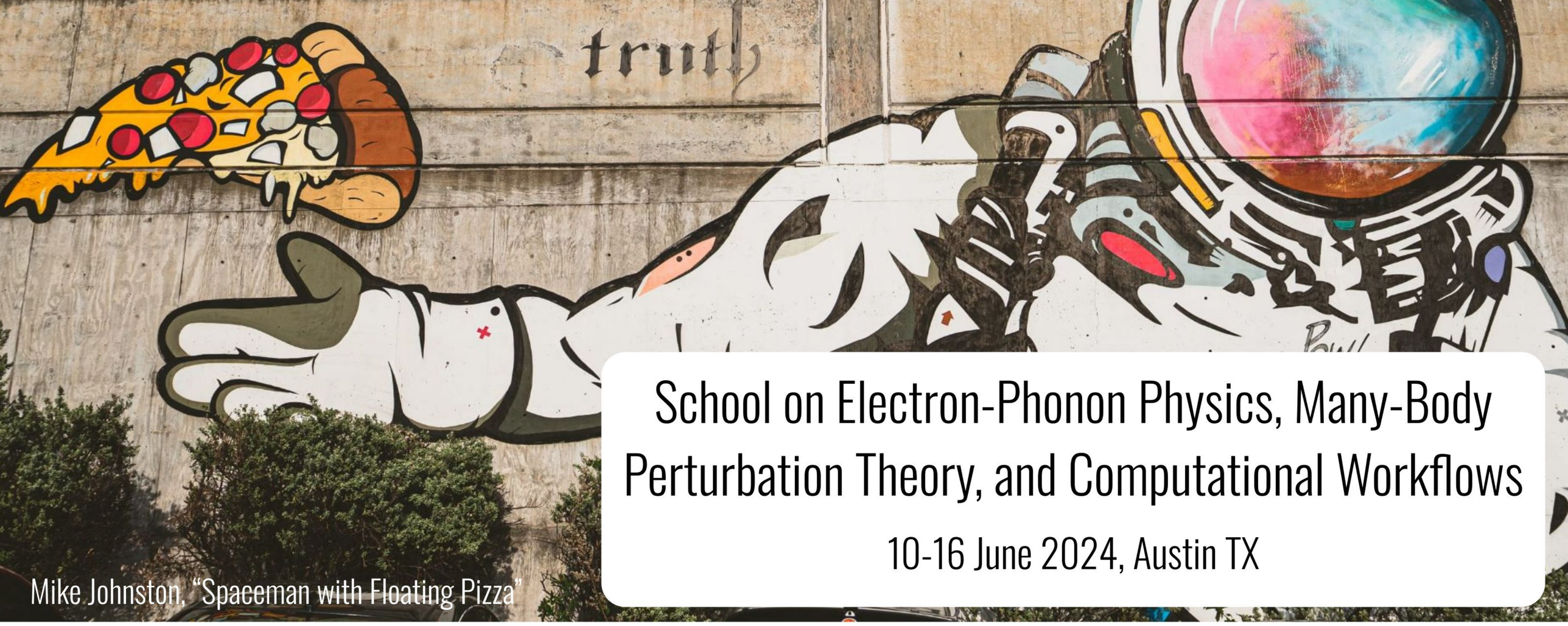

Mike Johnston, “Spaceman with Floating Pizza”

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

10-16 June 2024, Austin TX

U.S. DEPARTMENT OF ENERGY

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TEXAS ADVANCED COMPUTING CENTER

