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Winmostar tutorial
Quantum ESPRESSO
Basics
V7.003

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Contents

I. SCF calculation
II. Bands structure
III. Density of states
IV. Electron density

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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 calculation

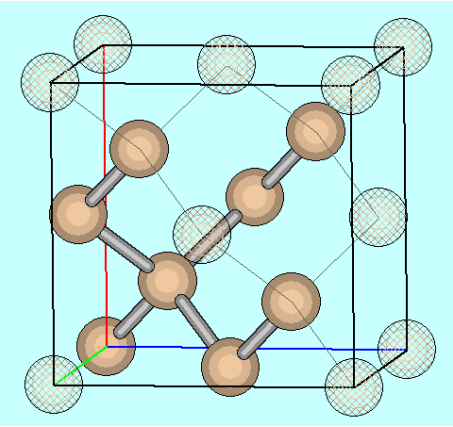
1. Click **File | Open**.
2. Select **si.cif.** (C:¥winmos7¥samples¥si.cif)

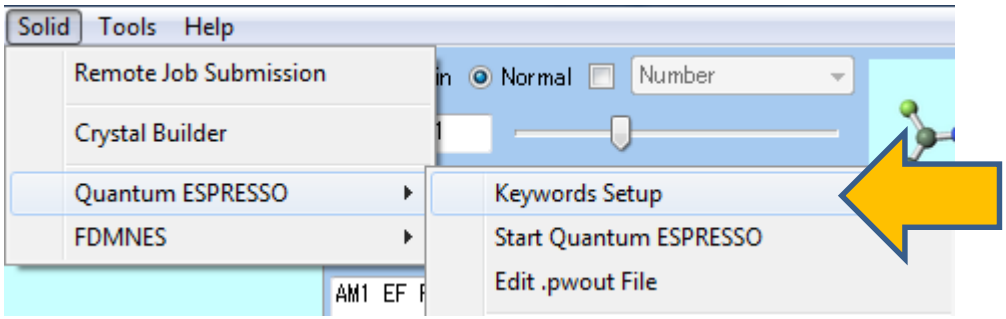
You can also make the same CIF file using Crystal Builder.
See crystal modeling tutorial and apply the following information.

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**.





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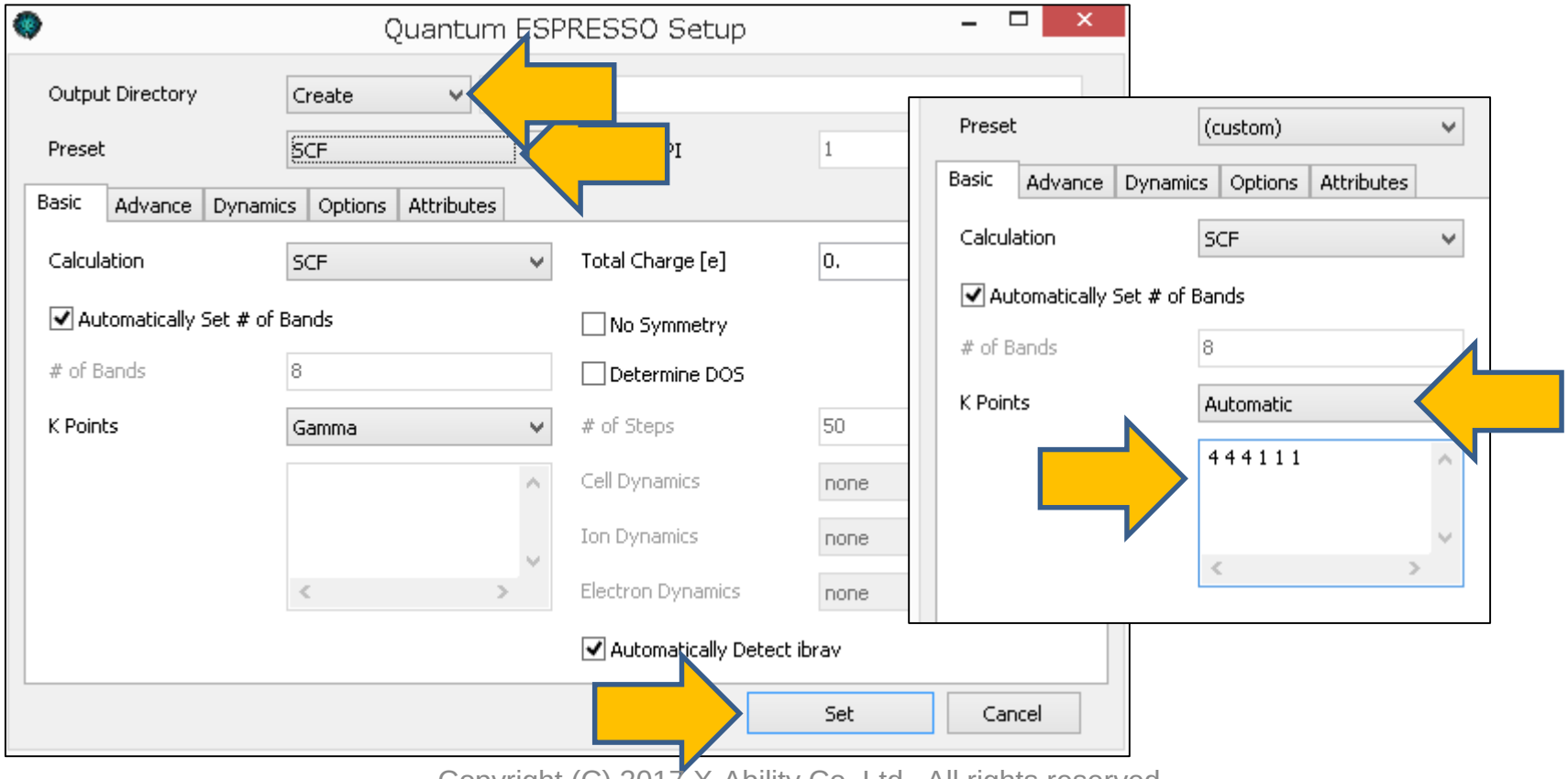
I. SCF calculation

