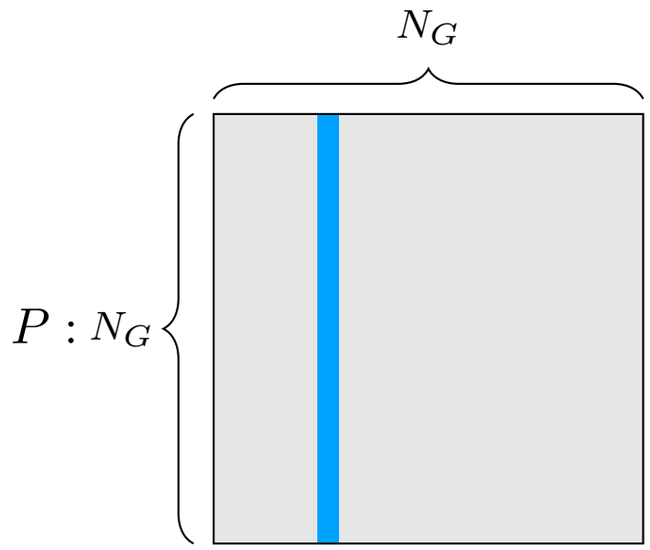
- *Isosurface* of square modulus at 1/10 of the maximum
- *Transparency* to indicate the norm (transparent: zero norm; opaque: max norm)
- *Dot*: real-space position associated with the DM column

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*)

$$P\Pi = QR$$

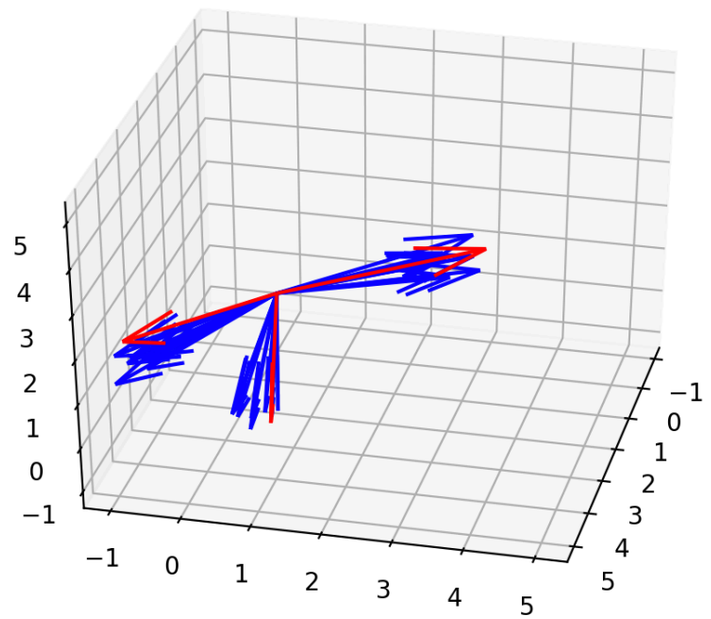
- *P*: density matrix (*input*)
- Π: permutation matrix (**swaps columns**)
- *Q*: orthogonal/unitary matrix (***columns* are orthogonal**: Q*Q=I)
- *R*: **upper-triangular matrix**
- Swaps chosen so that **diagonal elements of *R* are decreasing**: $|R_{11}| > |R_{22}| > \ldots$

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

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

ZGEQP3)

$$P\Pi = QR$$



ut)

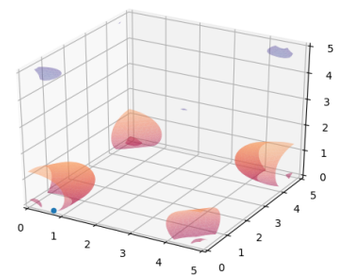
(swaps colu

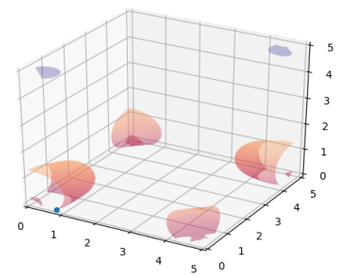
matrix (***colum***

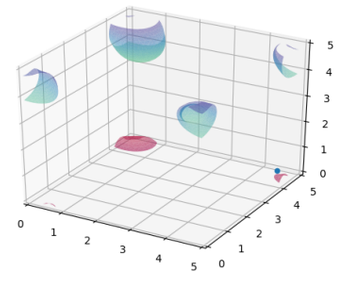
matrix

diagonal ele

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







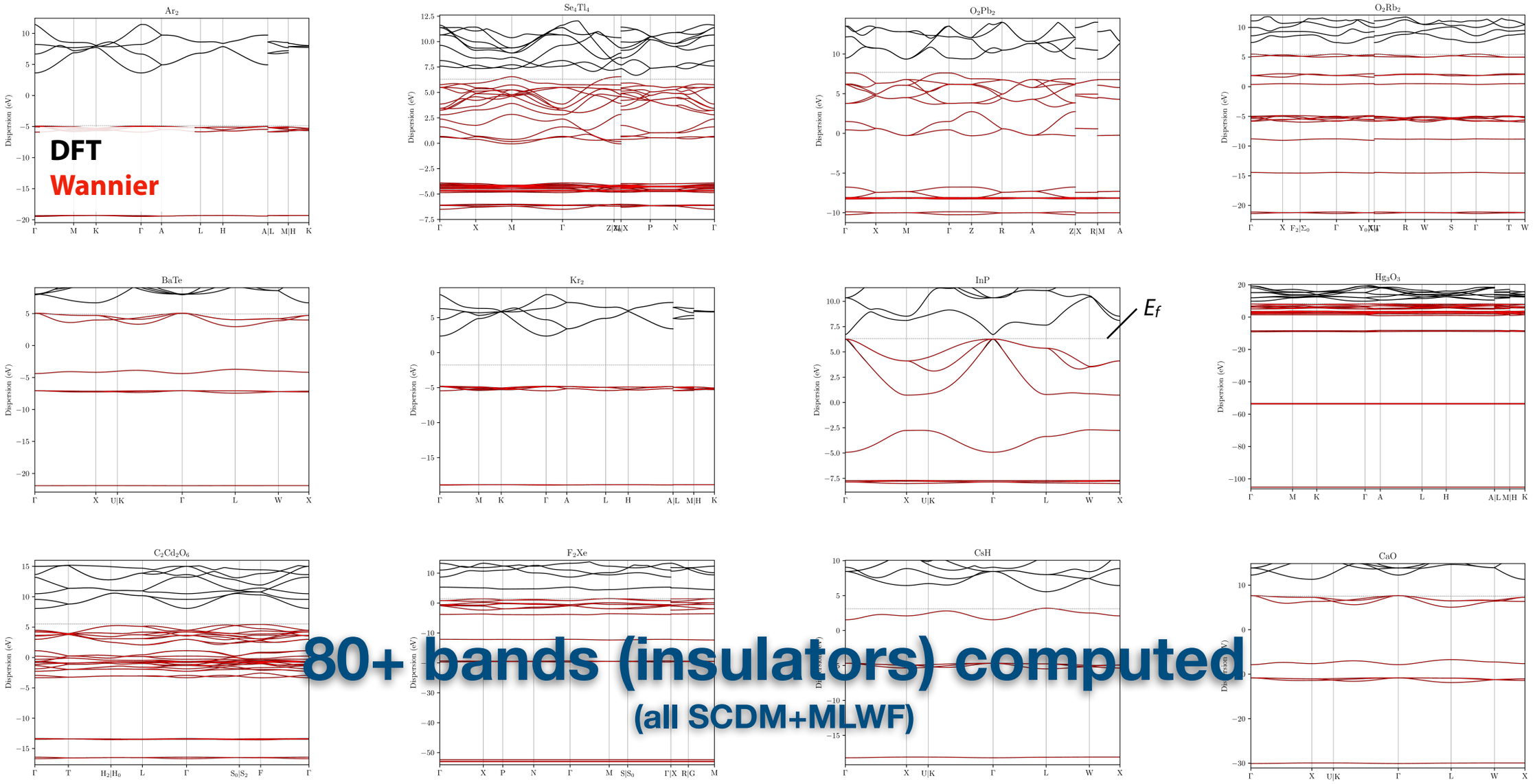
The rule for swaps finds the most representative ("most orthogonal") columns: SCDM

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)

Vitale, V., Pizzi, G., et al. Automated high-throughput Wannierisation,
npj Comput Mater 6, 66 (2020)

