

 winmostar tutorial

# Quantum ESPRESSO Phonon Calculation (DFPT Method)

V11.6.5

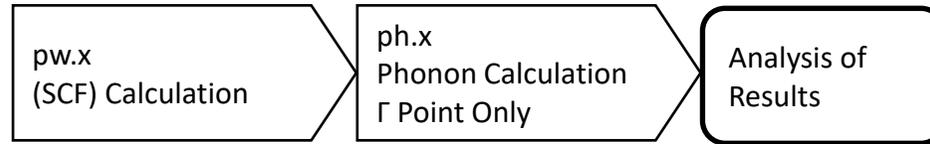
21 February 2024 X-Ability Co., Ltd.

# About This Manual

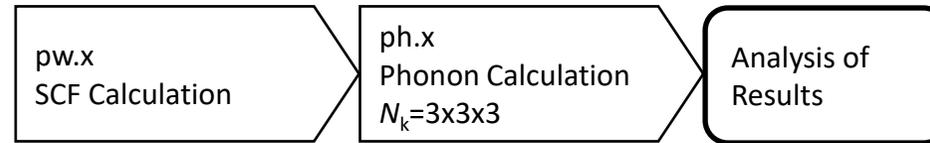
- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult [Beginner's Guide](#).
- For those who wish to explore the details of each feature, please refer to [Winmostar User Manual](#).
- Those who wish to practice the contents 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.
- The copyright for this document is held by X-Ability Co., Ltd. Any copying or duplication of the content in any form without the express permission of X-Ability Co., Ltd. is strictly prohibited.

# 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](https://qiita.com/xa_member)

# Preference of Operating Environment

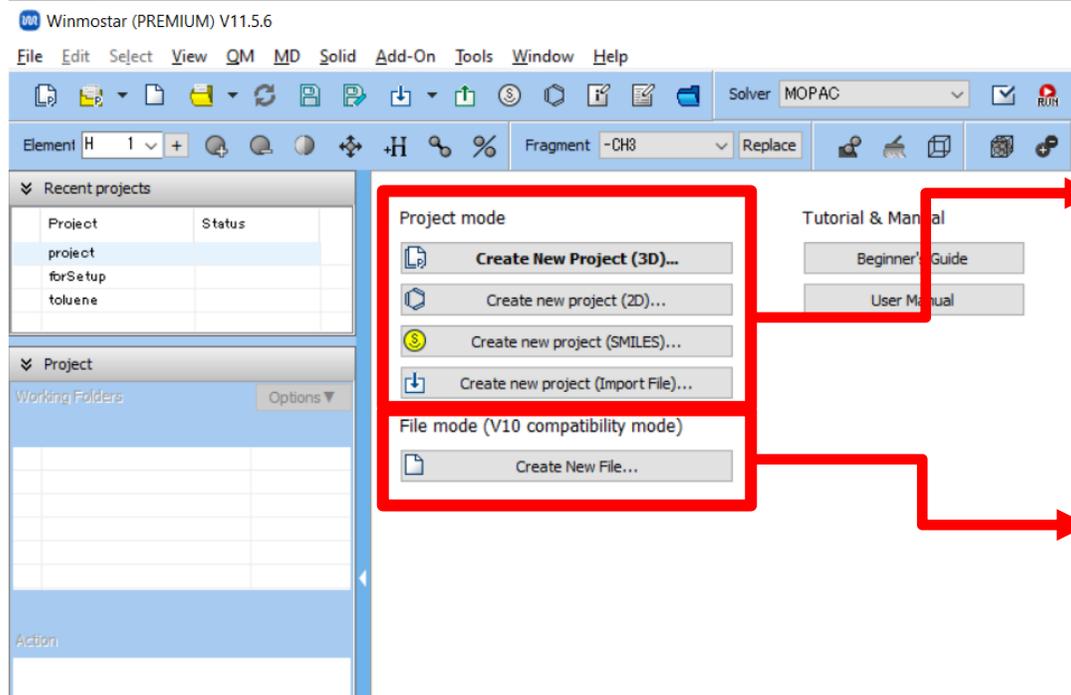
- For users of Winmostar version V11.5.0 or later on a 64-bit environment, please install and configure [CygwinWM version 2023/04/05 or later](#).
  - The CygwinWM version after 2023/04/05 includes the recommended version of 64-bit Quantum ESPRESSO.
- If the above does not apply to you or if you wish 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.

