UNIVERSITÀ DEGLI STUDI DI TRIESTE

EPFL

# Introduction to the hands-on tutorial:

# Wannier interpolation of band structures

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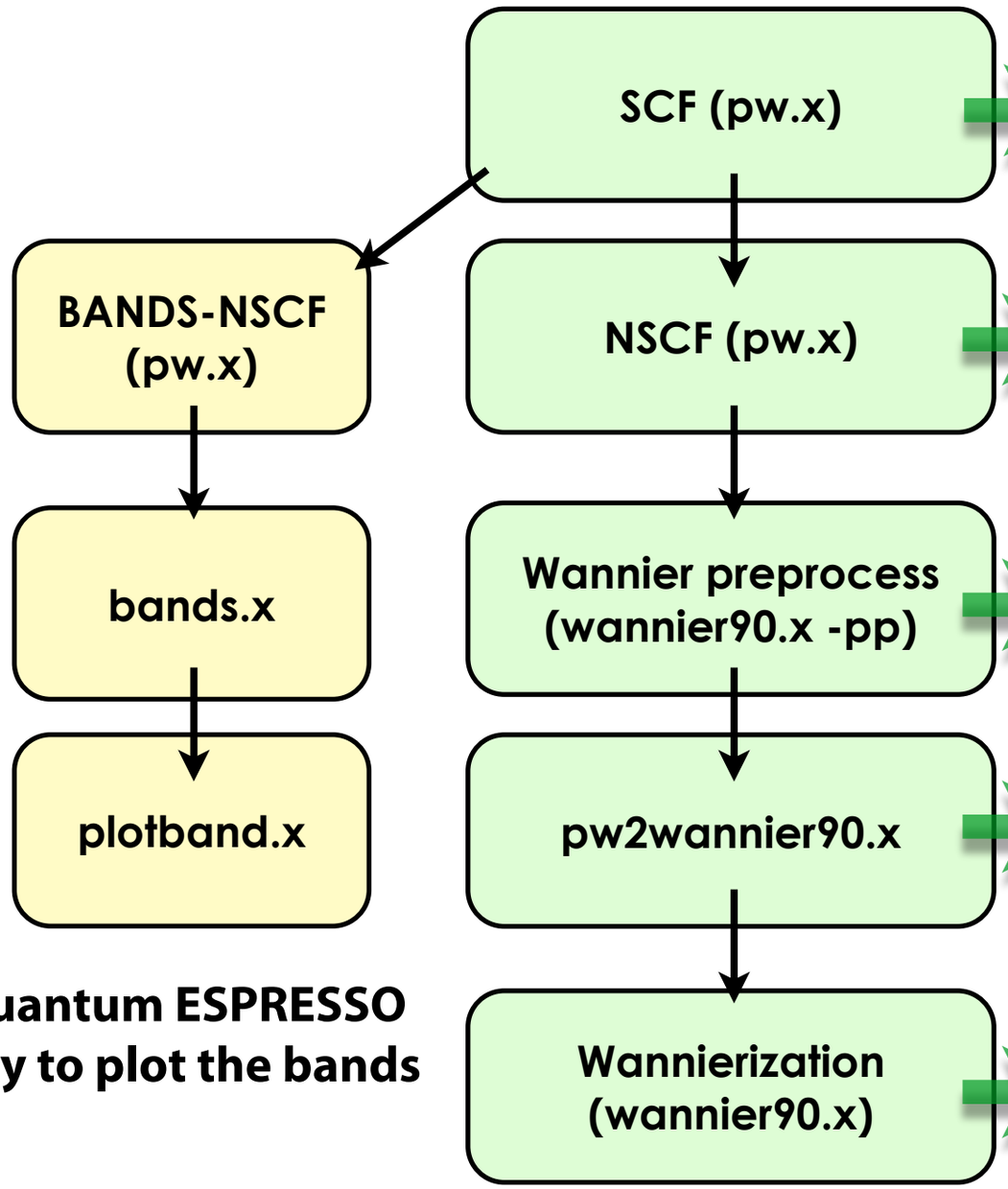
# Wannier90 "input data"

- 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)
- 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




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

# 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)

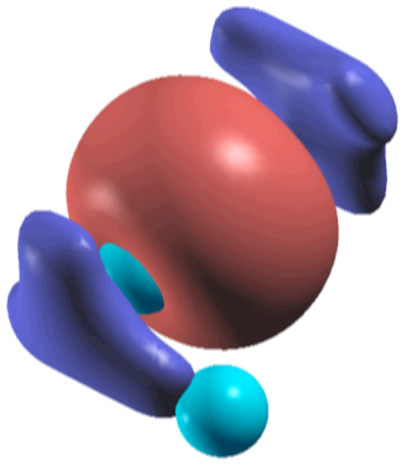

[1] Damle, A., Lin, L. & Ying, L. J. Compressed representation of Kohn–Sham orbitals via selected columns of the density matrix. J. Chem. Theory & Comp. 11, 1463–1469 (2015).

