winmostar tutorial

Quantum ESPRESSO Convergence Test

V11.6.5

8 April 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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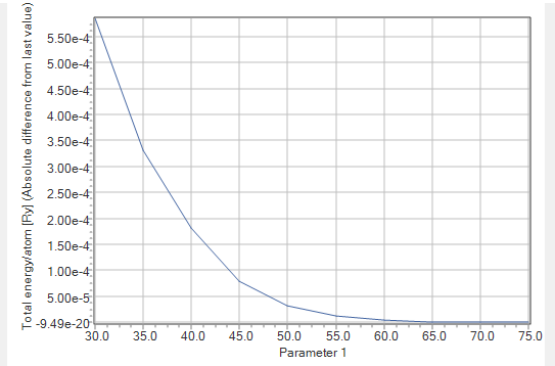
Overview

- This tutorial requires Winmostar V11 Professional Elite Edition.
- In this tutorial, we will conduct a convergence test by performing calculations on a Si crystal SCF calculation with varied cutoff energies and k-point numbers, introducing the procedure to find the optimal cutoff energy and k-point numbers.
- Firstly, we will scan the cutoff energy, followed by a scan of the k-point interval.
- In this manual, we will consider the calculation to have converged when the change in total energy from one parameter set to the next falls below a predetermined threshold (in this book, we set a relatively high precision threshold of 1 meV ≈ 0.00007 Ry ≈ 0.02 kcal/mol).



Note :

- The convergence behavior varies depending on the element, the pseudopotential used, and the type of functional.

◆ 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

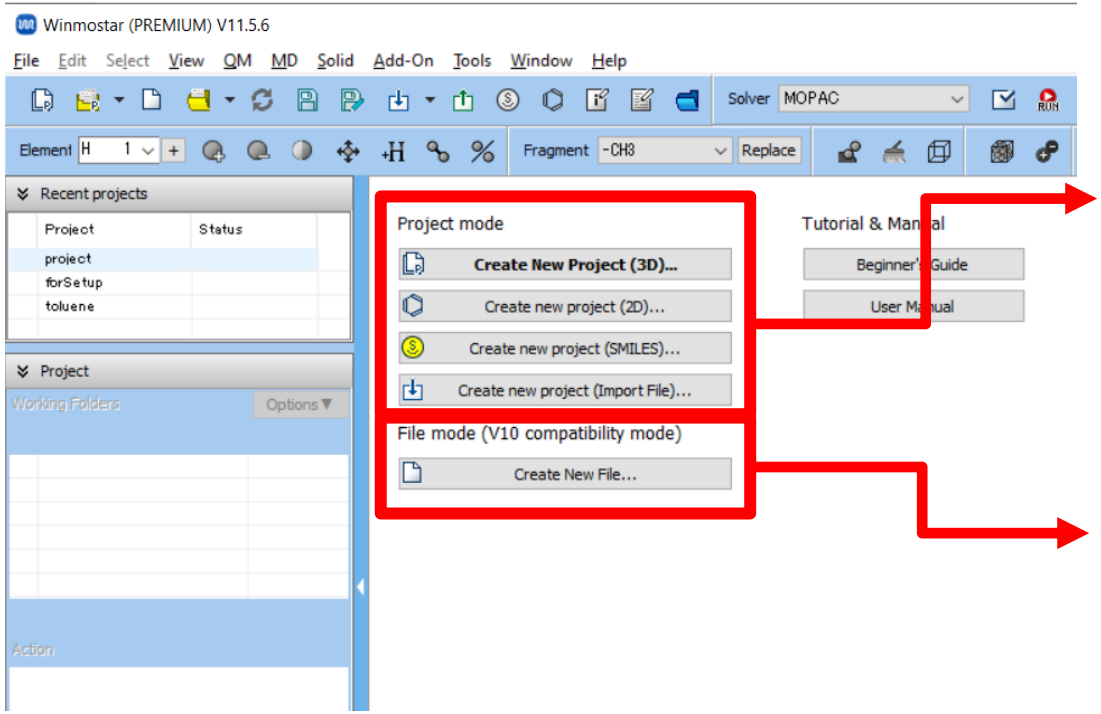
Preference of Operating Environment

- 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.

