winmostar tutorial

Quantum ESPRESSO Bulk Modulus

V11.6.5

3 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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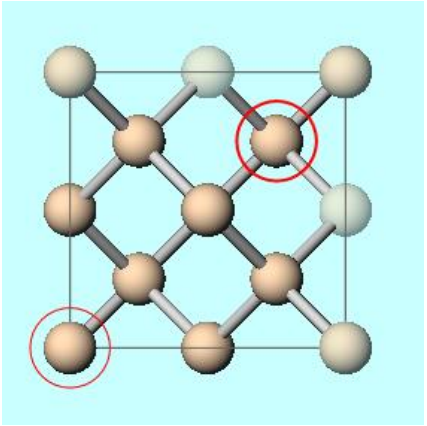
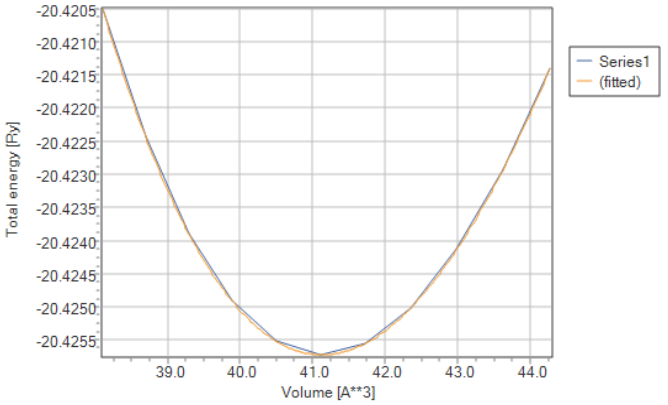
Overview

- This tutorial requires Winmostar V11 Professional Elite Edition.
- In this manual, we first carry out structural optimization calculations for Si crystals. Then, we generate multiple structures scaled from the optimized structure and execute self-consistent field (SCF) calculations consecutively on each, demonstrating the procedure to calculate the bulk modulus from the volume-energy diagram obtained thereby.





Note:

- The choice of k-points, type of pseudopotentials, and cutoff energy can impact the calculation results. In this tutorial, settings with reduced accuracy are used to obtain results more quickly.
- The appropriate range for scanning volumes may vary depending on the material.
- 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

