winmostar tutorial

Quantum ESPRESSO Phonon Calculation (DFPT Method)

V11.6.5

21 February 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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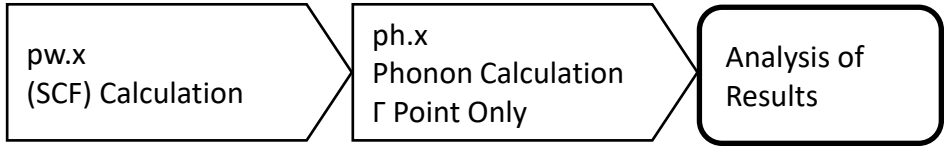
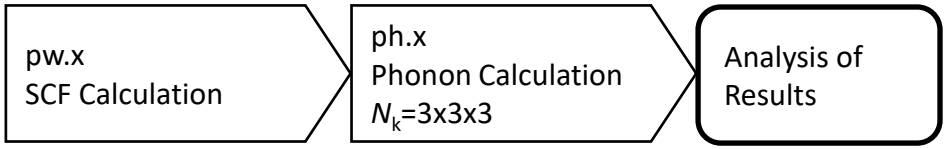
Overview

- Obtaining IR and Raman spectra of Si crystal from phonon calculations.



- Obtaining phonon bands and phonon DOS of Si crystal from phonon calculations.



Note:

- The choice of k-points, number of bands, type of pseudopotential, cutoff energy, and smearing width affect the calculation results.
- The k-point path (path) needs to be reset according to the targeted crystal structure. Refer to the recommended path for each crystal structure in the doc¥brillouin_zones.pdf located in the QE installation directory.

◆ 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

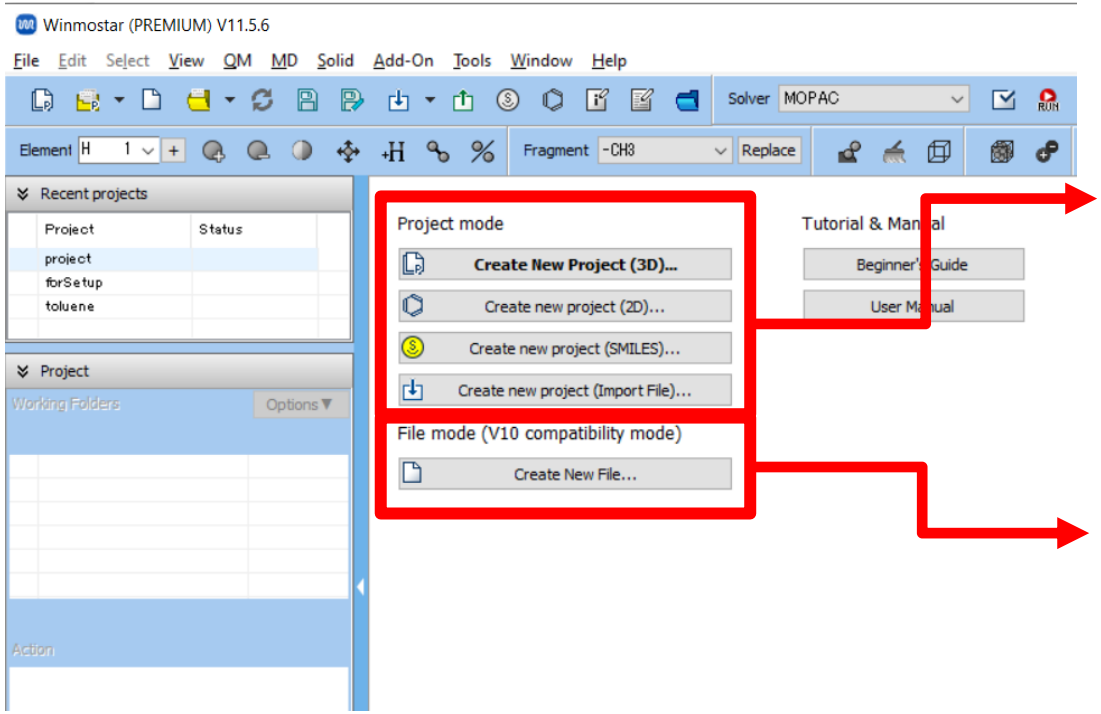
Preference of Operating Environment

- 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.
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