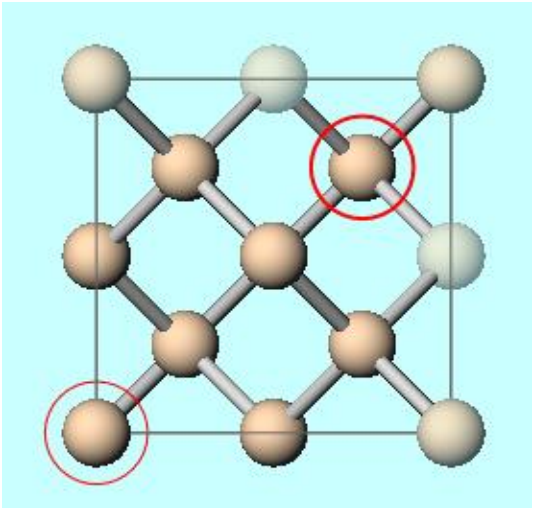
A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

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

For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Structure Building'.Here, we load an existing molecular structure file.

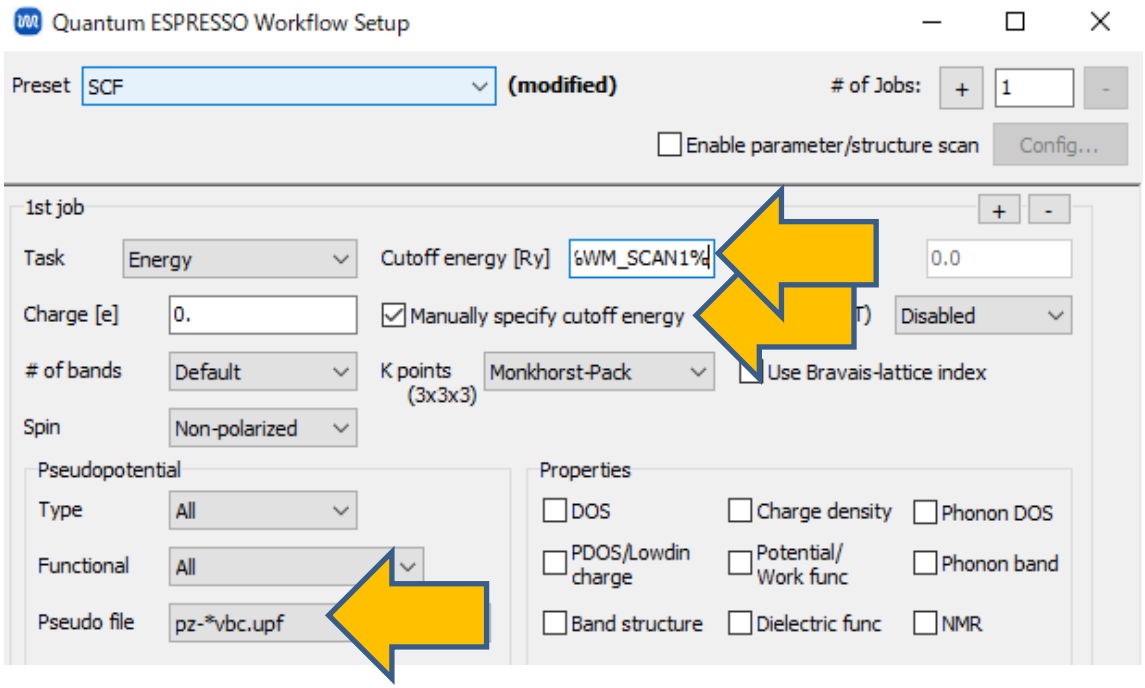
C. Click **File | Import | Sample File | si.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

