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Winmostar tutorial
Quantum ESPRESSO
Phonon
V8.007

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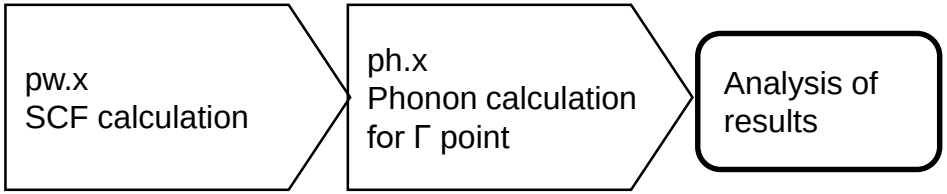
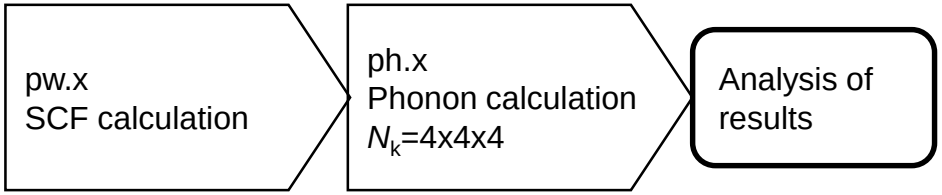
Summary

① Obtain IR and Raman spectrum of Si crystal from phonon calculation.



② Obtain phonon band of Si crystal and phonon DOS from phonon calculation.



Notes:

- Method for obtaining k points, number of bands, type of pseudopotential, cutoff energy, and settings for smearing will all affect calculation results. In this tutorial, we use a setting with reduced precision for faster processing.
- The path for k point needs to be set according to the target crystal structure. For recommended paths for crystal structures, please refer to file Doc¥Brrilouin_zonew.pdf in your install directory for QE.
- There are restrictions for the ph.x we use here (i.e. not available for GGA, Ultrasoft, etc.).

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Configuration

See Quantum ESPRESSO install manual
https://winmostar.com/en/QE_install_manual_en_win.pdf

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I. IR, Raman Spectrum

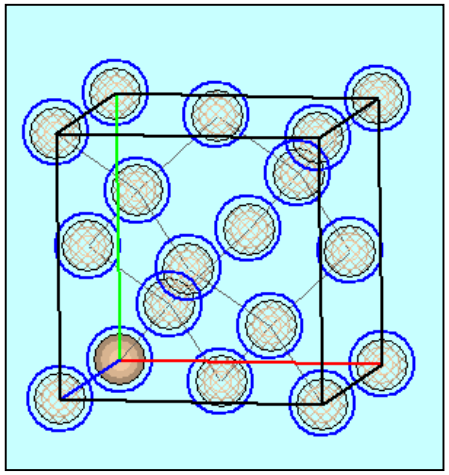
1. Click **File | Open**.
2. Select **si.cif.** (C:¥winmos8¥samples¥si.cif)

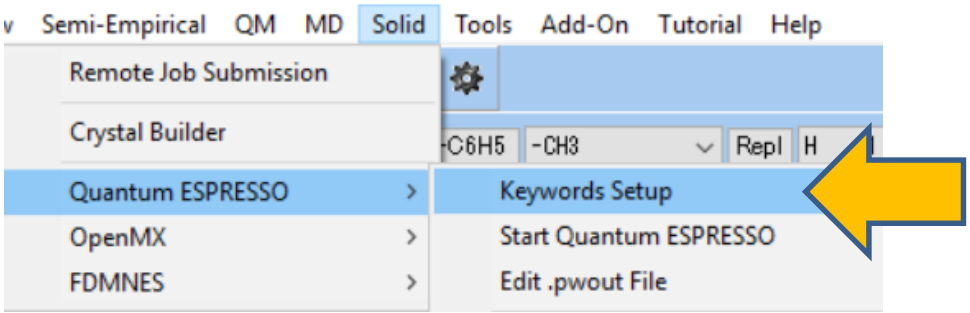
You can also make the same CIF file using Crystal Builder.
See crystal modeling tutorial and apply the following information.

To make Si unit cell

Crystal system：Cubic
Space group： Fm-3m (227)
Lattice constants：a=5.4309 Å
Fractional coordinates：Si (0.0 0.0 0.0)

