Hands on Aiidalab for muons (DFT+μ calculcations)

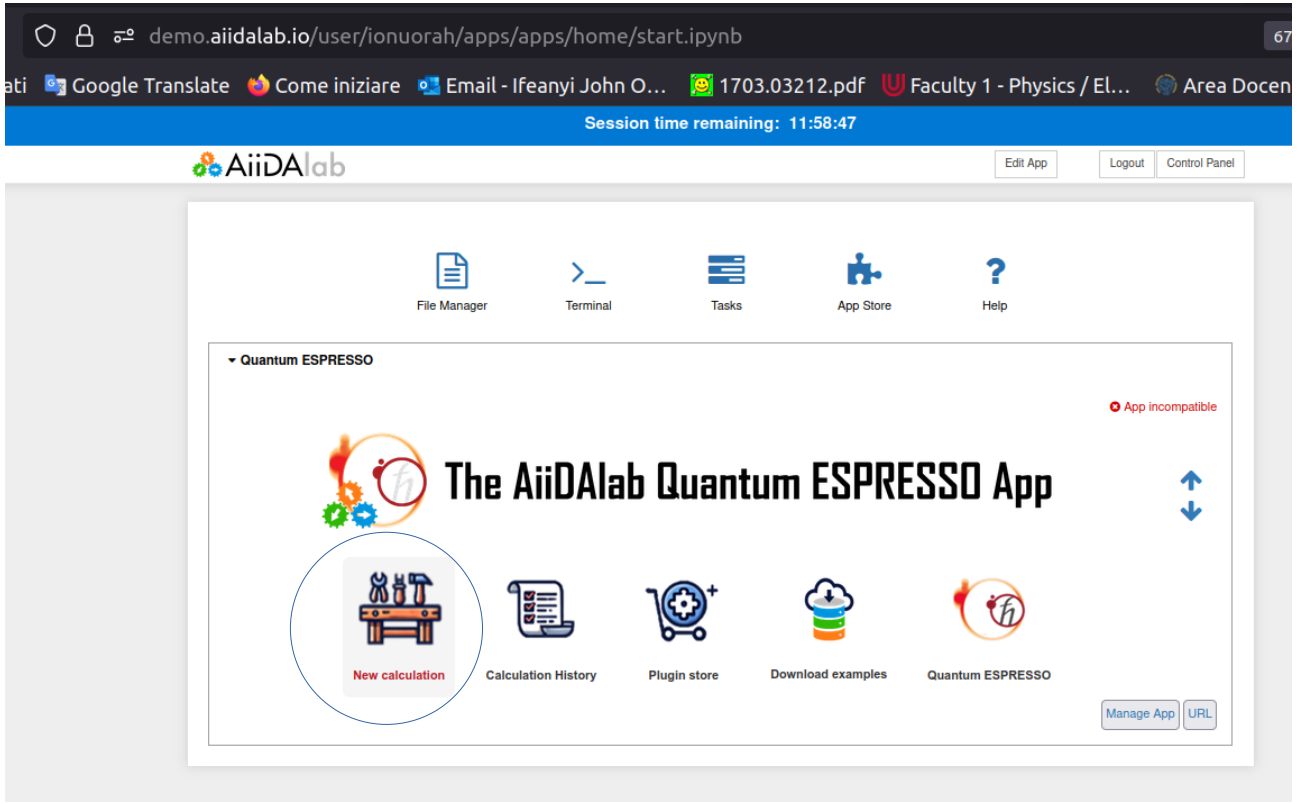
20^{h} July, 2025

Aiidalab Demo-version

- Demo version of Aiidalab (calculations only on 1 cpu – not recommended for large jobs)
- https:// demo.aiidalab.io

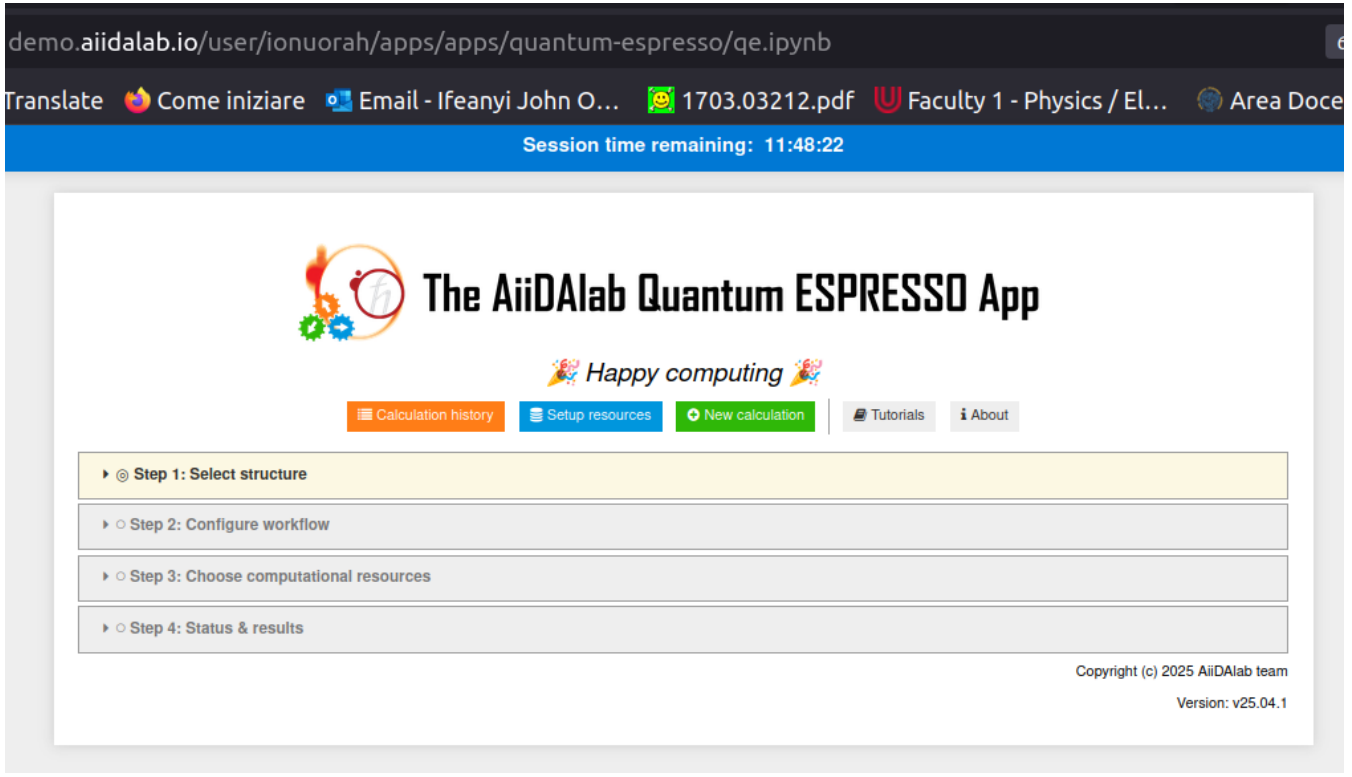
- Login with a github account (https://github.com/) signup to get one.
- Files (cifs) for the tutorial can be dowloaded from (http://bit.ly/4lZNPR1)
- This tutorial consists of 4 examples. Atleast, the first 2 is expected to be completed during the session.

Start-up page



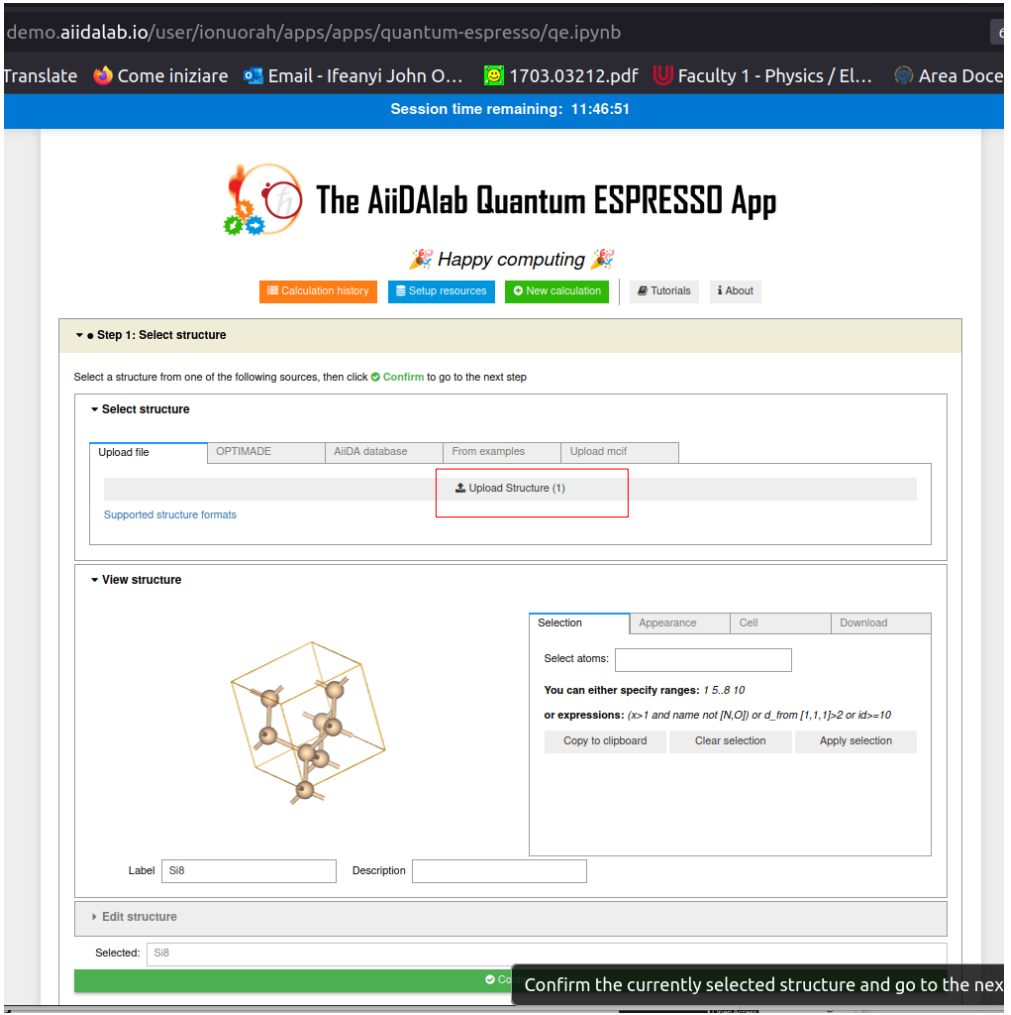
- At login, you are allowed to stay up to a max of 12 hours. Stored calculation results are also cleared.
- At start-up, there are icons for starting “**new calculation**”, **check “calculation history**” and “**Download examples**”
- The app uses the **Quantum ESPRESSO** DFT code
- To start the tutorial, lick on start a “**new calculation**”

Start a new calculation: **Example 1: "Band structure of Silicon"**



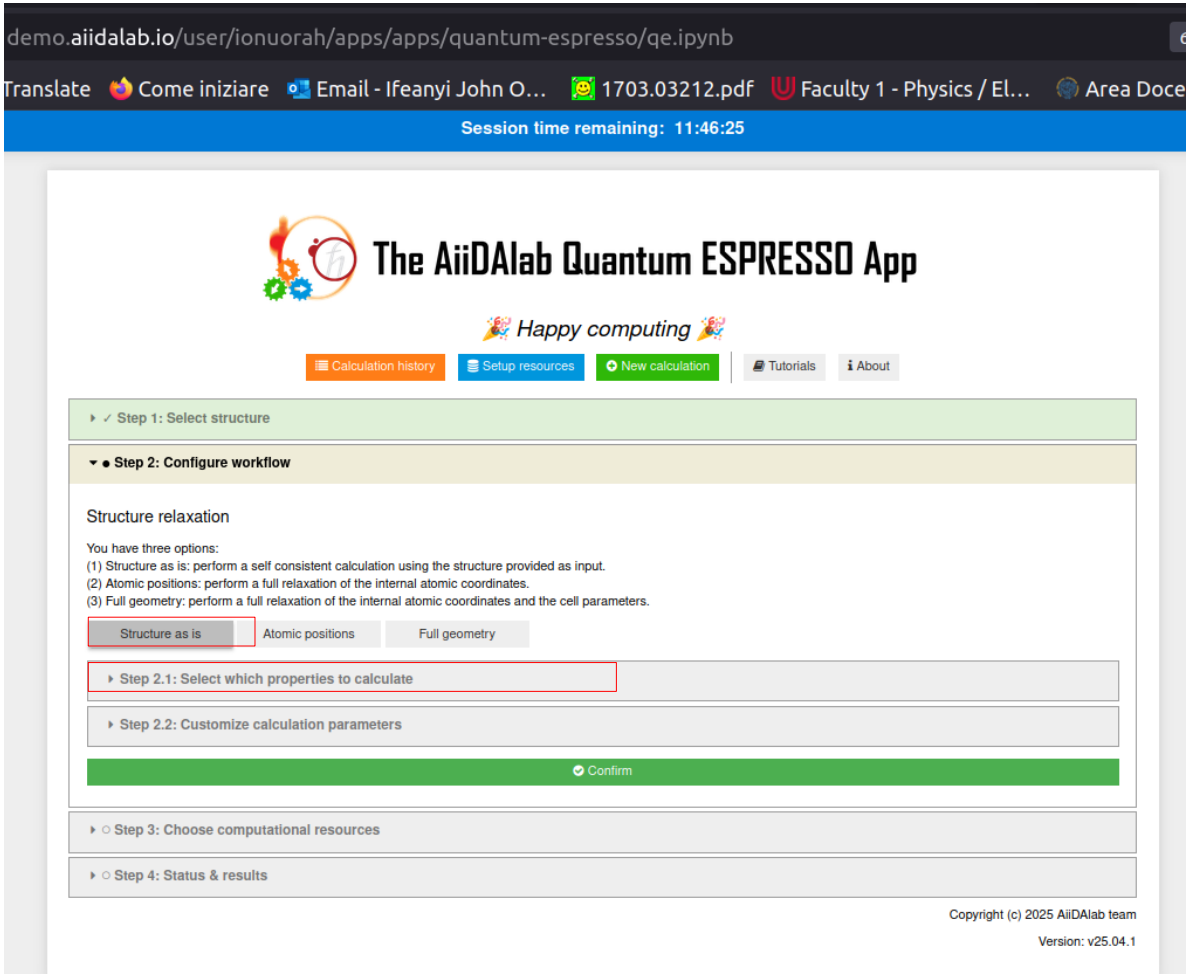
- In the **example 1 ,** we calculate the band structure of Silicon with DFT. This is aimed to allow us have a feel of the app before doing the DFT+μ calculations.
- To upload the Silicon structure, click on "**Select structure**"

Select and load structure



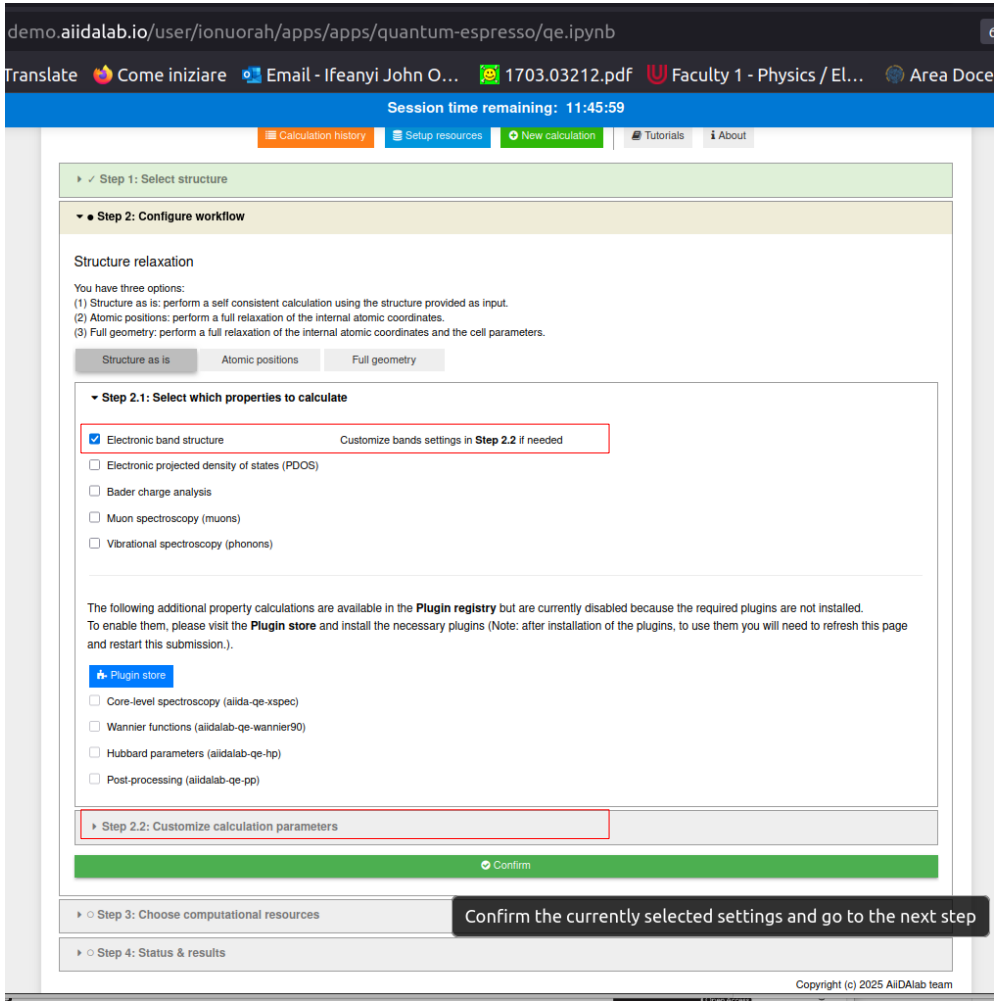
- Click on “**upload structure**”
- To upload the “Si.cif” structure file contained in the downloaded files for the tutorial
- Visualize the structure and click on “**confirm**” structure to continue

