winmostar tutorial

Quantum ESPRESSO Basic

V11.5.6

6 December, 2023 X-Ability Co., Ltd.

About This Document

- 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.
- 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 from Contact. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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Overview

- We will obtain the band structure, density of states, partial density of states, and electron density of Si crystals through first-principles calculations using Quantum ESPRESSO.

Procedure Overview:

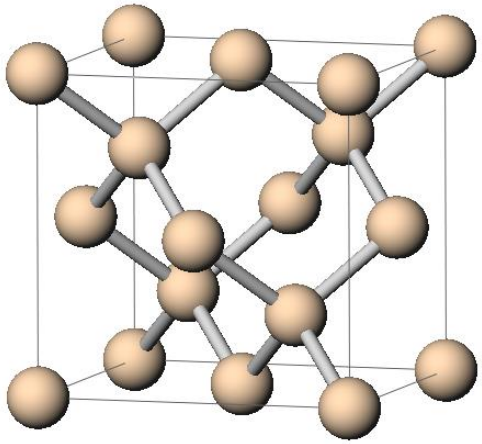
A. System Modeling

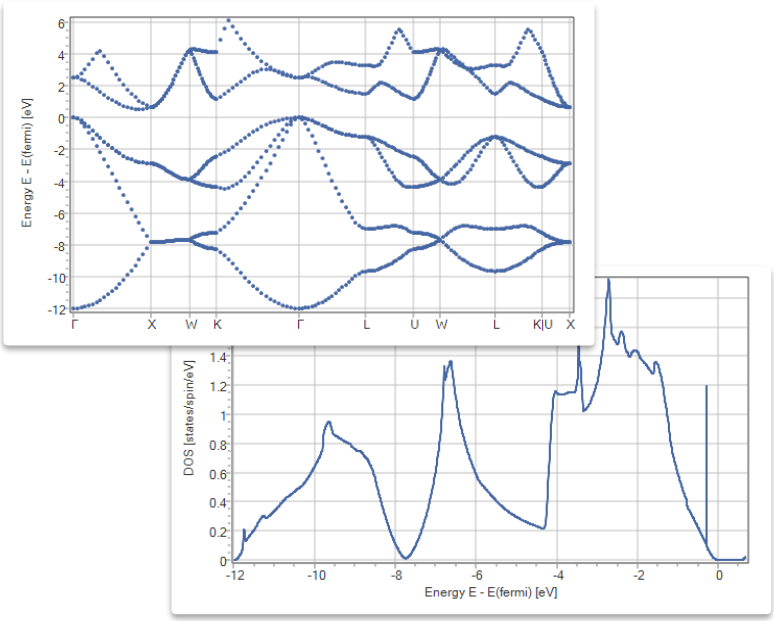
↓

B. Execution of Calculation

↓

C. Results Analysis





Operating Environment Settings

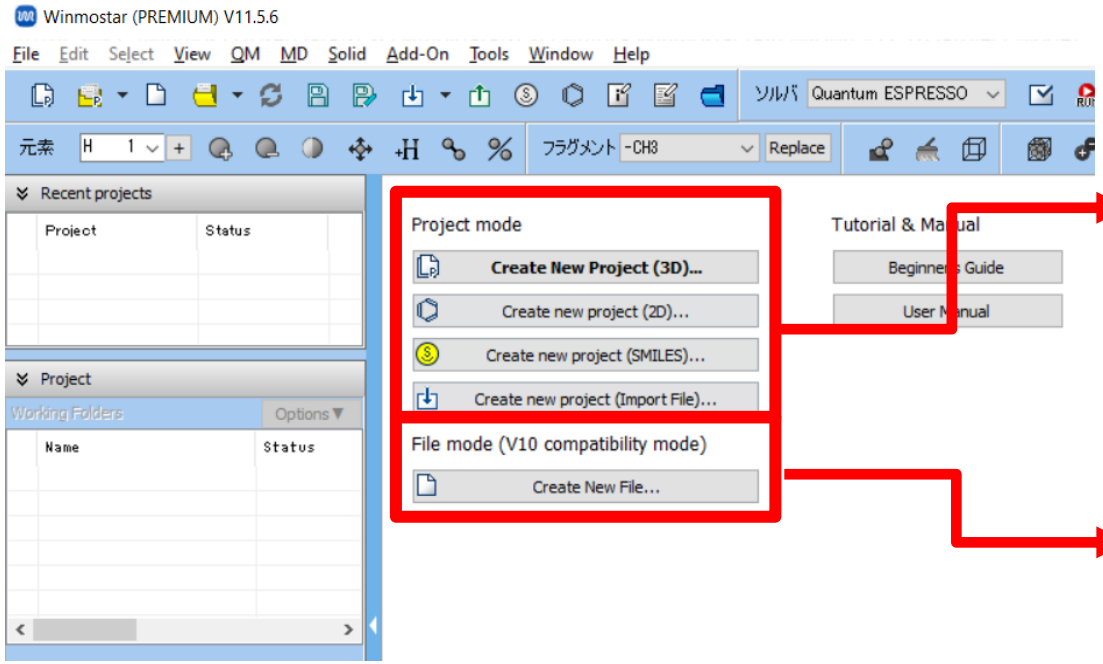
- Users utilizing Winmostar V11.5.0 or later in a 64-bit environment are advised to install and configure the CygwinWM version dated 2023/04/05 or later.
  - The CygwinWM version released after 2023/04/05 includes the recommended 64-bit version of Quantum ESPRESSO.

- 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 separately install and configure the Windows version of Quantum ESPRESSO.

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

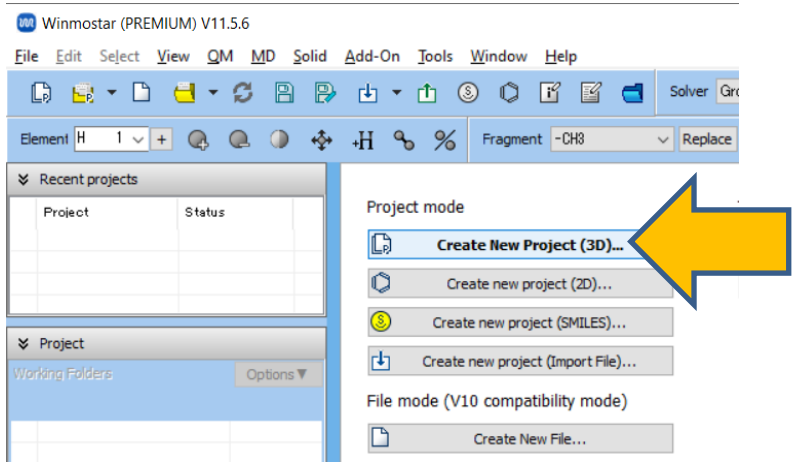
Users explicitly create and manage individual files.

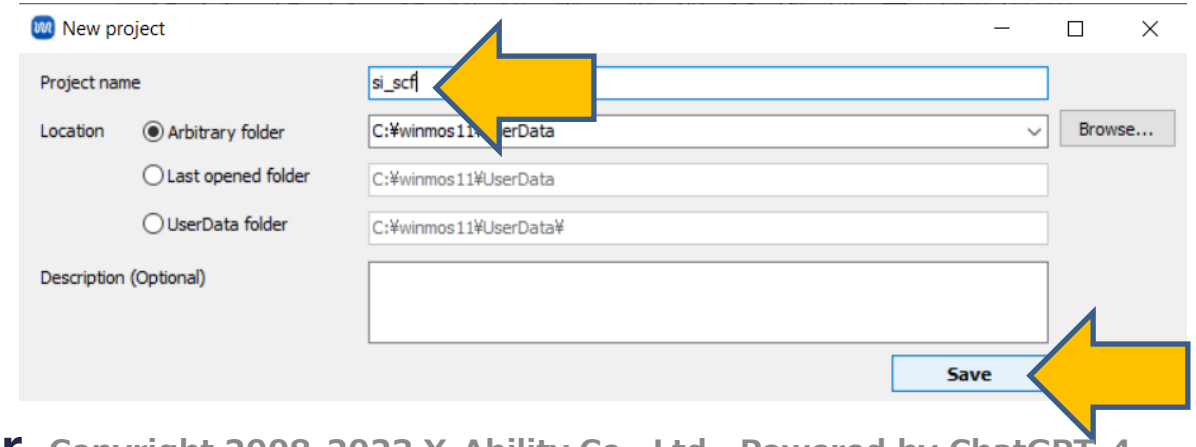
The operational procedure is the same as from V10 and earlier versions.