3. Click **Solid | Quantum ESPRESSO | Keywords Setup**.





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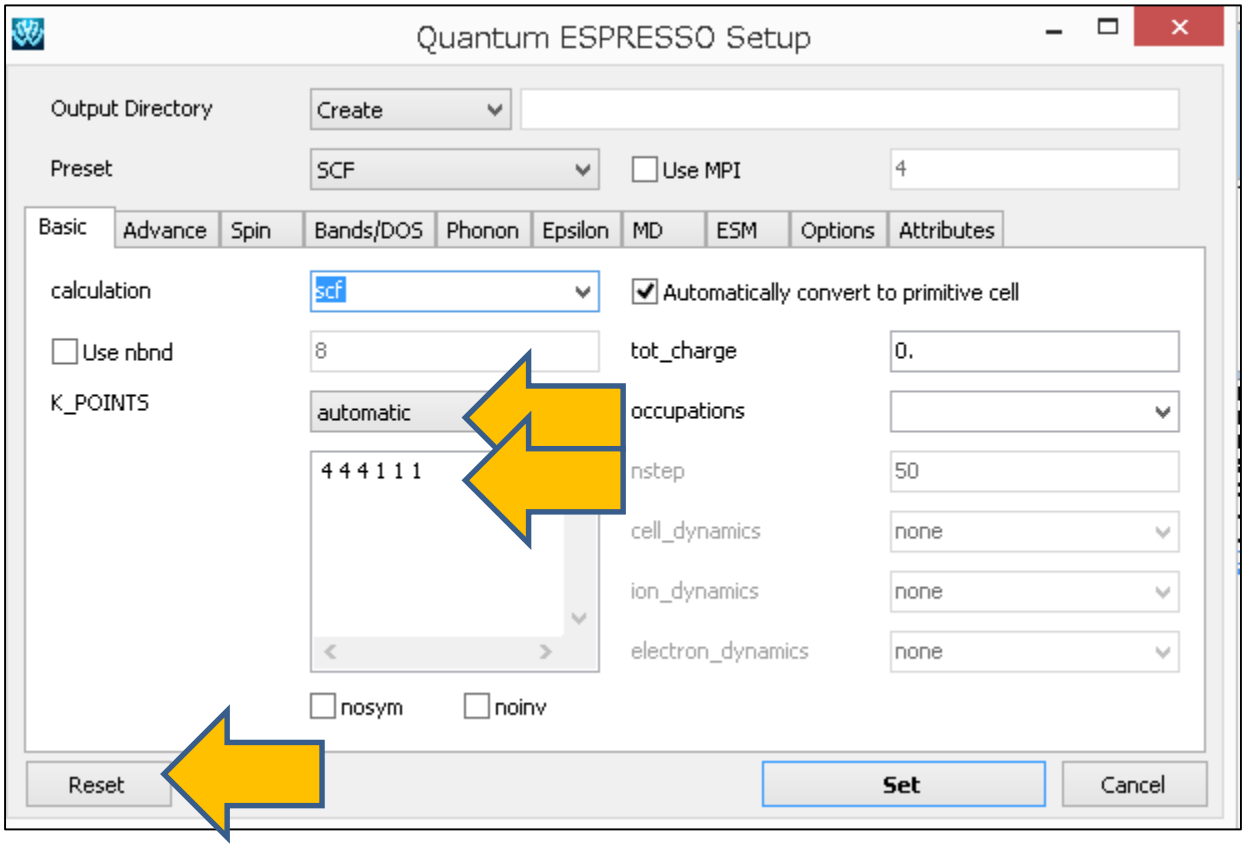
I. IR, Raman Spectrum

1. First, click **Reset**.
2. Set **K_POINTS** to **automatic**, then enter "**4 4 4 1 1 1**" (space separated) in the text box below.



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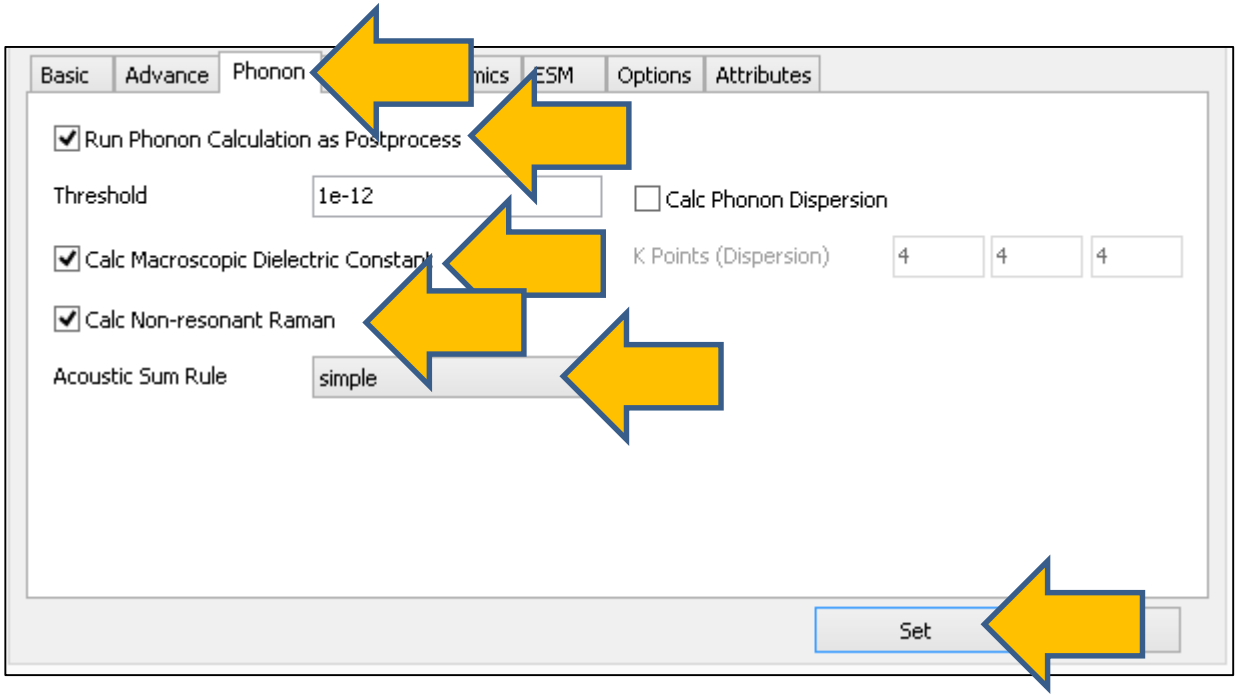
I. IR, Raman Spectrum

1. On Phonon tab, check **Run Phonon Calculation as Postprocess**, **Calc Macroscopic Dielectric Constant**, **Calc Non-resonant Raman**.
2. Set **Acoustic Sum Rule** to **simple**.
3. Click **Set**.



