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# Winmostar tutorial
## Quantum ESPRESSO
## Spin Polarization
V8.007

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2018/01/15

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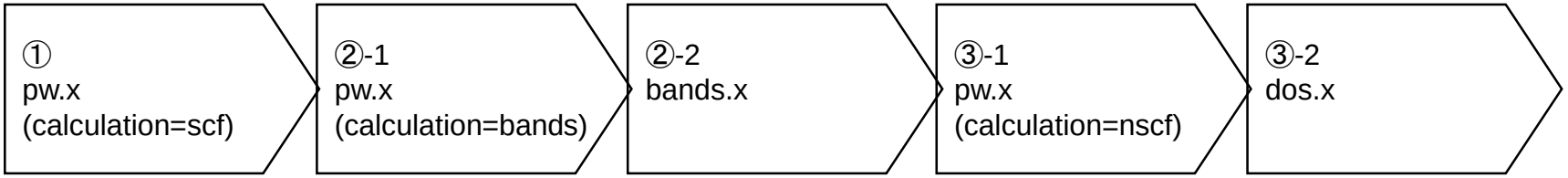
# Summary

- In this tutorial, we will perform SCF calculation on Fe crystal, then calculate the band structure and density of state (these processes will execute consecutively on Winmostar).




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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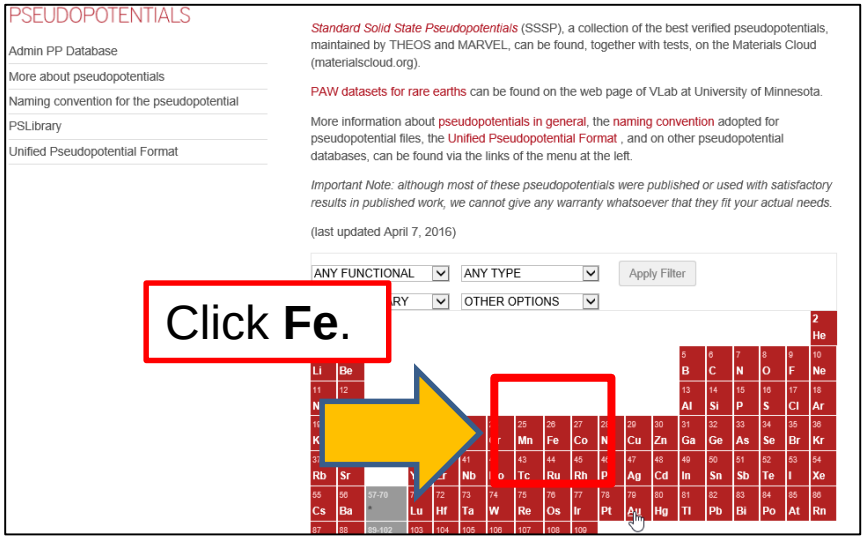
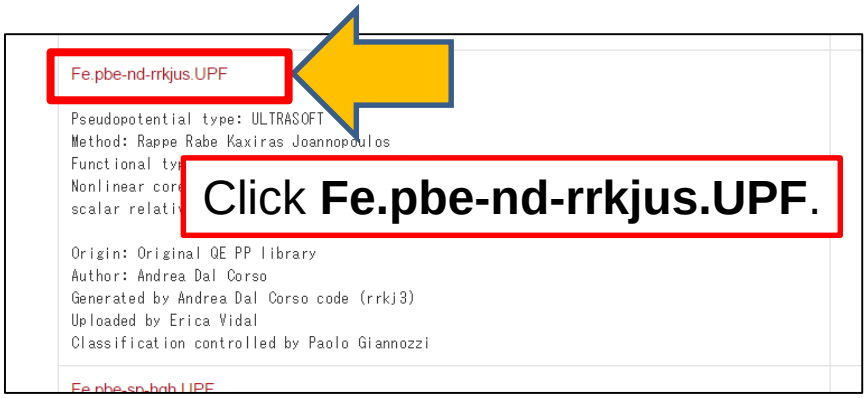
# Configuration

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

2. Via the following URL, download **Fe.pbe-nd-rrkjus.UPF** and move it into pseudo folder in Quantum ESPERSSO installation directory.
Then reopen Winmostar.
http://www.quantum-espresso.org/pseudopotentials/