A. System Modeling

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

B. Enter '`si_scf`' for **Project name** and click **Save**.





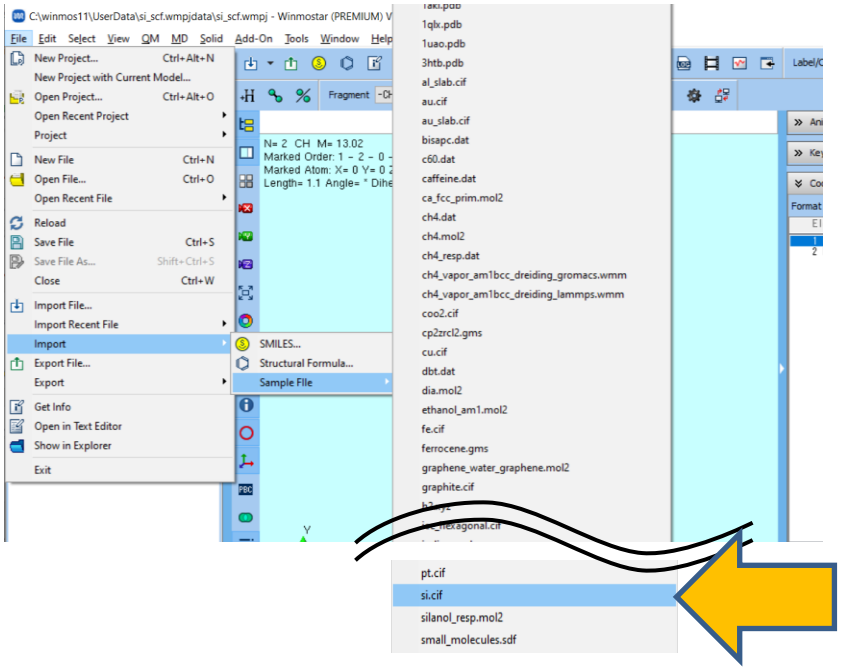
A. System Modeling

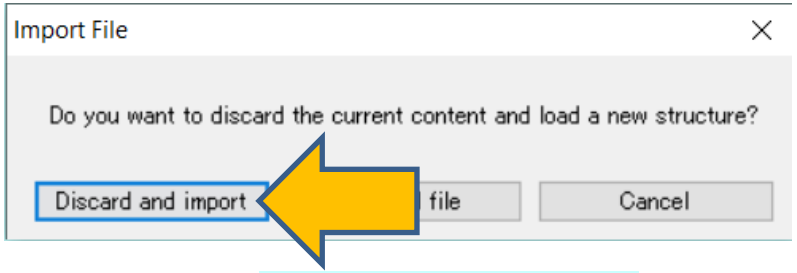
For details on creating an initial structure, please refer to Winmostar User Manual: 5. Methods for Creating Initial Structures.In this section, we will load an existing molecular structure file.

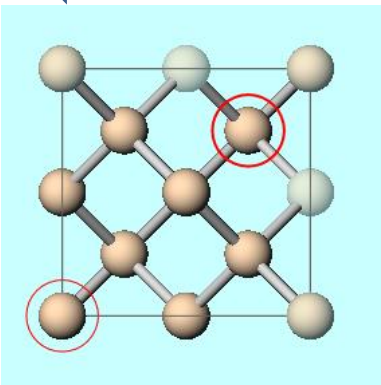
A. Click **File** | **Import** | **Sample File** | **si.cif**
   - If you wish to load a different file at this stage, use **File** | **Import File** instead.

B. In **Import File** dialog, click **Discard and import**.

C. Verify that the desired molecule appears in Viewport.





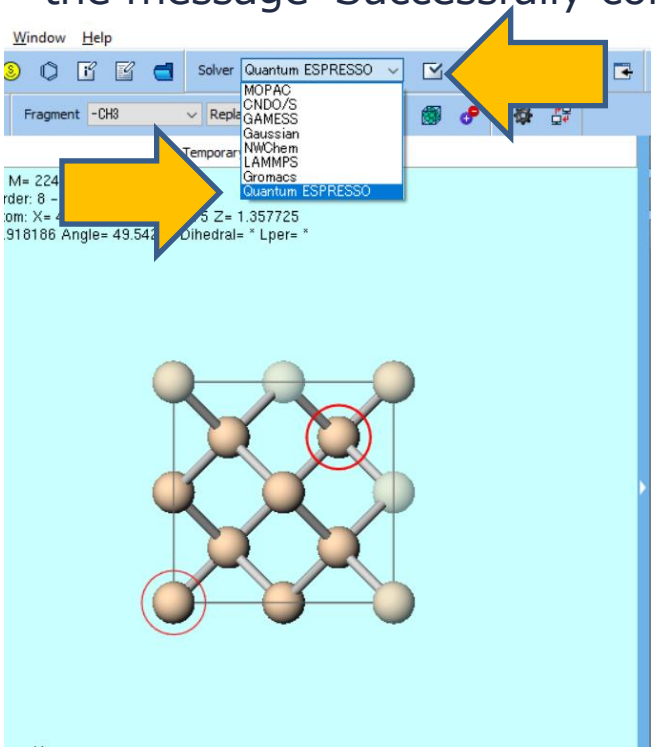


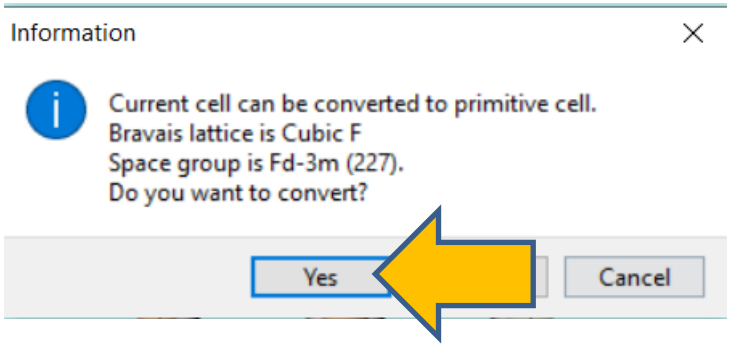
B. Execution of Calculation

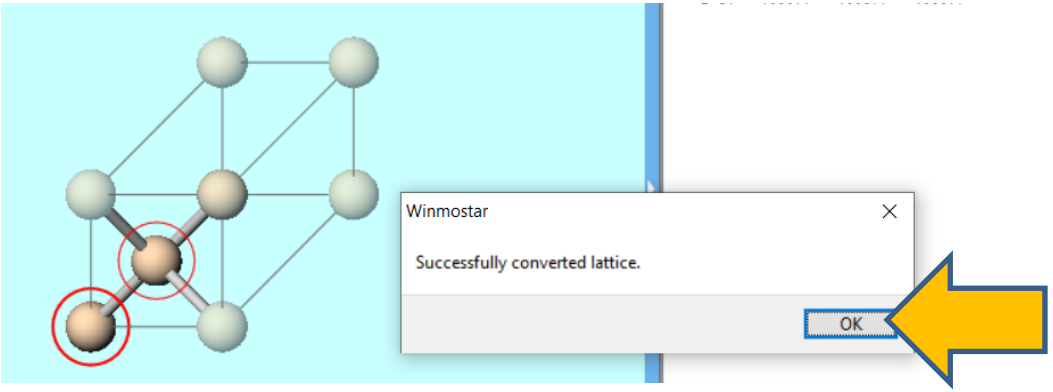
A. Select **Quantum ESPRESSO** from Toolbar's **Solver**.

B. Click **Workflow Setup**.

C. To reduce computation time, click **Yes** when asked if you want to convert to a primitive cell. The converted structure will appear in Viewport. Click **OK** when you see the message 'Successfully converted lattice'.

