winmostar tutorial

Quantum ESPRESSO Structural Optimization Calculation

V11.6.5

20 February 2024　X-Ability Co., Ltd.

About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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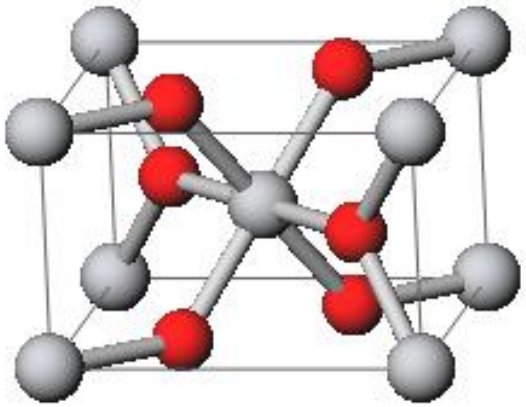
Overview

- This tutorial demonstrates the structural optimization calculation of a rutile-type TiO2 crystal, optimizing both the cell and atomic positions simultaneously.



Note:

- The choice of k-points, number of bands, type of pseudopotentials, and cutoff energy can significantly impact the calculation results.

◆ For a detailed explanation of Quantum ESPRESSO's calculation methods and settings, please see the following article from our company: https://qiita.com/xa_member

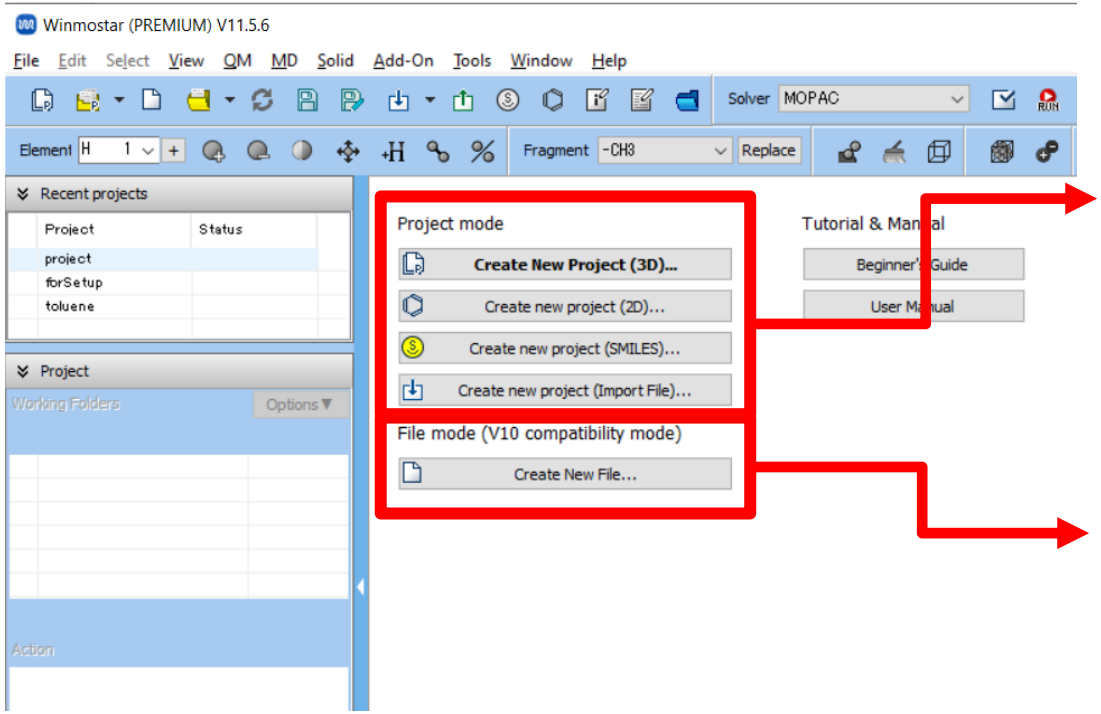
Preference of Operating Environment

- For users of Winmostar version V11.5.0 or later on a 64-bit environment, please install and configure CygwinWM version 2023/04/05 or later.
  - The CygwinWM version after 2023/04/05 includes the recommended version of 64-bit Quantum ESPRESSO.