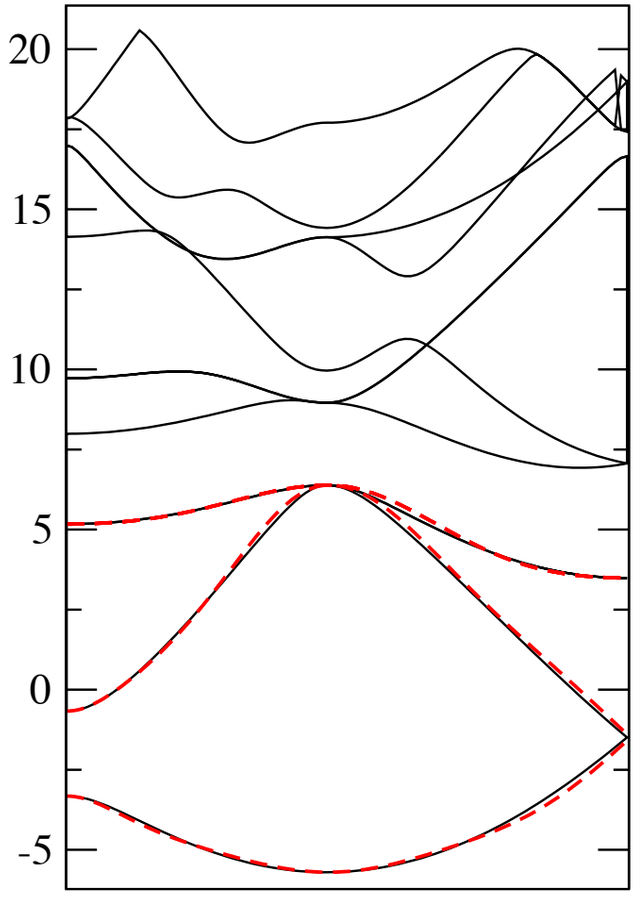
[2] Damle, A. & Lin, L. Disentanglement via entanglement: A unified method for Wannier localization. Mult. Scale. Model. & Simul. 16, 1392–1410 (2018).

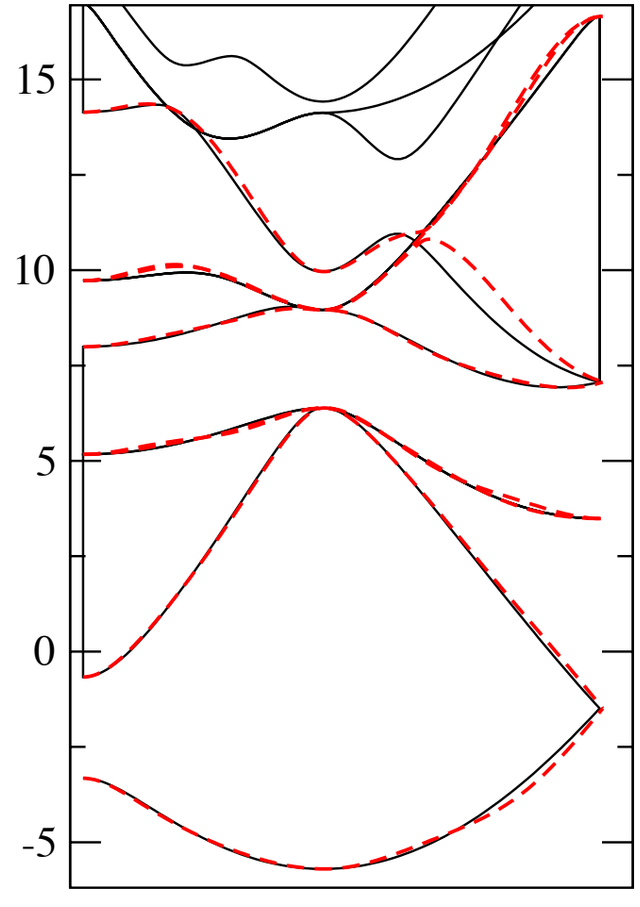
[3] Vitale, V., Pizzi, G., Marrazzo, A. et al. Automated high-throughput Wannierisation. npj Comput Mater 6, 66 (2020). https://doi.org/10.1038/s41524-020-0312-y

# 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

## Quantum ESPRESSO input generator and structure visualizer

▸ About the Quantum ESPRESSO input generator and structure visualizer

▸ Instructions

▸ Acknowledgements

### Upload your structure

Upload a crystal structure: Choose File no file selected

Select here the file format: Quantum ESPRESSO input [parser: qetools]

Select here the pseudopotential library: SSSP Efficiency PBEsol (version 1.1)

Select here the magnetism/smearing:[?] non-magnetic metal (fractional occupations)

Select here the k-points distance (1/Å)[?] (and smearing (eV) in case of fractional occupations): fine (0.20 1/Å, 0.2 eV)