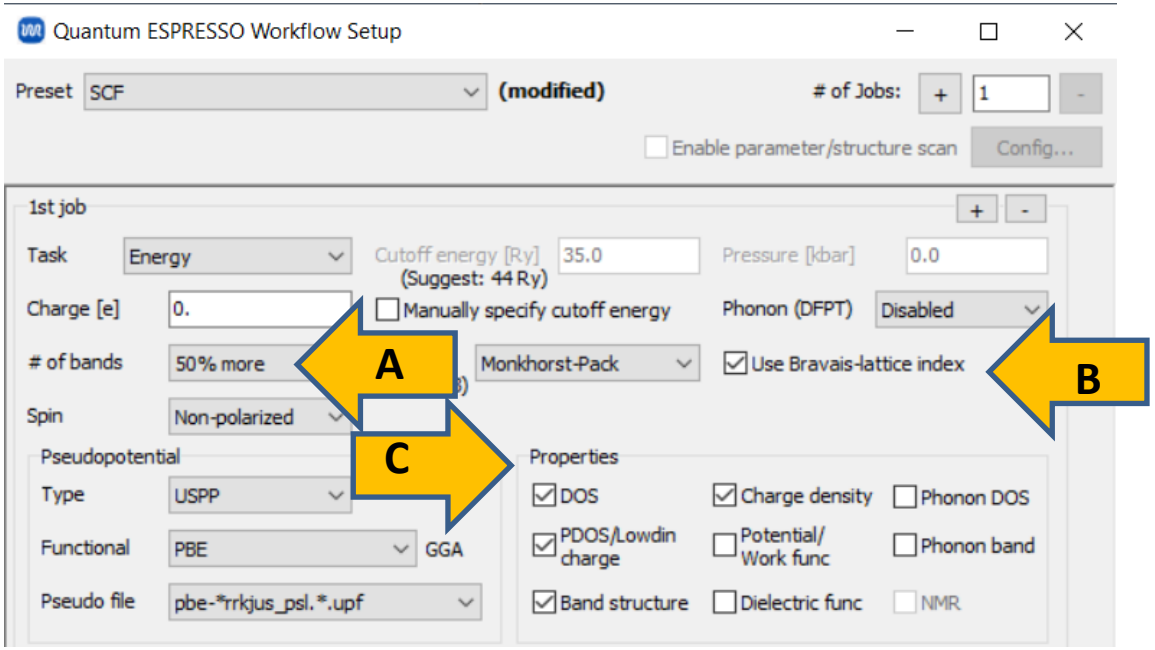






B. Execution of Calculation

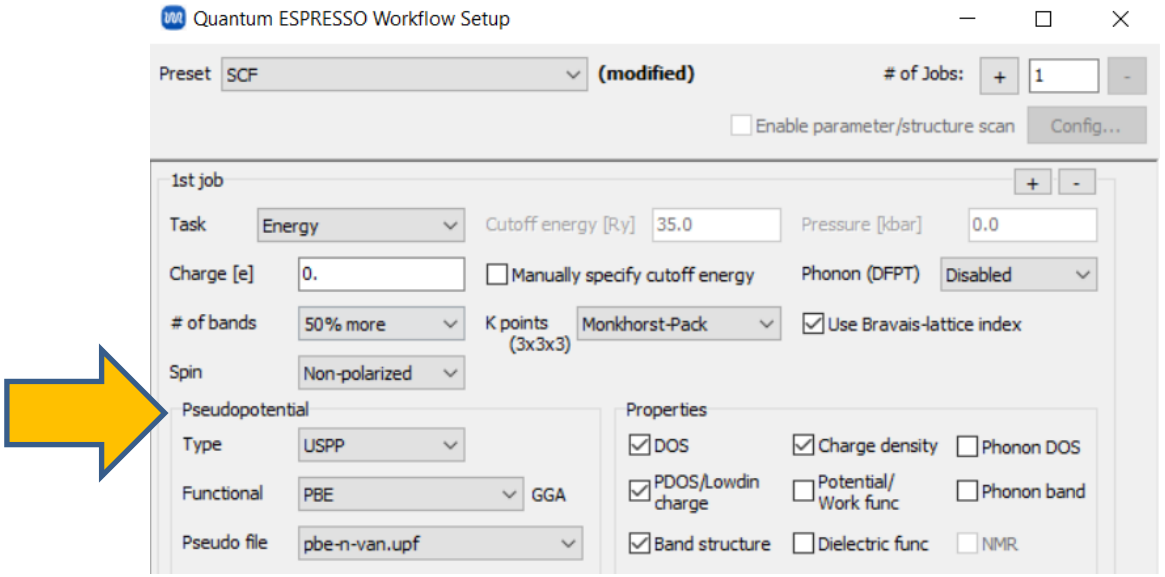
A. To output the band structure of the valence band, change **# of bands** to **50% more**.
B. Check **DOS**, **PDOS/Lowdin charge**, **Band structure**, and **Charge Density** in **Properties**.
C. As it is necessary for outputting the band structure in Winmostar, check **Use Bravais-lattice index**.



B. Execution of Calculation

A. Change **Pseudopotential Type** to '**USPP**', **Functional** to '**PBE**', and **Pseudo file** to '**pbe-n-van.upf**'.
   - The choices for '**Pseudo file**' are narrowed down based on **Type** and **Functional** selections. If you can infer the type of pseudopotential and functional from the notation of **Pseudo file**, please select **Pseudo file** directly.
   - If you want to add pseudopotential files, please refer to Quantum ESPRESSO Installation Manual for installation instructions.

B. Adjust computational conditions as necessary. (Not required in this manual)



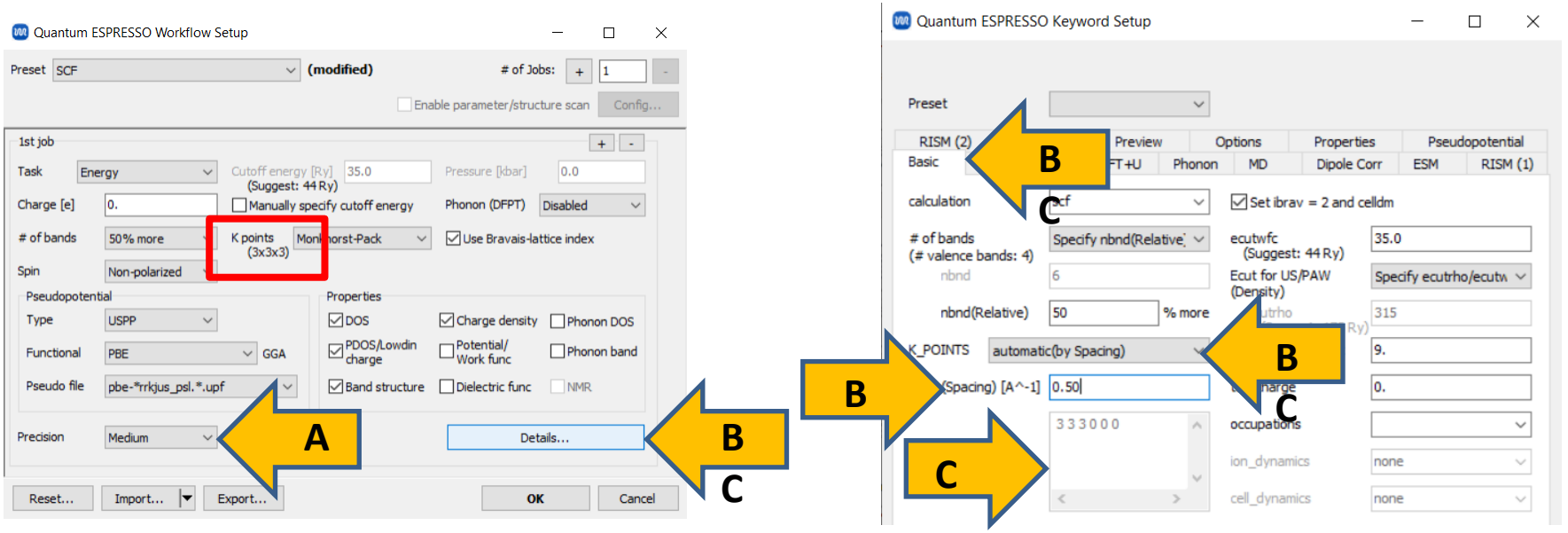
Supplement: Adjusting the Number of k-Points

To adjust the number of divisions in the Brillouin Zone using the Monkhorst-Pack method, follow these steps.

A. For rough adjustments: Change **Precision**. (The number of divisions will be displayed under **K points**.)

B. For finer adjustments: Click **Details**, go to **Basic** tab, change **K_POINTS** to 'automatic (by Spacing)', and adjust the value in **(Spacing)**.

C. For specific inputs: Click **Details**, go **Basic** tab, change **K_POINTS** to 'automatic', and adjust the values in the input fields located two lines below.



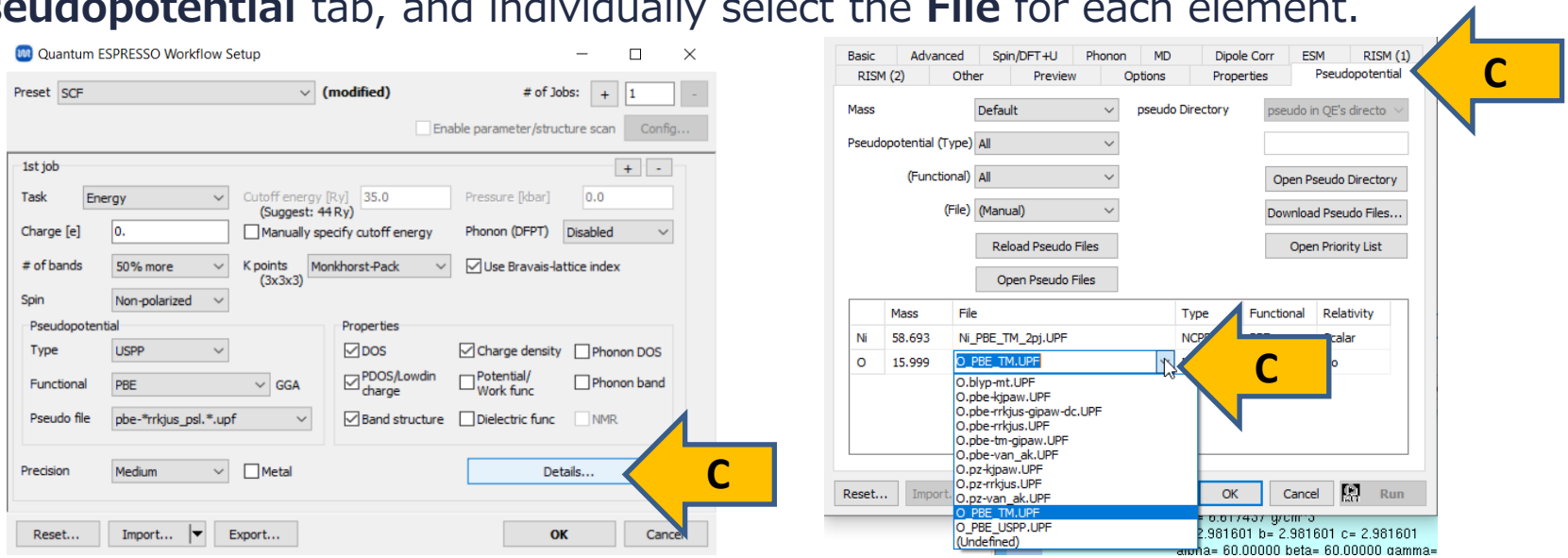
Supplement: If the Pseudopotential Files for Each Element are Not Available

If you do not have the necessary pseudopotential files for all elements in the substance you wish to calculate, perform one of the following operations.

