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Winmostar tutorial
Quantum ESPRESSO
Basics
V8.021

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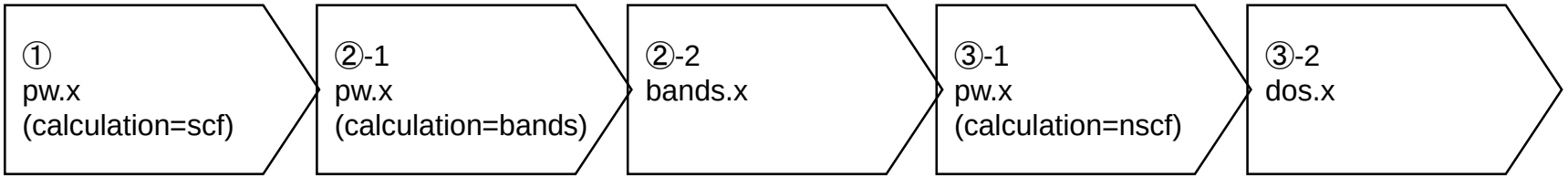
Summary

- In this tutorial, we will perform SCF calculation on a Si crystal, then calculate the band structure and density of state (these processes will execute consecutively on Winmostar). We will also show procedures to display potential DOS and electron density.



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.

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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. Creating the Model

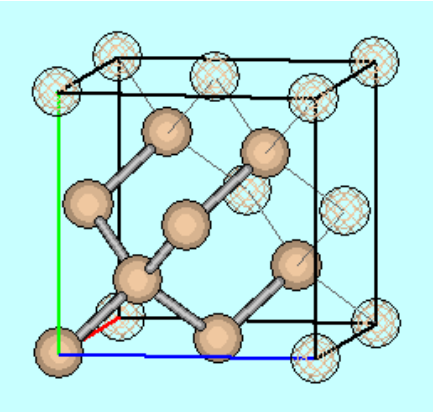
1. Click **File | Open**.
2. Select **si.cif.** (C:¥winmos8¥samples¥si.cif)

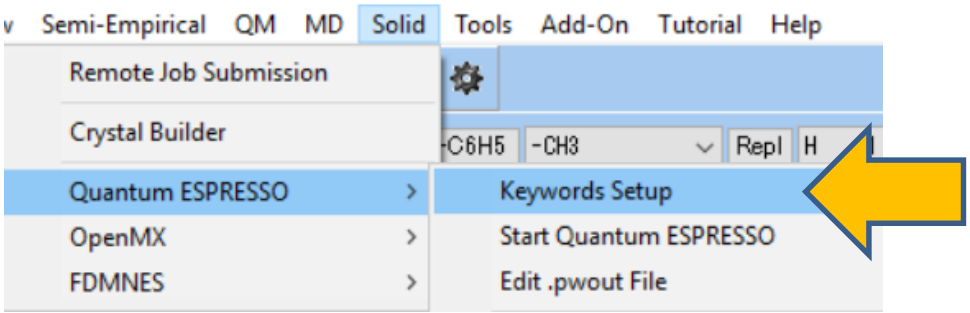
You can also make the same CIF file using Crystal Builder.
See crystal modeling tutorial and apply the following information.