Configure workflow: No structural relaxation



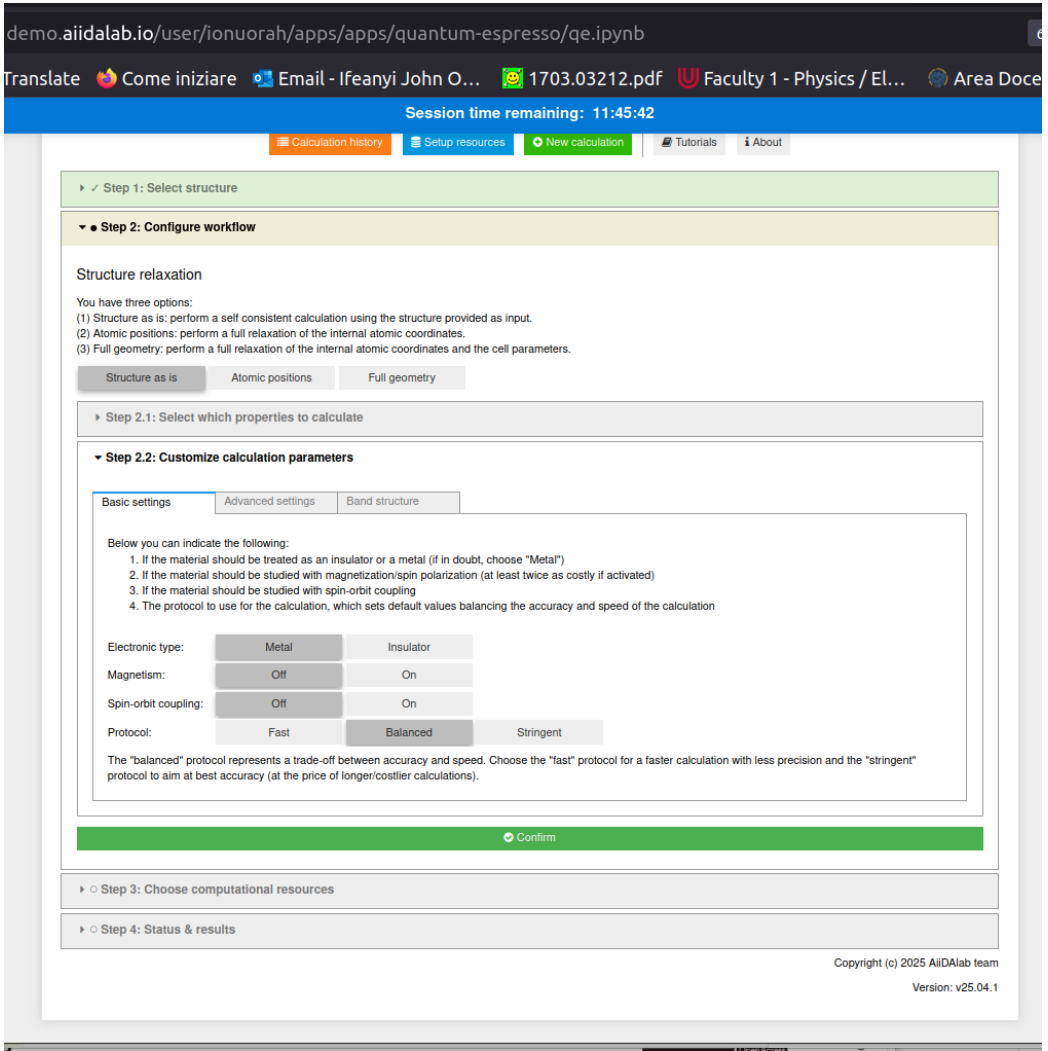
- Because of computational resource time we do not want to relax the structure (**full geometry**). Hence,
- Click “**structure as it is”**. To perform calculations with the exact uploaded structure.
- Then click on “**select which properties to calculate**”

Select properties to Calculate



- The list of available properties that can be calculated is listed.
- Select “**Electronic band structure**” to calculate the bands.
- then Click on “**Customize calculation parameters**” to open the Basic settings, see next slide

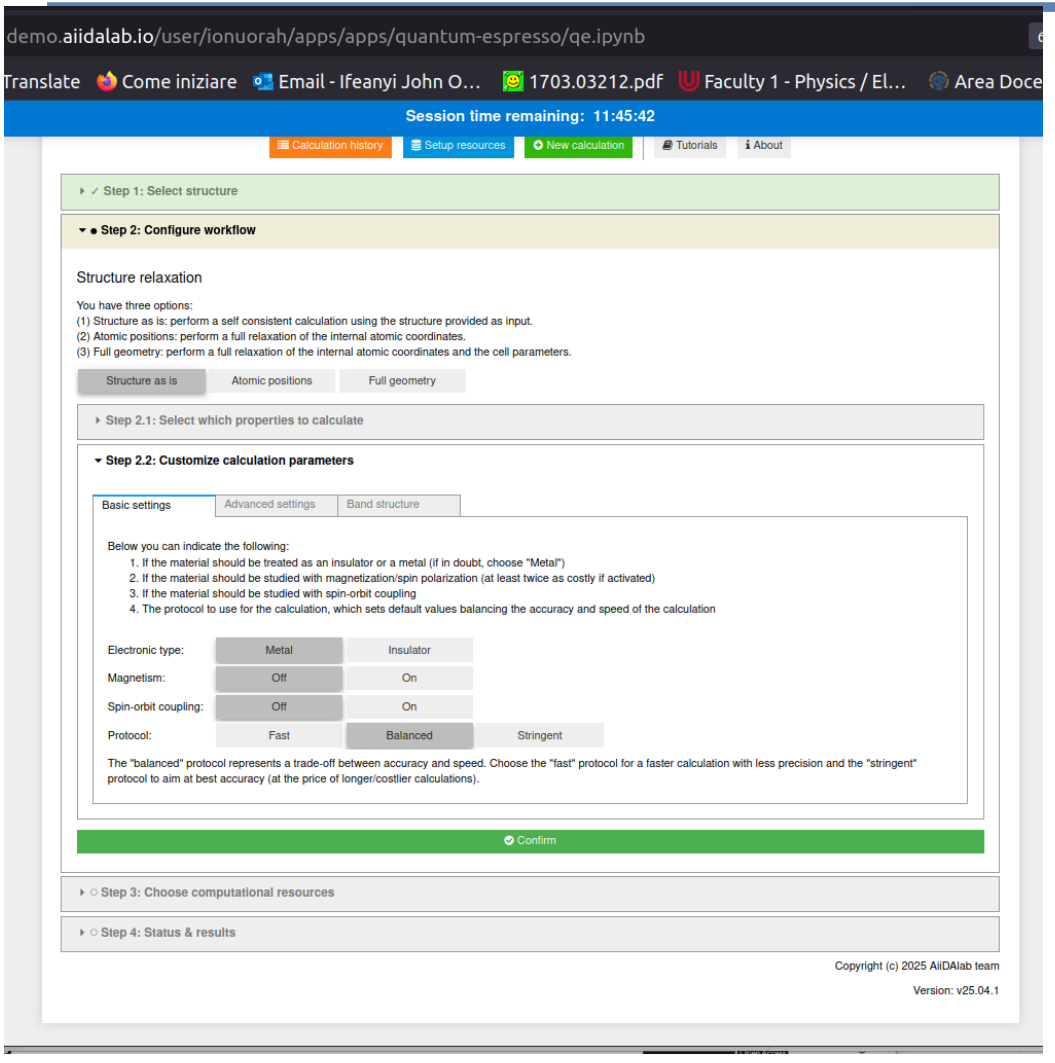
Basic-Settings of the Calculation



- Here we would use the default input settings for the example.
- Therefore click on “**confirm**” to move to the next step.
- **Note**: The input for the DFT calculations are set in this tab. In the next two slides, brief explanation is provided for reference purposes.
- To continue with the example for Si band structure, skip the next two slides on the “**input settings”**.

Tips for the **input settings(1):** Basic settings tab

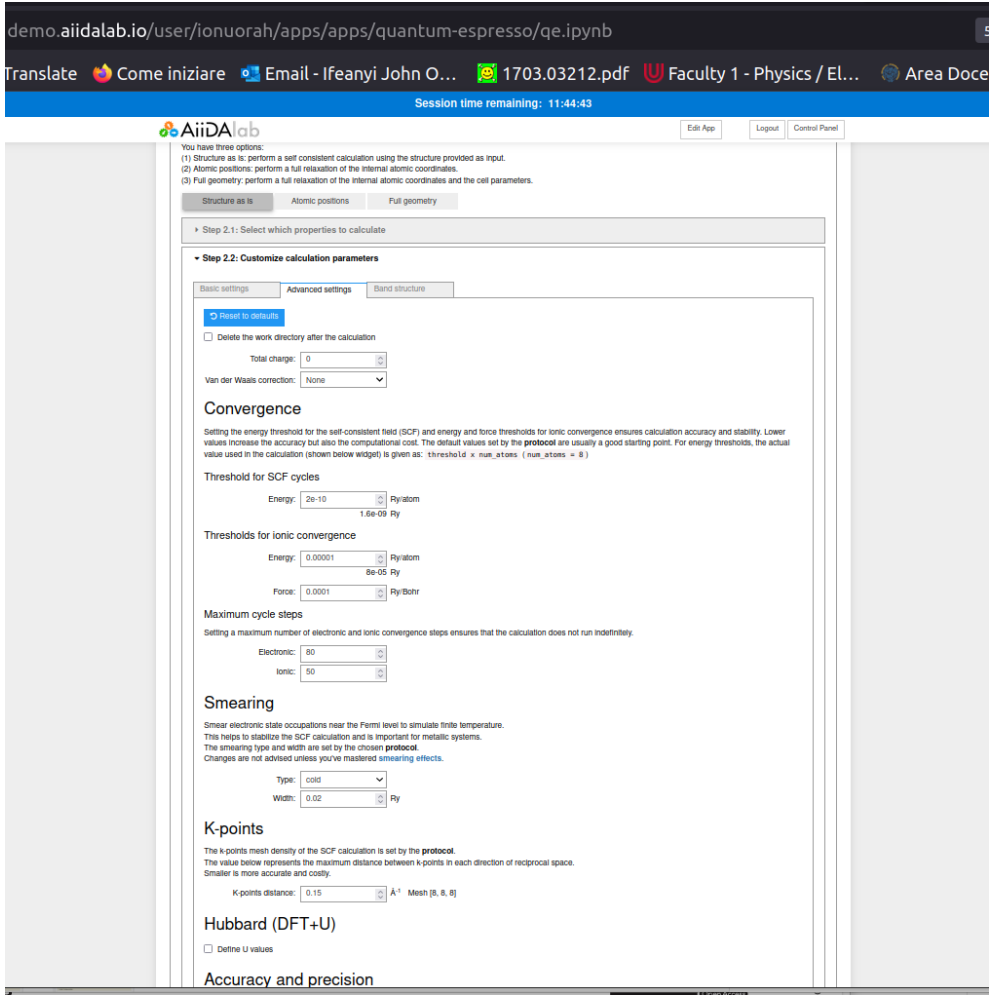
No action required!!!!



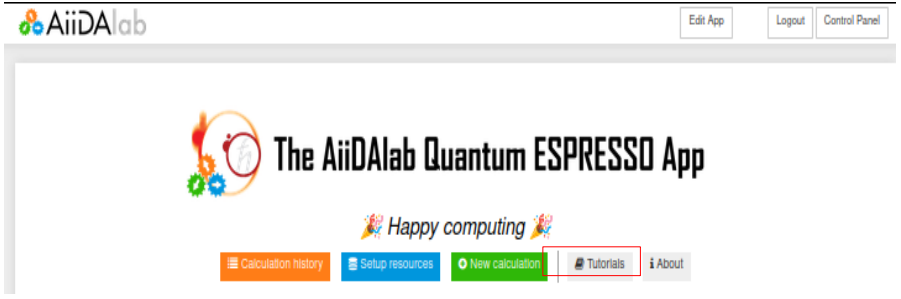
- Toggle the button, to go from “Metal” to “Insulator” for the appropriate case.
- If sample is magnetic, turn on magnetism and further settings in the “A**dvanced settings**” tab to set up the moment magnitude on the magnetic specie.
- Turn on spin-orbit coupling, to perform relativistic calculations.
- The protocol (**Fast, Balanced, Stringent**) controls the precision of the automatic settings of the input DFT parameters. The default “**balanced**” is sufficient for most calculations, considering computational resources and time. To see how the input parameters changes with each option, click on the “**Advanced settings**”.

Input settings(2): Advanced Settings tab

No action required!!!!

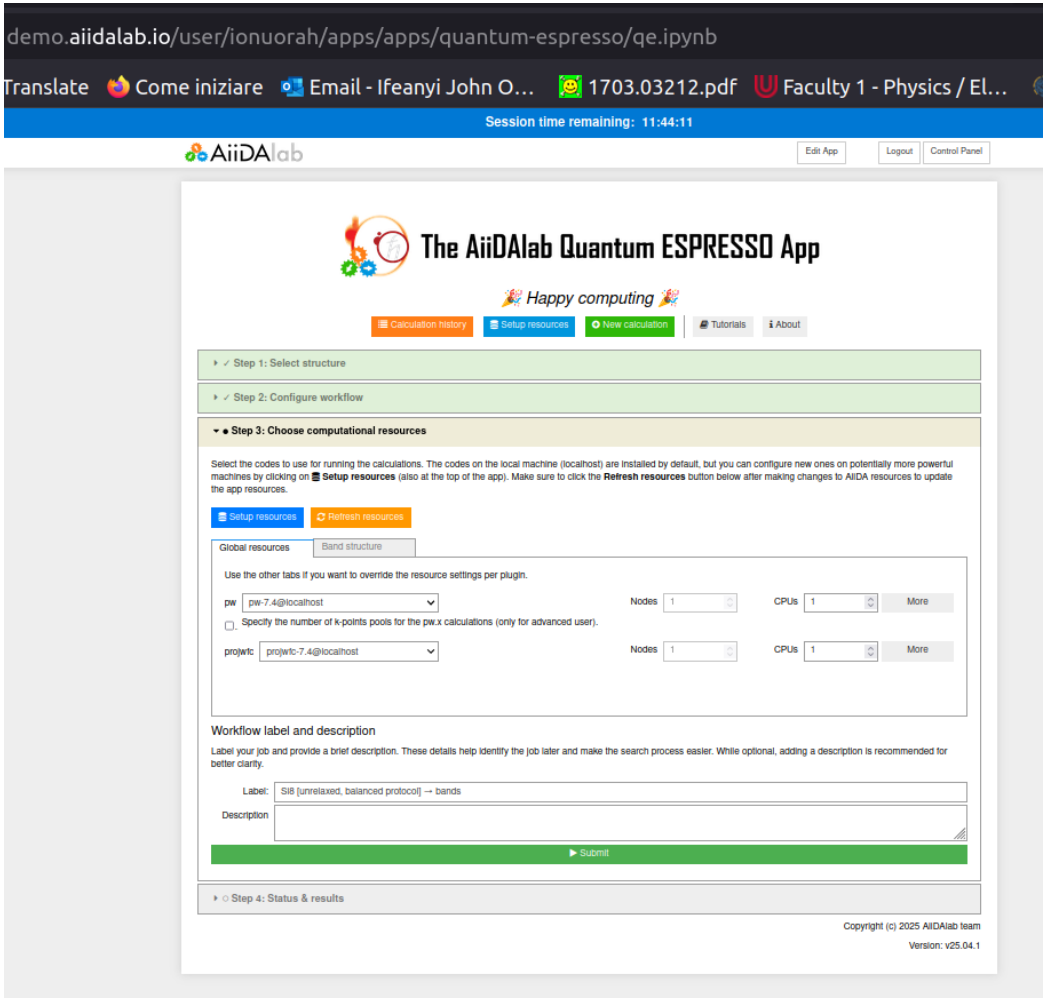


- The input parameters are described briefly with each button. However, more detailed documentation can also be accessed by toggling the "**Tutorials**" button at the top of the page on and off. See below



- DFT computing experience might be required to appropriately tune the input parameters. However for the purpose of this tutorial and mostly for all DFT+μ calculations. The default values at the "**balanced**" protocol are sufficient.

CPU resources



- Always use default, only 1 cpu is enabled in the demo-version.
- To continue with the calculation and run the job, click on “**Submit**”
- This opens the “**Status and result**” page

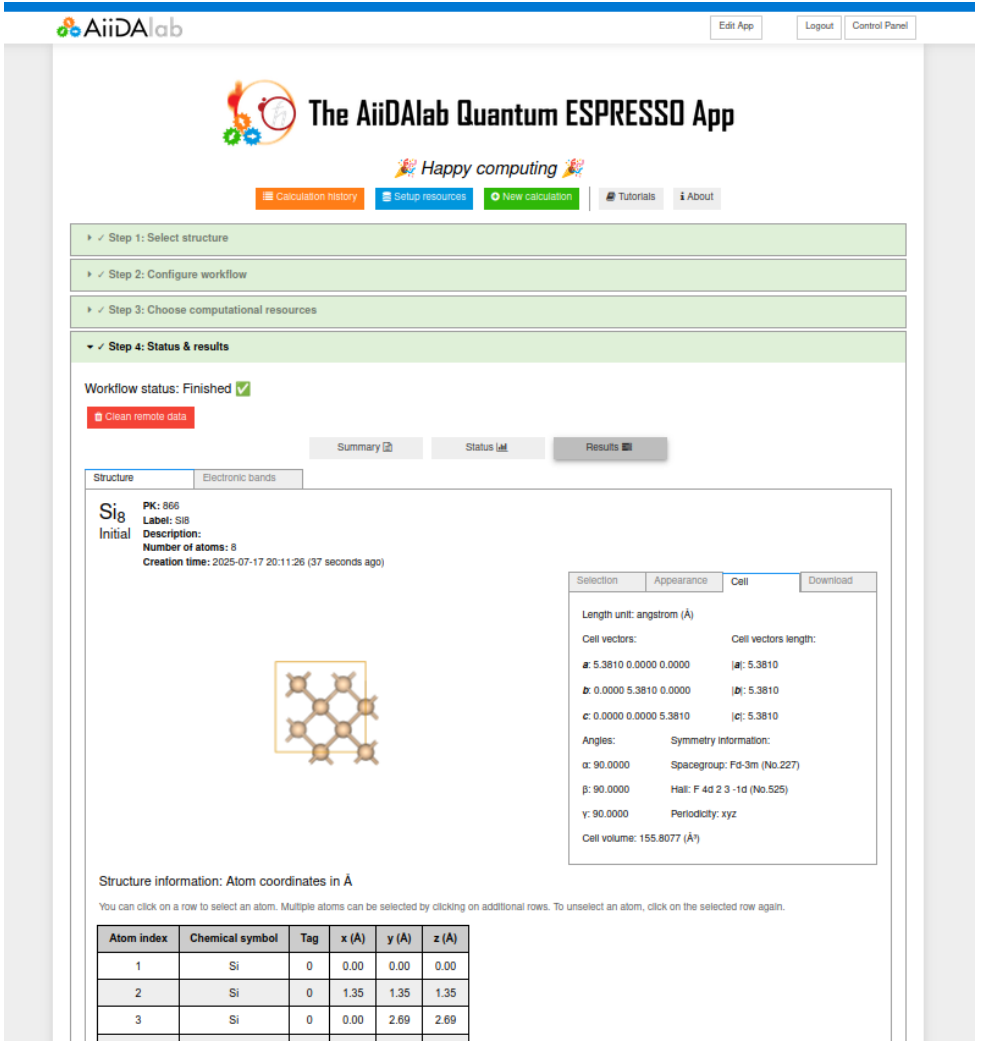
Calculation Status

- The status of the calculation is “**running**”
- Takes around 4 minutes to complete the calculation. Wait!
- At the end of the calculations the status will change to “**finished**”

