winmostar tutorial

Quantum ESPRESSO Dielectric Function

V11.6.5

1 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 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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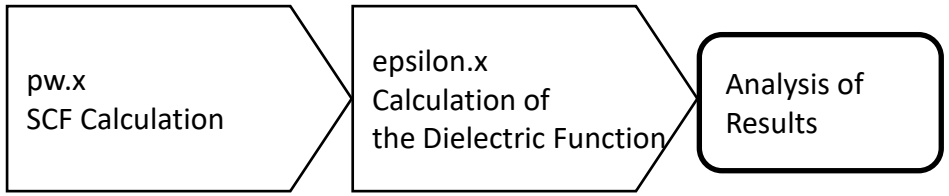
Overview

- This tutorial demonstrates how to obtain the dielectric function of a silicon crystal.



Note :

- The choice of k-points, number of bands, type of pseudopotential, cutoff energy, and smearing width will affect the calculation results. This tutorial uses settings that reduce accuracy to obtain results quickly.
- ◆ For a detailed explanation of the calculation methods and settings in Quantum ESPRESSO, please refer to our article at https://qiita.com/xa_member.

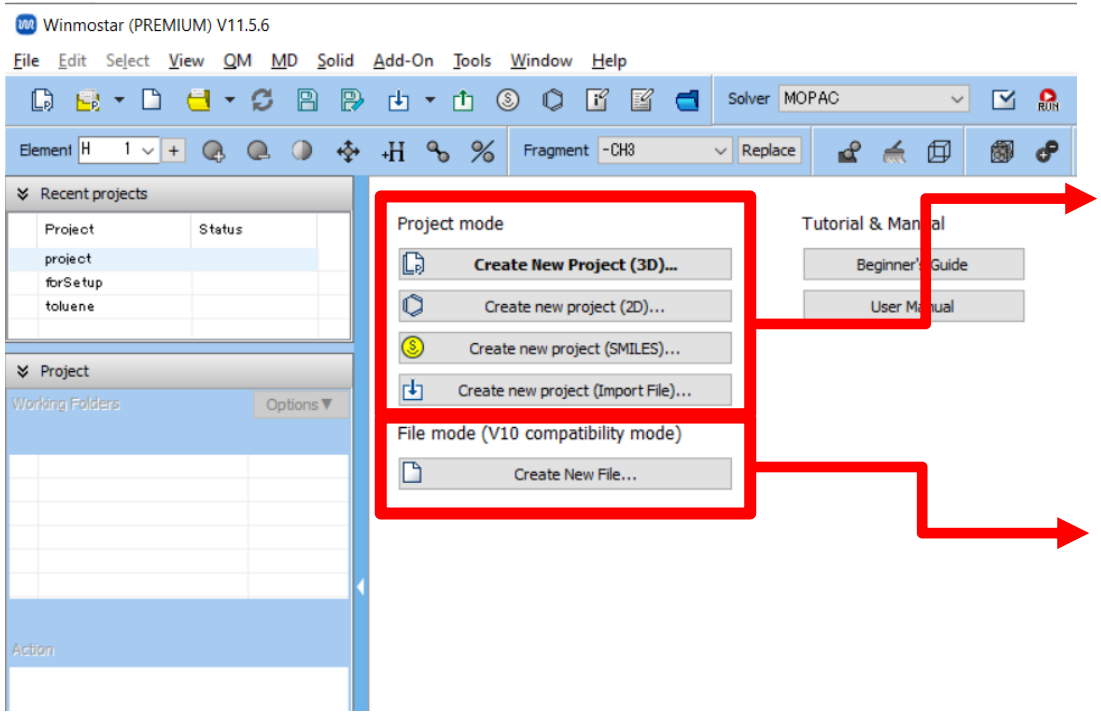
Preference of Operating Environment

- 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.
For operations in File Mode, please refer to [Quantum ESPRESSO tutorial for version 10].