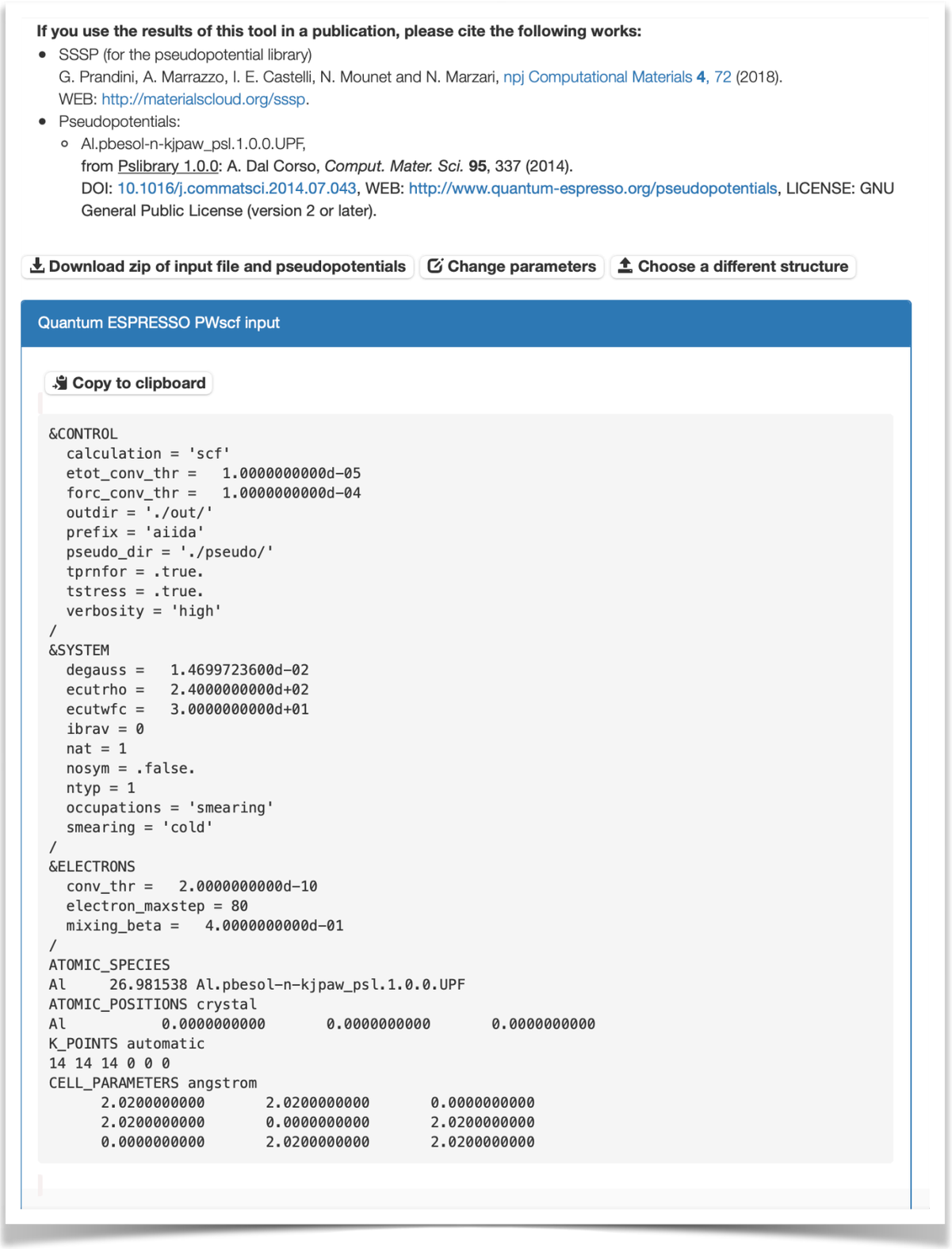
Refine cell (using spglib): No

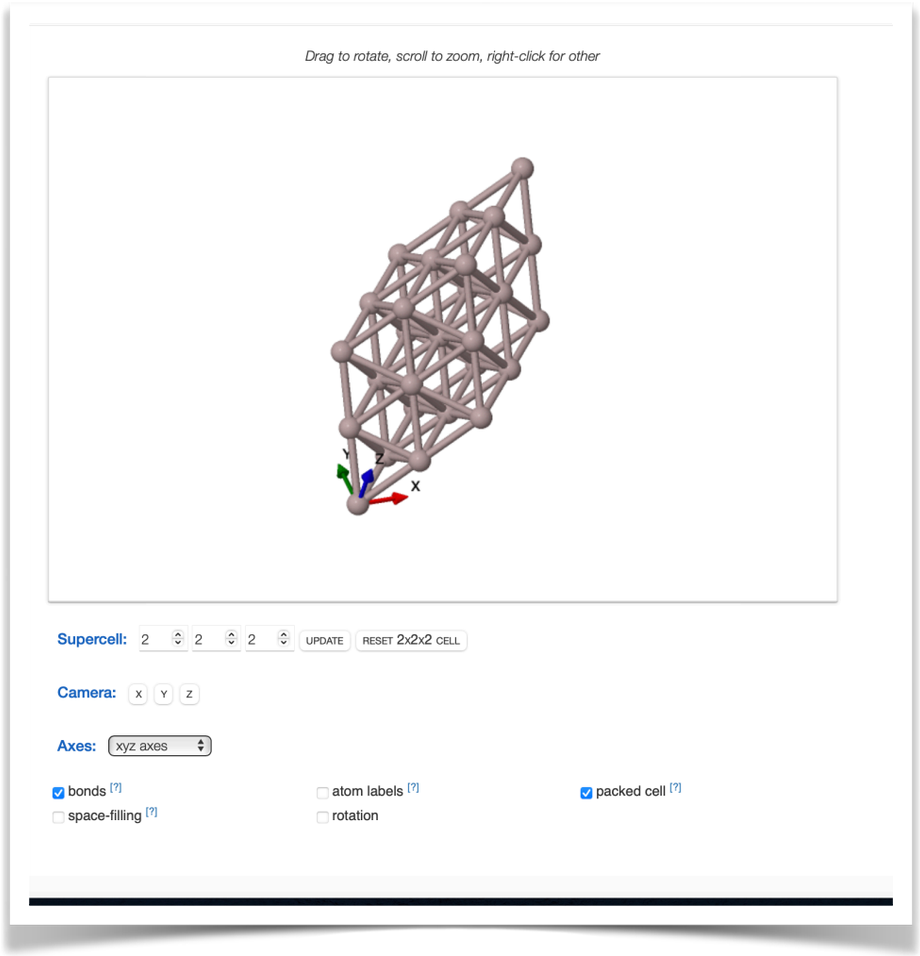
By continuing, you agree with the terms of use of this service.

Generate the PWscf input file

# The Quantum ESPRESSO input generator

