

Hands on Aiidalab for muons (DFT+ μ calculations)

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>



The screenshot shows the web interface of the Aiidalab demo server. At the top, there's a navigation bar with the Aiidalab logo, 'About', and 'FAQ' links. Below this, the main header features the Aiidalab logo (three interlocking gears) and the MARVEL logo (National Centre of Excellence in Materials Research). The central content area is titled 'Welcome to the AiiDALab demo server!' and includes a 'Login to AiiDALab' section with a 'Sign in with GitHub' button. A warning box states: 'This server is intended for temporary use only and is not suitable for production environments. All user data will be automatically deleted 12 hours after the first login.' Below the login section, there's a 'Getting started with AiiDALab' section with links to documentation and a video. The footer contains a citation for the work and a list of resources to learn more.

login to AiiDALab

Sign in with GitHub

Welcome to the AiiDALab demo server!

This AiiDALab server is deployed and maintained by the [AiiDALab team](#).

The goal of the server is to provide a platform for users to try out AiiDALab without the need to install it locally.

This server is intended for temporary use only and is not suitable for production environments. All user data will be automatically deleted 12 hours after the first login.

Login to AiiDALab

The service is available to anyone with GitHub credentials. Click the "Sign in with GitHub" button to login.

Getting started with AiiDALab

AiiDALab is a web environment to run materials simulation online. It is based on [Jupyter](#) as the web backend, and [AiiDA](#) as the workflow engine.

Some resources to learn AiiDALab:

- Our official documentation, for a more detailed introduction and hands on guide.
- An [AiiDALab introduction](#) video for an overview.

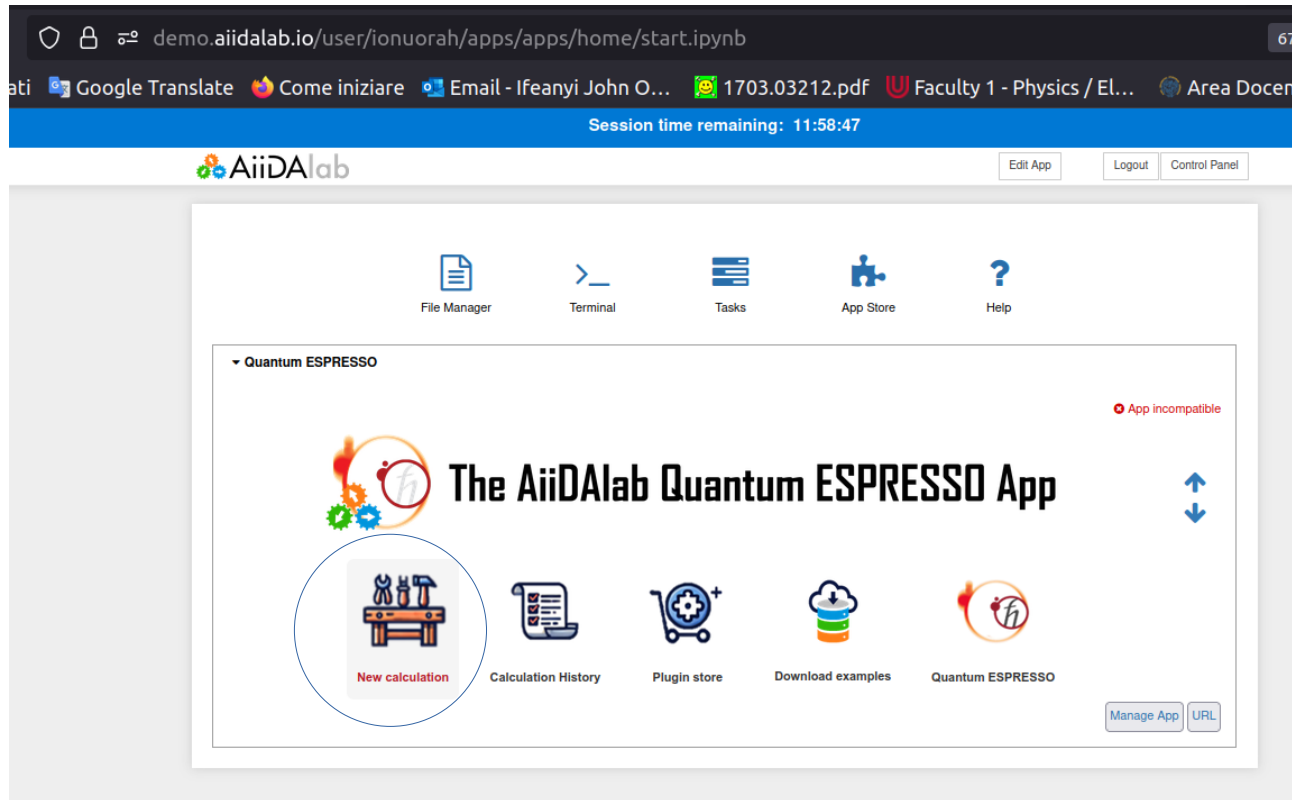
This work is or has been supported by the [MARVEL National Centre of Competence in Research](#) and funded by the [Swiss National Science Foundation](#), the [MARKETPLACE](#) project funded by [Horizon 2020](#) under the [H2020-NMBP-25-2017](#) call (Grant No. 760173), as well as by the [MaX European Centre of Excellence](#) funded by the [Horizon 2020](#) [EINFRA-5](#) program, Grant No. 676598, and other [Materials Cloud](#) partners.

We kindly ask you to cite the following publication if you use AiiDALab:

A. V. Yakutovich et al., *Comp. Mat. Sci.* 188, 110165 (2021) DOI:10.1016/j.commatsci.2020.110165

- ▶ Login with a github account (<https://github.com/>) signup to get one.
- ▶ Files (cifs) for the tutorial can be downloaded from (<http://bit.ly/4IZNPR1>)
- ▶ 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**”

The screenshot shows the AiiDALab Quantum ESPRESSO App interface in a web browser. The browser address bar shows the URL: `demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/qe.ipynb`. The browser's address bar also displays several tabs: "Translate", "Come iniziare", "Email - Ifeanyi John O...", "1703.03212.pdf", "Faculty 1 - Physics / EL...", and "Area Doc". A blue banner at the top of the app interface indicates "Session time remaining: 11:48:22". The main content area features the AiiDALab logo (a stylized 'h' inside a circle with gears) and the text "The AiiDALab Quantum ESPRESSO App". Below the logo is the phrase "Happy computing" with a small icon. A navigation bar contains four buttons: "Calculation history" (orange), "Setup resources" (blue), "New calculation" (green), and "Tutorials" (grey). To the right of these buttons is an "About" link. Below the navigation bar is a list of steps: "Step 1: Select structure" (highlighted in yellow), "Step 2: Configure workflow", "Step 3: Choose computational resources", and "Step 4: Status & results". At the bottom right of the interface, the copyright notice "Copyright (c) 2025 AiiDALab team" and the version "Version: v25.04.1" are displayed.

Select and load structure

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-esspresso/qe.ipynb

Translate Come iniziare Email - Ifeanyi John O... 1703.03212.pdf Faculty 1 - Physics / El... Area Doc

Session time remaining: 11:46:51

The AiiDALab Quantum ESPRESSO App

Happy computing

Calculation history Setup resources New calculation Tutorials About

▼ Step 1: Select structure

Select a structure from one of the following sources, then click **Confirm** to go to the next step

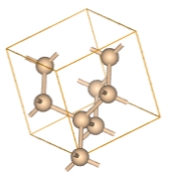
▼ Select structure

Upload file OPTIMADE AiiDA database From examples Upload mol

Upload Structure (1)

Supported structure formats

▼ View structure



Selection Appearance Cell Download

Select atoms:

You can either specify ranges: 1 5..8 10
or expressions: (x>1 and name not [N,O]) or d_from [1,1,1]>2 or kb=10

Copy to clipboard Clear selection Apply selection

Label Si8 Description

► Edit structure

Selected: Si8

Confirm the currently selected structure and go to the next step


- ▶ 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

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/qe.ipynb

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Session time remaining: 11:46:25



The AiiDALab Quantum ESPRESSO App

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

Step 2.2: Customize calculation parameters

Confirm

Step 3: Choose computational resources

Step 4: Status & results

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Version: v25.04.1

- ▶ 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

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/qe.ipynb

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Session time remaining: 11:45:59

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

☒ Electronic band structure Customize bands settings in Step 2.2 if needed

☐ Electronic projected density of states (PDOS)

☐ Bader charge analysis

☐ Muon spectroscopy (muons)

☐ Vibrational spectroscopy (phonons)

The following additional property calculations are available in the **Plugin registry** but are currently disabled because the required plugins are not installed. To enable them, please visit the **Plugin store** and install the necessary plugins (Note: after installation of the plugins, to use them you will need to refresh this page and restart this submission.).

Plugin store

☐ Core-level spectroscopy (aiida-qe-xspec)

☐ Wannier functions (aiidalab-qe-wannier90)

☐ Hubbard parameters (aiidalab-qe-hp)

☐ Post-processing (aiidalab-qe-pp)

Step 2.2: Customize calculation parameters

Confirm

Step 3: Choose computational resources

Step 4: Status & results

Confirm the currently selected settings and go to the next step

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- ▶ 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

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/qe.ipynb

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Session time remaining: 11:45:42

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

Step 2.2: Customize calculation parameters

Basic settings Advanced settings Band structure

Below you can indicate the following:

1. If the material should be treated as an insulator or a metal (if in doubt, choose "Metal")
2. If the material should be studied with magnetization/spin polarization (at least twice as costly if activated)
3. If the material should be studied with spin-orbit coupling
4. The protocol to use for the calculation, which sets default values balancing the accuracy and speed of the calculation

Electronic type:	Metal	Insulator	
Magnetism:	Off	On	
Spin-orbit coupling:	Off	On	
Protocol:	Fast	Balanced	Stringent

The "balanced" protocol represents a trade-off between accuracy and speed. Choose the "fast" protocol for a faster calculation with less precision and the "stringent" protocol to aim at best accuracy (at the price of longer/costlier calculations).

Confirm

Step 3: Choose computational resources

Step 4: Status & results

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Version: v25.04.1

- ▶ 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 “**Advanced 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**”.

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/qe.ipynb

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Session time remaining: 11:45:42

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

Step 2.2: Customize calculation parameters

Basic settings Advanced settings Band structure

Below you can indicate the following:

1. If the material should be treated as an insulator or a metal (if in doubt, choose "Metal")
2. If the material should be studied with magnetization/spin polarization (at least twice as costly if activated)
3. If the material should be studied with spin-orbit coupling
4. The protocol to use for the calculation, which sets default values balancing the accuracy and speed of the calculation

Electronic type: Metal Insulator

Magnetism: Off On

Spin-orbit coupling: Off On

Protocol: Fast Balanced Stringent

The "balanced" protocol represents a trade-off between accuracy and speed. Choose the "fast" protocol for a faster calculation with less precision and the "stringent" protocol to aim at best accuracy (at the price of longer/costlier calculations).

Confirm

Step 3: Choose computational resources

Step 4: Status & results

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Input settings(2): Advanced Settings tab

No action required!!!!

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/qe.ipynb

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Session time remaining: 11:44:43

AiiDA lab

Step 2.1: Select which properties to calculate

Step 2.2: Customize calculation parameters

Basic settings Advanced settings Band structure

Reset to defaults

☐ Delete the work directory after the calculation

Total charge: 0

Van der Waals correction: None

Convergence

Setting the energy threshold for the self-consistent field (SCF) and energy and force thresholds for ionic convergence ensures calculation accuracy and stability. Lower values increase the accuracy but also the computational cost. The default values set by the **protocol** are usually a good starting point. For energy thresholds, the actual value used in the calculation (shown below widget) is given as: $\text{threshold} \times \text{nat_atoms} \times (\text{nat_atoms} + 1)$

Threshold for SCF cycles

Energy: 2e-10 Ryatom 1.6e-09 Ry

Thresholds for ionic convergence

Energy: 0.00001 Ryatom 8e-05 Ry

Force: 0.0001 Ry/B0hr

Maximum cycle steps

Setting a maximum number of electronic and ionic convergence steps ensures that the calculation does not run indefinitely.

Electronic: 80

Ionic: 50

Smearing

Smear electronic state occupations near the Fermi level to simulate finite temperature. This helps to stabilize the SCF calculation and is important for metallic systems. The smearing type and width are set by the chosen **protocol**. Changes are not advised unless you've mastered **smearing effects**.

Type: cold

Width: 0.02 Ry

K-points

The k-points mesh density of the SCF calculation is set by the **protocol**. The value below represents the maximum distance between k-points in each direction of reciprocal space. Smaller is more accurate and costly.

K points distance: 0.15 Å⁻¹ Mesh [8, 8, 8]

Hubbard (DFT+U)

☐ Define U values

Accuracy and precision

- 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

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/qe.ipynb

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Session time remaining: 11:44:11

AiiDALab

The AiiDALab Quantum ESPRESSO App

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Step 3: Choose computational resources

Select the codes to use for running the calculations. The codes on the local machine (localhost) are installed by default, but you can configure new ones on potentially more powerful machines by clicking on **Setup resources** (also at the top of the app). Make sure to click the **Refresh resources** button below after making changes to AiiDA resources to update the app resources.