SCDM - entangled bands

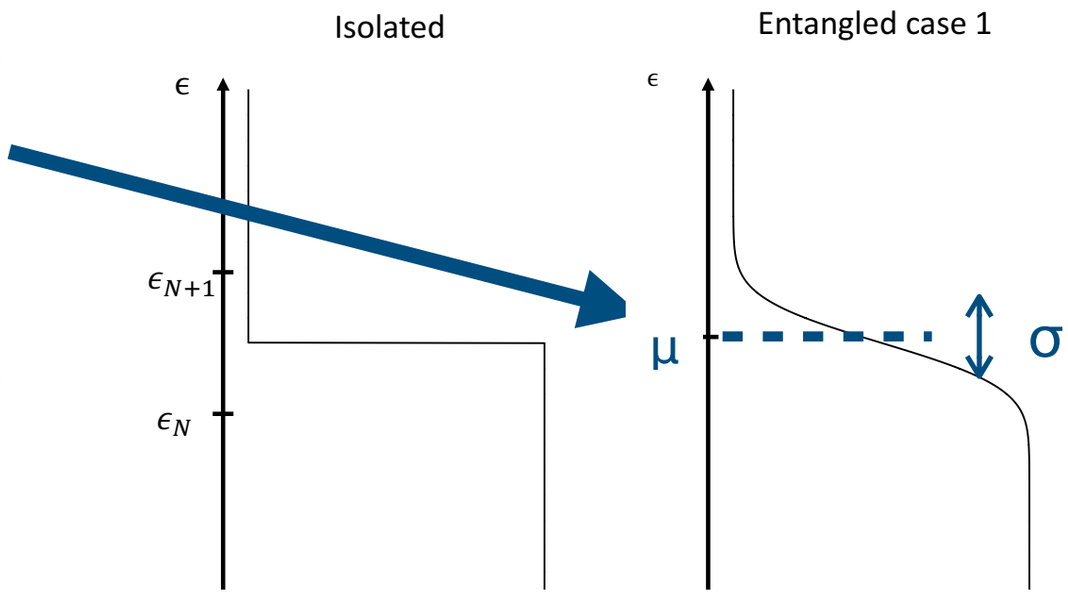
- We consider (formally) all eigenstates, and give a weight in the *quasi-density-matrix P*

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

- *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

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

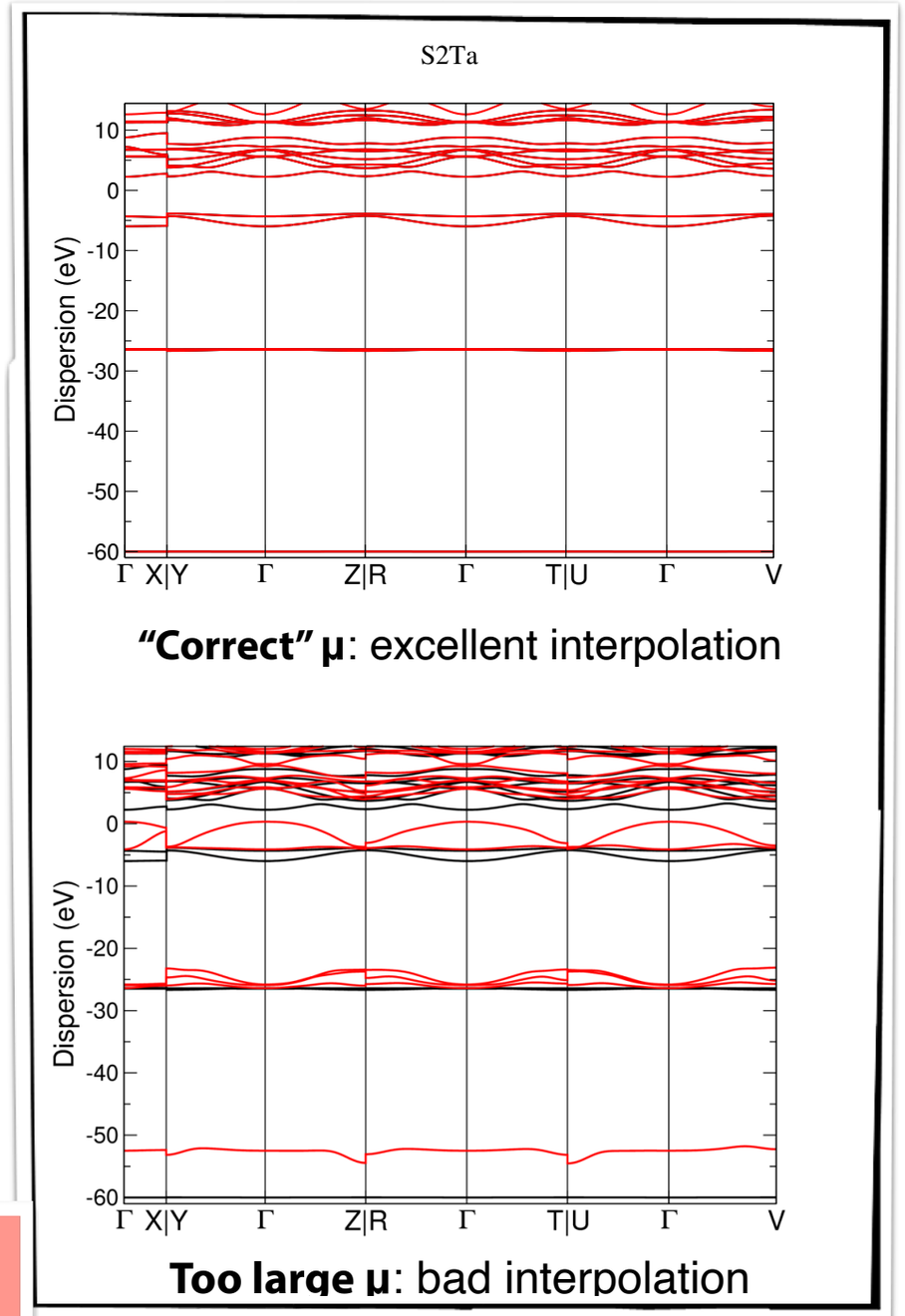
Arbitrary parameters to choose: μ and σ
(and *N*, the number of Wannier functions)



[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



“Correct” μ: excellent interpolation

Too large μ: bad interpolation

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)

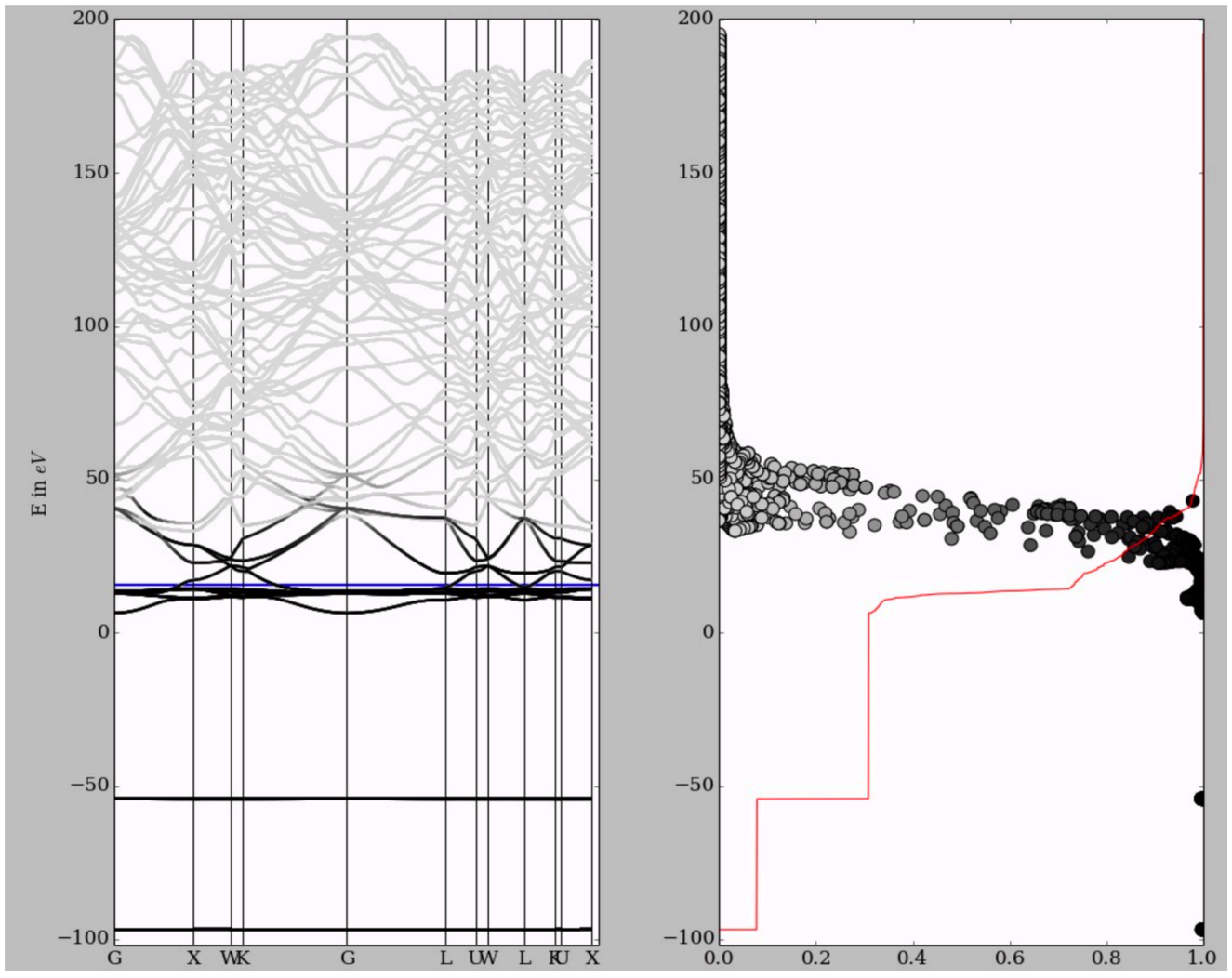


Image: courtesy of Daniel Marchand, EPFL

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

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:

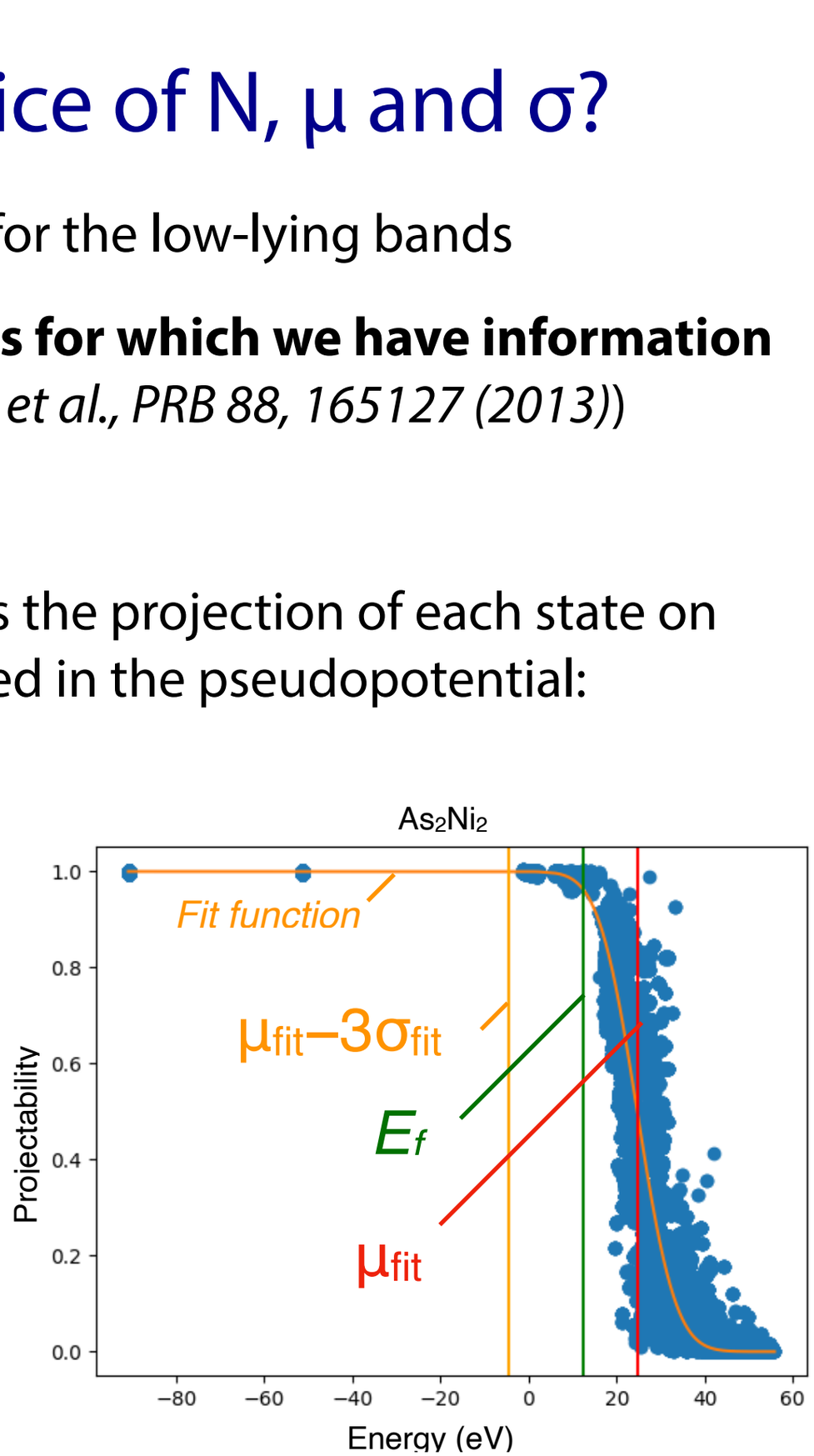
$$p(|\psi_{n,\mathbf{k}}\rangle) = \sum_i |\langle o_i|\psi_{n,\mathbf{k}}\rangle|^2$$

- 3: Fit the plot of the projectability vs. energy with

$$f(\varepsilon) = \frac{1}{2}\mathrm{erfc}\left(\frac{\varepsilon - \mu_{\mathrm{fit}}}{\sigma_{\mathrm{fit}}}\right)$$

- **4: choose the parameters μ and σ as follows**

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



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:

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

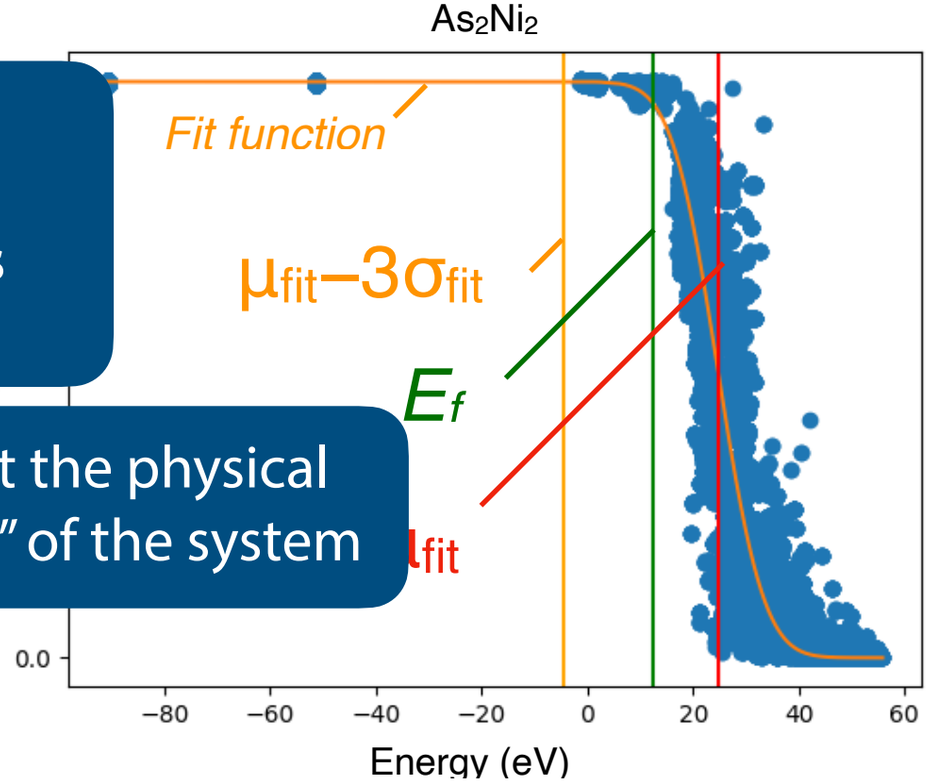
μ: when projectability≲0.9, weight≲10^{-3}

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

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

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

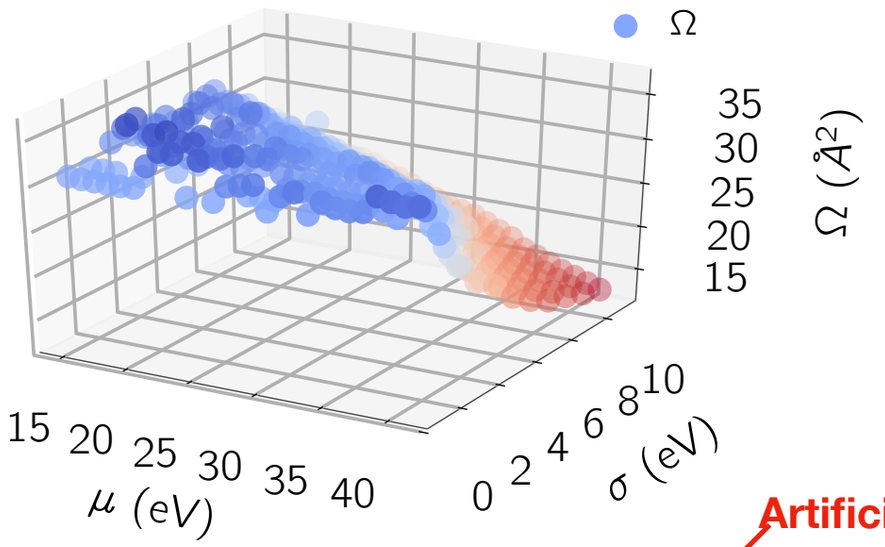
$$\mu = \mu_{\rm fit} - 3\sigma_{\rm fit}; \qquad \sigma = \sigma_{\rm fit}$$