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

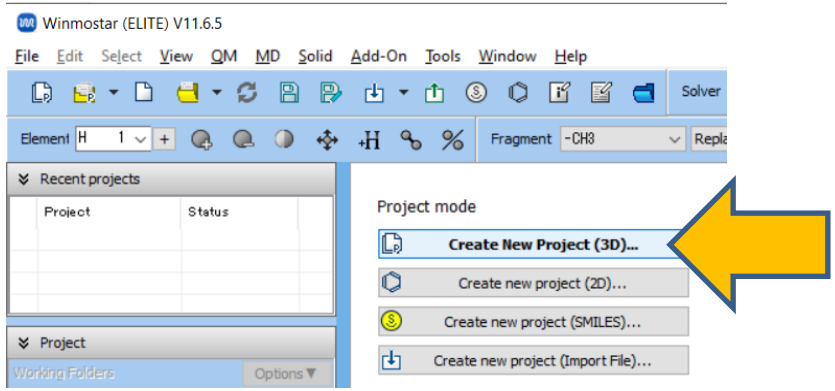
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

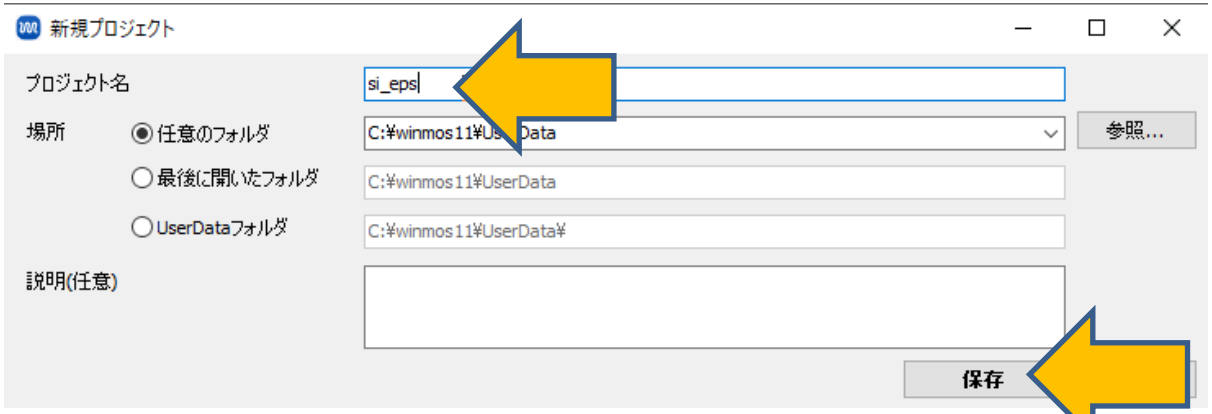
A. Modeling of the System

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 '`si_eps`' in **Project name** and click **Save**