ODEN

Lecture Tue.3

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

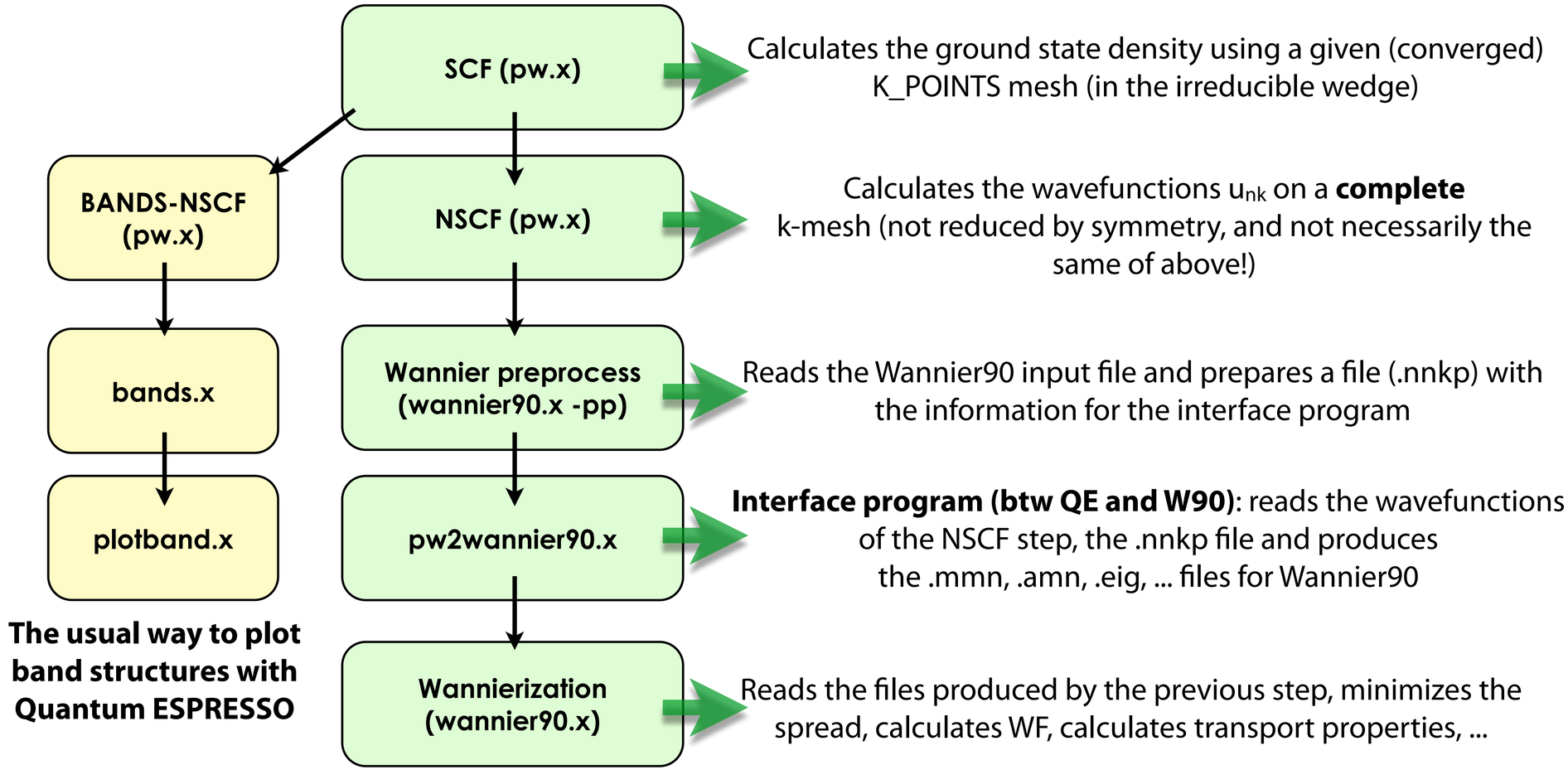
Antimo Marrazzo

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

Wannier90 "input data"

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

How to run a Wannier90 calculation



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

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)

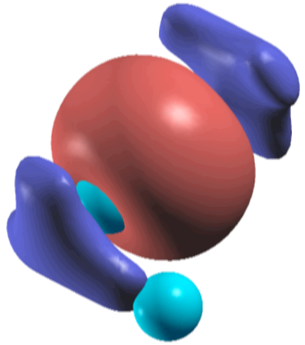
[1] Damle, A., Lin, L. & Ying, L. J. Compressed representation of Kohn–Sham orbitals via selected columns of the density matrix. J. Chem. Theory & Comp. 11, 1463–1469 (2015).