1. Set **Output Directory** to **Cubic**. Set **Preset** to **SCF**.
2. Set **K Points** to **Automatic** and input **4 4 4 1 1 1**.
3. Click **Set**.



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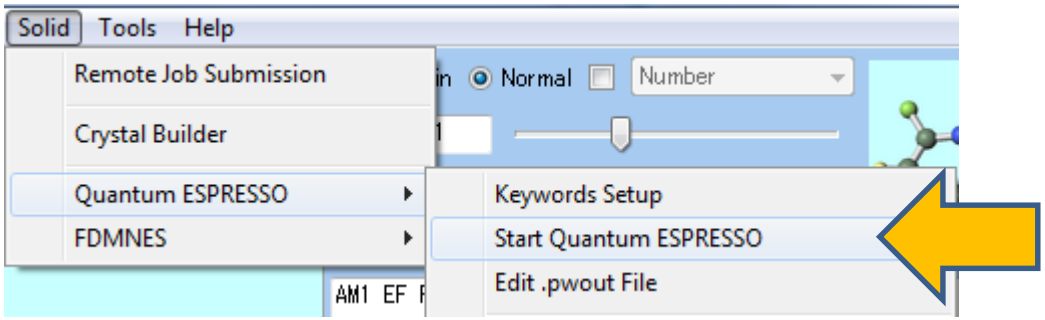
I. SCF calculation

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**.