Parameter choice validation: tungsten (W)

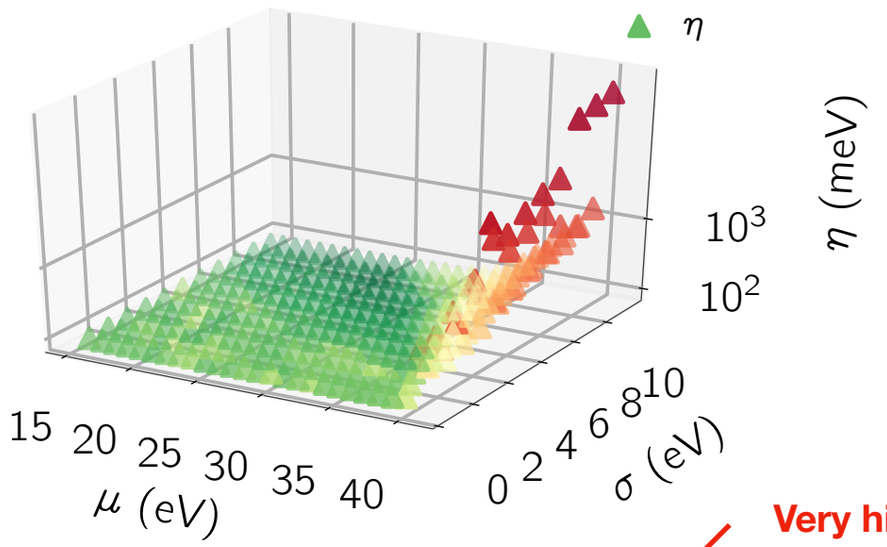
Spread

as a function of μ and σ



Bands distance

as a function of μ and σ

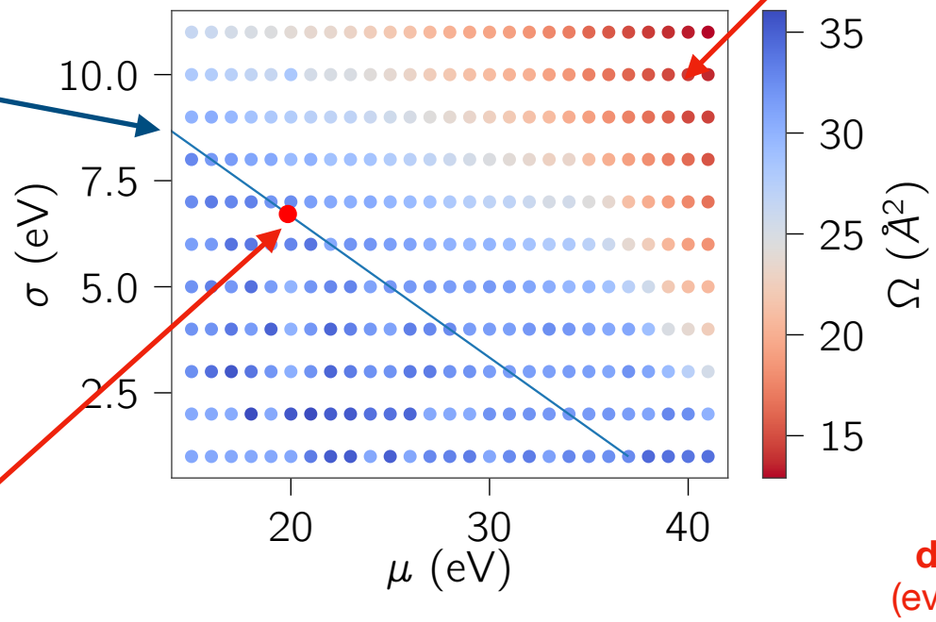


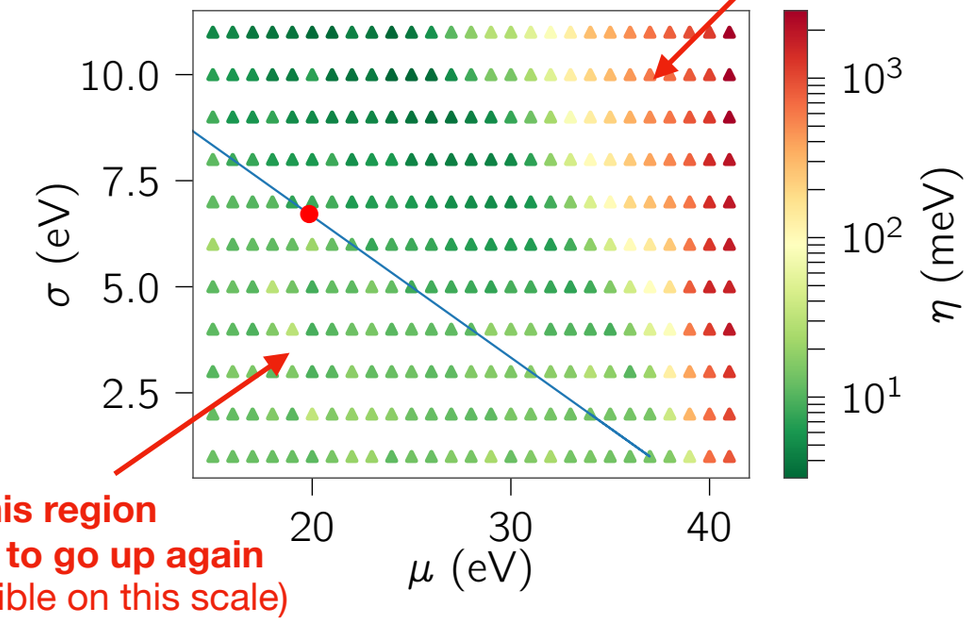
Artificially low total spread

Very high bands distance

$\mu = \mu_{fit} - 3\sigma$

Our protocol:
$\mu = \mu_{fit} - 3\sigma_{fit}$

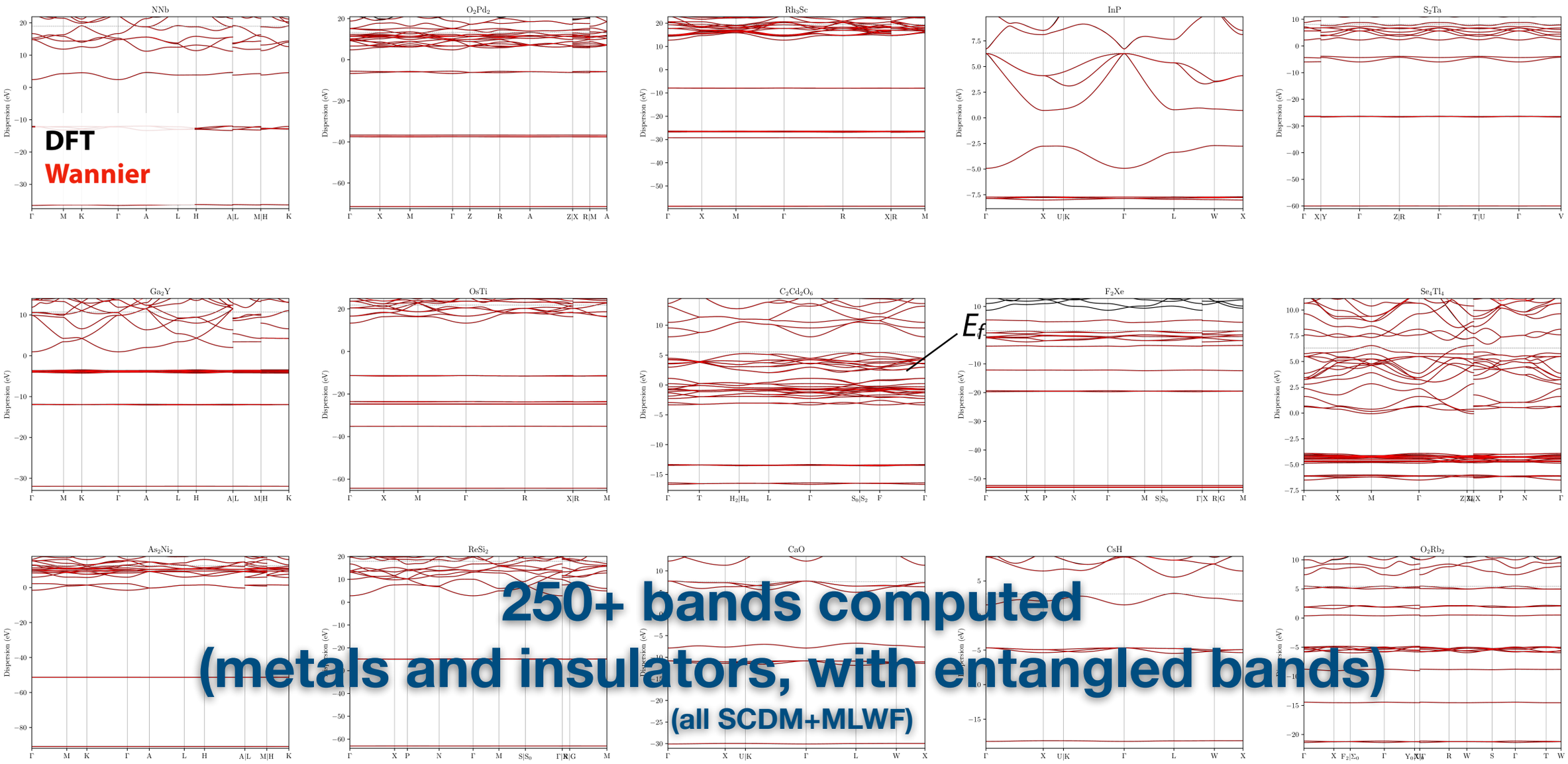




Also in this region distance starts to go up again
(even if not so visible on this scale)

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)

Vitale, V., Pizzi, G., et al. Automated high-throughput Wannierisation,