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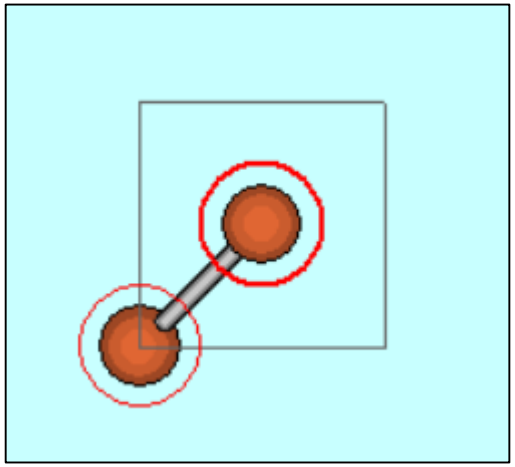
# I. Creating the Model

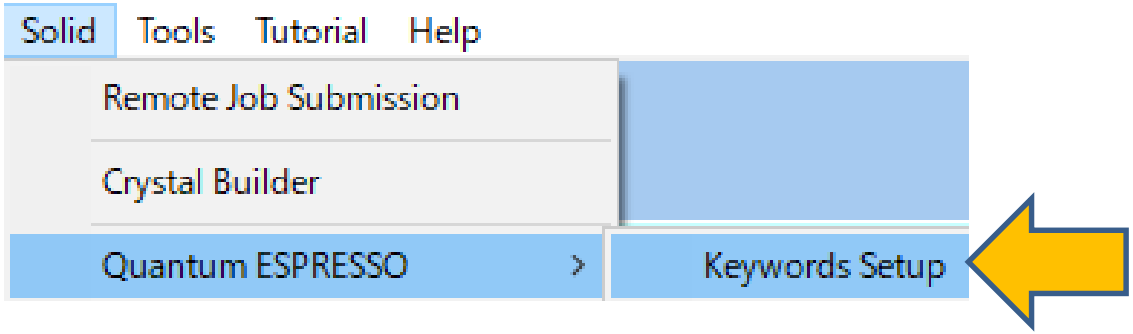
1. Click **File | Open**.
2. Open **fe.cif** in the sample directory. (C:¥winmos8¥samples¥fe.cif)

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

To make Fe unit cell
Crystal system: Cubic
Space group : Im-3m (229)
Lattice constants : a=2.8665 Å
Asymmetric unit: Fe (0.0 0.0 0.0)

