winmostar tutorial

Quantum ESPRESSO

Effective Screening Medium (ESM) Method

V11.9.5

30 Dec. 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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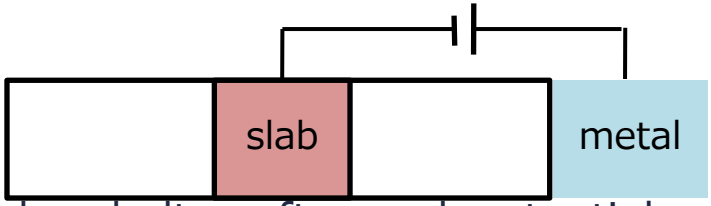
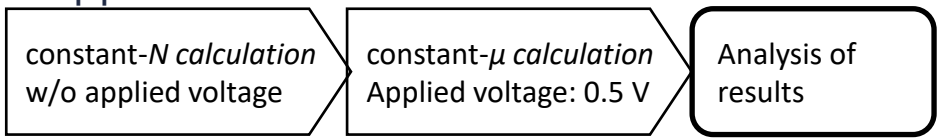
Overview

- This tutorial demonstrates an Effective Screening Medium (ESM) calculation using an aluminum monolayer (slab) as an electrode. The boundary condition representing a vacuum–slab–metal system (bc3) is applied.
- ※Because of the implementation of ESM in Quantum ESPRESSO, the boundary of the input supercell is internally mapped to the center of the simulation cell. This is illustrated in the figure below.



Using the PBE functional and ultrasoft pseudopotentials, we first perform a constant-N calculation (with no applied bias), followed by a constant-μ calculation with an applied voltage of 0.5 V. These calculations allow us to analyze the electronic structure and charge distribution of the Al slab under bias. We also confirm that a potential difference of approximately 0.5 V appears between the slab and the virtual electrode (metal).



Note :

- 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

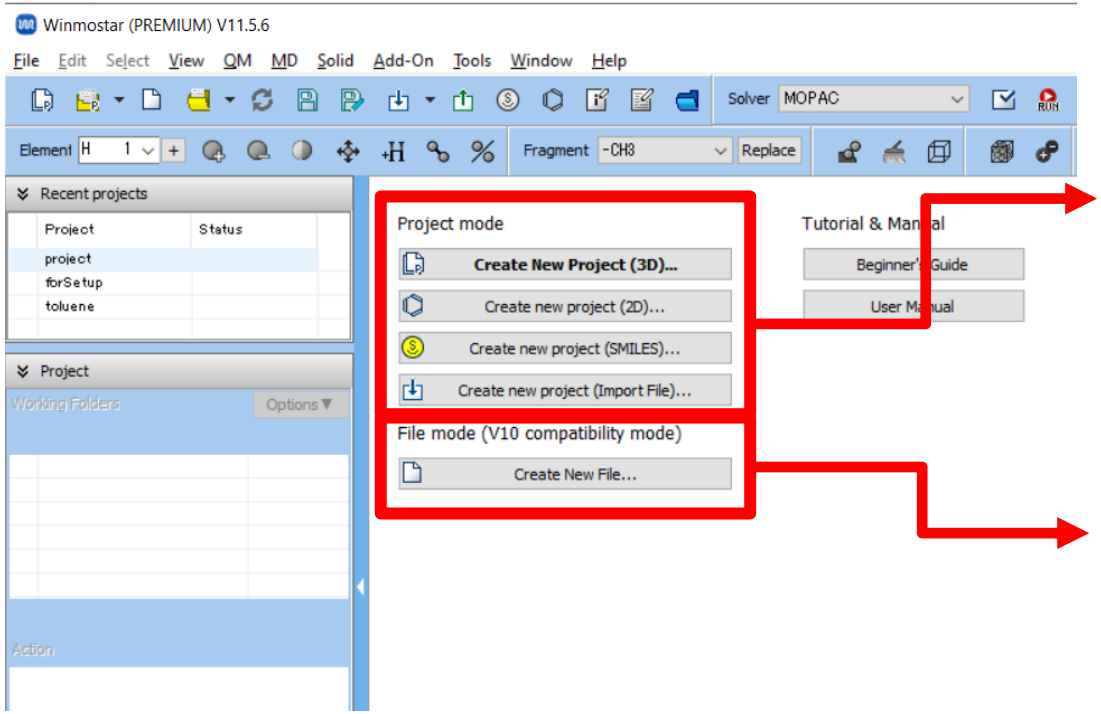
Preference of Operating Environment

- 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

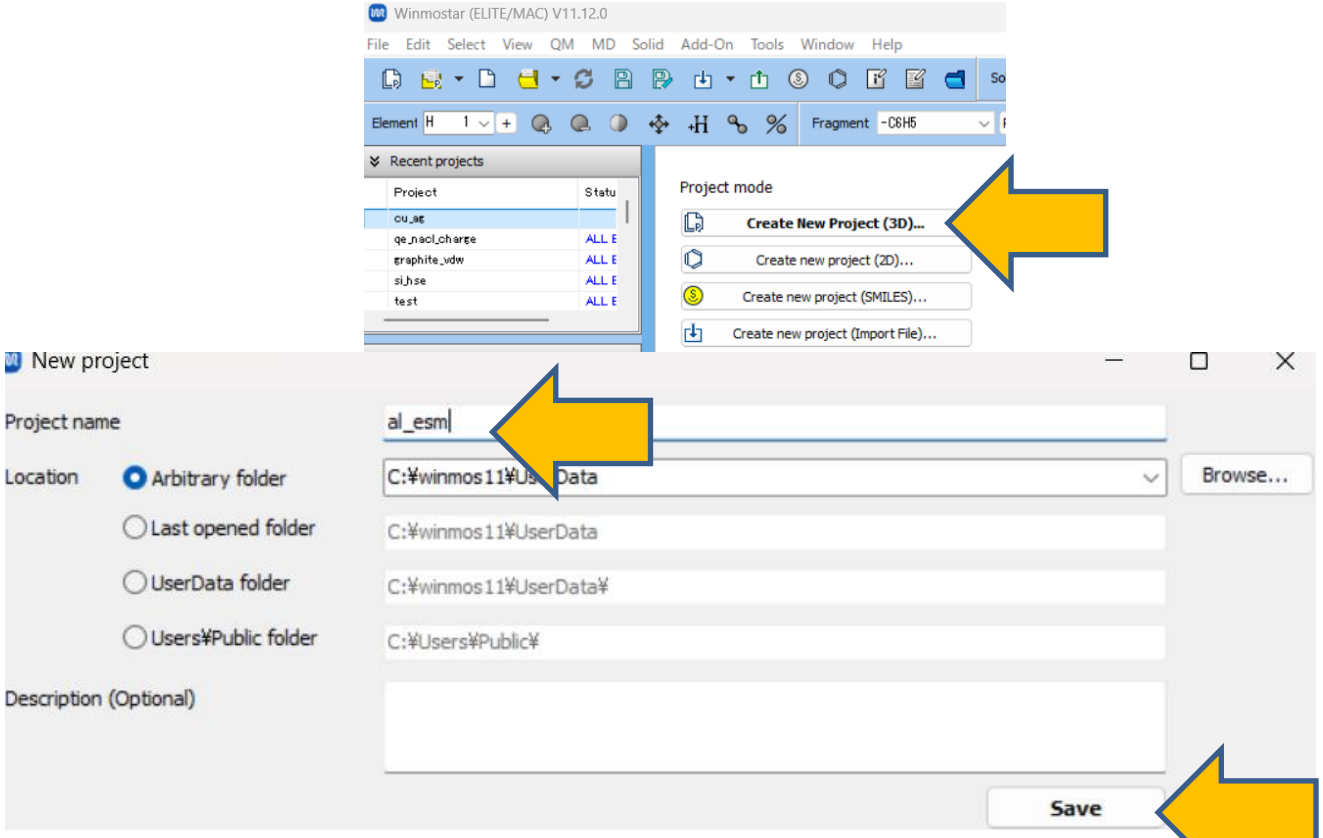
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System（constant-*N* calculation）