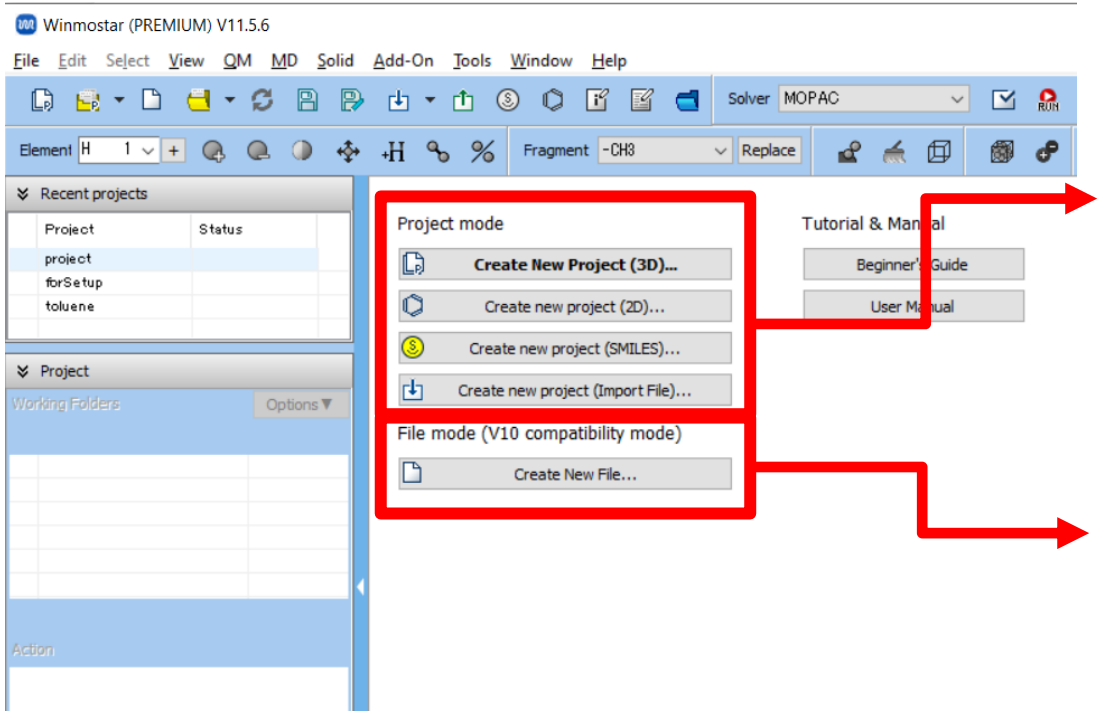
Preference of Operating Environment

- 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.



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 (Initial Structure)

- Please refer to QE Basic Tutorial for the basic operation method.
- For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Methods for Creating Initial Structures'.

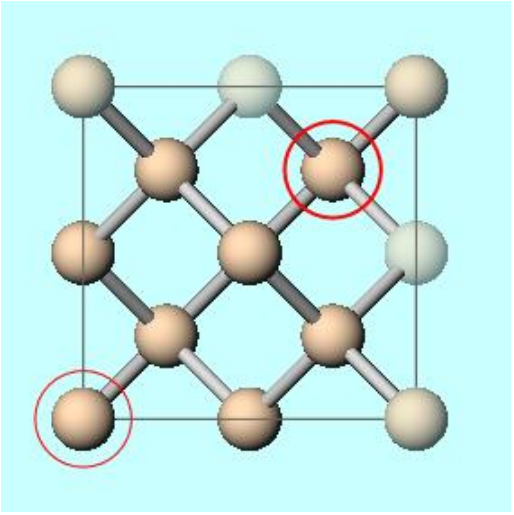
A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

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

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. Click **Discard and import** in **Import File**.

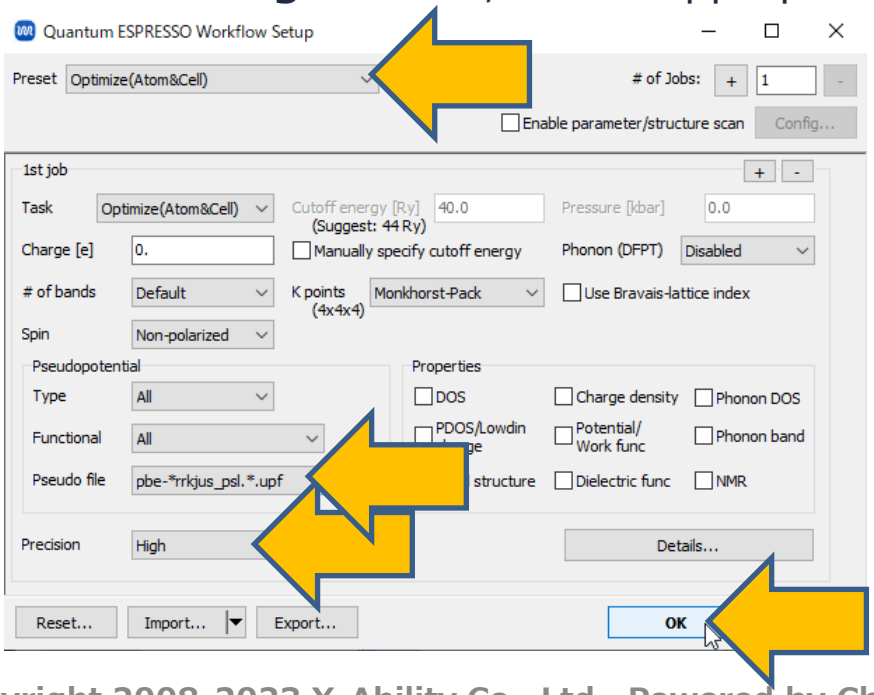


B. Execution of Calculation (Structural Optimization Calculation)

A. Select **Quantum ESPRESSO** from **Solver** in Toolbar and click **(Workflow Setup)**. If asked whether to convert to a primitive cell, click **Yes**.