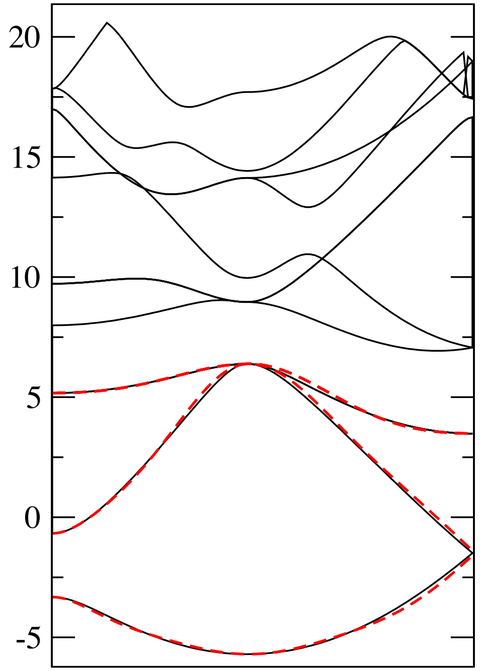
[2] Damle, A. & Lin, L. Disentanglement via entanglement: A unified method for Wannier localization. Mult. Scale. Model. & Simul. 16, 1392–1410 (2018).

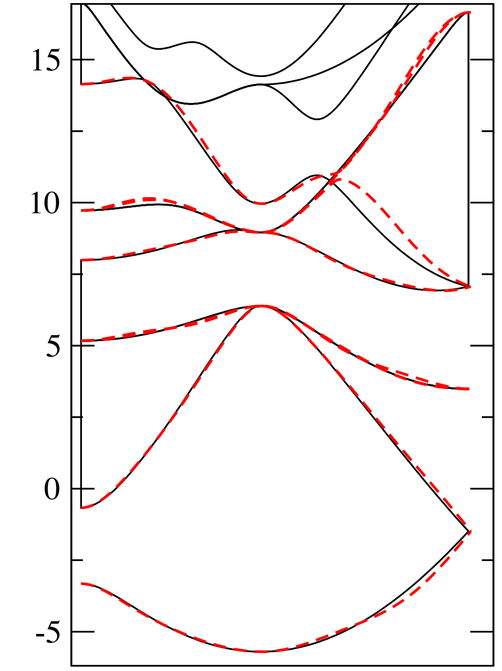
[3] Vitale, V., Pizzi, G., Marrazzo, A. et al. Automated high-throughput Wannierisation. npj Comput Mater 6, 66 (2020). https://doi.org/10.1038/s41524-020-0312-y