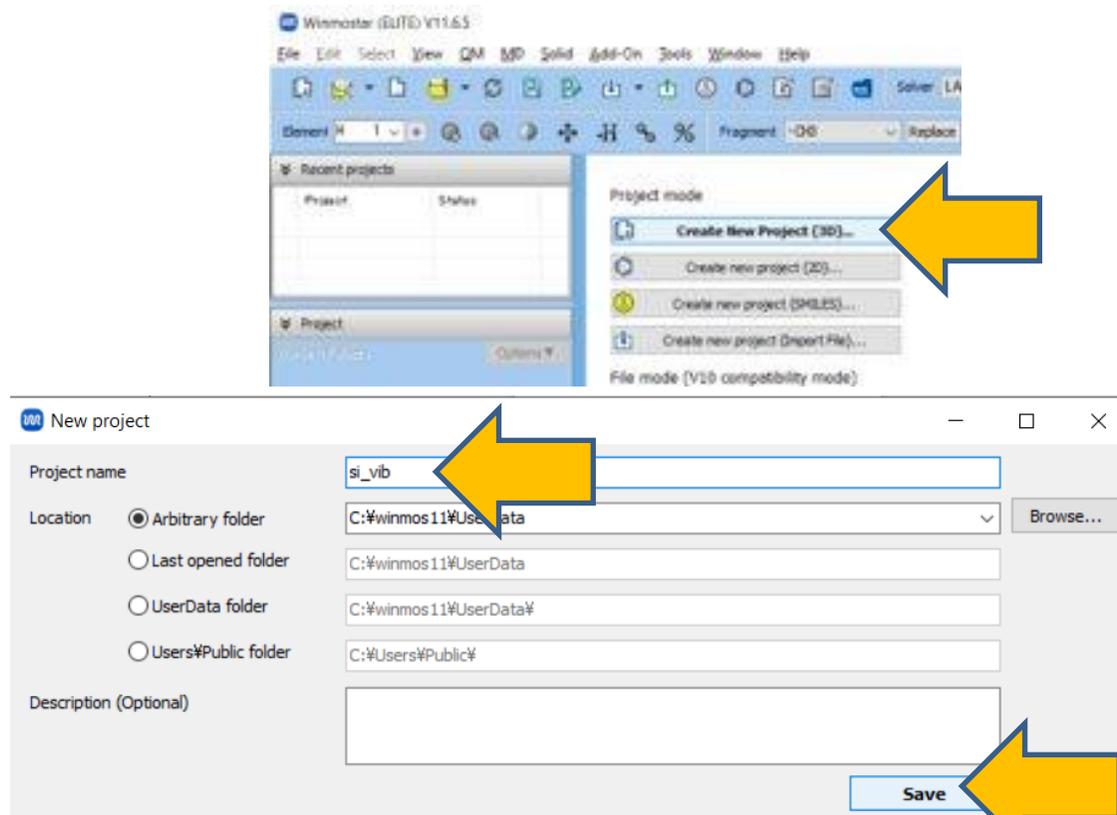
The operational procedure is the same as from V10 and earlier versions.