Calculation Status

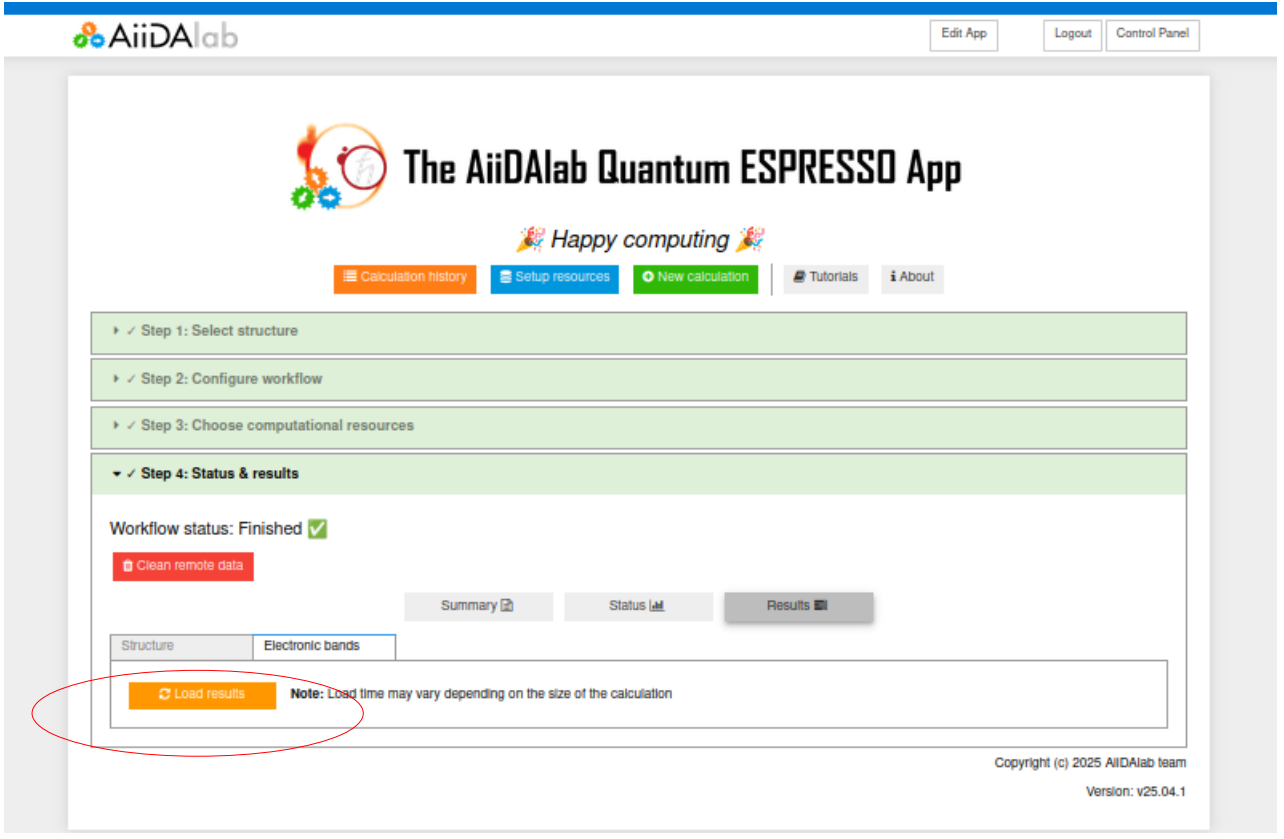
- The status is “**Finished**”
- Notice all menu boxes are now in green colour
- Click on the “**Result**” tab to see the structure and bands

Results



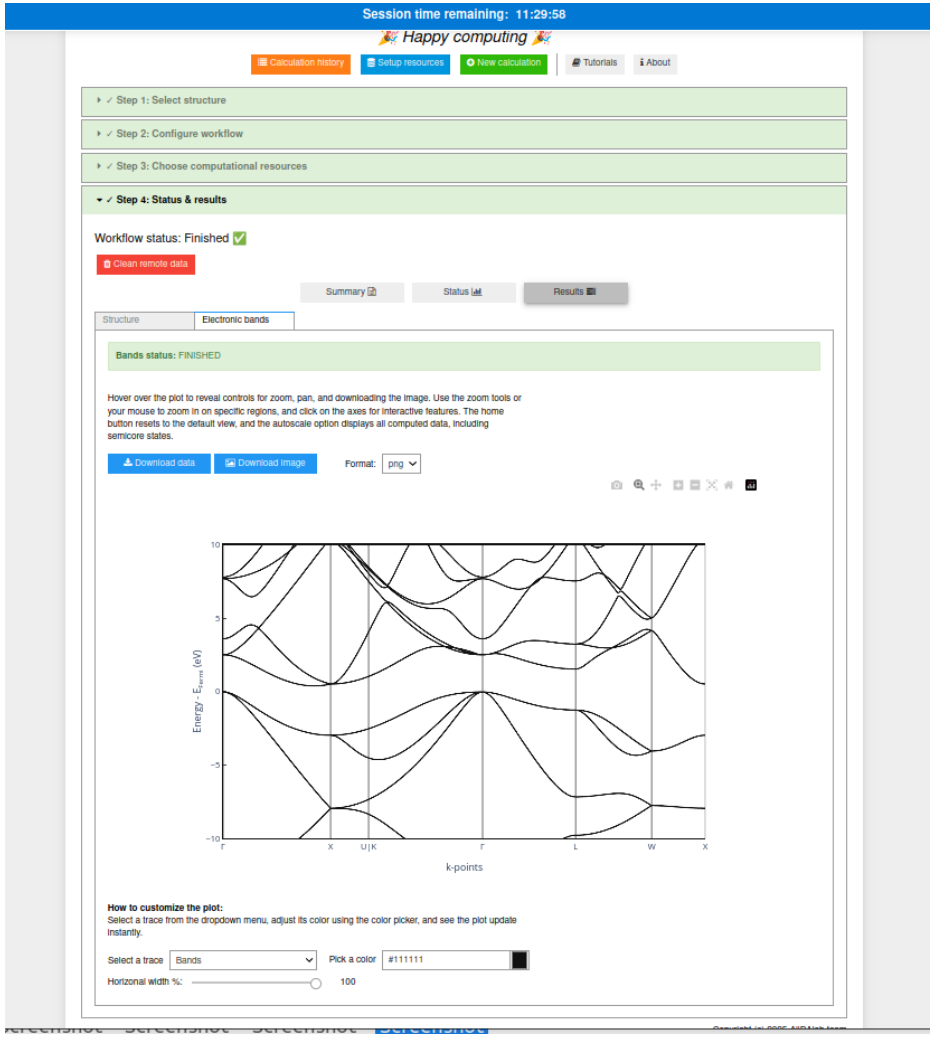
- The structure used for the calculations is displayed
- Click on the “**Electronic bands**” tab to see the band

Check and load “electronic band” results



- Click on “**load results**”

Visualize the Si electronic band



- Observe the band gap. The Fermi energy is at 0 (y-axis)
- The number of valence bands
- The end of example 1. By now we have a feel of how to use the app for calculations.

DFT+μ calculations

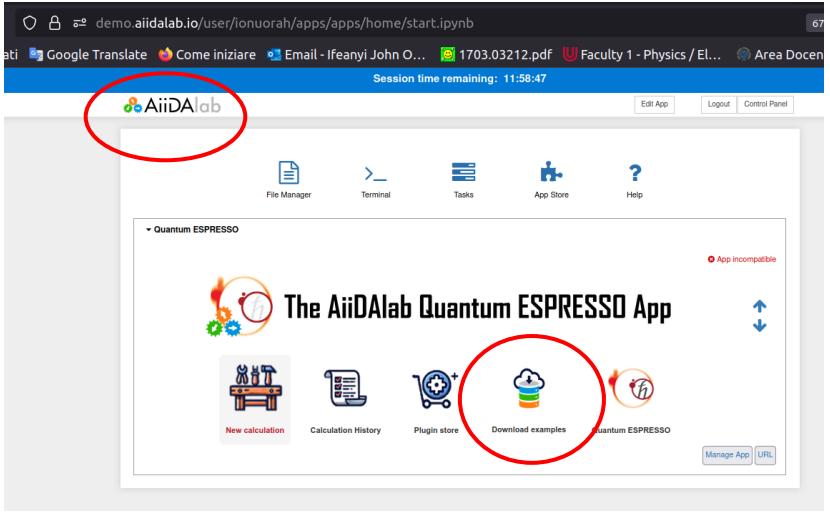
DFT+μ calculations

- Computationally intensive (large cells), we can't run proper calculations on-time in the demo-version.
- Will take probably more than 9 hours on the demo
- For this example, we will load already computed example, and visualize both the inputs and outputs. **No calculations** will be performed.

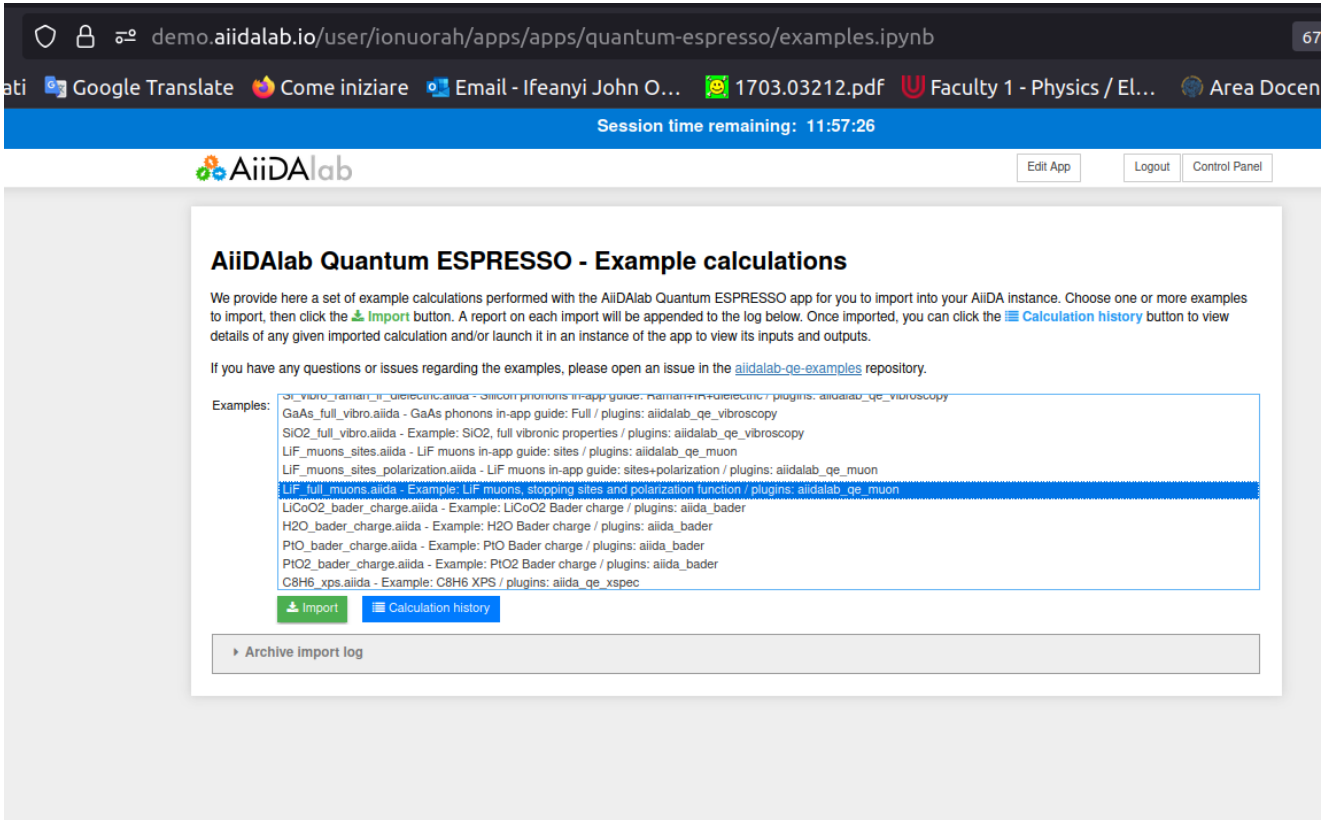
Example 2

Title: "Muon sites and ZF polarization in LiF"

- To return to the start-up page click the "**AiiDalab**" logo on the top left of the page
- And then accept to "**leave page**"
- From the start-up page click "**Download examples**"

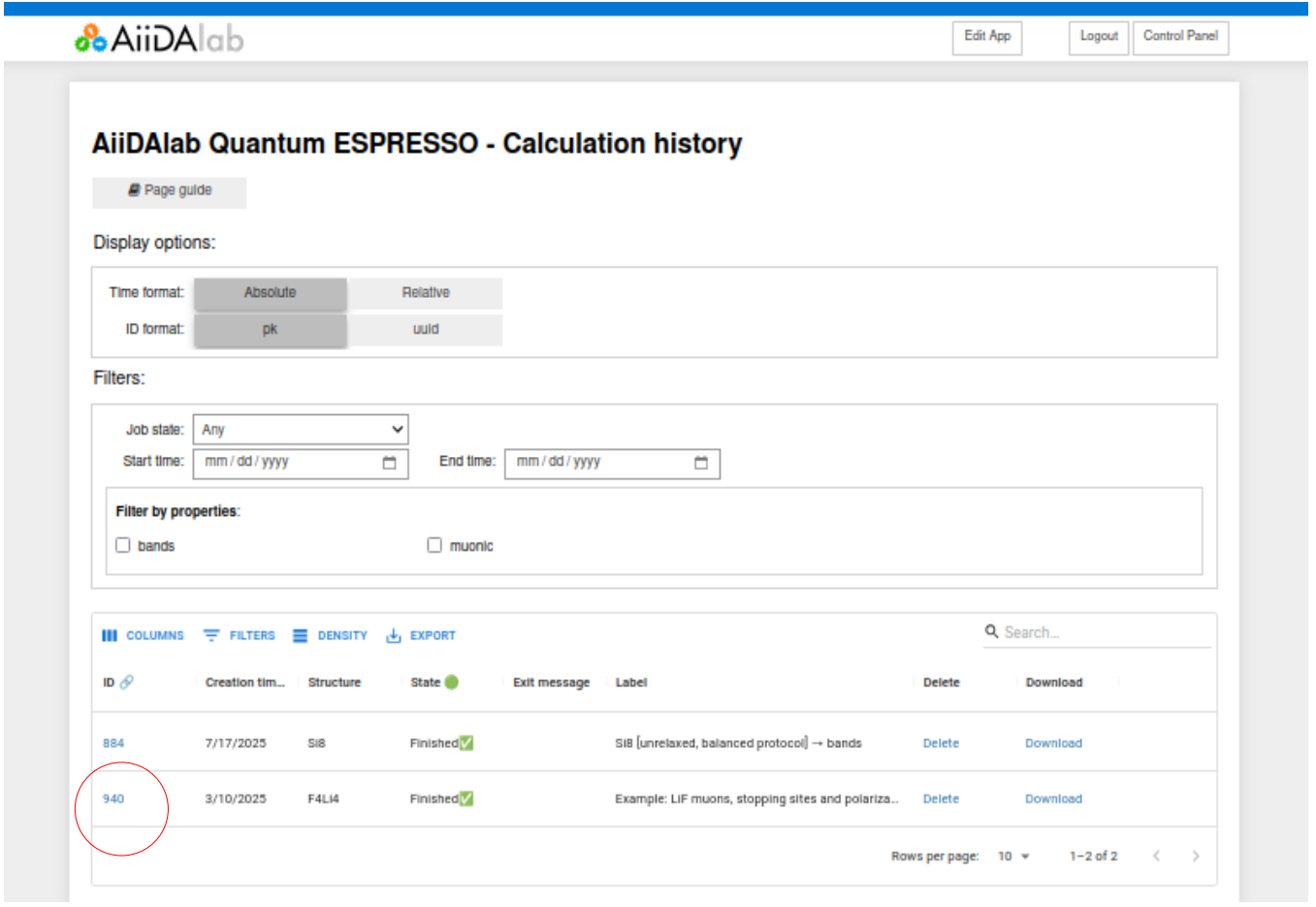


Select LiF example



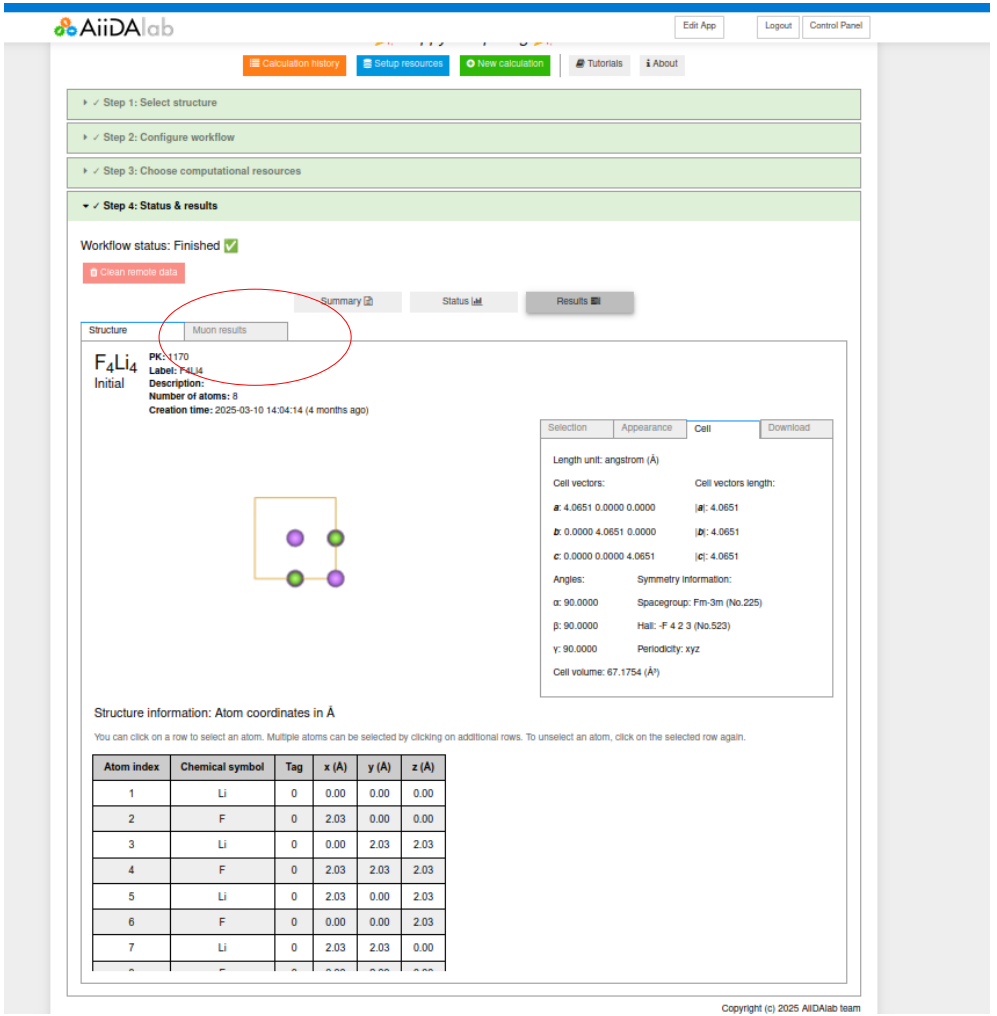
- Select the same highlighted LiF calculations.
- Click on “Import”
- Allow to load
- Then Click on the “**calculation history**” to see the list of calculations.