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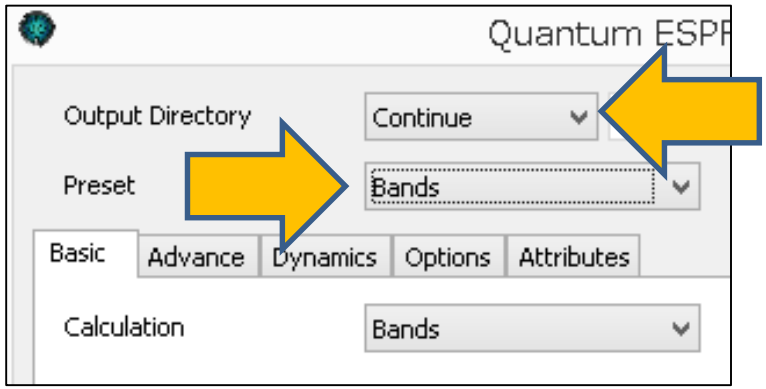
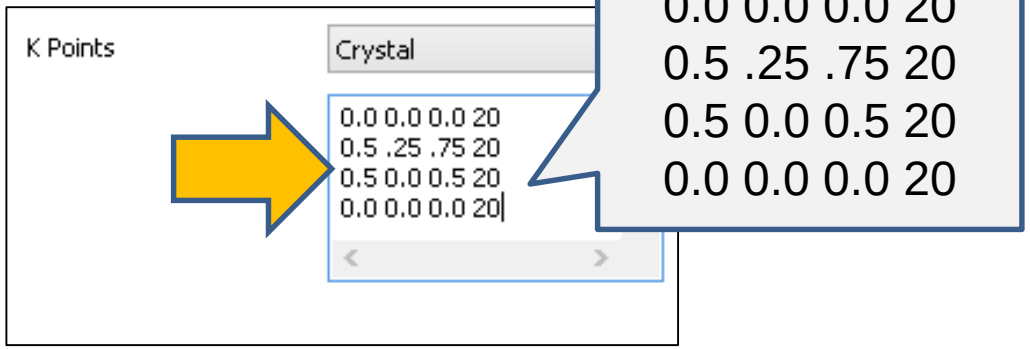
II. Bands Structure

1. After the SCF calculation, click **Solid | Quantum ESPRESSO | Keywords setting**.
2. Set **Output Directory** to **Continue**. Set **Preset** to **Bands**.
3. Input **K Points** like the picture.
4. Click **Set**.



K Points
(You can copy and paste.)



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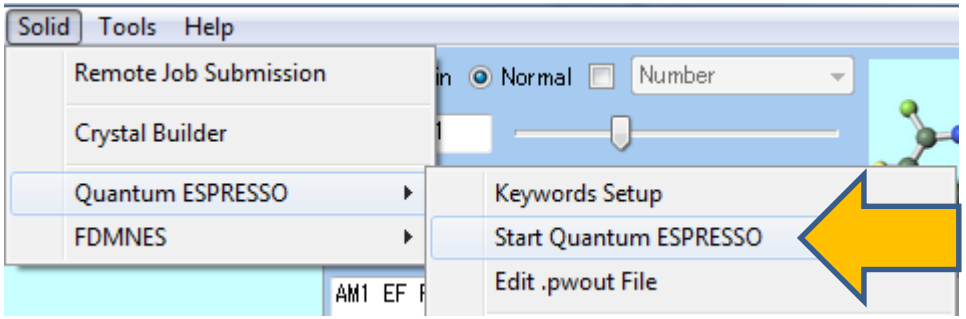
II. Bands Structure

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_bands.pwin**.