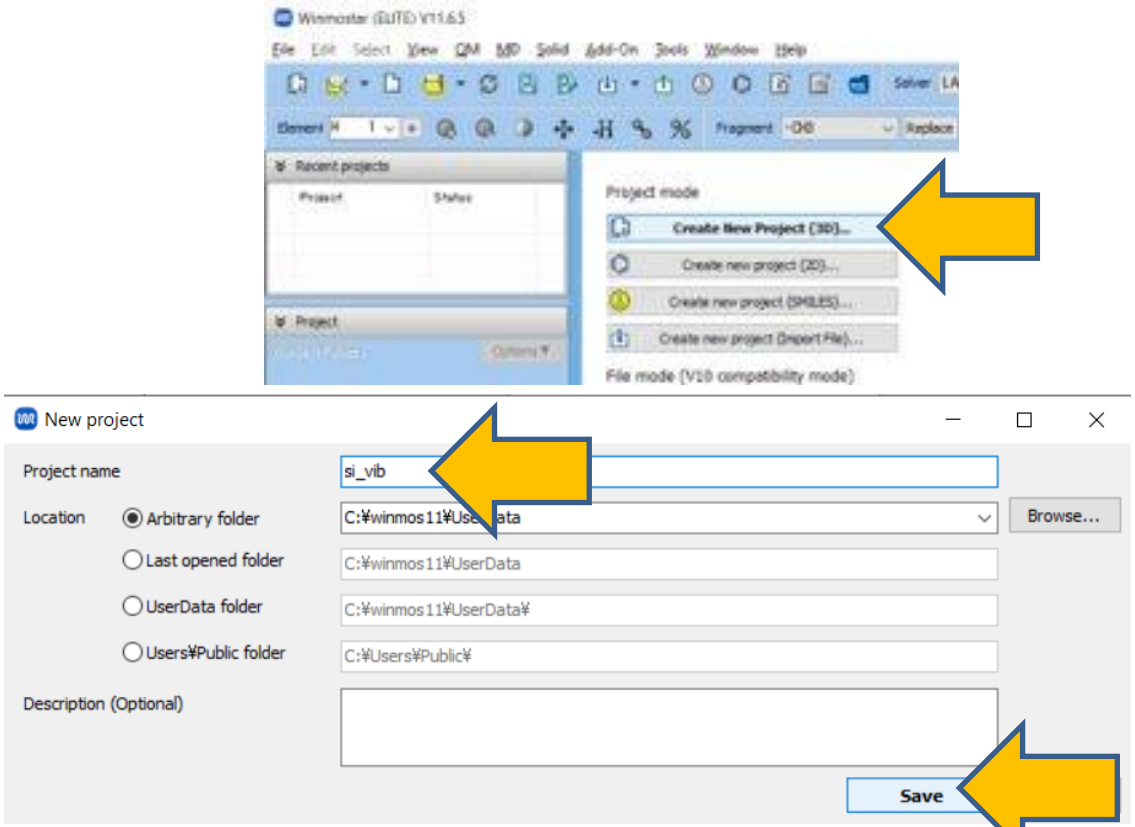
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

Please refer to QE Basic Tutorial for the basic operation method.

