winmostar tutorial

Quantum ESPRESSO Surface Reconstruction

V11.6.5

4 April 2024 X-Ability Co., Ltd.

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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 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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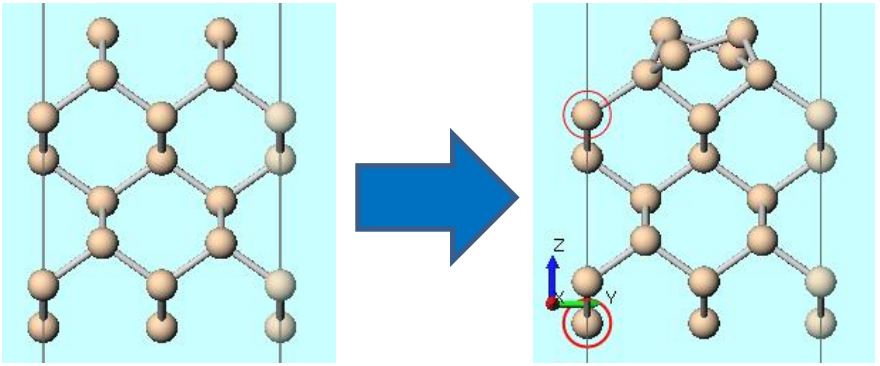
Overview

- In this manual, we conduct structural optimization calculations for the Si (001) surface and observe the surface reconstruction.
- Various reconstructed surface states of Si (001) are known, and in this tutorial, we obtain the asymmetric dimer p(2×2) structure among them.
- Due to the expected significant changes in atomic positions, the calculations are performed in stages from low to high precision to process efficiently.



Note :

- Depending on the calculation conditions, the result of the structural optimization calculation may converge to a different surface structure.
- The choice of k-points, type of pseudopotential, and cutoff energy can impact the calculation results. In this tutorial, settings with reduced accuracy are used to obtain results more quickly.
- 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

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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.

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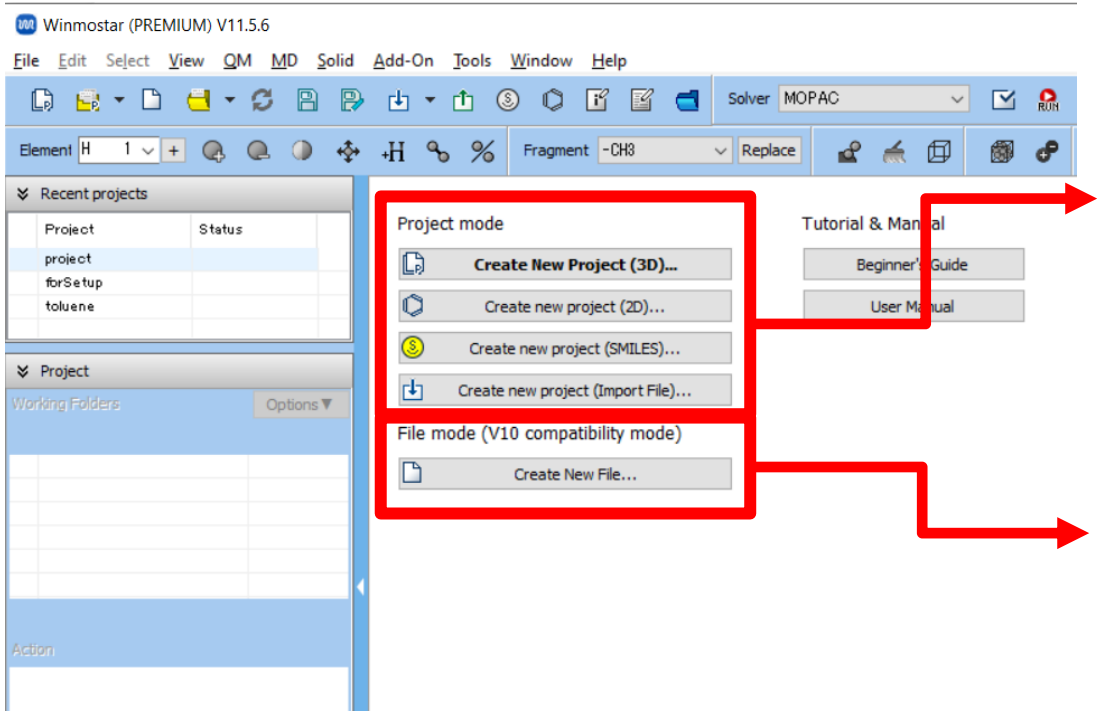
Operating Modes of Winmostar V11

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.