B. Change **Preset** to 'Optimize (Atom & Cell)', then change **Pseudo file** to 'pbe-rrkjus_psl.upf' and **Precision** to 'High'.
   - If you want to reduce the calculation accuracy to finish the calculation faster, set **Precision** to 'Medium'.

C. Click **OK**, then, in **Job Setting** window, make appropriate settings before clicking **Run**.

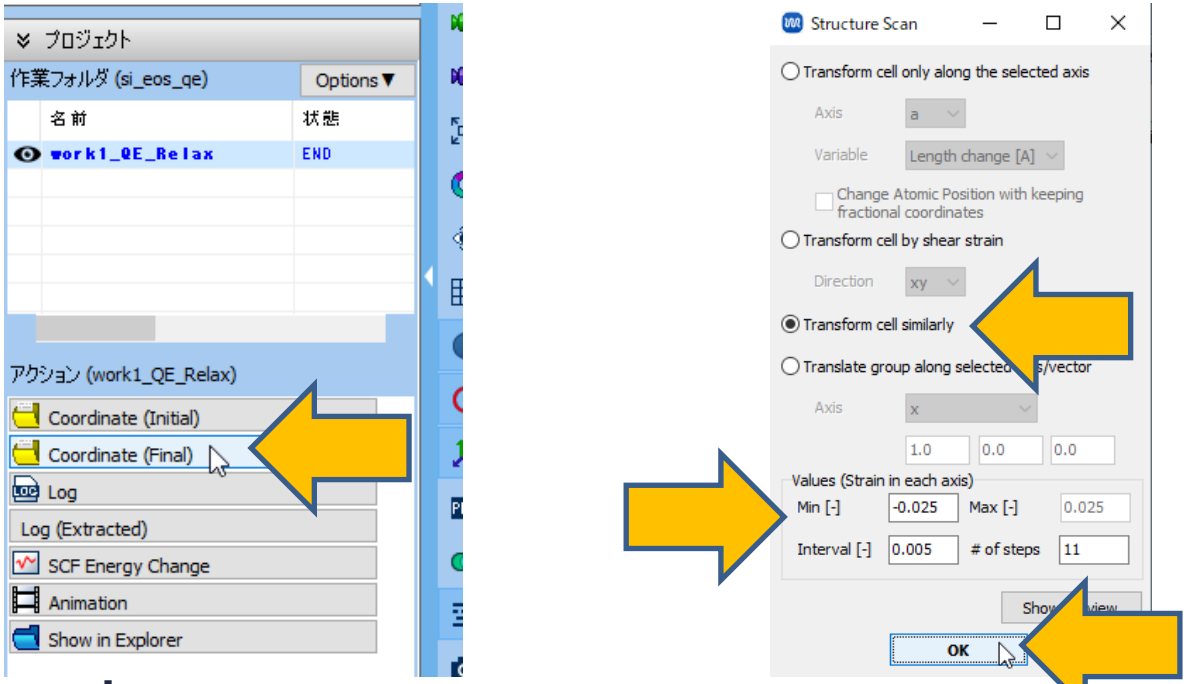


C. Modeling the System (Volume-Modified Structures)

A. Once **the status** of work1_QE_Relax changes to **END**, click **Coordinate (Final)** in **Action**.

B. Click **Tools | Structure Scan**. If prompted with '...Do you want to change to an output-ready format (wmm) and continue?', click **Yes**. If asked 'Do you want to overwrite and save changes?', click **No**.

C. Check the box for **Transform cell similarly** and enter '-0.025' in **Min** for **Value**, '0.005' for **Interval**, and '11' for **# of steps**, then click **OK**.