Setup resources Refresh resources

Global resources Band structure

Use the other tabs if you want to override the resource settings per plugin.

pw pw-7.4@localhost Nodes 1 CPUs 1 More

☐ Specify the number of k-points pools for the pw.x calculations (only for advanced user).

projwfc projwfc-7.4@localhost Nodes 1 CPUs 1 More

Workflow label and description

Label your job and provide a brief description. These details help identify the job later and make the search process easier. While optional, adding a description is recommended for better clarity.

Label: Si8 [unrelaxed, balanced protocol] -> bands

Description

Submit

Step 4: Status & results

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Version: v25.04.1

- ▶ 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 screenshot displays the AiiDALab Quantum ESPRESSO App interface. At the top, a blue header bar shows "Session time remaining: 11:42:24". Below the header, the AiiDALab logo is on the left, and "Edit App", "Logout", and "Control Panel" buttons are on the right. The main content area features the app title "The AiiDALab Quantum ESPRESSO App" and the slogan "Happy computing". A navigation bar includes "Calculation history", "Setup resources", "New calculation", "Tutorials", and "About". A progress bar shows four steps: "Step 1: Select structure", "Step 2: Configure workflow", "Step 3: Choose computational resources", and "Step 4: Status & results". The "Step 4" section is active, displaying "Workflow status: Running" in a red-bordered box. Below this is a "Kill workflow" button. A tabbed interface shows "Summary", "Status" (selected), and "Results". The "Status" tab contains a "Status overview" section with a "Collapse all" button and a "View in advanced panel" button. The overview lists two running jobs: "Quantum ESPRESSO app workflow | running | 1/2* jobs" and "Electronic band structure workflow | running | 1/2* jobs". A detailed log entry for the first job shows its process ID, state, UUID, and creation/modification times, noting that no log messages are recorded for this entry. A footer note states: "*Actual number of jobs may exceed estimated total due to error handling, dynamic sub-workflows, and/or other runtime adjustments". The bottom right corner of the interface shows the copyright notice "Copyright (c) 2025 AiiDALab team" and the version "Version: v25.04.1".

- ▶ 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 screenshot displays the AiiDA Quantum ESPRESSO App interface. At the top, the AiiDA logo and 'The AiiDALab Quantum ESPRESSO App' title are visible, along with a 'Happy computing' message. Navigation buttons include 'Calculation history', 'Setup resources', 'New calculation', 'Tutorials', and 'About'. The main workflow steps are listed: Step 1: Select structure, Step 2: Configure workflow, Step 3: Choose computational resources, and Step 4: Status & results. The 'Status & results' section shows 'Workflow status: Finished' with a green checkmark. Below this, there are tabs for 'Summary', 'Status', and 'Results'. The 'Status' tab is active, showing a 'Status overview' with a 'Collapse all' button and a 'View in advanced panel' button. The overview lists two completed jobs: 'Quantum ESPRESSO app workflow | finished | 2/2' jobs' and 'Electronic band structure workflow | finished | 2/2' jobs'. A detailed view of the selected job shows its UUID, state, and creation/modification times. A footer note states: '*Actual number of jobs may exceed estimated total due to error handling, dynamic sub-workflows, and/or other runtime adjustments'. The bottom right corner contains copyright information: 'Copyright (c) 2025 AiiDALab team' and 'Version: v25.04.1'.

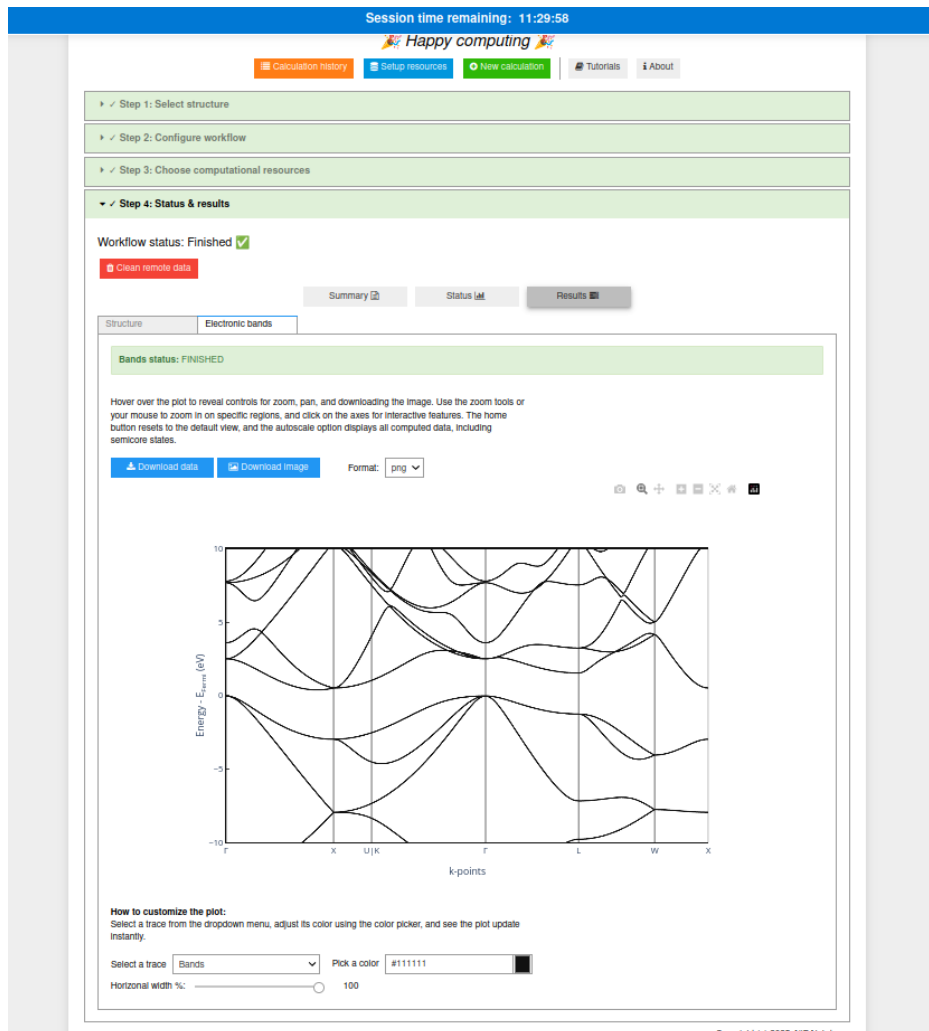
- ▶ The status is “**Finished**”
- ▶ Notice all menu boxes are now in green colour
- ▶ Click on the “**Result**” tab to see the structure and bands

Check and load “electronic band” results

- Click on “load results”

The screenshot displays the AiiDALab Quantum ESPRESSO App interface. At the top, the AiiDALab logo is on the left, and 'Edit App', 'Logout', and 'Control Panel' buttons are on the right. The main header features the app's logo, the title 'The AiiDALab Quantum ESPRESSO App', and the tagline 'Happy computing'. Below this are navigation buttons: 'Calculation history', 'Setup resources', 'New calculation', 'Tutorials', and 'About'. The workflow progress is shown as a series of steps: 'Step 1: Select structure', 'Step 2: Configure workflow', 'Step 3: Choose computational resources', and 'Step 4: Status & results' (which is expanded). Under 'Step 4', the 'Workflow status' is 'Finished' with a green checkmark. A 'Clean remote data' button is present. Below the status, there are three tabs: 'Summary', 'Status', and 'Results'. The 'Electronic bands' tab is selected, showing a 'Structure' tab and a 'Load results' button, which is circled in red. A note states: 'Note: Load time may vary depending on the size of the calculation'. The footer contains 'Copyright (c) 2025 AiiDALab team' and 'Version: v25.04.1'.

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

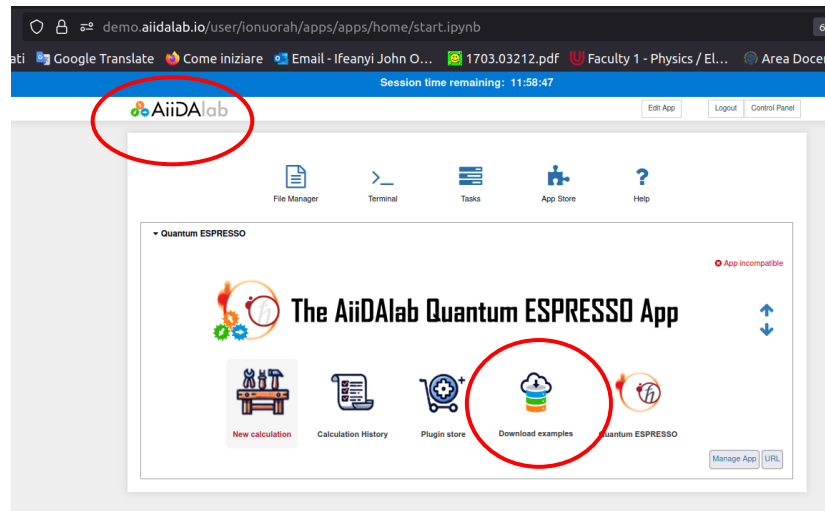
DFT+ μ calculations

- ▶ 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

The screenshot shows a web browser window with the URL `demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/examples.ipynb`. The browser's address bar and tabs are visible. Below the browser window, the AiiDA Lab interface is shown. It has a blue header bar with the AiiDA Lab logo on the left and buttons for 'Edit App', 'Logout', and 'Control Panel' on the right. The main content area is titled 'AiiDALab Quantum ESPRESSO - Example calculations'. It contains a paragraph explaining that the page provides example calculations for import into an AiiDA instance. Below this, there is a list of examples, each with a filename and a description. The example 'LiF_full_muons.aiida' is highlighted in blue. At the bottom of the examples list, there are two buttons: 'Import' and 'Calculation history'. Below the buttons, there is a button labeled 'Archive Import log'.

demo.aiidalab.io/user/ionuorah/apps/apps/quantum-espresso/examples.ipynb

Session time remaining: 11:57:26

AiiDALab

Edit App Logout Control Panel

AiiDALab Quantum ESPRESSO - Example calculations

We provide here a set of example calculations performed with the AiiDALab Quantum ESPRESSO app for you to import into your AiiDA instance. Choose one or more examples to import, then click the [Import](#) button. A report on each import will be appended to the log below. Once imported, you can click the [Calculation history](#) button to view details of any given imported calculation and/or launch it in an instance of the app to view its inputs and outputs.

If you have any questions or issues regarding the examples, please open an issue in the [aiidalab-qe-examples](#) repository.

Examples:

- `Si_vibro_amaro_qe_vibroscopy.aiida` - Silicon phonons in-app guide: amarof+qevibroscopy / plugins: aiidalab_qe_vibroscopy
- `GaAs_full_vibro.aiida` - GaAs phonons in-app guide: Full / plugins: aiidalab_qe_vibroscopy
- `SiO2_full_vibro.aiida` - Example: SiO2, full vibronic properties / plugins: aiidalab_qe_vibroscopy
- `LiF_muons_sites.aiida` - LiF muons in-app guide: sites / plugins: aiidalab_qe_muon
- `LiF_muons_sites_polarization.aiida` - LiF muons in-app guide: sites+polarization / plugins: aiidalab_qe_muon
- `LiF_full_muons.aiida` - Example: LiF muons, stopping sites and polarization function / plugins: aiidalab_qe_muon**
- `LiCoO2_bader_charge.aiida` - Example: LiCoO2 Bader charge / plugins: aiida_bader
- `H2O_bader_charge.aiida` - Example: H2O Bader charge / plugins: aiida_bader
- `PtO_bader_charge.aiida` - Example: PtO Bader charge / plugins: aiida_bader
- `PtO2_bader_charge.aiida` - Example: PtO2 Bader charge / plugins: aiida_bader
- `C8H6_xps.aiida` - Example: C8H6 XPS / plugins: aiida_qe_xspec

[Import](#) [Calculation history](#)

[Archive Import log](#)

- ▶ 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

AiiDAlab Quantum ESPRESSO - Calculation history

Page guide

Display options:

Time format: Absolute Relative

ID format: pk uuid

Filters:

Job state: Any

Start time: mm / dd / yyyy End time: mm / dd / yyyy

Filter by properties:

☐ bands ☐ muonic

COLUMNS FILTERS DENSITY EXPORT

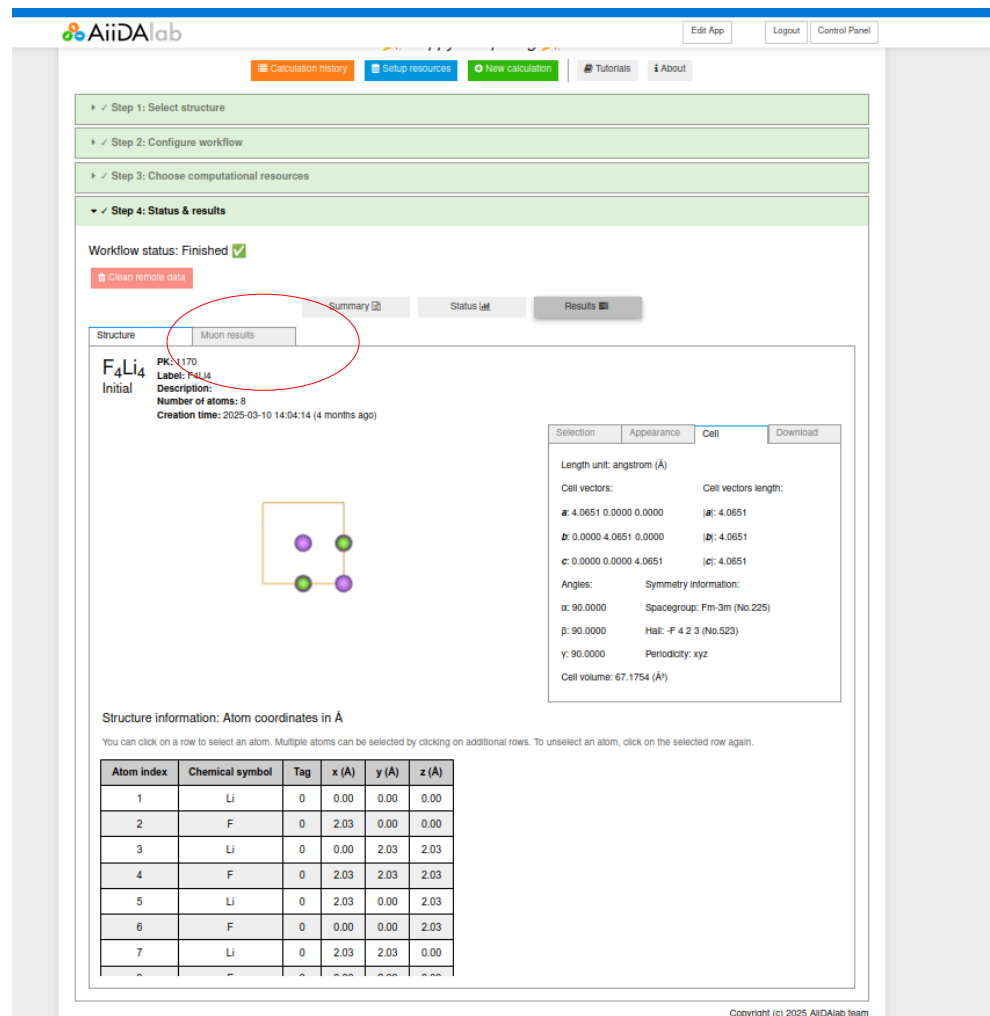
Search...

ID	Creation time	Structure	State	Exit message	Label	Delete	Download
884	7/17/2025	Si8	Finished	Si8 [unrelaxed, balanced protocol] → bands		Delete	Download
940	3/10/2025	F4Li4	Finished	Example: LiF muons, stopping sites and polariza...		Delete	Download

Rows per page: 10 1-2 of 2

- ▶ 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”



Workflow status: Finished ✓

[Clean remote data](#)

[Summary](#) [Status](#) [Results](#)

Structure [Muons results](#)

F₄Li₄
Initial
PK: 1170
Label: F4Li4
Description:
Number of atoms: 8
Creation time: 2025-03-10 14:04:14 (4 months ago)

Length unit: angstrom (Å)

Cell vectors:

Cell vectors length:

\mathbf{a} : 4.0651 0.0000 0.0000 $|\mathbf{a}|$: 4.0651
 \mathbf{b} : 0.0000 4.0651 0.0000 $|\mathbf{b}|$: 4.0651
 \mathbf{c} : 0.0000 0.0000 4.0651 $|\mathbf{c}|$: 4.0651

Angles:

Symmetry information:

α : 90.0000 Spacegroup: Fm-3m (No.225)
 β : 90.0000 Hall: -F 4 2 3 (No.523)
 γ : 90.0000 Periodicity: xyz
Cell volume: 67.1754 (Å³)

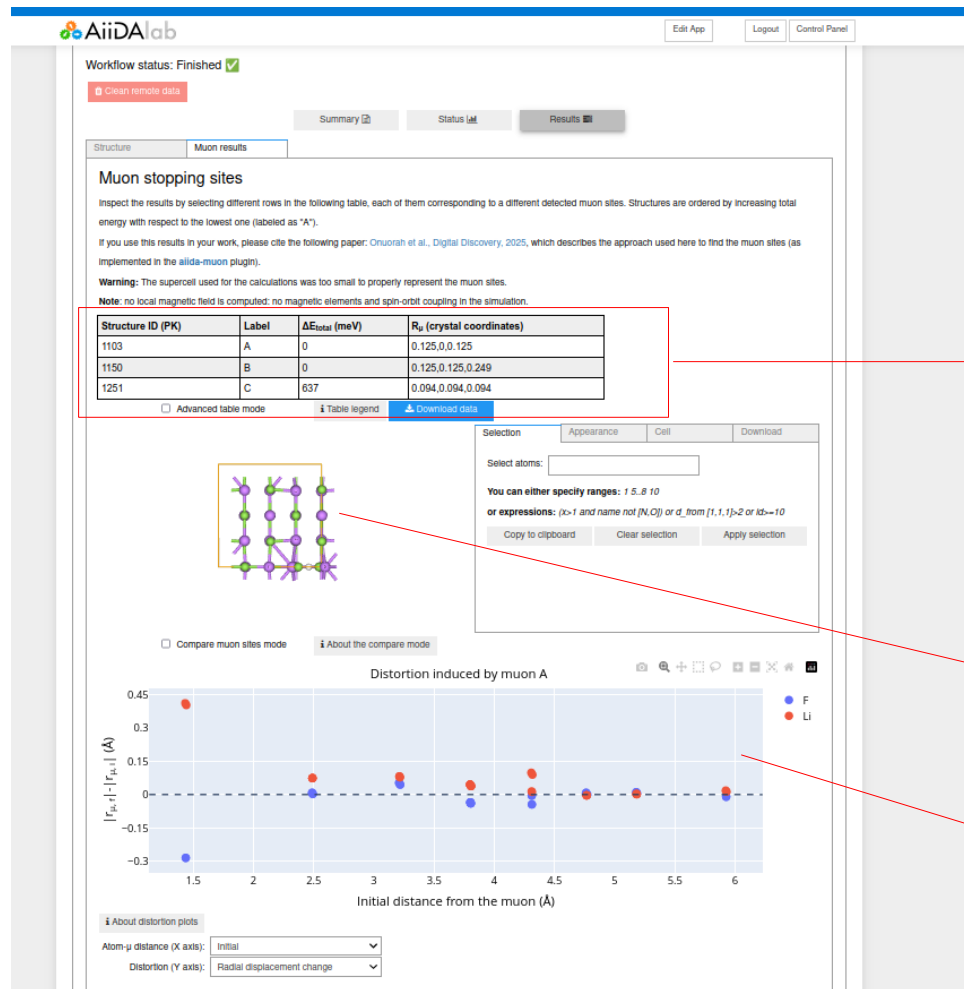
Structure information: Atom coordinates in Å

You can click on a row to select an atom. Multiple atoms can be selected by clicking on additional rows. To unselect an atom, click on the selected row again.

Atom index	Chemical symbol	Tag	x (Å)	y (Å)	z (Å)
1	Li	0	0.00	0.00	0.00
2	F	0	2.03	0.00	0.00
3	Li	0	0.00	2.03	2.03
4	F	0	2.03	2.03	2.03
5	Li	0	2.03	0.00	2.03
6	F	0	0.00	0.00	2.03
7	Li	0	2.03	2.03	0.00

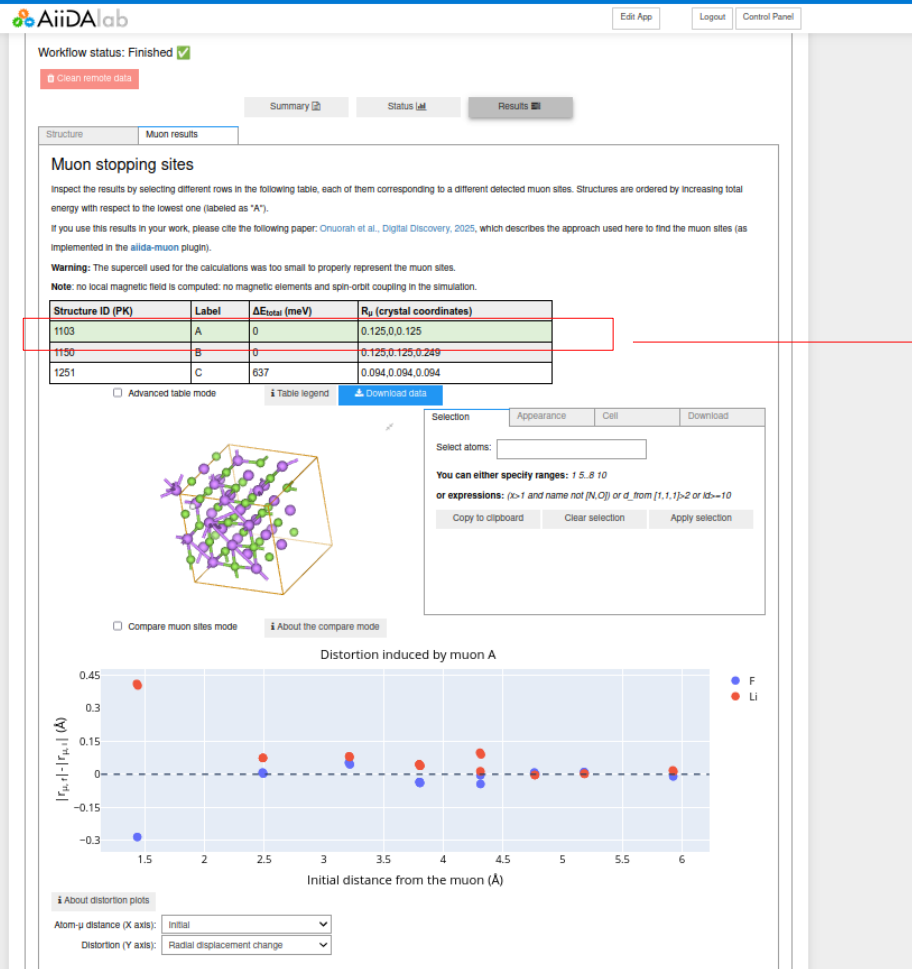
- ▶ Immediately, we can see the four task bars all in “green”, signifying that all the steps of the calculations are completed.
- ▶ The current open page is the “Result” → “structure” tab. This shows the LiF structure used as input to start the muon calculations.
- ▶ To visualize the muon results click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

Muon sites in LiF results(1)



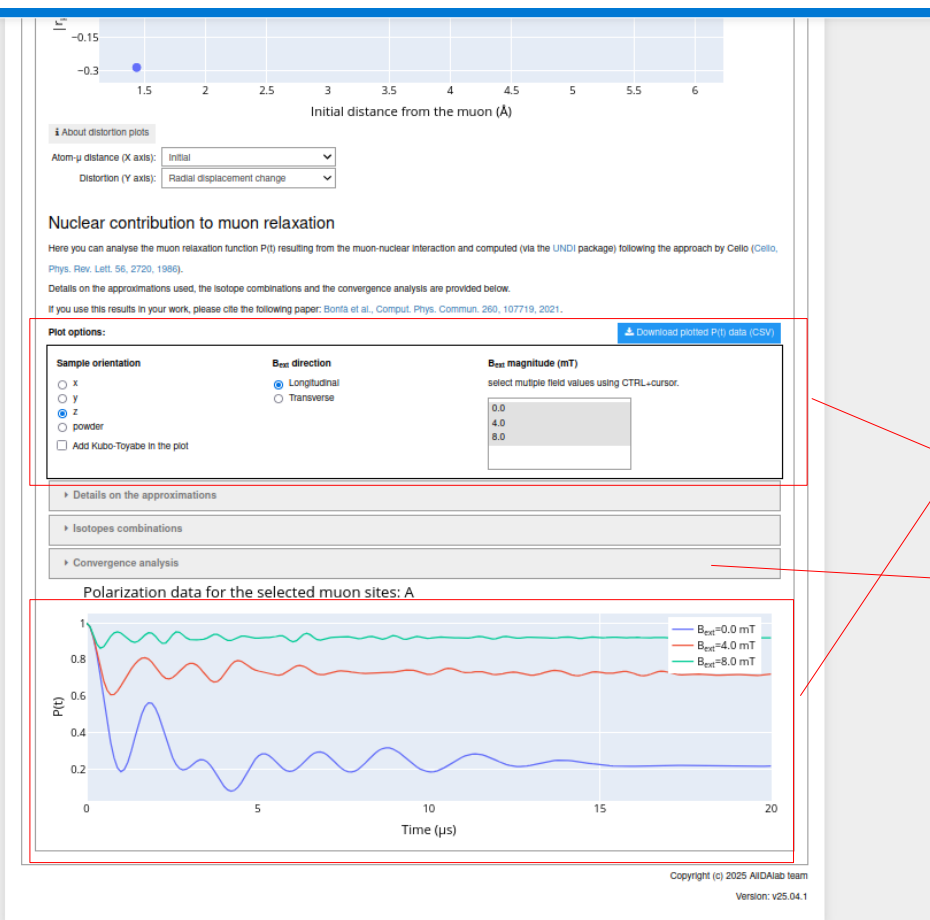
- ▶ In this slide and the next 3, tips on understanding the results are provided. No action is required before continuing the exercise.
- ▶ This tabulates the muon site positions obtained from the calculations. There are 3 sites with label A, B and C. Their relative total energies are given in the third 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 (metastable), likely not a candidate position.
- ▶ The positions in the supercell as well as unitcell can be visualized.
- ▶ This plot shows the displacement 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)