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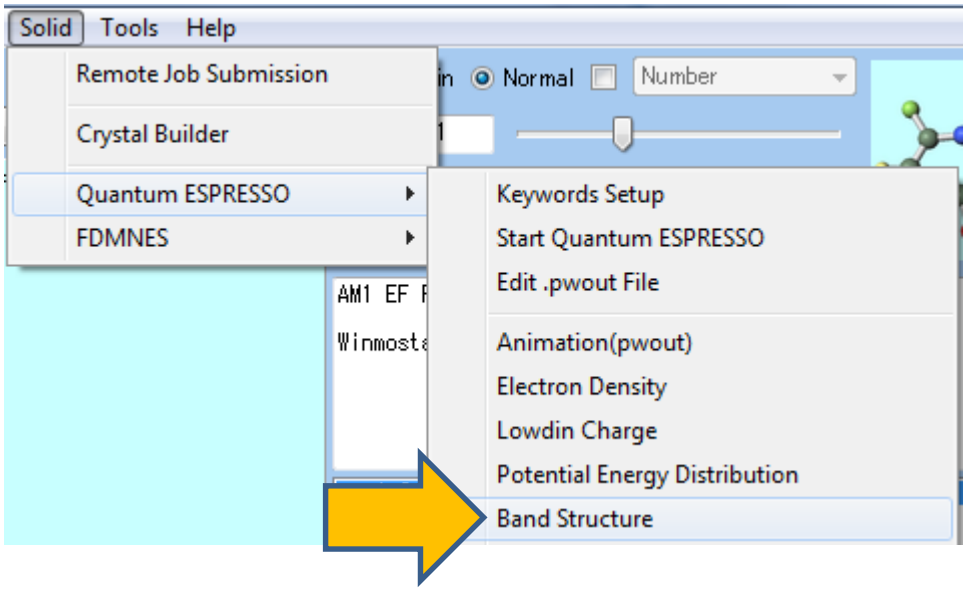
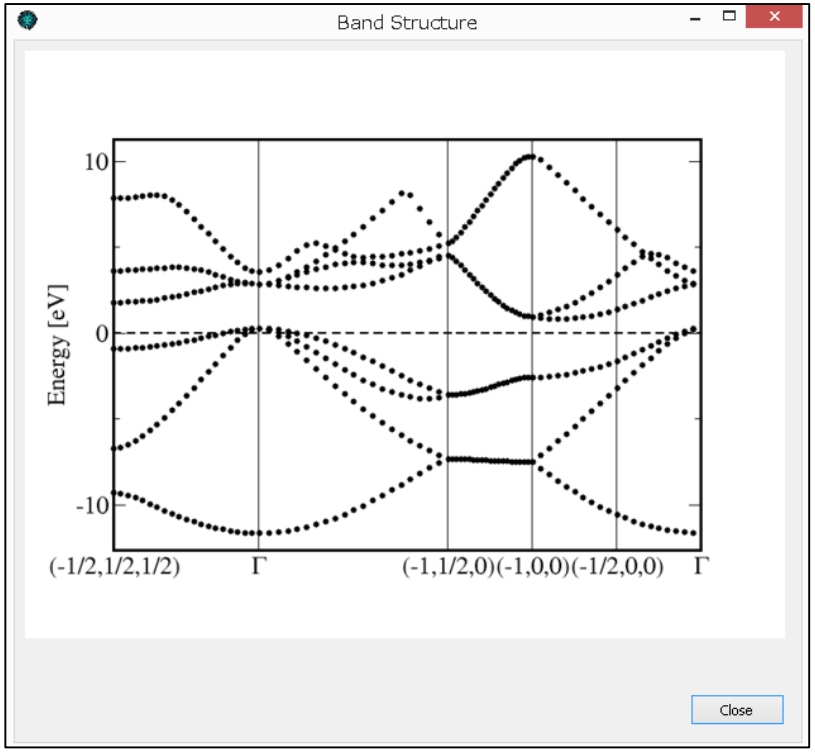
II. Bands Structure

1. After the calculation, click **Solid | Quantum ESPRESSO | Band Structure**.
2. Select a default folder.
3. New window will appear. The bands structure will be displayed.





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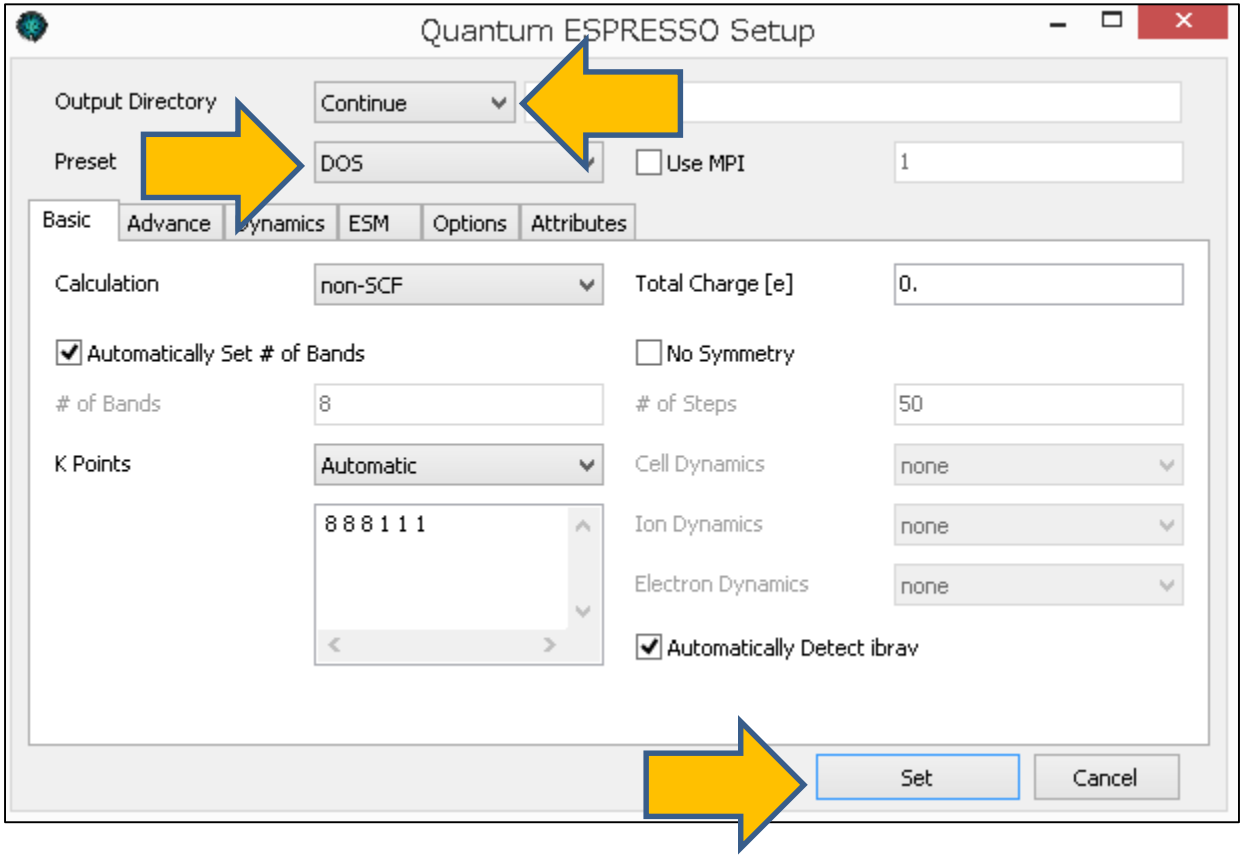
III. Density of States