- If the above does not apply to you or if you wish to use a version of Quantum ESPRESSO other than the recommended one, you will need to install and configure Windows version of Quantum ESPRESSO separately.

Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to Quantum ESPRESSO tutorial for version 10.



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

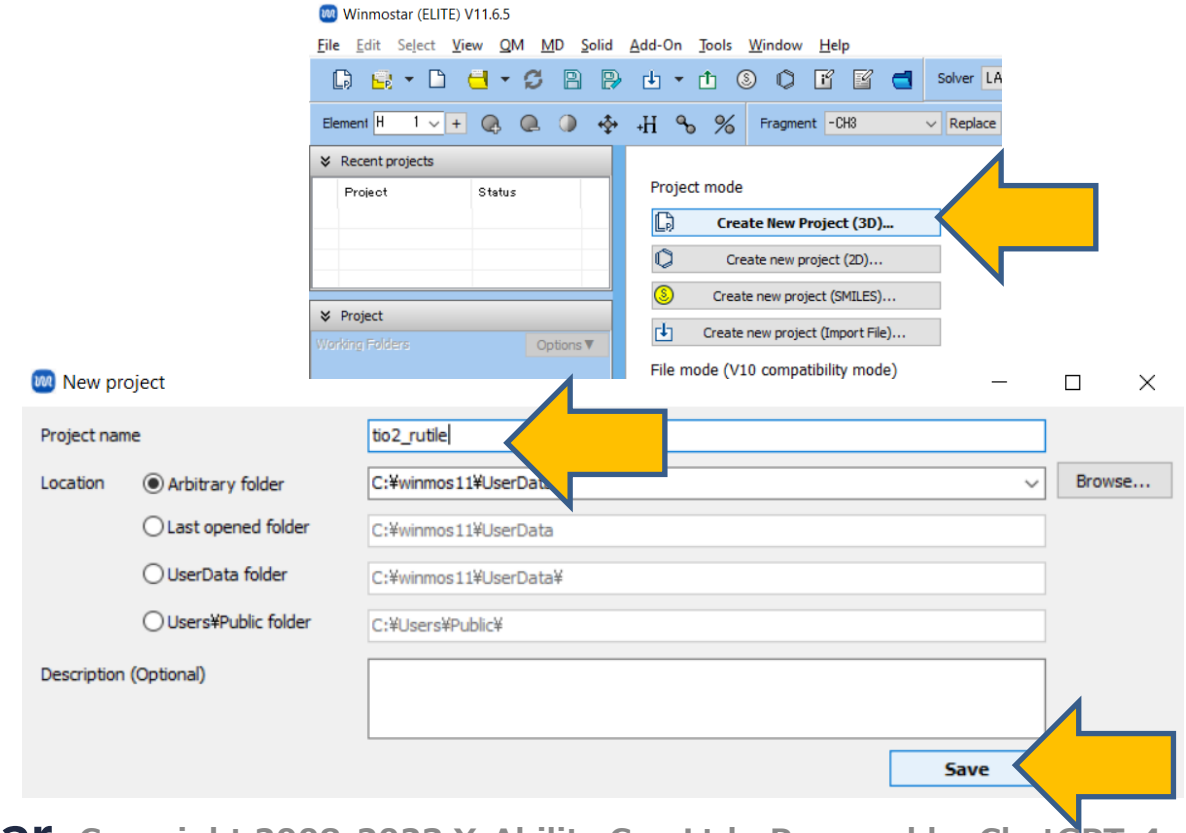
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

Please refer to QE Basic Tutorial for the basic operation method.