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

B. Enter '`si_vib`' in **Project name** and click **Save**.



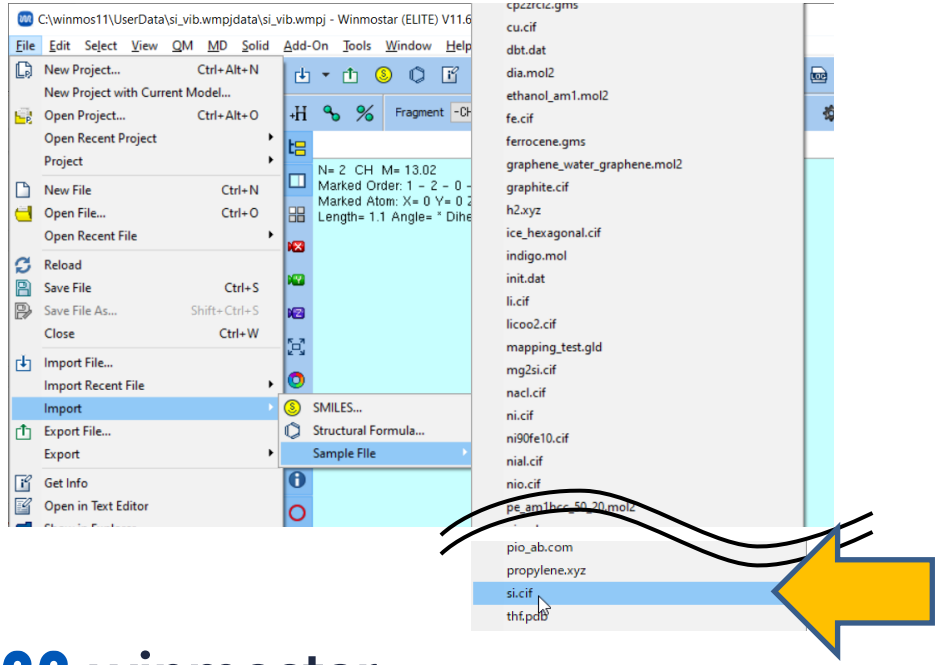
A. Modeling of the System

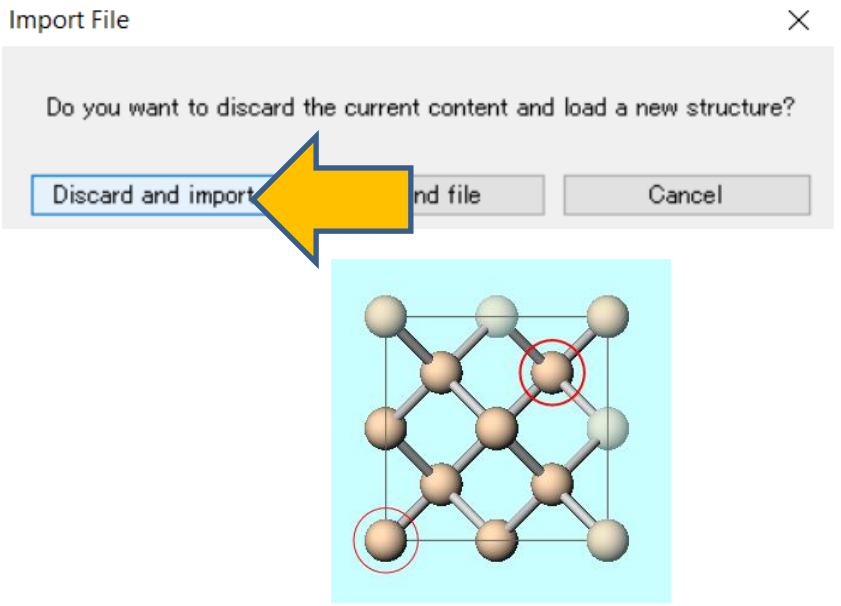
For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Methods for Creating Initial Structures'. Here, we will load an existing molecular structure file.

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**.

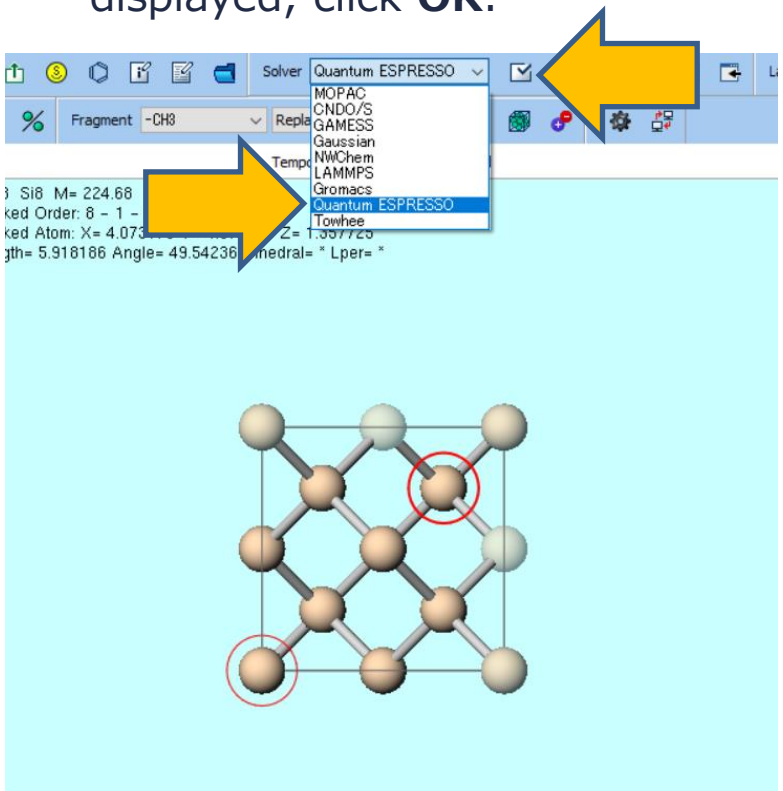
C. Confirm that the desired structure appears in Viewport.