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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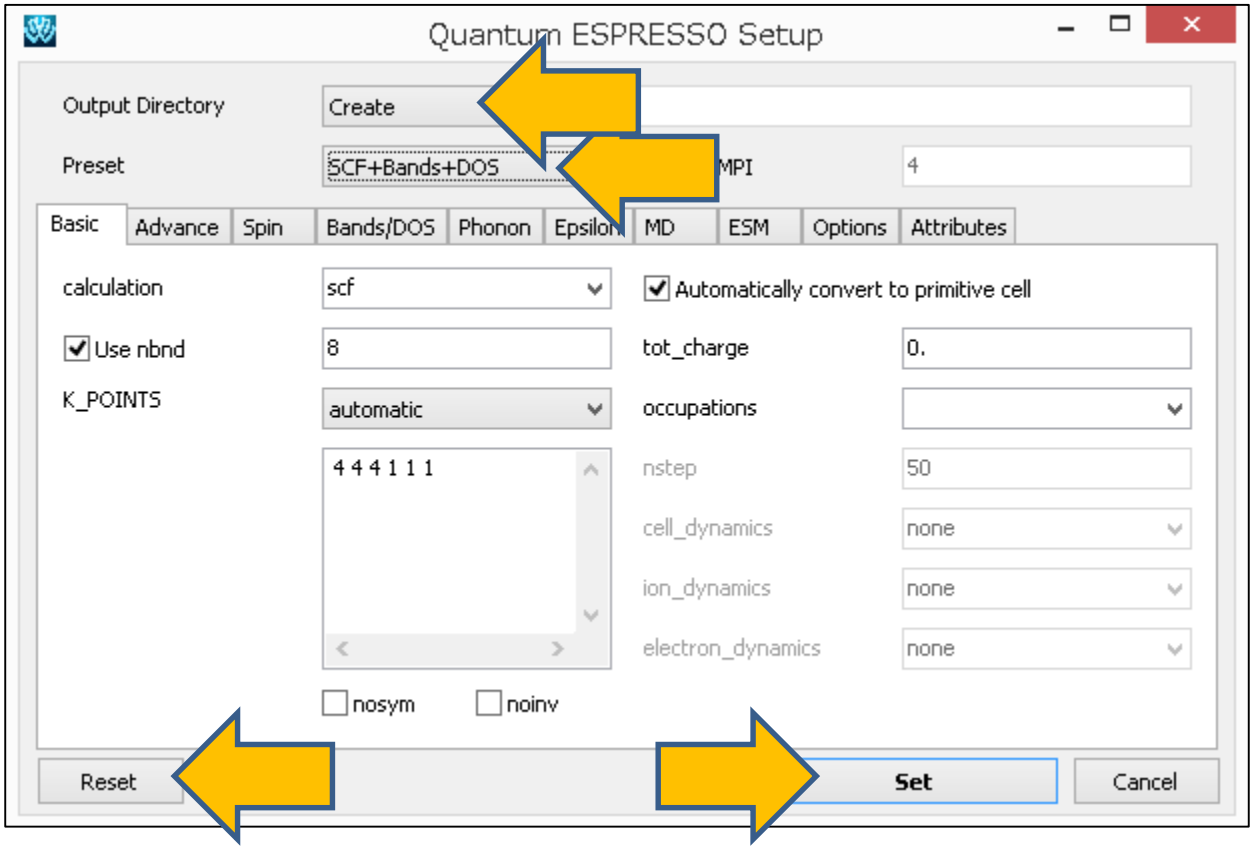
II. QE Calculation

1. First click **Reset**. Set **Preset** to **SCF+Bands+DOS**.
2. Click **Set**.



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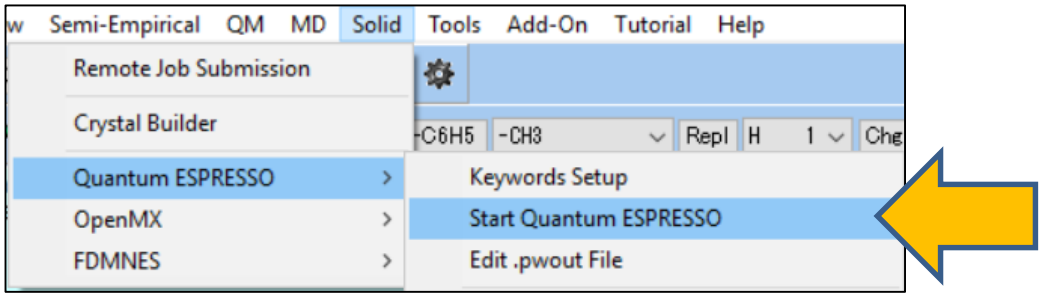
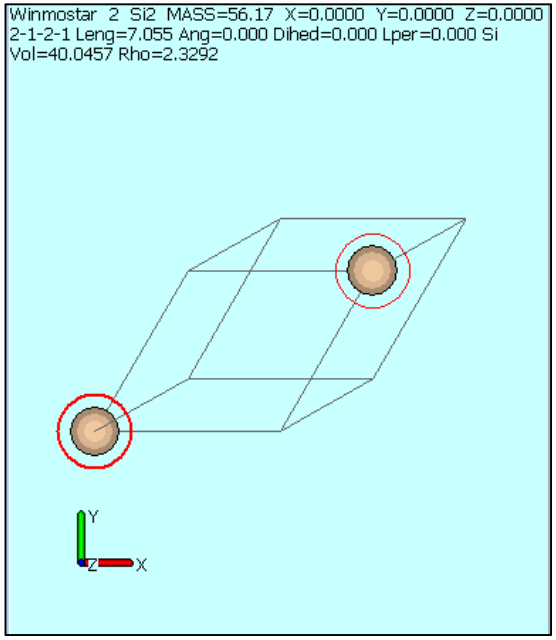
II. QE Calculation