A. Launch Winmostar and click **Create New Project (3D)**. (If it is already open, click **File | Close** first.)

B. Enter '`tio2_rutile`' in **Project name** and click **Save**.



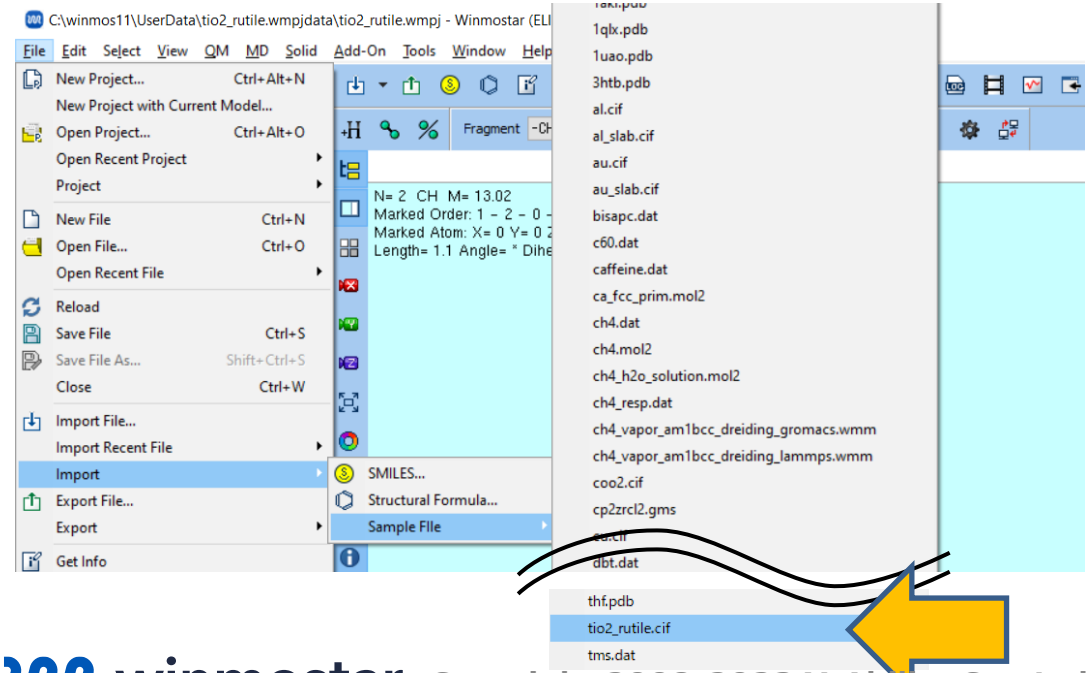
A. Modeling of the System

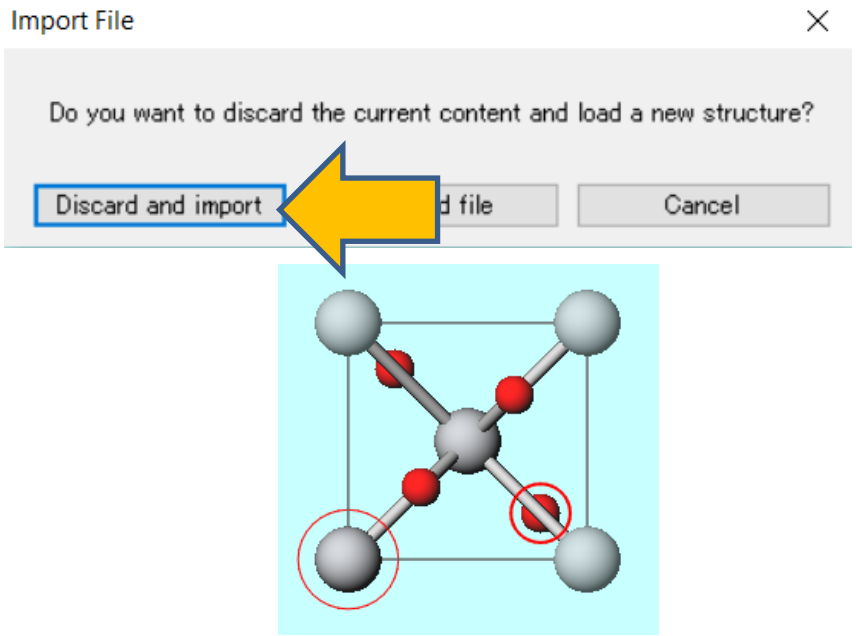
For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Methods for Creating Initial Structures'. Here, we will load an existing molecular structure file.