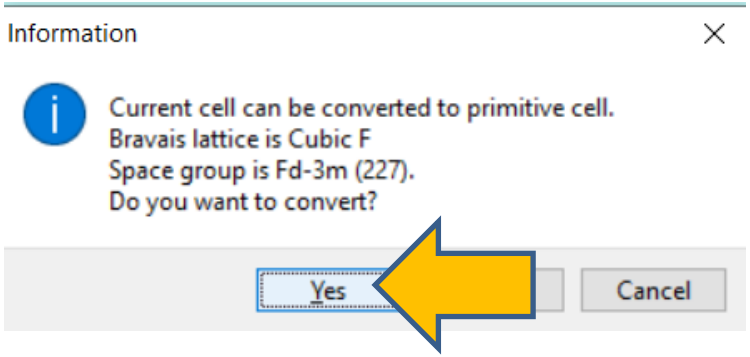


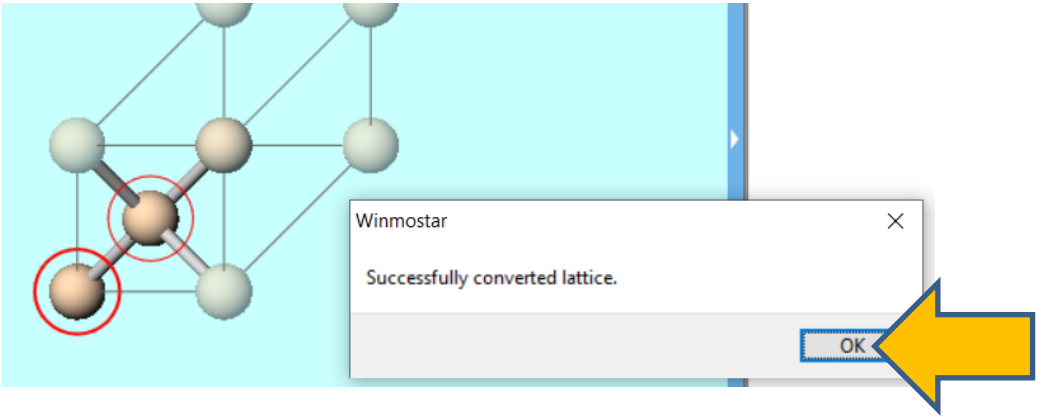


B. Execution of Calculation IR/Raman Spectra

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







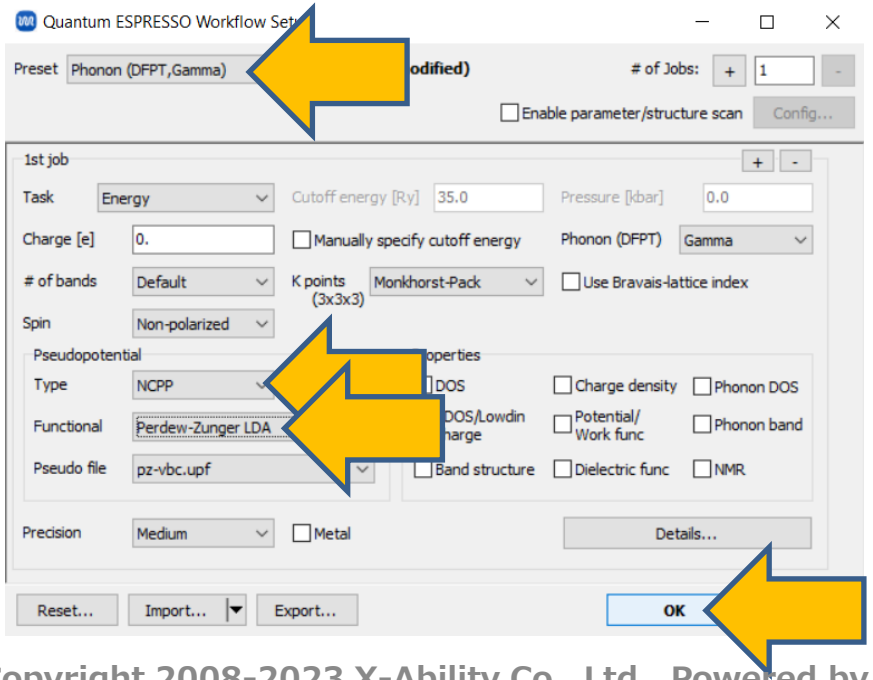
B. Execution of Calculation IR/Raman Spectra

A. Change **Preset** to **Phonon (DFPT, Gamma)**.

B. Change **Type of Pseudopotential** to **NCPP** and **Functional** to **Perdew-Zunger LDA**.(Because QE's **`ph.exe`** does not support GGA and Ultrasoft for Raman spectrum calculations).

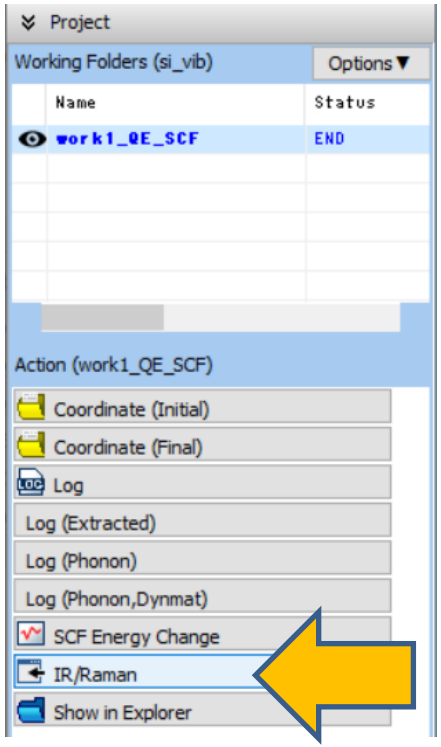
C. If you wish to reduce the computational precision to speed up the calculation, change **Precision** to 'Low'.