A. Obtain the appropriate pseudopotential files, click **Tools** | **Preference** | **Calculation** | **Open QE pseudo directory**, and copy the files into the opened folder.

B. If the appropriate pseudopotential files are available but not recognized due to slight differences in names, click **Tools** | **Preference** | **Calculation** | **Open priority list**, and add items in a recognizable format. You can use an asterisk (*) as a wildcard.

C. In **Quantum ESPRESSO Workflow Setup** window, click **Details**, go to **Pseudopotential** tab, and individually select the **File** for each element.



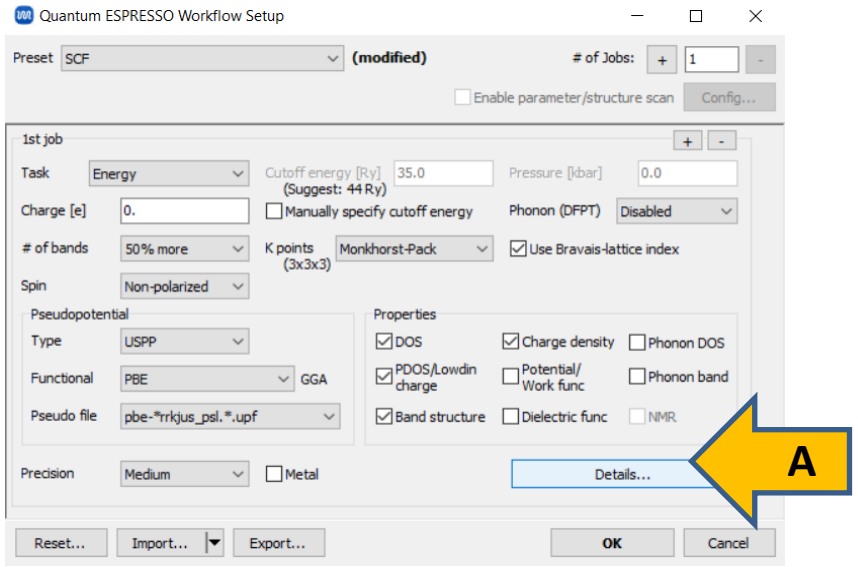
Supplement: Editing the Path of the Band Structure

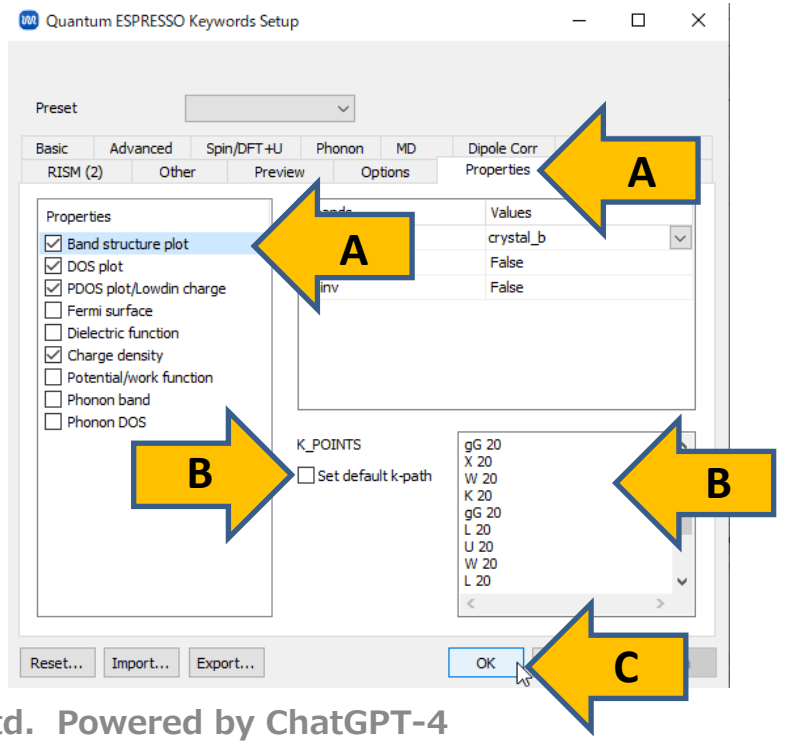
To edit the path of the band structure, follow these steps (not required in this manual).

A. Click **Details**, and in the opened **Quantum ESPRESSO Keywords Setup** window, click **Properties** tab. Then click the line for **Band structure plot** in **Properties**.

B. Uncheck **Set default k-path** and edit the path in the field to its right. The format follows the Quantum ESPRESSO K_POINTS syntax. Labels for special points can be found in the doc¥Brillouin_zones.pdf in the Quantum ESPRESSO installation folder.

C. After editing, click **OK**.





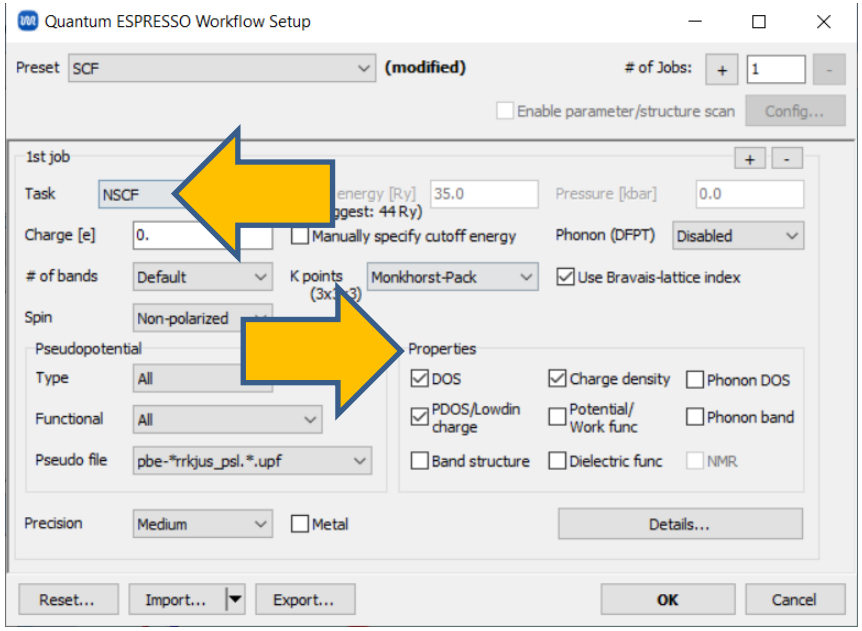
Supplement: Calculating Properties for Past Jobs Post-Hoc

To calculate properties such as the density of states for previously completed SCF or structure optimization calculations, follow these steps (not required in this manual).

A. Click **Workflow Setup**, and when prompted 'Do you want to continue from previous run?', click **Yes**. Then select the working folder of the completed SCF or structure optimization calculation and click **OK**.

