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Winmostar tutorial
Quantum ESPRESSO
Phonon
V7.025

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Contents

I. IR, Raman spectrum
II. Phonon dispersion
    dispersion curve・DOS

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Environment setting

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

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I. SCF & Dielectric Function

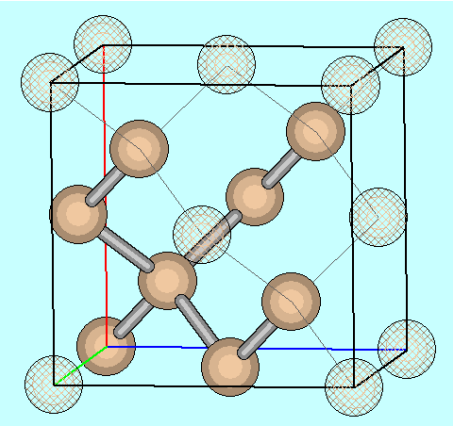
1. Click **File | Open**.
2. Select **si.cif.** (C:¥winmos7¥samples¥si.cif)

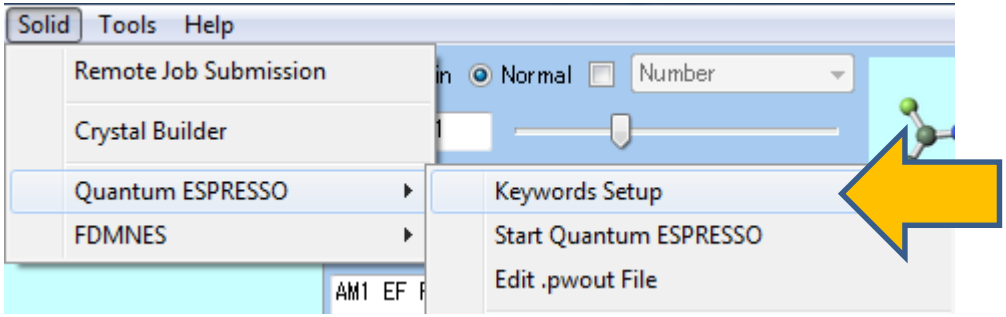
You can also make the same CIF file using Crystal Builder.
See crystal modeling tutorial and apply the following information.

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)

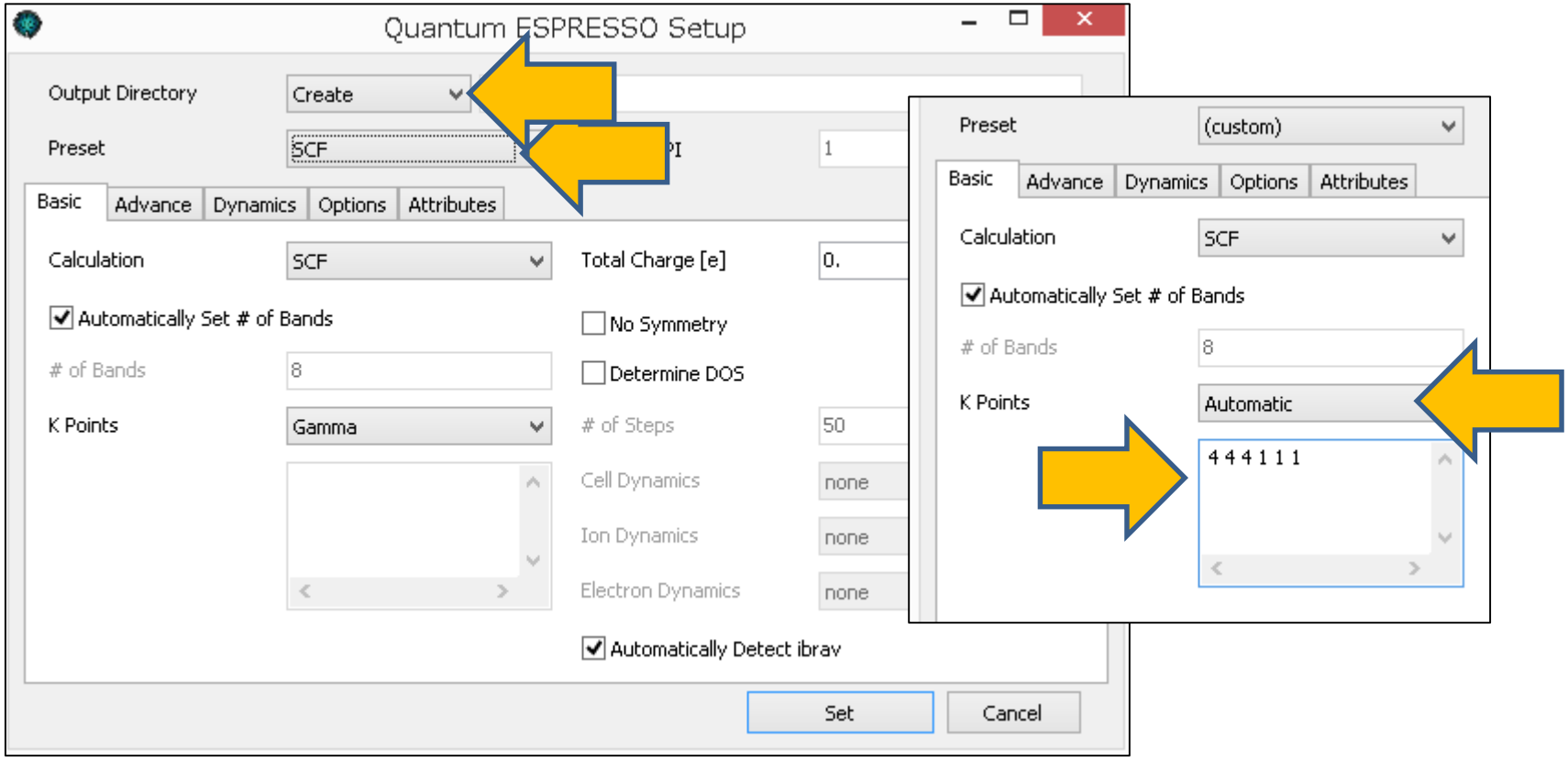
3. Click **Solid | Quantum ESPRESSO | Keywords Setup**.