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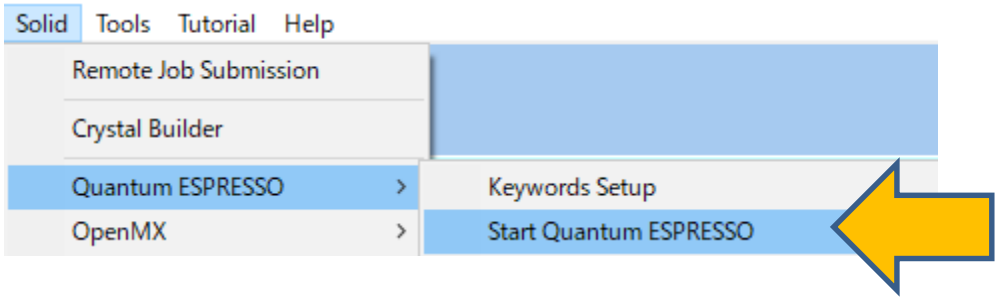
I. IR, Raman Spectrum

1. Click **Solid** | **Quantum ESPRESSO** | **Start Quantum ESPRESSO**.
2. Save as **si_vib.pwin**.



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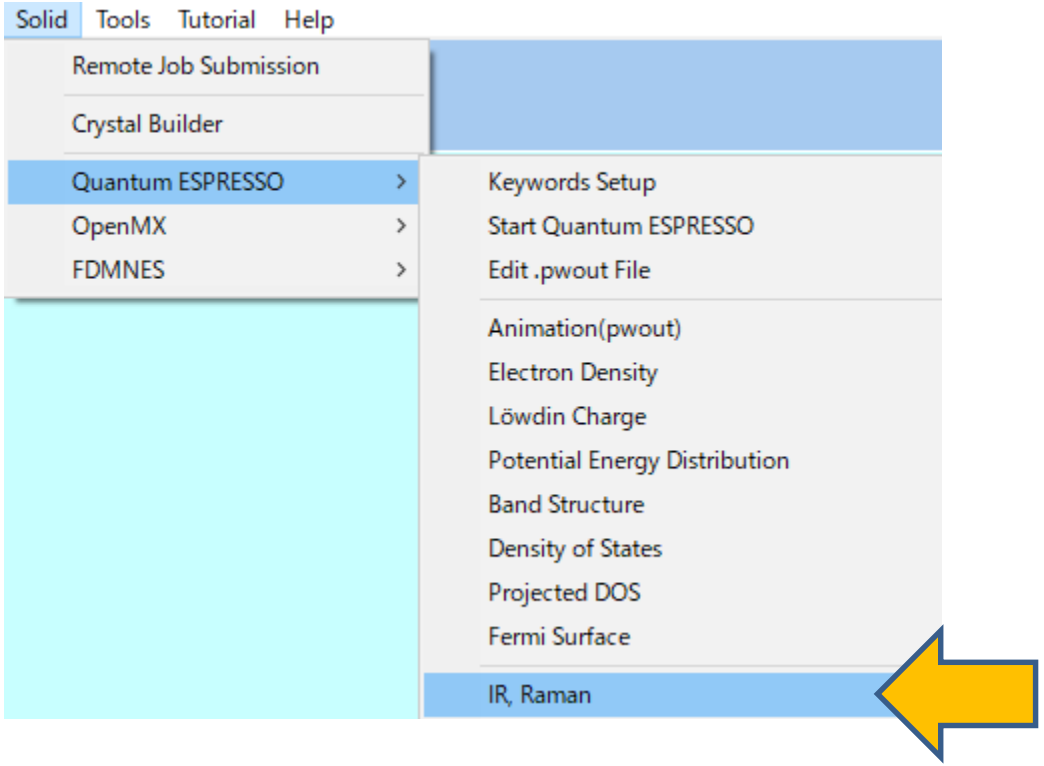
I. IR, Raman Spectrum

1. Click **Solid** | **Quantum ESPRESSO** | **IR, Raman**.
2. Select the QE working directory and output file which are suggested by default.



