# M winmostar tutorial Quantum ESPRESSO Structural Optimization Calculation

V11.6.5

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#### **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 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: <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.

For operations in File Mode, please refer to <u>Quantum ESPRESSO tutorial for version 10</u>.



#### A. Modeling of the System

Please refer to <u>QE Basic Tutorial</u> 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.

|            |             |                       | 🥺 Winmostar (ELITE) V11.6.5                                                                                               |
|------------|-------------|-----------------------|---------------------------------------------------------------------------------------------------------------------------|
|            |             |                       | <u>File Edit</u> Select <u>V</u> iew <u>Q</u> M <u>M</u> D <u>Solid A</u> dd-On <u>J</u> ools <u>W</u> indow <u>H</u> elp |
|            |             |                       | 🕼 🗟 🗝 🗂 🤩 🥵 🖪 🔛 🖶 🕇 🚯 🗘 🗭 🖆 🛃 Solver LA                                                                                   |
|            |             |                       | Element H 1 V + Q Q V V Fragment -CH3 V Replace                                                                           |
|            |             |                       | Projects     Project mode       Description     Status       Create New Project (3D)       Create new project (2D)        |
|            |             |                       | Create new project (SMILES)                                                                                               |
|            |             |                       | Working Folders Options V Create new project (unport Prej                                                                 |
|            | 阙 New pro   | oject                 | File mode (V10 compatibility mode) ×                                                                                      |
|            | Project nam | ne                    | tio2_rutile                                                                                                               |
|            | Location    | Arbitrary folder      | C:¥winmos11¥UserDat                                                                                                       |
|            |             | O Last opened folder  | er C:¥winmos11¥UserData                                                                                                   |
|            |             | O UserData folder     | C:¥winmos11¥UserData¥                                                                                                     |
|            |             | O Users¥Public folder | er C:¥Users¥Public¥                                                                                                       |
|            | Description | (Optional)            |                                                                                                                           |
|            |             |                       | Save                                                                                                                      |
| M winmosta |             | pyright 200           | 08-2023 X-Ability Co., Ltd. Powered by ChatGPT-4                                                                          |

### A. Modeling of the System

For detailed instructions on creating the initial structure, please refer to <u>Winmostar User</u> <u>Manual section 5, 'Methods for Creating Initial Structures</u>'. 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
- 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'.

(Workflow Setup).

E. Click **OK**, adjust settings as needed in **Job Setting** window, and then click **Run**.

|                                 | 🥺 Quantum E     | SPRESSO Workflow S   | <u></u>                         |                                    | - 🗆                      |  |  |
|---------------------------------|-----------------|----------------------|---------------------------------|------------------------------------|--------------------------|--|--|
|                                 | Preset Optimize | e(Atom&Cell)         |                                 |                                    | # of Jobs: + 1           |  |  |
| Solver Quantum ESPRESSO V       |                 |                      |                                 | Enable paramet                     | er/structure scan Config |  |  |
| MOPAC                           | 1st job         |                      |                                 |                                    | + -                      |  |  |
| CNDO/S                          | Task Op         | timize(Atom&Cell) 🗸  | Cutoff energy [Ry] 35           | .0 Pressure                        | [kbar] 0.0               |  |  |
| Gaussian Caresian               | Charge [e]      | 0.                   | Manually specify cuto           | off energy Phonon (D               | )FPT) Disabled ~         |  |  |
| T NWChem dited                  | # of bands      | Default $\lor$       | K points<br>(3x3x4) Monkhorst-P | Padk ∨ □Use Br                     | avais-lattice index      |  |  |
| LAMMPS<br>Gromaco               | Spin            | Non-polarized $\lor$ |                                 |                                    |                          |  |  |
| Quantum ESPRESSO                | Pseudopoten     | tial                 | Proper                          | ties                               |                          |  |  |
|                                 | Туре            | All 🗸                | DO                              | S Charge                           | density Phonon DOS       |  |  |
|                                 | Functional      | All                  | PD cha                          | OS/Lowdin Potentia<br>arge Work fu | al/ Phonon band          |  |  |
|                                 | Pseudo file     | pbe-*van_ak.upf      | Bar                             | nd structure 🗌 Dielectri           | ic func 🗌 NMR            |  |  |
|                                 | Precision       | Medium $\vee$        | Metal                           |                                    | Details                  |  |  |
|                                 |                 |                      |                                 |                                    |                          |  |  |
|                                 | Reset           | Import 🖛 E           | Export                          |                                    | ок                       |  |  |
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#### 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.

| Name       Status         Image: Status       ABORT         Image: Status       Image: Status         Image: Status       Image: Status       Image: Status         Image: Status       Image: Status <th>Working Folders (tio2_rutile)</th> <th>Options V</th> <th>100</th> <th>Select the working fo</th> <th>der which you w</th> <th>ant to continue</th> <th>the job from</th> <th></th> <th></th> <th></th>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Working Folders (tio2_rutile) | Options V                                                                      | 100                                                                                                                                                                      | Select the working fo | der which you w | ant to continue | the job from   |           |    |  |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|--------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|-----------------|-----------------|----------------|-----------|----|--|
| • vor k1_@E_Relax       ABORT       Output Location         [Displayed on viewport]       Name: work1_QE_Relax         Status: ABORT       Profile       Output Location: Local         Job Name: Exec1       Profile: Unknown Error(SCF)       Description: The maximum         Information       X         Information       X         Io you want to continue from previous run?       Mare                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Name                          | Status N2                                                                      |                                                                                                                                                                          |                       |                 |                 |                |           |    |  |
| Image: source of the second | 💿 work1_@E_Relax              | ABORT                                                                          |                                                                                                                                                                          | Name                  | Status          | Profile         | Output Locatio | n i i i n |    |  |
| Coordinate (Initial) Information X  Do you want to continue from previous run?  OK                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | <                             | [Displa<br>Name:<br>Status:<br>Profile<br>Outpu<br>Job Na<br>Profile<br>Descri | yed on viewport]<br>work1_QE_Relax<br>ABORT<br>: Local Job<br>t Location: Local<br>ime: Exec1<br>: Unknown Error(SCF)<br>ption: The maximum<br>of stens has been reached |                       |                 |                 |                |           |    |  |
| i) Do you want to continue from previous run?                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | Coordinate (Initial)          |                                                                                |                                                                                                                                                                          |                       |                 |                 |                |           |    |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Do you want                   | to continue from p                                                             | previous run?                                                                                                                                                            |                       |                 |                 |                | ок        | 1_ |  |

### **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.



structure optimization calculation is performed.

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#### **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.



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## 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.)
- If you are unable to proceed as instructed in this guide, please first consult <u>Frequently asked questions</u>.
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