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. You may be asked whether you save the file. Name the file and save. In this tutorial, we assume you named the file as **si_tutor.pwin**.

Note: After saving the file, the crystal structure will be converted to a Primitive Cell like the one shown below. You can choose to turn off automatic conversion by selecting **Solid | Quantum ESPRESSO | Quantum ESPRESSO Keyword Setup**, and checking off **Automatically convert to primitive cell**.





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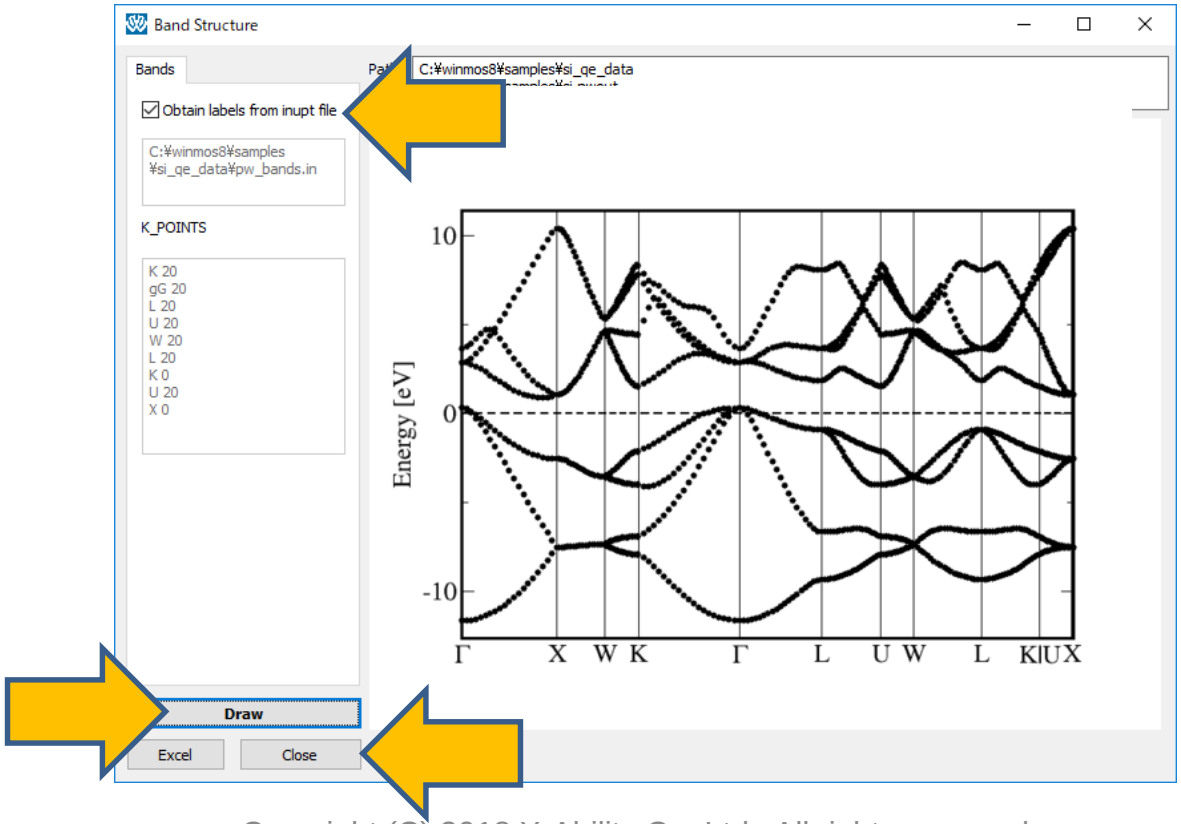
III. Analysis