1. Click **Solid | Quantum ESPRESSO | Keywords setting**.
2. Set **Output Directory** to **Continue**. Set **Preset** to **DOS**.
3. Click **Set**.



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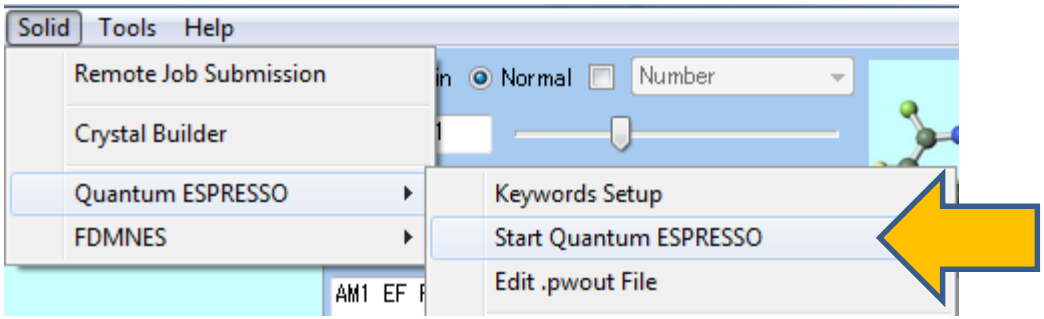
III. Density of States

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_dos.pwin**.