A. Click **File | Import | Sample File | tio2_rutile.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

B. In **Import File** dialog, click **Discard and import**.

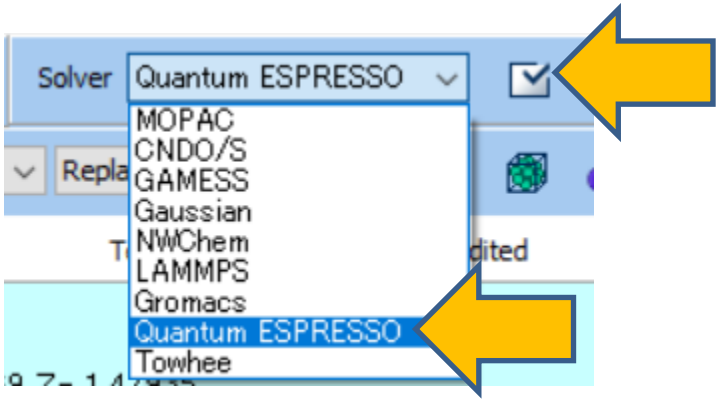
C. Confirm that the desired structure appears in Viewport.

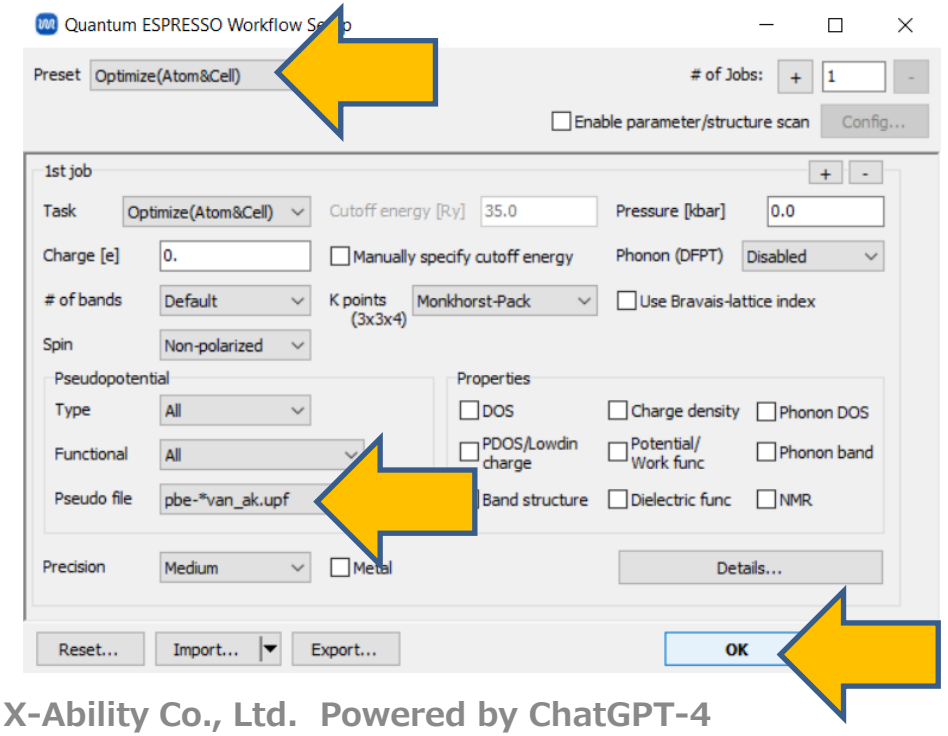




B. Execution of Calculation

A. Select **Quantum ESPRESSO** from **Solver** and click **(Workflow Setup)**.
B. Select **Optimize (Atom&Cell)** from **Preset**.
C. Change **Pseudo file** to **pbe-*van_ak.upf**.
D. If you wish to reduce the computational precision to speed up the calculation, change **Precision** to 'Low'.
E. Click **OK**, adjust settings as needed in **Job Setting** window, and then click **Run**.