1. After the calculation click **Solid | Quantum ESPRESSO | Band Structure**.
2. Select file suggested by default.
3. Click **Obtain labels from input file** to select file to be opened by default.
4. Click **Draw** to display the band diagram. Click **Close** when done.



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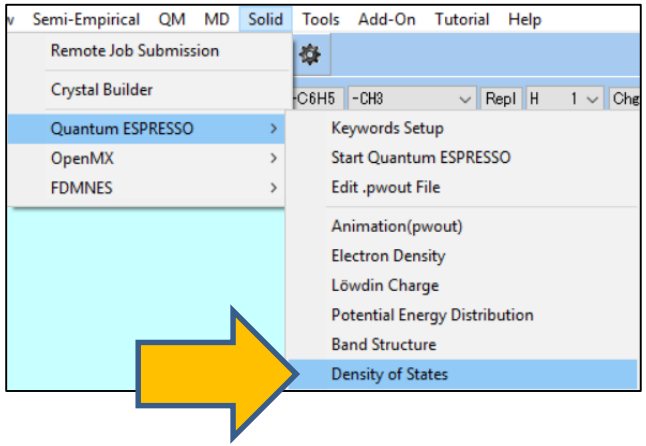
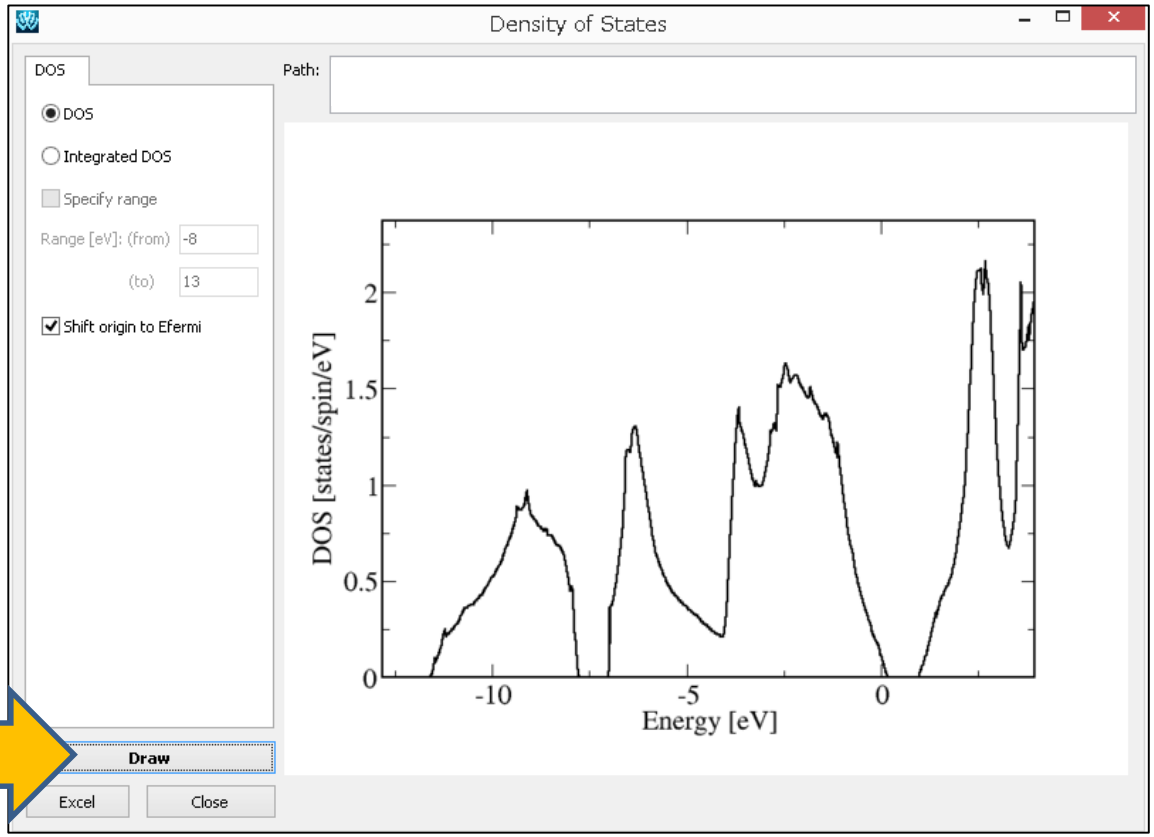
III. Analysis