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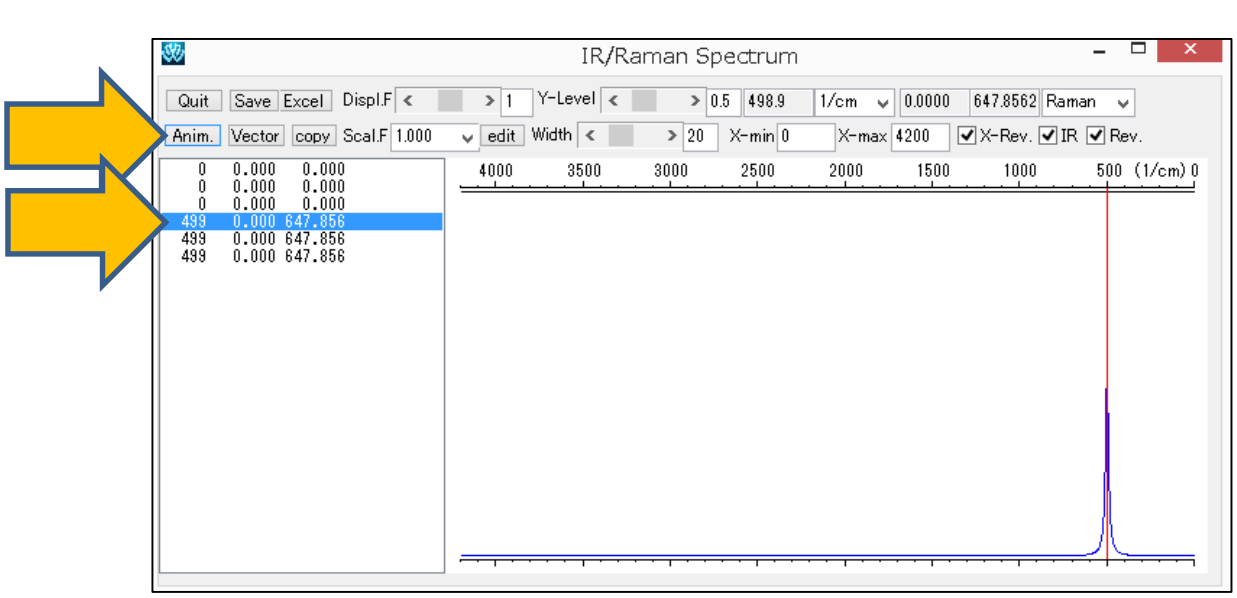
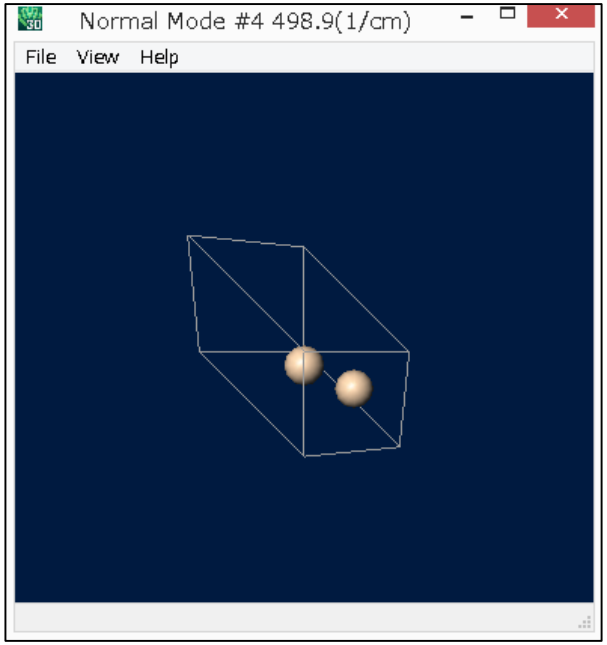
I. IR, Raman Spectrum

IR/Raman spectrum visualization window will appear.

1. Select the peak of the spectrum on the left side of the window.
2. Click **Anim** to visualize the vibration as an animation.





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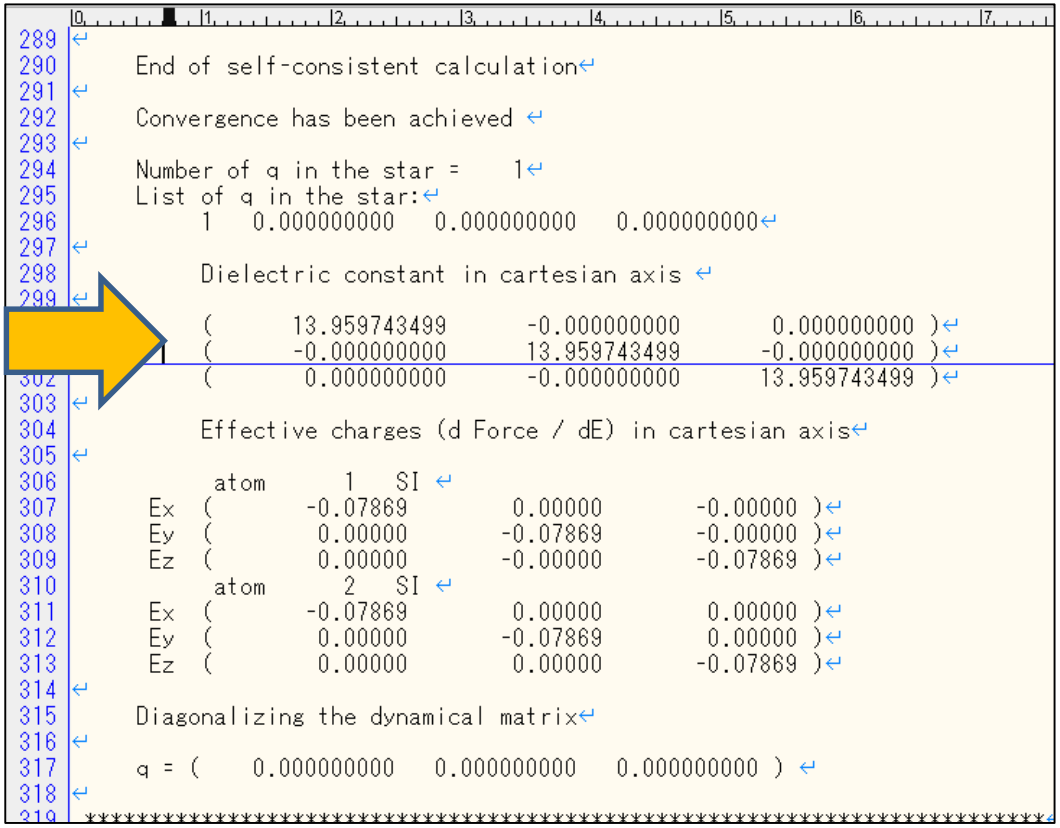
I. IR, Raman Spectrum