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





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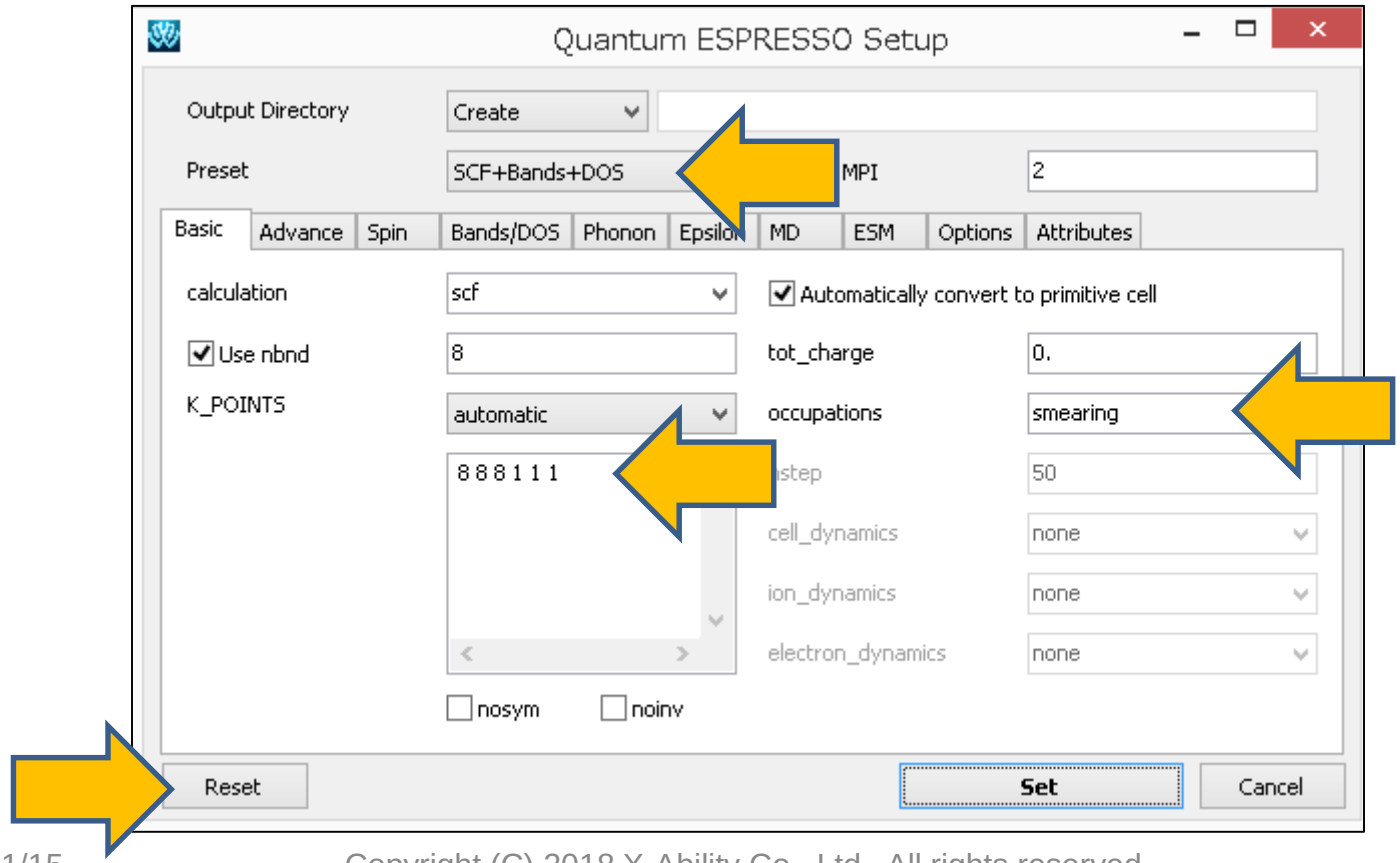
# II. QE Calculation

1. First click **Reset**. Set **Preset** to **SCF+Bands+DOS**.
2. In the text box under **K_POINTS**, enter "**8 8 8 1 1 1**" (space separated).
3. Set **occupations** to **smearing**.



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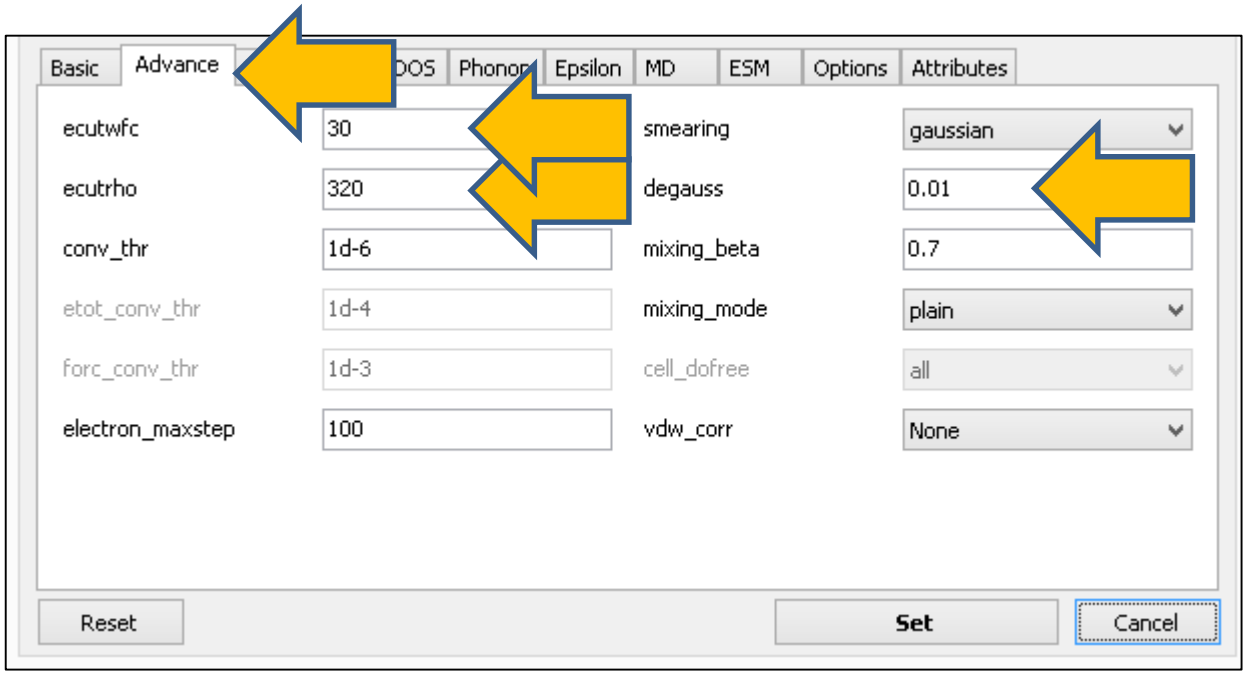
# II. QE Calculation