Calculation history



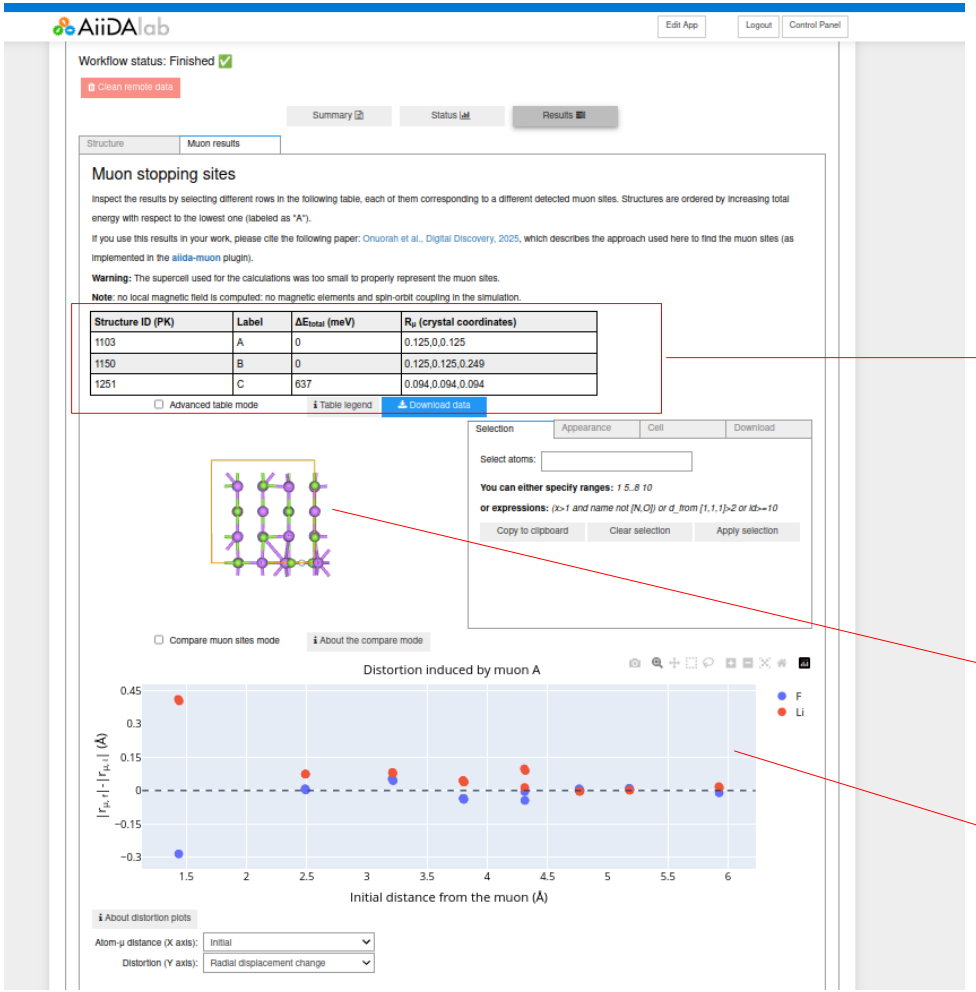
- Click on the LiF job number to load the (F4Li4) calculations.
- This will open, the results (“structure”) tab of the LiF calculations. See next slide

Pre-loaded DFT+μ calculations for LiF: “Results”



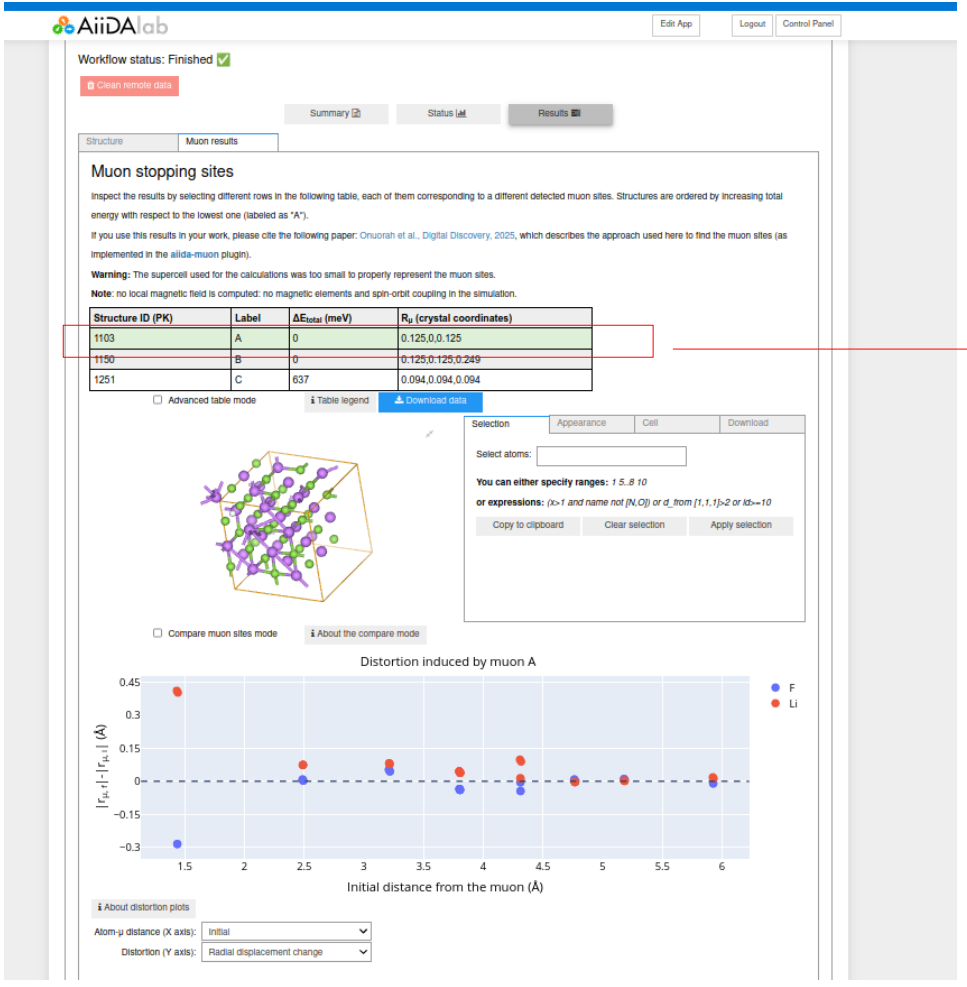
- Immediately, we can see the four task bars all in “green”, signifying that all the steps of the calculations are completed.
- The current open page is the “Result” → “structure” tab. This shows the LiF structure used as input to start the muon calculations.
- To visualize the muon results click on the “**Muon results**” tab

Muon sites in LiF results(1)



- In this slide and the next 3, tips on understanding the results are provided. No action is required before continuing the exercise.
- This tabulates the muon site positions obtained from the calculations. There are 3 sites with label A, B and C. Their relative total energies are given in the third column. Site A and B (so called F-mu-F site) are symmetry equivalent, with lowest energy and true position of the muon. Site C has high energy (mestable), likely not a candidate position.
- The positions in the supercell as well as unitcell can be visualized.
- This plot shows the diplacement distance from equilibrium of the Li and F atomic sites due to the muon. The displacement is largest close to the muon.

Still on muon sites in LiF results(2)

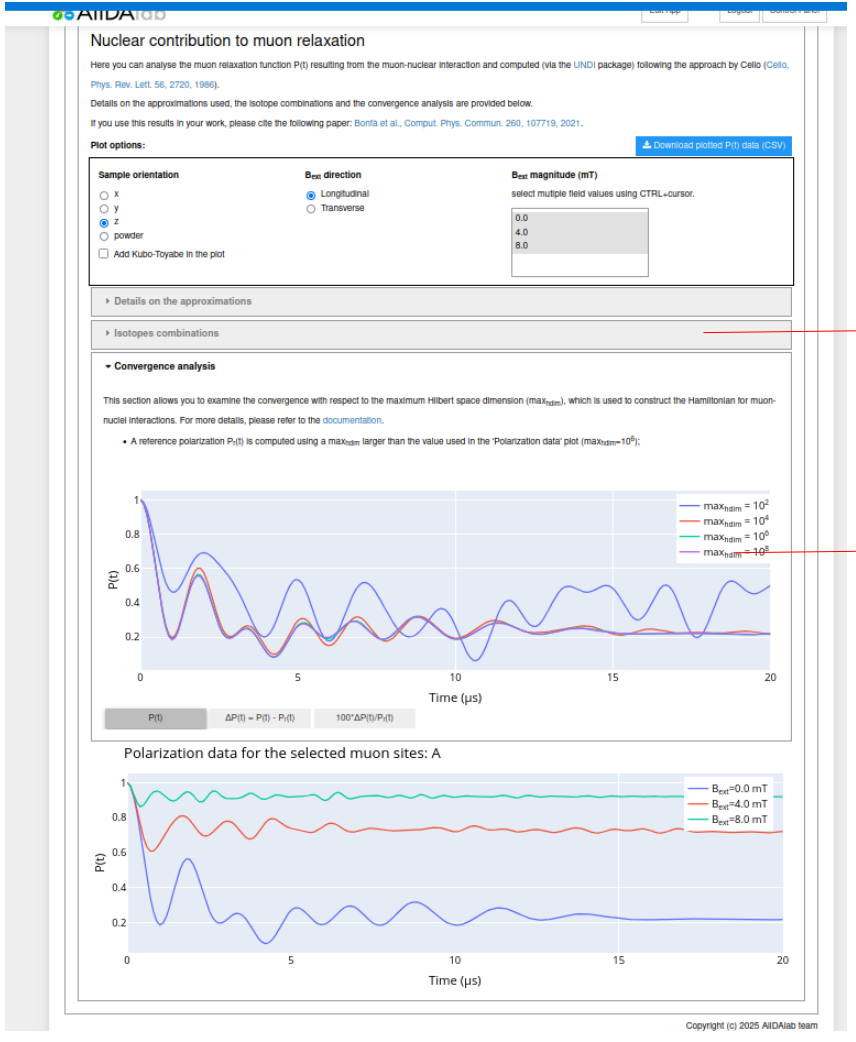


- Here just to say that we can select by clicking on the muon site one after the other (see green line for site A) in the table to access separately its position in the structure and its other properties in the “muon result” tab.

Still on muon sites in LiF results(3)

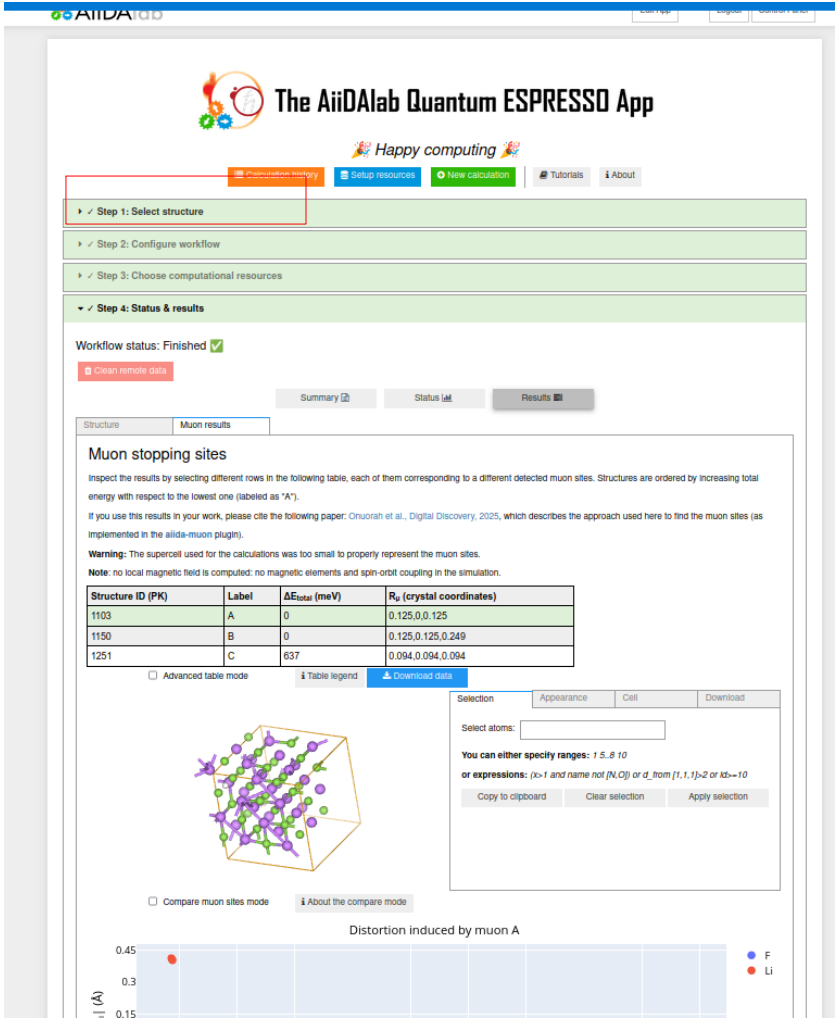
- Also, the “**nuclear contribution to the muon relaxation**” results is shown. The citation of the method utilized is shown in the description or with the lectures on muon relaxation.
- The plot of the muon polarization from the nuclear contribution at zero field and applied field.
- Use this box to change the direction and type of field desired in the plot.
- Click and open the “convergence analysis” drop-down tab to see the convergence of the simulation against the size of the Hilbert space used for the calculations. See next slide

Still on muon sites in LiF results(4)



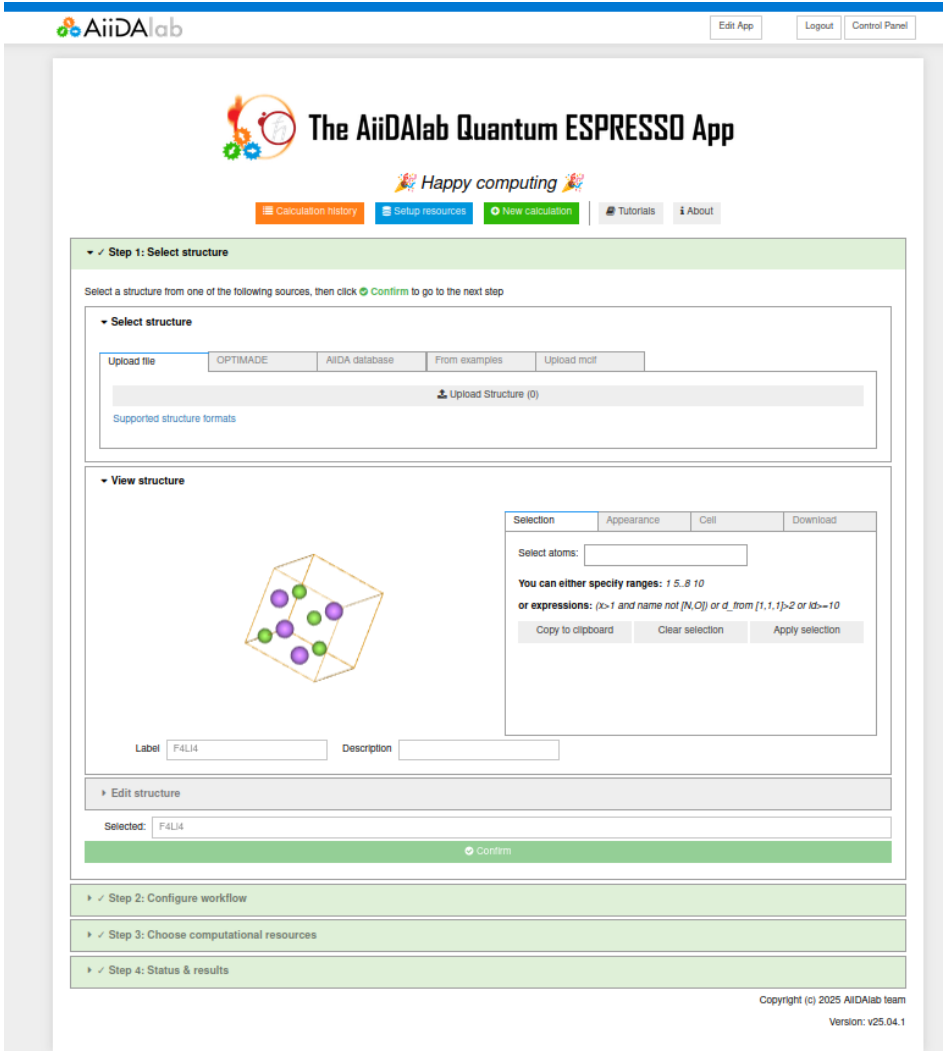
- Click and open to see the isotope combination used for the simulation.
- The convergence analysis plot.