I. IR, Raman spectrum

1. Set **Output Directory** to **Create**, **Preset** to **SCF**.
2. Set **K Points** to **Automatic**, ”**4 4 4 1 1 1**” (space separated) below.



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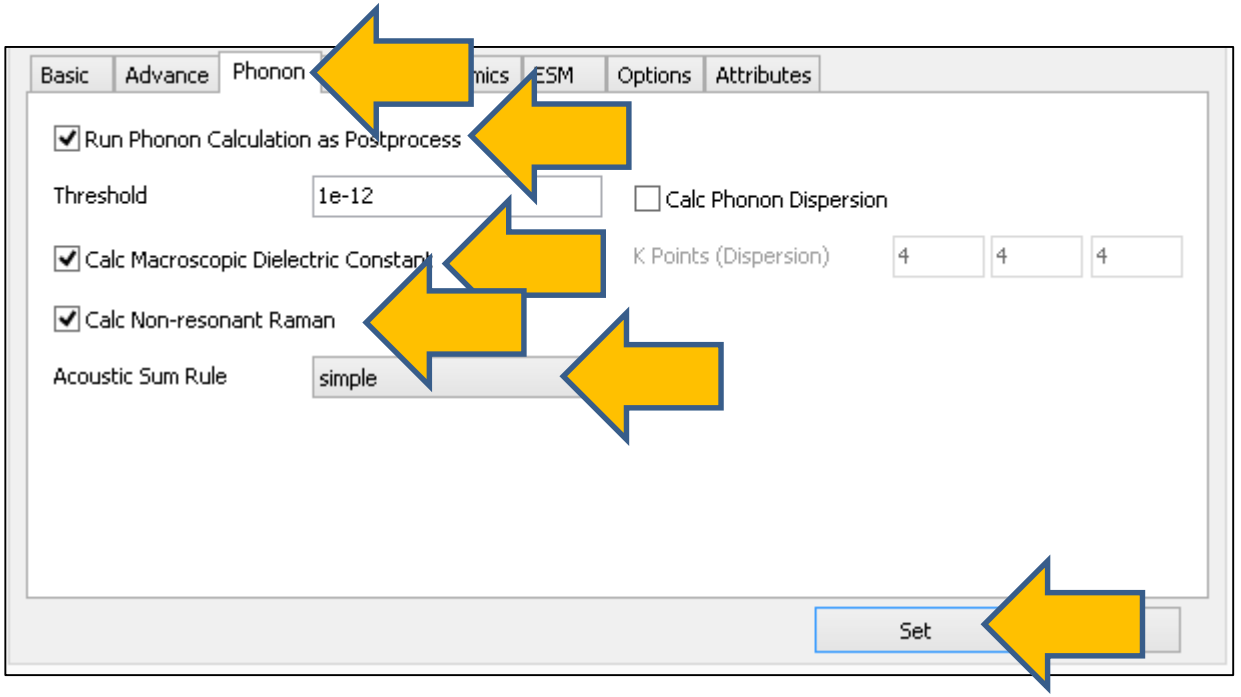
I. IR, Raman spectrum

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



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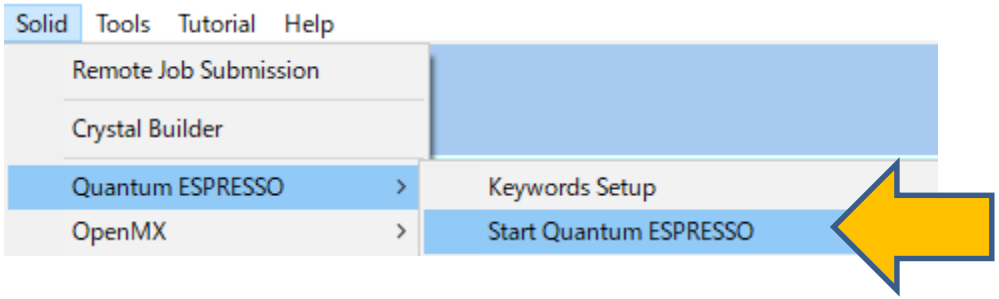
I. IR, Raman spectrum

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



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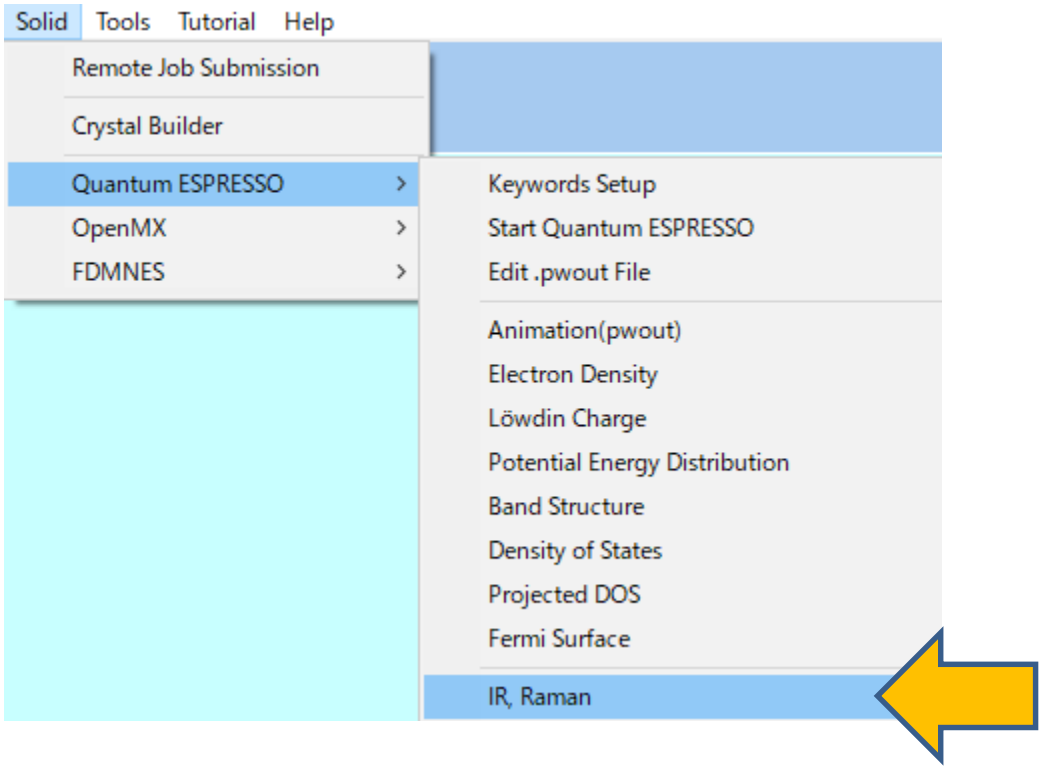
I. IR, Raman spectrum