- 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 'al_esm' in **Project name** and click **Save**.

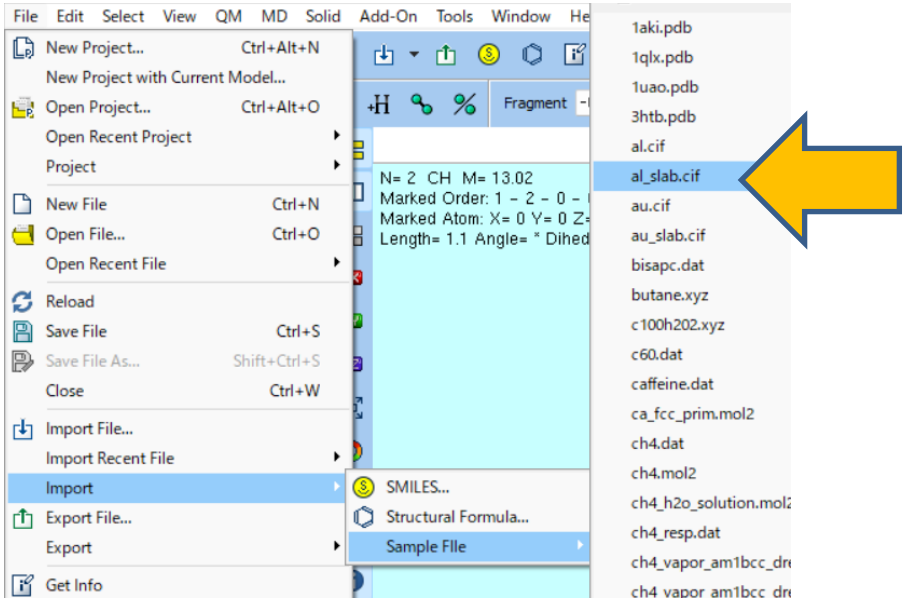


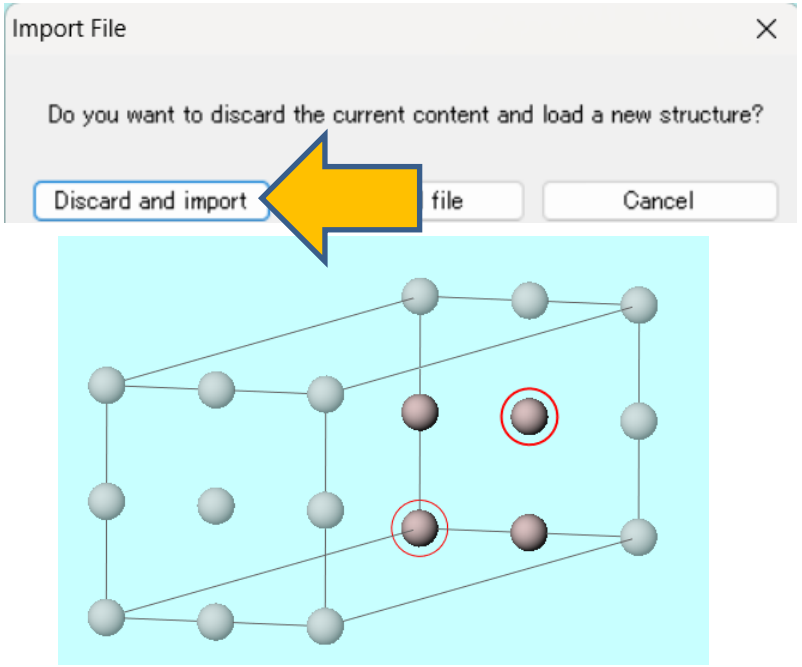
A. Modeling of the System（constant-*N* calculation）

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

A. Click **File | Import | Sample File | al_slab.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**.



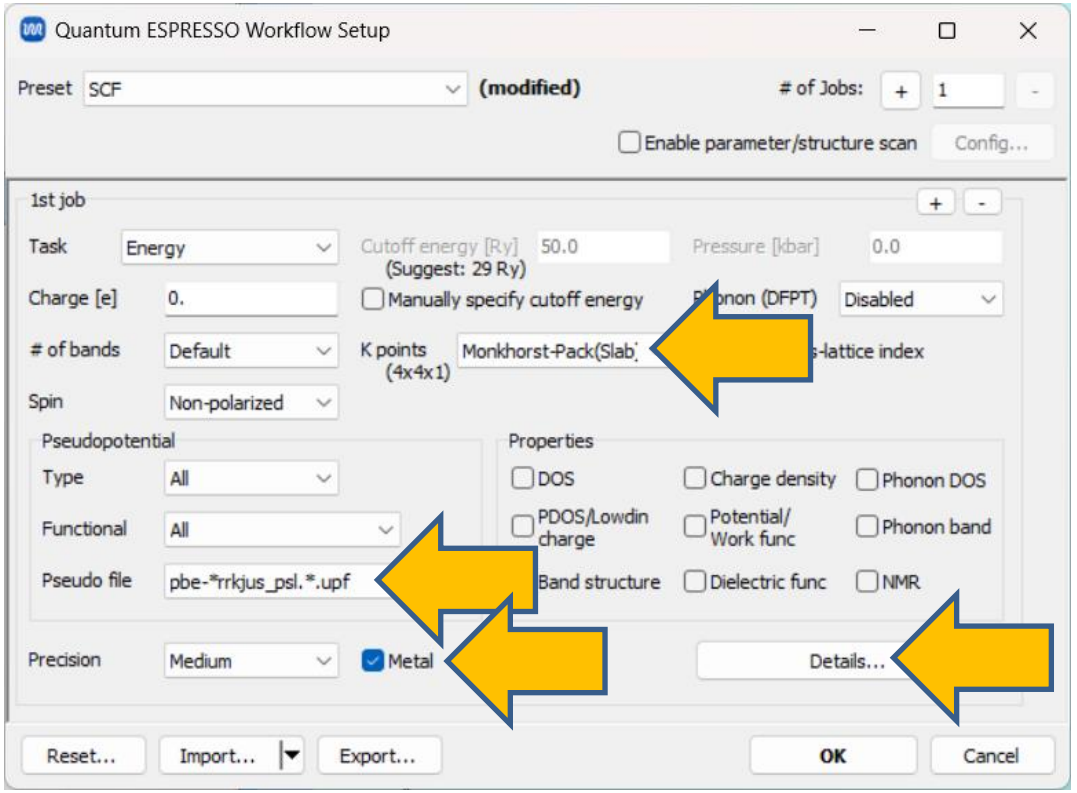


B. Execution of Calculation (constant-*N* calculation)

A. Select **Quantum ESPRESSO** from **Solver** in Toolbar and click **(Workflow Setup)**. If asked whether to convert to a primitive cell, click **No**.