Still on muon sites in LiF results(5) and visualize input structure



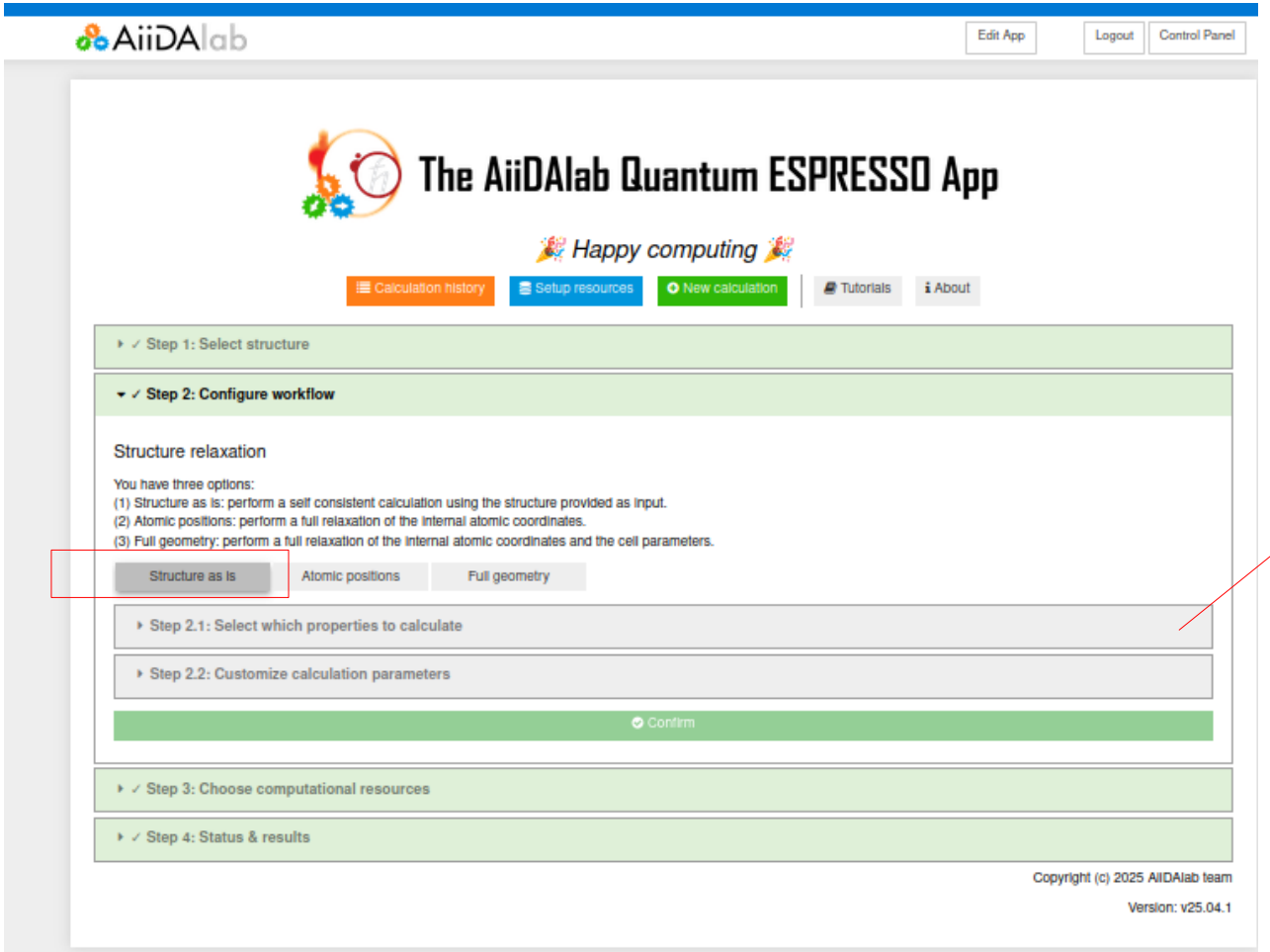
- On the muon results tab scroll all the way up
- To access the inputs of the calculation and visualize the starting structure click on "**Select structure**" drop-down tab

Select Structure Menu



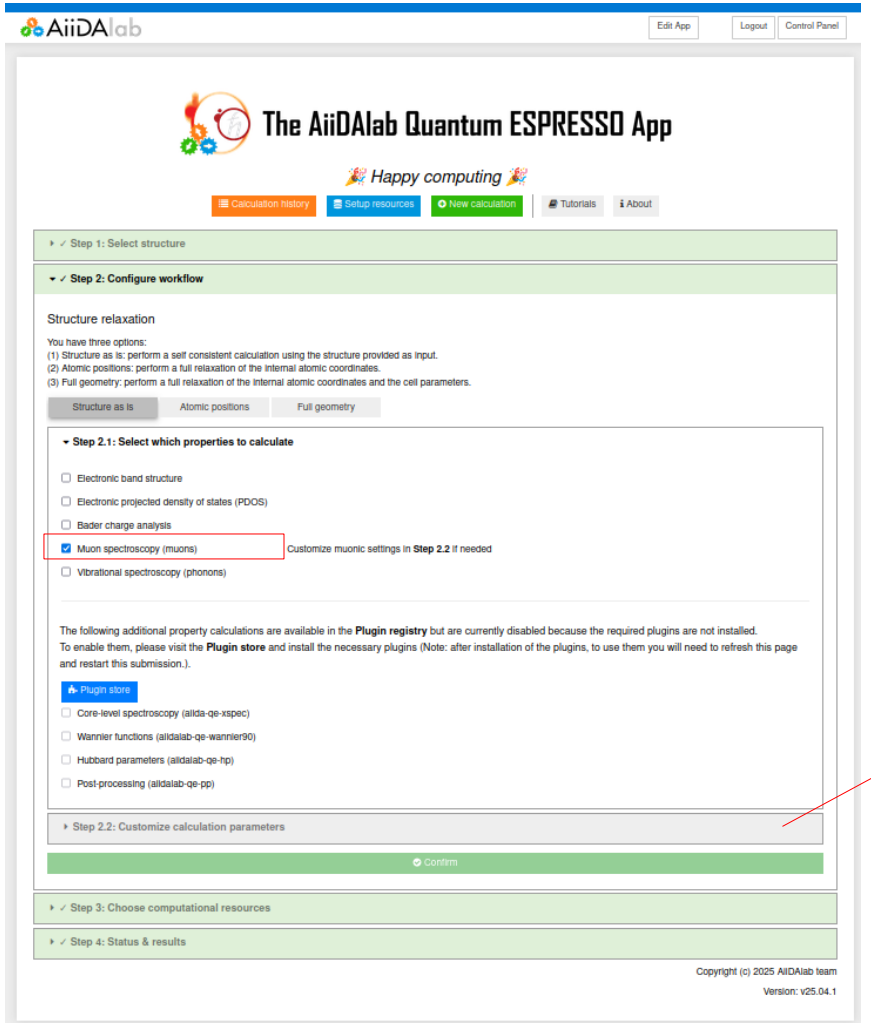
- Visualize the structure
- A LiF cif file was uploaded to start the calculations.
- Notice that the “confirm” button is disabled, showing that it is a calculation loaded from the history.
- To see the settings used for the calculation click on “**Configure workflow**” drop-down menu.

Configure Workflow



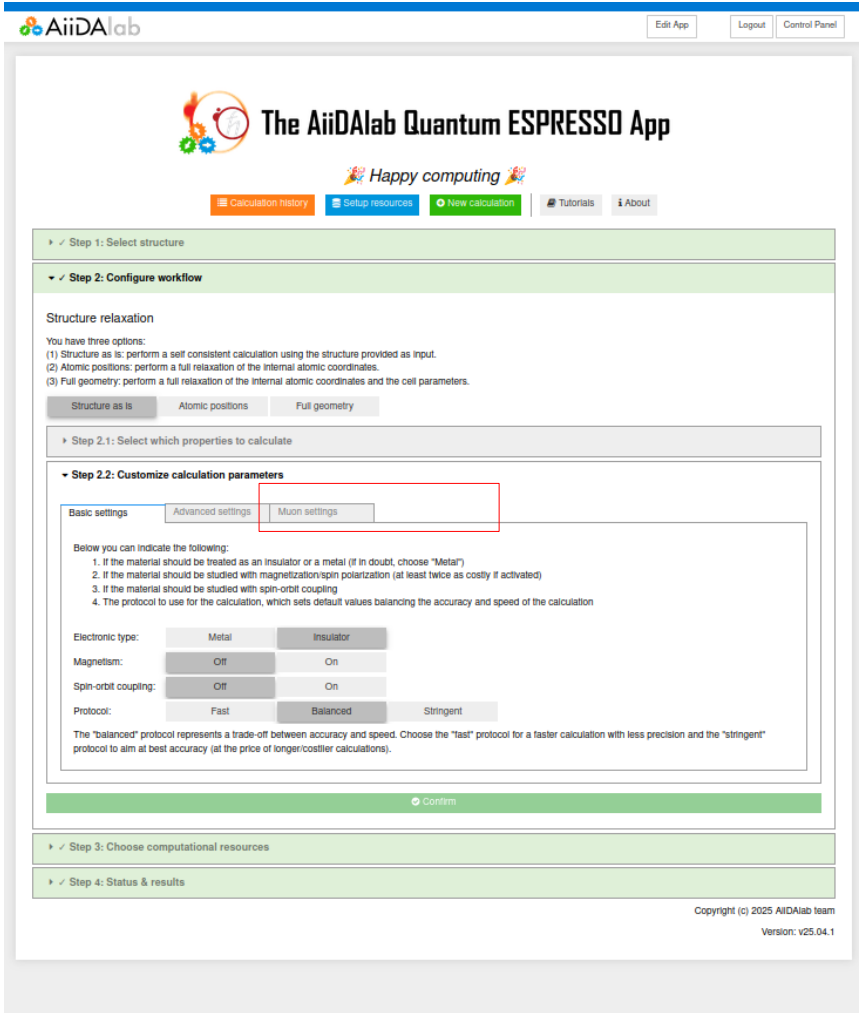
- With the “Structure as it is” the input structure was not relaxed here, this is because it was relaxed later with the DFT+μ calculations.
- Click on “**Select which properties to calculate**”

Select which properties to calculate



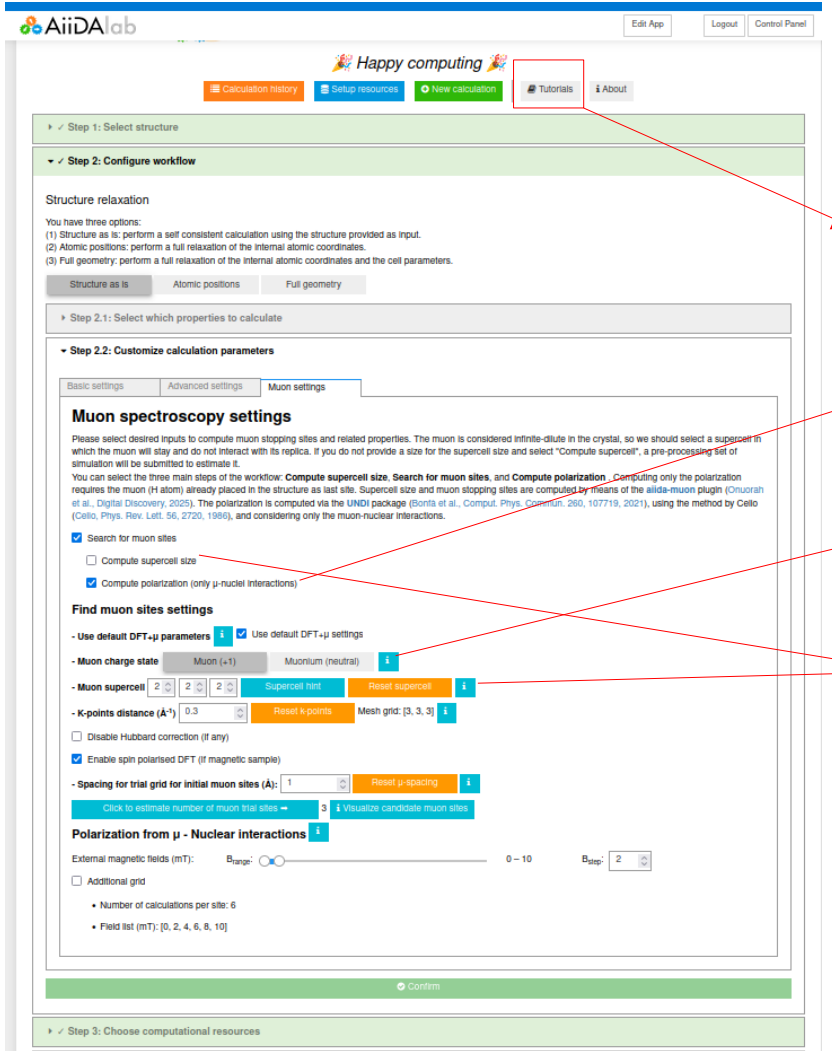
- The “Muon spectroscopy (muons)” was selected to perform the DFT+μ calculations.
- To access the input settings used for the muon calculation click on “**Customize calculation parameters**”

Customize Calculation parameters



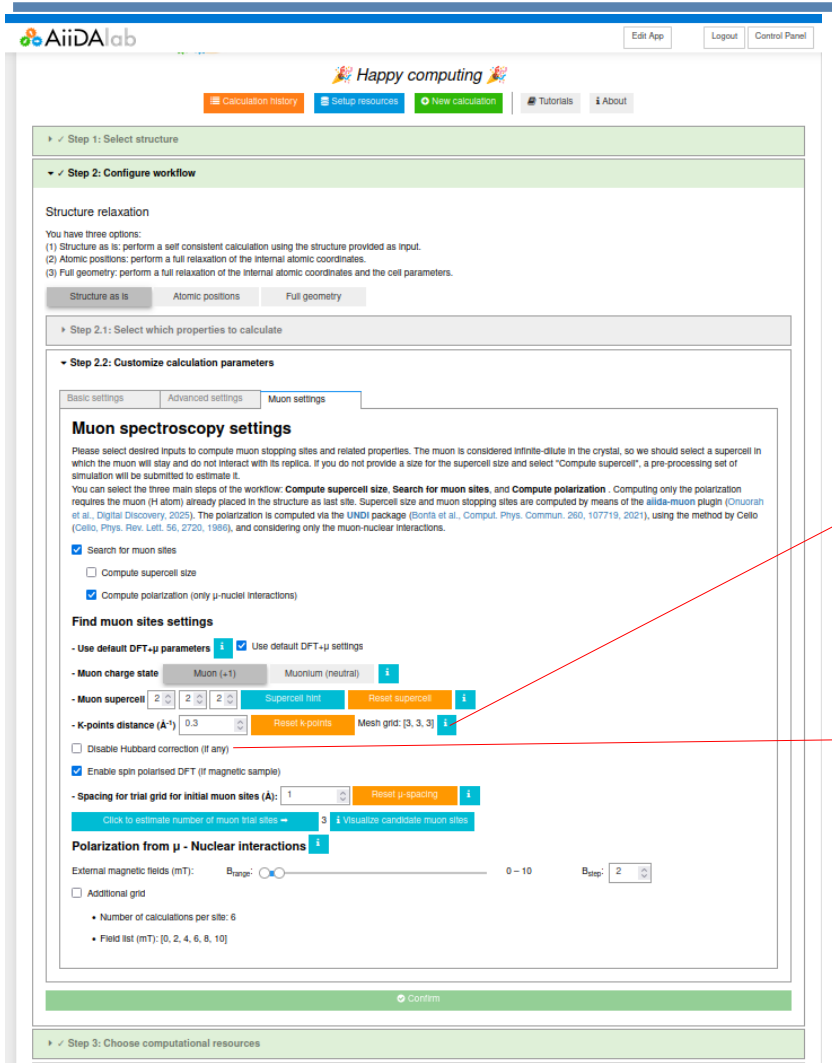
- The settings in this tab should be familiar with the Si example above. However, there is a new tab "**Muon settings**" that comes on with activating the muon calculations.
- **Note:** For DFT+μ calculations, the default for the basic and advanced settings can always be used, any required specific input settings will be overriden in the "**Muon settings**"
- Click on the "**Muon settings**" tab

Muon settings (1)



- This tab contains settings for DFT+μ calculations. Most of the input settings should be familiar from the lecture. In this page and the next 2 pages, we go through it once again.
- Toggling the tutorial button on/off provides more detailed description of the input parameters
- Uncheck this button if you don't want the workflow to compute the nuclear contribution to muon relaxation.
- For selecting the appropriate muon charge state for the calculations.
- **Supercell size**: Remember a large enough cell is required to suppress the impact of the periodic images of the muon in the impurity treatment approach. Appropriate supercell size can be computed automatically with the workflow by checking the "**compute supercell size**" or this can be selected manually e.g a 2x2x2 cell of the unit cell was used for the LiF calculations. Also there is a button in the manual section "**supercell hint**" which when clicked, suggest supercell size.

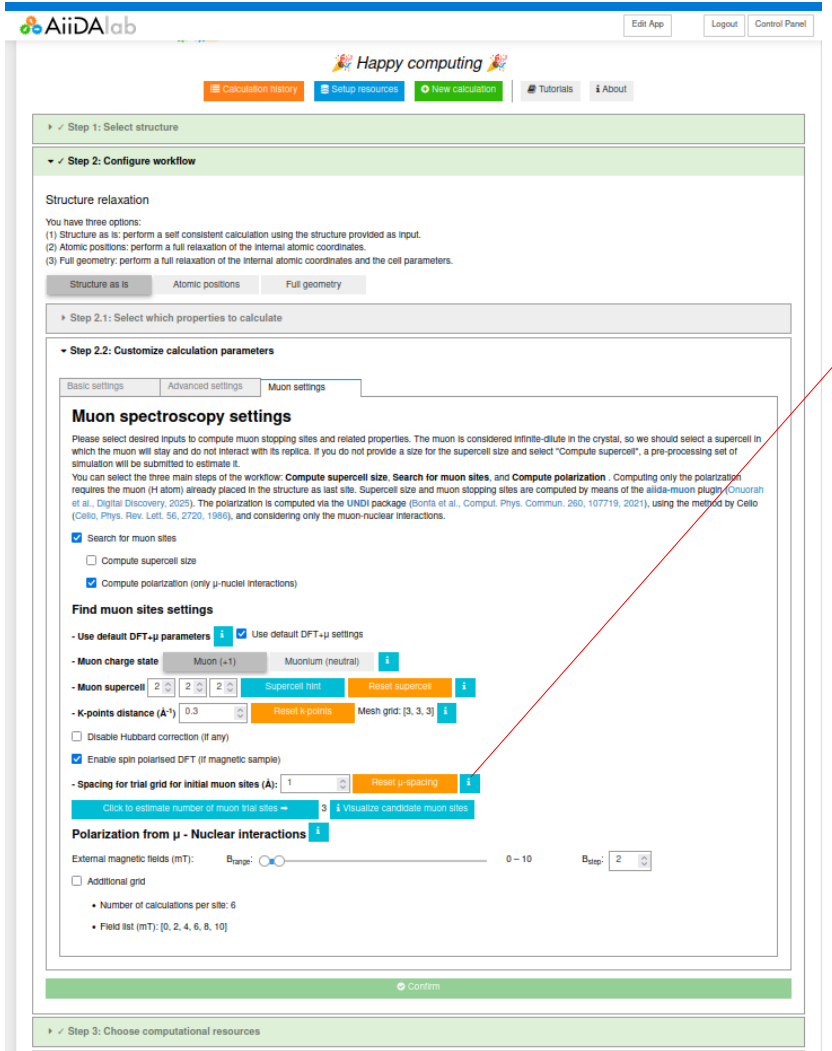
Still on muon settings (2)



- **K-points distance**: This is the spacing that determines the grid of the k-points used for the Brioullion zone integration in solving the Kohn-Sham equations.