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



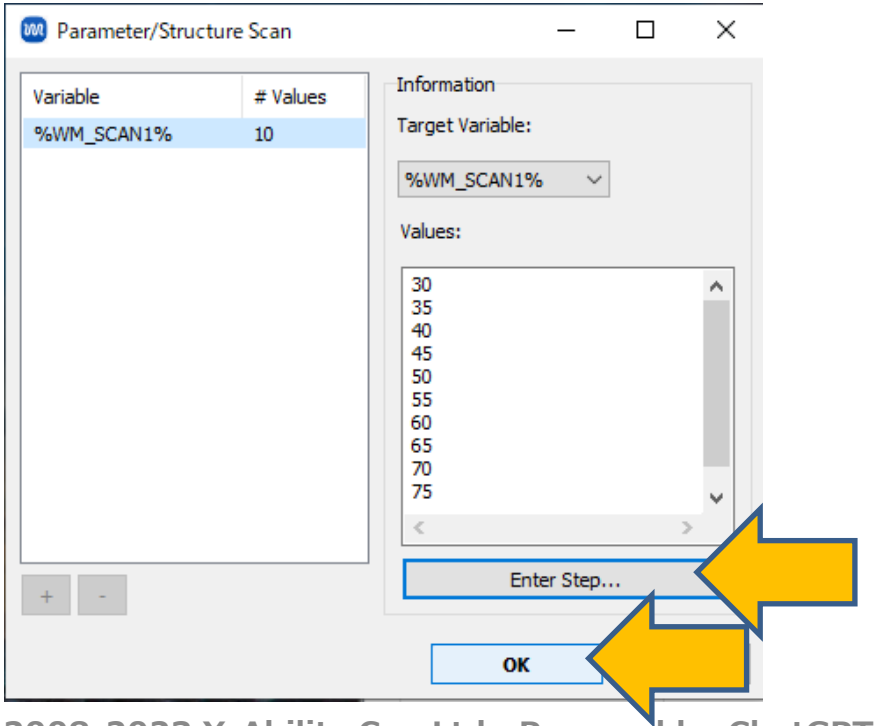
B. Execution of Calculation (Scanning of Cutoff Energy)

A. Select **Quantum ESPRESSO** from **Solver**, and then click **(Workflow Setup)**.
B. Click **Yes** when asked, 'Current cell can be converted to primitive cell···Do you want to convert?'
C. Change **Pseudo file** to **pz-*vbc.upf**.
D. Check **Manually specify cutoff energy** and enter '`%WM_SCAN1%`' as **Cutoff energy**.



B. Execution of Calculation (Scanning of Cutoff Energy)

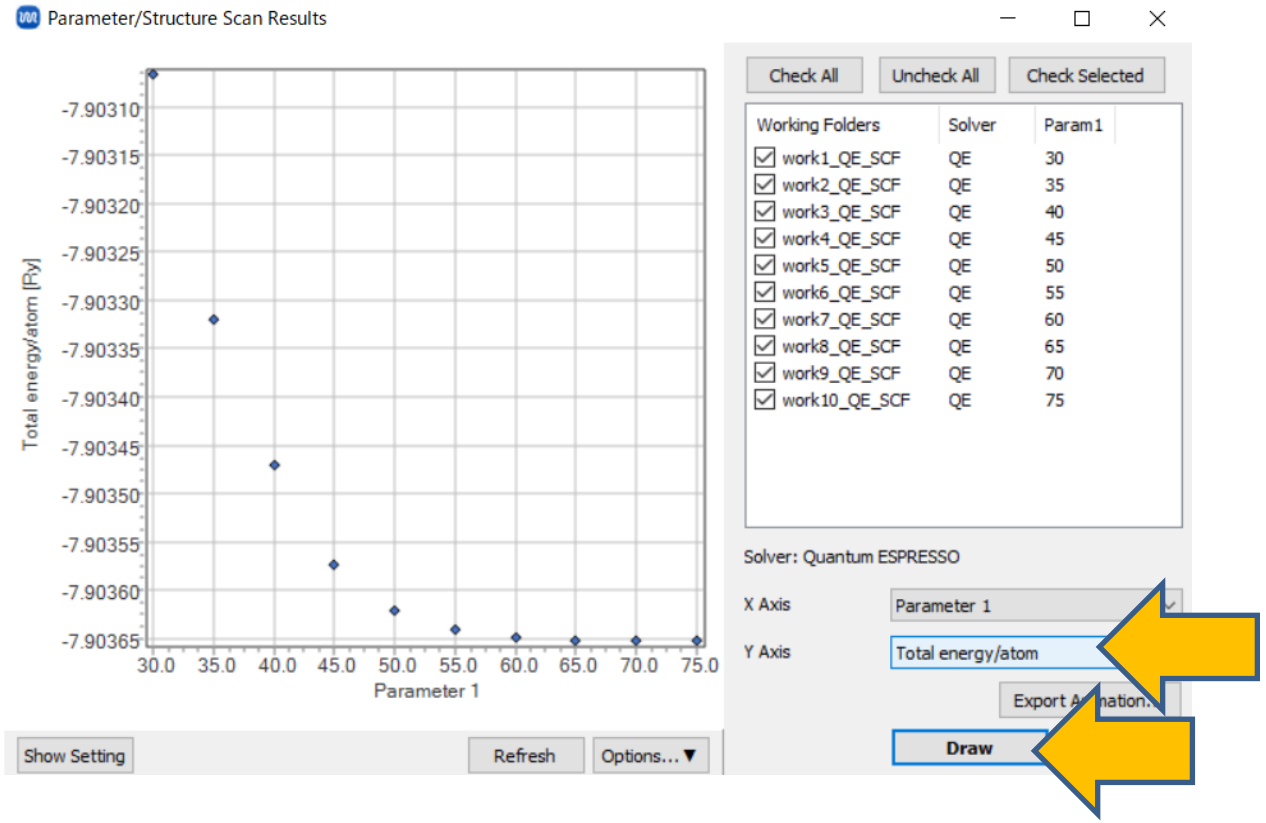
A. Check **Enable parameter/structure scan** and click **Config**.
B. Click **Enter Step**, and enter '30' for Minimum Value, '5' for Interval, and '10' for Number of steps.
C. Click **OK** to close **Parameter/Structure Scan** window.
D. In **Quantum ESPRESSO Workflow Setup** window, click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.