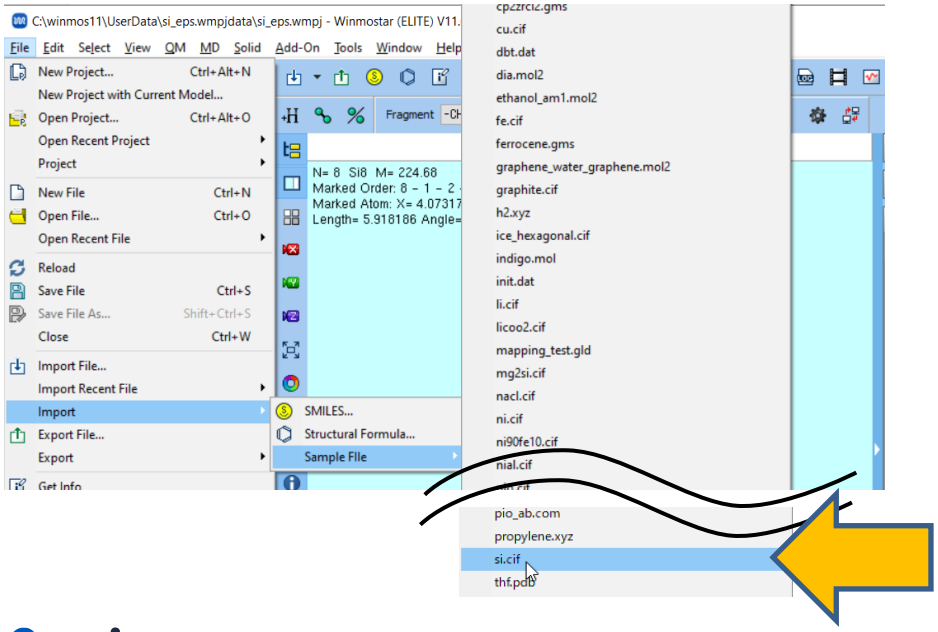
A. Modeling of the System

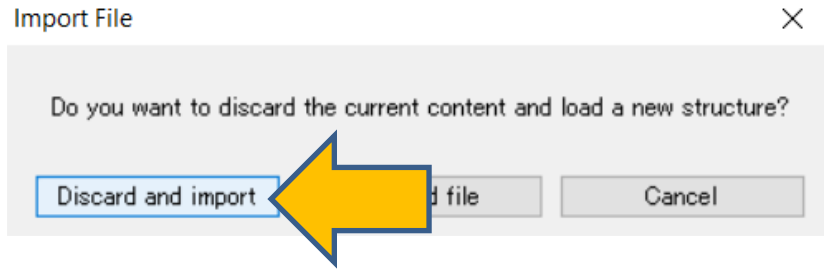
For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Methods for Creating Initial Structures'.Here, we load an existing molecular structure file.

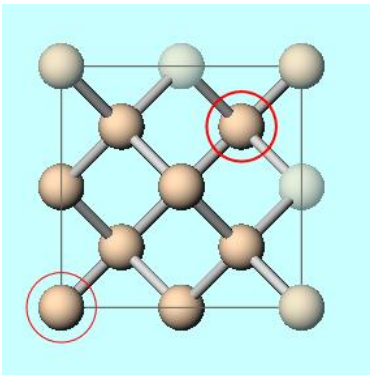
A. Click **File | Import | Sample File | si.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