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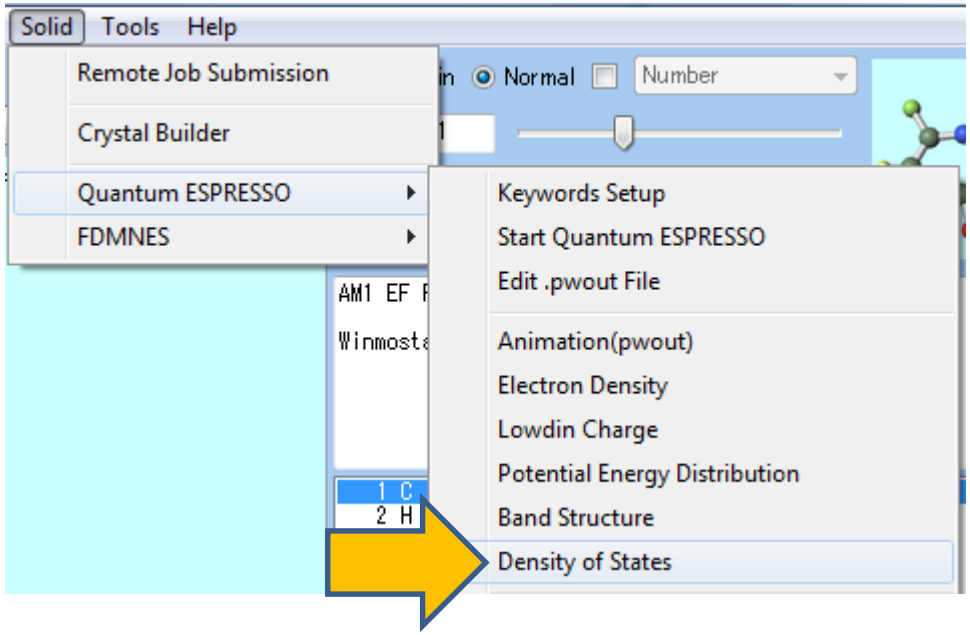
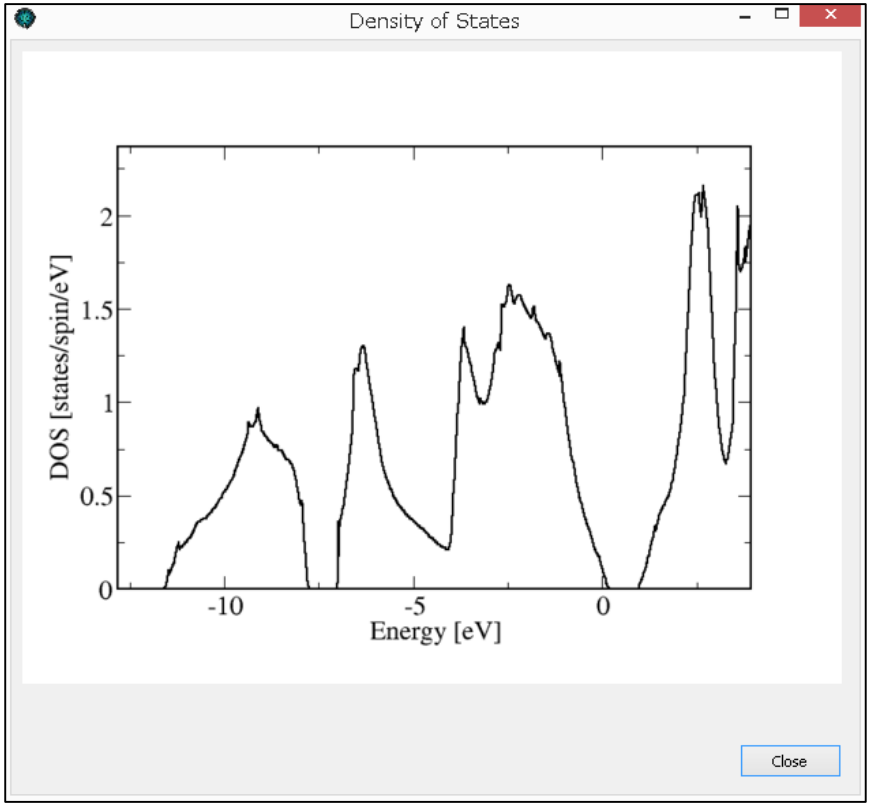
III. Density of States