B. Change **Task** to 'NSCF', and in **Properties**, check the items you want to calculate.

C. Click **OK**, and then click **Run** in **Job Setting** window.

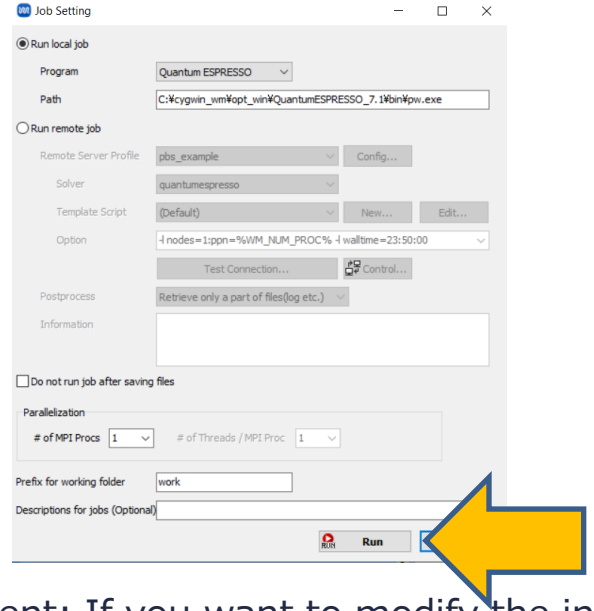


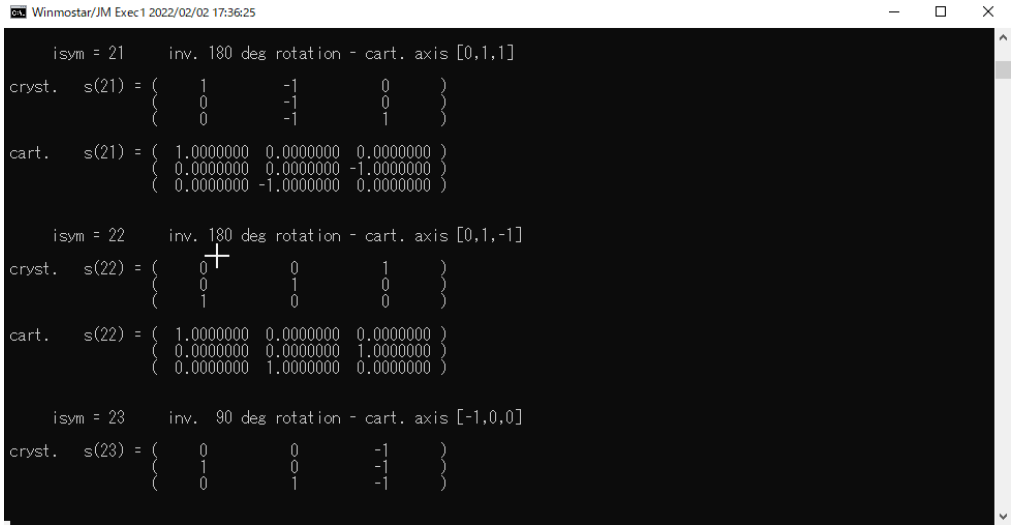
B. Execution of Calculation

(If working with remote jobs, please proceed here first.)

A. Click **OK** at the bottom right of **Quantum ESPRESSO Workflow Setup** window.

B. Click **Run** in **Job Setting** window. **Winmostar Job Manager** will start in the background, and a black console window, as shown in the right figure, will appear, indicating the start of the calculation.



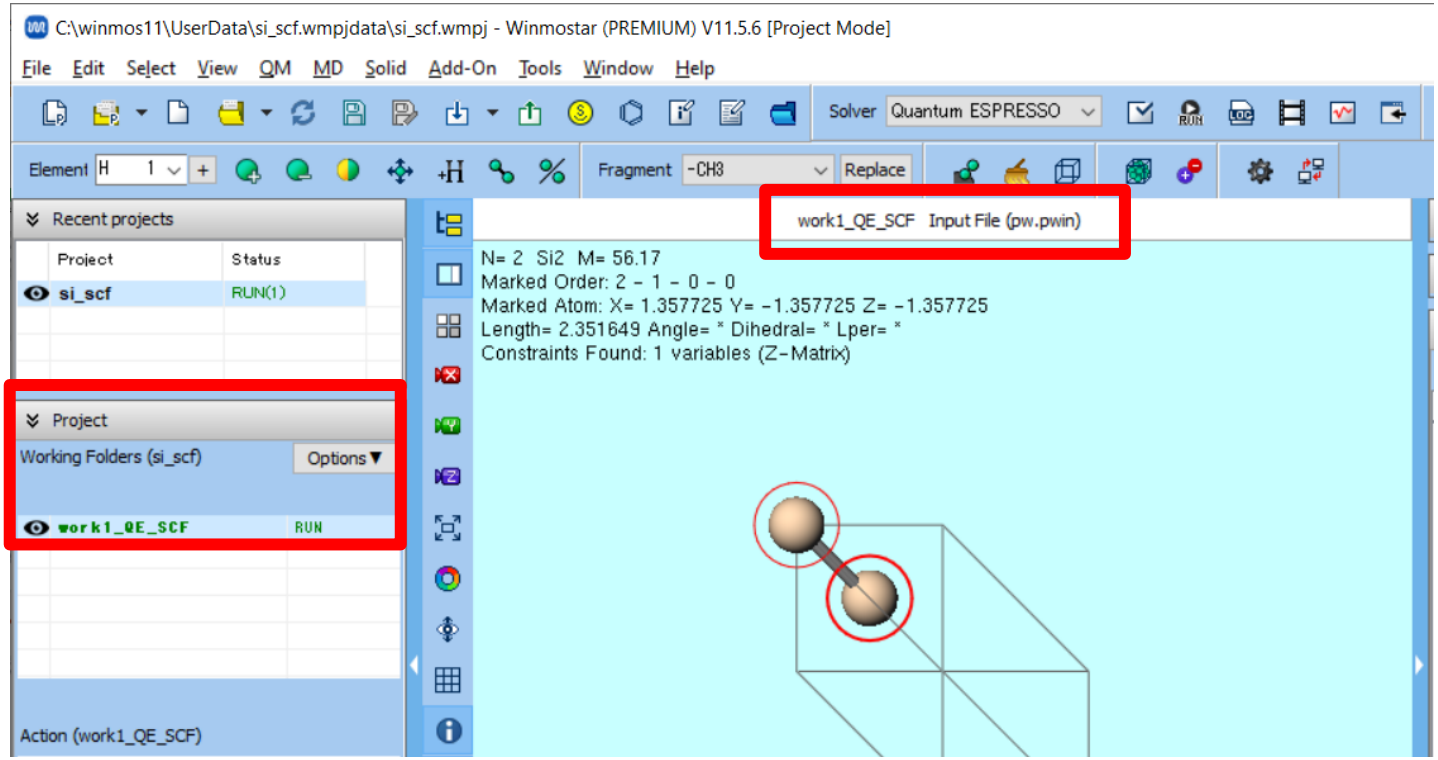


Supplement: If you want to modify the input files yourself or copy them to a remote server for use, check **Do not run job after saving files** in **Job Setting** window and click **Run**. To run the calculation after saving, click **File** | **Project** | **Selected Woking Folder** | **Run**.

B. Execution of Calculation

A. Upon returning to the main window (it's fine even if a calculation is running), **Project Area** will show the working folder for the job set up in **Quantum ESPRESSO Workflow Setup** window.

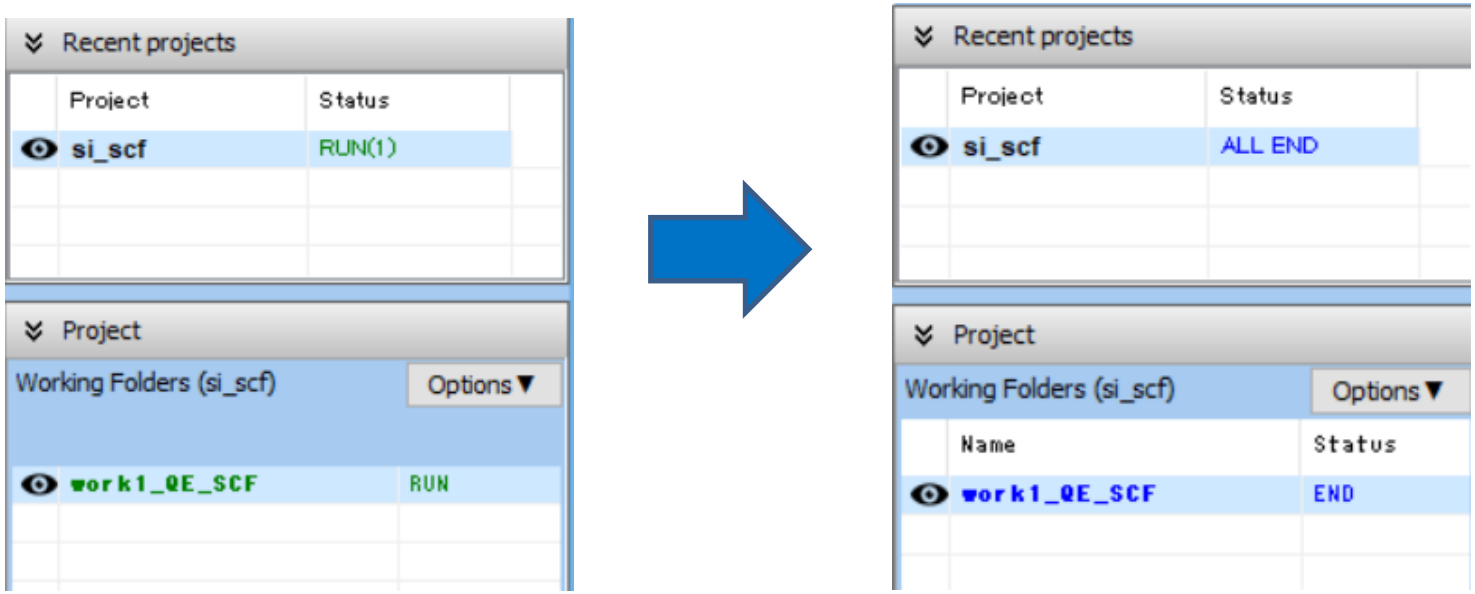
B. In Viewport, the input file from the first working folder (work1_QE_SCF) will automatically open. You can also confirm this at the top of **Viewport**.