C. Analysis of Results (Scanning of Cutoff Energy)

A. Once **the status** of work folders from work1_QE_SCF to work10_QE_SCF changes to **END** or **END(-)**, click **File | Project | Parameter/Structure Scan Results**.

B. Select **Total energy/atom** for **Y Axis** and click **Draw** to display the total energy per atom for each parameter (in this case, Cutoff energy).

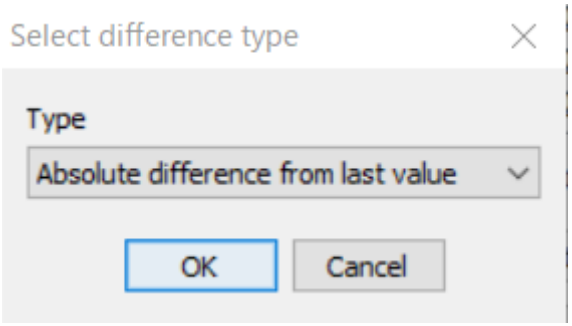


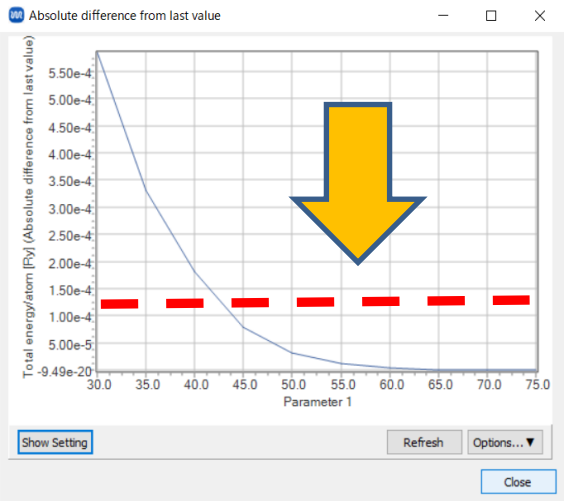
C. Analysis of Results (Scanning of Cutoff Energy)

A. Click **Options | Calculate Differences from First/Last Value** in the bottom right of the graph. Select 'Absolute difference from last value' as **Type** and click **OK** (since higher accuracy is achieved as the scanned parameter increases, the difference from the last value is chosen). The change in total energy per atom when varying the parameter will be displayed.

B. In this manual, we determine convergence at 50 Ry, where the graph values fall below the threshold of approximately 0.00007 Ry.
   - As stated at the beginning of this manual, we have adopted a threshold that requires relatively high precision.