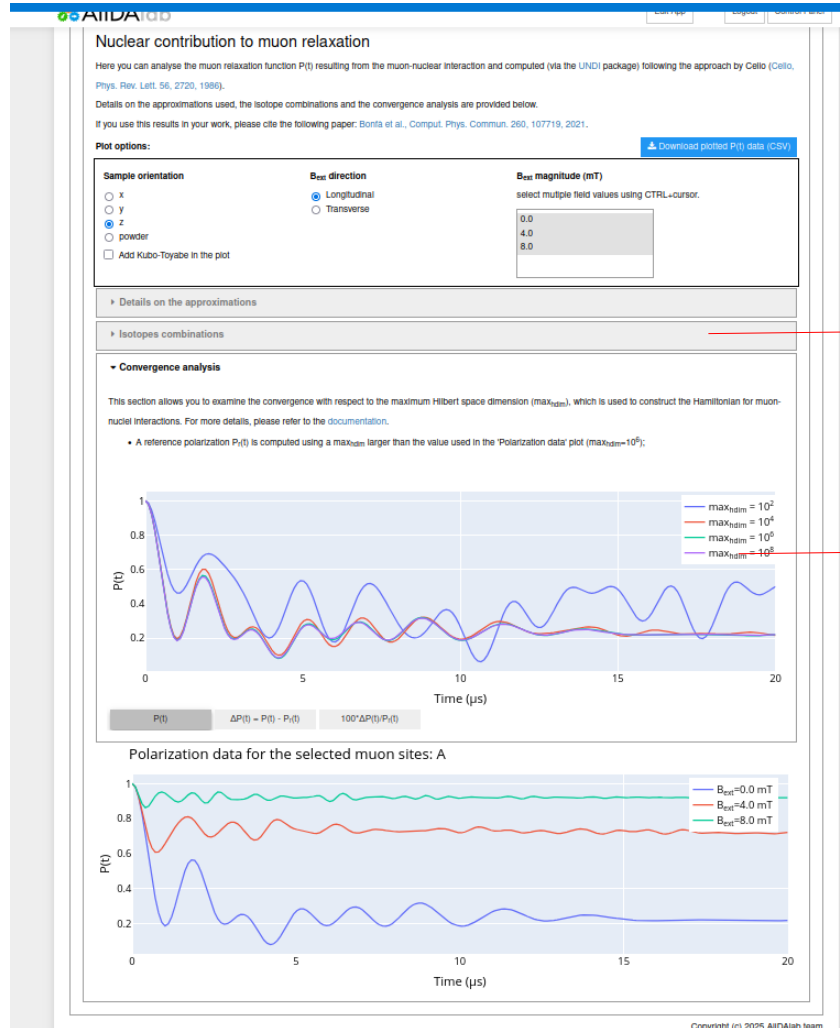
- Here just to say that we can select by clicking on the muon site one after the other (see green line for site A) in the table to access separately its position in the structure and its other properties in the “muon result” tab.

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

The AiiDA Quantum ESPRESSO App

Happy computing

Production ready | Setup resources | New calculation | Tutorials | About

Step 1: Select structure

Step 2: Configure workflow

Step 3: Choose computational resources

Step 4: Status & results

Workflow status: Finished ✓

Clean remote data

Summary | Status | Results

Structure | Muon results

Muon stopping sites

Inspect the results by selecting different rows in the following table, each of them corresponding to a different detected muon sites. Structures are ordered by increasing total energy with respect to the lowest one (labeled as "A").

If you use this results in your work, please cite the following paper: [Orunah et al., Digital Discovery, 2025](#), which describes the approach used here to find the muon sites (as implemented in the `aiida-muon` plugin).

Warning: The supercell used for the calculations was too small to properly represent the muon sites.

Note: no local magnetic field is computed: no magnetic elements and spin-orbit coupling in the simulation.

Structure ID (PK)	Label	ΔE_{total} (meV)	R_0 (crystal coordinates)
1103	A	0	0.125,0.0.125
1150	B	0	0.125,0.125,0.349
1251	C	837	0.094,0.094,0.094

☐ Advanced table mode | ☐ Table legend | [Download data](#)

☐ Compare muon sites mode | [About the compare mode](#)

Selection | Appearance | Cell | Download

Select atoms:

You can either specify ranges: `1 ≤ 8 10`
or expressions: `(x>1 and name not [N,O]) or d_from [1,1,1]>2 or kb=10`


Distortion induced by muon A


d (Å)

● F
● Li

- ▶ 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


 Edit App Logout Control Panel

 The AiiDA Lab Quantum ESPRESSO App

Happy computing

Calculation history Setup resources New calculation Tutorials About

✓ Step 1: Select structure

Select a structure from one of the following sources, then click  Confirm to go to the next step

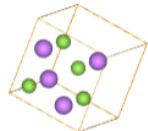
Select structure

Upload file OPTIMADE AiiDA database From examples Upload mol

Upload Structure (0)

Supported structure formats

View structure



Selection Appearance Cell Download

Select atoms:

You can either specify ranges: $x: 5..8$ 10
or expressions: $(x>1 \text{ and name not } [N,O])$ or $d_from [1,1,1]>2$ or $id==10$

Copy to clipboard Clear selection Apply selection

Label Description

Edit structure

Selected:

Confirm

➤ Step 2: Configure workflow

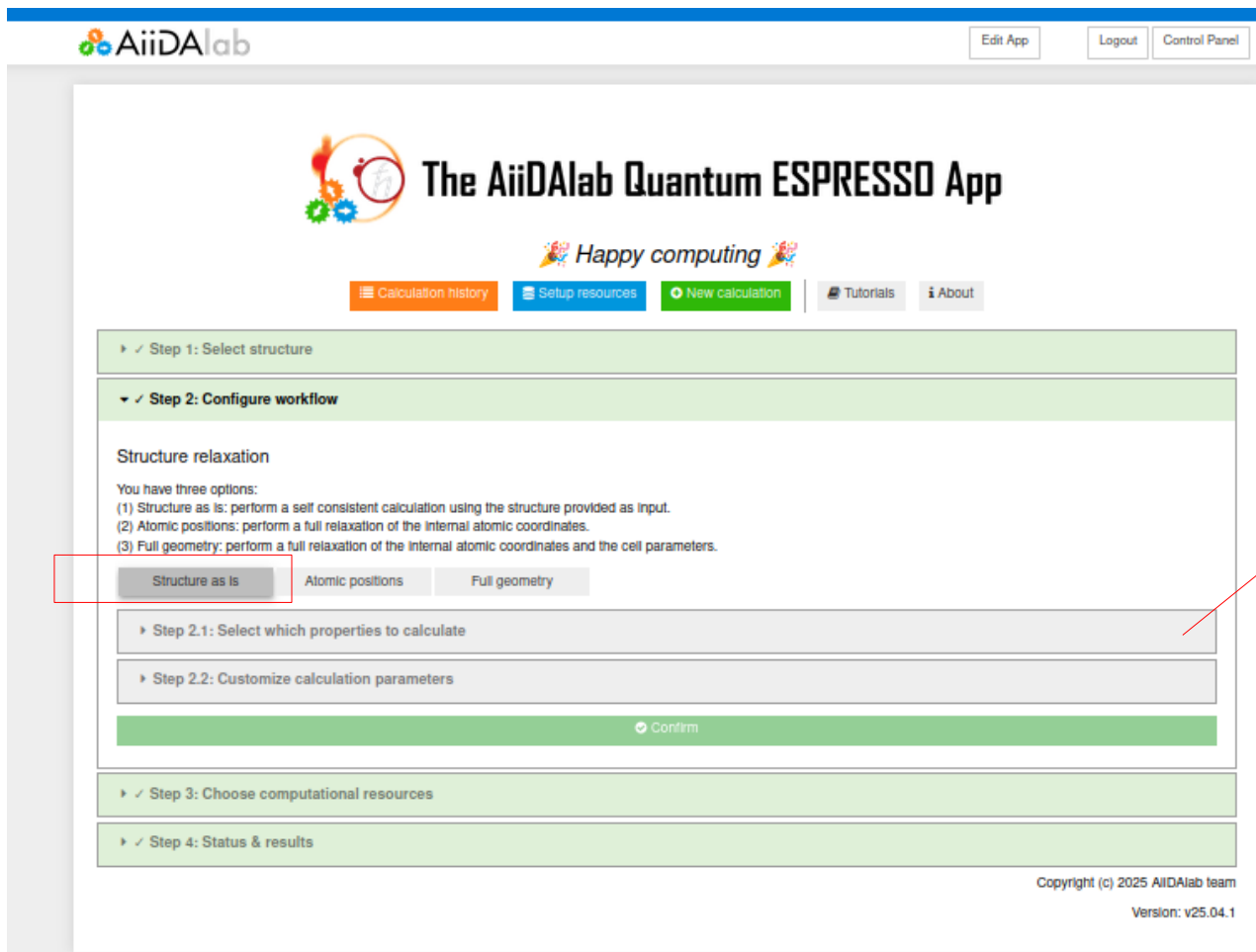
➤ Step 3: Choose computational resources

➤ Step 4: Status & results

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Version: v25.04.1

- ▶ 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



The screenshot displays the AiiDA Quantum ESPRESSO App interface. At the top, there is a navigation bar with the AiiDA logo, 'Edit App', 'Logout', and 'Control Panel' buttons. Below this, the main header features the app's logo and title, 'The AiiDA Quantum ESPRESSO App', along with the slogan 'Happy computing'. A secondary navigation bar includes buttons for 'Calculation history', 'Setup resources', 'New calculation', 'Tutorials', and 'About'.

The main content area is divided into four steps, each in a green bar:

- Step 1: Select structure
- Step 2: Configure workflow (expanded)
 - Structure relaxation
 - You have three options:
 - (1) Structure as is: perform a self consistent calculation using the structure provided as input.
 - (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
 - (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.
 - Three buttons are shown: 'Structure as is' (highlighted with a red box), 'Atomic positions', and 'Full geometry'.
 - Step 2.1: Select which properties to calculate
 - Step 2.2: Customize calculation parameters
 - A green 'Confirm' button.
- Step 3: Choose computational resources
- Step 4: Status & results

At the bottom right, the footer text reads: 'Copyright (c) 2025 AiiDA team' and 'Version: v25.04.1'.

- ▶ 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 AiiDA Quantum ESPRESSO App

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

- ☐ Electronic band structure
- ☐ Electronic projected density of states (PDOS)
- ☐ Bader charge analysis
- ☒ Muon spectroscopy (muons) Customize muonic settings in Step 2.2 if needed
- ☐ Vibrational spectroscopy (phonons)

The following additional property calculations are available in the **Plugin registry** but are currently disabled because the required plugins are not installed. To enable them, please visit the **Plugin store** and install the necessary plugins (Note: after installation of the plugins, to use them you will need to refresh this page and restart this submission.).

Plugin store

- ☐ Core-level spectroscopy (aiida-qe-xspec)
- ☐ Wannier functions (aiida-qe-wannier90)
- ☐ Hubbard parameters (aiida-qe-hp)
- ☐ Post-processing (aiida-qe-pp)

Step 2.2: Customize calculation parameters

Confirm

Step 3: Choose computational resources

Step 4: Status & results

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Version: v25.04.1

- ▶ 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 screenshot displays the AiiDALab Quantum ESPRESSO App interface. At the top, there's a header with the AiiDALab logo, 'Edit App', 'Logout', and 'Control Panel' buttons. Below the header, a navigation bar includes 'Calculation history', 'Setup resources', 'New calculation', 'Tutorials', and 'About'. The main content area is divided into steps: 'Step 1: Select structure', 'Step 2: Configure workflow', 'Step 3: Choose computational resources', and 'Step 4: Status & results'. Under 'Step 2: Configure workflow', there's a 'Structure relaxation' section with three options: 'Structure as is', 'Atomic positions', and 'Full geometry'. Below this is 'Step 2.1: Select which properties to calculate'. The current step is 'Step 2.2: Customize calculation parameters', which has three sub-tabs: 'Basic settings', 'Advanced settings', and 'Muon settings'. The 'Muon settings' tab is highlighted with a red box. It contains instructions on how to indicate material properties and a table for selecting calculation parameters. The table has rows for 'Electronic type', 'Magnetism', 'Spin-orbit coupling', and 'Protocol', each with two columns of options. A 'Confirm' button is at the bottom of the settings section. The footer shows 'Copyright (c) 2025 AiiDALab team' and 'Version: v25.04.1'.

AiiDALab

The AiiDALab Quantum ESPRESSO App

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

Step 2.2: Customize calculation parameters

Basic settings Advanced settings Muon settings

Below you can indicate the following:

1. If the material should be treated as an insulator or a metal (if in doubt, choose "Metal")
2. If the material should be studied with magnetization/spin polarization (at least twice as costly if activated)
3. If the material should be studied with spin-orbit coupling
4. The protocol to use for the calculation, which sets default values balancing the accuracy and speed of the calculation

Electronic type:	Metal	Insulator	
Magnetism:	Off	On	
Spin-orbit coupling:	Off	On	
Protocol:	Fast	Balanced	Stringent

The "balanced" protocol represents a trade-off between accuracy and speed. Choose the "fast" protocol for a faster calculation with less precision and the "stringent" protocol to aim at best accuracy (at the price of longer/costlier calculations).