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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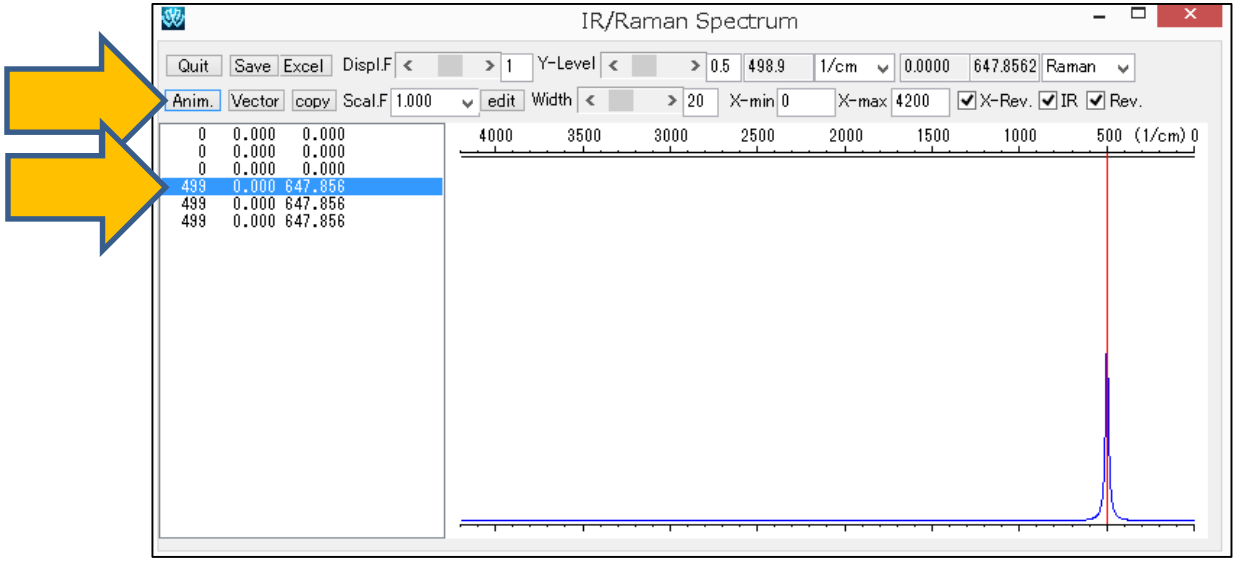
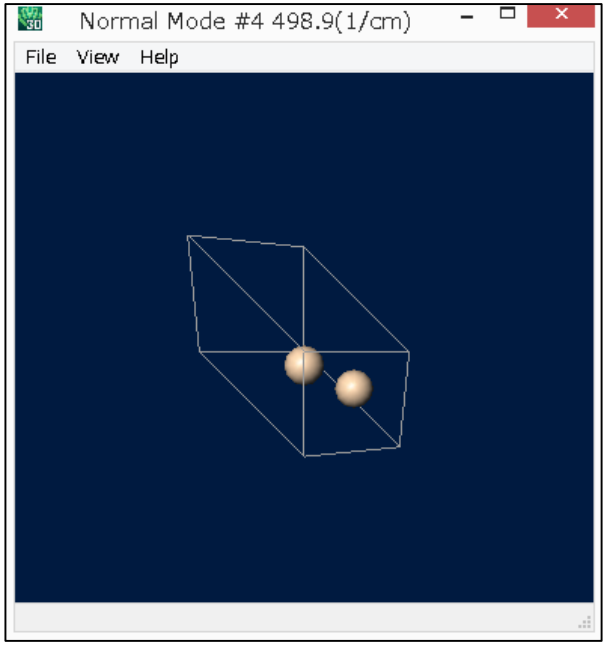
I. IR, Raman spectrum

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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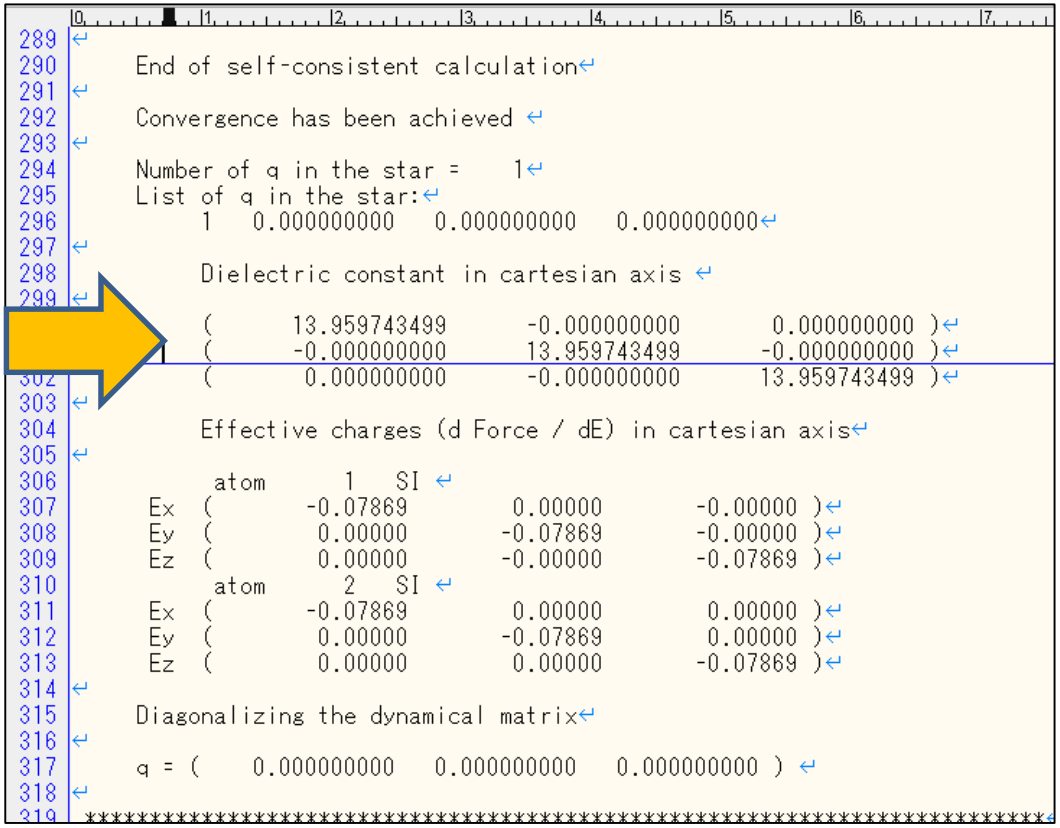
I. IR, Raman spectrum