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A. Modeling of the System (Bulk Crystal)

- 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'.

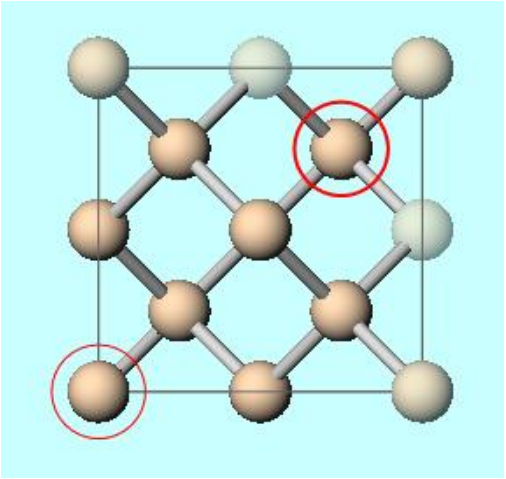
A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

B. Enter '`si_surf`' 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. In **Import File** dialog, click **Discard and import**.



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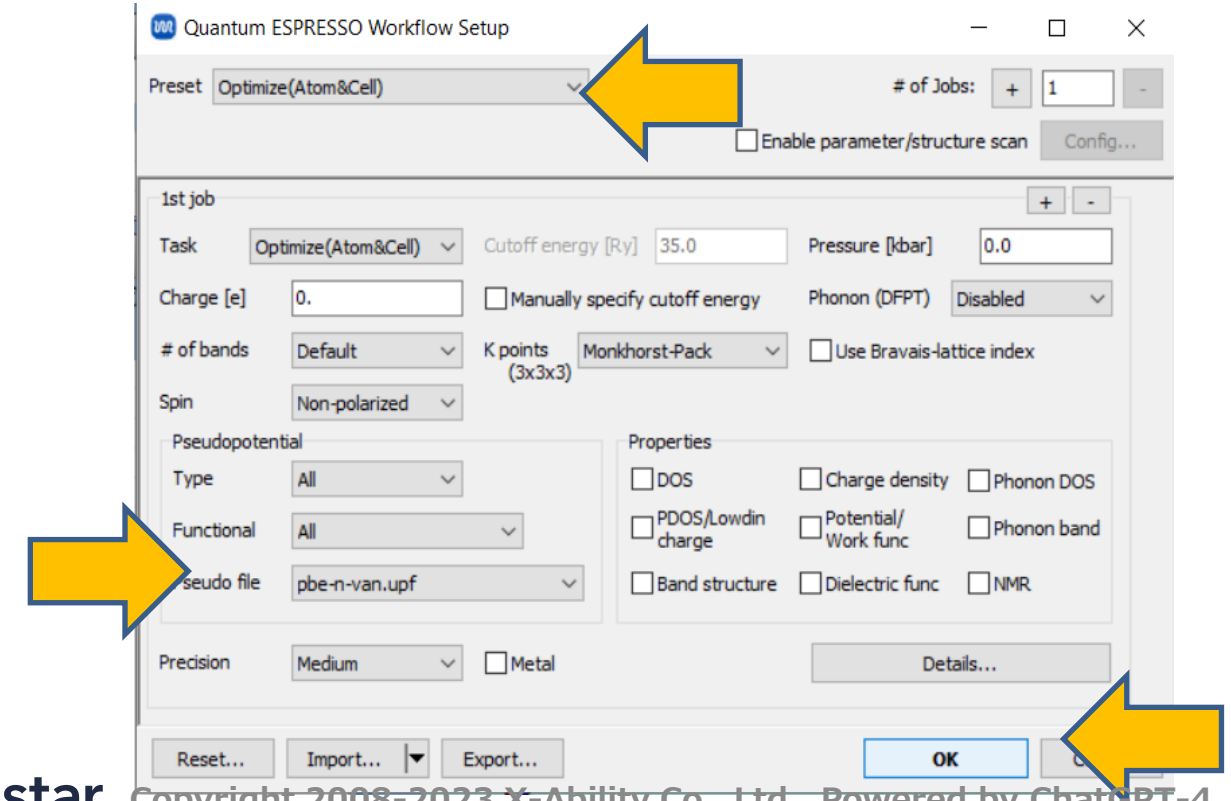
B. Execution of Calculation (Bulk Crystal)

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)' and change **Pseudo file** to 'pbe-n-van.upf'.
C. Click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.