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




- 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**

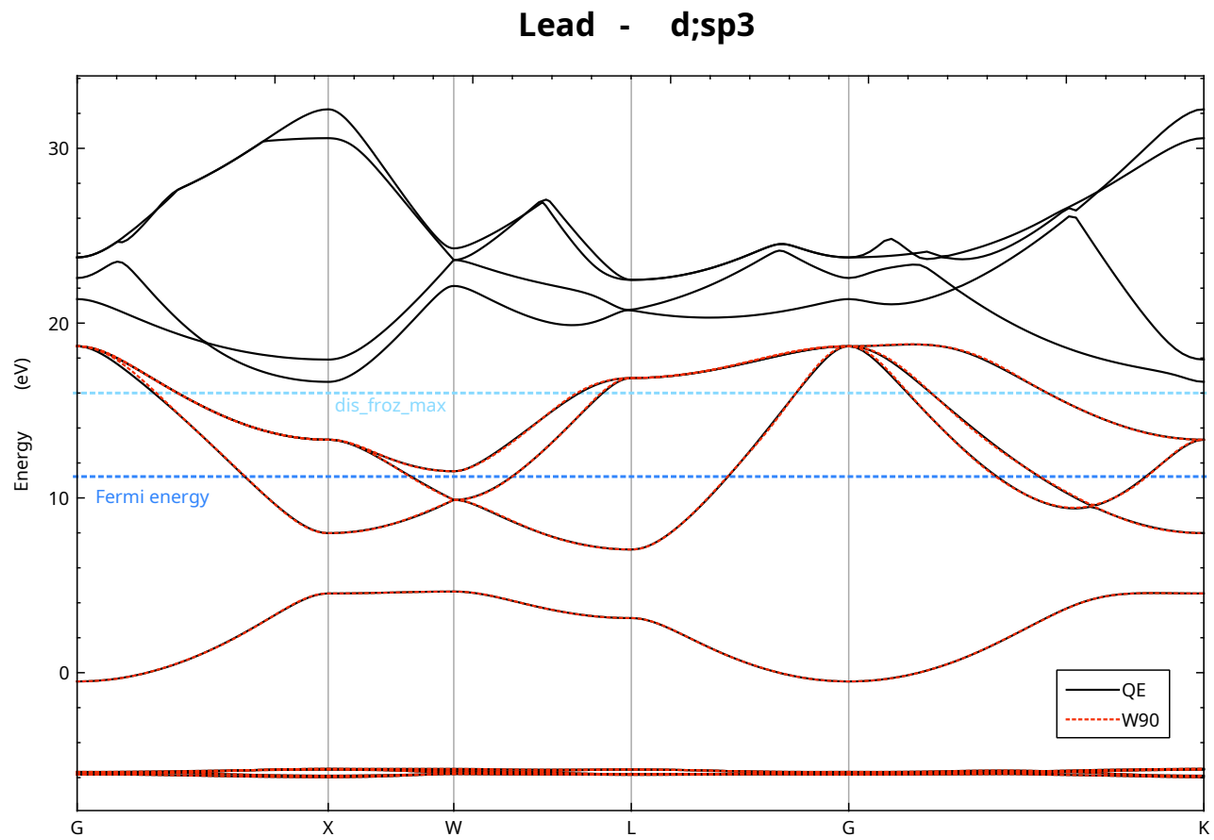
# Example of input file (ex1)

```
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
```