npj Comput Mater 6, 66 (2020)

SCDM - results for entangled bands

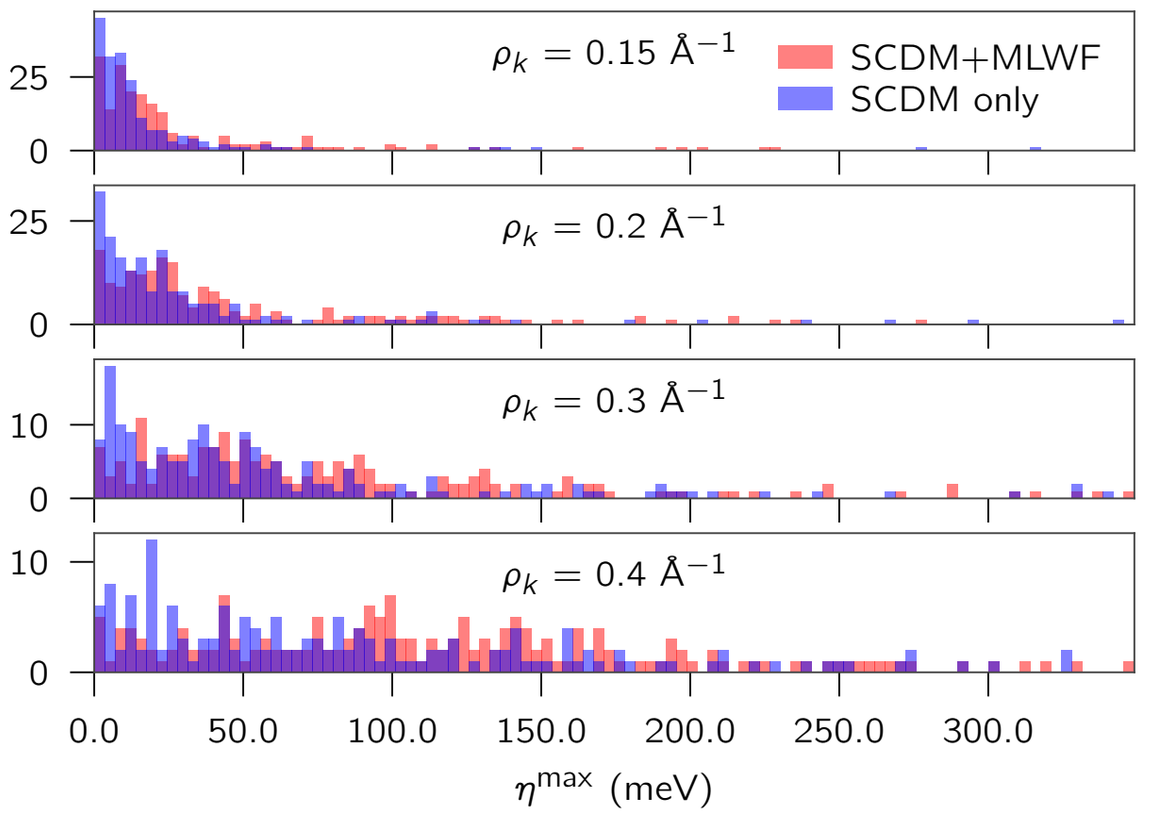
- To assess quality of Wannierisation and interpolation: we define a **bands distance** (between DFT bands and interpolated bands)

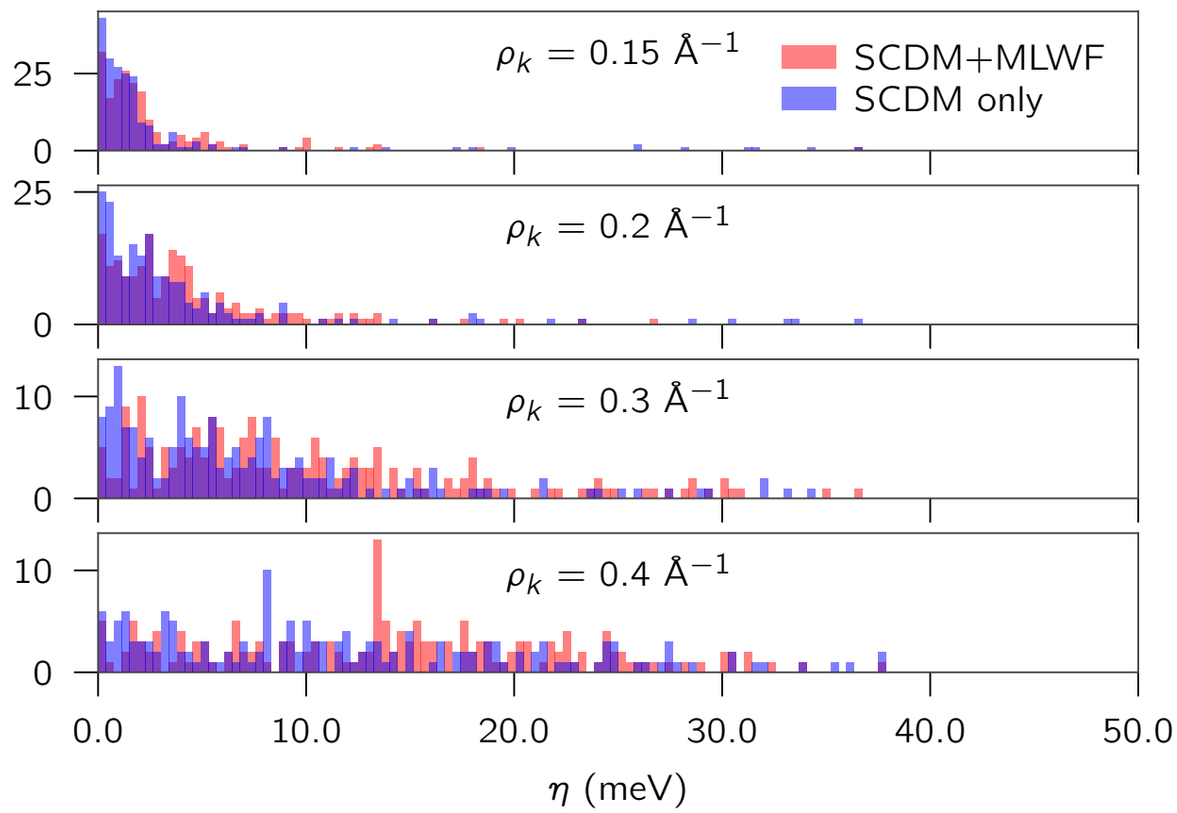
$$\eta = \sqrt{\sum_{n\mathbf{k}} \left(\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} - \varepsilon_{n\mathbf{k}}^{\mathrm{Wan}}\right)^2}, \qquad \eta^{\max} = \max_{n\mathbf{k}} \left(\left|\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} - \varepsilon_{n\mathbf{k}}^{\mathrm{Wan}}\right|\right)$$