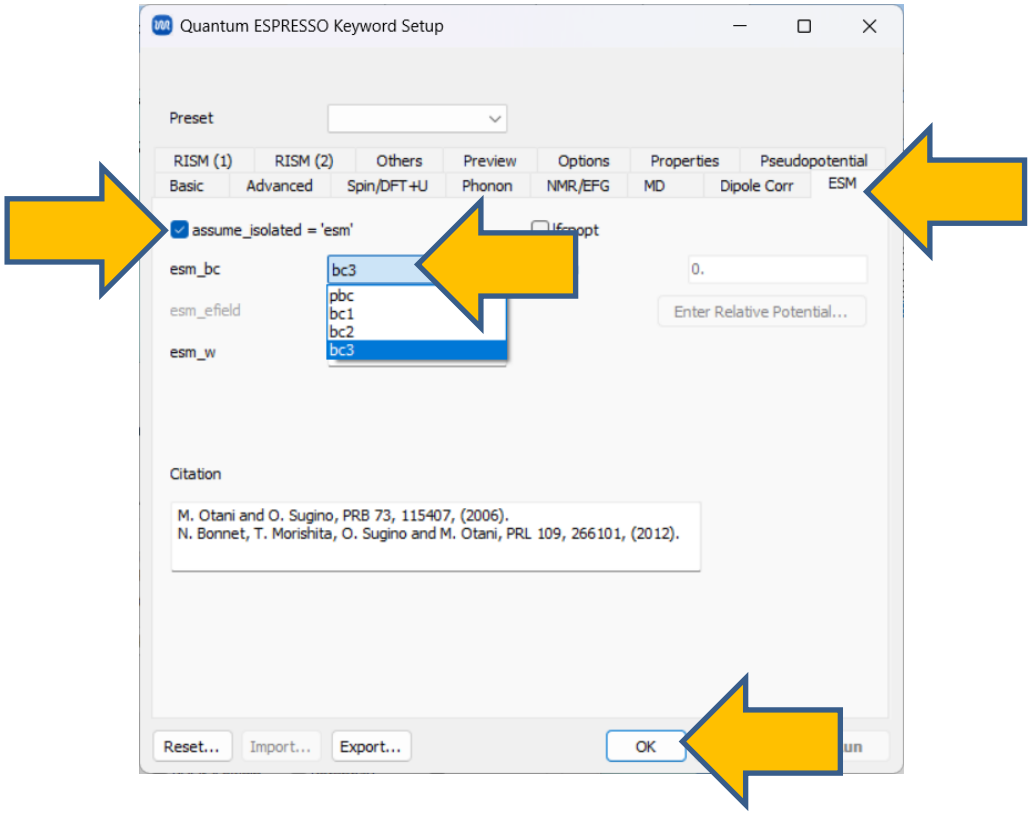
B. Change the **K points** setting to **Monkhorst-Pack (Slab)**, enable the **Metal** option, and select **pbe-*rrkjus_psl.*.upf** in **Pseudo file**.

C. Click **Details**



B. Execution of Calculation (constant-*N* calculation)

A. Select the **ESM** tab, enable the **assume_isolated = 'esm'** setting, and change the **esm_bc** parameter to **bc3**.
B. Click **OK**
C. Click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.

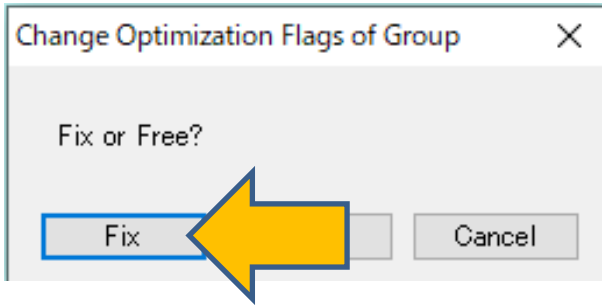


C. Modeling of the System (constant-μ calculation)

A. Click **Select | Select All**.

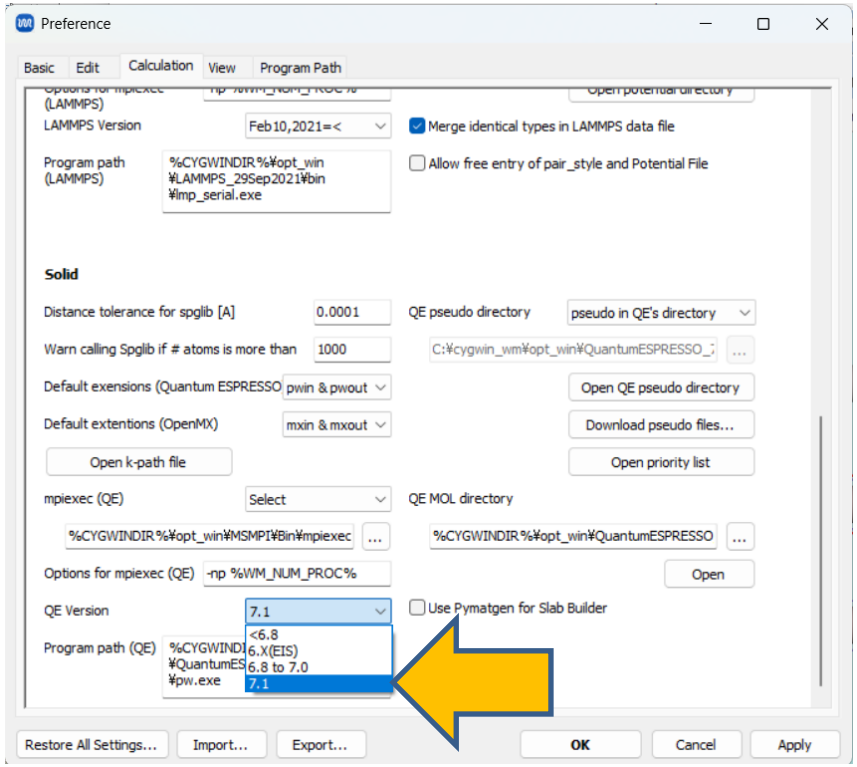
B. Click  **(Modify Selected Group) | Change Optimization Flags of Group** and then click **Fix.**

- In the charge optimization calculation, the structure optimization routine is reused. By assigning fixed optimization flags to all atoms, the atomic positions are held fixed while only the charges are optimized.