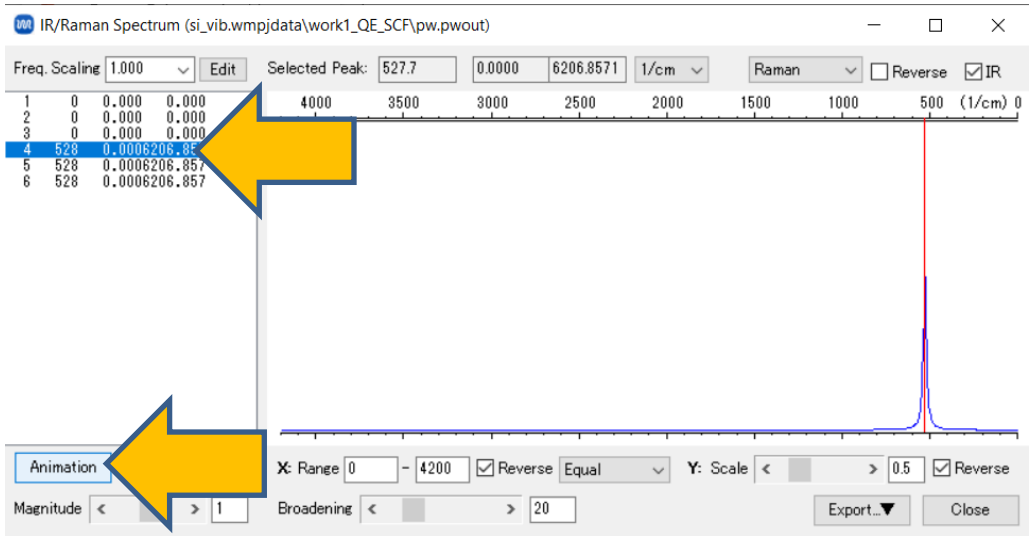
D. Click **OK**, adjust settings as needed in **Job Setting** window, and then click **Run**.

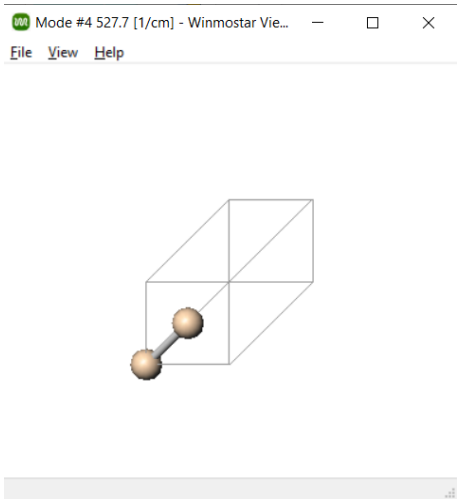


C. Analysis of Results IR/Raman Spectra

A. After the calculation is completed and the status of the working folder changes to **END (blue)**, click **IR/Raman** in **Action** to display IR/Raman spectrum.
B. In **IR/Raman Spectrum window**, click on the peak you want to visualize.
C. Click **Animation** button to display the animation of the vibrational mode.





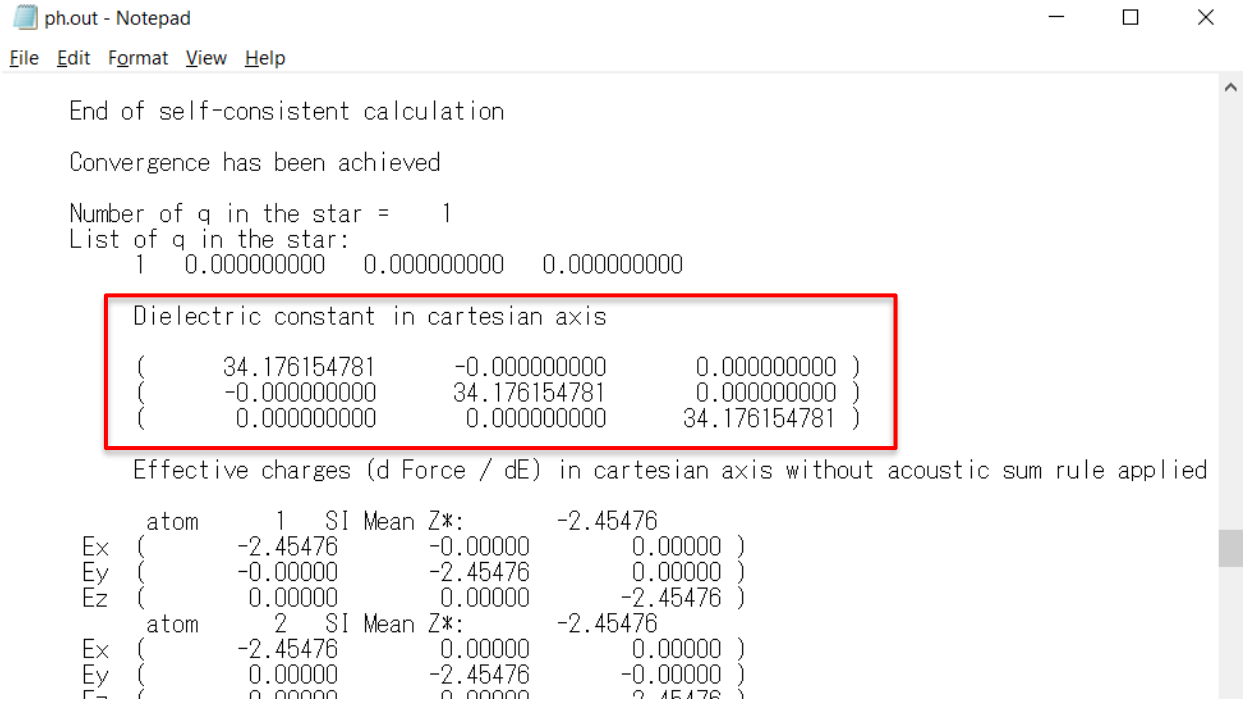


C. Analysis of Results IR/Raman Spectra

A. Click **Log (Phonon)** in **Action** to open the log file of the phonon calculation.

B. The dielectric constant is displayed after the last occurrence of 'Dielectric constant in cartesian axis.'

Note: Increasing the number of k-point divisions brings the results closer to experimental values, but for the sake of calculation speed, the number of k-points has been reduced in this book. Please refer to QE Basic Tutorial for how to adjust the number of k-point divisions.