In the **Advance** tab, set **ecutwfc** (Cutoff Energy of Wave Function) to “**30**”, **ecutrho** (Charge Density) “**320**”, and **degauss** to “**0.01**”.



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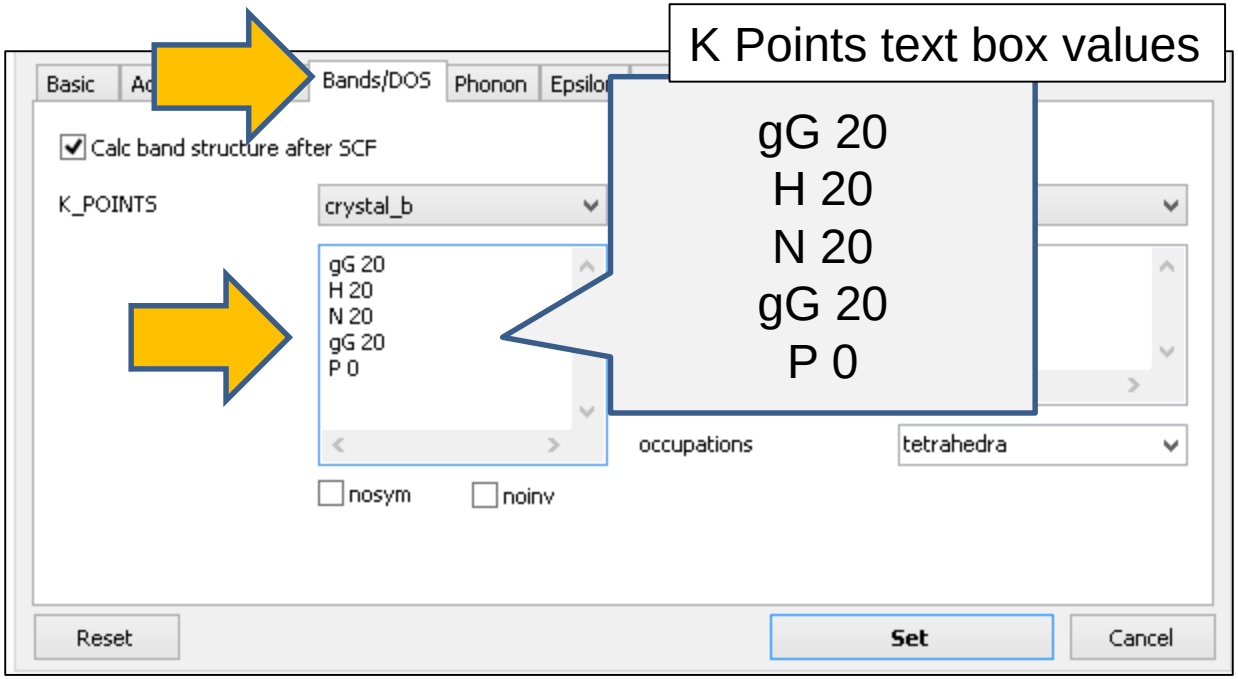
# II. QE Calculation

In the **Bands/DOS** tab, copy the values below in the text box under **K_POINTS**.