- The correction of the conventional DFT energies in strongly correlated electron systems with the Hubbard formalism is implemented automatically and will be used when required (magnetic samples with more than 1 element and hosts transition metal elements). However, this feature can be turned off by checking the box “ **Disable Hubbard correction (if any)**”.

Still on muon settings (3)



- **Spacing for trlal initial grid**: Remember to start the search for the muon sites, the void in the lattice is sampled and the uniform grid sampling is used. This spacing parameter defines how far the muon is spaced from one another in the grid. Thus it determines the number of initial muon positions and in turn number of supercells to be calculated. Here, spacing parameter value should be chosen ensuring to strike a balance between accuracy of the calculations and available computational resources.

- In all, for the "**muon settings**", except for the supercell size (unless the compute supercell is selected) and the muon charge states, the default input parameters are all sufficient for DFT+μ calculations.

- Next, to the computer resources, click on "**Choose computational resources**"

Computational resources menu

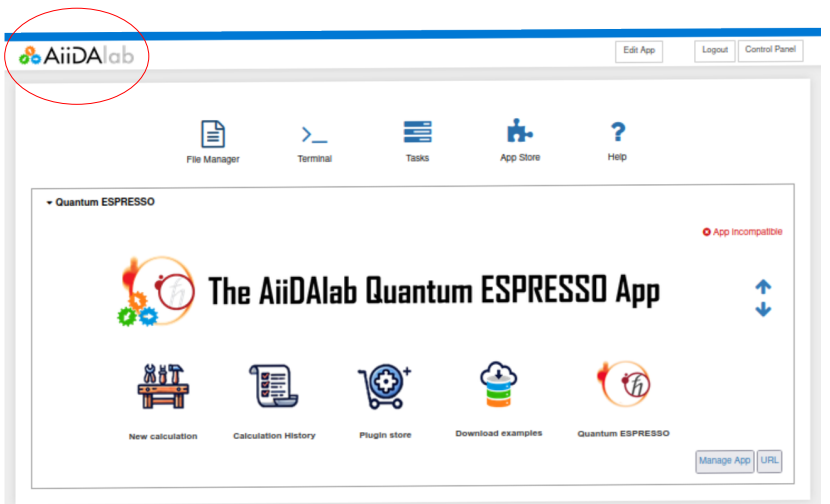
- Here the resources required for the calculation can be set. But remember for this demo only 1 cpu is available.
- The submit button is blocked because it is a calculation from history.
- Notice the error message in red on why this step is blocked. Ignore, as we are not performing the calculations.
- At this point we have seen all the parts of the calculations.
- End of the exercise,

Example 3: Muon sites and local field in magnetic MnF_2

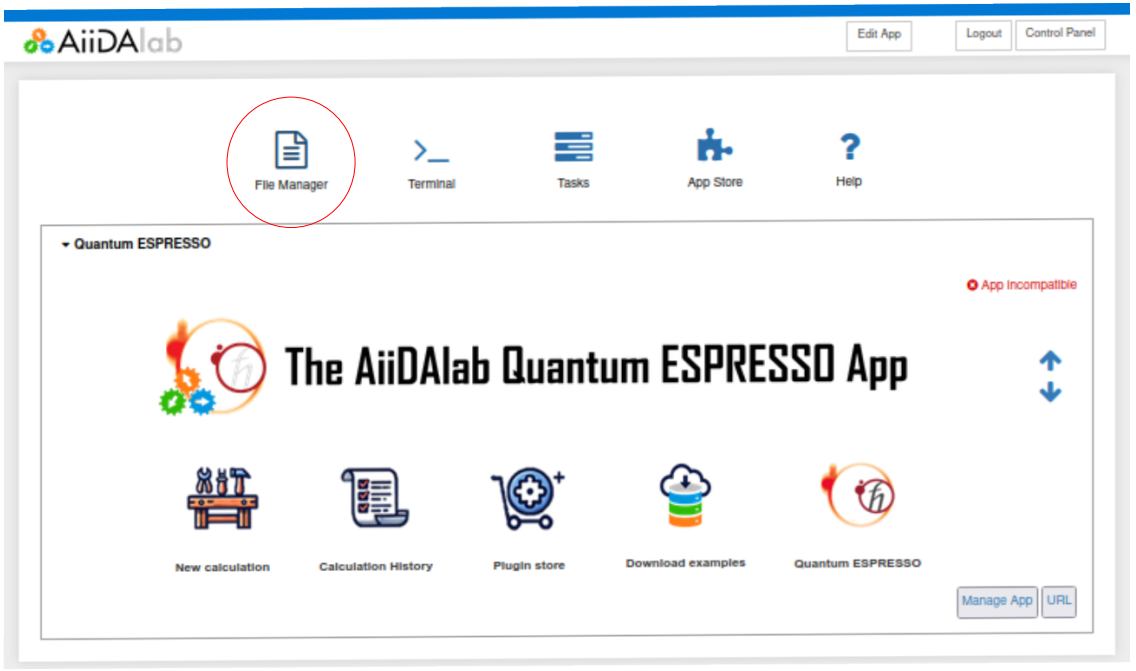
- Here we see an example of DFT+μ calculations in MnF_2. Remember precise (with supercell) DFT+μ calculations is not practical with the demo-version. Hence we will again load from already completed calculation, but in this case the archive data is in the downloaded files.

- This sample is magnetic and such to compute the muon local field contributions ($\mathbf{B}_\mu = \mathbf{B}_{dip} + \mathbf{B}_C$), the description of the magnetic structure (mcif file – see MnF2.mcif in the downloaded files), as well as the muon site(s) are required.

- For this tutorial, return to the start-up page by clicking the “Aiidalab” logo.

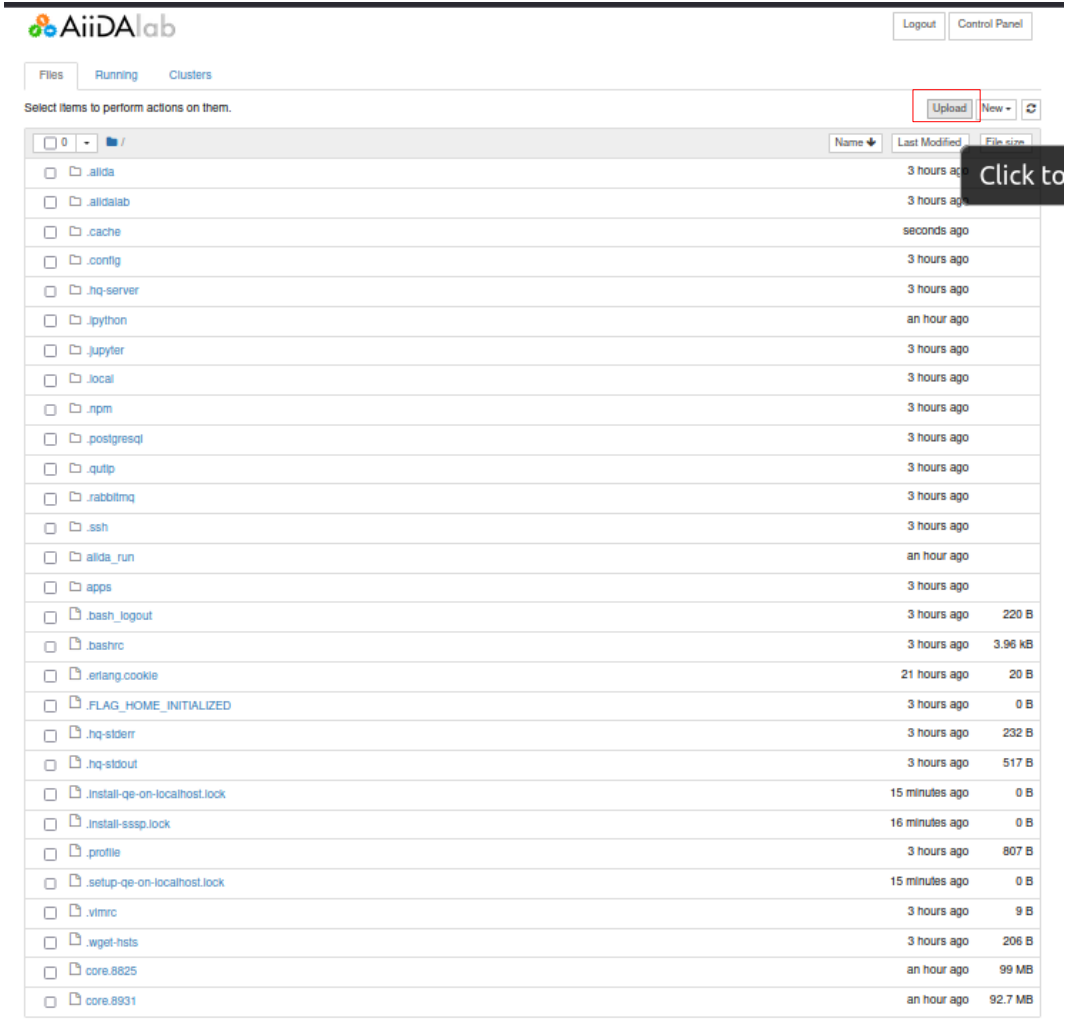


Load the aiida archive data for MnF_2



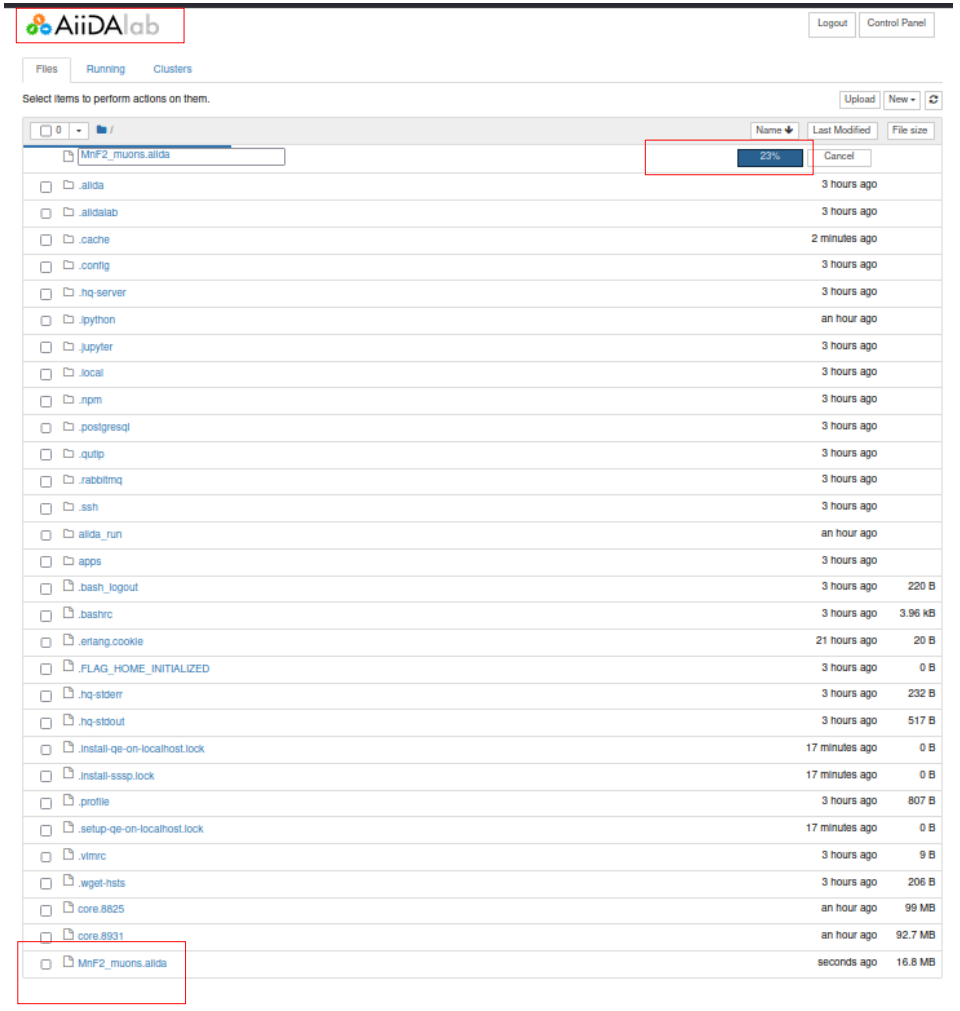
- On the startup page click on "**File manager**"

Load the aiida archive data for MnF_2



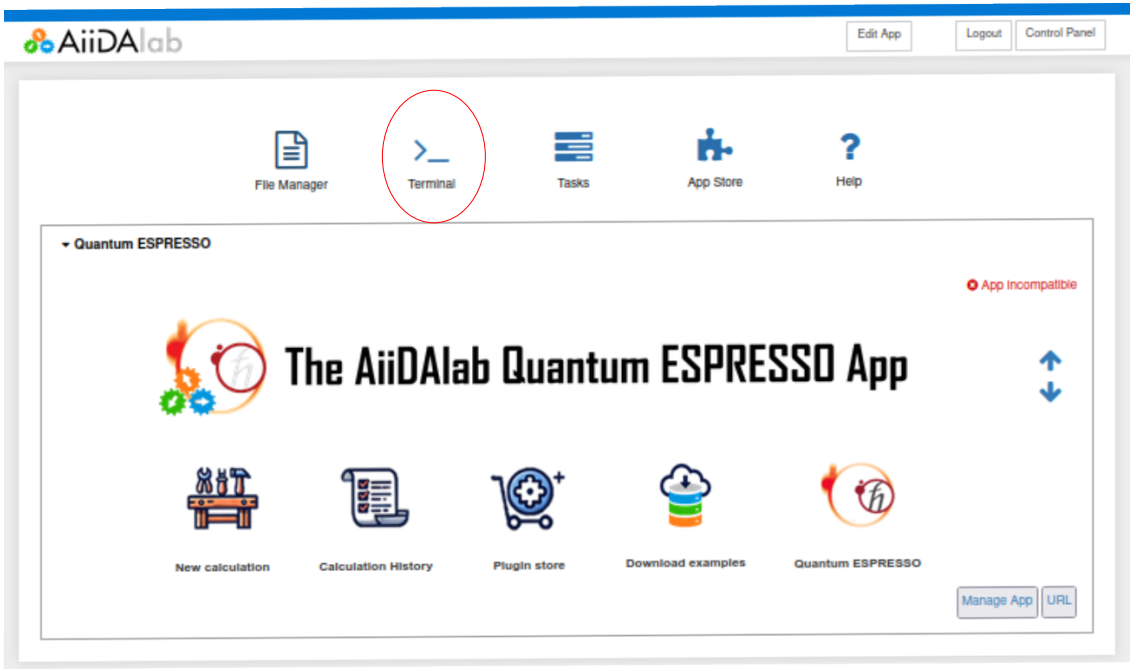
- Upload the zip file “**MnF2_muons.aiida**” that was downloaded at the start of this tutorial by clicking “**upload**”.
- Go to next page for the upload status

Load the aiida archive data for MnF_2



- It will complain of file size but, still click "**ok**".
- This takes few minutes but you can always see the upload status percentage bar.
- At the end of the upload, you should be able to see the file "**MnF2_muons.aiida**" as last in the list of file
- If this is done, click on the "**Aiidalab**" logo to return to the startup page

Import the MnF_2 data to the calculation history



- Click on the “terminal”
- It will open it on a new tab

Import the MnF_2 data to the calculation history

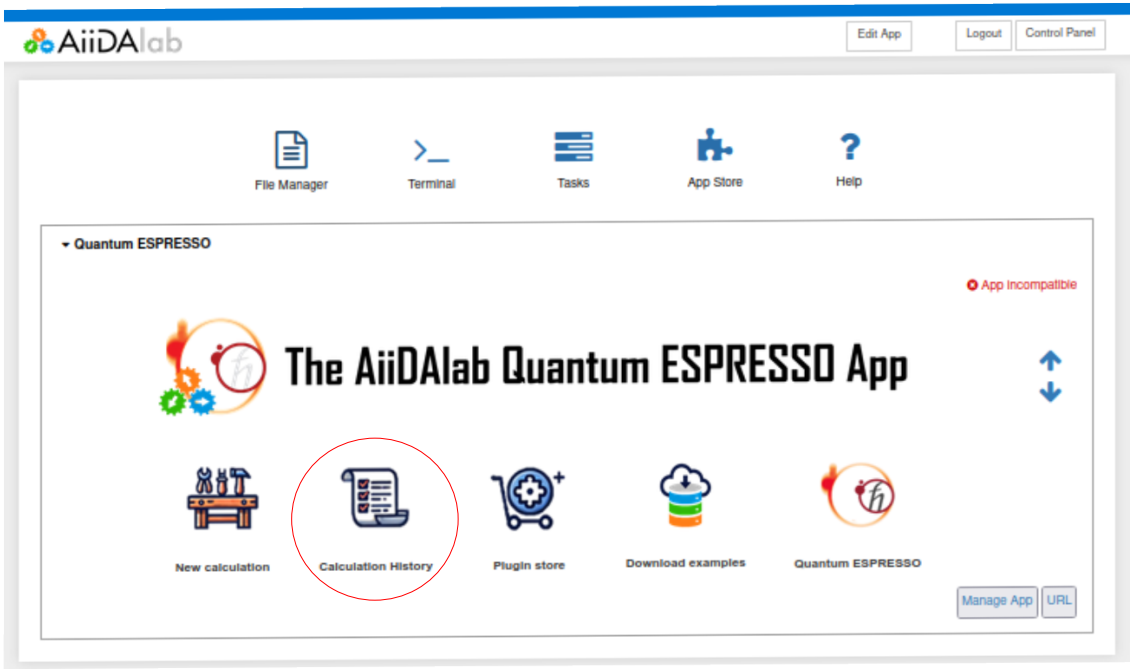
AiiDAlab

```
(base) jovyan@jupyter-ionuorah:~$ verdi archive import MnF2_muons.aiida
```

- On the terminal, type this command "**verdi archive import MnF2_muons.aiida**" and press "**enter**" to import the dataset.
- If successful, your screen will look like below. Then go back to the startup page (click aiidalab logo).