Confirm

Step 3: Choose computational resources

Step 4: Status & results

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Version: v25.04.1

- ▶ 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 overridden in the “**Muon settings**”
- ▶ Click on the “**Muon settings**” tab

Muon settings (1)

The screenshot shows the AiiDAlab web interface. At the top, there's a navigation bar with 'Edit App', 'Logout', and 'Control Panel'. Below it, a 'Happy computing' banner is followed by tabs: 'Calculation history', 'Setup resources', 'New calculation', 'Tutorials' (highlighted with a red box), and 'About'. The main content area is divided into steps: 'Step 1: Select structure', 'Step 2: Configure workflow', and 'Step 3: Choose computational resources'. Under 'Step 2: Configure workflow', there's a 'Structure relaxation' section with three options: 'Structure as is', 'Atomic positions', and 'Full geometry'. Below this is 'Step 2.1: Select which properties to calculate'. The main section is 'Step 2.2: Customize calculation parameters', which has three sub-tabs: 'Basic settings', 'Advanced settings', and 'Muon settings' (selected). The 'Muon settings' tab contains 'Muon spectroscopy settings' and 'Find muon sites settings'. The 'Muon spectroscopy settings' section includes a text block about selecting inputs for muon stopping sites, a 'Search for muon sites' checkbox (checked), a 'Compute supercell size' checkbox (unchecked), and a 'Compute polarization (only μ -nuclear interactions)' checkbox (checked). The 'Find muon sites settings' section includes a 'Use default DFT- μ parameters' checkbox (checked), a 'Muon charge state' dropdown (set to 'Muonium (+1)'), a 'Muon supercell' input (set to '2x2x2'), a 'Supercell hint' button, a 'Reset supercell' button, a 'K-points distance (Å⁻¹)' input (set to '0.3'), a 'Reset k-points' button, a 'Mesh grid' dropdown (set to '[3, 3, 3]'), a 'Disable Hubbard correction (if any)' checkbox (unchecked), an 'Enable spin polarization DFT (if magnetic sample)' checkbox (checked), a 'Spacing for trial grid for initial muon sites (Å)' input (set to '1'), a 'Reset μ -spacing' button, a 'Click to estimate number of muon trial sites' button (set to '3'), and a 'Visualize candidate muon sites' button. The 'Polarization from μ - Nuclear interactions' section includes a 'Polarization from μ - Nuclear interactions' dropdown (set to 'Nuclear interactions'), an 'External magnetic fields (mT)' slider (set to '0 - 10'), a 'B_{range}' dropdown (set to '2'), an 'Additional grid' checkbox (unchecked), a 'Number of calculations per site' input (set to '6'), and a 'Field list (mT)' input (set to '[0, 2, 4, 6, 8, 10]'). At the bottom, there's a 'Confirm' button.

- ▶ 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)

AiiDAlab

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

Step 2.2: Customize calculation parameters

Basic settings Advanced settings Muon settings

Muon spectroscopy settings

Please select desired inputs to compute muon stopping sites and related properties. The muon is considered infinite-dilute in the crystal, so we should select a supercell in which the muon will stay and do not interact with its replica. If you do not provide a size for the supercell size and select "Compute supercell", a pre-processing set of simulation will be submitted to estimate it.

You can select the three main steps of the workflow: **Compute supercell size**, **Search for muon sites**, and **Compute polarization**. Computing only the polarization requires the muon (H atom) already placed in the structure as last site. Supercell size and muon stopping sites are computed by means of the **aiida-muon** plugin (Omurrah et al., Digital Discovery, 2025). The polarization is computed via the UNDI package (Soris et al., Comput. Phys. Commun. 260, 107719, 2021), using the method by Celis (Celis, Phys. Rev. Lett. 56, 2720, 1986), and considering only the muon-nuclear interactions.

☒ Search for muon sites

☐ Compute supercell size

☒ Compute polarization (only μ -nuclei interactions)

Find muon sites settings

- Use default DFT- μ parameters ☒ Use default DFT- μ settings

- Muon charge state: Muon (+1) Muonium (neutral)

- Muon supercell: 2 2 2 Supercell hint Reset supercell

- K-points distance (\AA^{-1}): 0.3 Reset k-points Mesh grid: [3, 3, 3]

☐ Disable Hubbard correction (if any)

☒ Enable spin polarised DFT (if magnetic sample)

- Spacing for trial grid for initial muon sites (\AA): 1 Reset μ -spacing

Click to estimate number of muon trial sites: 3 Visualize candidate muon sites

Polarization from μ - Nuclear interactions

External magnetic fields (mT): B_{range} 0 - 10 B_{step} 2

☐ Additional grid

- Number of calculations per site: 6
- Field list (mT): [0, 2, 4, 6, 8, 10]

Confirm

Step 3: Choose computational resources

- ▶ **K-points distance:** This is the spacing that determines the grid of the k-points used for the Bricoullion 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)

AiiDAlab

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Structure relaxation

You have three options:

- (1) Structure as is: perform a self-consistent calculation using the structure provided as input.
- (2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
- (3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is Atomic positions Full geometry

Step 2.1: Select which properties to calculate

Step 2.2: Customize calculation parameters

Basic settings Advanced settings Muon settings

Muon spectroscopy settings

Please select desired inputs to compute muon stopping sites and related properties. The muon is considered infinite-dilute in the crystal, so we should select a supercell in which the muon will stay and do not interact with its replica. If you do not provide a size for the supercell size and select "Compute supercell", a pre-processing set of simulation will be submitted to estimate it.

You can select the three main steps of the workflow: **Compute supercell size**, **Search for muon sites**, and **Compute polarization**. Computing only the polarization requires the muon (H atom) already placed in the structure as last site. Supercell size and muon stopping sites are computed by means of the **aiida-muon** plugin (Omura et al., Digital Discovery, 2022). The polarization is computed via the UNDI package (Santis et al., Comput. Phys. Commun. 260, 107719, 2021), using the method by Celis (Cello, Phys. Rev. Lett. 56, 2720, 1986), and considering only the muon-nuclear interactions.

☒ Search for muon sites

☐ Compute supercell size

☒ Compute polarization (only μ -nuclei interactions)

Find muon sites settings

☒ Use default DFT+ μ parameters ☒ Use default DFT+ μ settings

- Muon charge state Muon (+1) Muonium (neutral)

- Muon supercell 2 2 2 **Supercell hint** **Reset supercell**

- K-points distance (\AA^{-1}) 0.3 **Reset k-points** Mesh grid: [3, 3, 3]

☐ Disable Hubbard correction (if any)

☒ Enable spin polarised DFT (if magnetic sample)

- Spacing for trial grid for initial muon sites (\AA) 1 **Reset μ -spacing**

Click to estimate number of muon trial sites 3 **Visualize candidate muon sites**

Polarization from μ - Nuclear interactions

External magnetic fields (mT): B_{range} 0 - 10 B_{step} 2

☐ Additional grid

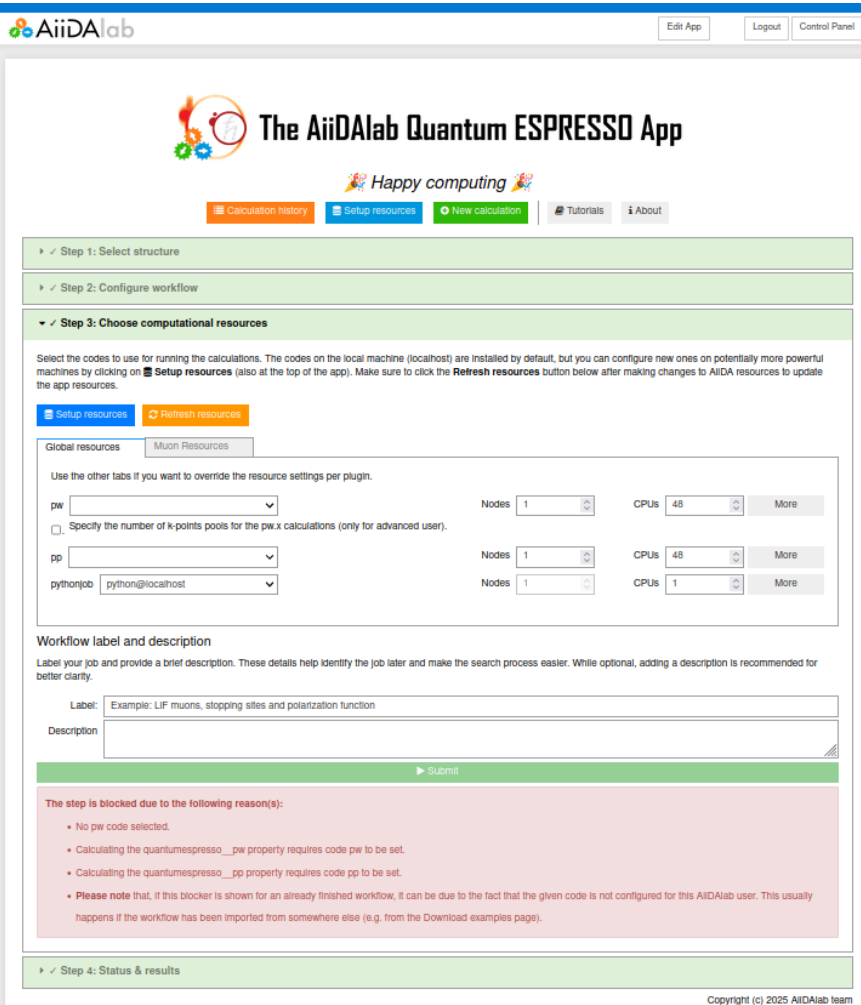
- Number of calculations per site: 6
- Field list (mT): [0, 2, 4, 6, 8, 10]

Confirm

Step 3: Choose computational resources

- **Spacing for trial 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



AiiDALab

Edit App Logout Control Panel

The AiiDALab Quantum ESPRESSO App

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure

Step 2: Configure workflow

Step 3: Choose computational resources

Select the codes to use for running the calculations. The codes on the local machine (localhost) are installed by default, but you can configure new ones on potentially more powerful machines by clicking on **Setup resources** (also at the top of the app). Make sure to click the **Refresh resources** button below after making changes to AiiDALab resources to update the app resources.

Setup resources Refresh resources

Global resources Muon Resources

Use the other tabs if you want to override the resource settings per plugin.

pw Nodes 1 CPUs 48 More

☐ Specify the number of k-points pools for the pw.x calculations (only for advanced user).

pp Nodes 1 CPUs 48 More

pythonjob python@localhost Nodes 1 CPUs 1 More

Workflow label and description

Label your job and provide a brief description. These details help identify the job later and make the search process easier. While optional, adding a description is recommended for better clarity.

Label: Example: LIF muons, stopping sites and polarization function

Description

Submit

The step is blocked due to the following reason(s):

- No pw code selected.
- Calculating the quantum.espresso__pw property requires code pw to be set.
- Calculating the quantum.espresso__pp property requires code pp to be set.
- Please note that, if this blocker is shown for an already finished workflow, it can be due to the fact that the given code is not configured for this AiiDALab user. This usually happens if the workflow has been imported from somewhere else (e.g. from the Download examples page).