B. Execution of Calculation

A. Based on the progress of the calculation, the status of each working folder in **Working Folders section of Project Area** changes from **PEND (black)** → **RUN (green)** → **END (blue)**.

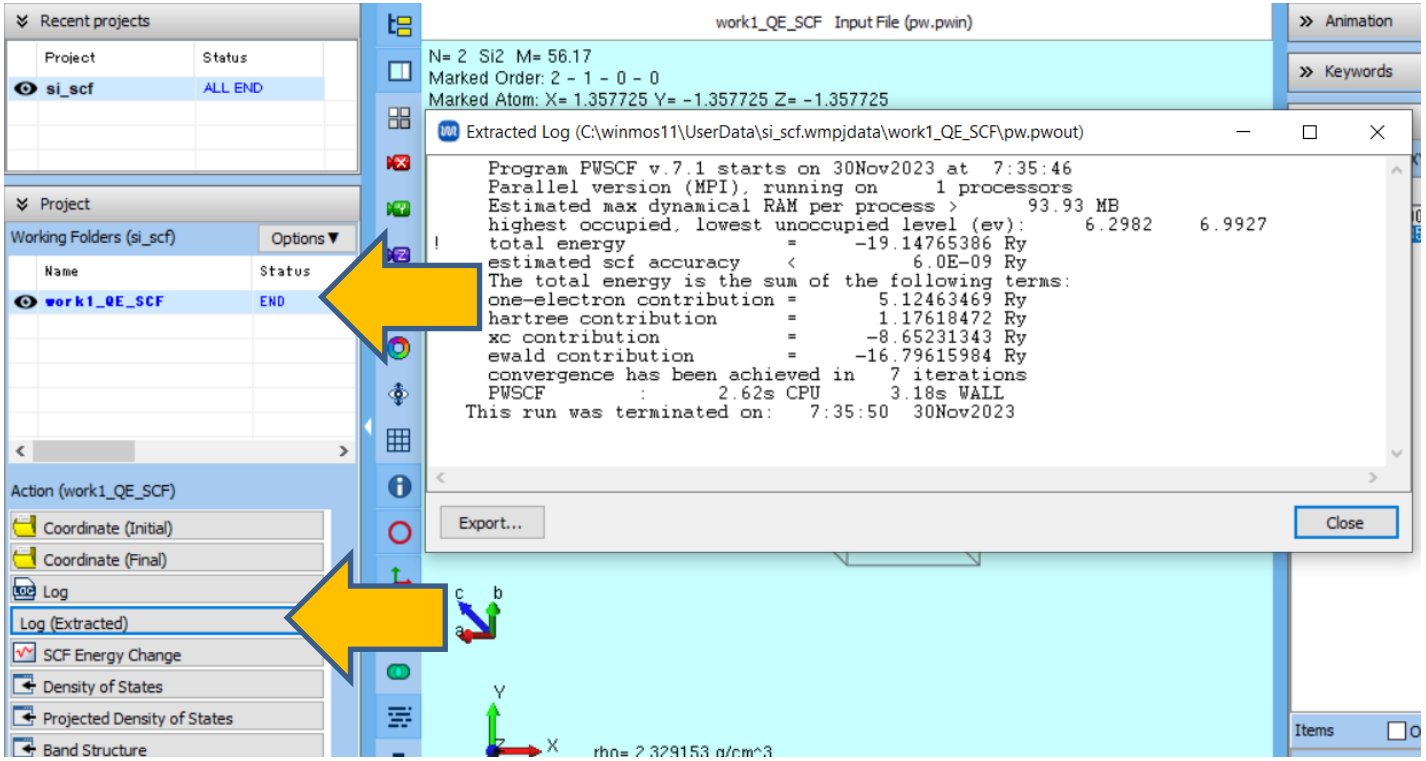
B. Wait until the status of all work folders changes to **END (blue)**. During this time, the status of **the recently used project** 'si_scf' will also change to ALL **END (blue)**.



B. Execution of Calculation

A. If you want to view the main contents of each calculation's log, select the relevant calculation's working folder in **Working Folders section of Project Area**, then click **Log(Extracted)** under **Action**. (This feature is exclusive to the Professional Premium Edition.)

B. If you wish to view the complete log, click **Log**.



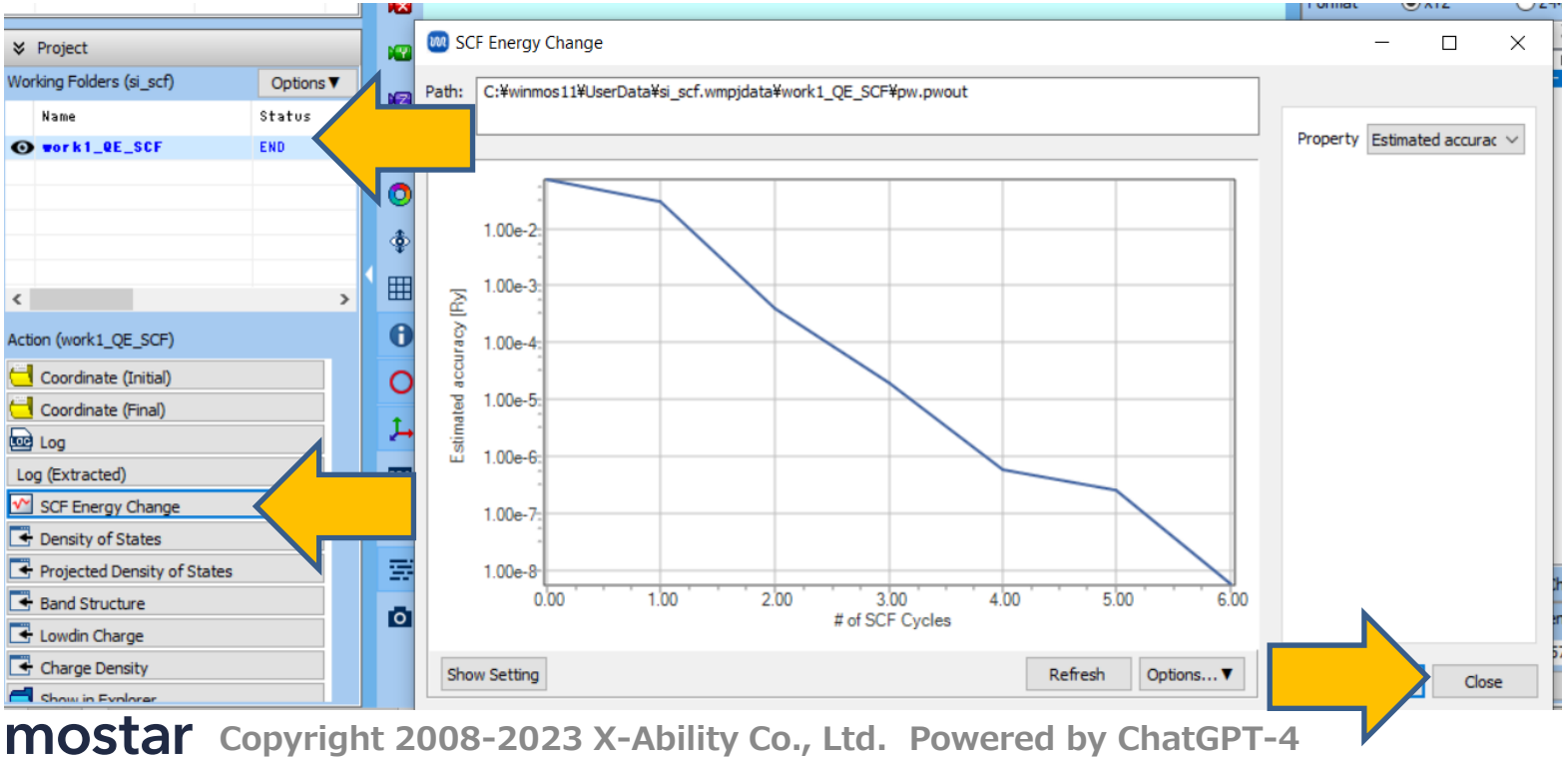
C. Result Analysis　SCF Energy Change

From here on, you may skip any analysis items that are not of interest.

A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').