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

C. Confirm that the desired structure appears in Viewport.

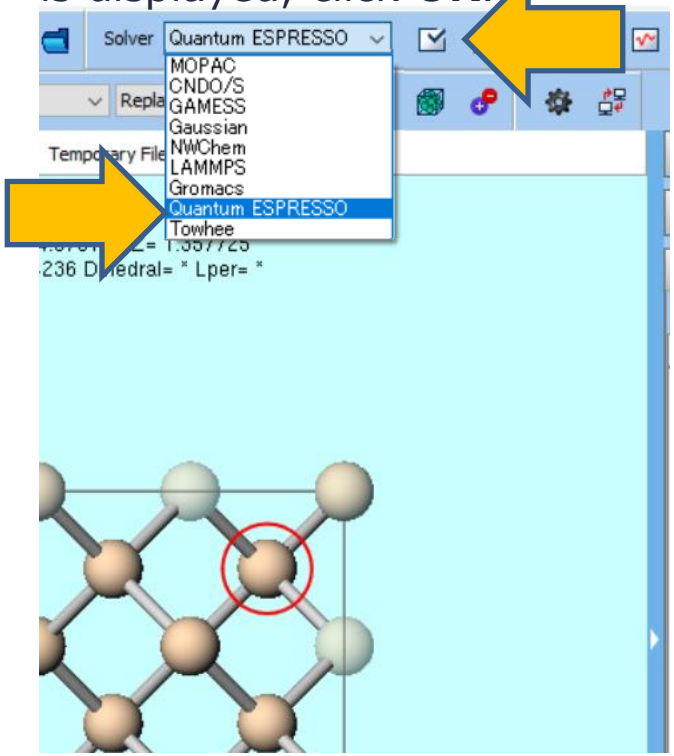


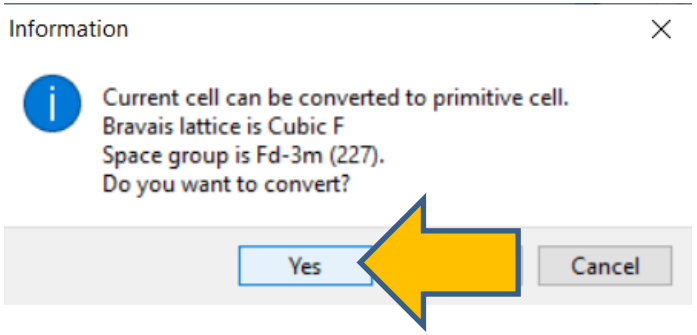




B. Execution of Calculation

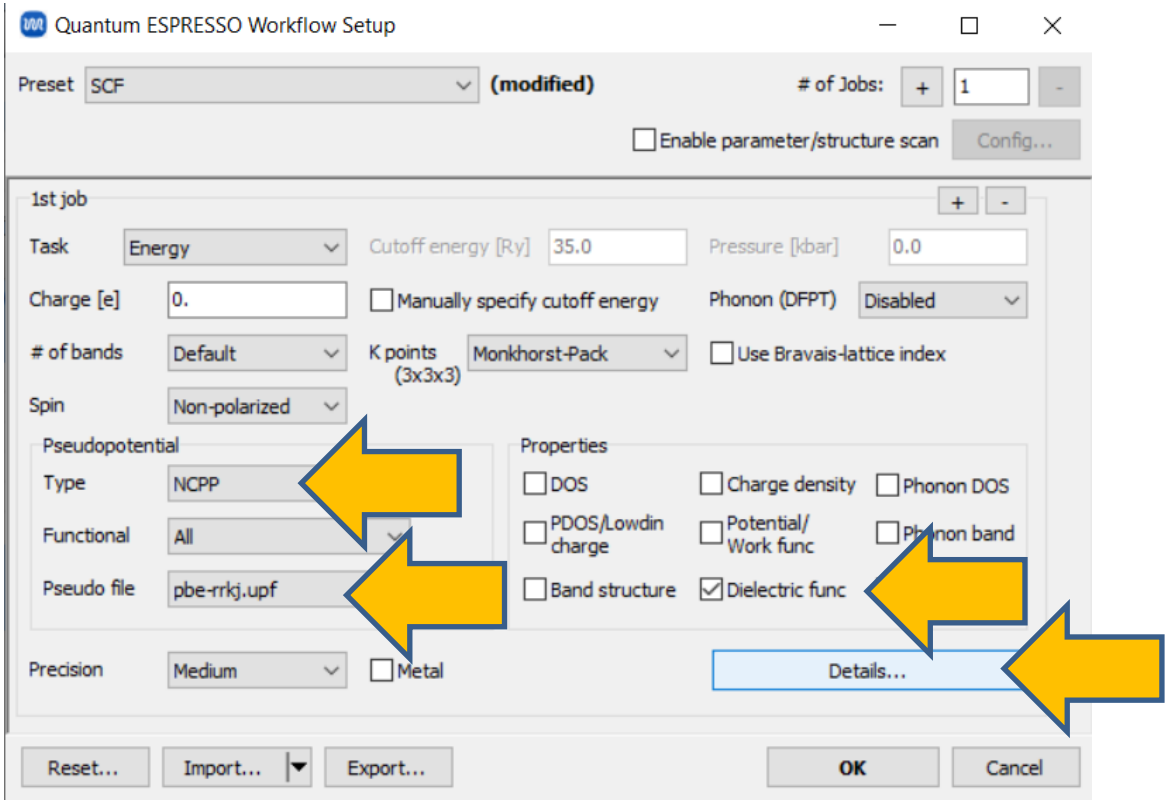
A. Select **Quantum ESPRESSO** from toolbar's **Solver**.
B. Click **(Workflow Setup)**.
C. To reduce computation time, if asked whether to convert to a primitive cell, click **Yes**. The converted structure will appear in Viewport. When 'Successfully converted lattice' is displayed, click **OK**.





B. Execution of Calculation

A. Change **Type** of **Pseudopotential** to **NCPP** and **Pseudo file** to **pbe-*rrkj.upf** (because QE's `epsilon.x` does not support Ultrasoft).
B. Check **Dielectric func** under **Properties**.
C. Click **Details**.