1. After the calculation, click **Solid | Quantum ESPRESSO | Density of States**.
2. Select the default set folder.





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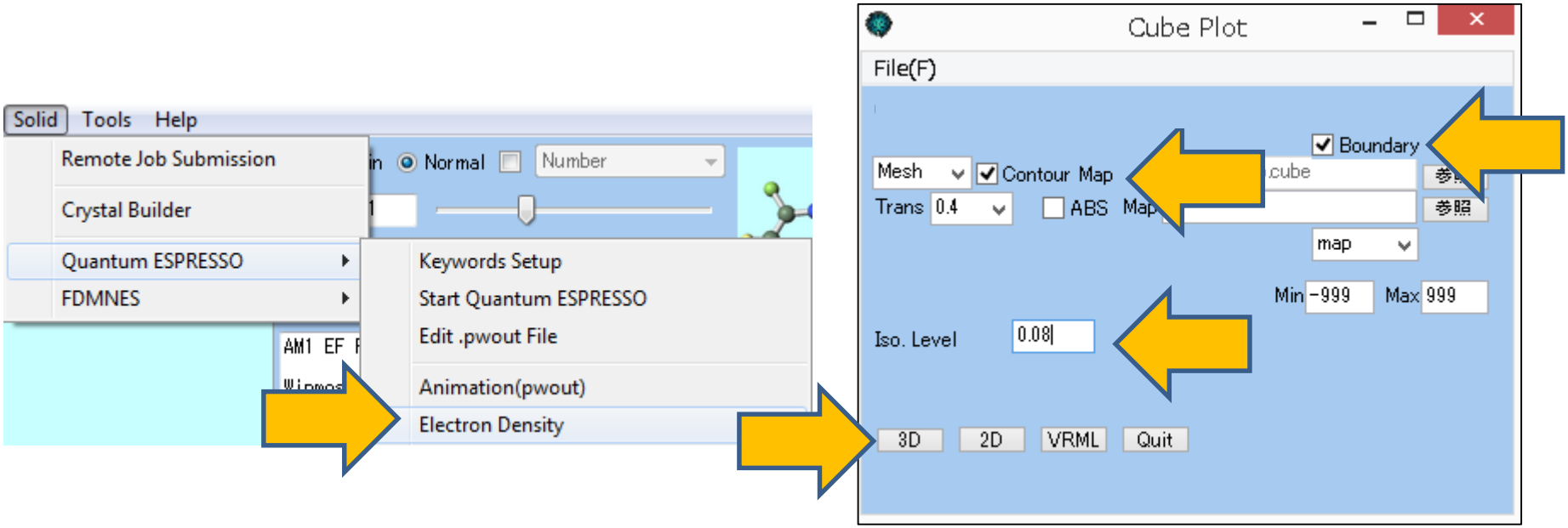
IV. Visualization of electron density

1. Click **Solid | Quantum ESPRESSO | Electron Density**.
2. Select a default folder.
3. Check **Contour Map** and **Boundary**. Input **Iso. Level** = **0.08**.
4. Click **3D**.



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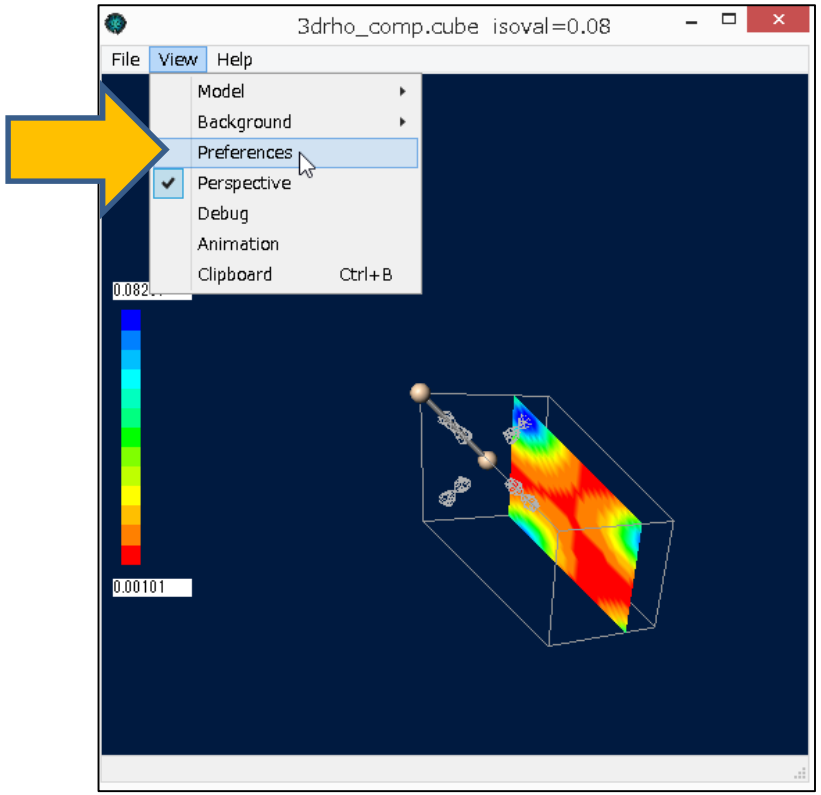
IV. Visualization of electron density

1. Visualization window will appear.
2. Click **View | Preferences**.



The unit cell in this graphics is not **cubic** because the conventional cell was converted to the primitive cell to reduce computational costs.

You can avoid this conversion
if you uncheck **Automatically Detect ibrav**
in Quantum ESPRESSO keyword setting window.

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IV. Visualization of electron density

Move **X**, **Y** and **Z** slider to adjust the position of counter map.