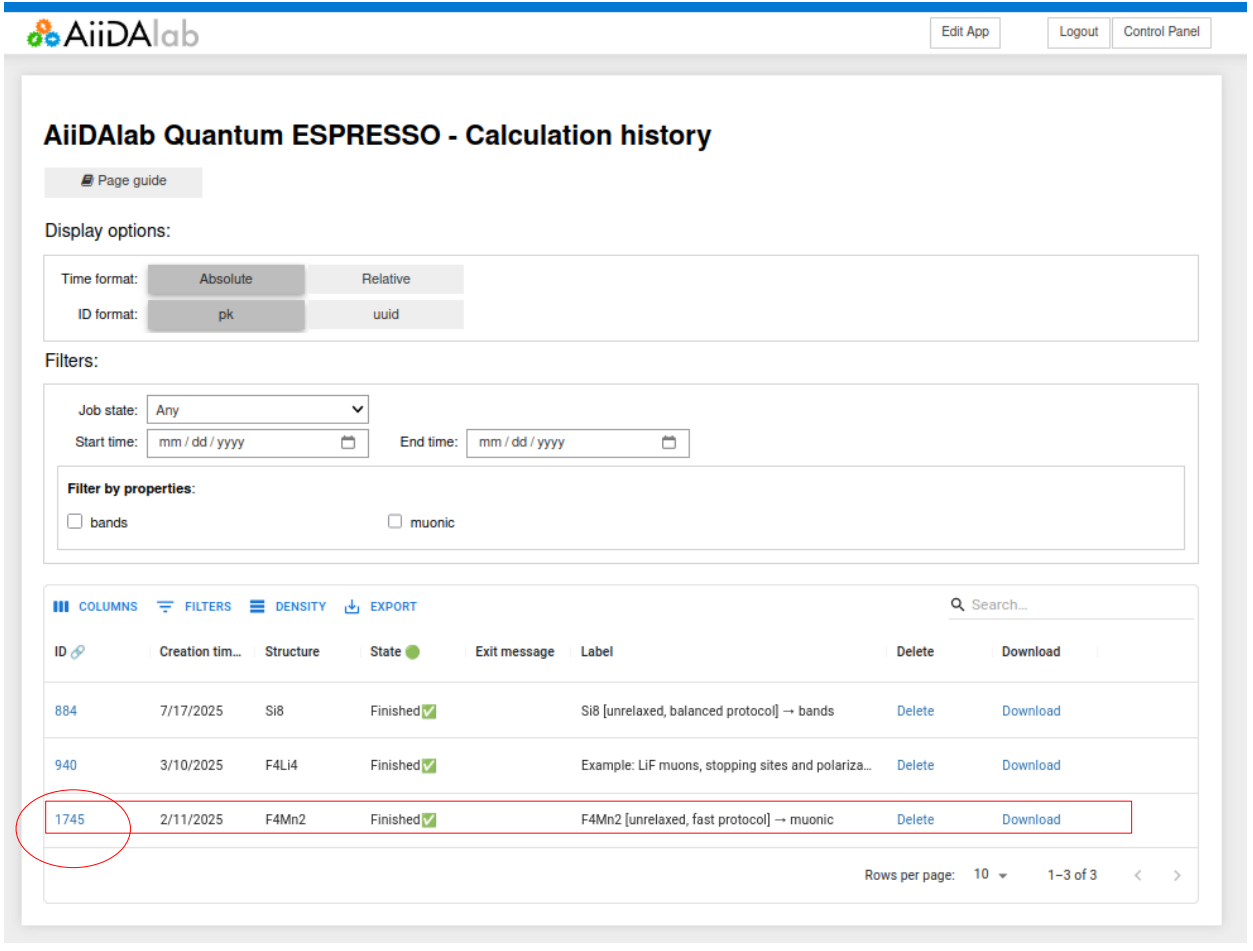
```
(base) jovyan@jupyter-ionuorah:~$ verdi archive import MnF2_muons.aiida
Report: starting import: MnF2_muons.aiida
Report: Parameters
------------------------------  ----------------
Archive                         MnF2_muons.aiida
New Node Extras                 keep
Merge Node Extras (in database)  (k)eep
Merge Node Extras (in archive)   do (n)ot create
Merge Node Extras (in both)      (l)eave existing
Merge Comments                  leave
Computer Authintos              exclude

Report: Skipping 1 existing User(s)
Report: Skipping 1 existing Computer(s)
Report: Adding 1 new computer(s)
Report: Collecting Node(s) ...
Report: Skipping 2 existing Node(s)
Report: Adding 898 new node(s)
Report: Adding 376 new log(s)
Report: Gathering existing 'create' Link(s)
Report: Added 198 new 'create' Link(s)
Report: Gathering existing 'return' Link(s)
Report: Added 177 new 'return' Link(s)
Report: Gathering existing 'input_calc' Link(s)
Report: Added 684 new 'input_calc' Link(s)
Report: Gathering existing 'input_work' Link(s)
Report: Added 594 new 'input_work' Link(s)
Report: Gathering existing 'call_calc' Link(s)
Report: Added 69 new 'call_calc' Link(s)
Report: Gathering existing 'call_work' Link(s)
Report: Added 29 new 'call_work' Link(s)
Report: Created new import Group: PK=18, label=20250717-210751
Report: Checking keys against repository ...
Report: Skipping 10 existing repository files
Report: Adding 538 new repository files
Report: Committing transaction to database...
Success: imported archive MnF2_muons.aiida
(base) jovyan@jupyter-ionuorah:~$
```

Open the calculation history



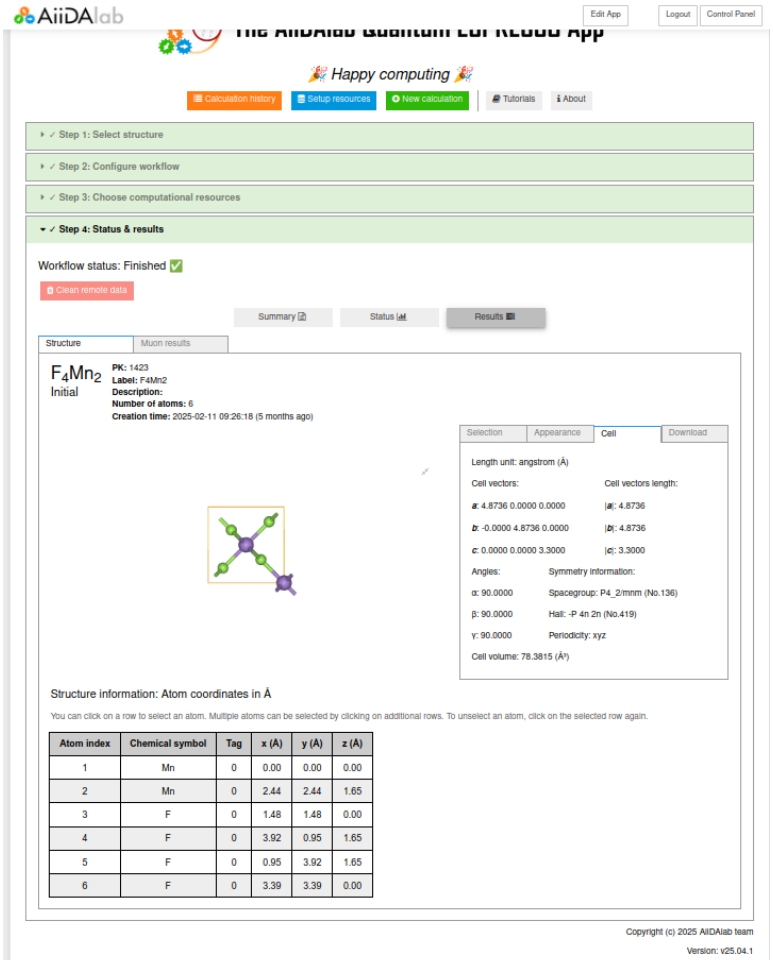
- Click on the “**calculation history**” to open it

The calculation history



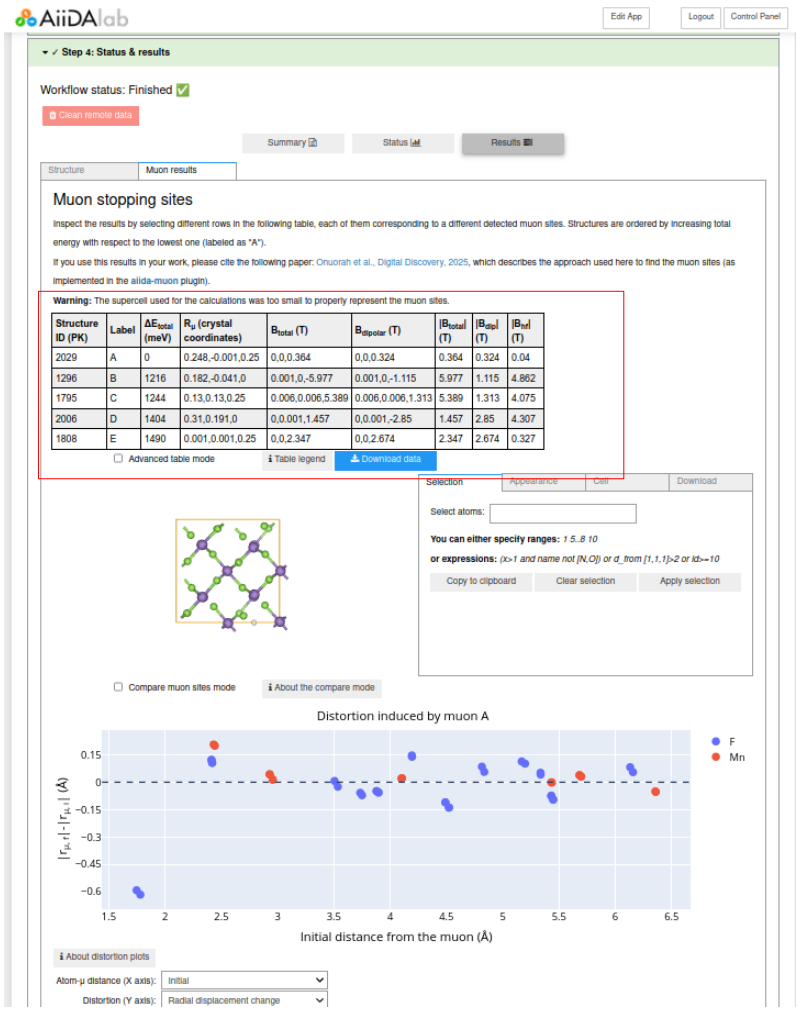
- Now we can see the new MnF_2 data in the history. To open the calculations, click on the calculation ID.
- This will open the Results tab of MnF_2 like we have seen in example-2 for LiF.

MnF_2 loaded calculation data: “Result” tab



- Just like for example 2, click on “**Muon results**” to see the DFT+μ results.

MnF_2 loaded calculation data: “Result” tab

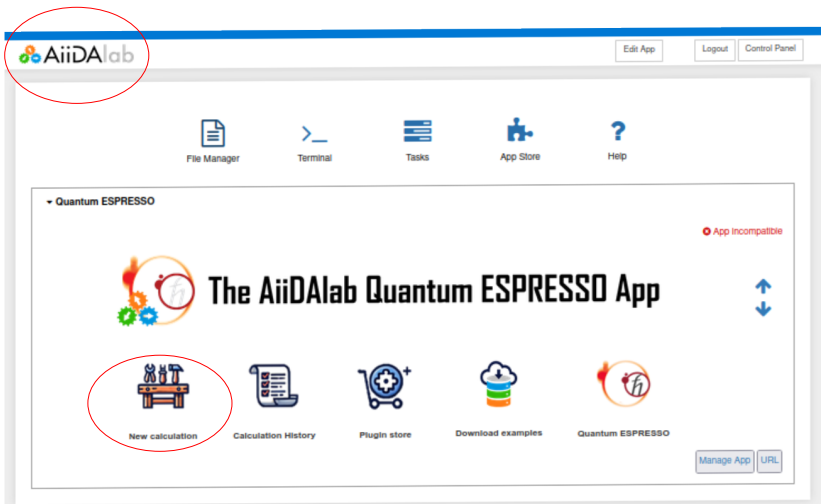


- The different section of the results is like we have seen in example 2 for LiF. In addition, because the sample is magnetic, the muon result table also contains the different contribution of the muon local field.
- E.g, For lowest energy site A (I.e the F-mu-F site), the dipolar contribution is 0.324 T, the contact term is vanishing 0.04 T, while the total is 0.354 T.
- The other sections of the results and inputs are similar as we have seen in example 2.
- **The end** of this exercise.

(Optional) Example 4: Band structure of Fe

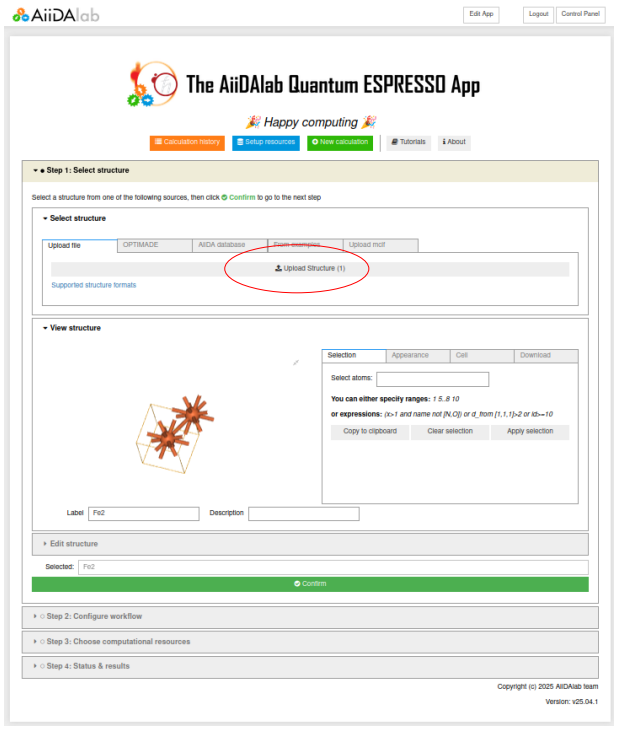
- In this example, the aim is to compare the electronic band structure of Fe assuming a non-magnetic and then a magnetic Fe-bcc sample with DFT calculations.
- To start the calculations return to the start-up page and click on new calculations.

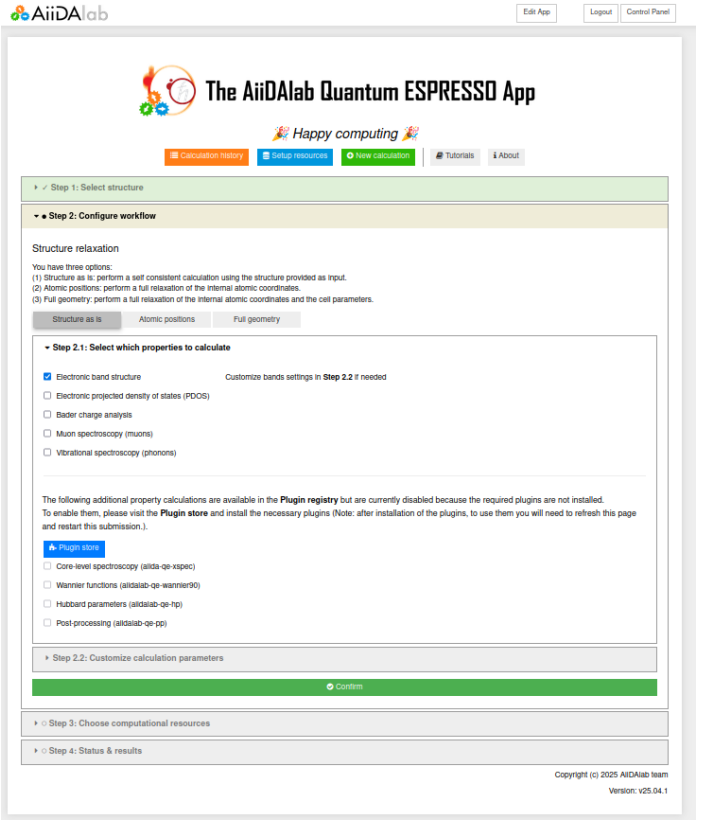
Notes

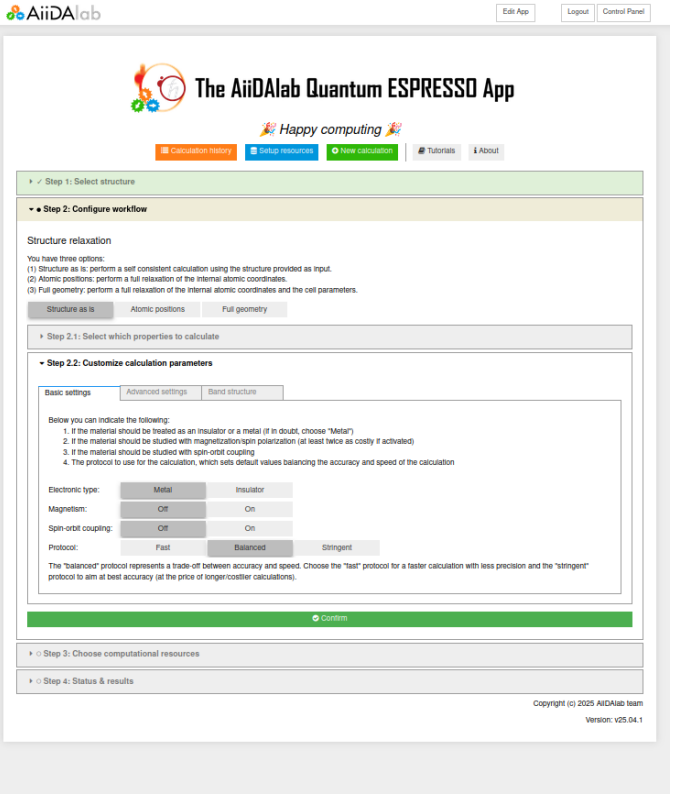


- The steps for the calculations are similar for Si in example 1
- Open two new calculations, one for the non-magnetic Fe and the other for the magnetic Fe. For the input structure use the “Fe_bcc.cif” file from the downloaded files.
- For the **non-magnetic Fe**, the default parameters are used for the calculations while for the **magnetic Fe**, “**magnetism**” has to be turned on in the “**Customize calculation parameters**” → “**Basic settings**” tab.