Dielectric constant has been calculated with IR and Raman spectrum.
Open **ph.out** in **si_vib_qe_data** folder where **si_vib.pwin** was saved.



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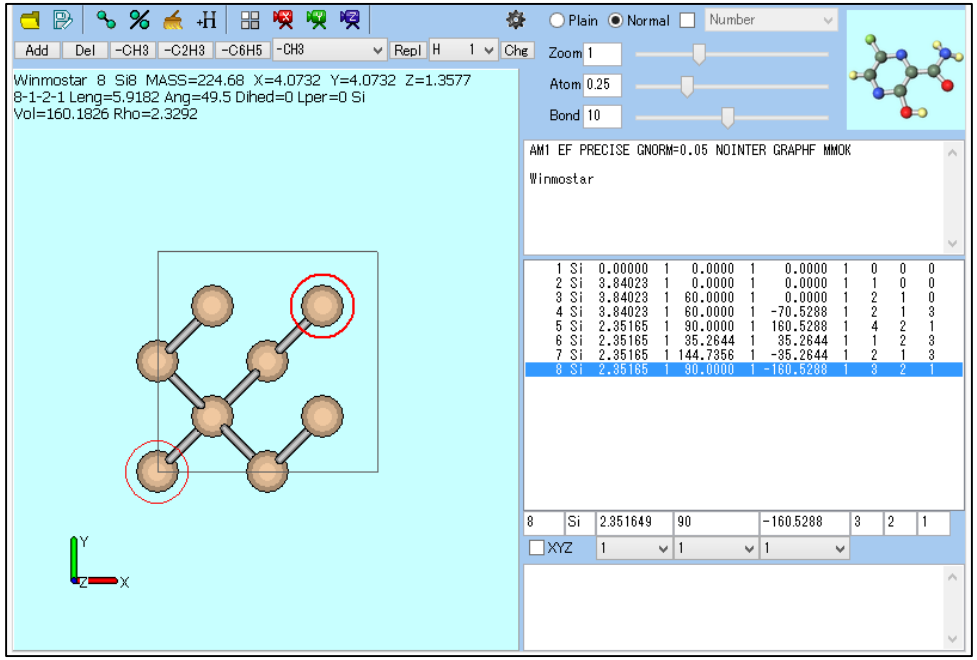
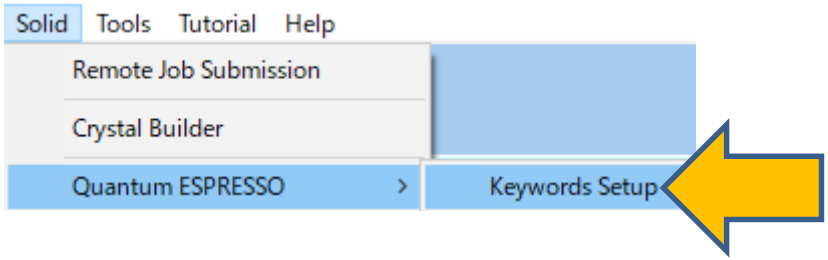
II. Phonon Dispersion

1. Re-open the initial structure of Si crystal.
2. Click **Solid** | **Quantum ESPRESSO** | **Keywords Setup**.





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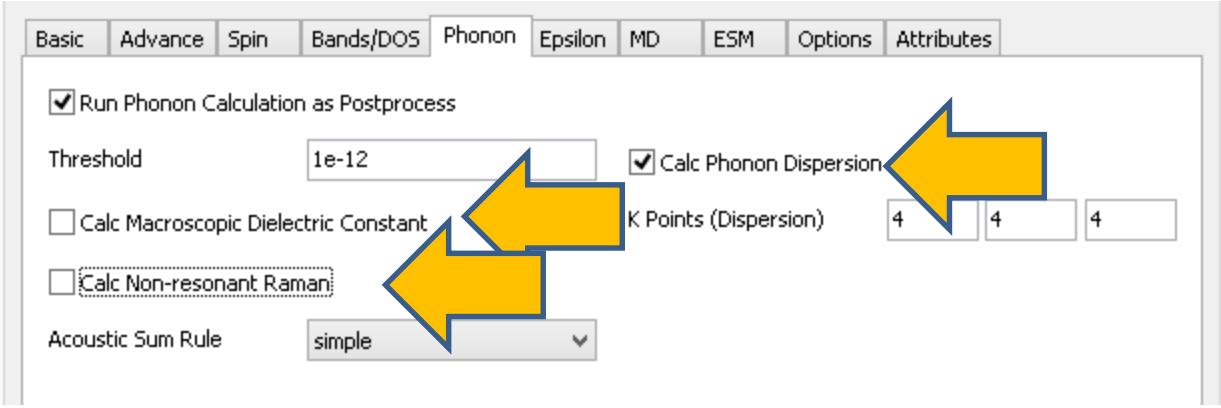
II. Phonon Dispersion

1. In the **Phonon** tab, uncheck **Calc Microscopic Dielectric Constant** and **Calc Non-resonant Raman**, then check the box for **Calc Phonon Dispersion**.
2. Click **Set**.