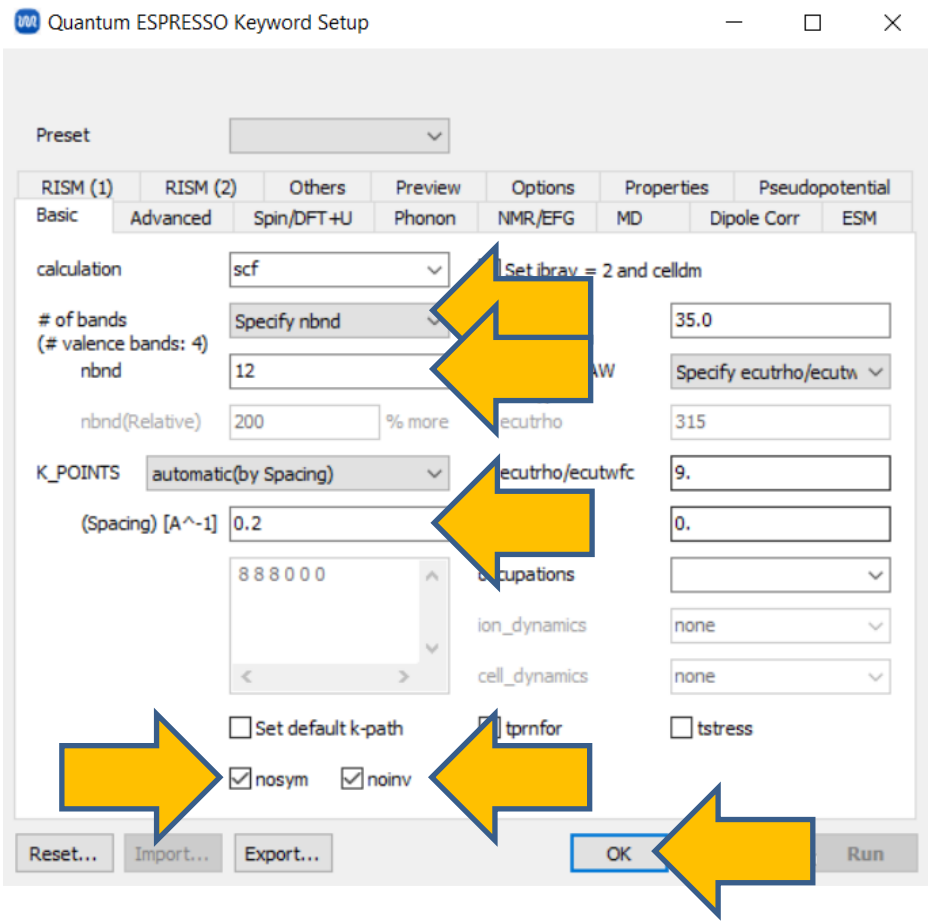
B. Execution of Calculation

A. In **Basic** tab, make the following changes:
   A. Change **# of bands** to **Specify nbnd**.
   B. Enter '12' for **nbnd**.
   C. Enter '0.2' for **K_POINTS (Spacing)**.
   D. Check **nosym** and **noinv**.