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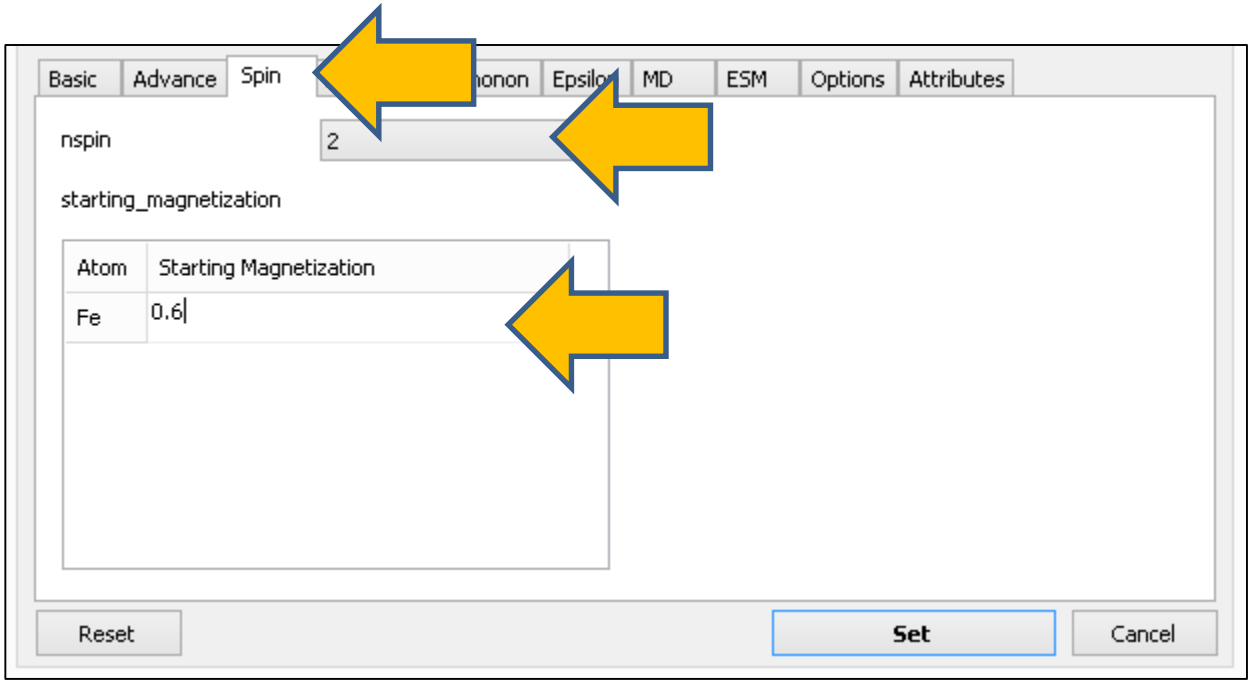
# II. QE Calculation