D. Execution of Calculation Phonon Dispersion

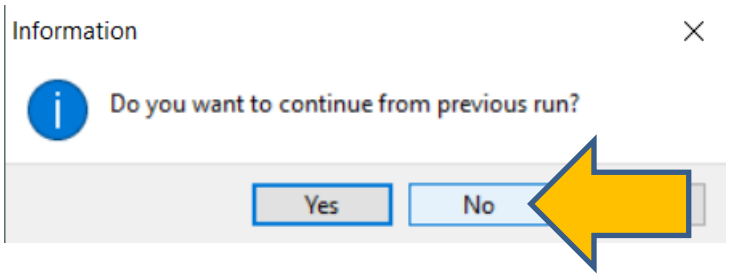
A. Click  **(Workflow Setup)**.

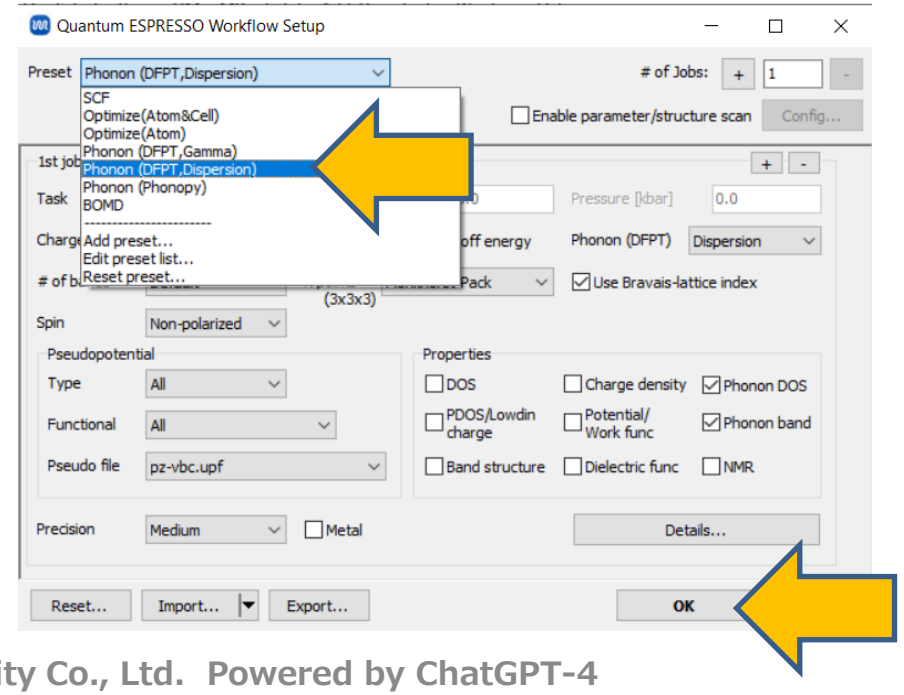
B. If prompted with 'Do you want to continue from previous run?', click **No**.