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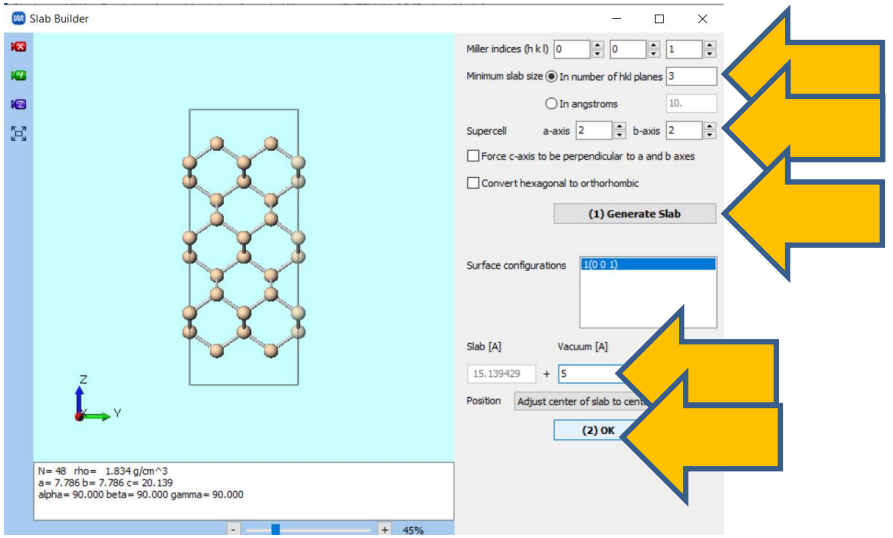
C. Modeling of the System (Slab)

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

B. Click **Solid | Convert Lattice**, and if prompted with '...Do you want to change to an output-ready format (wmm) and continue?', click **Yes**. If asked '...Do you want to convert to conventional cell?', click **Yes**.

C. Click **Solid | Slab Builder**, set **In number of hkl planes** value of **Minimum slab size** to '3', and change both **a-axis** and **b-axis** of **Supercell** to '2', then click **(1) Generate Slab**.