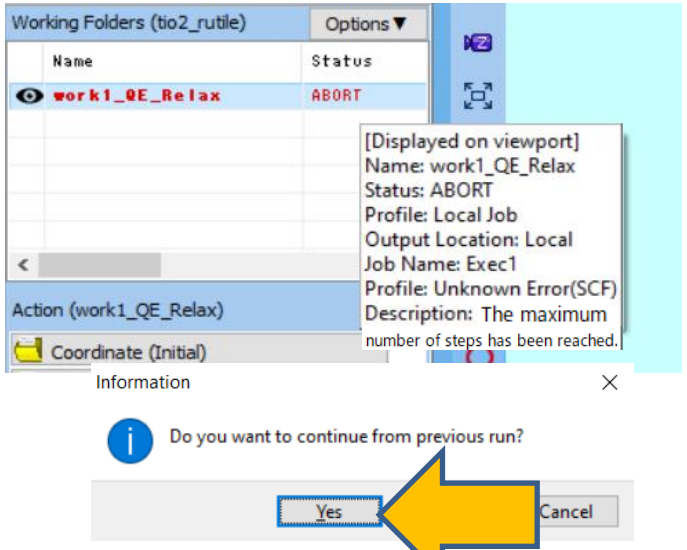
Supplement: Continuing Structure Optimization Calculation When Convergence is Not Achieved

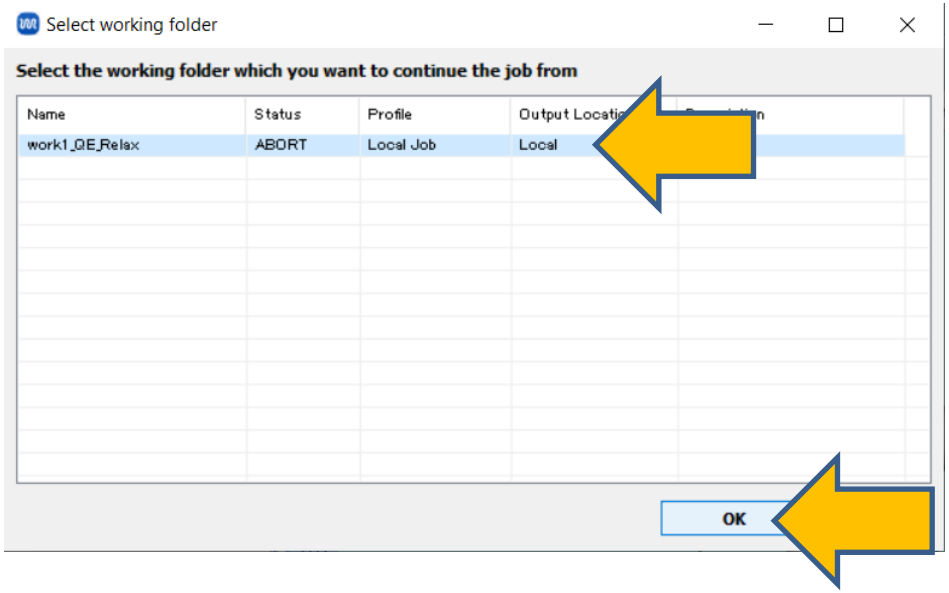
A. If the SCF calculation does not converge, **the status** will be displayed as **ABORT**. Hovering the cursor over work1_QE_Relax will display the error message 'The maximum number of steps has been reached.'

B. Click **(Workflow Setup)**, and if asked 'Do you want to continue from previous run?', click **Yes**.

C. When 'Select working folder' appears, select the original job and click **OK**. If a warning is displayed, click **Yes**.