# 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.

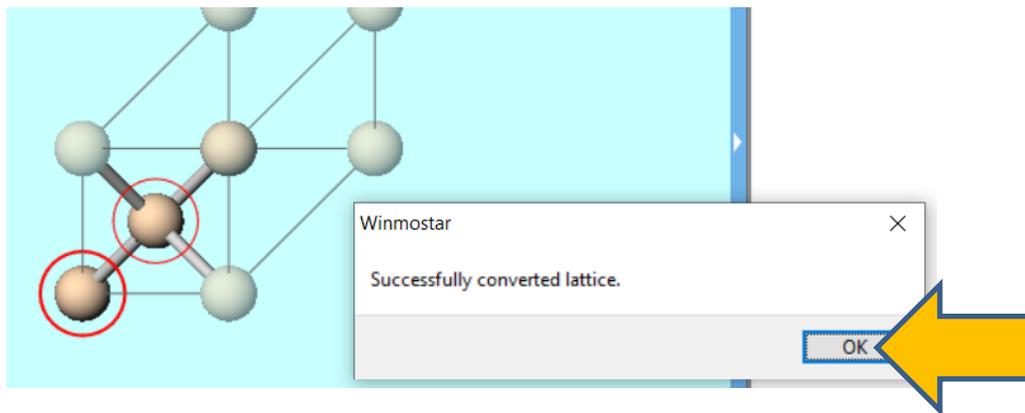
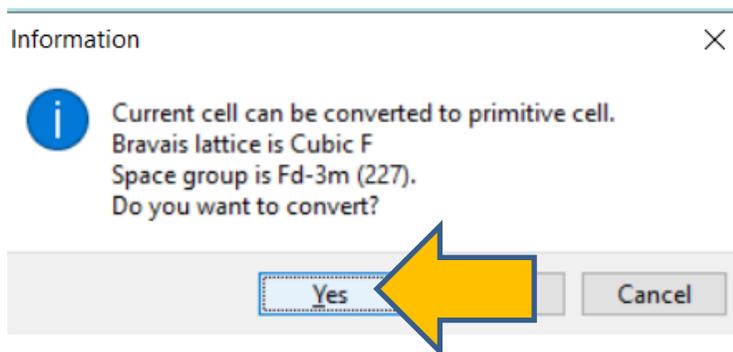
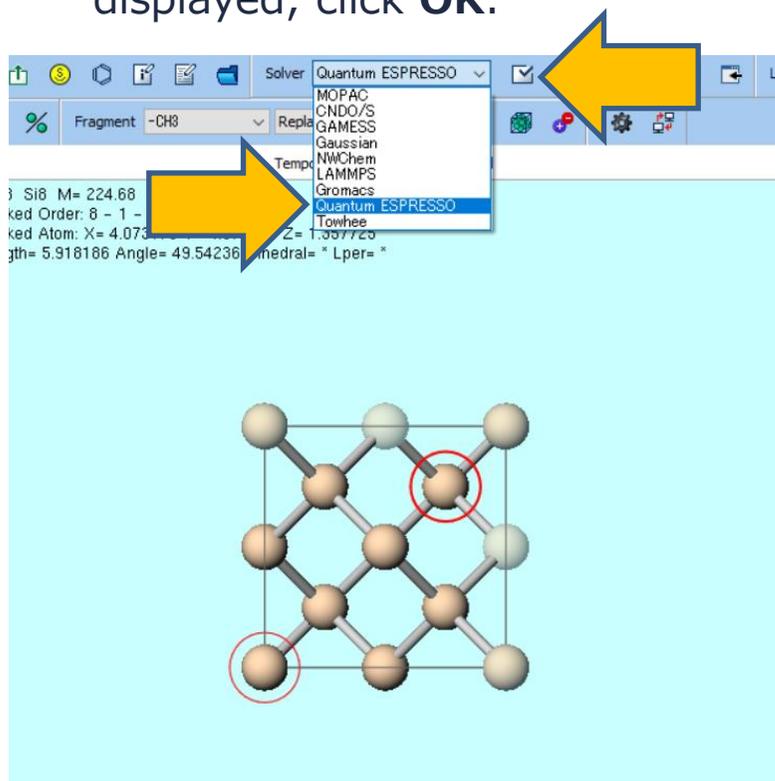
B. In **Import File** dialog, click **Discard and import**.

C. Confirm that the desired structure appears in Viewport.

The image shows a screenshot of the Winmostar software interface. On the left, the 'File' menu is open, and the 'Import' option is selected, leading to a submenu where 'Sample File' is chosen. A yellow arrow points from the 'Sample File' option to the 'Import File' dialog box. The dialog box contains the question 'Do you want to discard the current content and load a new structure?' and two buttons: 'Discard and import' and 'Cancel'. A yellow arrow points to the 'Discard and import' button. Below the dialog box, a 3D ball-and-stick model of a crystal structure is shown in a viewport. A yellow arrow points from the 'si.cif' file in the file list to the 3D model. The file list on the right includes files like 'cu.cif', 'dbt.dat', 'dia.mol2', 'ethanol\_am1.mol2', 'fe.cif', 'ferrocene.gms', 'graphene\_water\_graphene.mol2', 'graphite.cif', 'h2.xyz', 'ice\_hexagonal.cif', 'indigo.mol', 'init.dat', 'li.cif', 'licoo2.cif', 'mapping\_test.gld', 'mg2si.cif', 'nacl.cif', 'ni.cif', 'ni90fe10.cif', 'nial.cif', 'nio.cif', 'pe\_am1ther\_50\_20.mol2', 'pio\_ab.com', 'propylene.xyz', 'si.cif', and 'thf.pdb'.