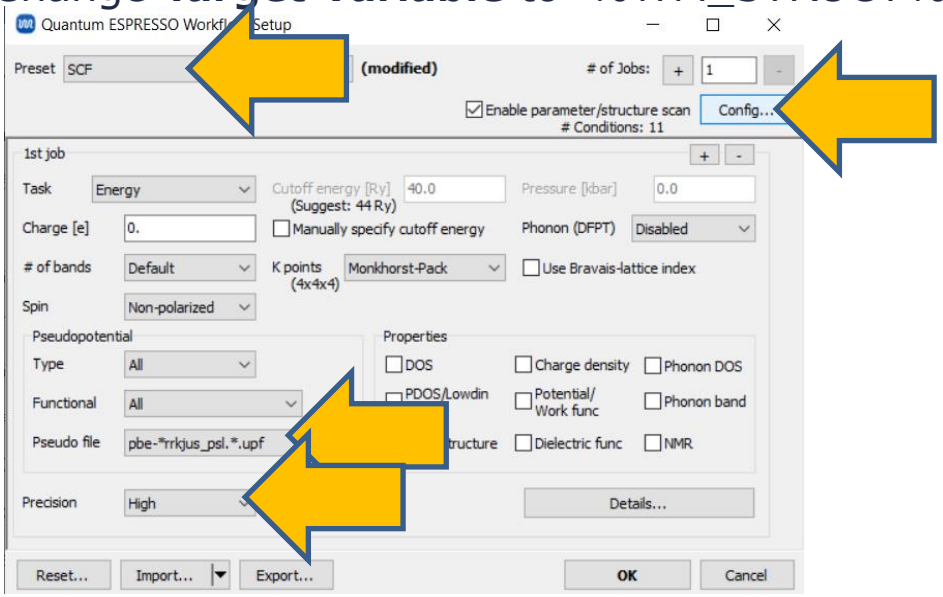
D. Execution of Calculation (Volume-Modified Calculations)

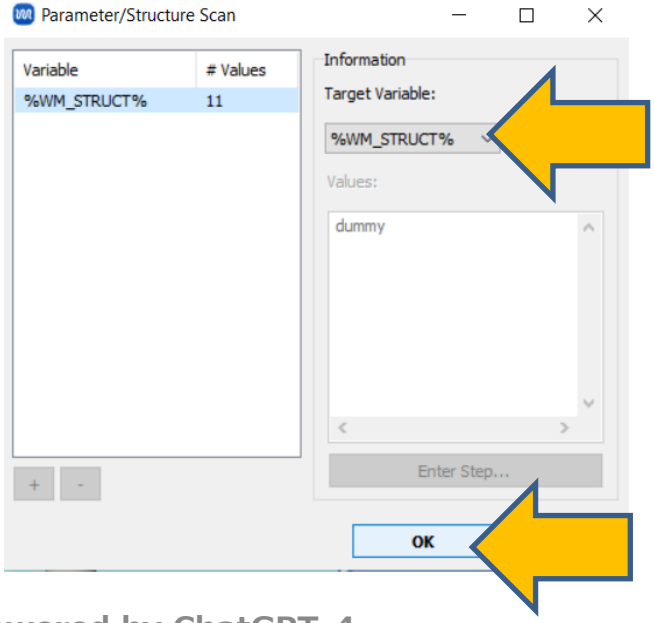
A. Click **(Workflow Setup)** in Toolbar. If asked 'Do you want to contune from previous run?', click **No**.

B. Change **Preset** to 'SCF', then change **Pseudo file** to 'pbe-rrkjus_psl.upf' and **Precision** to 'High'.
   - If you want to reduce the calculation accuracy to finish the calculation faster, set **Precision** to 'Medium'.