D. Adjust the calculation conditions in the Workflow Setup window just like the first job and execute the job.

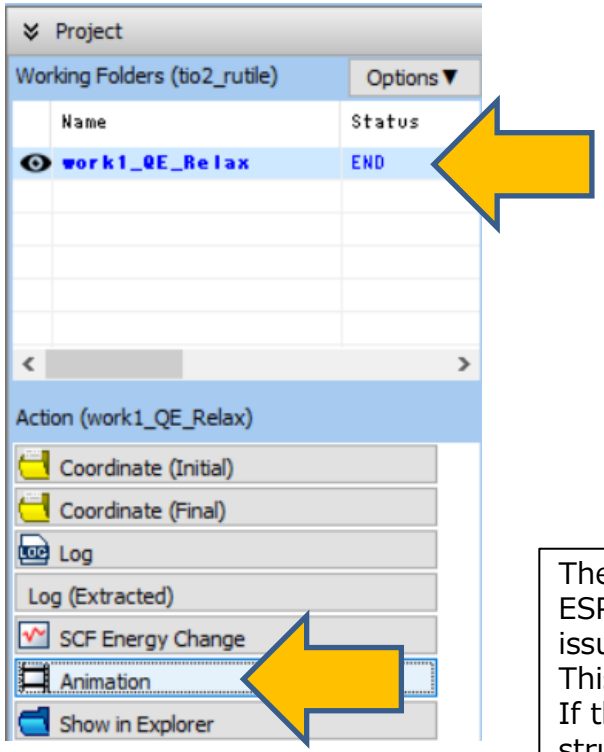


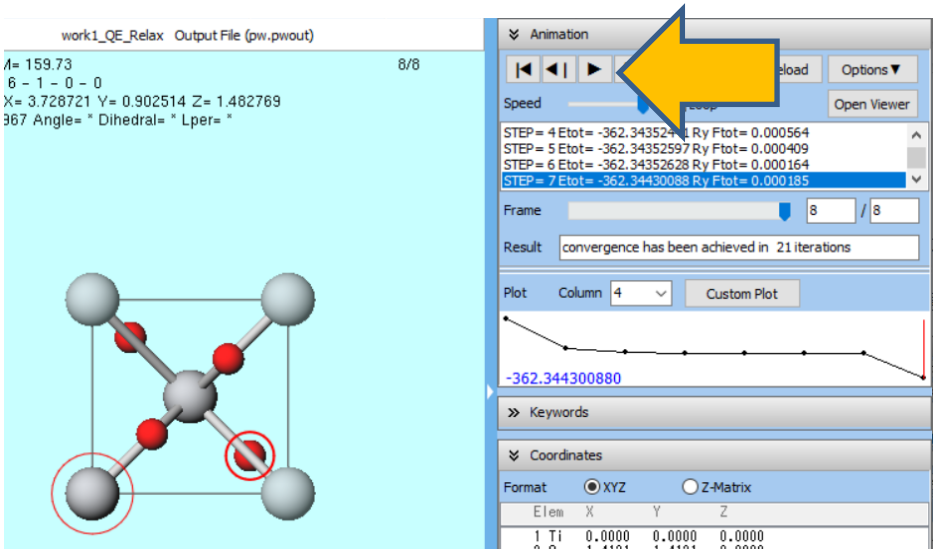


C. Analysis of Results

A. After **the state** of **work1_QE_Relax** folder changes to **END(blue)** in **Working Folders**, click work1_QE_Relax in **Working Folders** and click **Animation** in **Action** menu to bring up Animation panel on the right side of Main Window.

B. Clicking ▶ **(play)** button allows you to observe the optimization of both the cell and atomic positions on the main screen.