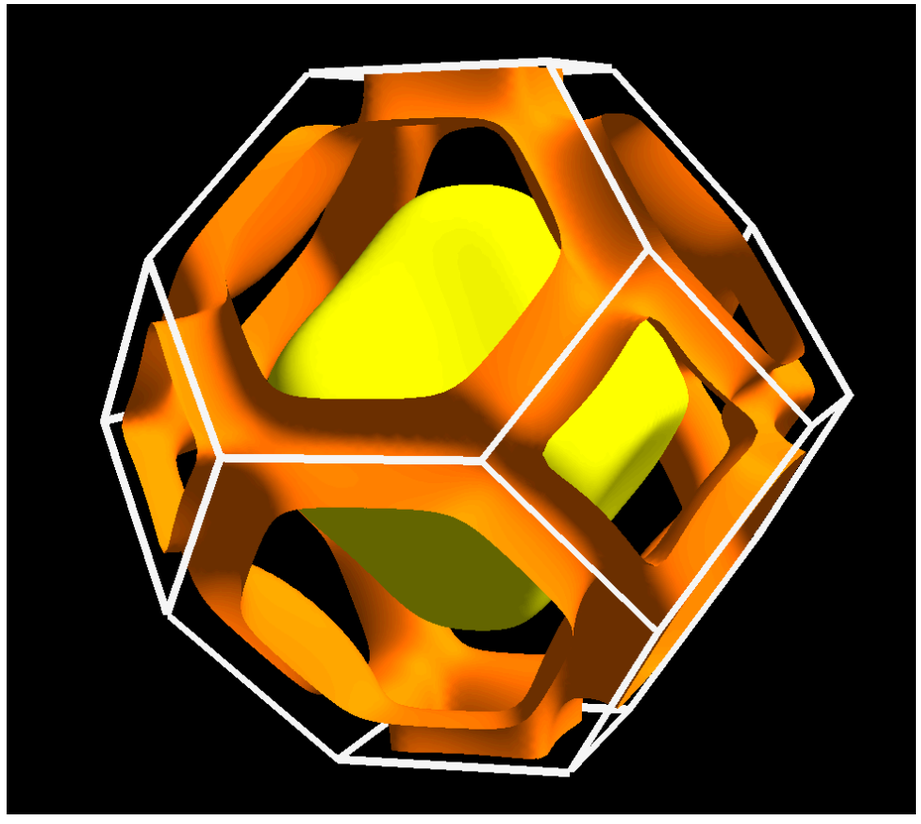
```
mp_grid  =  XXX XXX XXX
begin kpoints
XXX
XXX
XXX
end kpoints

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

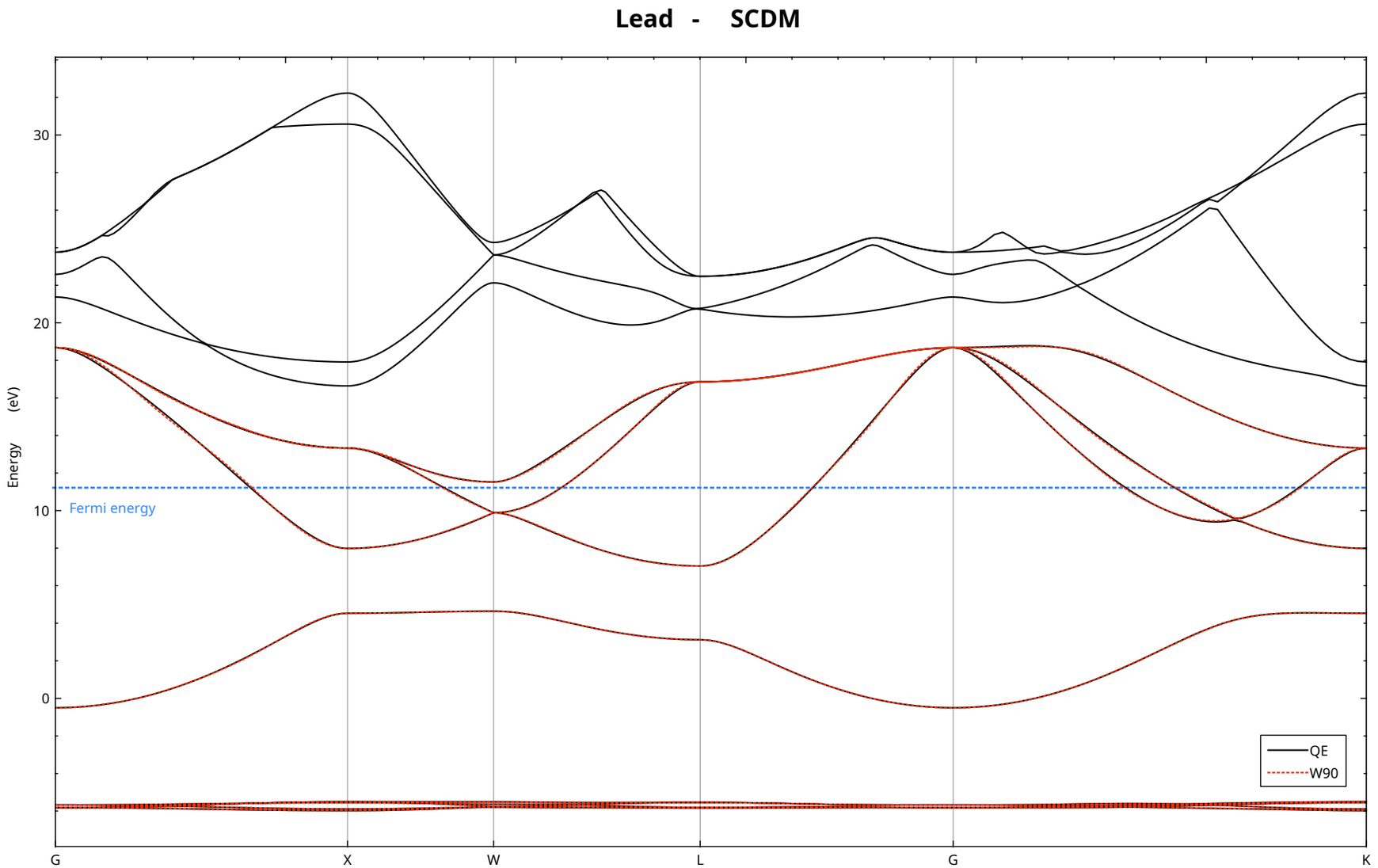



- Show the Fermi surface of lead
  - Requires a very dense grid of points in the BZ! ~$50^3$=125000
  - Wannier interpolation essential to compute it efficiently