D. Change **Vacuum** to '5' and click **(2) OK**.



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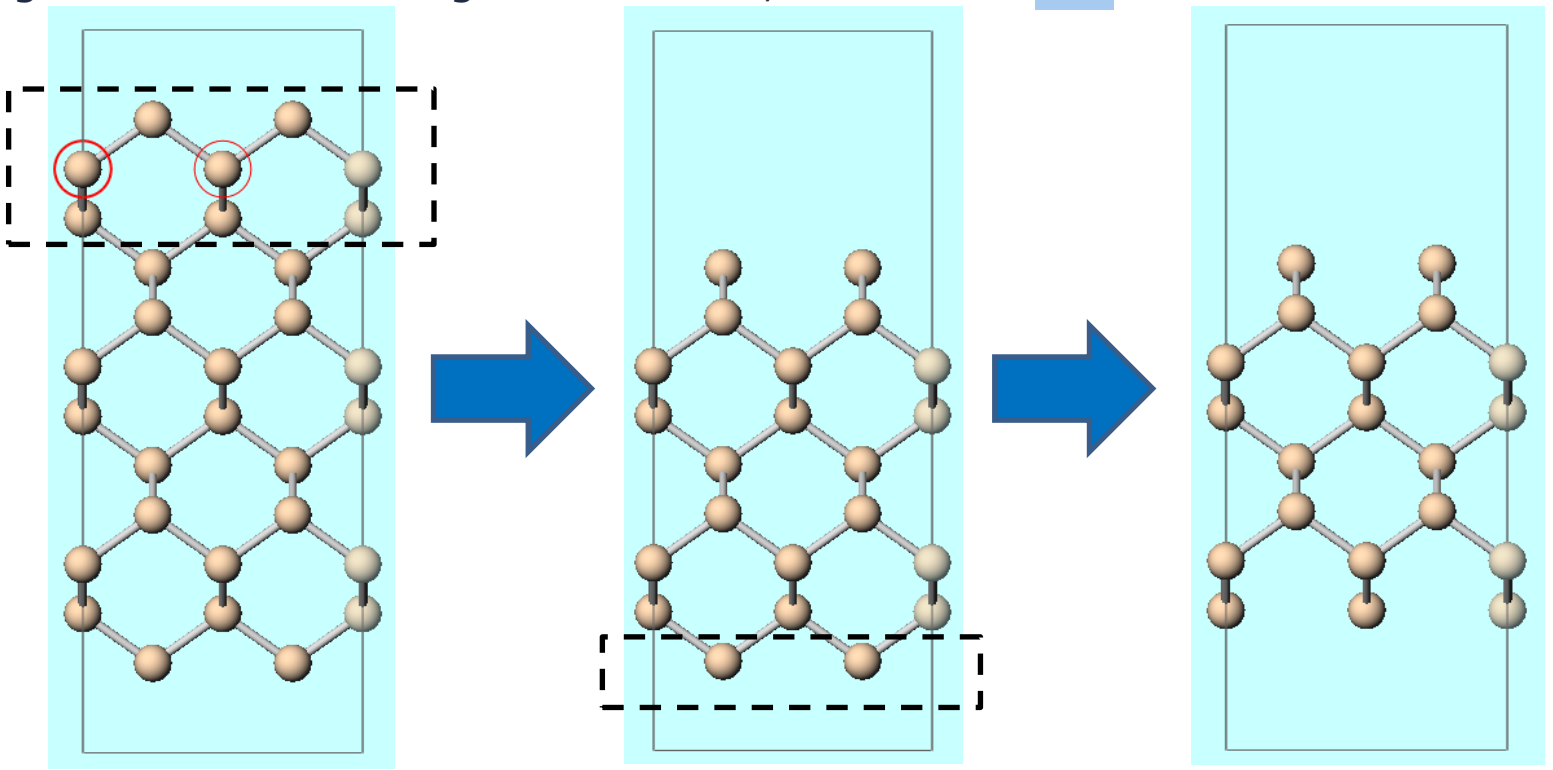
C. Modeling of the System (Slab)

A. Click **Align View to X-Axis** followed by **Fit to Window**.

B. As shown in the figure below (left), select the top 3 atomic layers using Ctrl+Drag to make a rectangular selection, then click **Delete Atom** and click **Delete**.

C. As shown in the figurebelow (middle), select the bottom 1 atomic layer using Ctrl+Drag to make a rectangular selection, then click **Delete Atom** and click **Delete**.



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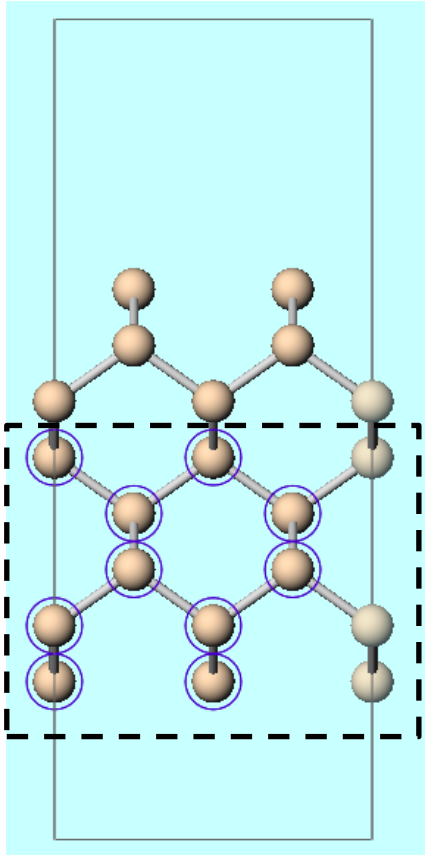
C. Modeling of the System (Slab)

A. As shown in the figure below (left), select the bottom 5 atomic layers using Ctrl+Drag to make a rectangular selection, then click **Modify Selected Group | Change Optimization Flags of Group** and click **Fix**.