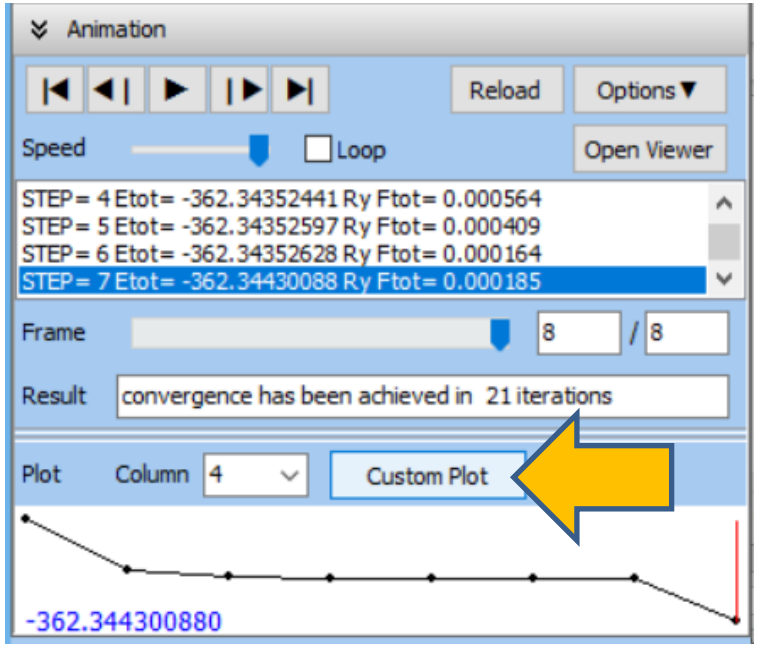


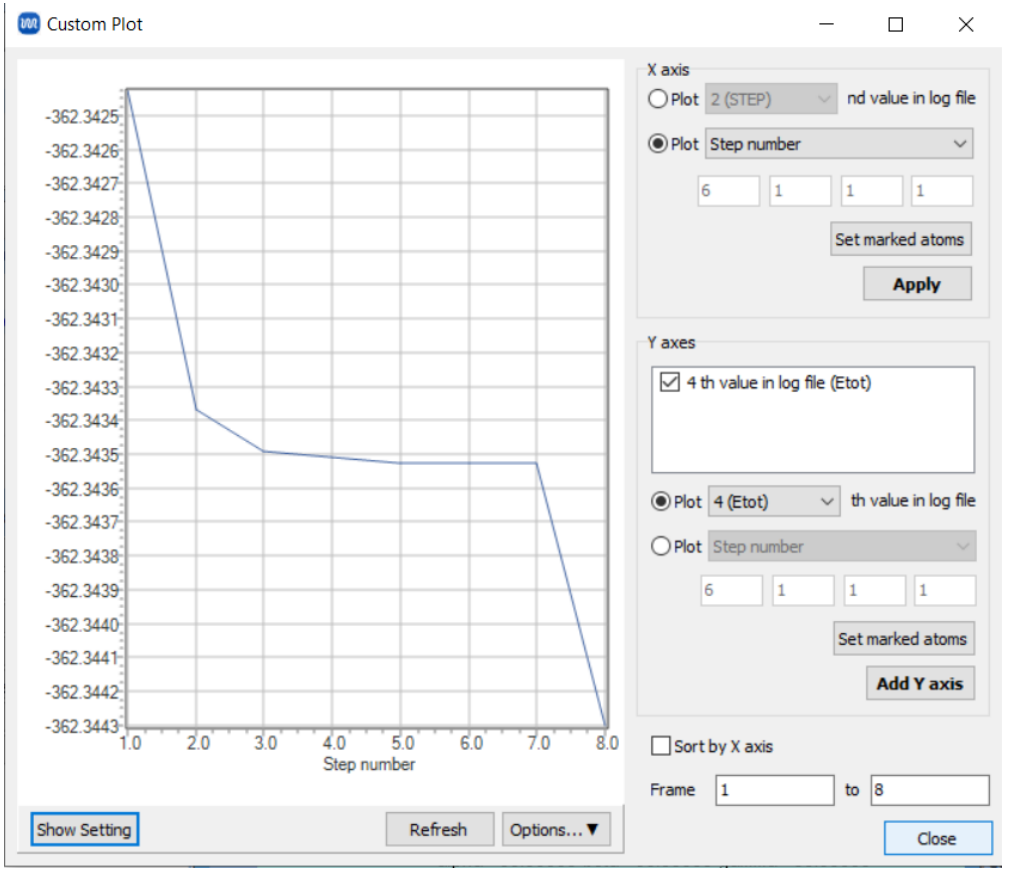


The slight discontinuity in energy change at the end occurs because Quantum ESPRESSO redraws the set of plane waves used only for the final calculation to avoid issues related to Pulay stress.
This jump in energy can be somewhat mitigated by increasing the cutoff energy.
If the initial structure significantly differs from the final structure, a subsequent structure optimization calculation is performed.