Average bands distance *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



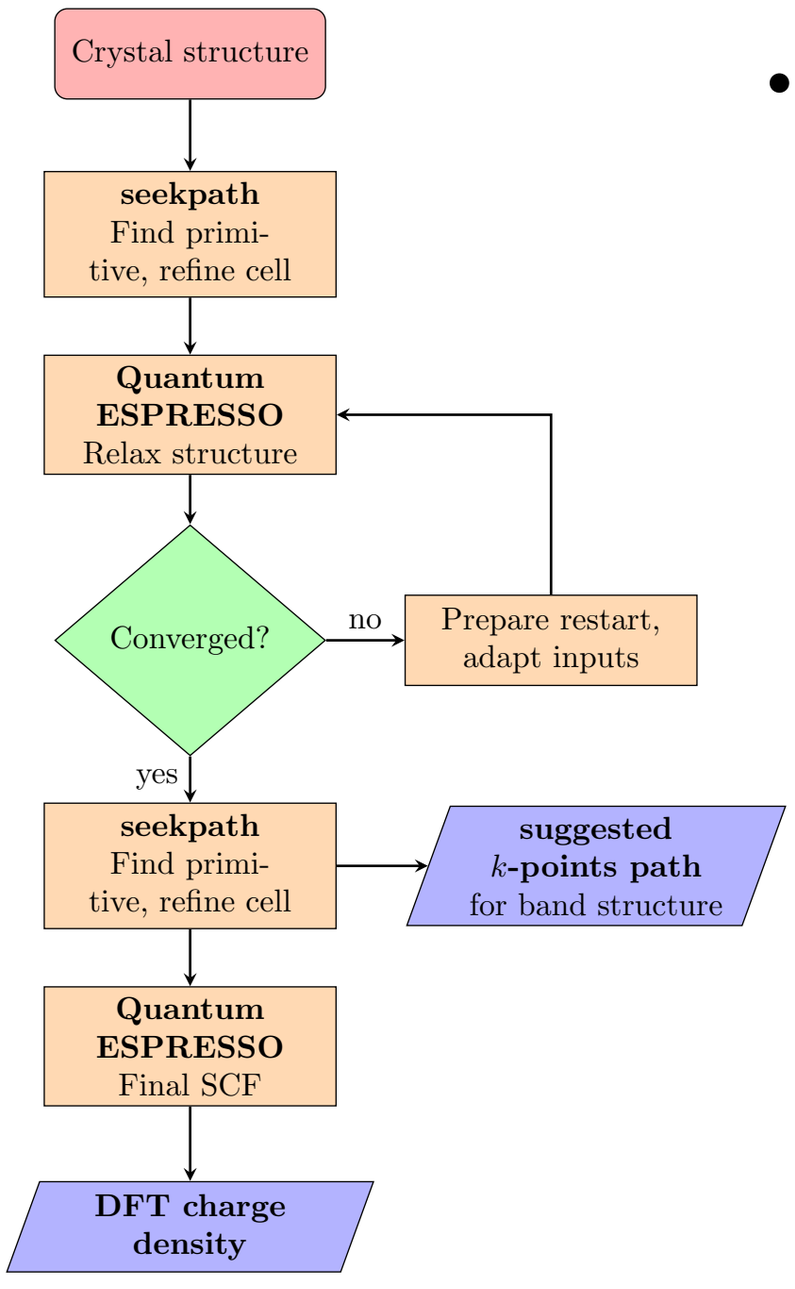


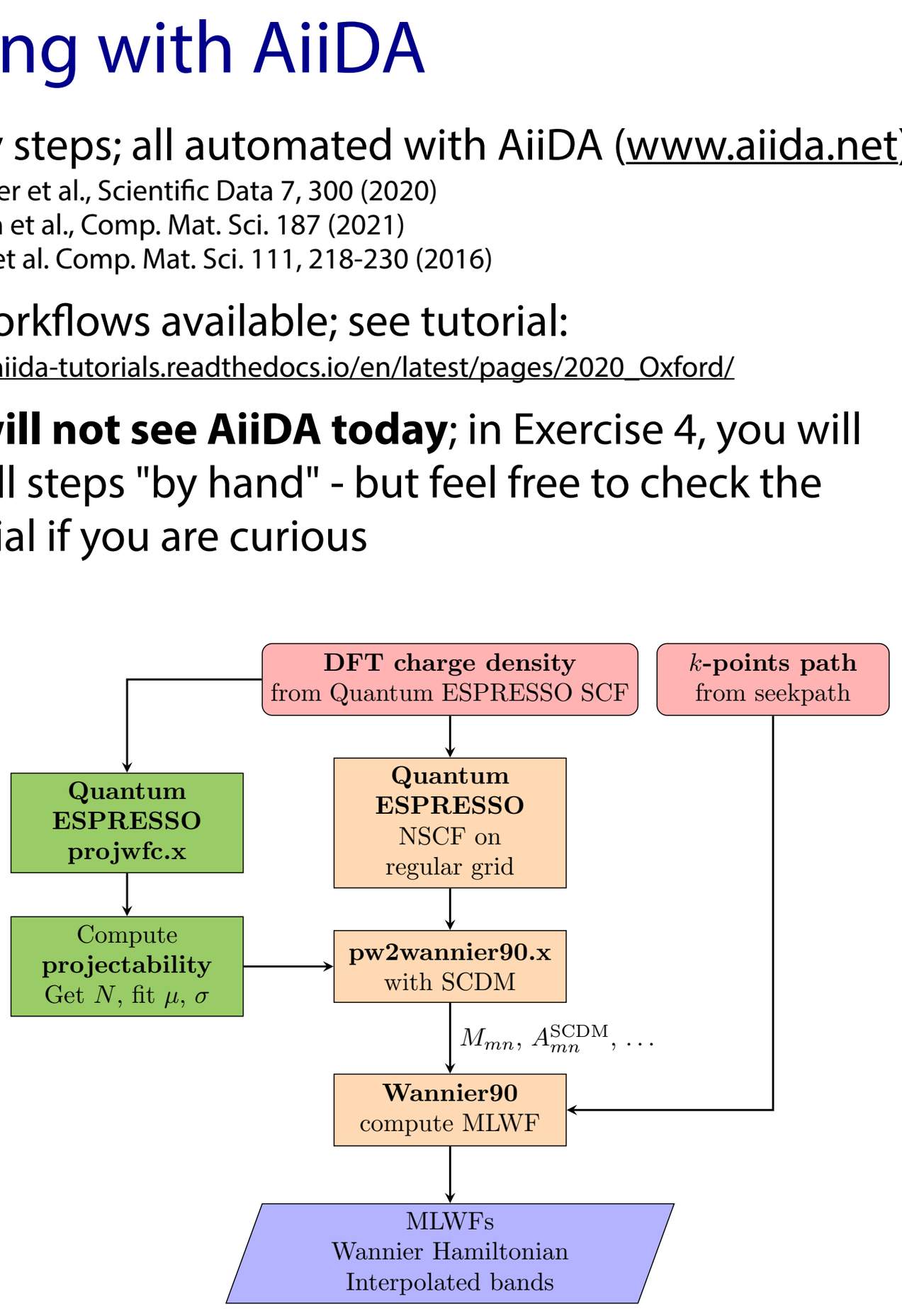
- Good results require a density of at least 0.2 Å^{-1} or more dense
- **For insulators**, SCDM-only already provides very good results; MLWF improves them
- In general, very small band distances (i.e. very good interpolation)

Vitale, V., Pizzi, G., et al. Automated high-throughput Wannierisation,
npj Comput Mater 6, 66 (2020)