B. Click **Select | Select None**.



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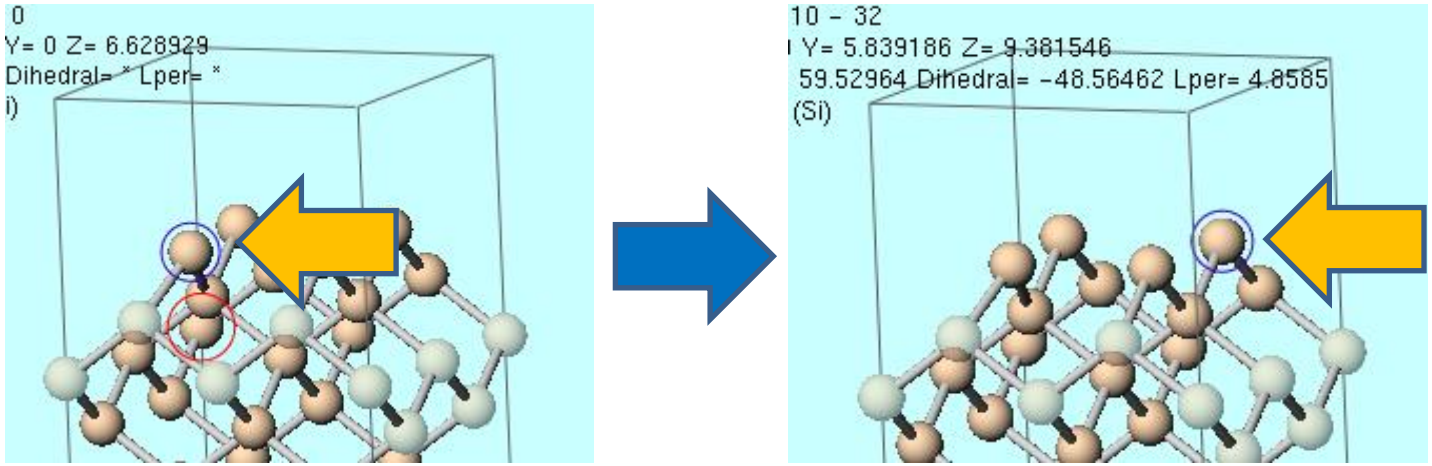
C. Modeling of the System (Slab)

A. Drag in Viewport, moving the camera so that all four atoms on the topmost surface are visible as shown in the figure below (left).

B. As shown in the figure below (left), Ctrl+click on one of the atoms on the topmost surface, click **Modify Selected Group | Translate (Numerical)**, change the value of **Y** to '0.5', and click **OK**.

C. Click Select | Select None.

D. As shown in the figure below (right), Ctrl+click on the atom diagonally opposite to the one selected in step 2, click **Modify Selected Group | Translate (Numerical)**, change the value of **Y** to '-0.5', and click **OK**.



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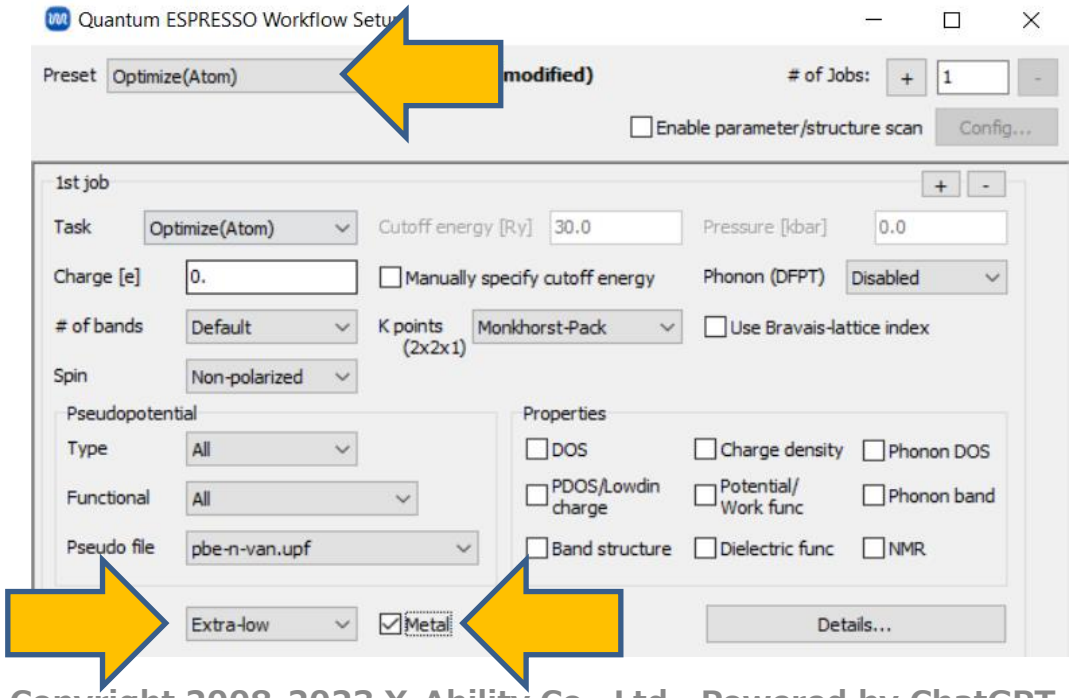
D. Execution of Calculation (Slab, Low Precision)