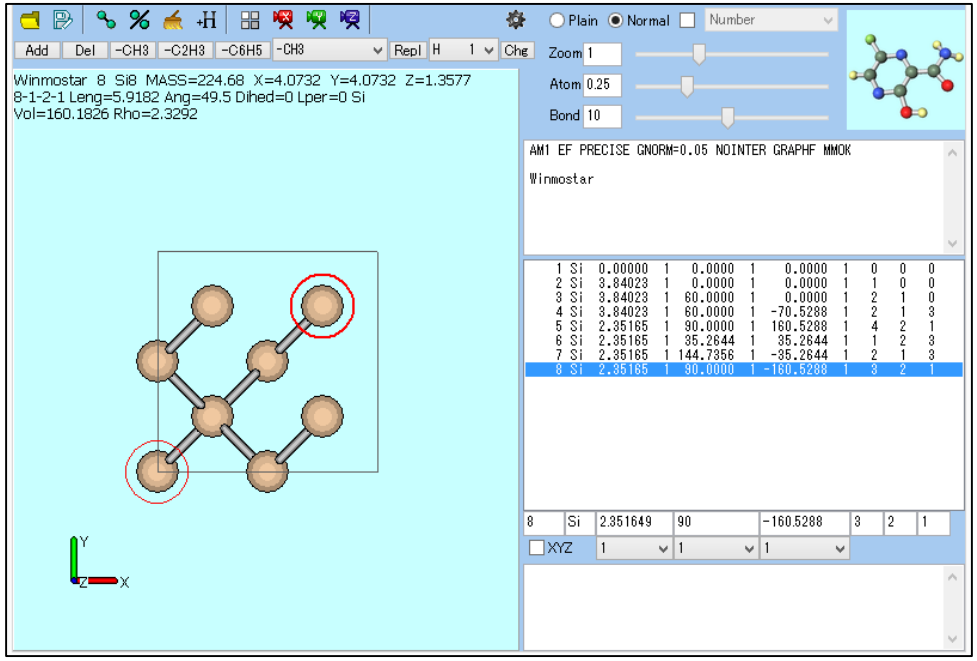
Dielectric constant has been calculated with IR and Raman spectrum.
Open **ph.out** in **si_vib_qe_data** folder where **si_vib.pwin** was saved.

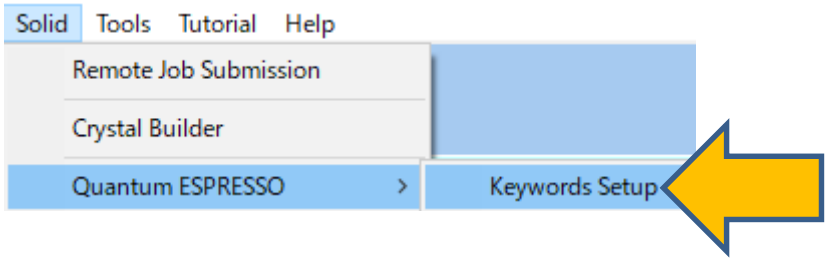


```
289
290      End of self-consistent calculation
291
292      Convergence has been achieved
293
294      Number of q in the star =    1
295      List of q in the star:
296           1   0.000000000   0.000000000   0.000000000
297
298           Dielectric constant in cartesian axis
299
300           (      13.959743499      -0.000000000       0.000000000 )
301           (      -0.000000000      13.959743499      -0.000000000 )
302           (       0.000000000      -0.000000000      13.959743499 )
303
304           Effective charges (d Force / dE) in cartesian axis
305
306            atom      1   SI
307       Ex  (       -0.07869         0.00000        -0.00000 )
308       Ey  (        0.00000        -0.07869        -0.00000 )
309       Ez  (        0.00000        -0.00000        -0.07869 )
310            atom      2   SI
311       Ex  (       -0.07869         0.00000         0.00000 )
312       Ey  (        0.00000        -0.07869         0.00000 )
313       Ez  (        0.00000         0.00000        -0.07869 )
314
315      Diagonalizing the dynamical matrix
316
317      q = (    0.000000000   0.000000000   0.000000000 )
318
319 ********************************************************************************
```