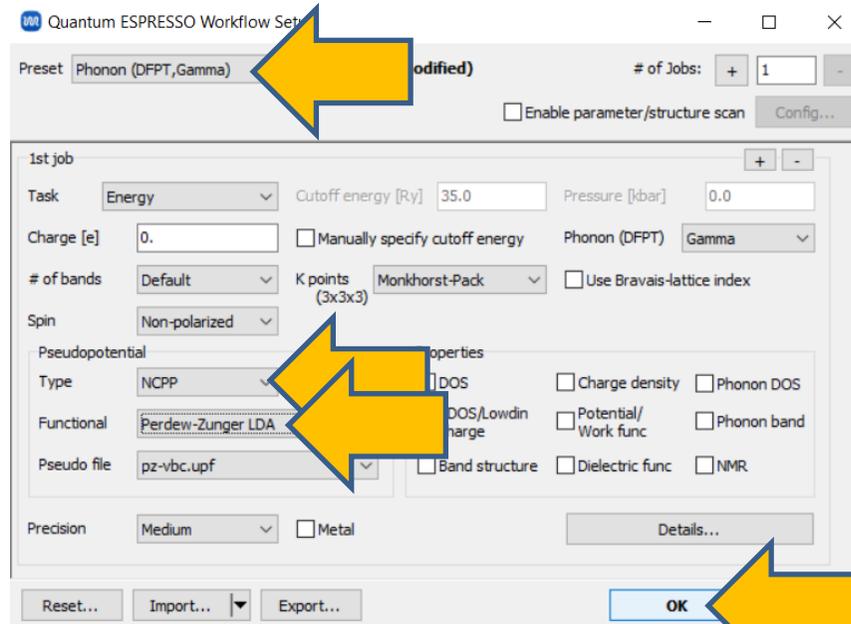
# B. Execution of Calculation IR/Raman Spectra

- 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**.