A. Click **(Workflow Setup)** and if prompted with 'Do you want to continue from previous run?', click **No**.

B. Change **Preset** to 'Optimize (Atom)' and **Precision** to 'Extra-Low', and check the box for **Metal**.
   - Surface states appearing in the band gap worsen the convergence of SCF, so set it to Metal and apply smearing.

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



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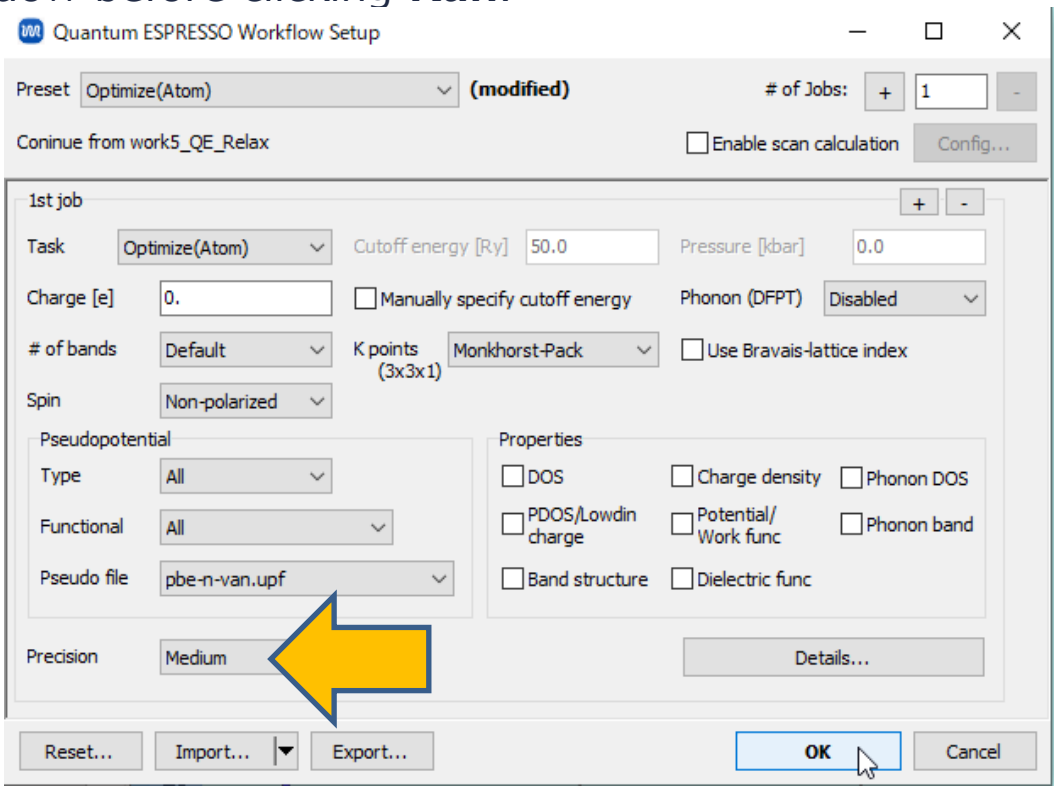
D. Execution of Calculation (Slab, High Precision)

A. Once **the status** of work2_QE_Relax changes to **END**, click **(Workflow Setup)** and if prompted with 'Do you want to continue from previous run?', click **Yes**.