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

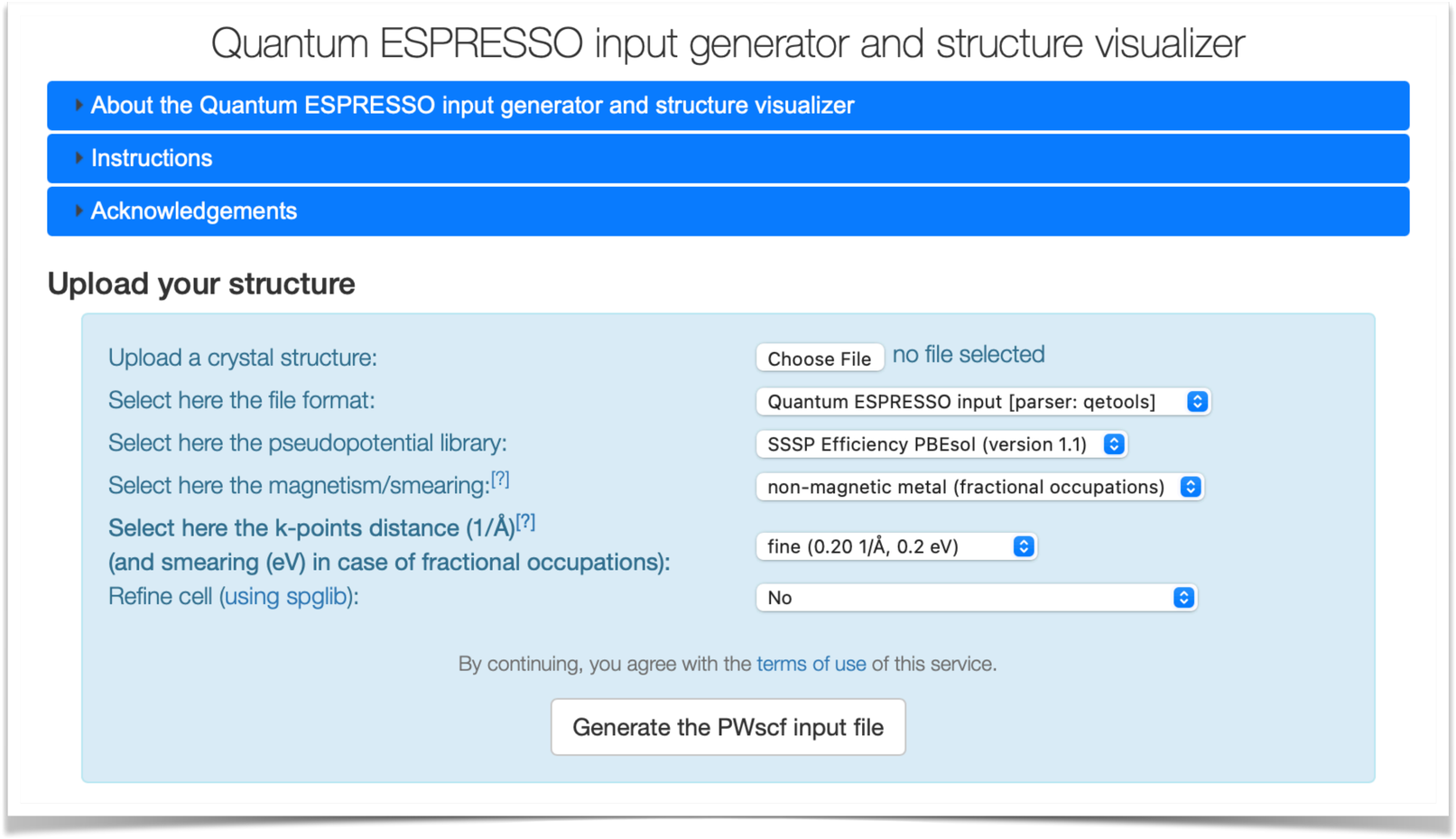
→ Definition of atomic positions

→ 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:

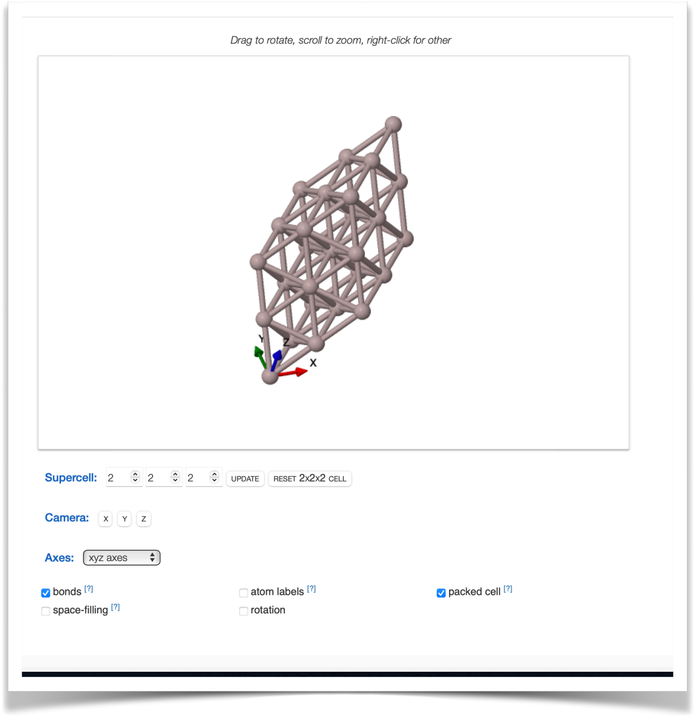
- SSSP (for the pseudopotential library)
  G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet and N. Marzari, npj Computational Materials **4**, 72 (2018).
  WEB: http://materialscloud.org/sssp.
- Pseudopotentials:
  - Al.pbesol-n-kjpaw_psl.1.0.0.UPF,
    from Pslibrary 1.0.0: A. Dal Corso, *Comput. 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*, A. Marrazzo* *et al.*, npj Comp. Mat. 4, 72 (2018)