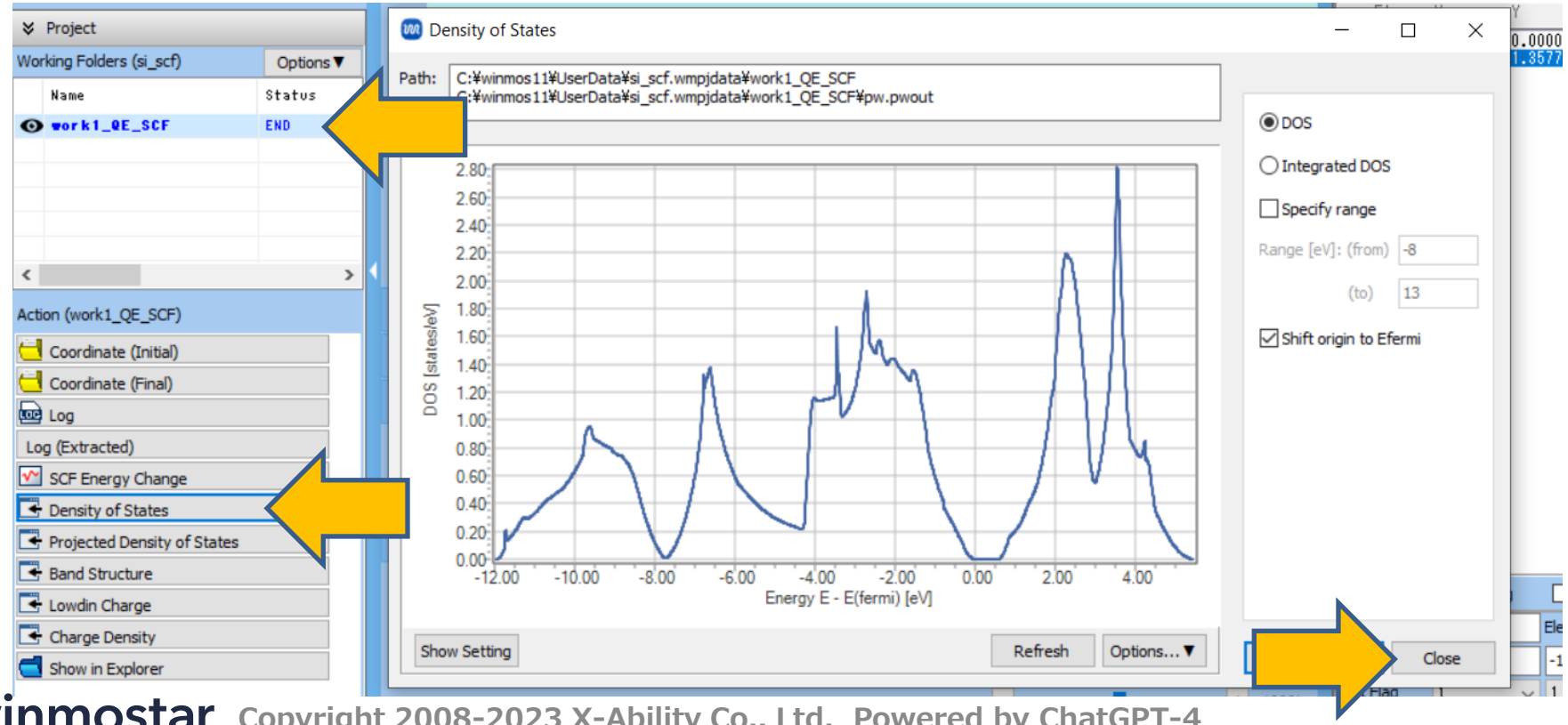
B. When you click **SCF Energy Change** in **Action**, **SCF Energy Change** window will open, displaying the plot of Estimated accuracy from the Quantum ESPRESSO log.

C. After reviewing, click **Close**.



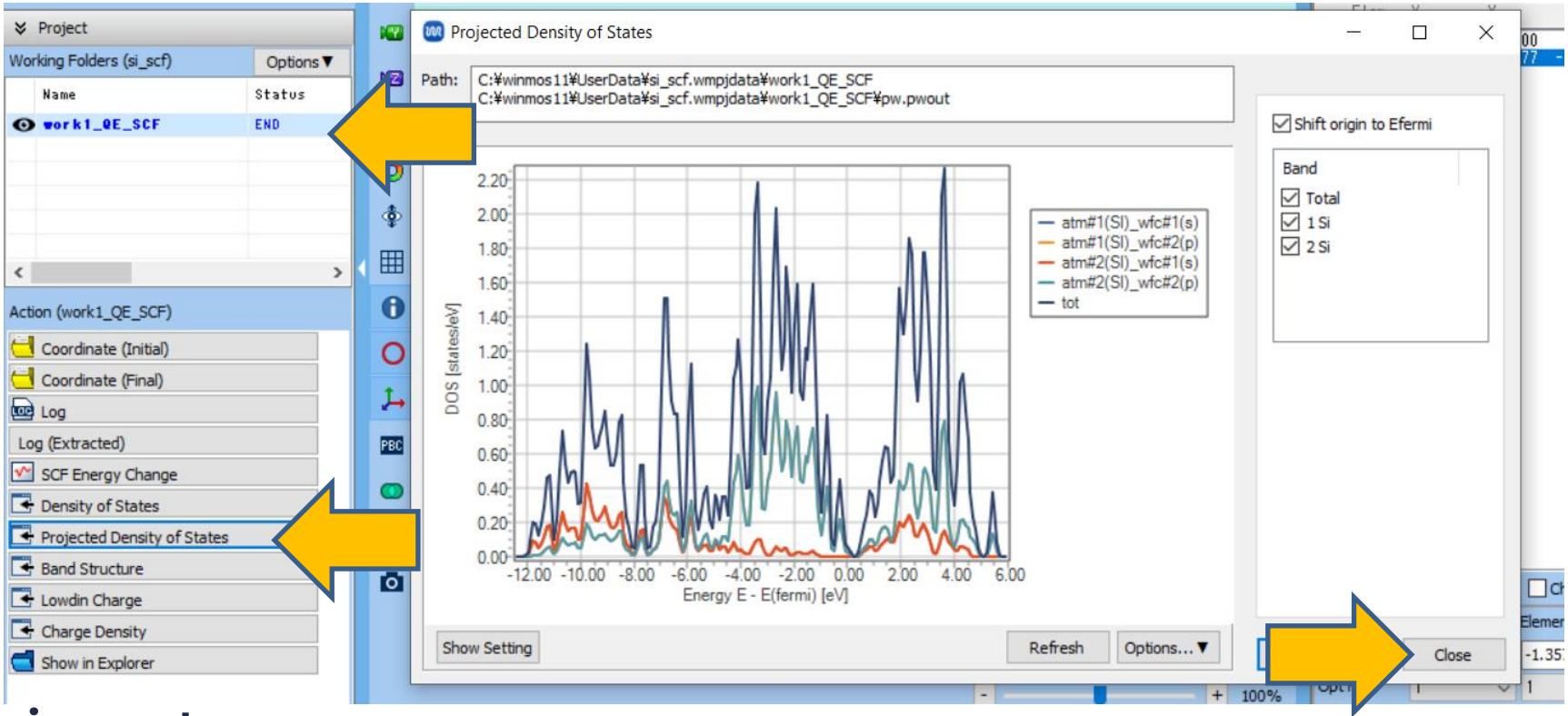
C. Result Analysis　Density of States

A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').
B. When you click **Density of States** in **Action**, **Density of States** window will open, displaying the plot of the density of states..
C. After reviewing, click **Close**.



C. Result Analysis　Partial Density of States

A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').
B. When you click **Projected Density of States** in **Action**, **Projected Density of States** window will open, displaying the plot of the partial density of states.
C. After reviewing, click **Close**.