1. Click **Spin** tab.
2. Set **nspin** to **2**.
3. Set **Starting Magnetization** of **Fe** atom to **0.6**.



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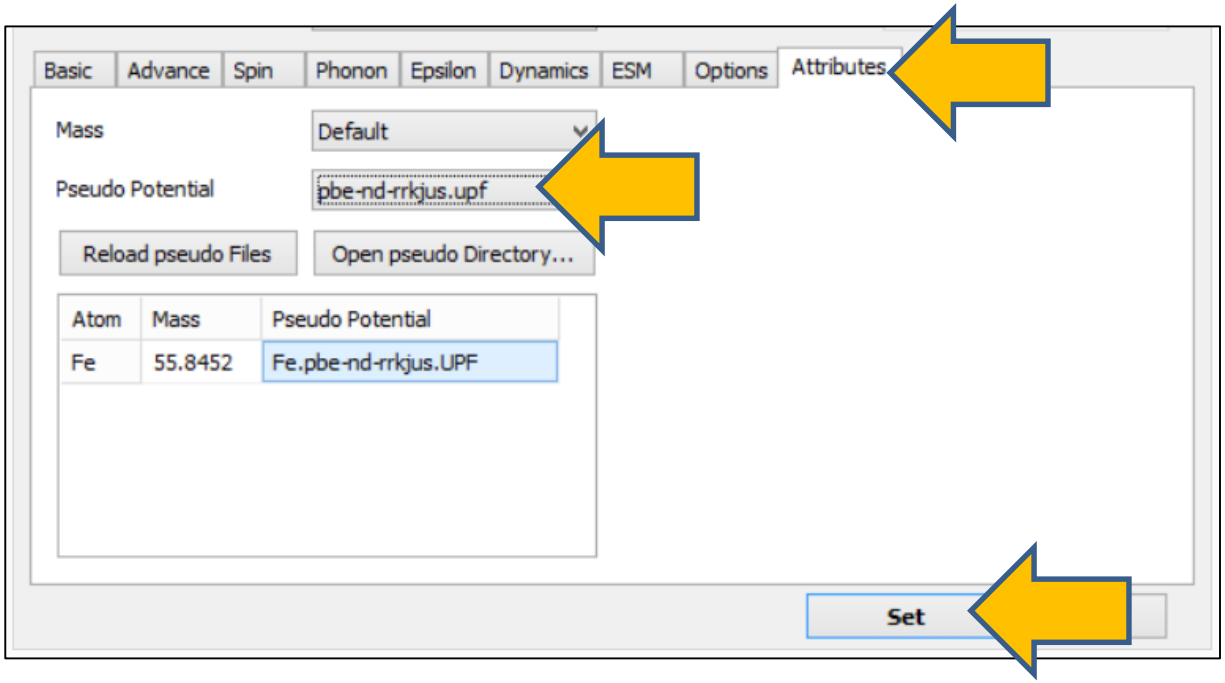
# II. QE Calculation

1. On **Attributes** tab, set **Pseudo Potential** to **pbe-nd-rrkjus.upf**.
2. Click **Set**.

If "pbe-nd-rrkjus.upf“ is not found, follow the instructions in Page 3 to save the pseudo file in pseudo folder. Then click **Reload pseudo Files**.



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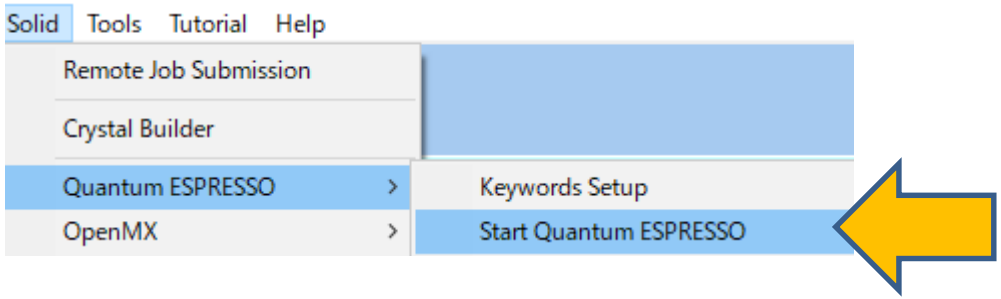
# II. QE Calculation