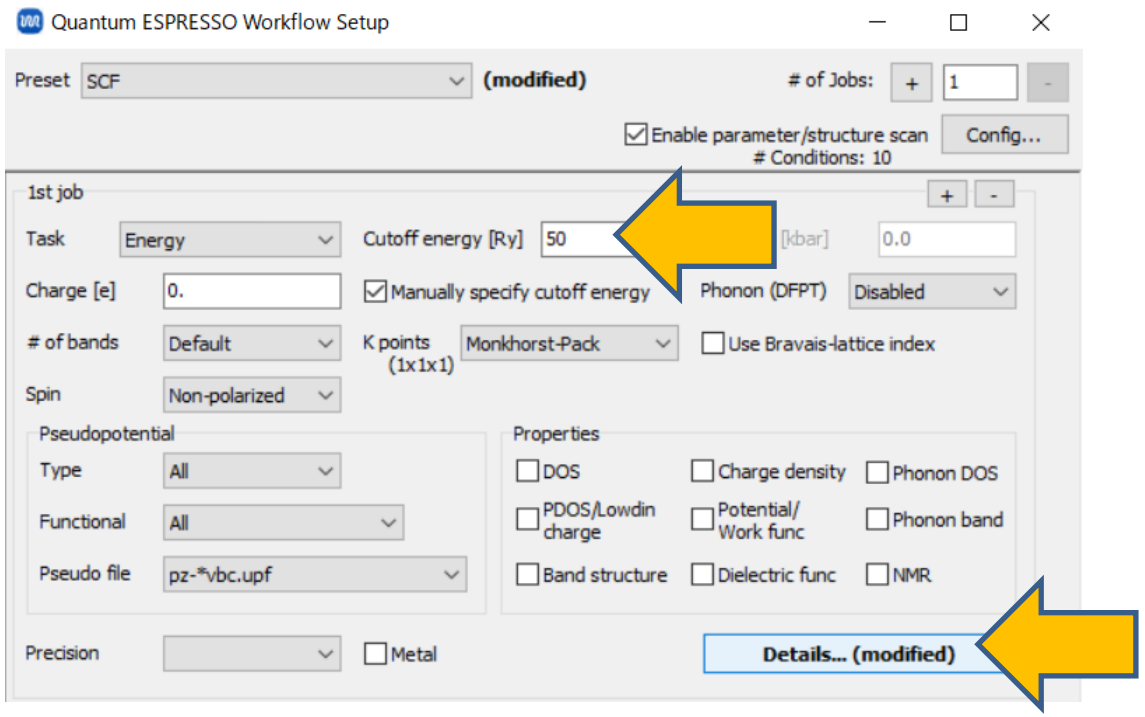
C. After reviewing the graph, click **Close**, and then click **Cancel** to close **Parameter/Structure Scan Result** window.