II. Phonon dispersion

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





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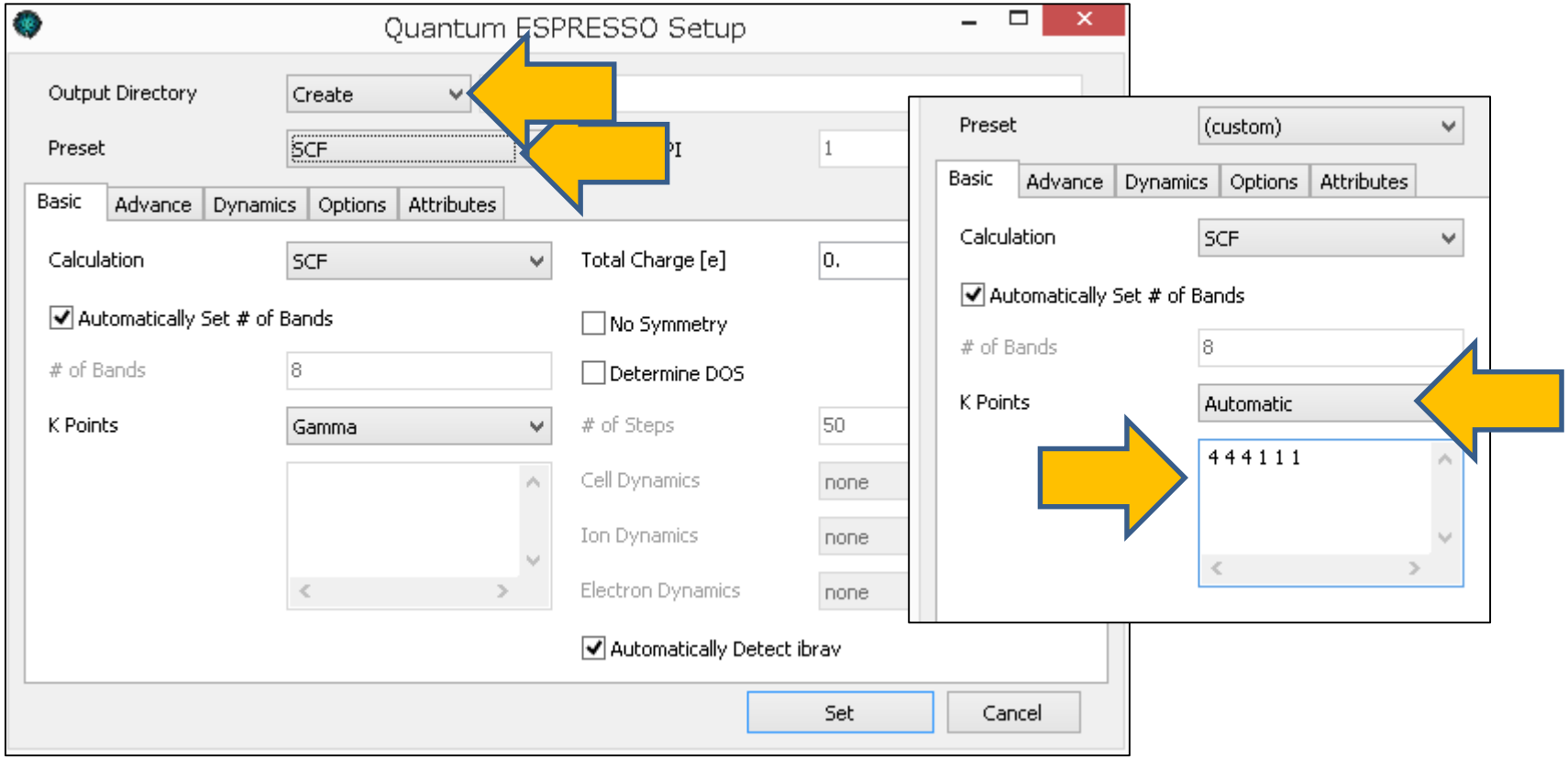
II. Phonon dispersion

1. Set **Output Directory** to **Create**, **Preset** to **SCF**.
2. Set **K Points** to **Automatic**, ”**4 4 4 1 1 1**”(space separated) below.



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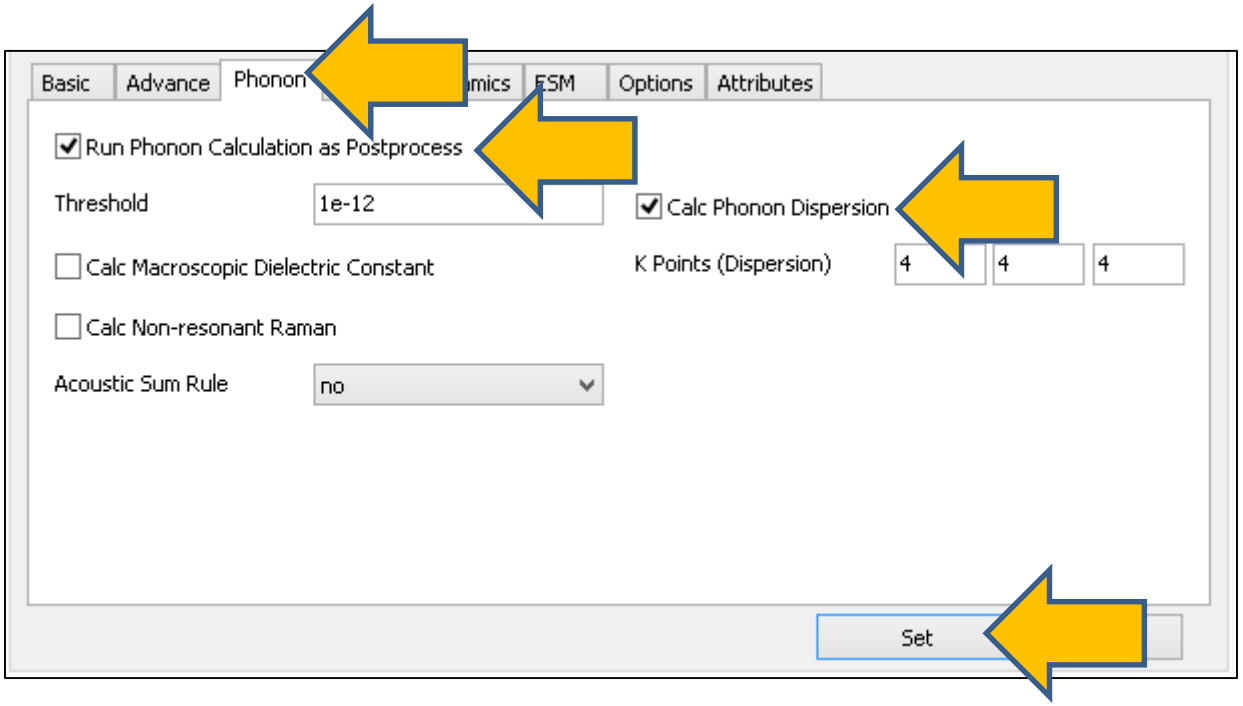
II. Phonon dispersion