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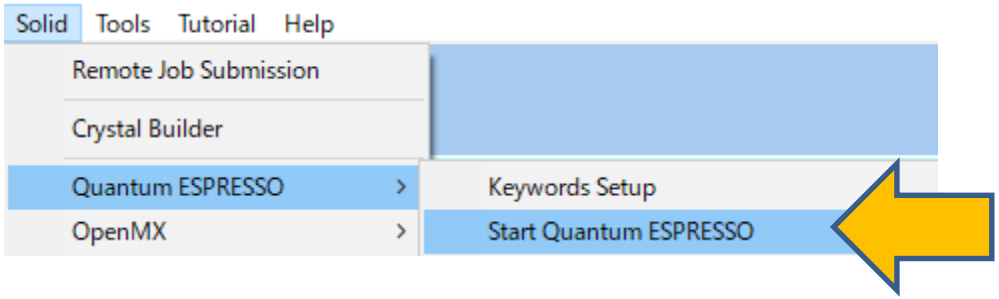
II. Phonon Dispersion

1. Click **Solid** | **Quantum ESPRESSO** | **Start Quantum ESPRESSO**.
2. Save as **si_disp.pwin**.



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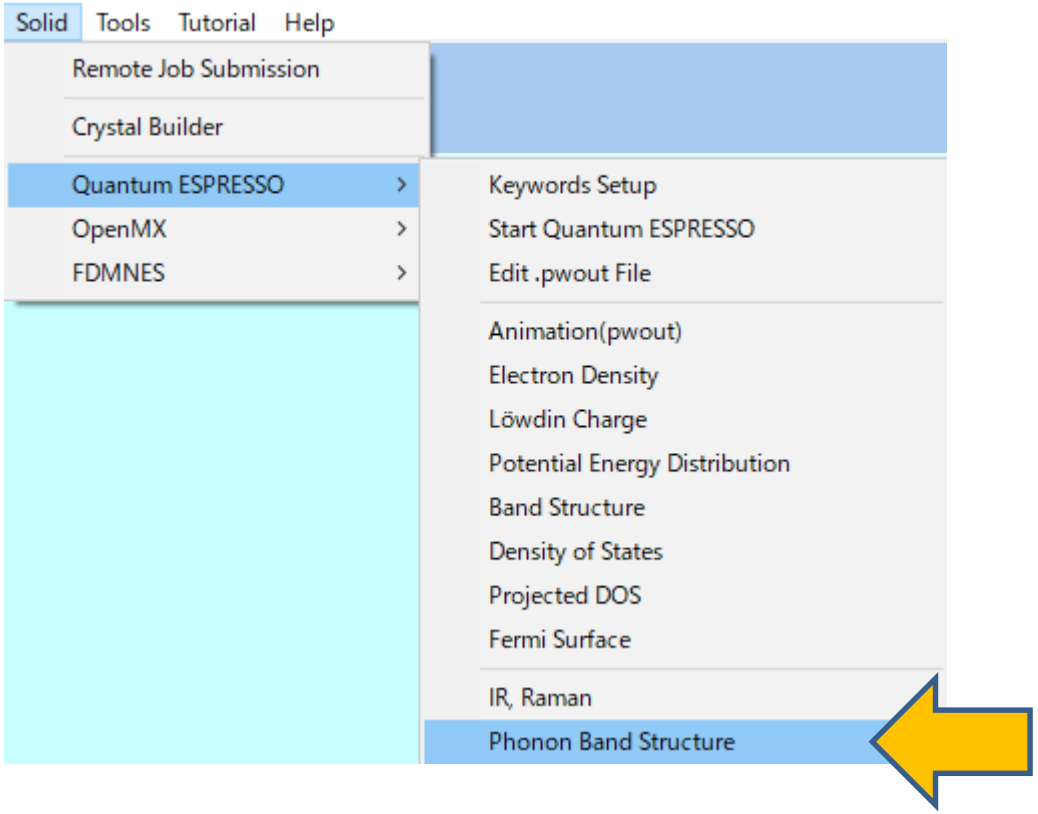
II. Phonon Dispersion

1. Click | **Quantum ESPRESSO** | **Phonon Band Structure**.
2. Select QE working directory which is suggested by default.