How to run and input file

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

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

  wannier90.x ex1 (for the Wannierization step)

- Input file format: very simple, there are *no* namelists but only:
  - Variables (order is not important; not case sensitive)
    num_wann = 4
    mp_grid : 6 6 6
  - Blocks
    begin atoms_frac
    Si -0.25 0.75 -0.25
    Si 0.00 0.00 0.00
    end atoms_frac
- Default units: lengths are **angstrom** (bohr are also accepted), energies are **eV**

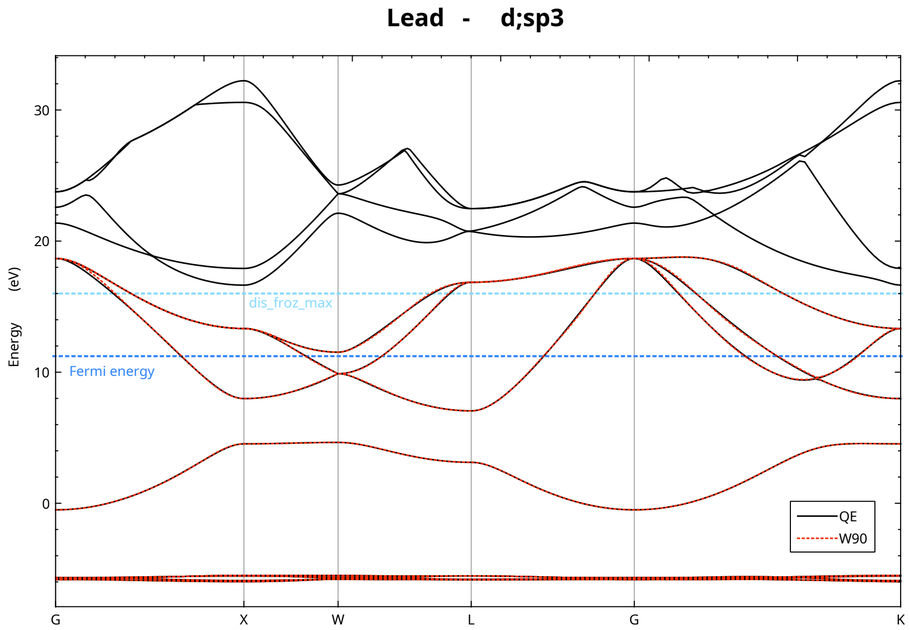
Example of input file (ex1)

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

! restart            =  plot
wannier_plot         =  true
wannier_plot_supercell =  3