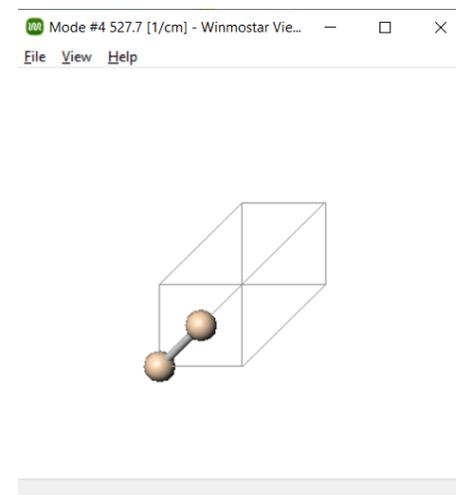
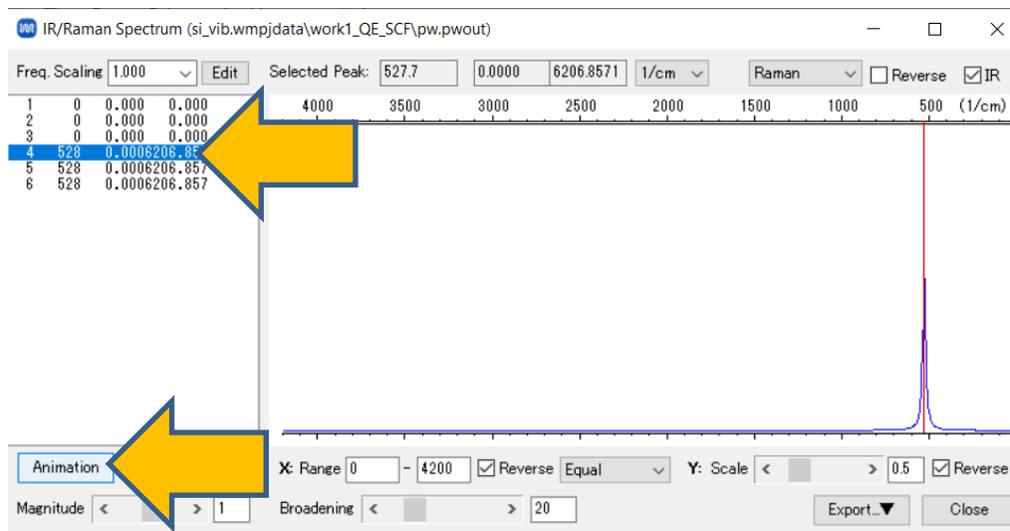
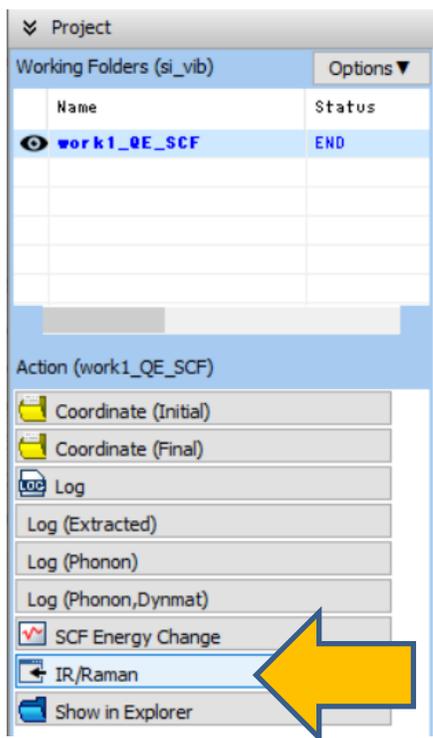
# B. Execution of Calculation IR/Raman Spectra

- 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.

```
ph.out - Notepad
File Edit Format View Help

End of self-consistent calculation

Convergence has been achieved

Number of q in the star = 1
List of q in the star:
  1  0.000000000  0.000000000  0.000000000

Dielectric constant in cartesian axis

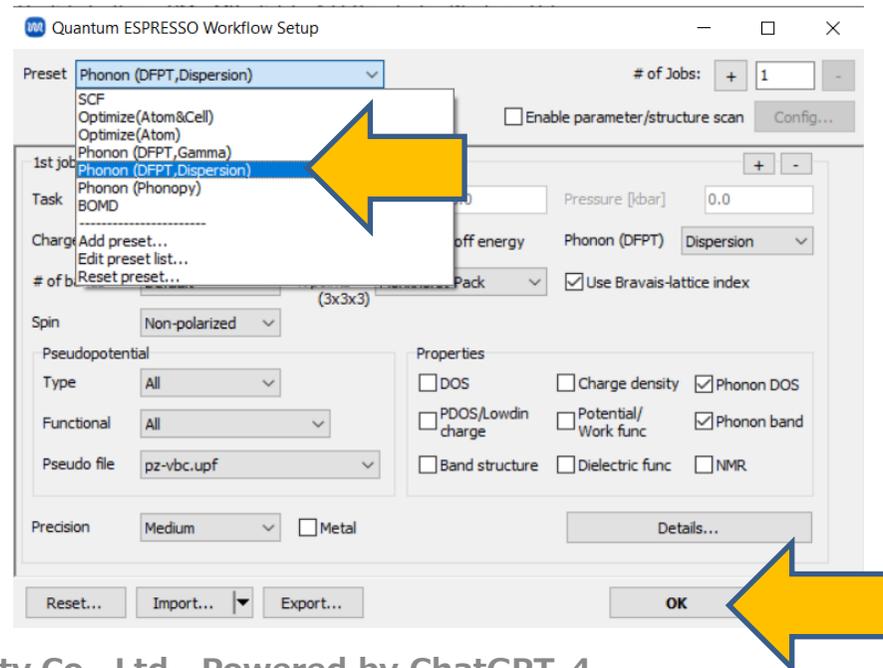