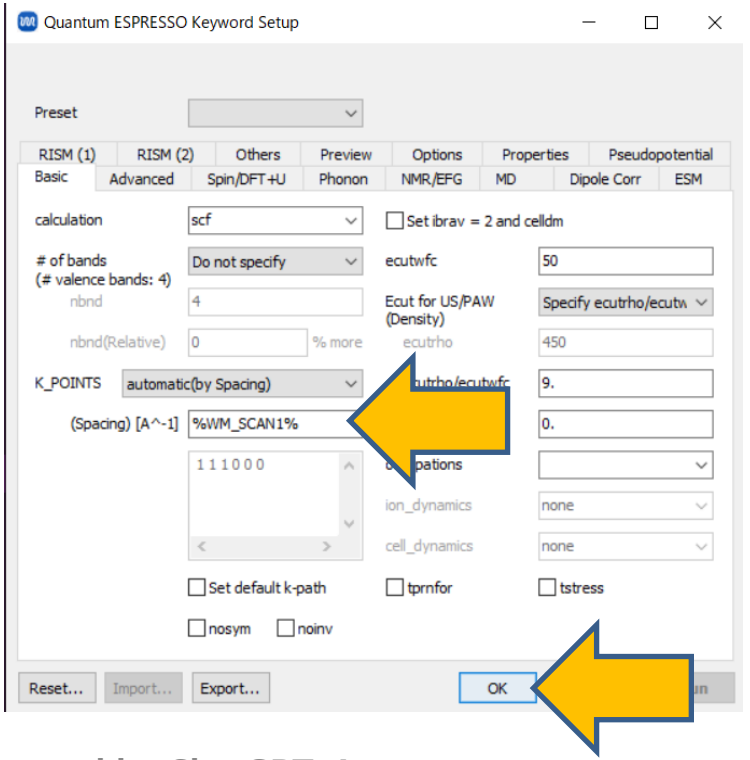




D. Execution of Calculation (Scanning of k-Point Numbers)

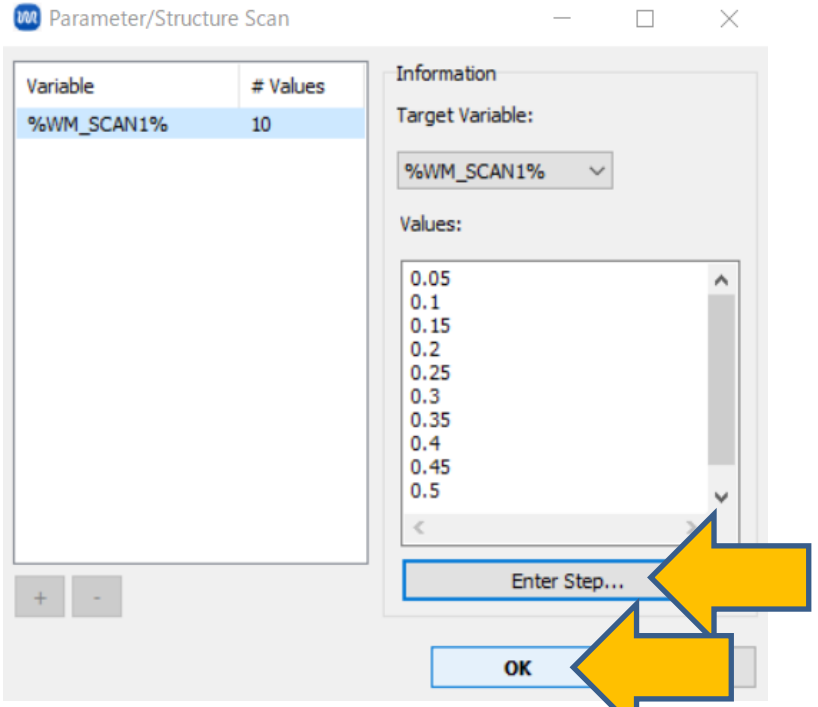
A. Click **(Workflow Settings)** and click **No** when asked 'Do you want to continue from previous run?'.
B. Enter the value determined on P. 10 for **Cutoff energy** ('50').
C. Click **Details**, enter '%WM_SCAN1%' for **K_POINTS** (Spacing), and click **OK**.





D. Execution of Calculation (Scanning of k-Point Numbers)

A. Click **Config** next to **Enable parameter/structure scan**.
B. Click **Enter Step**, and enter '0.05' for Minimum Value, '0.05' for Interval, and '10' for Number of steps.
C. Click **OK** to close **Parameter/Structure Scan** window.
D. In **Quantum ESPRESSO Workflow Setup** window, click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.