C. Check the box for **Enable parameter/structure scan** and click **Config**.

D. Change **Target Variable** to '%WM_STRUCT%' and click **OK**.

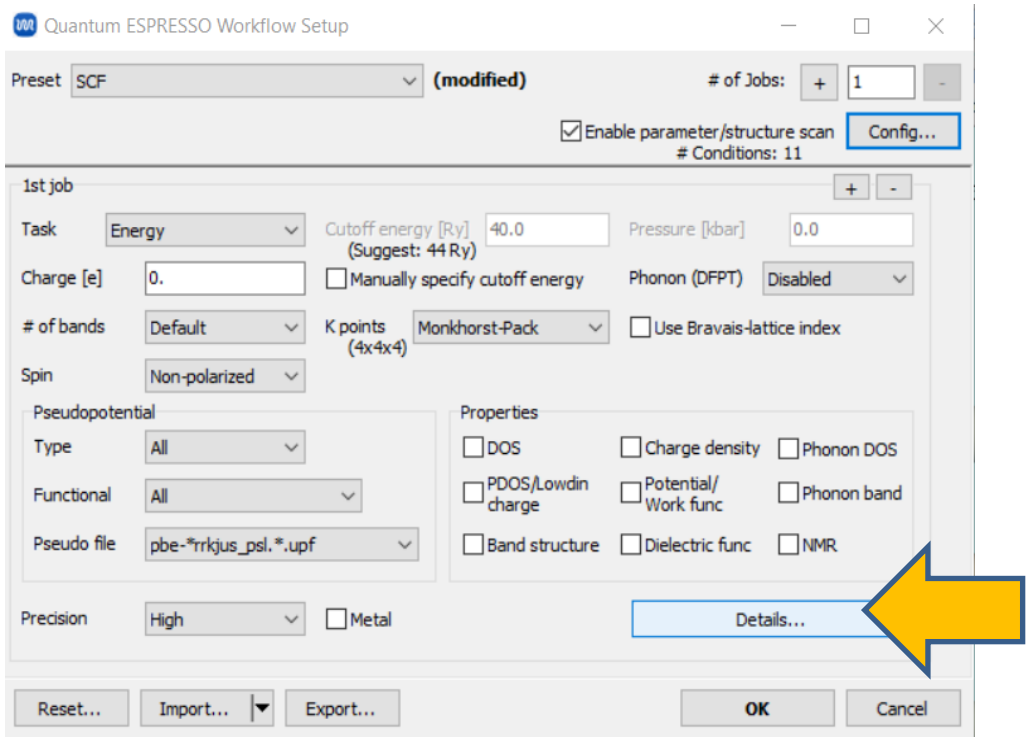


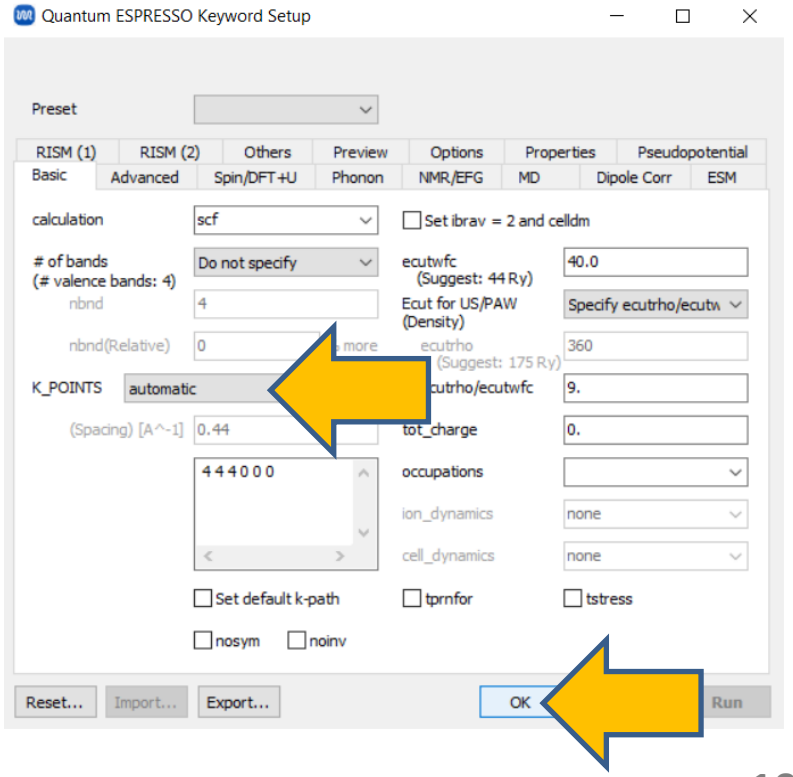


D. Execution of Calculation (Volume-Modified Calculations)

A. To perform calculations on structures of varying volumes