C. In **Quantum ESPRESSO Workflow Setup** window, select **Phonon (DFPT, Dispersion)** from **Preset**.

D. If you wish to reduce the computational precision to speed up the calculation, change **Precision** to 'Low'.

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

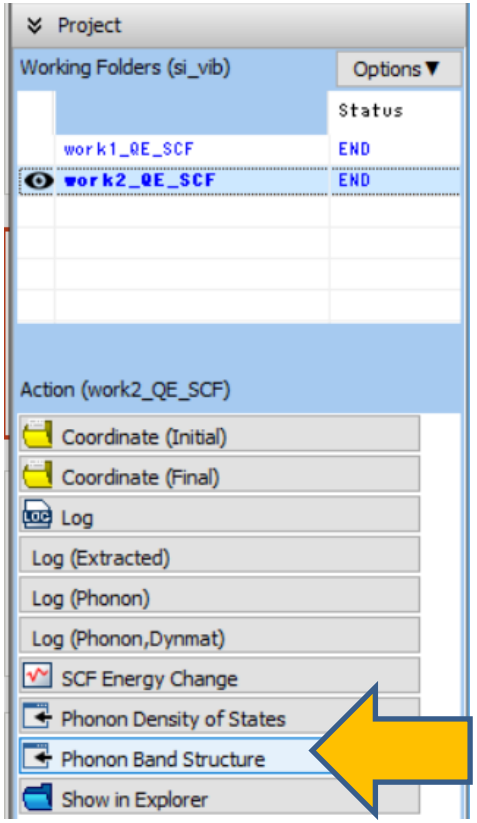


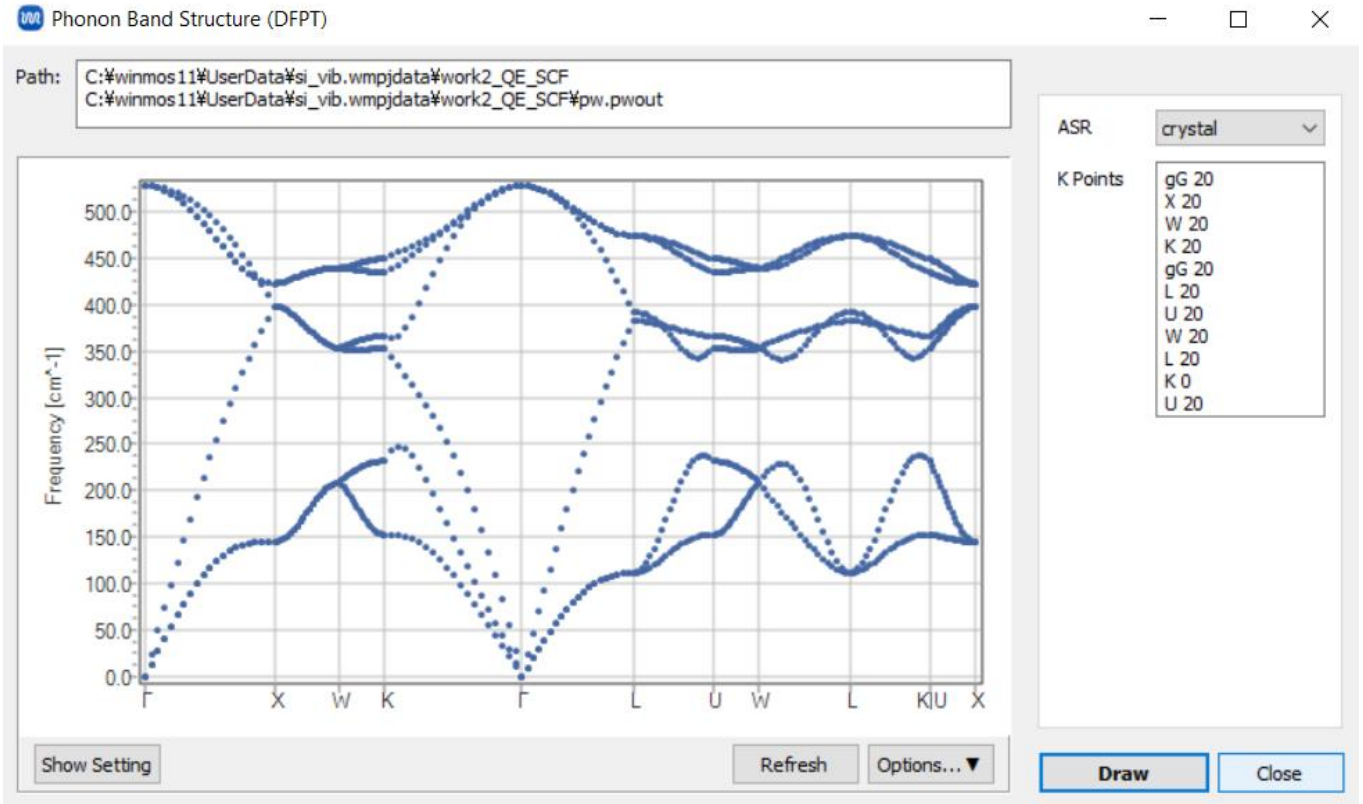


E. Analysis of Results Phonon Dispersion

A. After the calculation is completed and the status of the working folder changes to **END (blue)**, click **Phonon Band Structure** in **Action** to open Phonon Band Structure window, where the phonon dispersion curves can be obtained.