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



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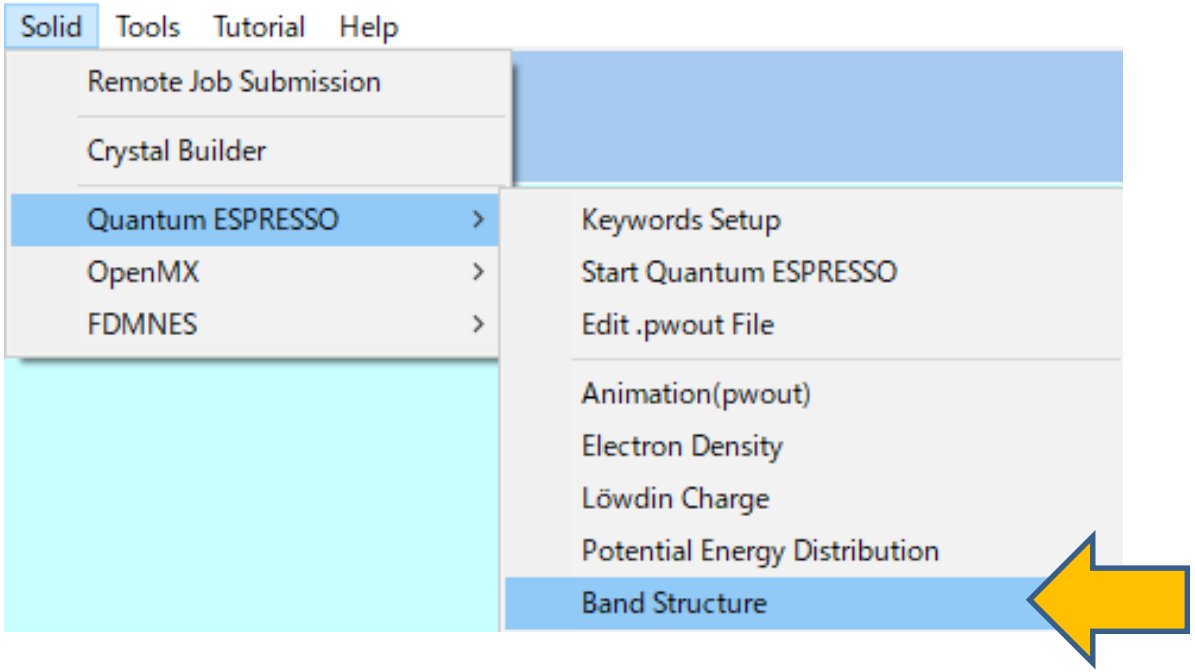
# III. Analysis

1. After the calculation, click **Solid** | **Quantum ESPRESSO** | **Band Structure**. Open directory and file suggested by default.



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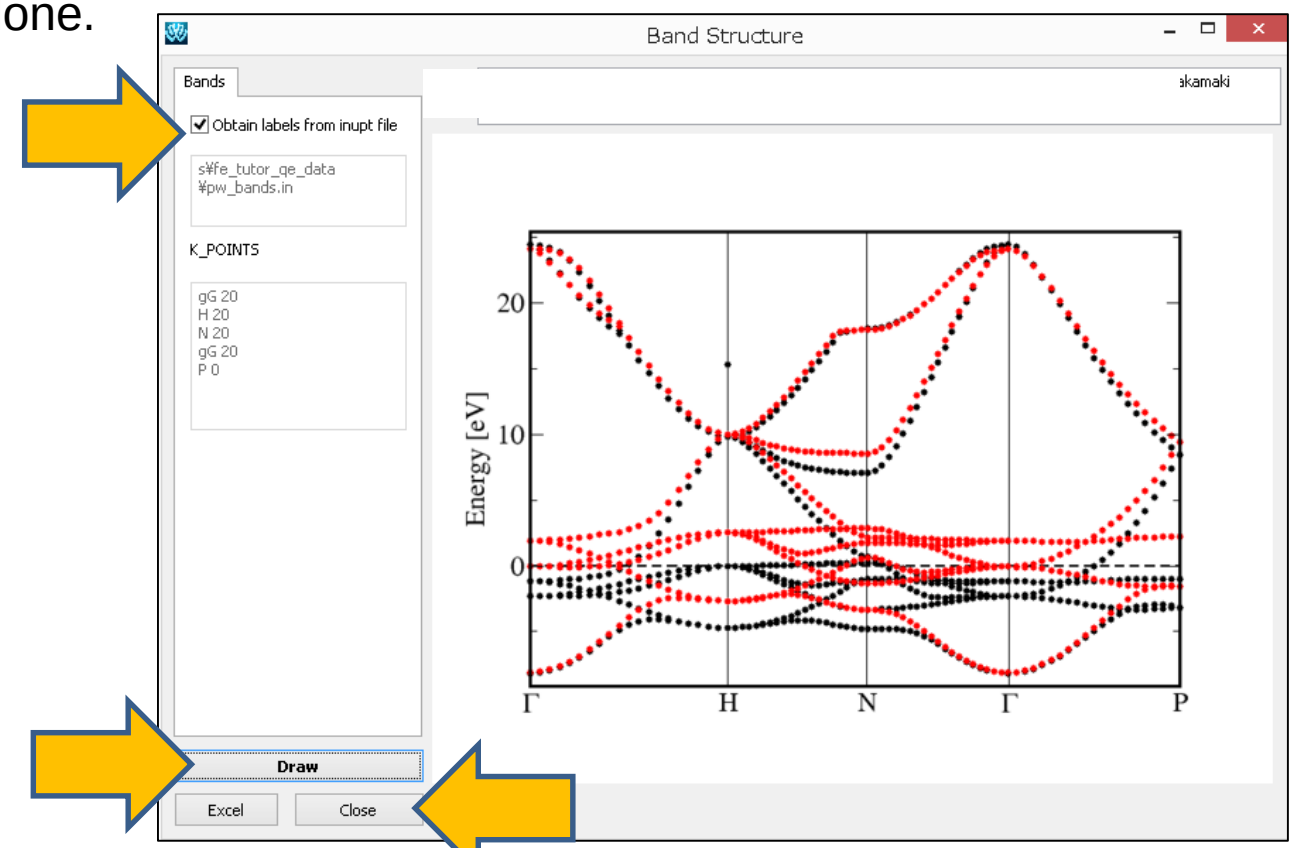
# III. Analysis