with the same number of k-points, click **Details** and change **K_POINTS** to 'automatic', then click **OK**.
   – If you wish to calculate stress as well, also check the box for **tstress**.

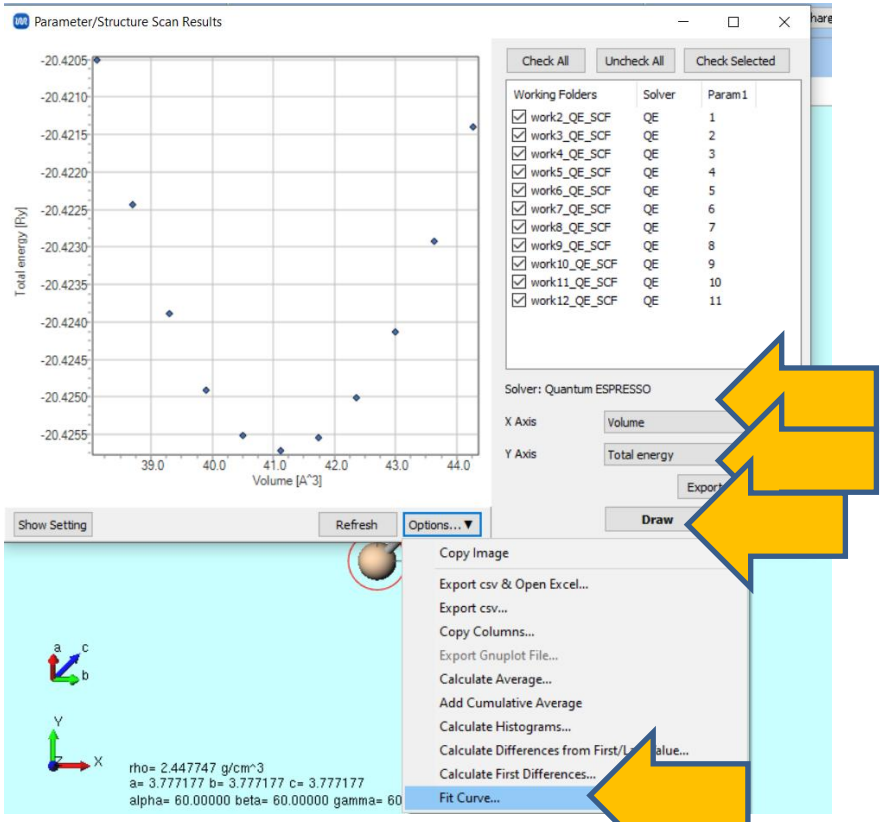
B. In **Quantum ESPRESSO Workflow Setup** window, click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.