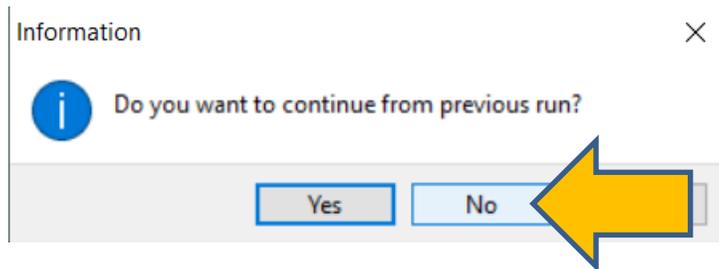
( 34.176154781 -0.000000000  0.000000000 )
( -0.000000000  34.176154781  0.000000000 )
( 0.000000000  0.000000000  34.176154781 )

Effective charges (d Force / dE) in cartesian axis without acoustic sum rule applied

atom 1 SI Mean Z*: -2.45476
Ex ( -2.45476 -0.00000 -0.00000 )
Ey ( -0.00000 -2.45476 0.00000 )
Ez ( 0.00000 0.00000 -2.45476 )
atom 2 SI Mean Z*: -2.45476
Ex ( -2.45476 0.00000 0.00000 )
Ey ( 0.00000 -2.45476 -0.00000 )
Ez ( 0.00000 0.00000 -2.45476 )
```