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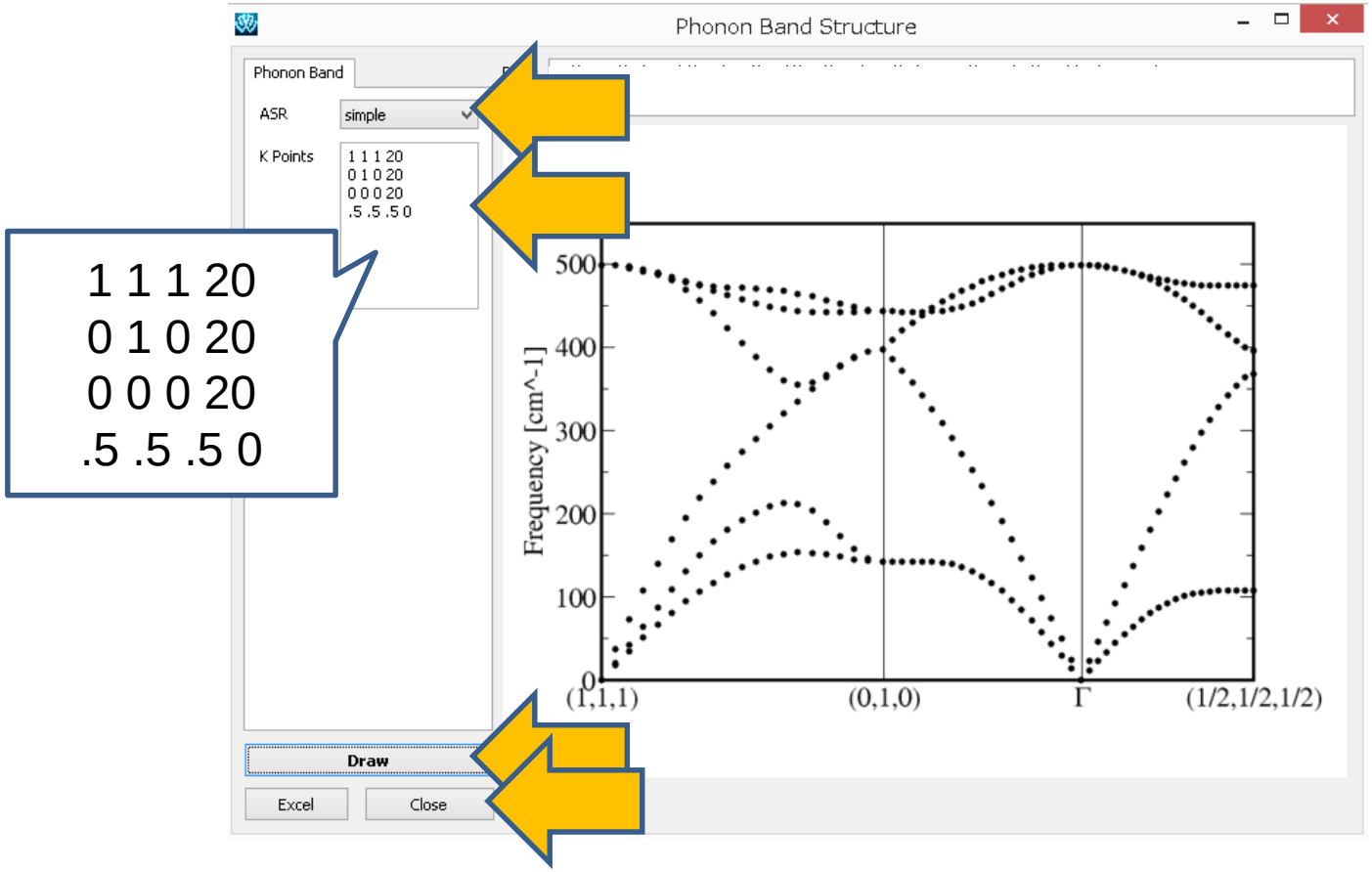
II. Phonon Dispersion

1. Set **ASR** to **Simple**, then set **K Points** as shown below.
2. Clicking **Draw** will display the phonon band structure. Click **Close** when done.