# Exercise 4: automatic projections with SCDM

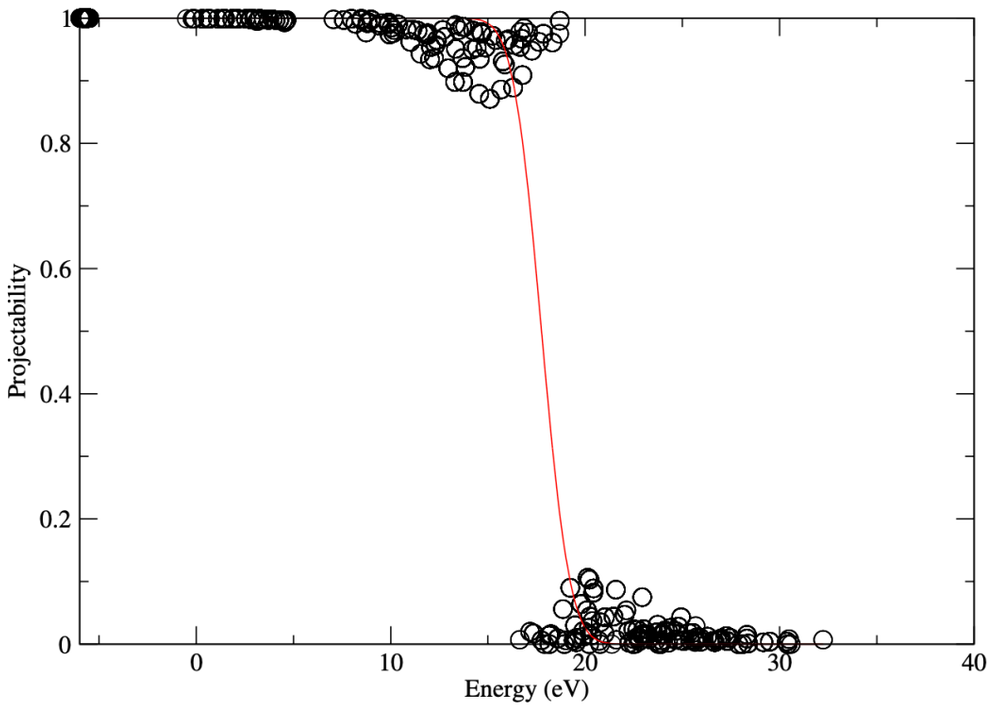
- Obtain the Wannier functions and the band structure of lead **without having to explicitly specify the projections!**

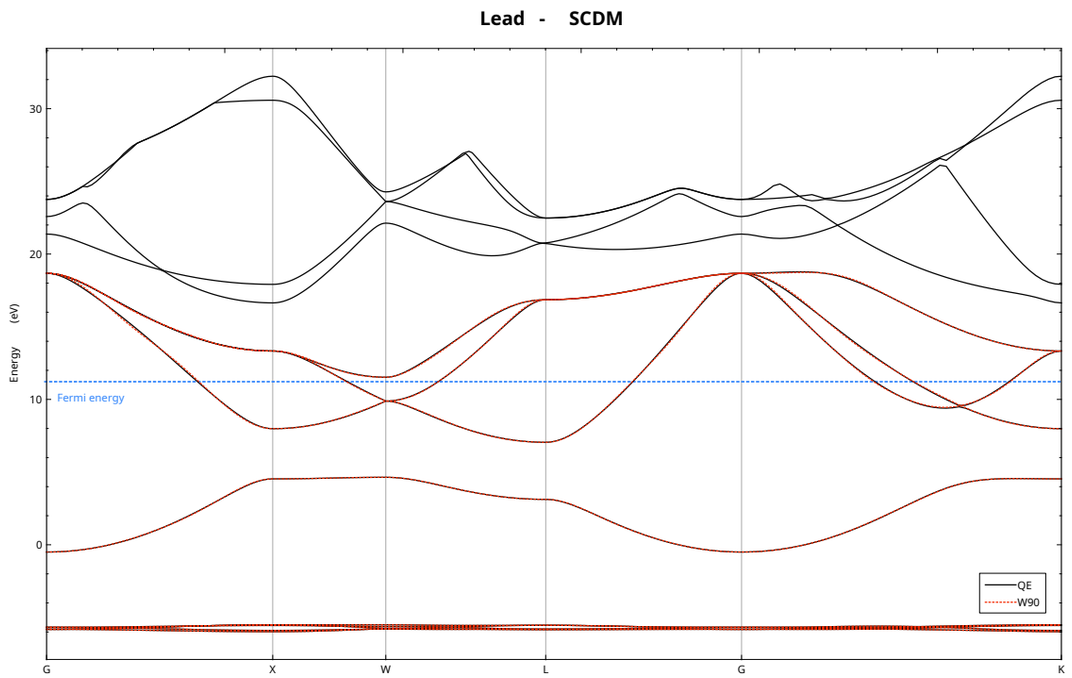


# Exercise 4: automatic projections with SCDM

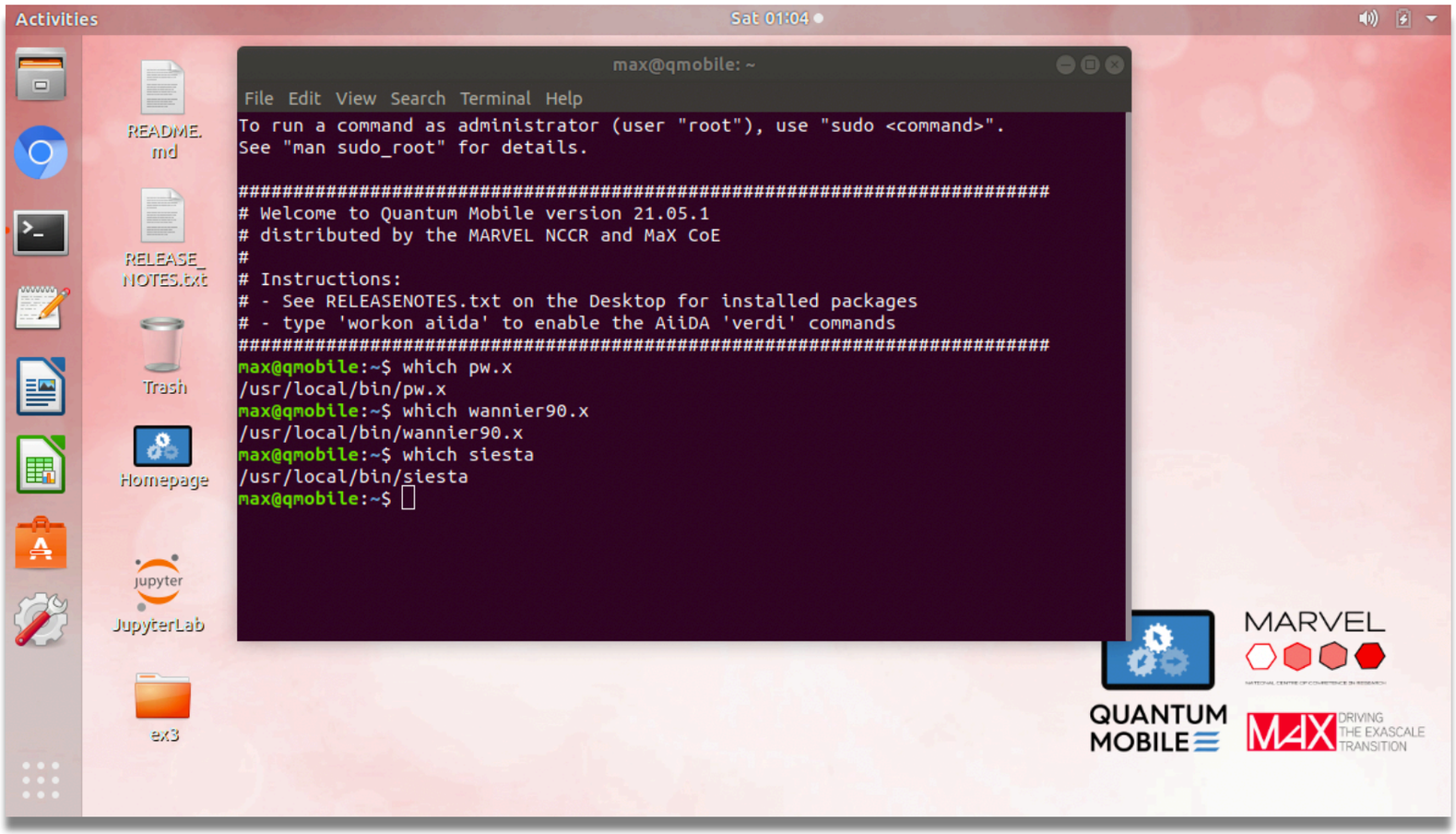