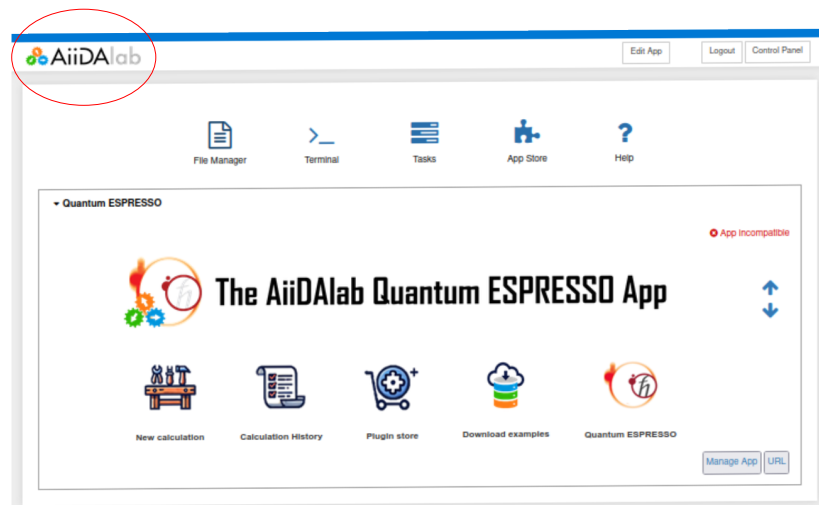
Step 4: Status & results

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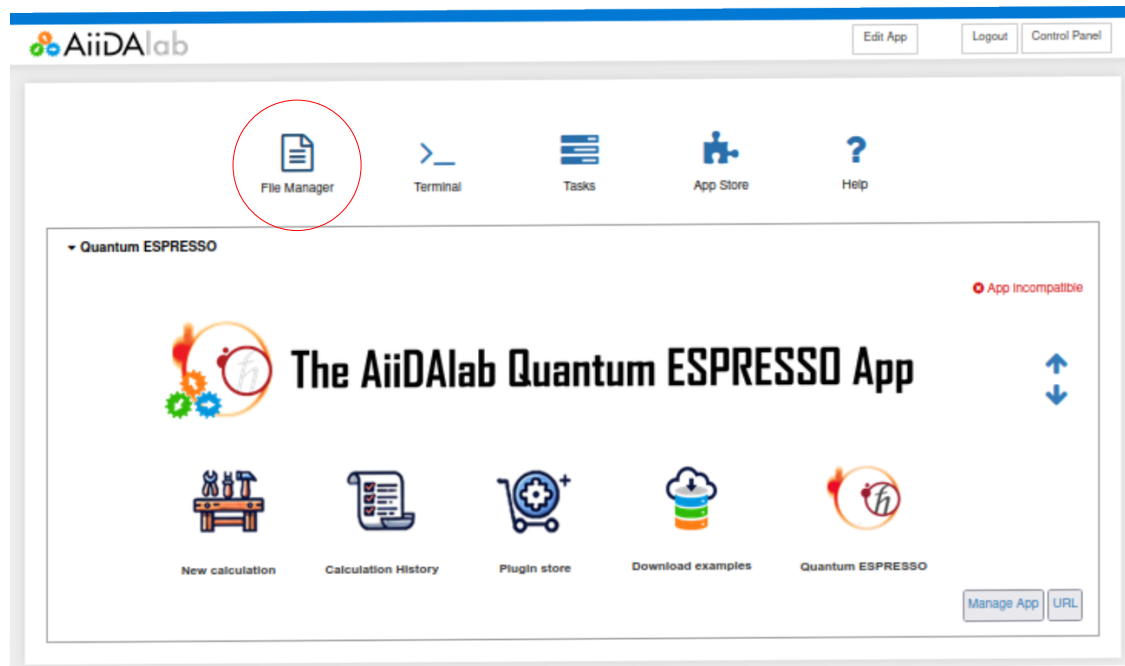
- ▶ Here the resources required for the calculation can be set. But remember for this demo only 1 cpu is available.
- ▶ The submit button is blocked because it is a calculation from history.
- ▶ Notice the error message in red on why this step is blocked. Ignore, as we are not performing the calculations.
- ▶ 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 ($\mathbf{B}_\mu = \mathbf{B}_{\text{dip}} + \mathbf{B}_C$), the description of the magnetic structure (mcif file – see $\text{MnF}_2.\text{mcif}$ 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.

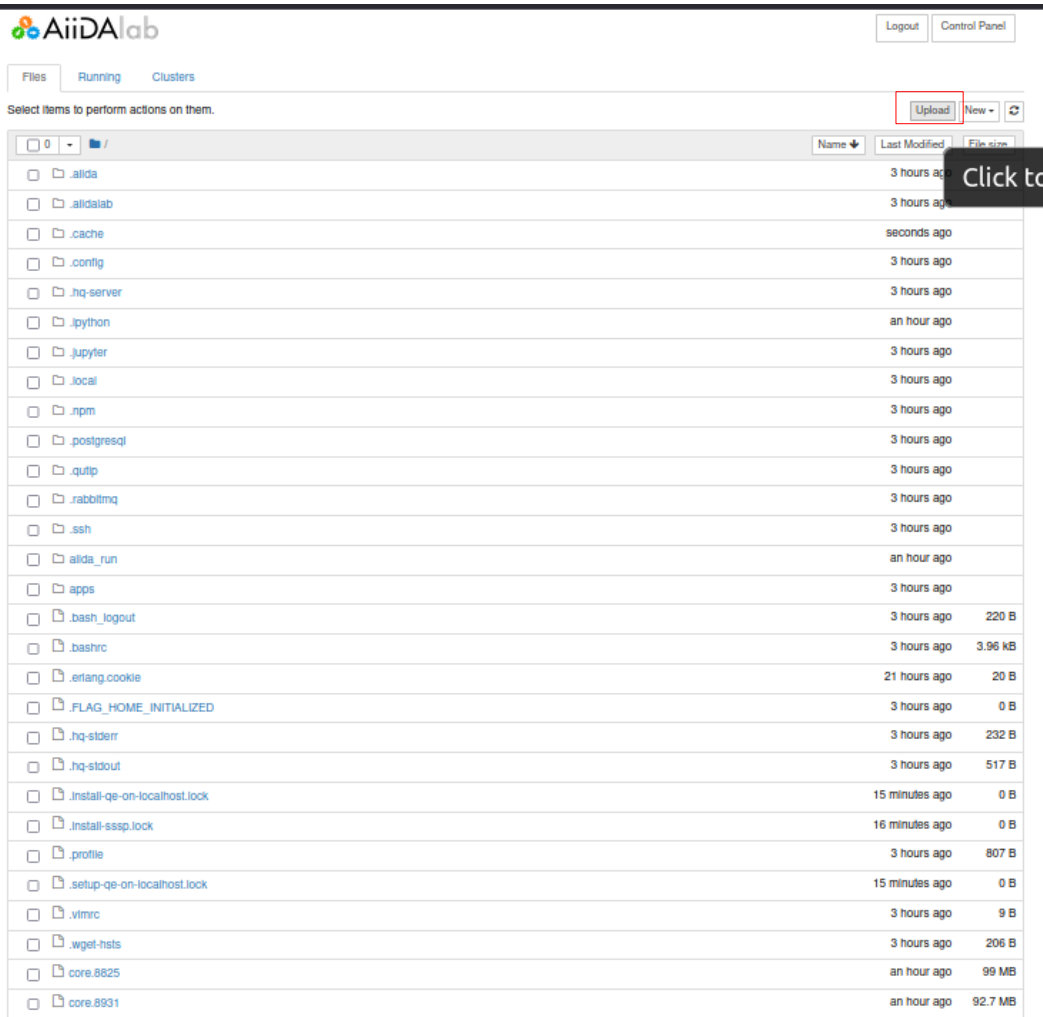


Load the aiida archive data for MnF_2



- On the startup page click on **“File manager”**

Load the aiida archive data for MnF₂



The screenshot shows the AiiDA Lab web interface. At the top, there's a header with the AiiDA Lab logo, a 'Logout' button, and a 'Control Panel' button. Below the header, there are tabs for 'Files', 'Running', and 'Clusters'. The 'Files' tab is active, and it shows a list of files and directories. A red box highlights the 'Upload' button in the top right corner of the file list. A black box with the text 'Click to' is overlaid on the 'Upload' button. The file list has columns for 'Name', 'Last Modified', and 'File size'. The files are listed in a table format.

Name	Last Modified	File size
.aiida	3 hours ago	
.aiidalab	3 hours ago	
.cache	seconds ago	
.config	3 hours ago	
.hq-server	3 hours ago	
.ipython	an hour ago	
.jupyter	3 hours ago	
.local	3 hours ago	
.npm	3 hours ago	
.postgresql	3 hours ago	
.qutip	3 hours ago	
.rabbitmq	3 hours ago	
.ssh	3 hours ago	
.aiida_run	an hour ago	
.apps	3 hours ago	
.bash_logout	3 hours ago	220 B
.bashrc	3 hours ago	3.96 kB
.erlang.cookie	21 hours ago	20 B
.FLAG_HOME_INITIALIZED	3 hours ago	0 B
.hq-stderr	3 hours ago	232 B
.hq-stdout	3 hours ago	517 B
.install-qe-on-localhost.lock	15 minutes ago	0 B
.install-sssp.lock	16 minutes ago	0 B
.profile	3 hours ago	807 B
.setup-qe-on-localhost.lock	15 minutes ago	0 B
.vimrc	3 hours ago	9 B
.wget-hsts	3 hours ago	206 B
core.8825	an hour ago	99 MB
core.8931	an hour ago	92.7 MB

- ▶ 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

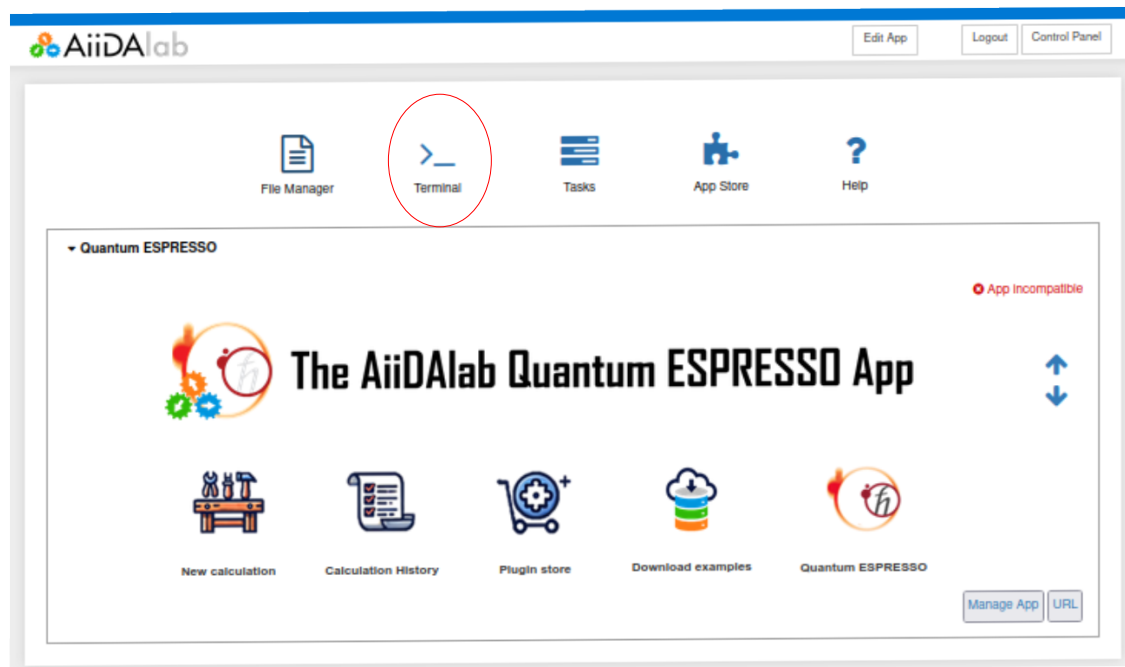
Load the aiida archive data for MnF₂

The screenshot shows the AiiDA Lab web interface. At the top left is the AiiDA Lab logo. To its right are 'Logout' and 'Control Panel' buttons. Below the logo are tabs for 'Files', 'Running', and 'Clusters'. A message says 'Select items to perform actions on them.' followed by 'Upload' and 'New' buttons. The main area is a file list table with columns for Name, Last Modified, and File size. The file 'MnF2_muons.aiida' is highlighted with a red box, and its upload progress bar is also highlighted with a red box, showing 23%. At the bottom of the list, the file 'MnF2_muons.aiida' is also highlighted with a red box.

Name	Last Modified	File size
MnF2_muons.aiida	23%	
.aiida	3 hours ago	
.aiidaib	3 hours ago	
.cache	2 minutes ago	
.config	3 hours ago	
.hq-server	3 hours ago	
.ipython	an hour ago	
.jupyter	3 hours ago	
.local	3 hours ago	
.npm	3 hours ago	
.postgresql	3 hours ago	
.qutp	3 hours ago	
.rabbitmq	3 hours ago	
.ssh	3 hours ago	
aiida_run	an hour ago	
apps	3 hours ago	
.bash_logout	3 hours ago	220 B
.bashrc	3 hours ago	3.96 kB
.erlang.cookie	21 hours ago	20 B
.FLAG_HOME_INITIALIZED	3 hours ago	0 B
.hq-stderr	3 hours ago	232 B
.hq-stdout	3 hours ago	517 B
.install-qe-on-localhost.lock	17 minutes ago	0 B
.install-sssp.lock	17 minutes ago	0 B
.profile	3 hours ago	807 B
.setup-qe-on-localhost.lock	17 minutes ago	0 B
.vimrc	3 hours ago	9 B
.wget-hsts	3 hours ago	206 B
core.8825	an hour ago	99 MB
core.8831	an hour ago	92.7 MB
MnF2_muons.aiida	seconds ago	16.8 MB

- ▶ 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 MnF₂ data to the calculation history