C. Analysis of Results

A. Clicking **Custom Plot** button opens **Custom Plot** window.

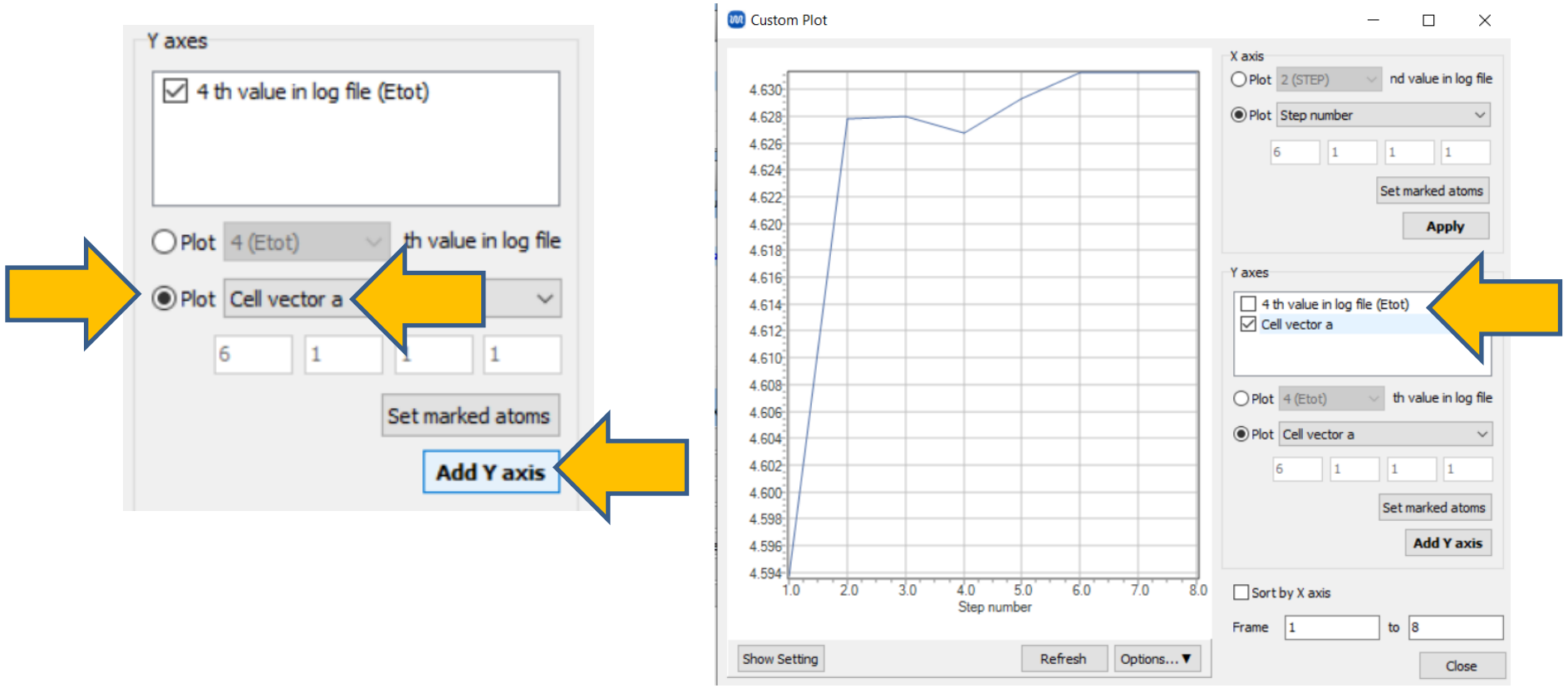




C. Analysis of Results

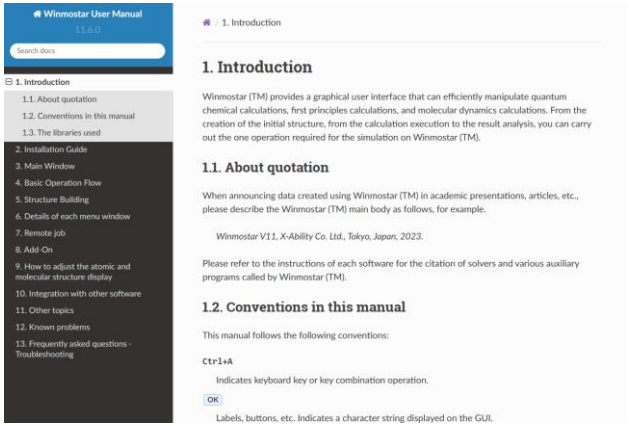
A. Check the second **Plot** in **Y axes** and select **Cell vector a** from the dropdown. Then, click **Add Y axes** button to add **Cell vector a** to the list.

B. Uncheck the default checked item, **4th value in log file (Etot)**, in **Y axes** list to plot the optimization of the lattice constant in the a-axis direction.



Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

Scenes from Winmostar Training Session

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