- Goals:
  - Understand how to run Wannier90 without an explicit specification of the initial projections
  - Understand the simulation steps involved in SCDM
  - Use the projectability approach to get the values for the

## SCDM parameters



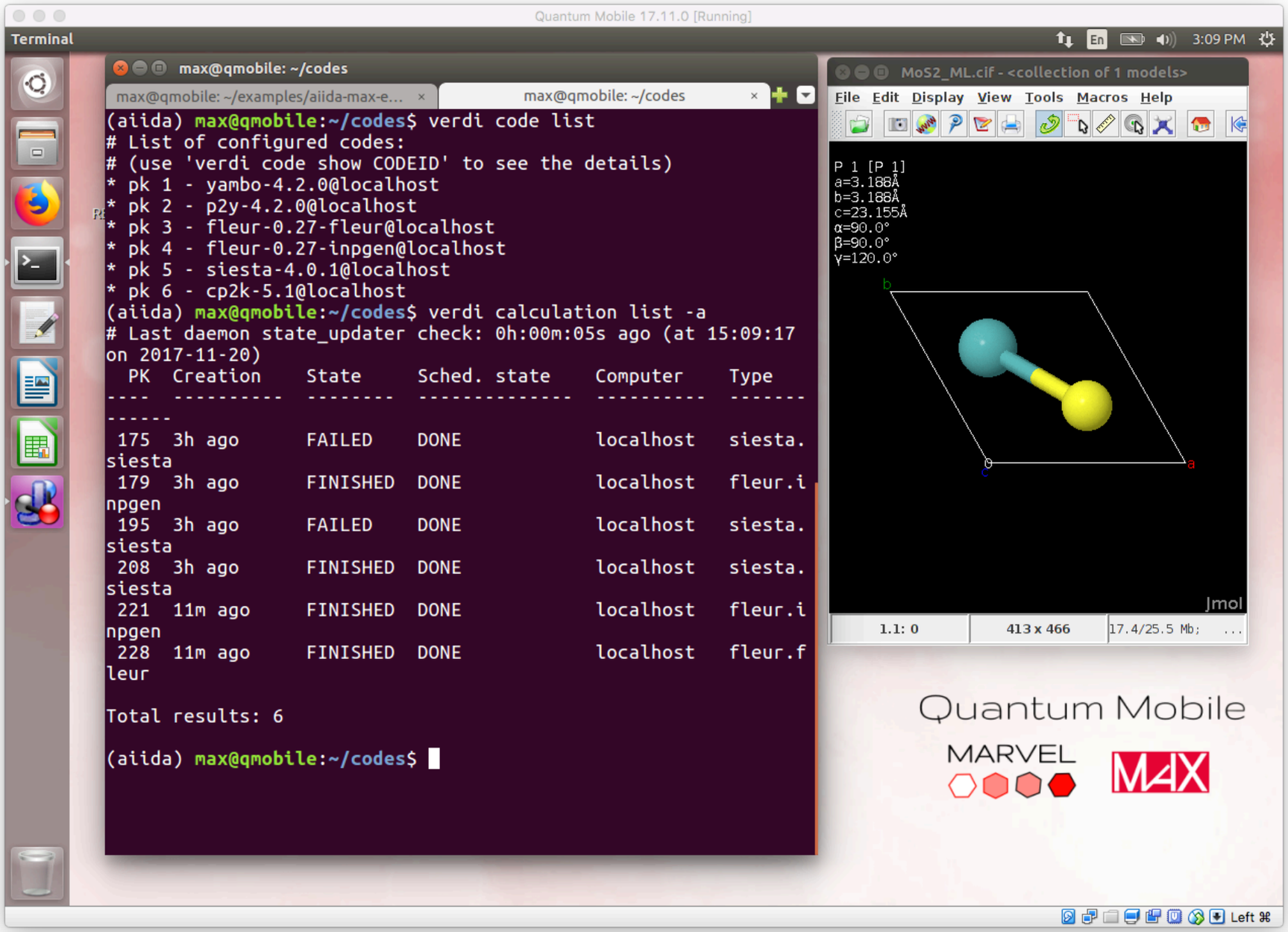
# If you want to continue at home:
# Quantum Mobile: A VM for quantum simulations




- 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 :-)
- **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://epw2022.oden.utexas.edu/74-schedule
- Or also inside **/work2/06868/giustino/EP-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/EP-SCHOOL/Tue.4.Marrazzo.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