Automating 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

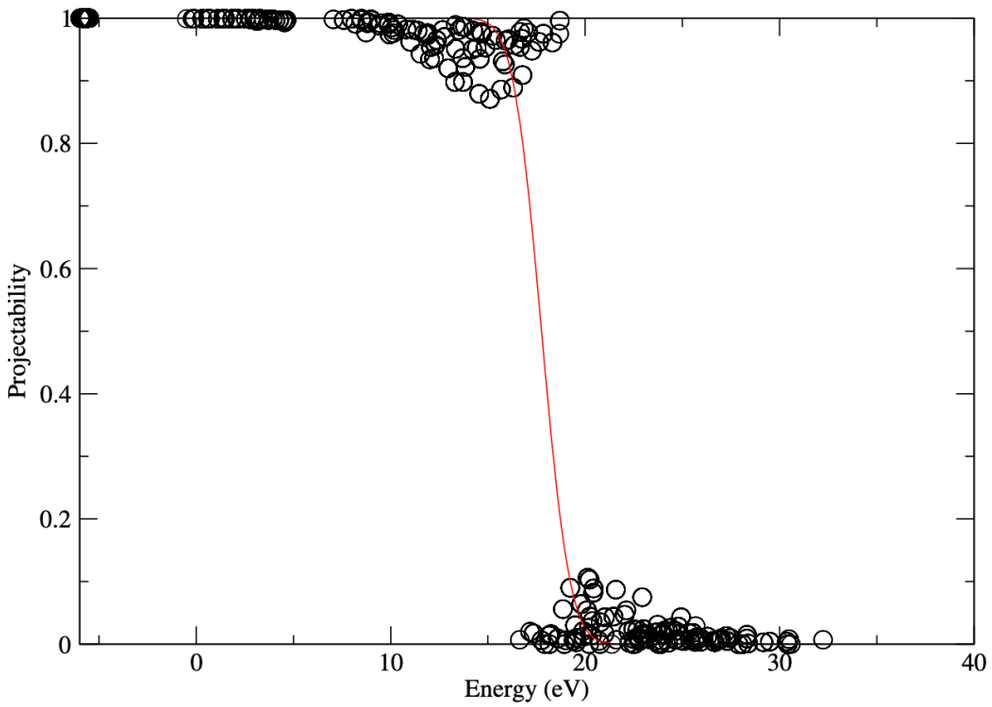


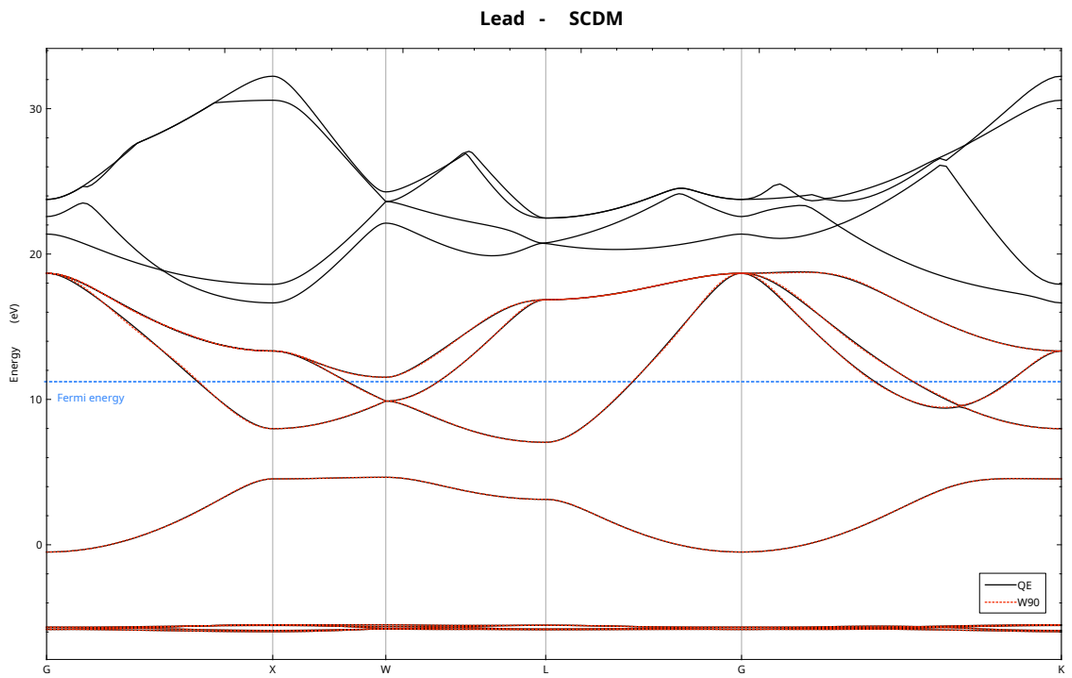


Exercise 4: automatic projections with SCDM

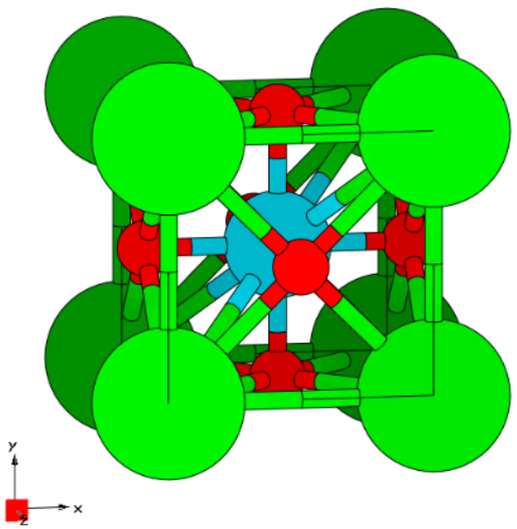
- Goals:
  - Understand how to run Wannier90 without an explicit specification of the initial projections
  - Understand the simulation steps involved in SCDM
  - Use the projectability approach to get the values for the