B. Select work2_QE_Relax in 'Select working folder' and click **OK**.

C. Change **Precision** to 'Medium', click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.



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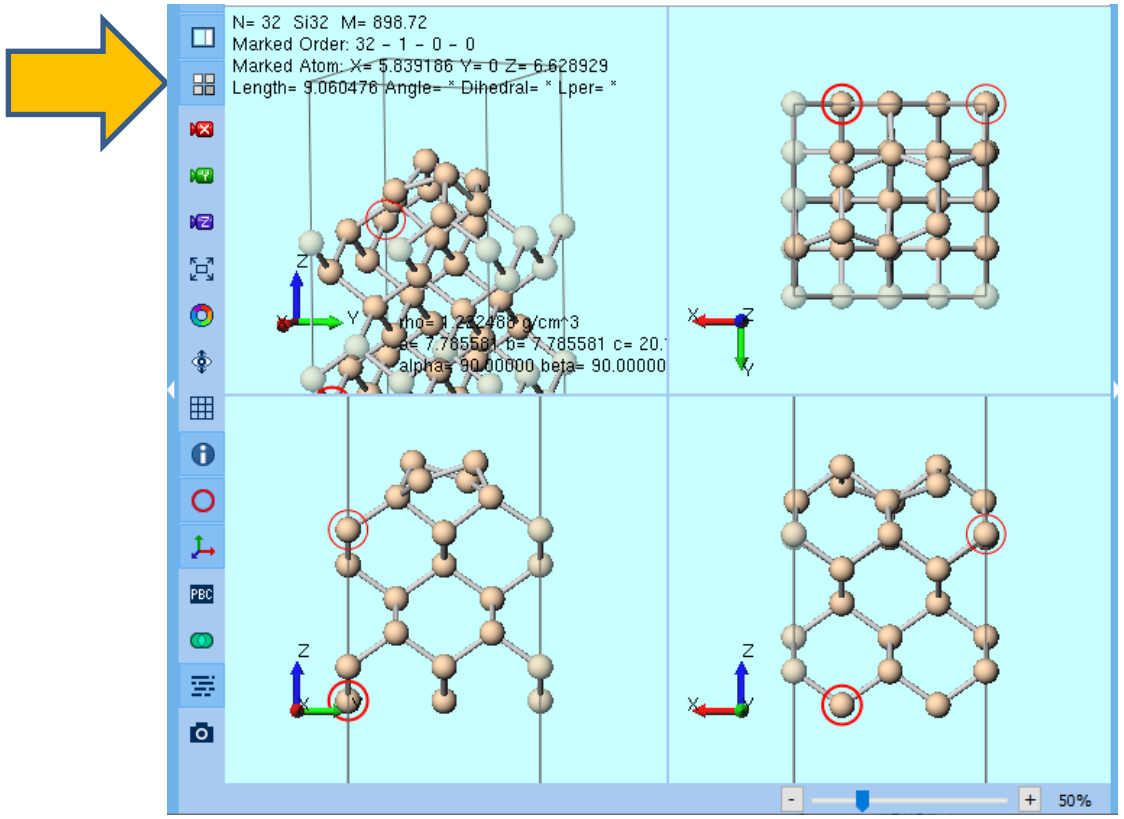
E. Result Analysis

A. Once **the status** of work3_QE_Relax changes to **END**, click **Coordinate (Final)** in Action.

B. Click **Show Multi-View**. In Viewport, adjust the display range appropriately by Shift+Dragging. To cancel the tri-view, click **Show Multi-View** again.



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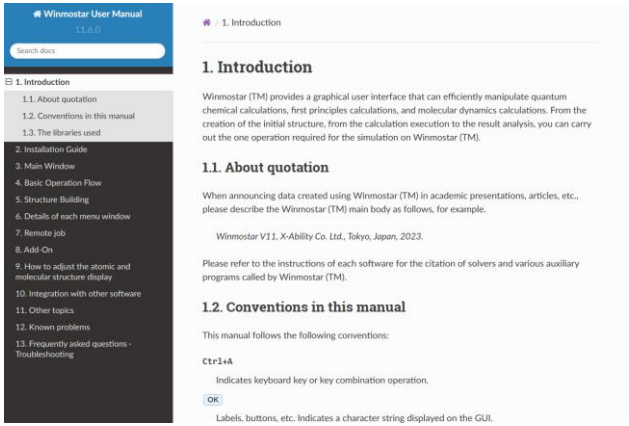
Finally

- 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 Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
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