D. Execution of Calculation (constant-*μ* calculation)

A. The keyword settings required for constant-μ calculations vary depending on the version of Quantum ESPRESSO being used. To ensure compatibility, click **Preference**, open the **Calculation** tab, and select the correct **QE version**. Then click **OK** to apply the setting.
(For Winmostar V11.5.0 or later with the default QE path, select “7.1” to use the bundled QE 7.1 via CygwinWM. If you are using QE 5.2.1, select “<6.8”.)



D. Execution of Calculation (constant-μ calculation)

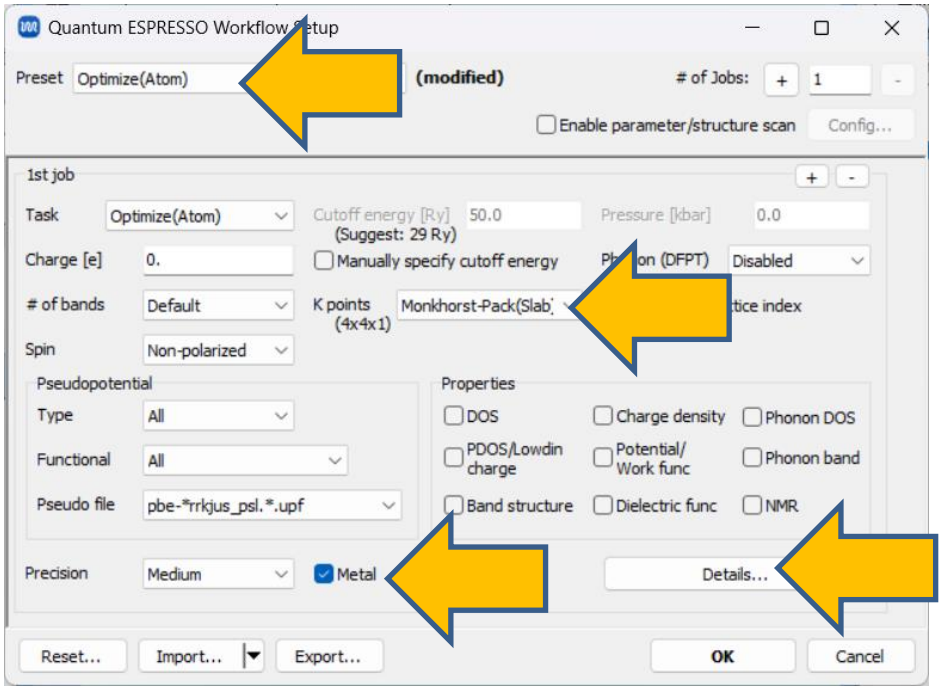
A. After **the status** of **Working Folders work1_QE_SCF** changes to **END (blue)** , Click **(Workflow Setup)** in Toolbar.. If asked 'Do you want to continue from previous run?', click **No**.

B. If asked to convert to a primitive cell, click **No**.

C. Change **Preset** to 'Optimize(Atom)', The settings for the constant-N calculation will be reset.

D. Set **K points** to **Monkhorst-Pack (Slab)**, and check the **Metal** option.

E. Click **Details**.

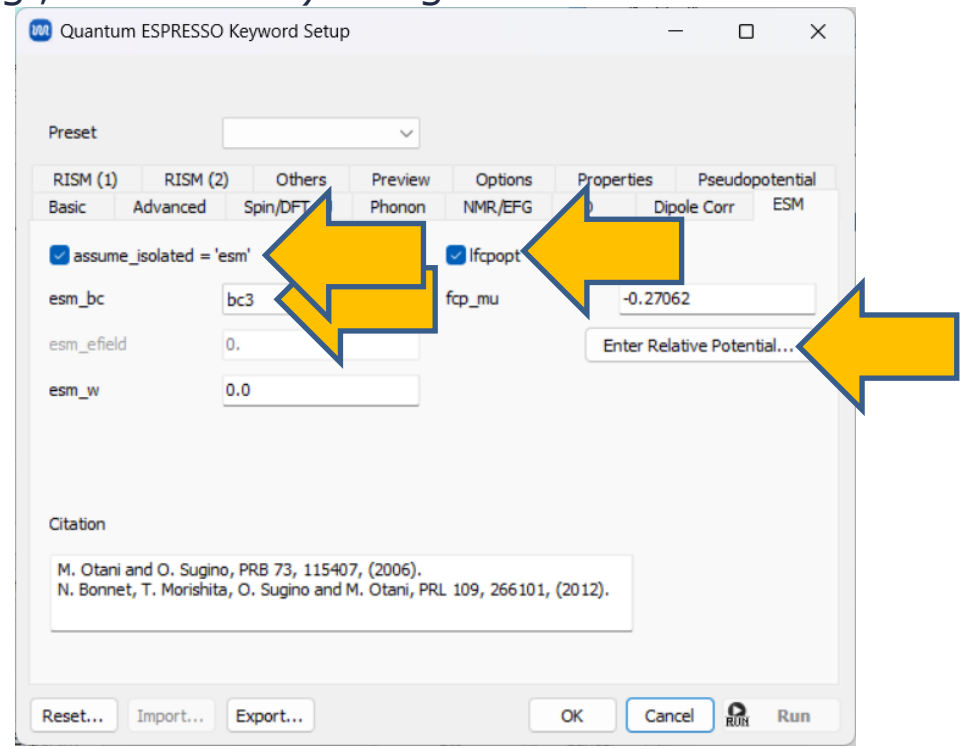


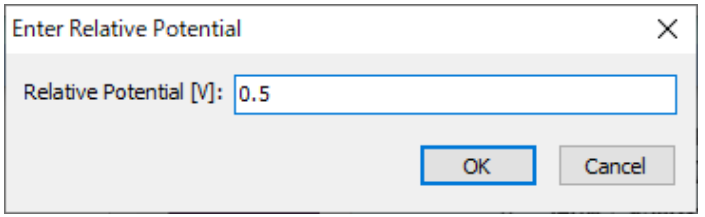
D. Execution of Calculation (constant-μ calculation)

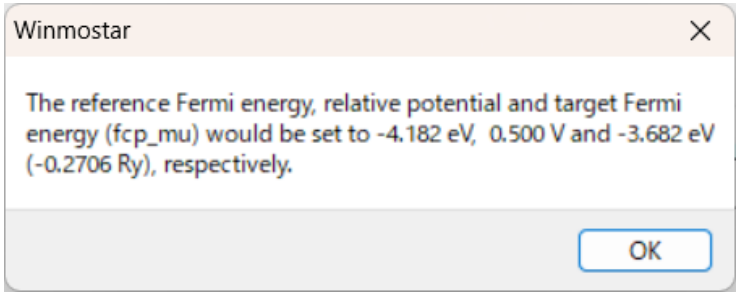
A. Select the **ESM** tab, enable the **assume_isolated = 'esm'** setting, and change the **esm_bc** parameter to **bc3**.