1. On **Phonon** tab, check **Run Phonon Calculation as Postprocess**, **Calc Phonon Dispersion**.
2. Click **Set**.



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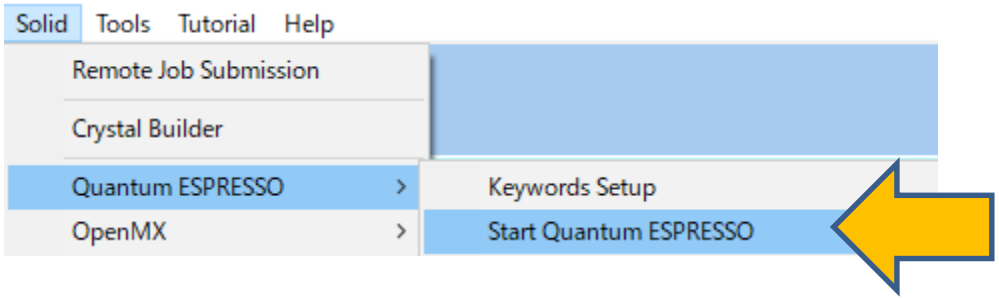
II. Phonon dispersion

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



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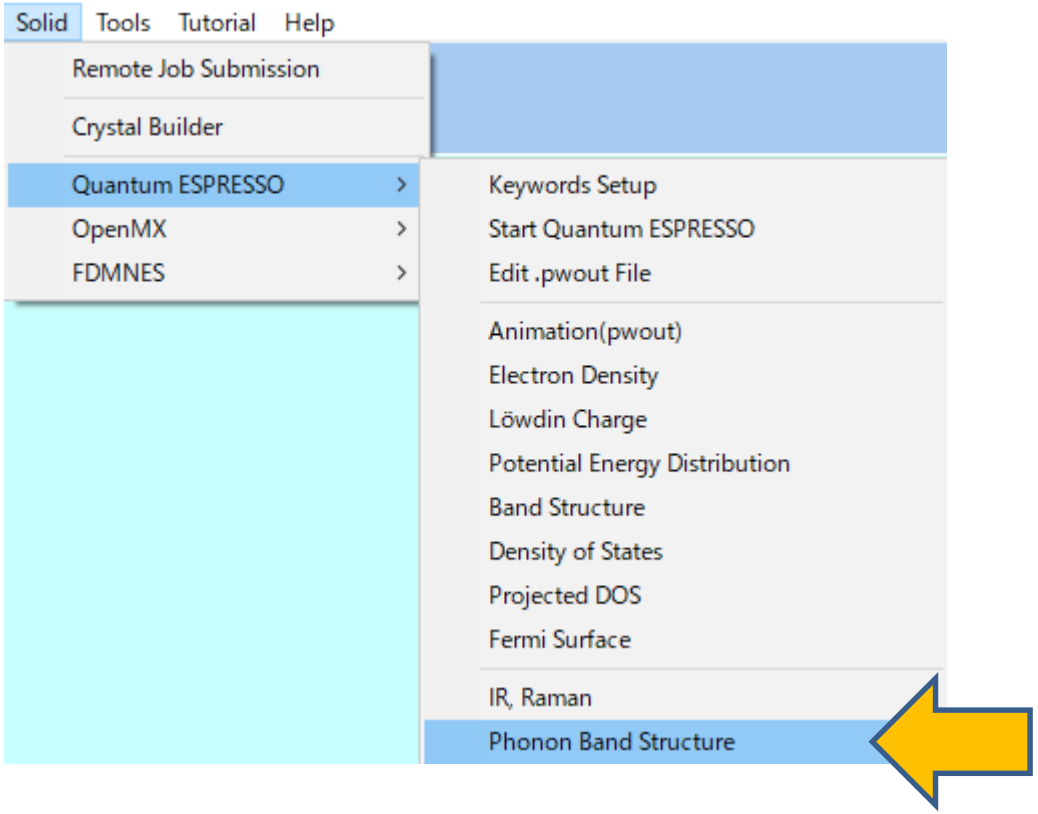
II. Phonon dispersion

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



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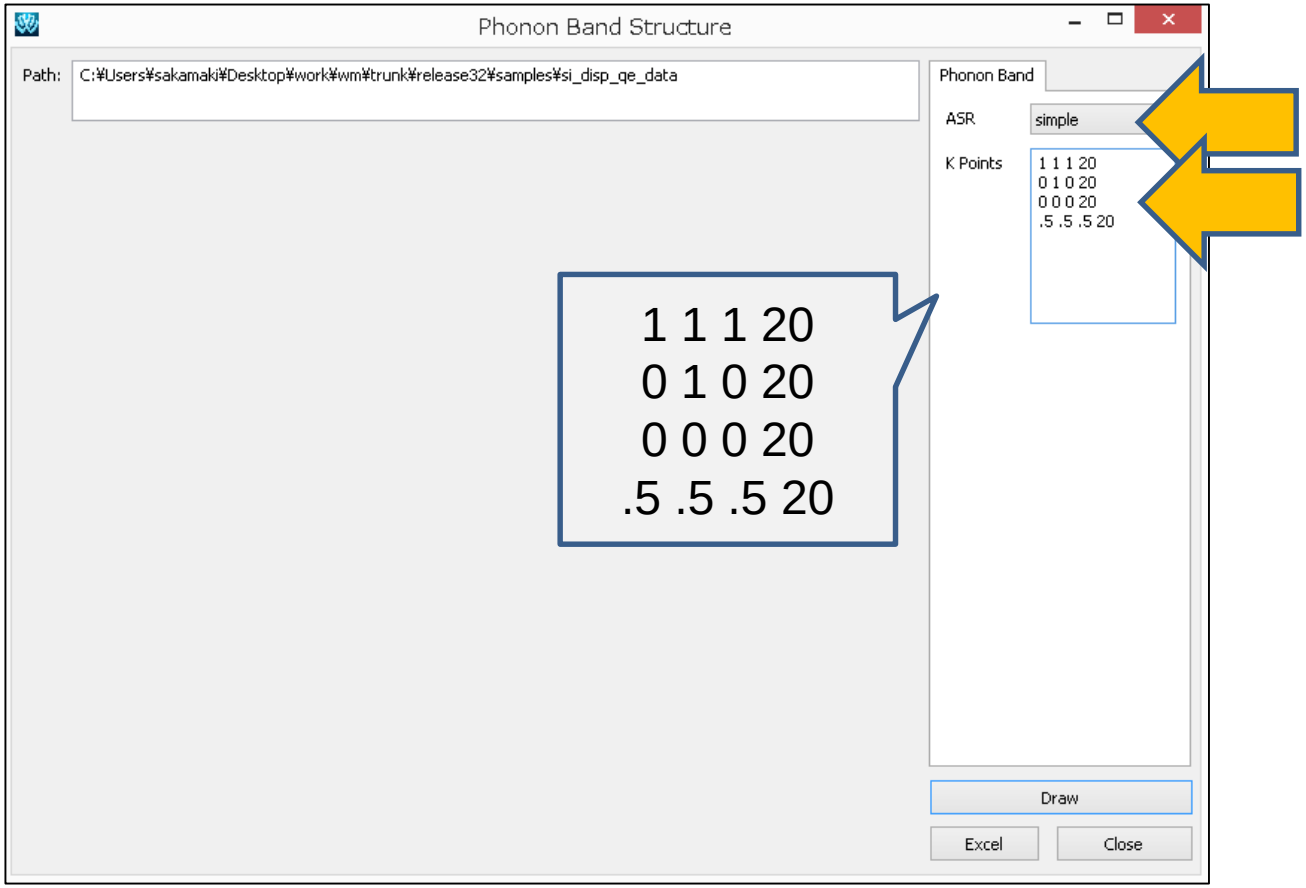
II. Phonon dispersion

