# **M** 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 <u>Beginner's Guide</u>.
- For those who wish to explore the details of each feature, please refer to <u>Winmostar User Manual.</u>
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - <u>Winmostar Introductory Training Session</u>: This guide only introduces the operation methods of the Basic Tutorial.
  - <u>Winmostar Basic Training Session</u>: 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.
  - <u>Individual Training Session</u>: 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 <u>Frequently asked questions</u>.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using <u>Contact page</u>. 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: <u>https://qiita.com/xa\_member</u>

# **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 <u>the recommended one</u>, you will need to install and configure <u>Windows version of Quantum ESPRESSO</u> separately.

# **Operating Modes of Winmostar V11**

V11 offers two operating modes: **Project Mode** and **File Mode**. This manual focuses on operations in Project Mode.



# A. Modeling of the System (Initial Structure)

- Please refer to <u>QE Basic Tutorial</u> for the basic operation method.
- For detailed instructions on creating the initial structure, please refer to <u>Winmostar User Manual section 5, 'Methods for Creating Initial Structures'</u>.
- A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.
- B. Enter <code>'si\_eos\_qe'</code> 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)

Run.

- 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 'pberrkjus\_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

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### 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**.

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#### **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**.

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# **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**.
- Once you confirm that the blue line (E(V) curve) and the orange line (fitted curve) Β. 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

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