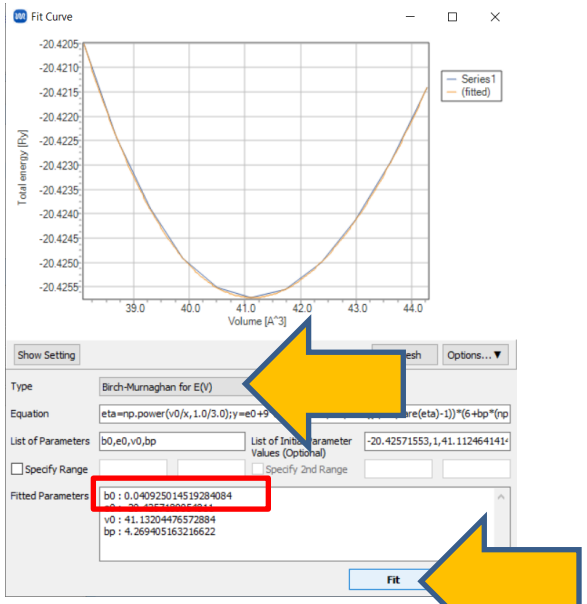
E. Analysis of Results

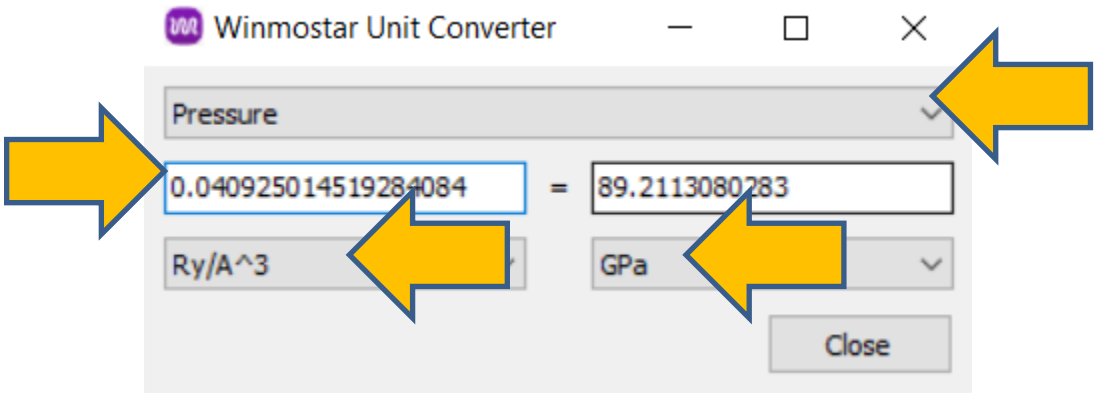
A. Once **the status** of work2 to work12 changes to **END**, click **File | Project | Parameter/Structure Scan Results**.
B. Select 'Volume' for **X Axis** and 'Total energy' for **Y Axis**, then click **Draw**.
C. Click **Fit Curve** in **Options**.



E. Analysis of Results

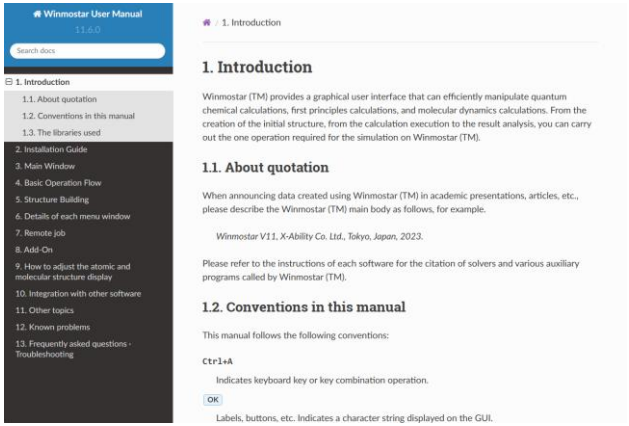
A. Change **Type** to 'Birch-Murnaghan for E(V)' and click **Fit**.
B. Once you confirm that the blue line (E(V) curve) and the orange line (fitted curve) approximately overlap on the graph, copy the value of 'b0: ' from **Fitted Parameters**.
C. Return to Main window, click on **Tools | Unit Converter**, change the physical quantity to 'Pressure', the unit on the left to 'Ry/A^3', and the unit on the right to 'GPa'. Then paste the value of b0 copied in step 2 into the left field, and the bulk modulus in GPa will be displayed in the right field.





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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