1. Set **ASR** to **Simple**.
2. Set **K Points** as shown below.



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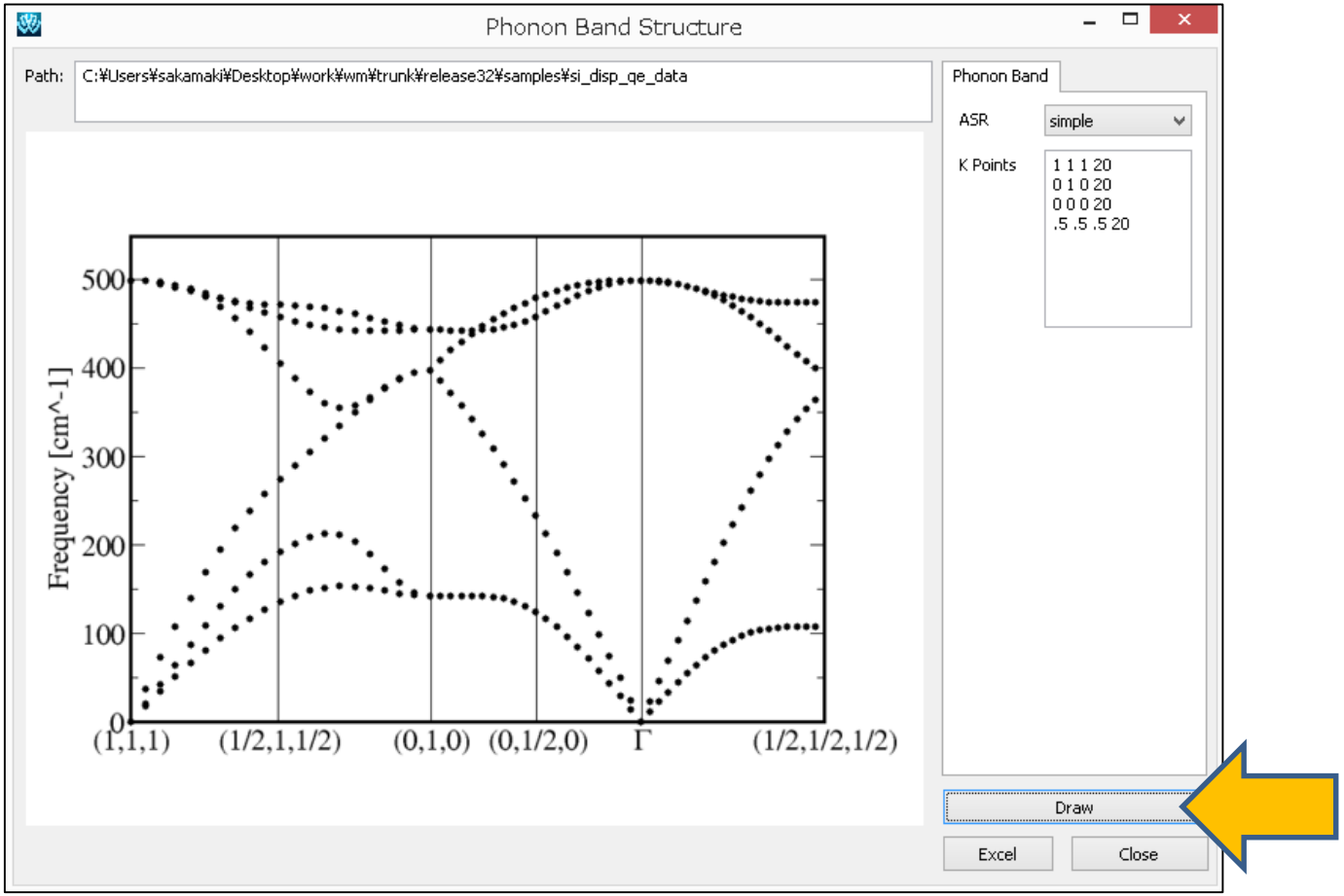
II. Phonon dispersion

Click **Draw** to draw phonon dispersion.