B. If you want to reduce the computational accuracy to finish the calculation faster, change **(Spacing)** to '0.5'.

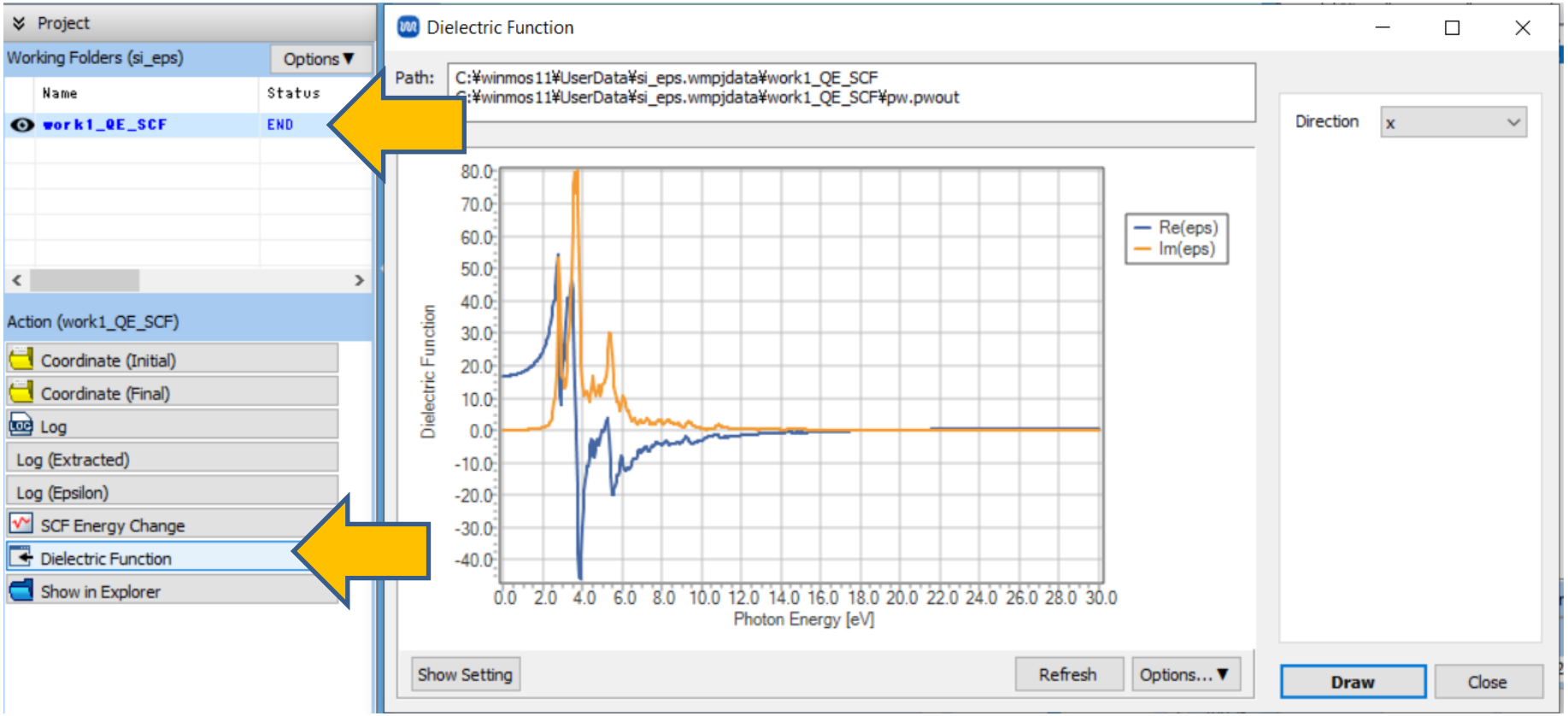
C. Click **OK**.

D. Click **OK** in **Quantum ESPRESSO Workflow Setup** window, then after setting **Job Setting** as needed, click **Run**.



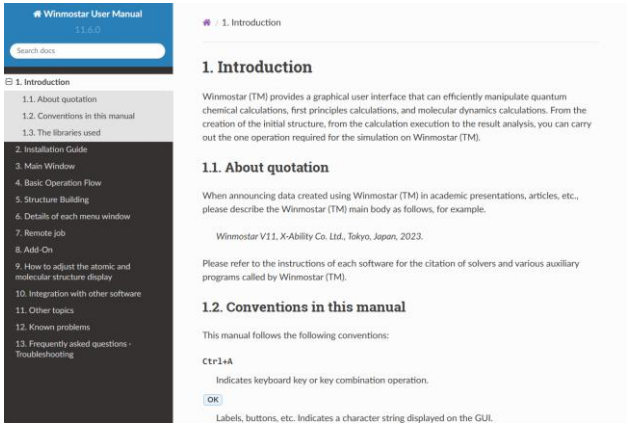
C. Analysis of Results

A. After **the status** of **the work folder work1_QE_SCF** changes to **END（blue）**, click work1_QE_SCF in **Working Folders** and click **Dielectric Function** in **Action**.



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.)
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