B. Check the **lfcopt** option, then click **Enter Relative Potential**.

C. You will be prompted to select the output file used as the Relative Potential. Open the log file from the constant-N calculation folder (e.g., work1_QE_SCF¥pw.pwout). Then, enter **0.5** as the Relative Potential and click **OK**. When the message “The reference Fermi energy⋯” appears, click “**OK**”. Finally, note down the value assigned to **fcp_mu** (e.g., “-0.27062”) using a text editor such as Notepad.

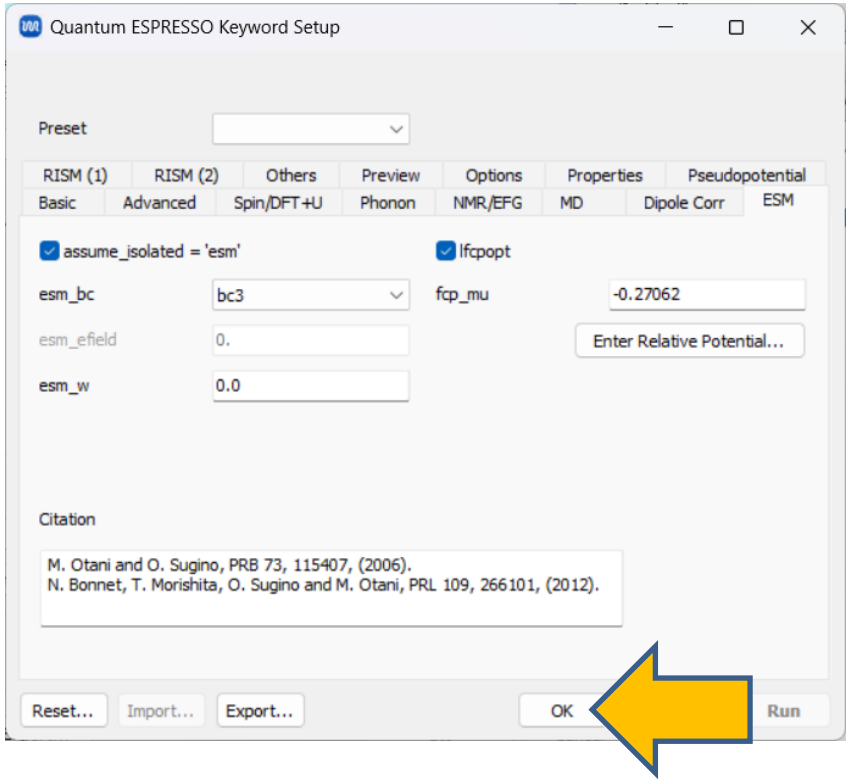


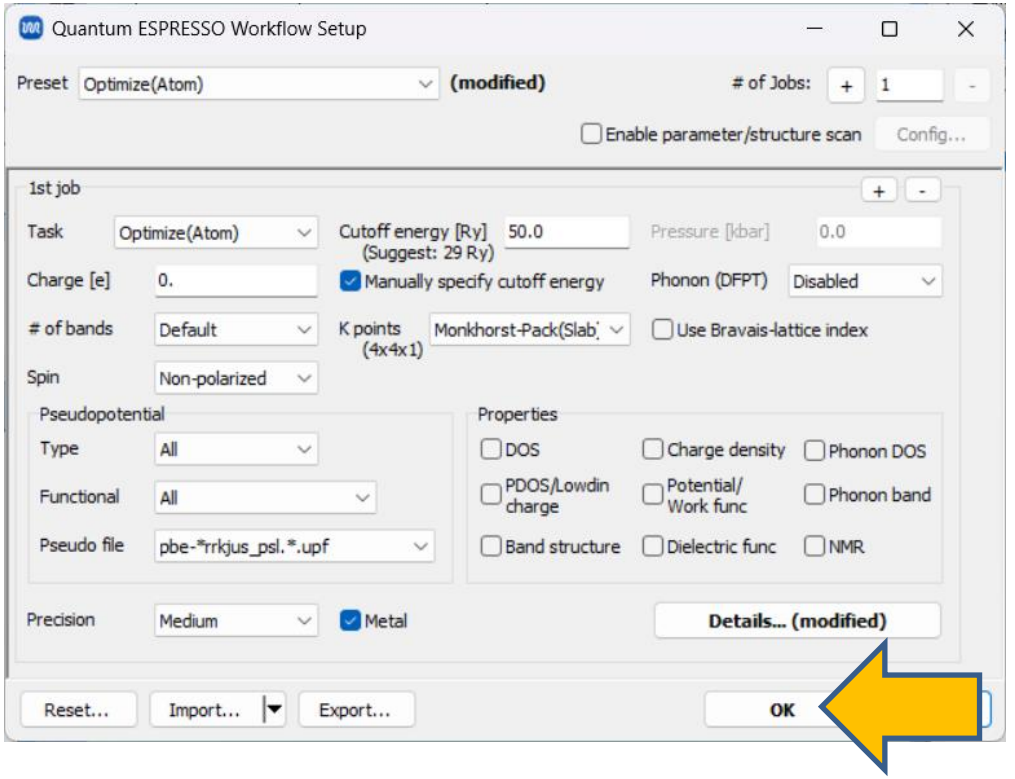




D. Execution of Calculation (constant-μ calculation)

A. Click **OK** to close the **Quantum ESPRESSO Keyword Setup** window. Then, click **OK** in the **Quantum ESPRESSO Workflow Setup** window. In the **Job Setting** window, configure the settings as needed and click **Run** to start the calculation.



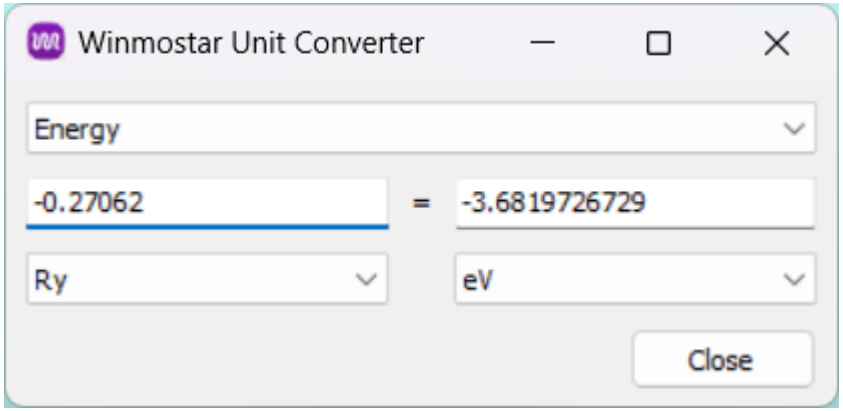


D. Execution of Calculation (constant-μ calculation)

Since the target Fermi energy (**fcp_mu**) is written in Rydberg units in the input file but output in electron volts (eV) in the log file, it is important to check and note the value in eV here.