1. Check **Obtain labels from input file**.
2. Open file suggested by default.
3. Click **Draw** to draw the band structures of up and down spin. Click close when done.



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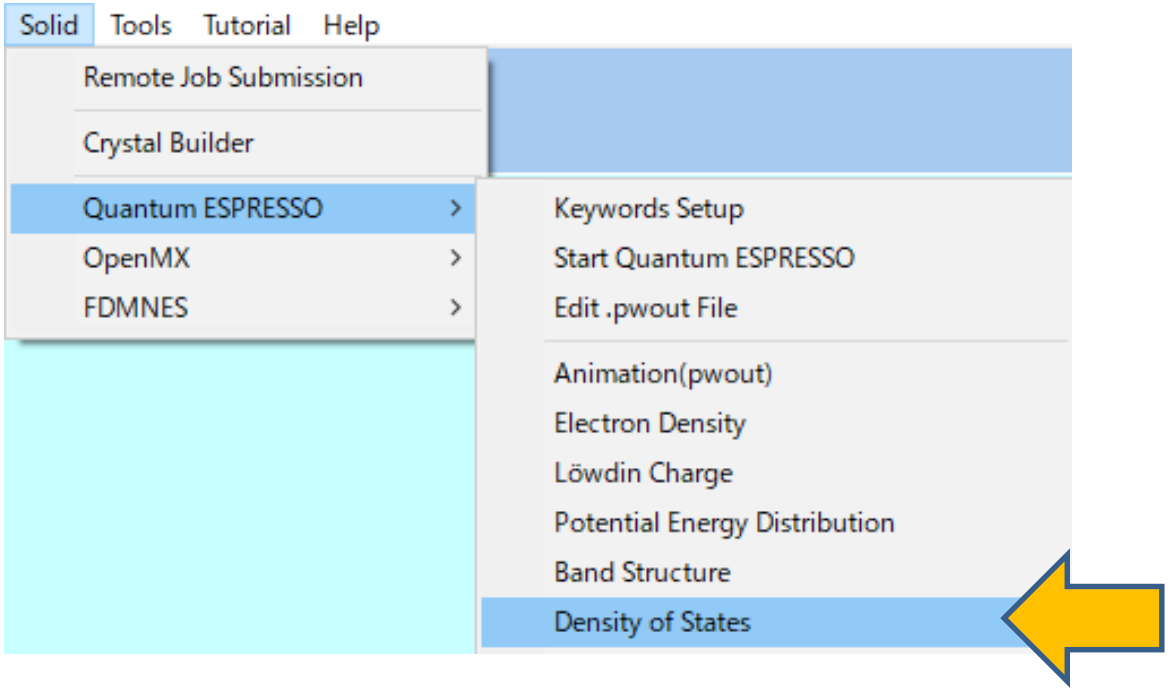
# III. Analysis

After the calculation, click **Solid** | **Quantum ESPRESSO** | **Density of States**. Open the directory and file suggested by default.



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# III. Analysis

Click **Draw** to draw DOS of up and down spin.