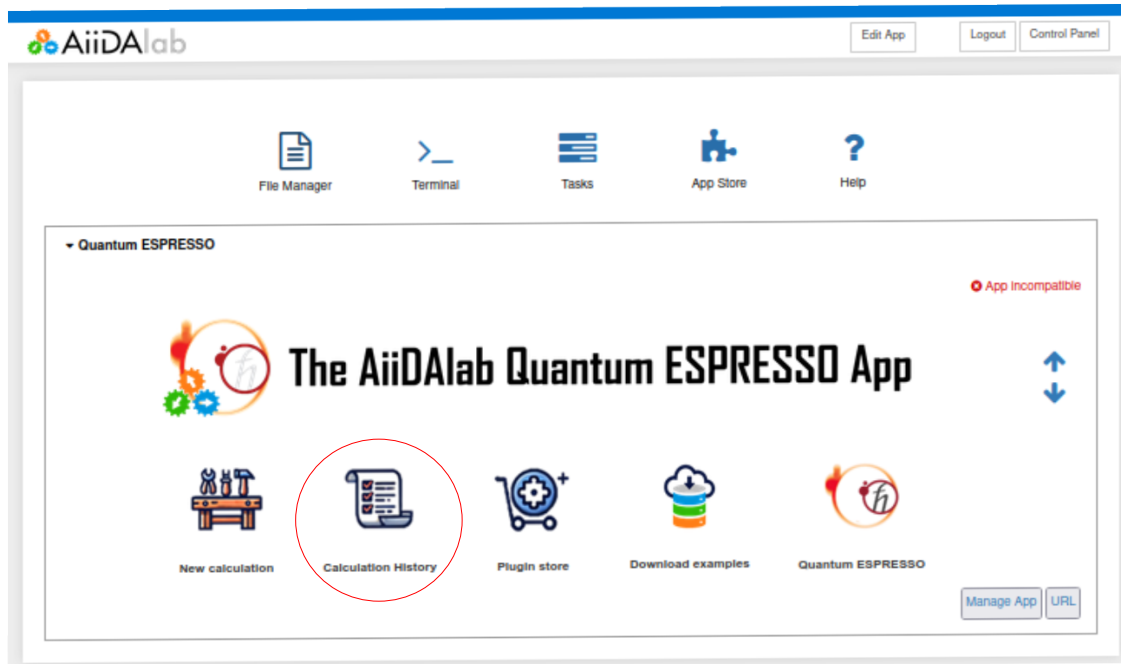
```
(base) jovyan@jupyter-ionuorah:~$ verdi archive import MnF2_muons.aiida
```

- ▶ 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 aiiadalab 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 Authinfos      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 3/6 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

AiiDALab

Page guide

Display options:

Time format: Absolute Relative
ID format: pk uuid

Filters:

Job state: Any
Start time: mm / dd / yyyy End time: mm / dd / yyyy

Filter by properties:
☐ bands ☐ muonic

ID	Creation time	Structure	State	Exit message	Label	Delete	Download
884	7/17/2025	Si8	Finished	Si8 [unrelaxed, balanced protocol] → bands		Delete	Download
940	3/10/2025	F4Li4	Finished	Example: LiF muons, stopping sites and polariza...		Delete	Download
1745	2/11/2025	F4Mn2	Finished	F4Mn2 [unrelaxed, fast protocol] → muonic		Delete	Download

Rows per page: 10 1-3 of 3

- ▶ 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.

MnF₂ loaded calculation data: “Result” tab

AiiDA Lab THE AIIDA LAB QUANTUM COMPUTING APP

Happy computing

Calculation history Setup resources New calculation Tutorials About

Step 1: Select structure
Step 2: Configure workflow
Step 3: Choose computational resources
Step 4: Status & results

Workflow status: Finished ☒


Clean remote data

Summary Status Results

Structure Muon results

F₄Mn₂
PK: 1423
Label: F4Mn2
Description:
Number of atoms: 6
Creation time: 2025-02-11 09:26:18 (5 months ago)

Initial



Selection Appearance Cell Download

Length unit: angstrom (Å)

Cell vectors: \mathbf{a} : 4.8736 0.0000 0.0000 \mathbf{b} : -0.0000 4.8736 0.0000 \mathbf{c} : 0.0000 0.0000 3.3000

Cell vectors length: $|\mathbf{a}|$: 4.8736 $|\mathbf{b}|$: 4.8736 $|\mathbf{c}|$: 3.3000

Angles: α : 90.0000 β : 90.0000 γ : 90.0000

Symmetry information: Spacegroup: P4₂mm (No.136) Hall: -P 4n 2n (No.419) Periodicity: xyz

Cell volume: 78.3815 (Å³)

Structure information: Atom coordinates in Å

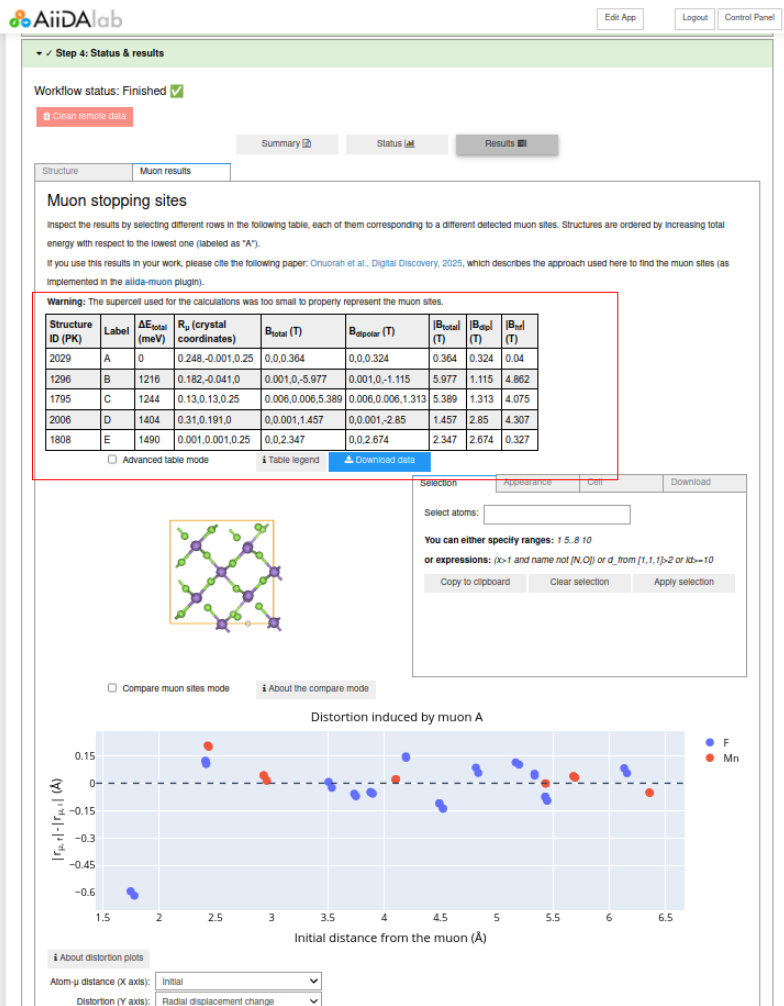
You can click on a row to select an atom. Multiple atoms can be selected by clicking on additional rows. To unselect an atom, click on the selected row again.

Atom index	Chemical symbol	Tag	x (Å)	y (Å)	z (Å)
1	Mn	0	0.00	0.00	0.00
2	Mn	0	2.44	2.44	1.65
3	F	0	1.48	1.48	0.00
4	F	0	3.92	0.95	1.65
5	F	0	0.95	3.92	1.65
6	F	0	3.39	3.39	0.00

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

MnF₂ loaded calculation data: “Result” tab



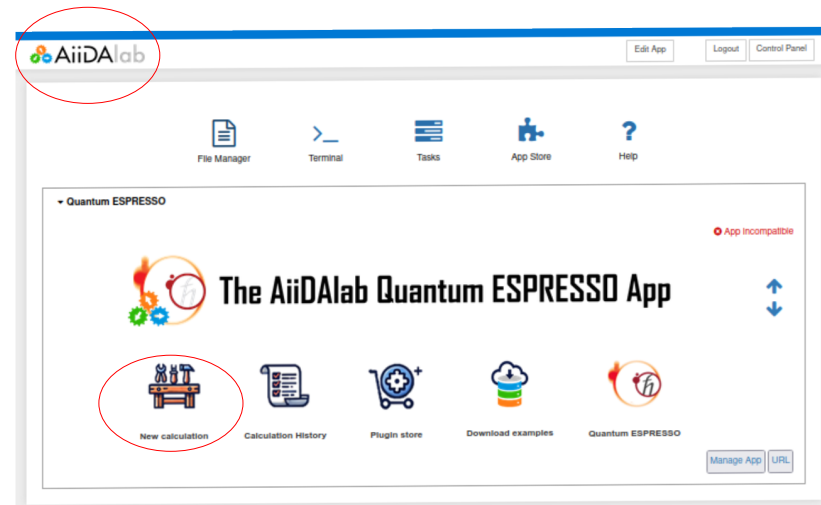
- ▶ The different section of the results is like we have seen in example 2 for LiF. In addition, because the sample is magnetic, the muon result table also contains the different contribution of the muon local field.
- ▶ E.g, For lowest energy site A (I.e the F-mu-F site), the dipolar contribution is 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)

AiiDA

lab

⚙️ Edit App

👤 Logout

🔧 Control Panel

The AiiDA

lab Quantum ESPRESSO App

Happy computing

📊 Calculation history

🔧 Setup resources

🚀 New calculation

📖 Tutorials

📄 About

• Step 1: Select structure

Select a structure from one of the following sources, then click [Confirm](#) to go to the next step

• Select structure

Upload file

OPTIMADE

AiiDA database

From examples

Upload mol

Supported structure formats

⬆️ Upload Structure (1)

• View structure

Selection

Appearance

Cell

Download

Select atoms:

You can either specify ranges: `1:5,8-10`
or expressions: `(x>1 and name not N_O) or d_from(1,1,1)-2 or d<=10`

Copy to clipboard

Clear selection

Apply selection

Label: Fe2

Description:

• Edit structure

Selected: Fe2

⏹️ Confirm

• Step 2: Configure workflow

• Step 3: Choose computational resources

• Step 4: Status & results

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AiiDA

lab

⚙️ Edit App

👤 Logout

🔧 Control Panel

The AiiDA

lab Quantum ESPRESSO App

Happy computing

📊 Calculation history

🔧 Setup resources

🚀 New calculation

📖 Tutorials

📄 About

• Step 1: Select structure

• Step 2: Configure workflow

Structure relaxation

You have three options:
(1) Structure as is: perform a self consistent calculation using the structure provided as input.
(2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
(3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is

Atomic positions

Full geometry

• Step 2.1: Select which properties to calculate

☒ Electronic band structure

Customize bands settings in Step 2.2 if needed

☐ Electronic projected density of states (PDOS)

☐ Bader charge analysis

☐ Muon spectroscopy (muons)

☐ Vibrational spectroscopy (phonons)

The following additional property calculations are available in the **Plugin registry** but are currently disabled because the required plugins are not installed. To enable them, please visit the **Plugin store** and install the necessary plugins (Note: after installation of the plugins, to use them you will need to refresh this page and restart this submission.).

➡️ Plugin store

☐ Core-level spectroscopy (aiida-qc-xspec)

☐ Wannier functions (aiida-qc-wannier90)

☐ Hubbard parameters (aiida-qc-tp)

☐ Post-processing (aiida-qc-pp)

• Step 2.2: Customize calculation parameters

⏹️ Confirm

• Step 3: Choose computational resources

• Step 4: Status & results

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⚙️ Edit App

👤 Logout

🔧 Control Panel

The AiiDA

lab Quantum ESPRESSO App

Happy computing

📊 Calculation history

🔧 Setup resources

🚀 New calculation

📖 Tutorials

📄 About

• Step 1: Select structure

• Step 2: Configure workflow

Structure relaxation

You have three options:
(1) Structure as is: perform a self consistent calculation using the structure provided as input.
(2) Atomic positions: perform a full relaxation of the internal atomic coordinates.
(3) Full geometry: perform a full relaxation of the internal atomic coordinates and the cell parameters.

Structure as is

Atomic positions

Full geometry

• Step 2.1: Select which properties to calculate

• Step 2.2: Customize calculation parameters

Basic settings

Advanced settings

Band structure

Below you can indicate the following:
1. If the material should be treated as an insulator or a metal (if in doubt, choose "Metal")
2. If the material should be studied with magnetization spin polarization (at least twice as costly if activated)
3. If the material should be studied with spin-orbit coupling
4. The protocol to use for the calculation, which sets default values balancing the accuracy and speed of the calculation

Electronic type:

Metal

Insulator

Magnetism:

Off

On

Spin-orbit coupling:

Off

On

Protocol:

Fast

Balanced

Stringent

The "balanced" protocol represents a trade-off between accuracy and speed. Choose the "fast" protocol for a faster calculation with less precision and the "stringent" protocol to aim at best accuracy (at the price of longer/costlier calculations).

⏹️ Confirm

• Step 3: Choose computational resources

• Step 4: Status & results

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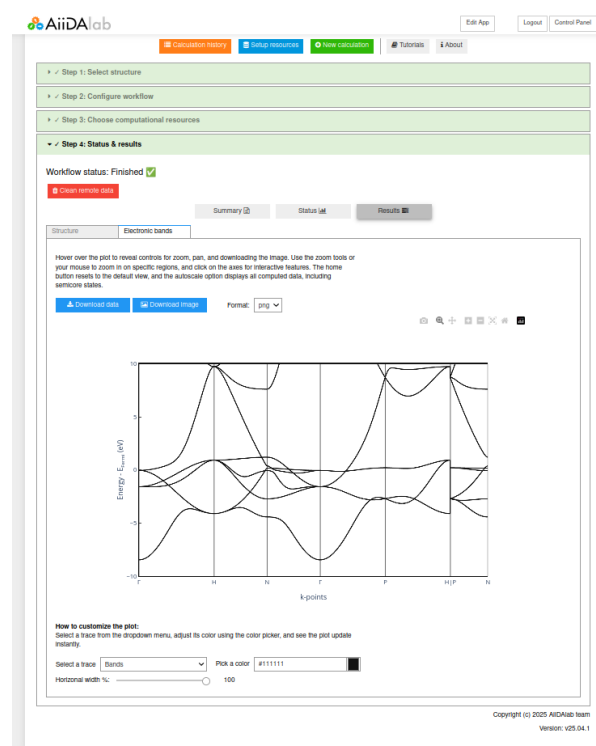
lab team

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Still on non-magnetic Fe calculation steps (2)

The AiiDA Quantum ESPRESSO App interface, Step 3: Choose computational resources. The interface shows a sidebar with navigation links: Calculation history, Setup resources, New calculation, Tutorials, and About. The main content area is titled "Step 3: Choose computational resources" and includes a "Global resources" section with a "Band structure" tab. Below this, there are input fields for "pw" (set to "pw-7.4@localhost") and "project" (set to "project-7.4@localhost"). There are also input fields for "Nodes" (set to 1) and "CPUs" (set to 1). A "Workflow label and description" section is at the bottom, with a "Label" field containing "Pw2 [unrelaxed, balanced protocol] -> bands" and a "Description" field. A green "Submit" button is at the bottom right.