A. Click **Tools** | **Unit Converter**

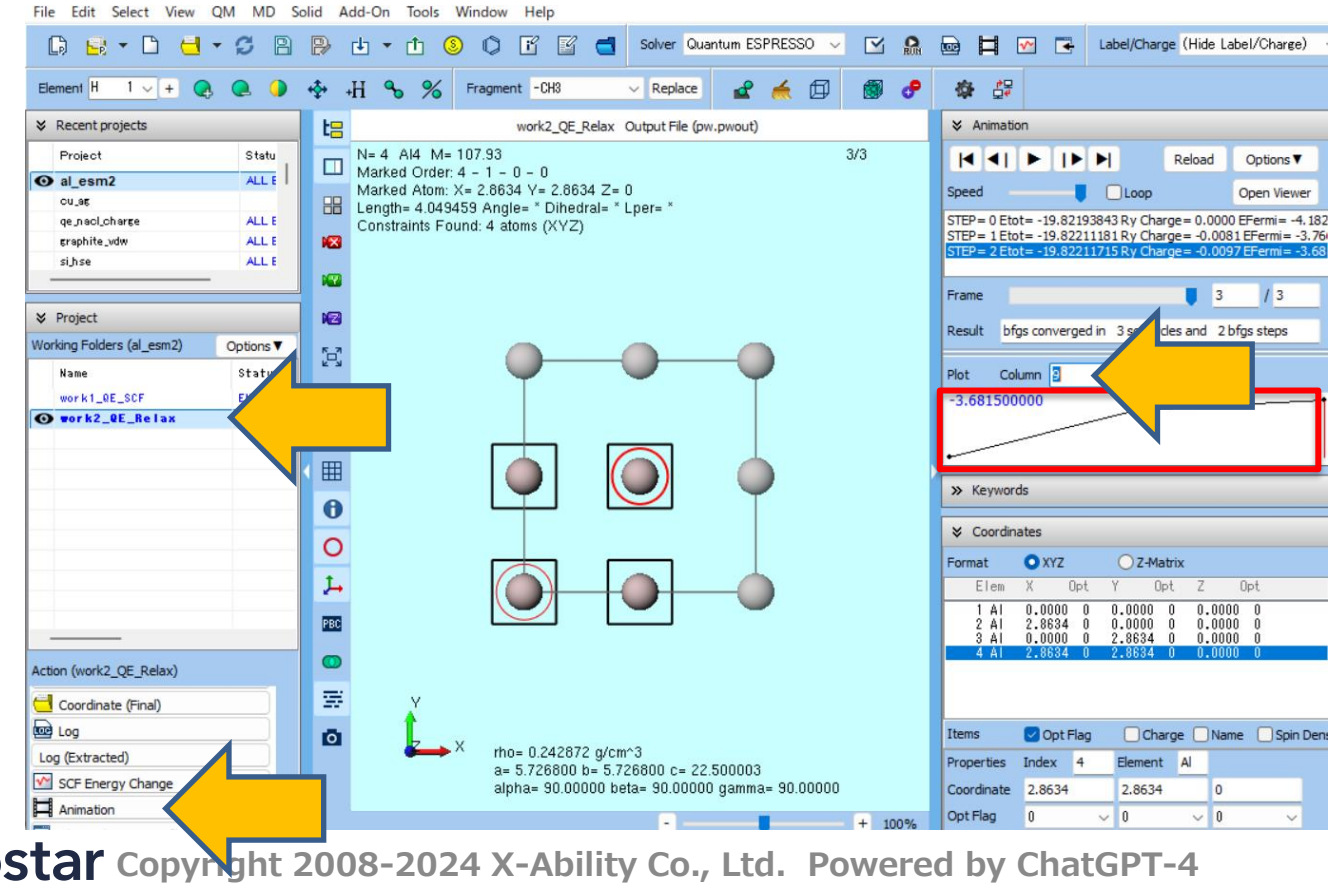
B. Set the physical quantity to **Energy**, change the left unit to **Ry** and the right unit to **eV**, then paste the previously copied **fcp_mu** value into the left input field. The value shown on the right represents the target Fermi energy for the constant-μ calculation.



E. Analysis of Results

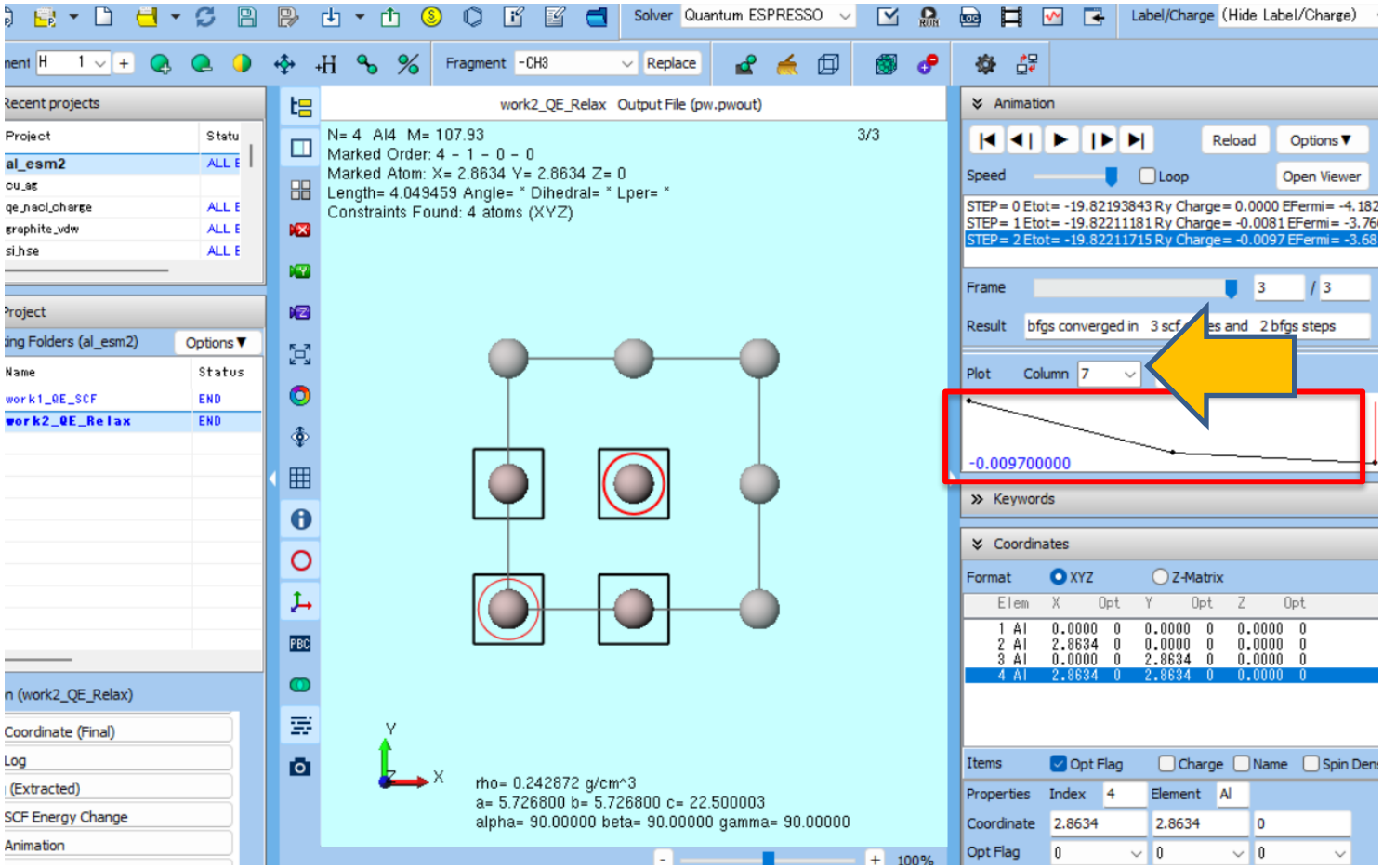
A. After the status of **work2_QE_Relax** changes to **END（blue）**, In the **Working Folders** section, click **work2_QE_Relax**, then go to the **Action** menu and select **Animation**.