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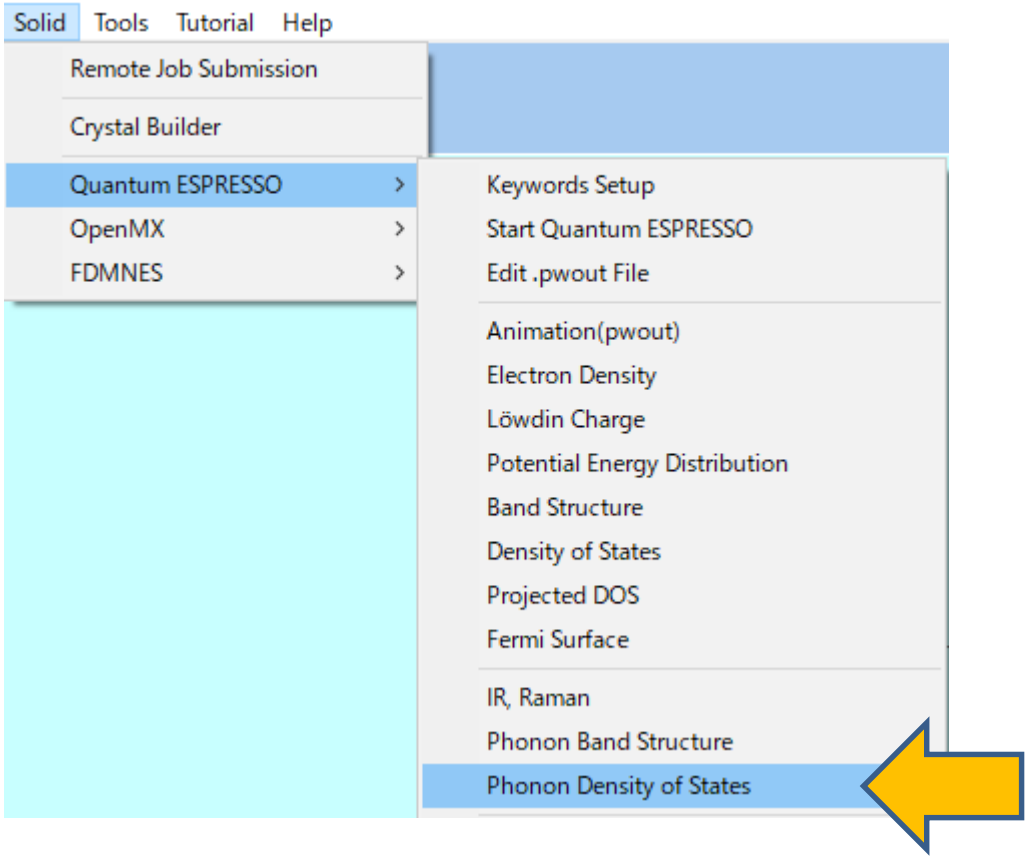
II. Phonon dispersion

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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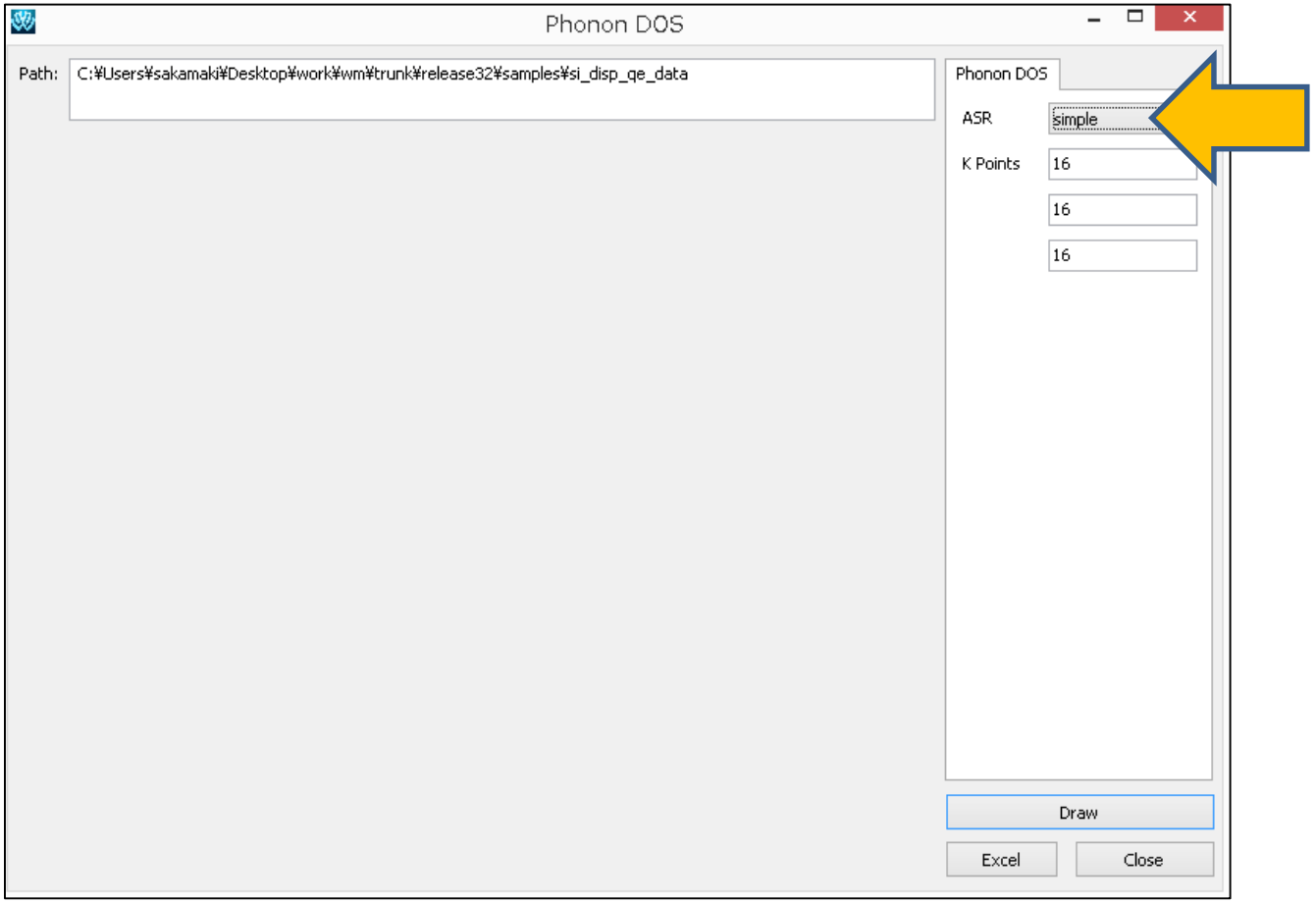
II. Phonon dispersion

Set **ASR** to **simple**.



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II. Phonon dispersion

Click **Draw** to draw phonon density of states.