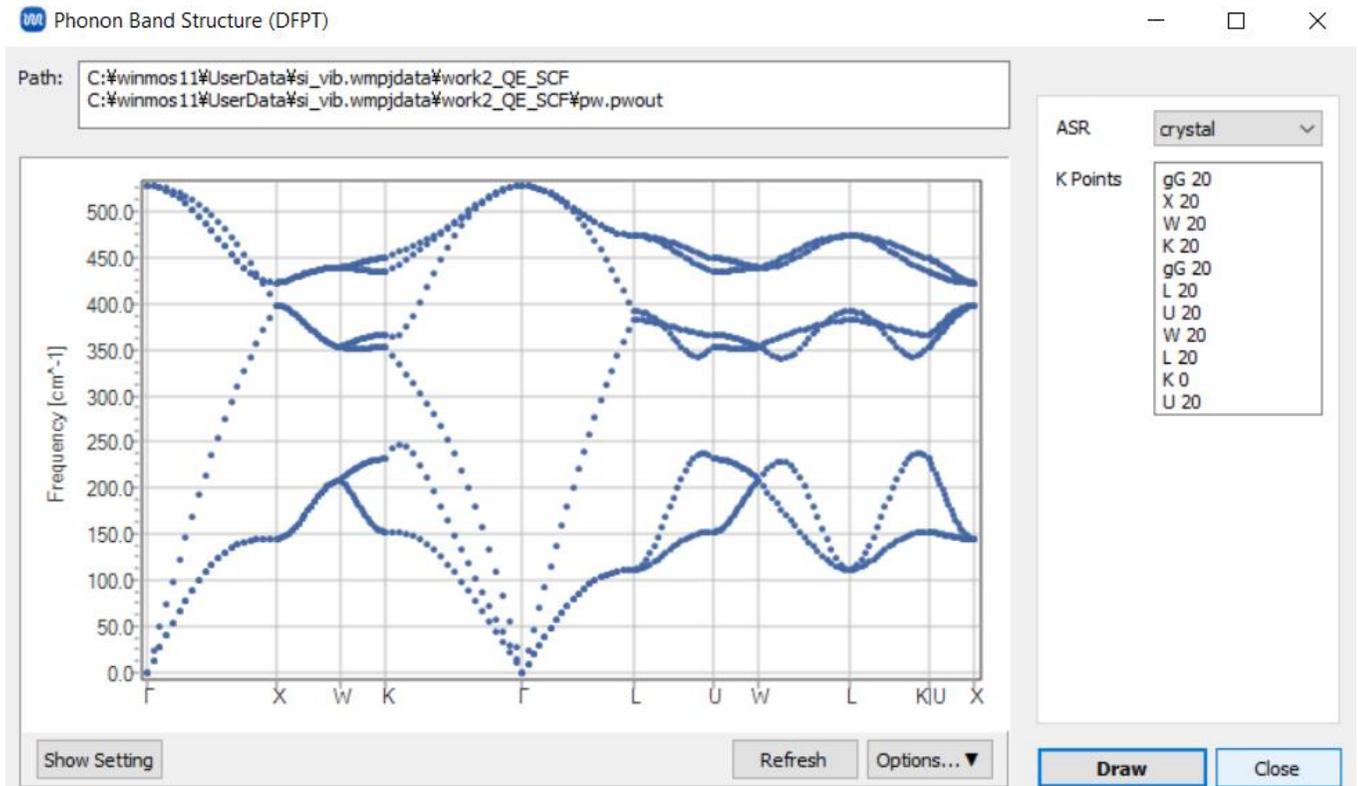
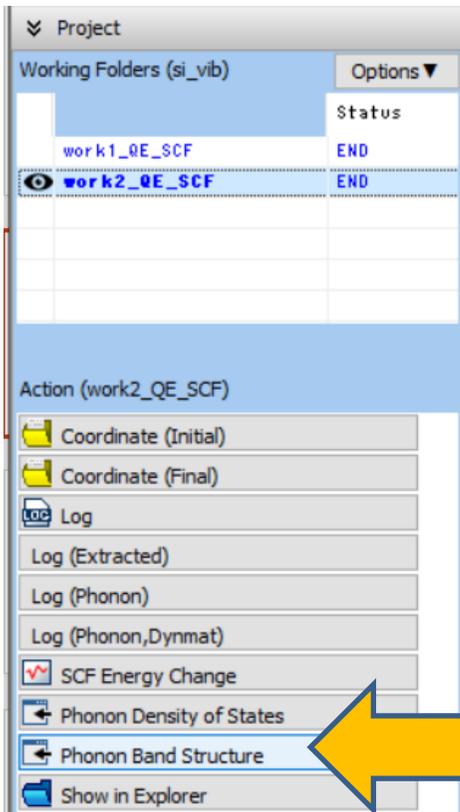
# D. Execution of Calculation Phonon Dispersion