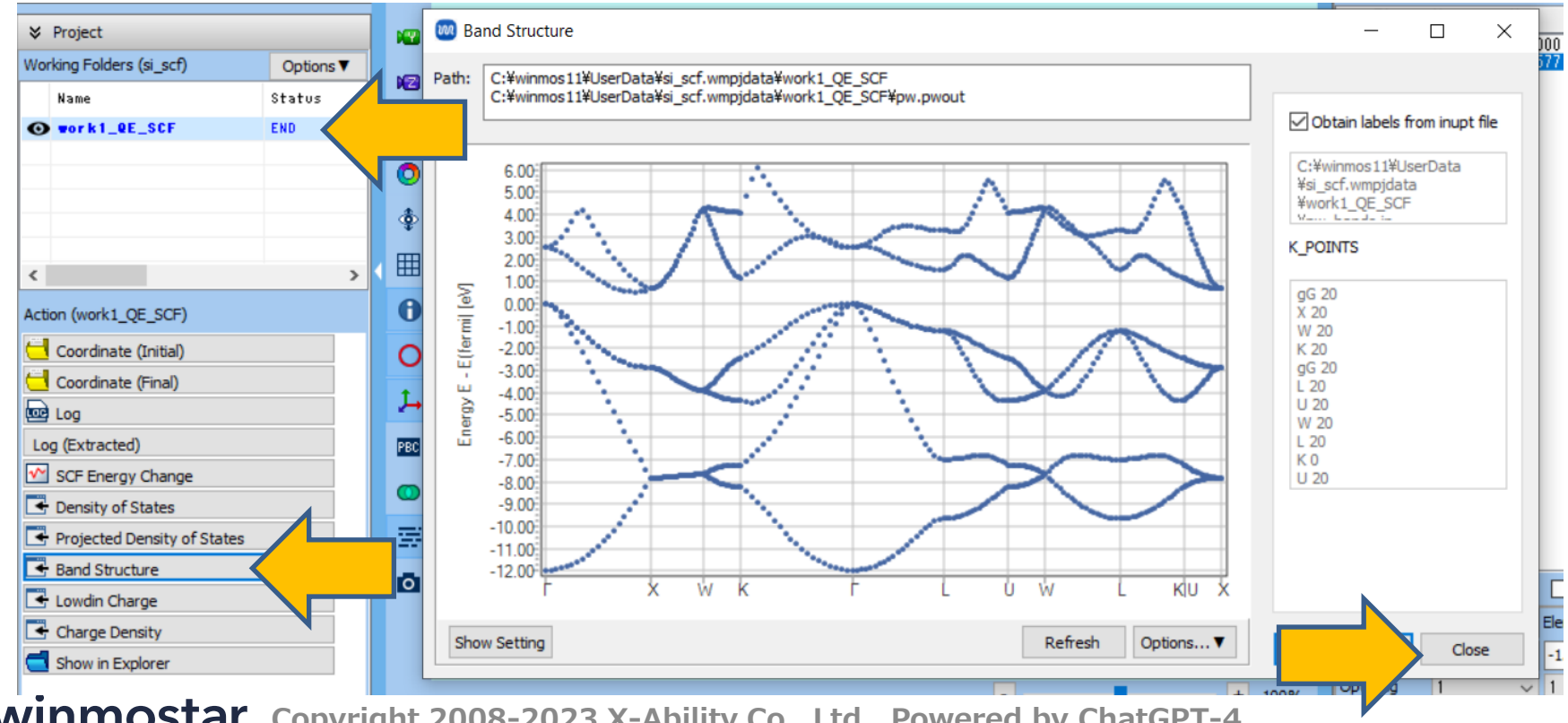


C. Result Analysis　Band Structure

A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').

B. When you click **Band Structure** in **Action**, **Band Structure** window will open, displaying the plot of the band structure.

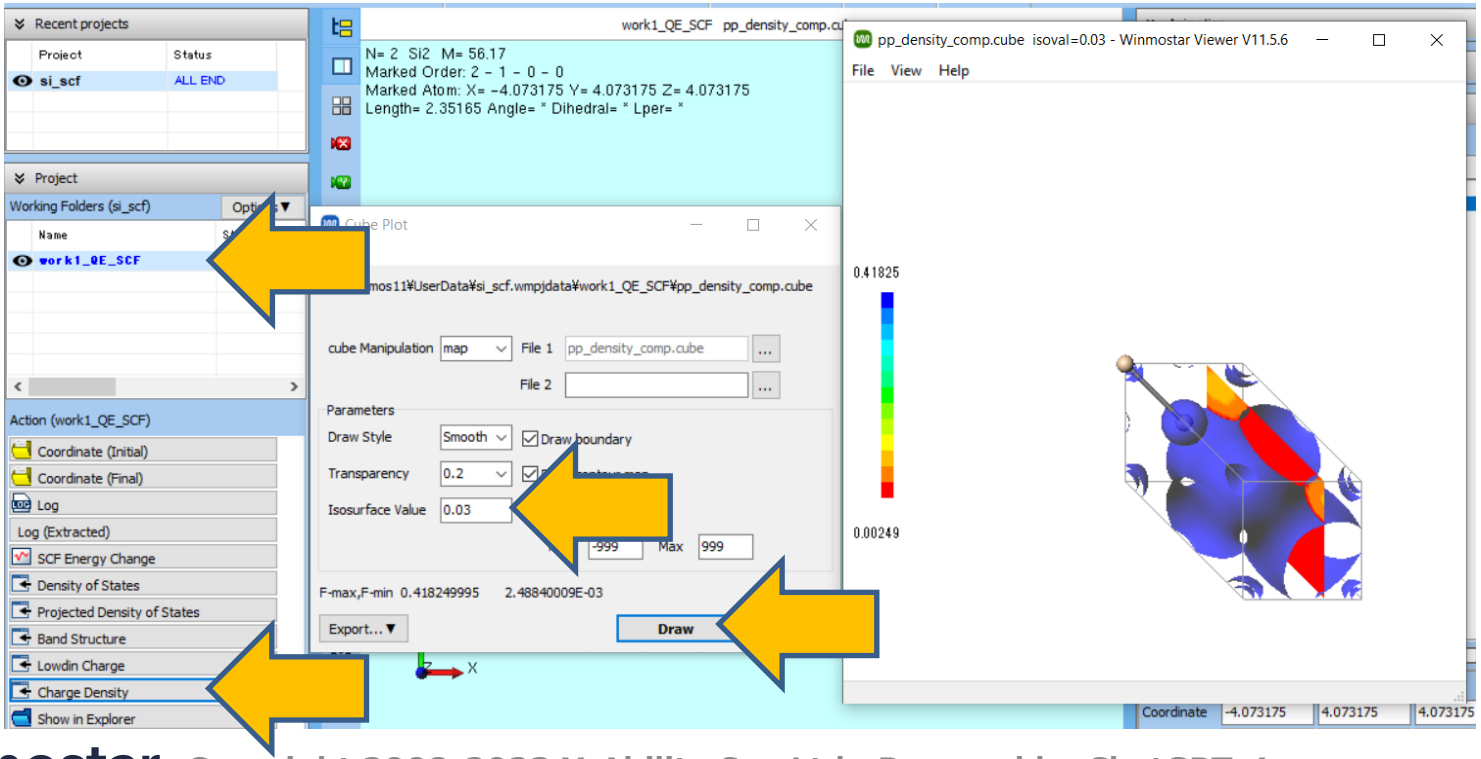
C. After reviewing, click **Close**.



C. Result Analysis　Electron Density

A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').

B. When you click **Charge Density** in **Action**, after automatic processing for a few seconds, **Winmostar Viewer** will start and the electron density will be displayed in 3D. If you want to change the settings of the isosurface, modify **Isosurface Value** in **Cube Plot** window and click **Draw**.

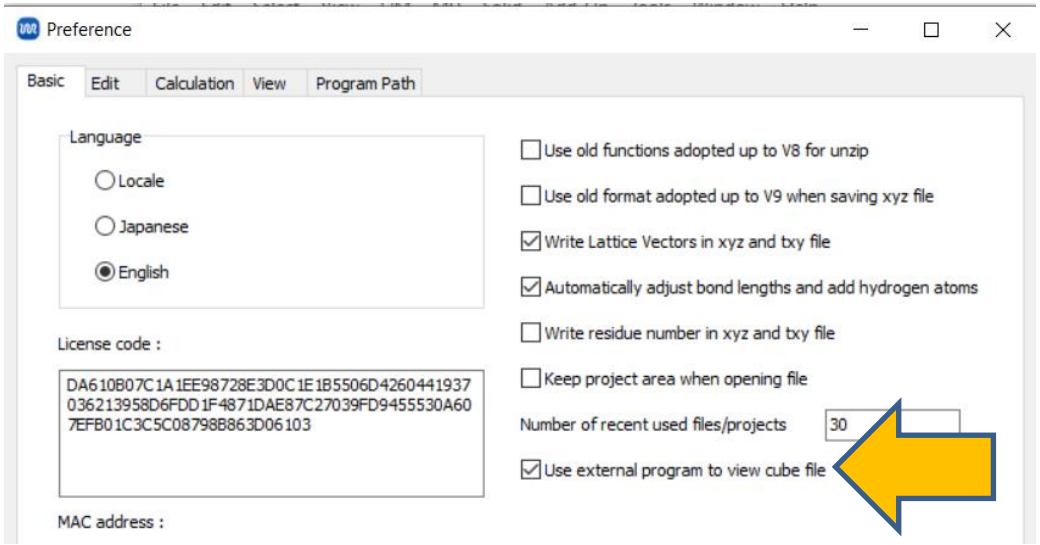


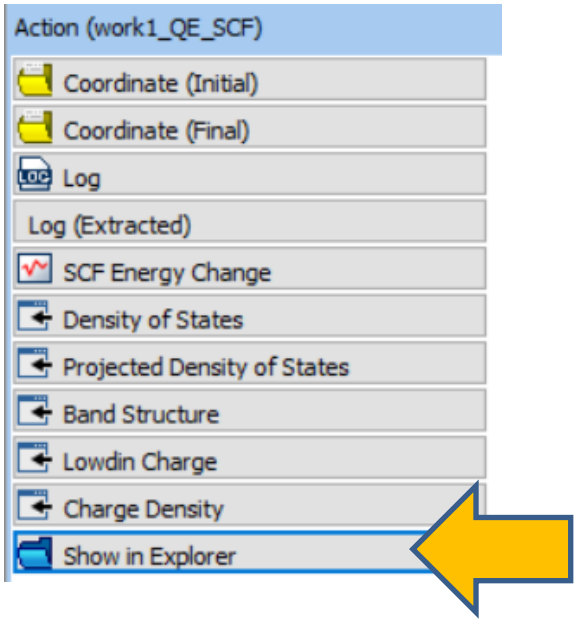
Supplement: Visualization of Electron Density Using Programs Other Than Winmostar

It is possible to visualize the electron density using other programs like VESTA.

A. By checking the box for **tools** | **Preference** | **Basic** | **Use external program to view cube file** and selecting the executable file of VESTA in **Program path** | **Cube Viewer**, VESTA will open as per the procedure on page 23.

B. Click **Show in Explorer** under **Action**, and explicitly open the '`pp_density_comp.cube`' file in the working folder with VESTA or a similar program.





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