1. Click **Solid | Quantum ESPRESSO | Density of States**.
2. Select directory and file suggested by default.
3. Click **Draw** in the new pop-up window to display DOS.





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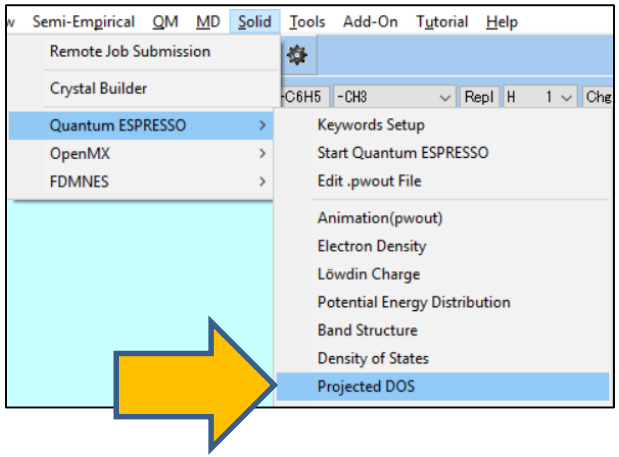
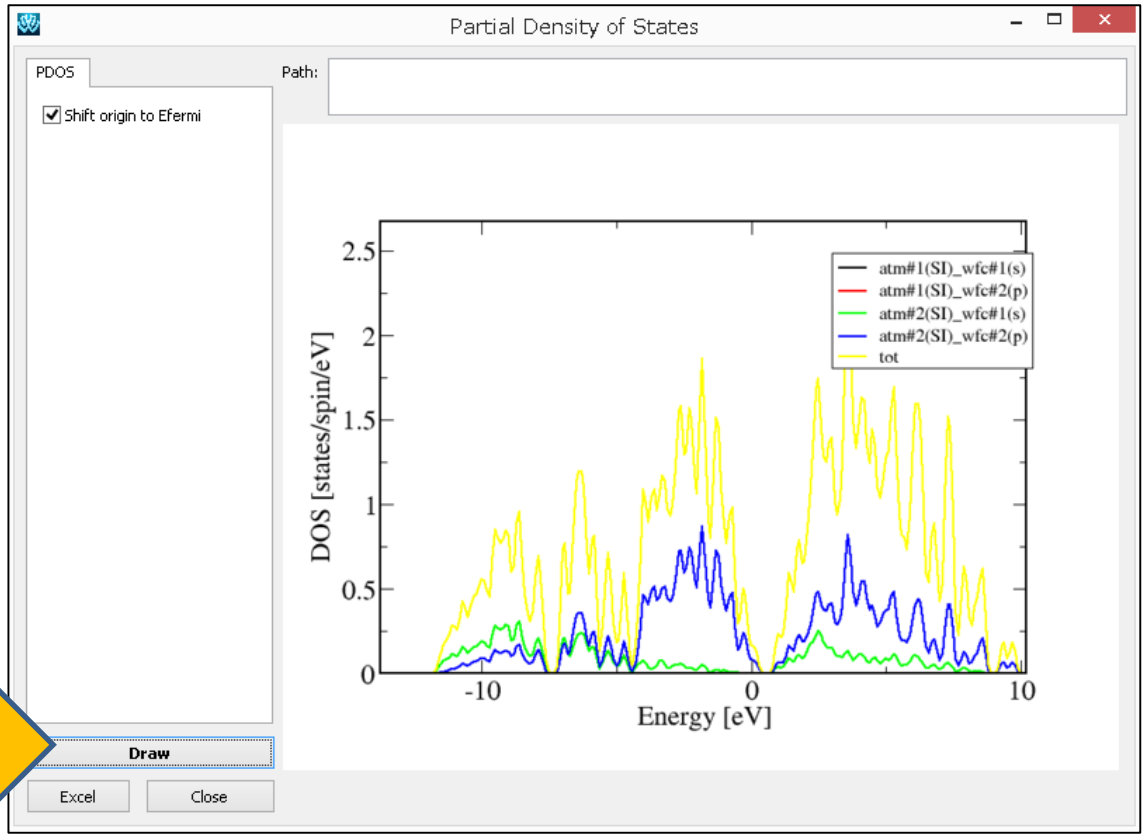
III. Analysis