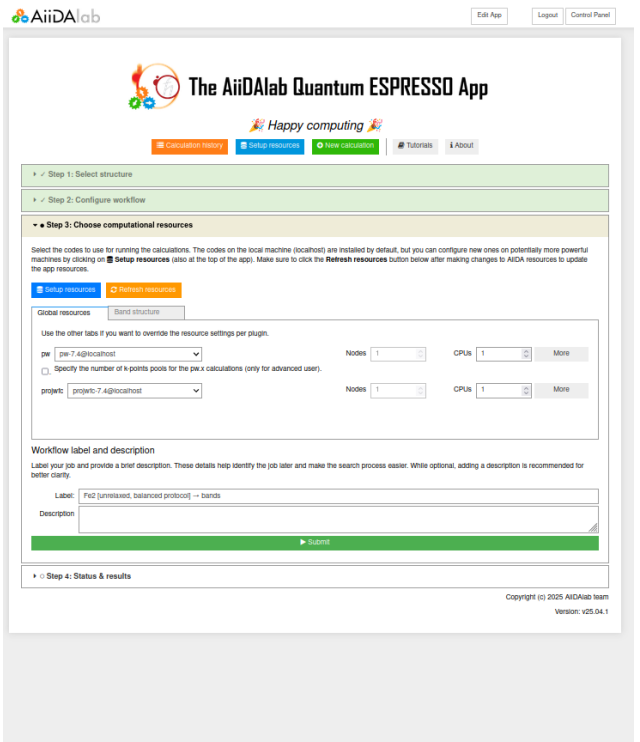
Non-magnetic Fe calculation steps (1)

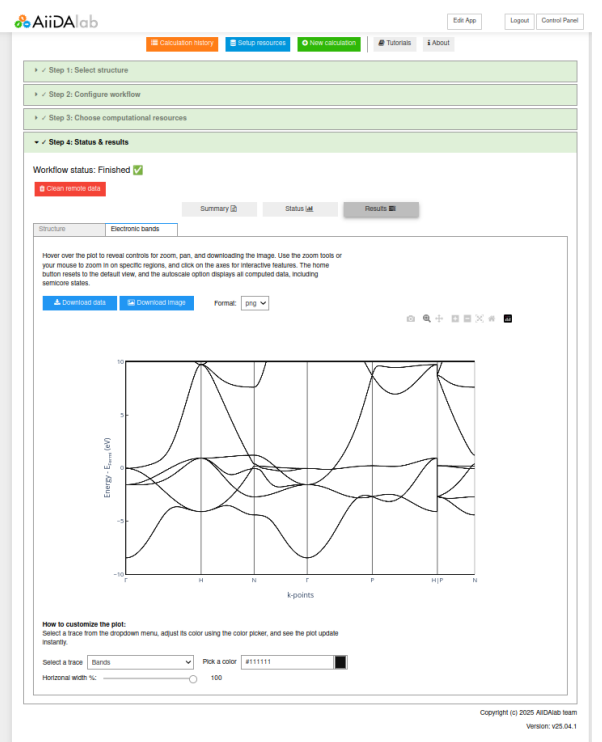






Still on non-magnetic Fe calculation steps (2)

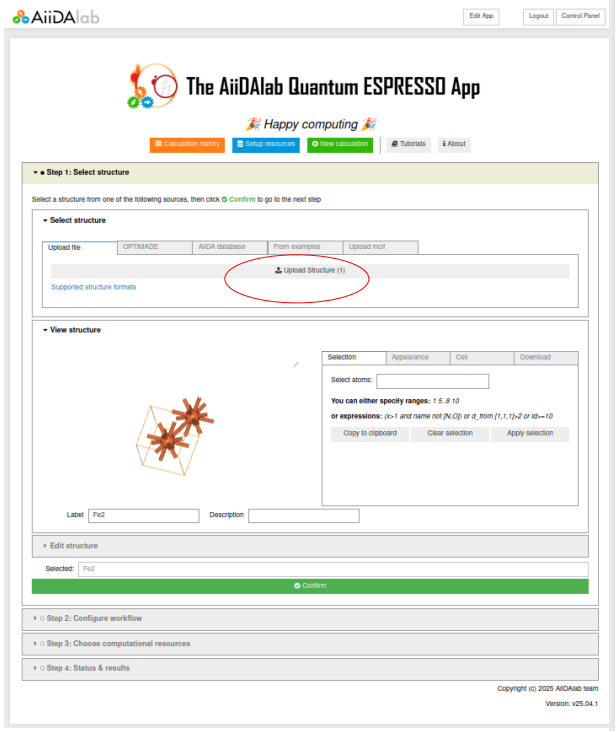


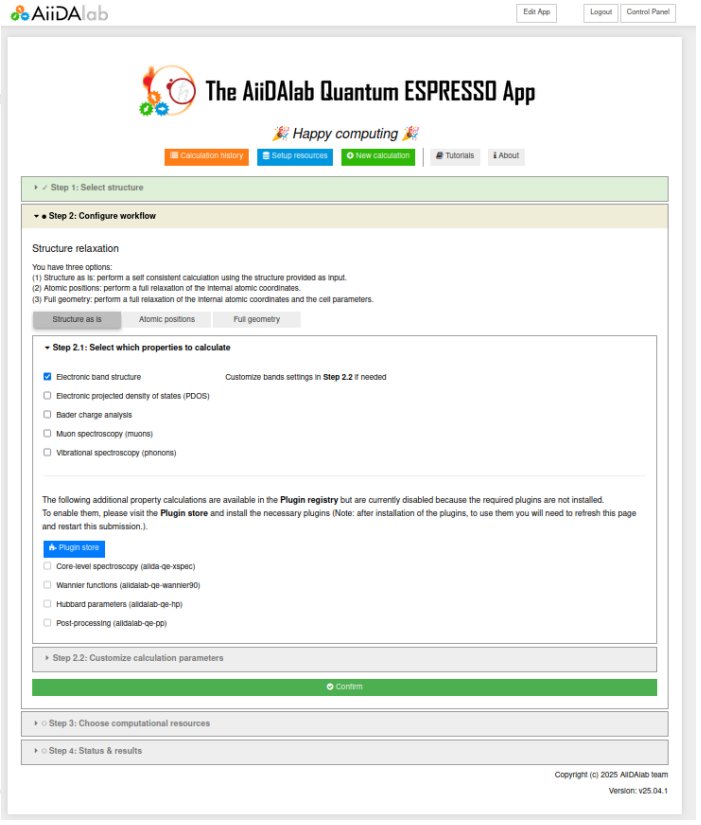


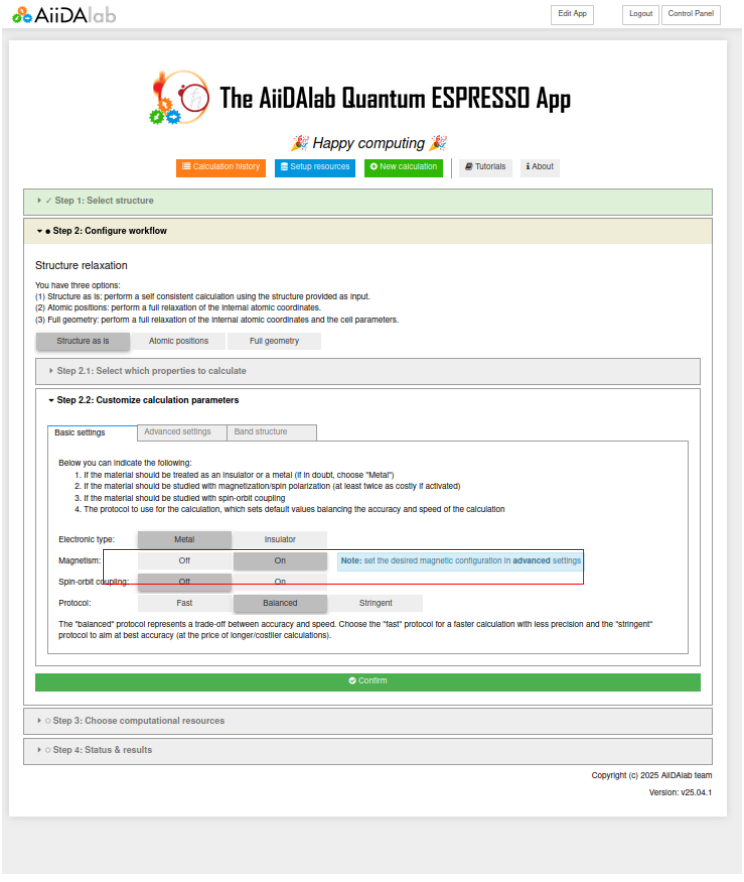
- When the calculations are “Finished”, the results can then be loaded. “Results” → “Electronic band” → “load results”

- The electronic band structure of the non-magnetic Fe. We compare this later with the magnetic case.

Magnetic Fe calculation steps (1)

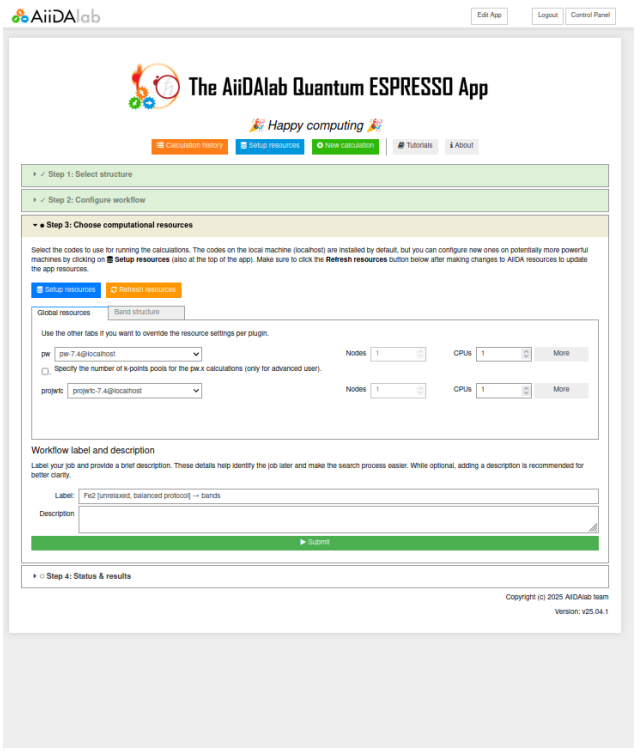


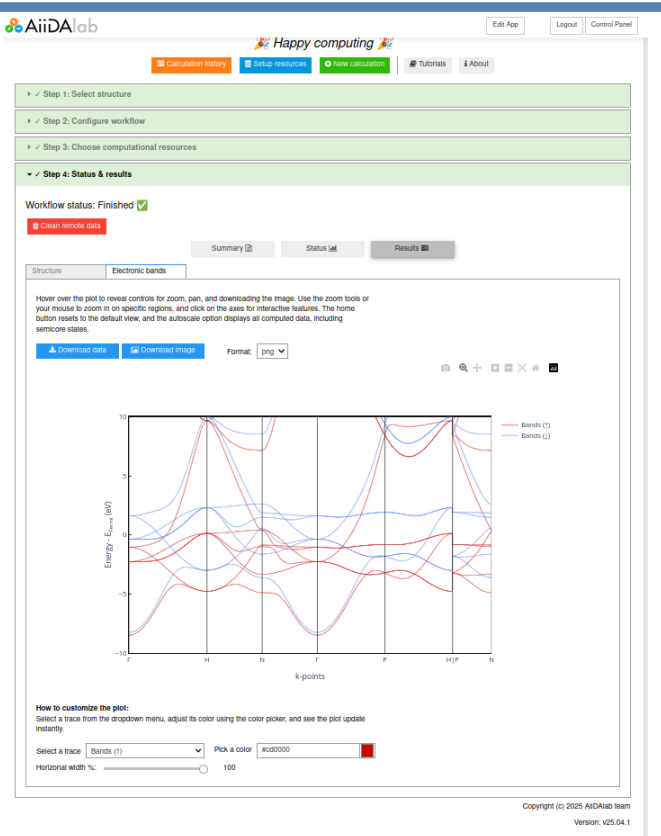




- Note here for the magnetism on. There is a note to set the desired configuration in the advanced settings. Here we use the default, since we desire a ferromagnetic order.

Still on magnetic Fe calculation steps (2)



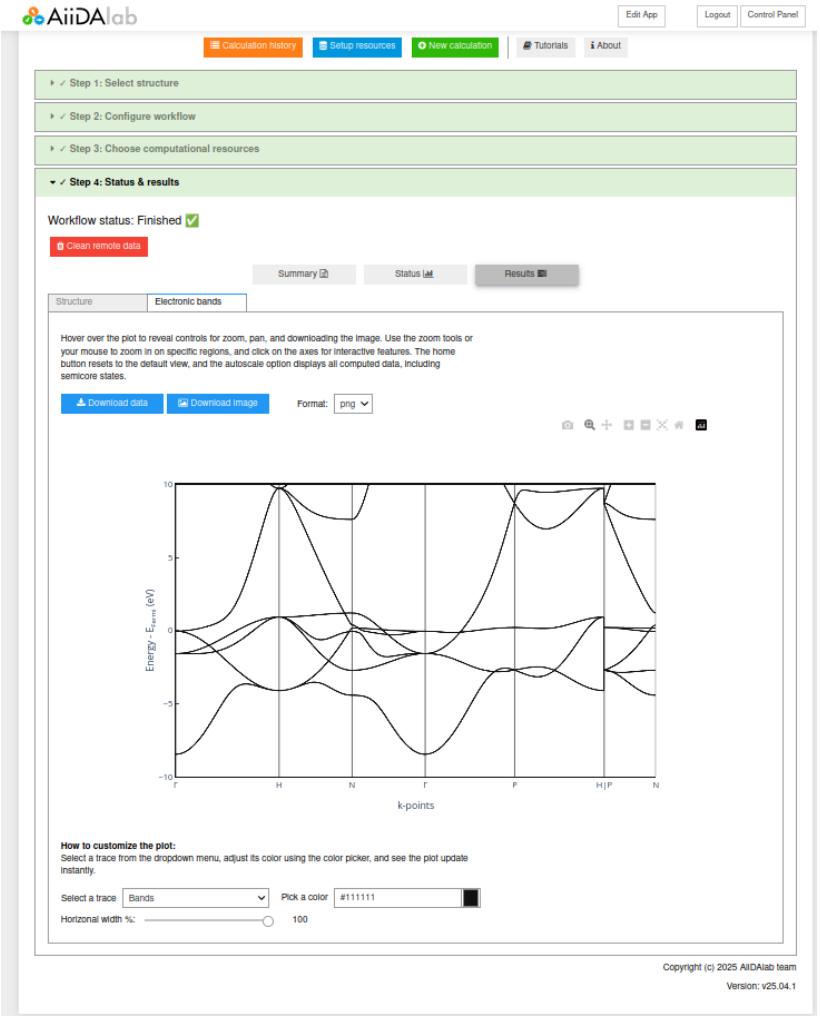


- When the calculations are “Finished”, the results can then be loaded. “Results”→ “Electronic band”→ “load results”

- The electronic band structure of the magnetic Fe. We compare this later with the non-magnetic case in the next slide.

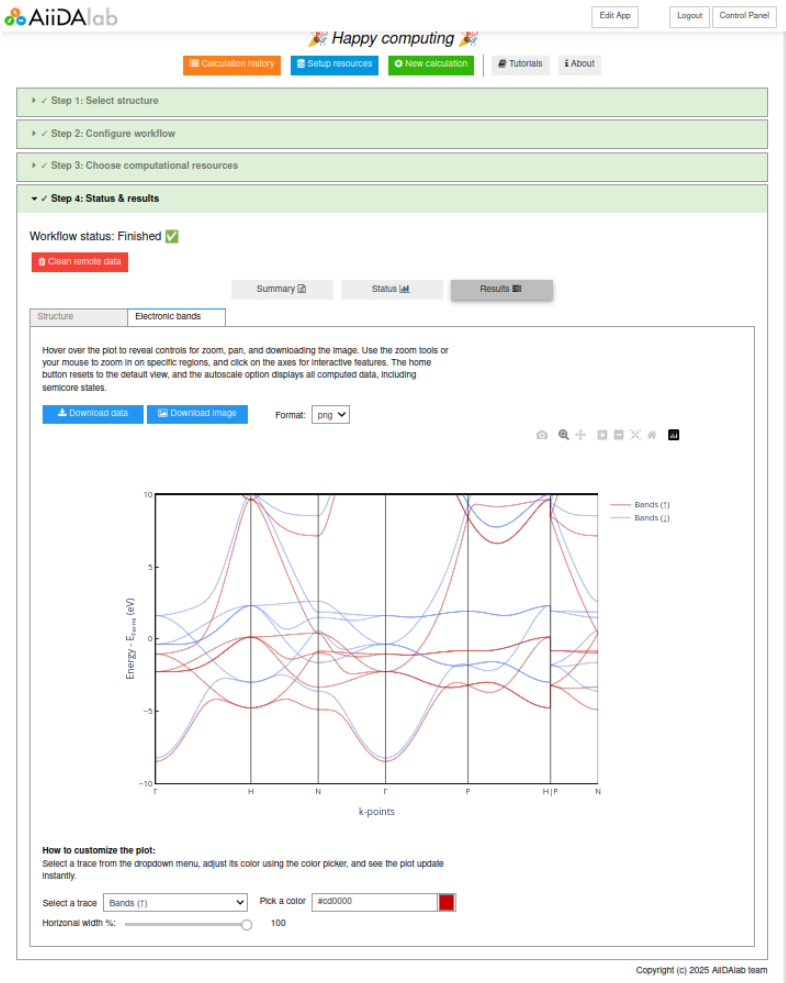
Compare electronic bands

Non-magnetic Fe



- Notice the spin polarized bands for the magnetic case.
- Both are metallic, see the lines crossing the Fermi energy at 0 (y-axis)
- In the next slide we access the total energy of the calculations to determine the ground state configuration.

Magnetic Fe



Compare DFT total energies

Non-magnetic Fe

- To access this page, in the status and results tab, click status, then the dropdown till “SCF cycle-finished”. With the cursor on the black background page of the Quantum espresso output page, scroll up till you arrive at the point seen on the images.
- The Ferromagnetic Fe is the ground state as it
- The end

Magnetic Fe