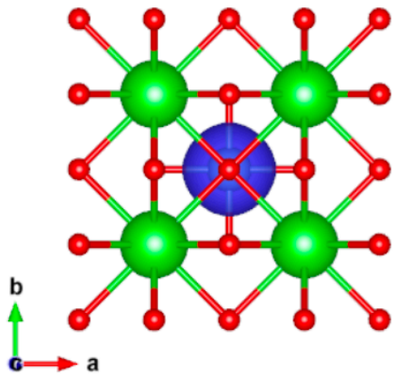
SCDM parameters



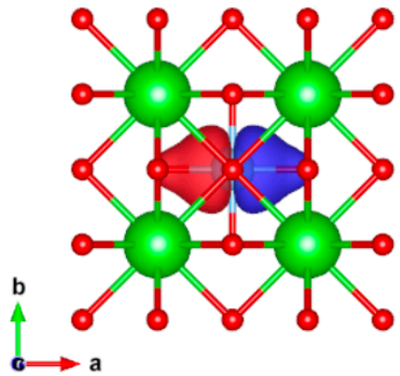


Exercise 5: cubic $BaTiO_3$

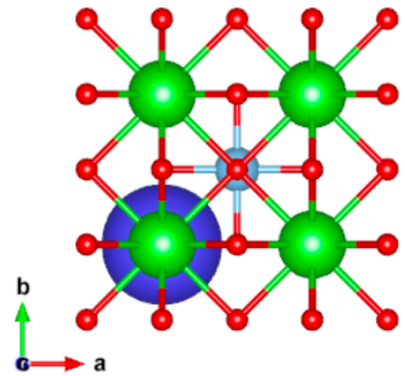




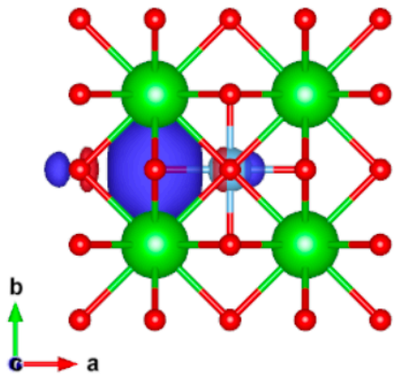
(a) Exclude bands = 2-20.
Ti:s



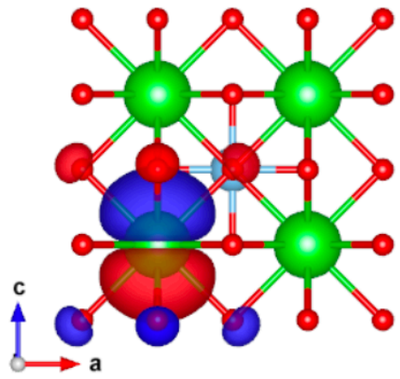
(b) Exclude bands = 1,5-20.
Ti:p



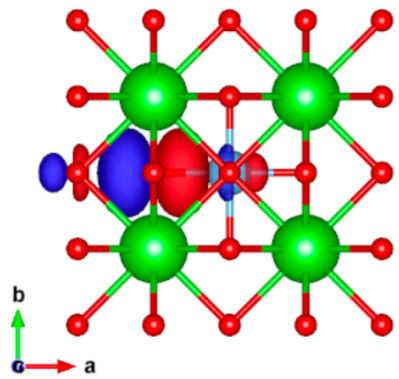
(c) Exclude bands = 1-4,6-20.
Ba:s



(d) Exclude bands = 1-5,9-20.
O:s

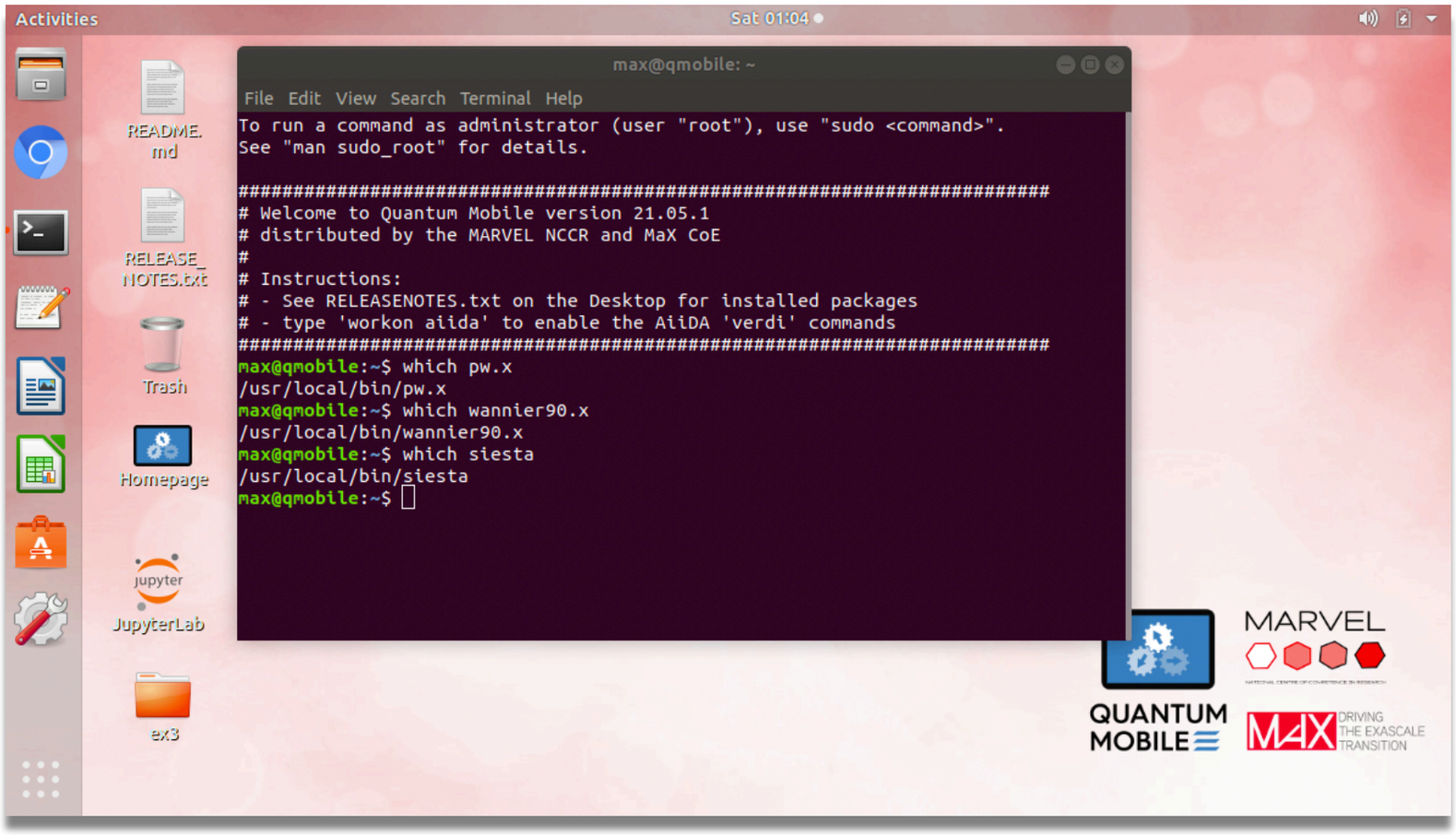


(e) Exclude bands = 1-8,12-20.
Ba:p



(f) Exclude bands = 1-11.
O:p

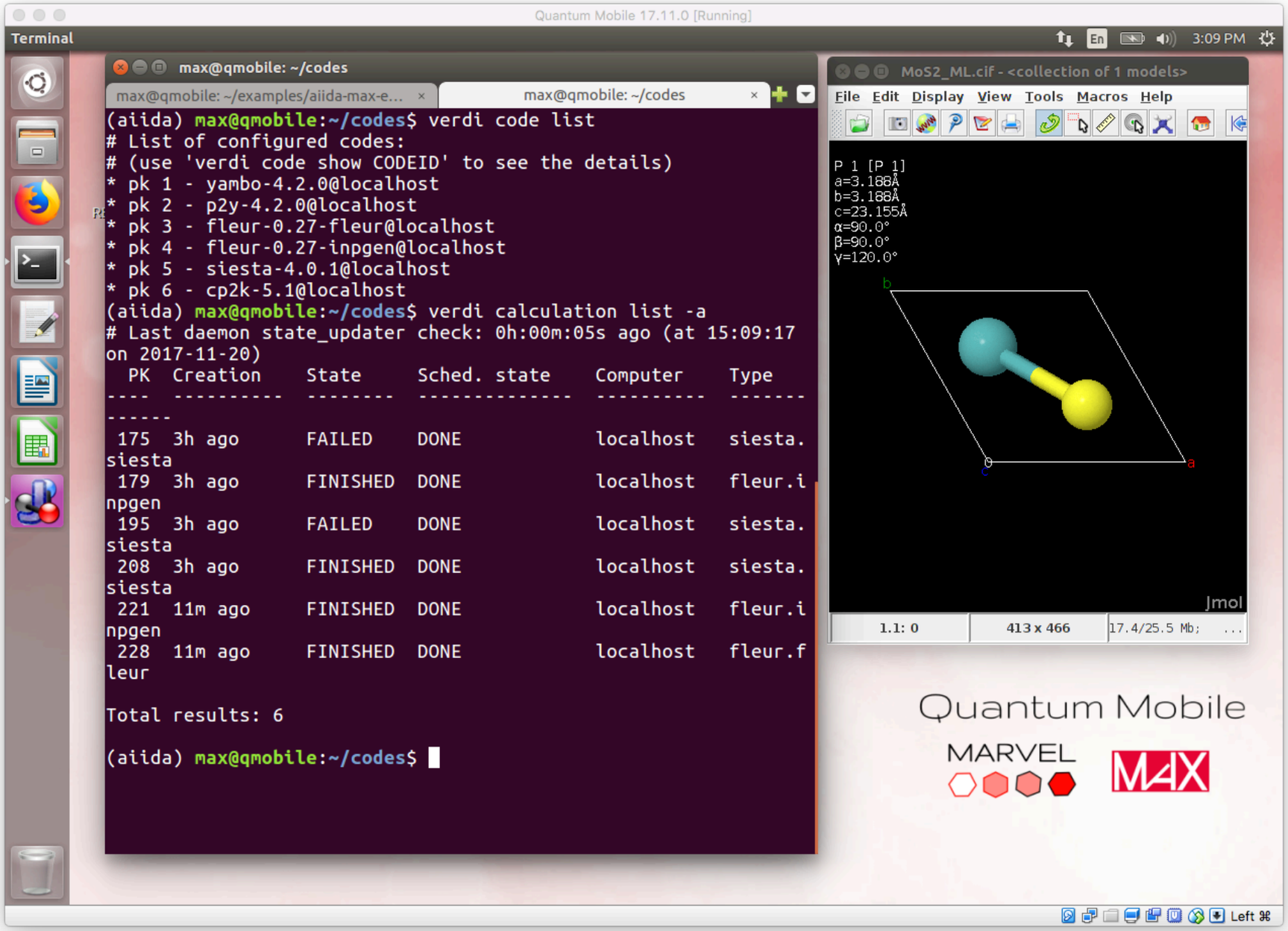
If you want to continue at home:
Quantum Mobile: A VM for quantum simulations



- VM based on Ubuntu Linux
- Comes with quantum codes:
  - **Quantum ESPRESSO**
  - **Yambo**
  - **Fleur**
  - **Siesta**
  - **cp2k**
  - **Wannier90**
  - **…**
- Contains also AiiDA, preconfigured to use these codes
- **Just download and start running!** No need to spend time on installation, compilation, ...

Quantum Mobile:
https://www.materialscloud.org/quantum-mobile

If you want to continue at home:
Quantum Mobile: A VM for quantum simulations



- **All codes ready to be used through AiiDA**
- Visualization tools (xcrysden, …)
- Useful for:
  - exercises, courses, …
  - running simulations without any setup
  - experimenting with new codes
  - Production simulations

Quantum Mobile:
https://www.materialscloud.org/work/quantum-mobile

Getting help

- **Today**: ask me, Junfeng, and all other tutors of the school

- **From tomorrow on...**: www.wannier.org
  - User guide, tutorials (with solutions)
  - Register to the Wannier90 mailing list *(do it today!)*
  - Read the source code!

Practical information

- You can find the PDF with the instructions online: https://epw2021.oden.utexas.edu/74-schedule
- Or also inside **/work2/06868/giustino/EPW-SCHOOL/**
- Before starting the tutorials, copy the files above in your scratch; you can go to it with: **cd $SCRATCH**
- To untar: **tar xf FILENAME.tar**
  - For instance: **tar xf /work2/06868/giustino/EPW-SCHOOL/Mon.4.Pizzi.tar**
- You will need to submit to the queue in order to be able to run
  - Don't fill the queue for too long, be considerate for others
  - Use parameters and commands suggested in the PDF