The AiiDA Quantum ESPRESSO App interface, Step 4: Status & results. The interface shows a sidebar with navigation links: Calculation history, Setup resources, New calculation, Tutorials, and About. The main content area is titled "Step 4: Status & results" and includes a "Workflow status: Running" indicator. Below this, there is a "Status overview" section with a "Collapse all" button and a list of workflows. A "View to advanced panel" button is also present. The "Advanced status view" section shows details for the "Quantum ESPRESSO app workflow" and "Electronic band structure workflow".



- 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)

The image displays three sequential screenshots of the AiiDALab Quantum ESPRESSO App interface, illustrating the initial steps for a magnetic Fe calculation.

Screenshot 1 (Left): Step 1: Select structure

- The interface shows the "Select structure" step.
- Under "Select structure", the "Upload structure (1)" button is highlighted with a red circle.
- Below, the "View structure" section shows a 3D model of a crystal structure (Fe₂) and a table for selecting atoms.
- The "Label" field is set to "Fe2".

Screenshot 2 (Middle): Step 2: Configure workflow

- The interface shows the "Configure workflow" step.
- Under "Structure relaxation", the "Structure as is" tab is selected.
- In the "Step 2.1: Select which properties to calculate" section, the "Electronic band structure" checkbox is checked.
- The "Step 2.2: Customize calculation parameters" section is visible at the bottom.

Screenshot 3 (Right): Step 2: Configure workflow (continued)

- The interface shows the "Customize calculation parameters" section.
- Under "Basic settings", the "Magnetism" section is expanded.
- The "Magnetism" dropdown is set to "On".
- The "Spin-orbit coupling" dropdown is set to "On".
- A red box highlights the "Magnetism" and "Spin-orbit coupling" settings, with a note: "Note: set the desired magnetic configuration in advanced settings".

- 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)

The screenshot shows the 'Step 3: Choose computational resources' section of the AiiDA Quantum ESPRESSO App. It includes a 'Global resources' section with a 'Band structure' tab. Below this, there are input fields for 'pw' (set to 'pw-7.4@localhost') and 'project' (set to 'project-7.4@localhost'). There are also dropdowns for 'Nodes' and 'CPU' (both set to 1). A 'Submit' button is at the bottom of the section. The interface also shows a 'Workflow label and description' section with a 'Label' field containing 'Pw2 [unrelaxed, balanced protocol] -> bands'.

The screenshot shows the 'Step 4: Status & results' section of the AiiDA Quantum ESPRESSO App. It displays the 'Workflow status: Running' and a 'Status overview' section. The 'Status overview' shows a list of jobs, including 'Quantum ESPRESSO app workflow' and 'Electronic band structure workflow'. A 'View in advanced panel' button is visible. The 'Advanced status view' section shows details for the 'Electronic band structure workflow', including the process ID, state, and a report of the calculation results.

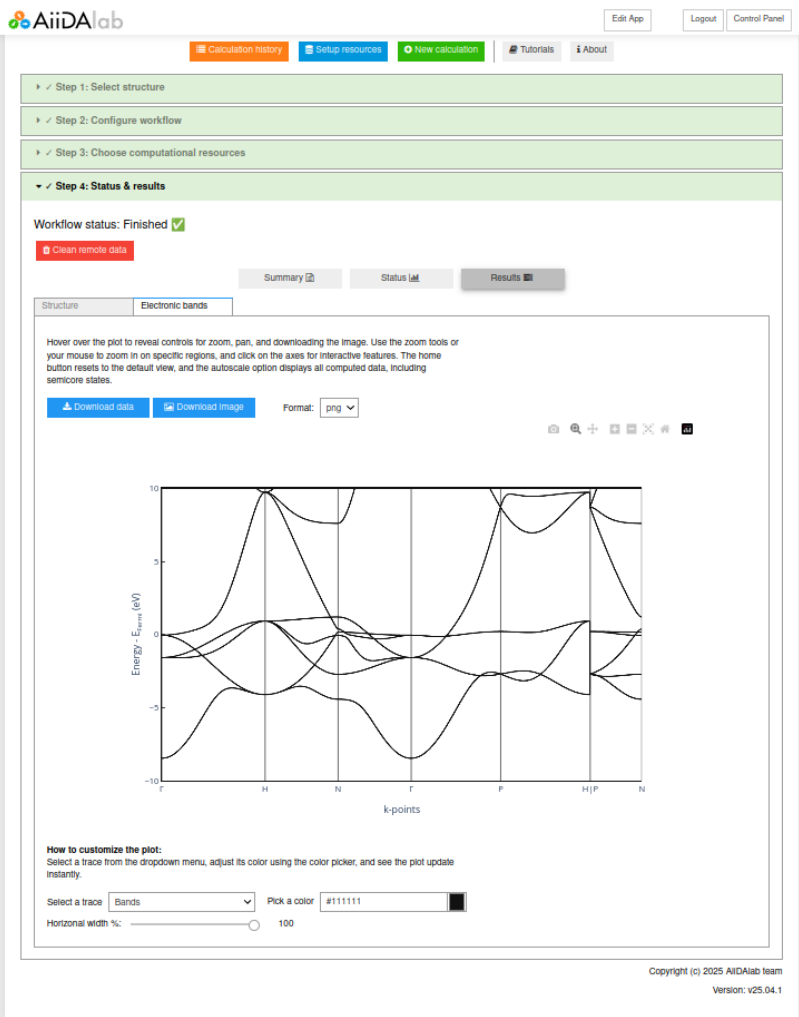
The screenshot shows the 'Step 4: Status & results' section of the AiiDA Quantum ESPRESSO App, specifically the 'Electronic bands' plot. The plot shows the energy E_{eV} versus the k-points. The plot includes two sets of bands: 'Bands (1)' (red lines) and 'Bands (2)' (blue lines). The plot is titled 'Electronic bands' and includes a 'Download data' button and a 'Download image' button. The plot also includes a 'Format' dropdown menu set to 'png'. The plot shows a clear band gap between the two sets of bands.

- ▶ 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.

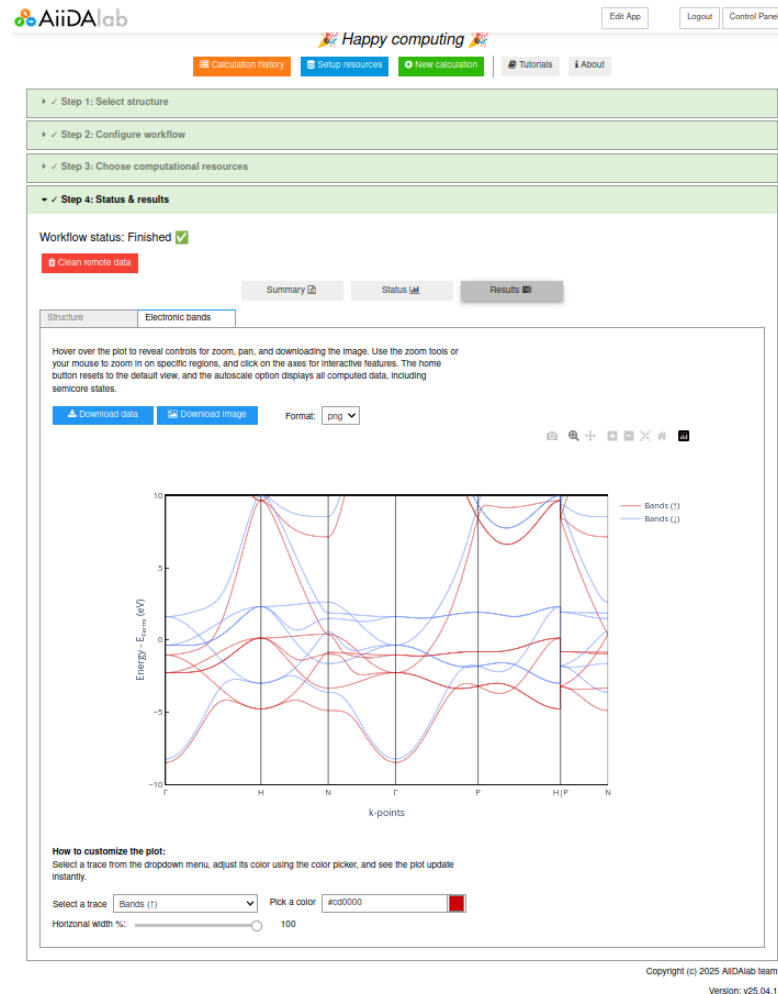
Non-magnetic Fe

Compare electronic bands

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.



Compare DFT total energies

Non-magnetic Fe

Magnetic Fe

The AiiDALab Quantum ESPRESSO App

Happy computing

Calculation history | Setup resources | New calculation | Tutorials | About

Step 1: Select structure
Step 2: Configure workflow
Step 3: Choose computational resources
Step 4: Status & results

Workflow status: Finished ✓

Clean remote data

Summary | Status | Results

Status overview

Collapse all

- Quantum ESPRESSO app workflow | finished | 2/2* jobs
- Electronic band structure workflow | finished | 2/2* jobs
- SCF workflow | finished | 1/1* job
- SCF cycle | finished
- Bands workflow | finished | 1/1* job

View in advanced panel

CalcJob: uid: 46a47b94-b8fe-4143-0329-1c47d3341e42 (pk: 2222)
(aidda.calculations.quantum espresso pw)

aidda.out

```
k = 0.0000 0.0000 0.8248 ( 1144 PWs) bands (ev):  
-68.8972 -35.2742 -35.2726 -35.2726 13.7173 13.7194 18.08  
18.7142 27.2096 27.6325 27.6325  
  
occupation numbers  
1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 0.00  
0.0000 0.0000 0.0000 0.0000  
  
the Fermi energy is 17.8057 ev  
  
total energy = -326.87661764 Ry  
total all-electron energy = -2543.282329 Ry  
estimated scf accuracy < 3.0E-11 Ry  
smearing contrib. (-TS) = -0.00169157 Ry  
internal energy Escf+TS = -326.87492607 Ry  
  
The total energy is Fe-ETS. E is the sum of the following  
one-electron contribution = -118.98654595 Ry  
hartree contribution = 65.54228028 Ry  
xc contribution = -34.34853773 Ry  
paw contribution = 177.89041671 Ry
```

*Actual number of jobs may exceed estimated total due to error handling, dynamic sub-workflows, and/or other runtime adjustments

Advanced status view

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► 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

The AiiDALab Quantum ESPRESSO App

Happy computing

Calculation history | Setup resources | New calculation | Tutorials | About

Step 1: Select structure
Step 2: Configure workflow
Step 3: Choose computational resources
Step 4: Status & results

Workflow status: Finished ✓

Clean remote data

Summary | Status | Results

Status overview

Collapse all

- Quantum ESPRESSO app workflow | finished | 2/2* jobs
- Electronic band structure workflow | finished | 2/2* jobs
- SCF workflow | finished | 1/1* job
- SCF cycle | finished
- Bands workflow | finished | 1/1* job

View in advanced panel

CalcJob: uid: cfaae9b2-bbf1-44c1-8822-9f3b0314320f (pk: 2267)
(aidda.calculations.quantum espresso pw)

aidda.out

```
occupation numbers  
1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 0.00  
0.0000 0.0000 0.0000 0.0000  
  
the Fermi energy is 17.7230 ev  
  
total energy = -326.91447233 Ry  
total all-electron energy = -2543.240183 Ry  
estimated scf accuracy < 1.9E-11 Ry  
smearing contrib. (-TS) = 0.00062446 Ry  
internal energy Escf+TS = -326.91509679 Ry  
  
The total energy is Fe-ETS. E is the sum of the following  
one-electron contribution = -111.08246962 Ry  
hartree contribution = 65.75371179 Ry  
xc contribution = -34.48489553 Ry  
ewald contribution = -173.09851671 Ry  
one-center paw contrib. = -74.08301692 Ry  
-> PAW hartree energy AE = 208.21312956 Ry  
-> PAW hartree energy PS = -207.34258015 Ry  
-> PAW xc energy AE = -108.91329147 Ry
```

*Actual number of jobs may exceed estimated total due to error handling, dynamic sub-workflows, and/or other runtime adjustments

Advanced status view

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