B. Change the **Column** setting in the **Animation** control area to “9” to display a graph of the Fermi energy variation. Confirm that the value asymptotically approaches the result obtained in the previous step.



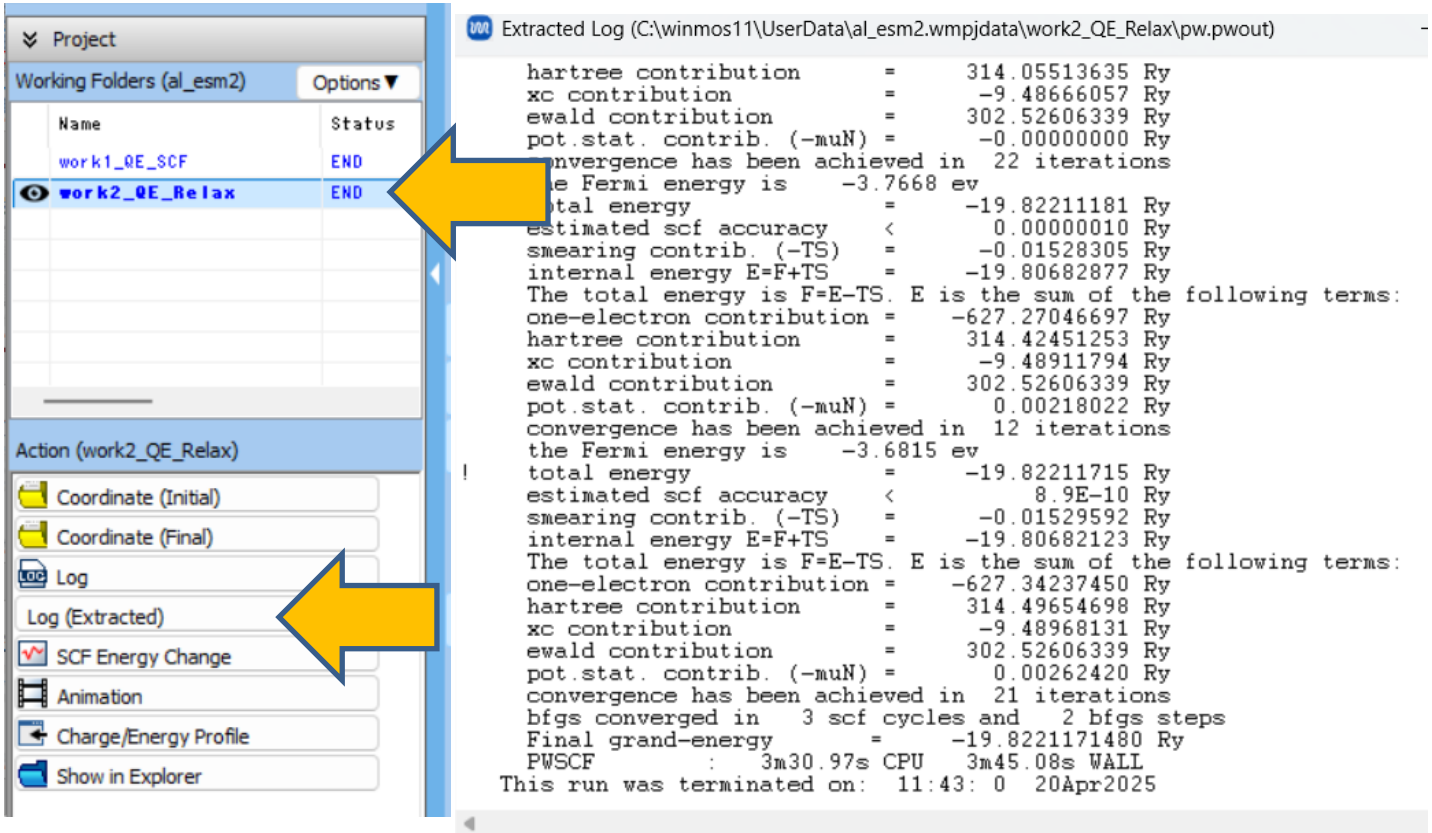
E. Analysis of Results

A. Change the **Column** setting in the **Animation** control area to “7” to display a graph of the charge variation.



E. Analysis of Results

A. In the **Working Folders** section, click **work2_QE_Relax**, then go to the **Action** menu and select either **Log** (full log file) or **Log (Extracted)** (summary view). Check the final values such as the total energy and Fermi energy for the Al slab from the log output.