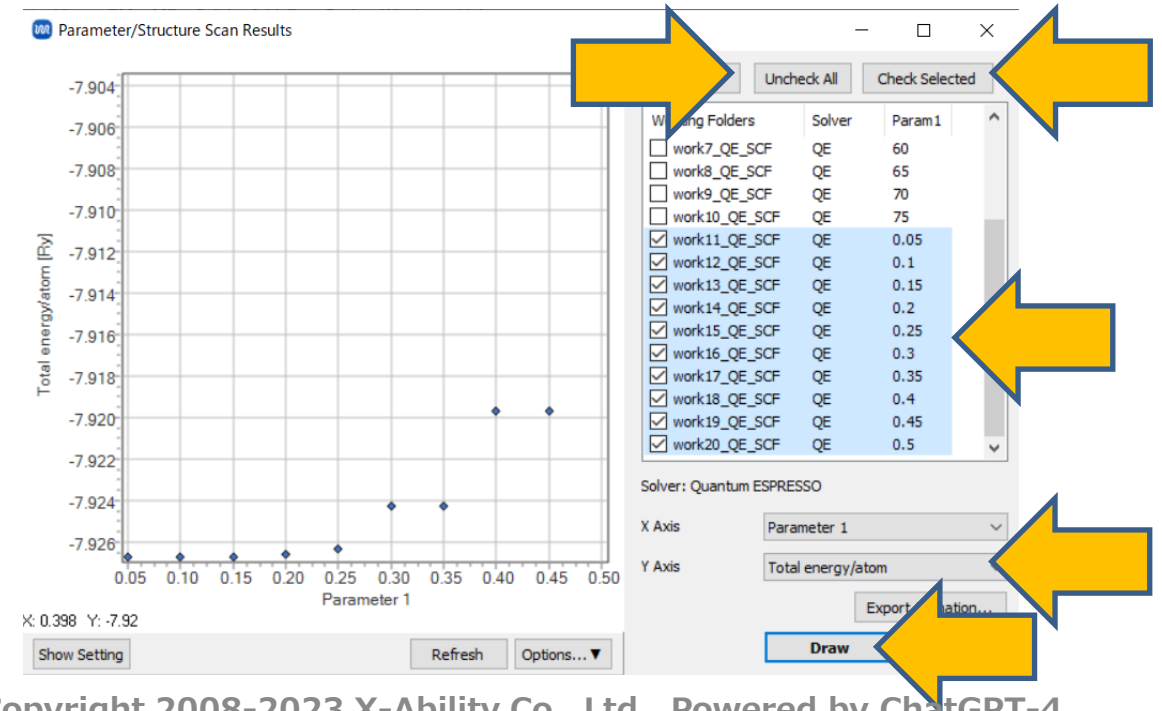


E. Analysis of Results (Scanning of k-Point Numbers)

A. Once **the status** of work folders from work11_QE_SCF to work20_QE_SCF changes to **END** or **END(-)**,Click **File | Project | Parameter/Structure Scan Results**.

B. Click **Uncheck All**, then select work11 to work20 from the list of **Working Folders** by Shift+clicking for multiple selection, and click **Check Selected**.

C. Select **Total energy/atom** for **Y Axis** and click **Draw** to display the total energy per atom for each parameter (in this case, K spacing).

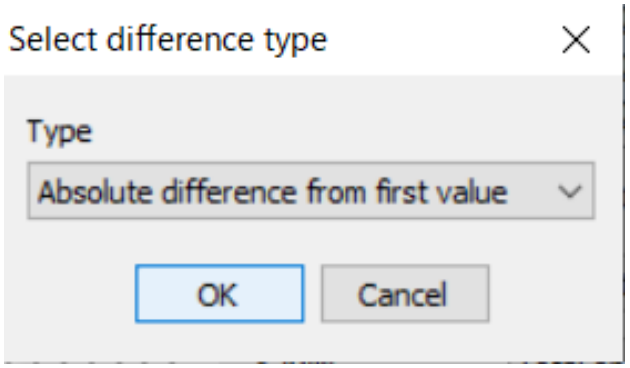


E. Analysis of Results (Scanning of k-Point Numbers)

A. Click **Options | Calculate Differences from First/Last Value** in the bottom right of the graph. Select **Absolute difference from first value** as **Type** and click **OK** (since higher accuracy is achieved as the scanned parameter decreases, the difference from the first value is chosen).

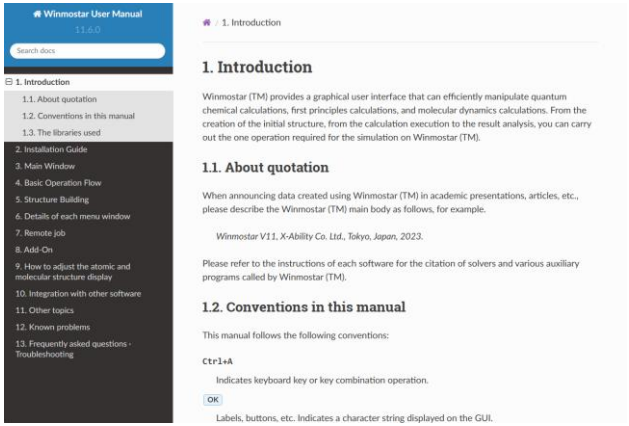
B. As the vertical axis shows significant changes making it difficult to read the values, click **Show Setting** in the bottom left of the graph, and check **Logarithm** for **Y Axis**. Similar to P.10, the calculations in this book determine convergence at a k-point Spacing of 0.15 Å^-1.

   – As stated at the beginning of this book, a relatively high precision threshold has been adopted.



Finally

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



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
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