- Click  (**Workflow Setup**).
- If prompted with 'Do you want to continue from previous run?', click **No**.
- In **Quantum ESPRESSO Workflow Setup** window, select **Phonon (DFPT, Dispersion)** from **Preset**.
- If you wish to reduce the computational precision to speed up the calculation, change **Precision** to 'Low'.
- Click **OK**, adjust settings as needed in **Job Setting** window, and then click **Run**.



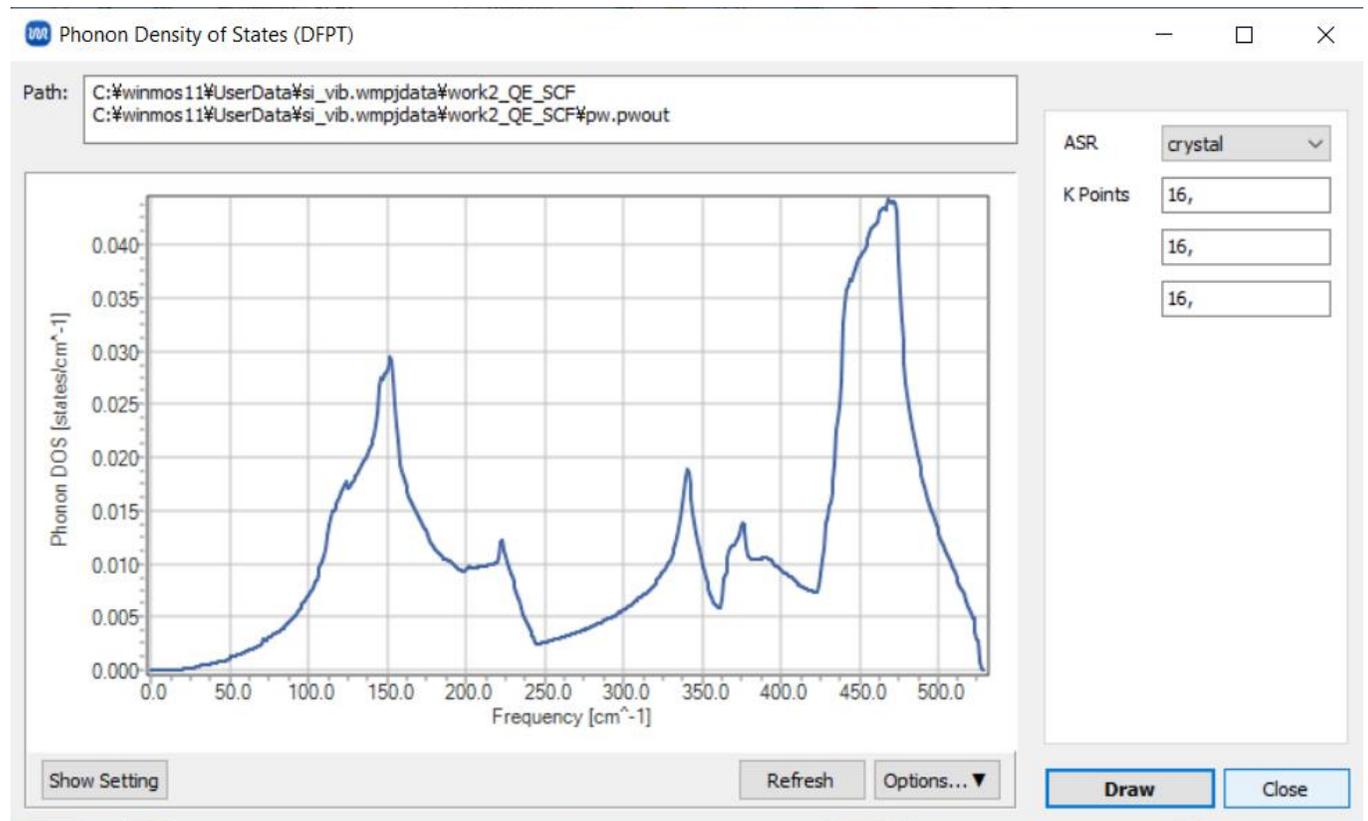
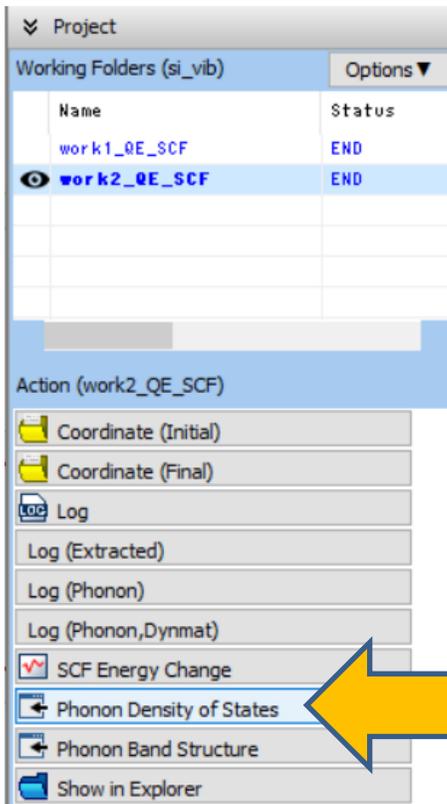
# E. Analysis of Results Phonon Dispersion

- 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.



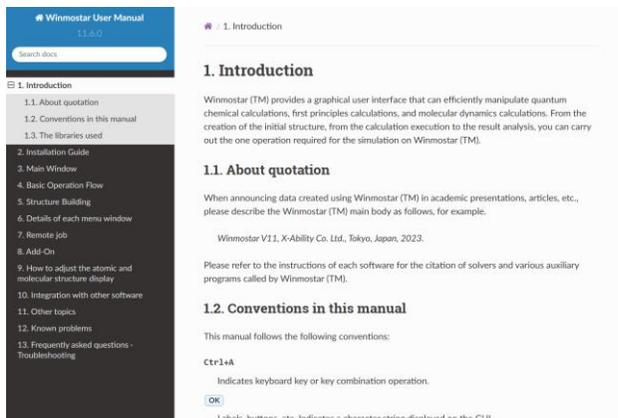
# E. Analysis of Results Phonon Dispersion

- Click **Phonon Density of States** in **Action** to open Phonon Density of States window, where the phonon density of states can be obtained.
- 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](#)

- 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](#).
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through [Contact page](#), detailing the steps to reproduce the issue and attaching any generated files at that time.