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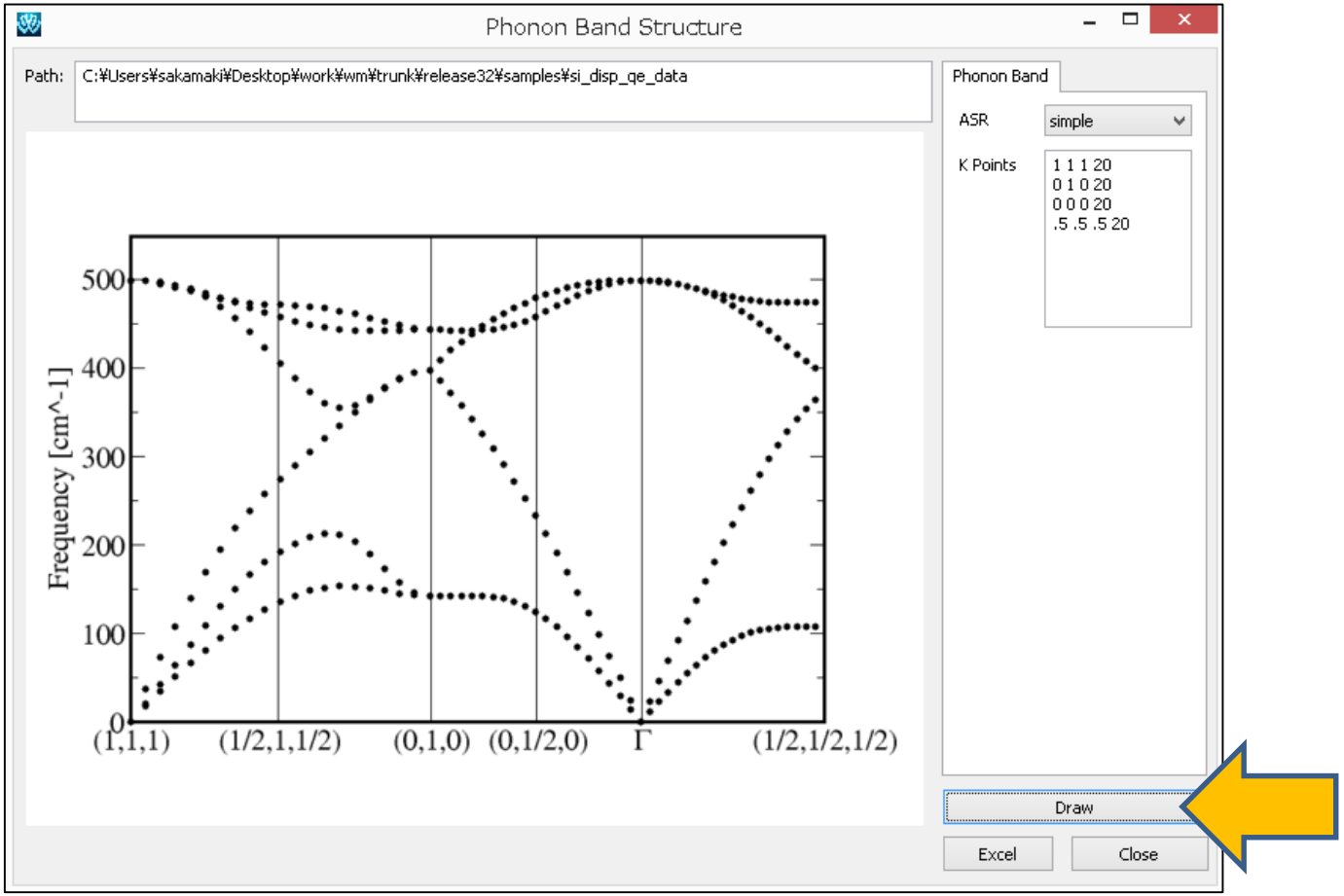
II. Phonon Dispersion

Click **Draw** to draw phonon dispersion.



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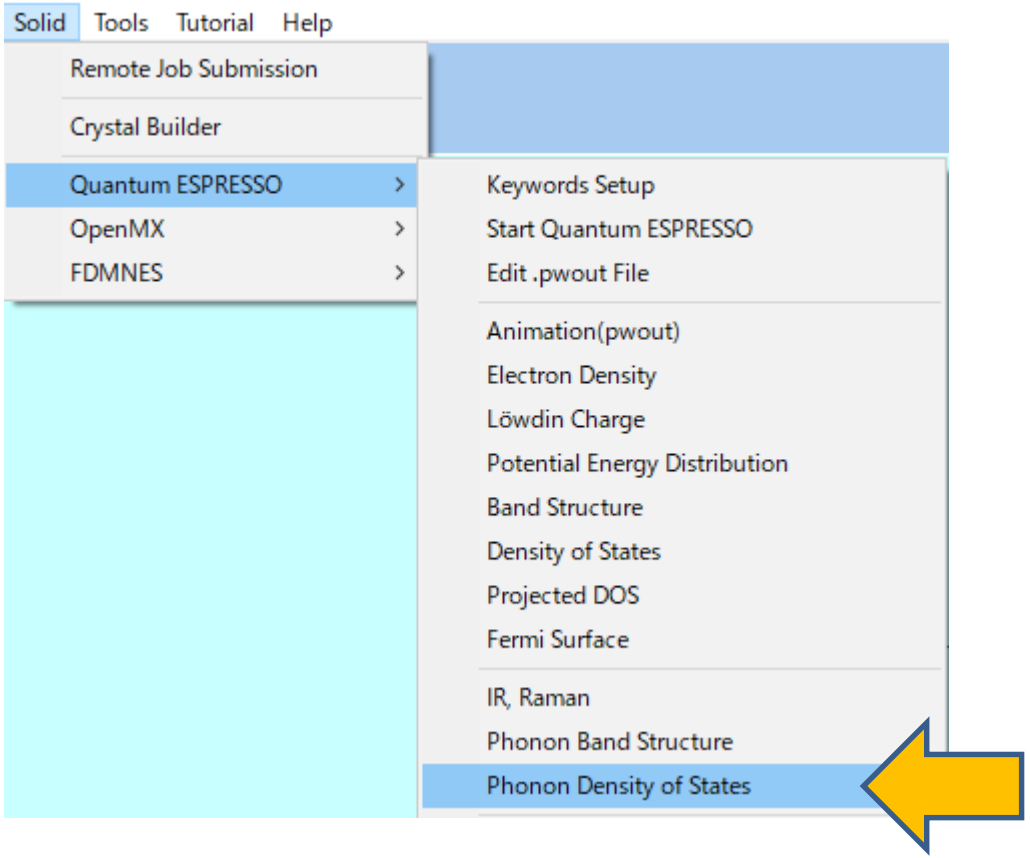
II. Phonon Dispersion

1. Click **Solid** | **Quantum ESPRESSO** | **Phonon Density of States**.
2. Select a working directory of QE. Here, the suggested directory by default should be selected.



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II. Phonon Dispersion

1. Set **ASR** to **simple**.
2. Click **Draw** to draw phonon density of states.