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

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

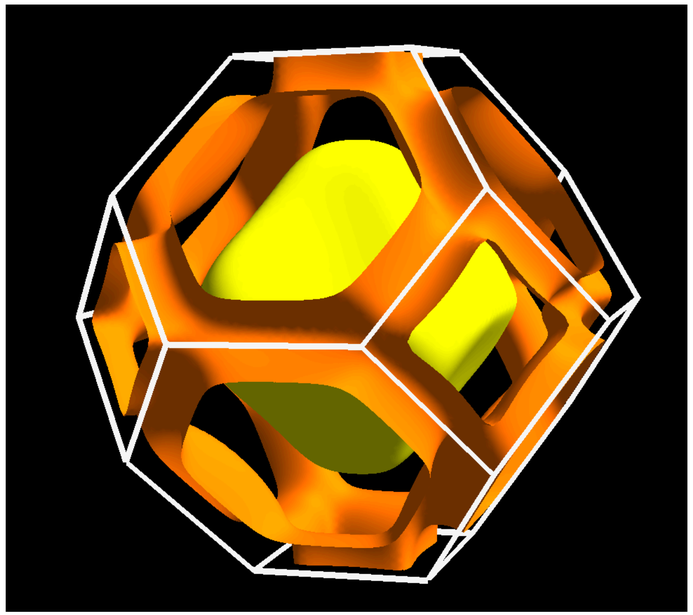
```
mp_grid  =  XXX XXX XXX
begin kpoints
XXX
XXX
XXX
end kpoints

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

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

Exercise 3: band structure and Fermi surface of lead

- Interpolate the band structure of lead



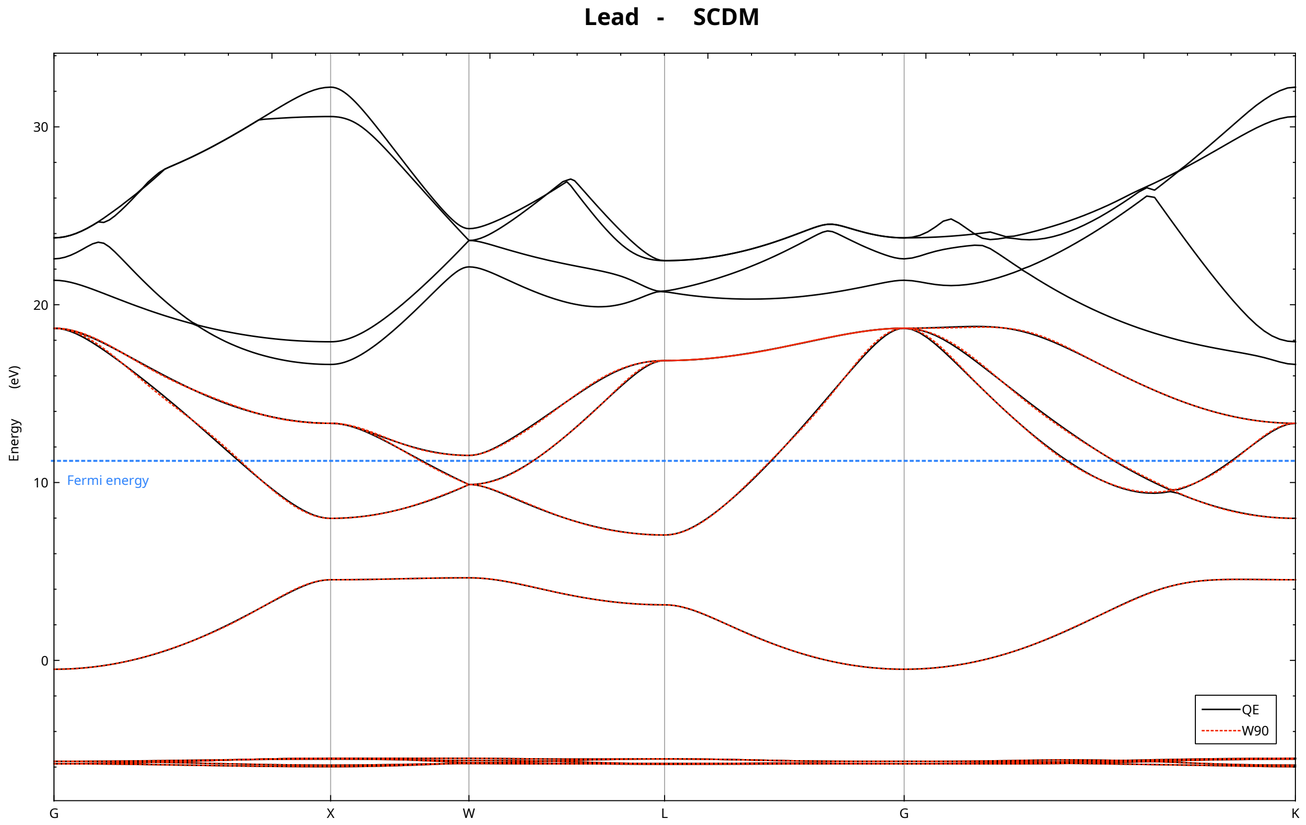
- Show the Fermi surface of lead



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

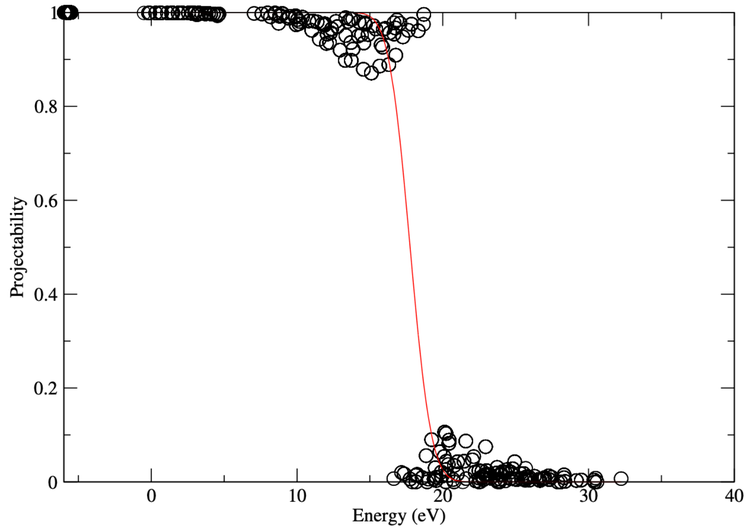
Exercise 4: automatic projections with SCDM

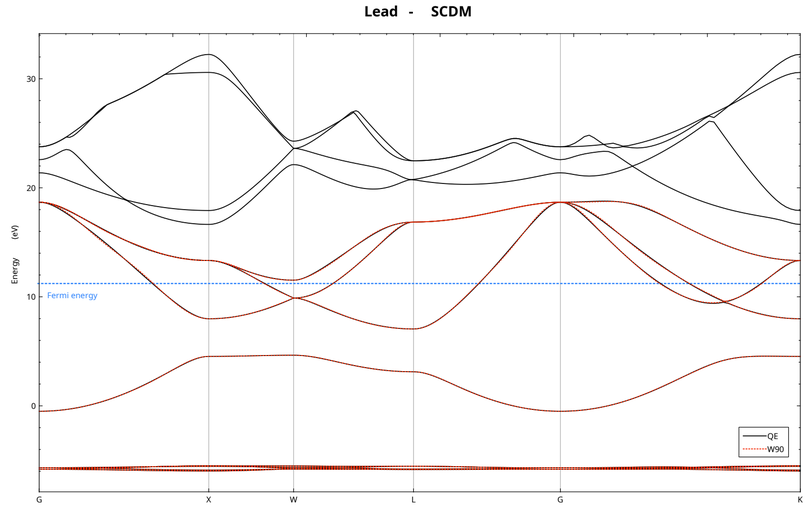
- Obtain the Wannier functions and the band structure of lead **without having to explicitly specify the projections!**



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





Accuracy and convergence

- Two major parameters control the quality (and computational cost) of your Wannier functions (WFs):
  - Spread minimization
  - K-point grid for the initial (e.g., DFT) Hamiltonian eigenstates

➡ Starting point for the spread minimization (i.e., projections) is crucial to avoid being trapped in local minima

➡ Lower spread -> more localized WFs -> coarser initial k-points grids are needed

➡ Accuracy of band interpolation is a proxy for the quality of the underlying WFs

➡ Check also the Im/Re ratio: MLWFs should be real at the global minimum (for collinear composite bands without spin-orbit coupling)

Getting help

- **Today (and until Saturday morning)**: ask me or Junfeng :-)
- **From tomorrow on**: www.wannier.org

  - User guide, tutorials (with solutions)
  - Register to the Wannier90 mailing list
  - Actually read the source code!

Practical information

- You can find the PDF with the instructions online: https://epw2024.oden.utexas.edu/74-schedule
- Or also inside **/work2/05193/sabyadk/stampede3/EPWSchool2024/tutorials**
- Before starting the tutorials, copy the files above in your scratch; you can go to there with: **cd $SCRATCH**
- To untar: **tar -xvf FILENAME.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