1. Click **Solid | Quantum ESPRESSO | Projected DOS**.
2. Select directory and file suggested by default.
3. Click **Draw** in the new pop-up window to display PDOS.





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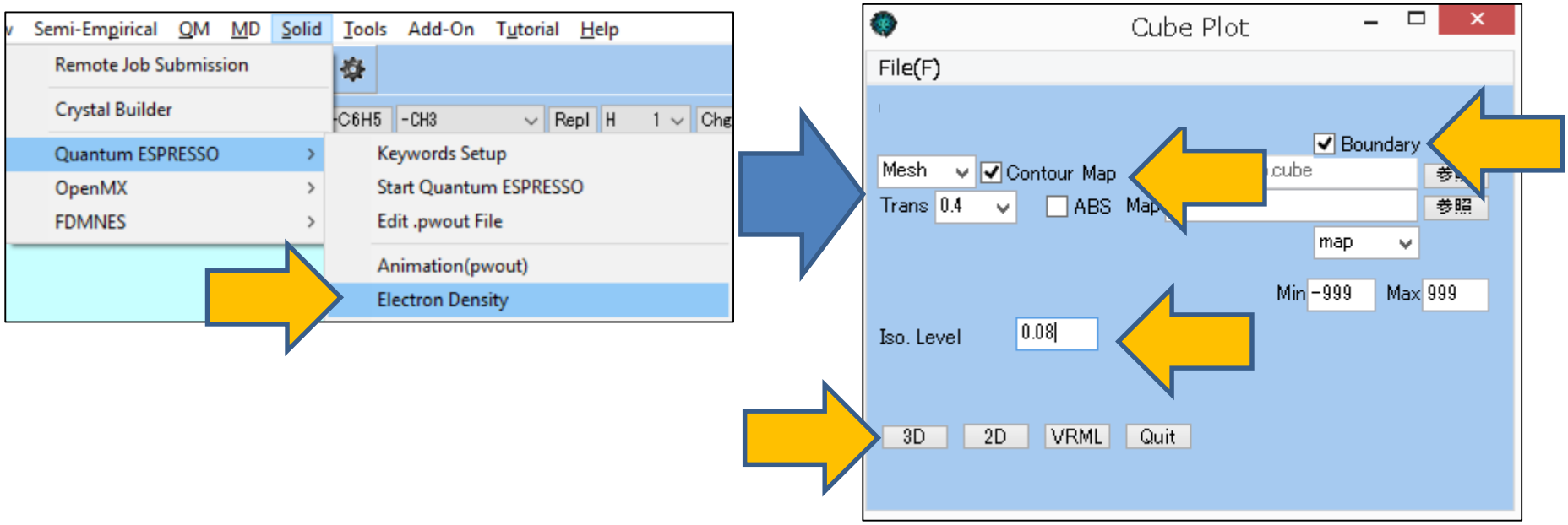
III. Analysis

1. Click **Solid | Quantum ESPRESSO | Electron Density**.
2. Select directory suggested by default.
3. Check boxes for **Contour Map** and **Boundary**, and set **Iso. Level** to **0.08**.
4. Click **3D**.



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III. Analysis

1. In the Winmostar 3D window, click **View | Preferences**.
2. Move the **X**, **Y**, and **Z** sliders and select surface to display for contour map.