B. Click **Close** after reviewing.

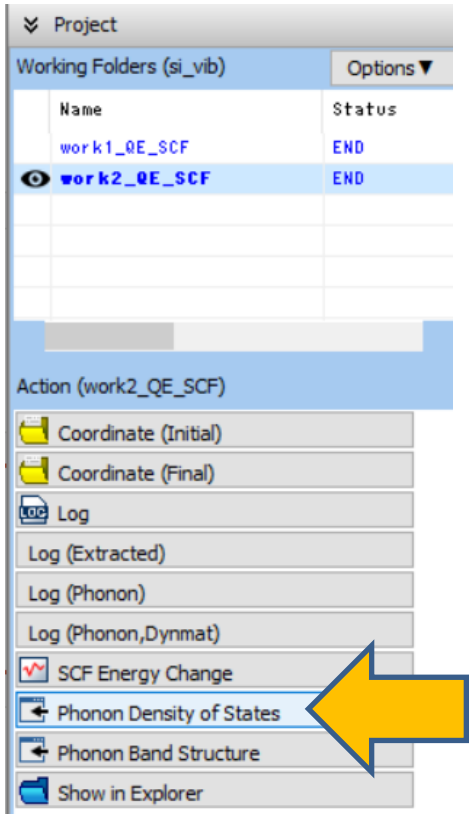


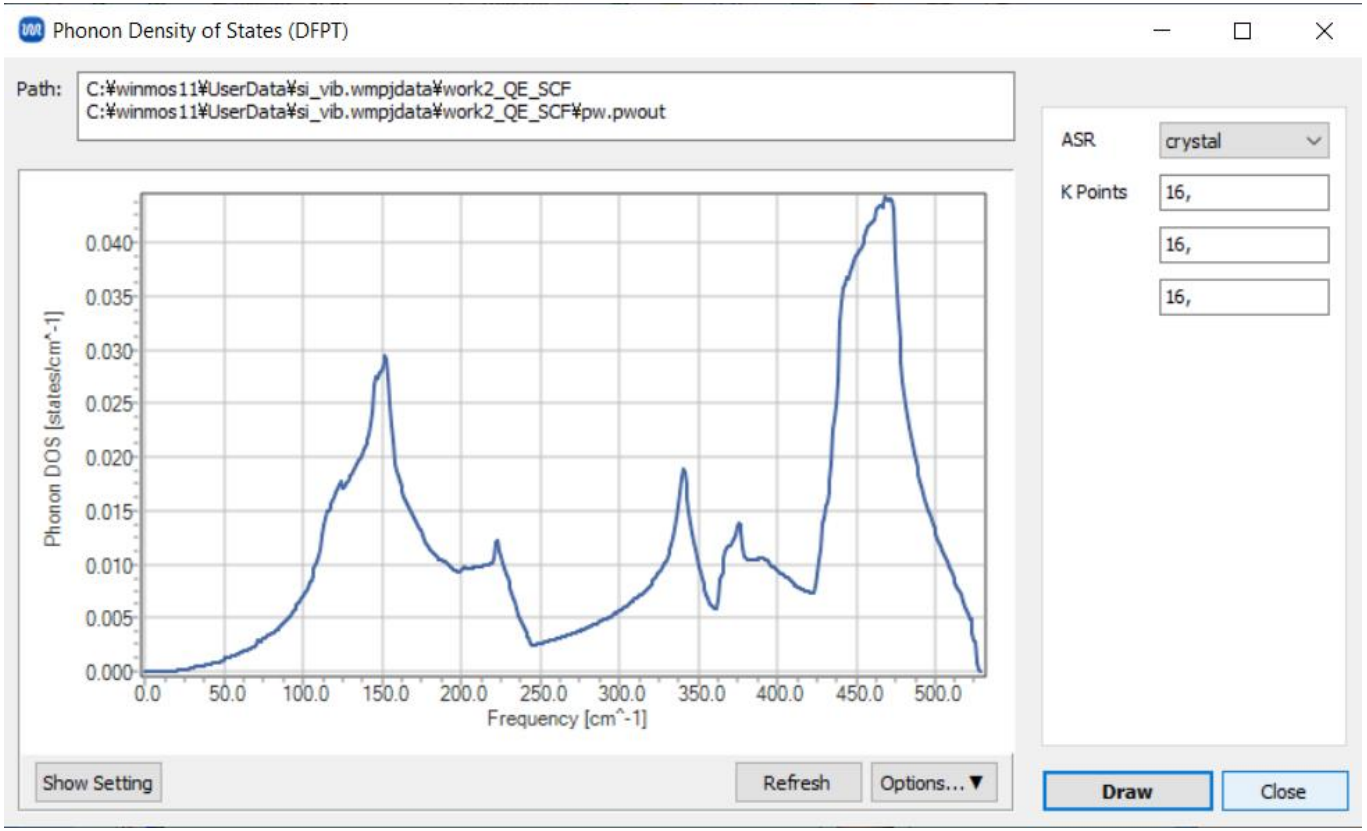


E. Analysis of Results Phonon Dispersion

A. Click **Phonon Density of States** in **Action** to open Phonon Density of States window, where the phonon density of states can be obtained.

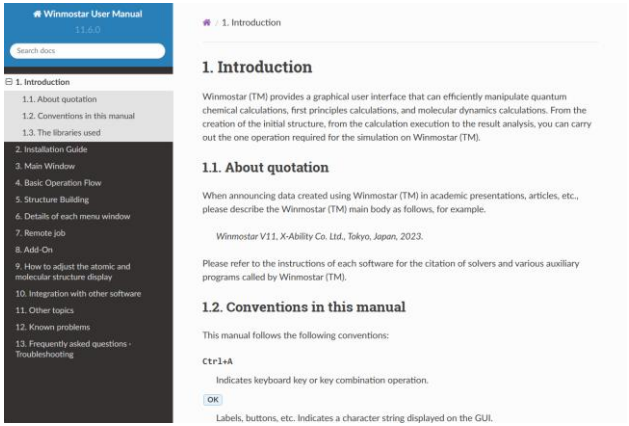
B. Click **Close** after reviewing.





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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