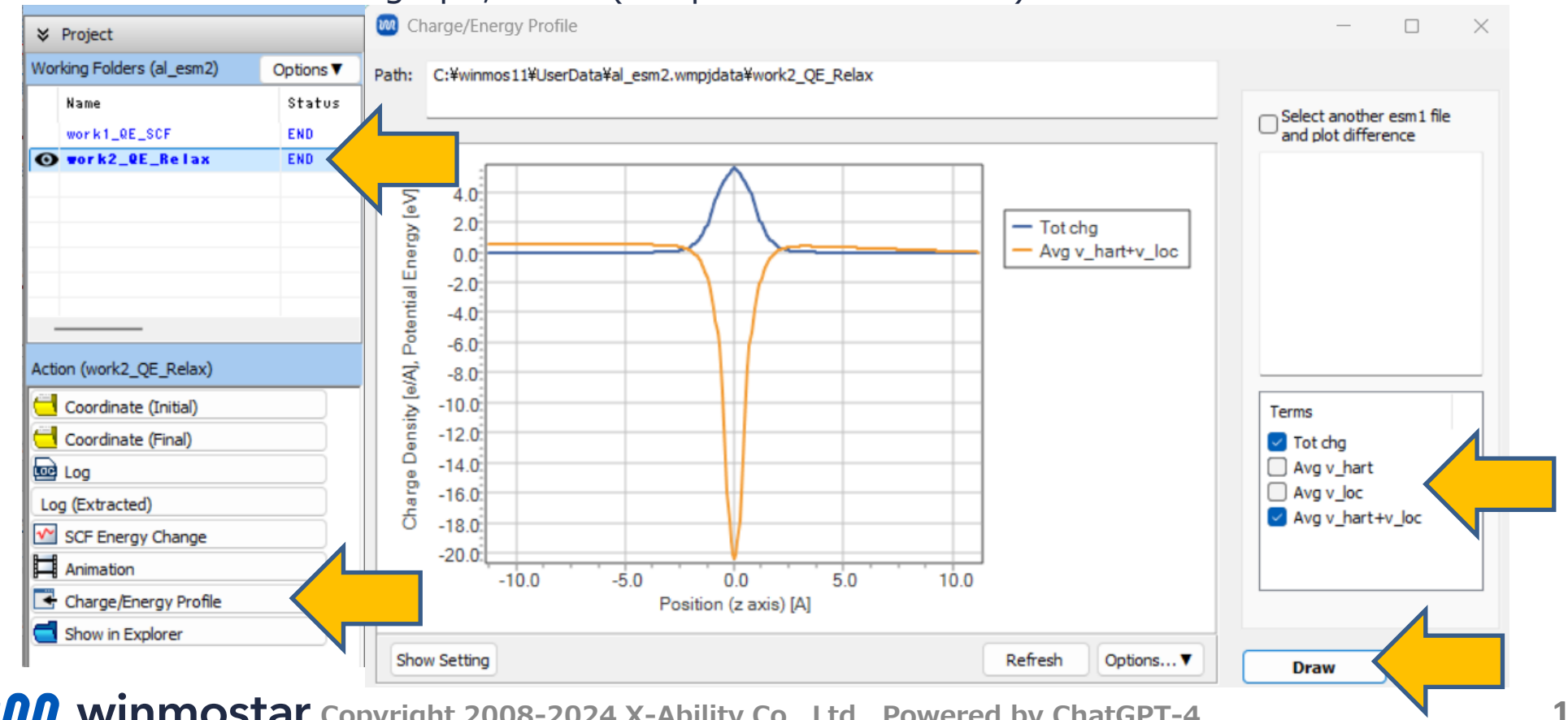


E. Analysis of Results

A. In the **Working Folders**, click **work2_QE_Relax**, then select **Charge/Energy Profile** from the “Action” menu.

B. In the **Terms** section, check only **Tot chg** (charge) and **Avg v_hart+v_loc** (potential), then click **Draw**.

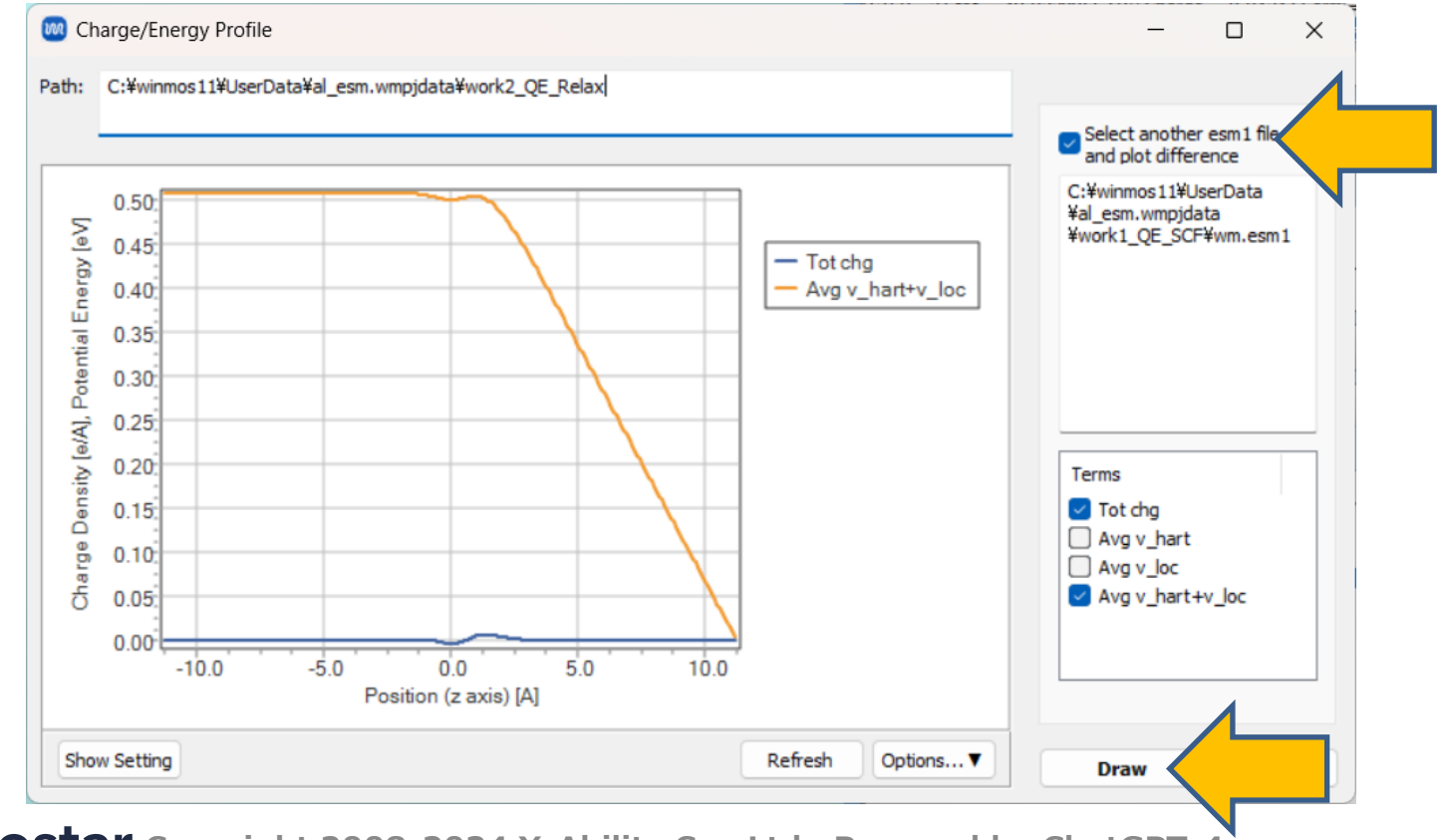
- Note that in this graph, z = 0 (the position of the slab) is centered.



E. Analysis of Results

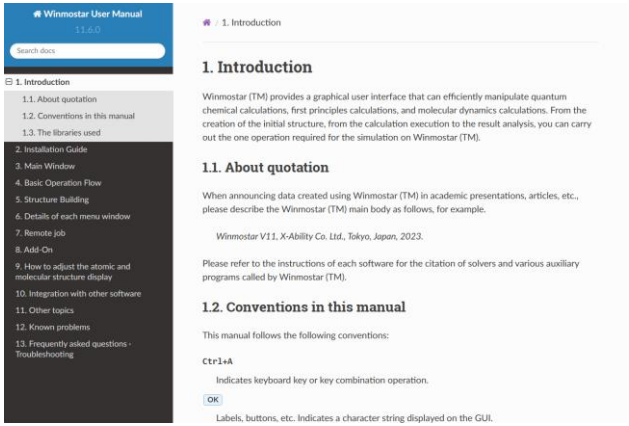
A. To plot the difference in charge or potential between the constant-N and constant-μ calculations, check **Select another esm1 file and plot difference**, then select the wm.esm1 file from the constant-N calculation folder (e.g., work1_QE_SCF¥wm.esm1).

B. Click **Draw**.



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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