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Winmostar tutorial
Quantum ESPRESSO
Spin Polarization
V7.025

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Contents

I. SCF calculation
II. Bands calculation
III. Fermi surface

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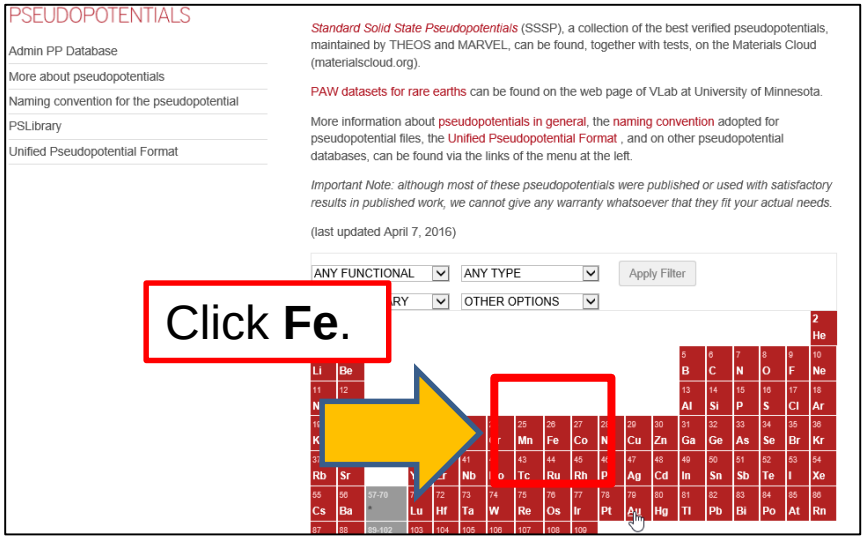
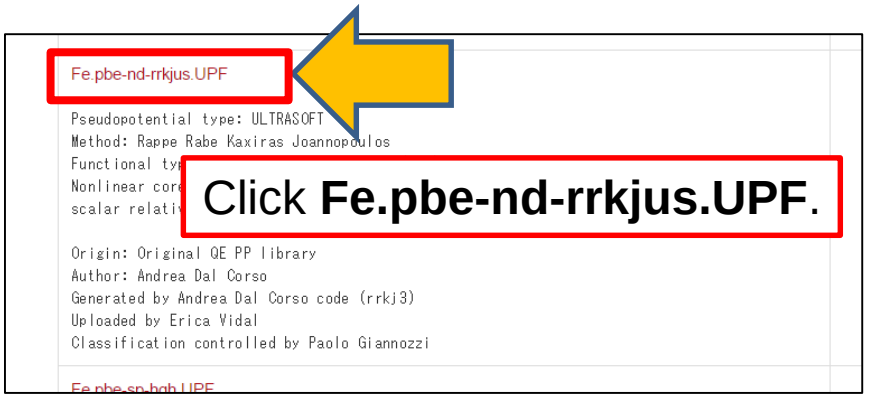
Environment setting

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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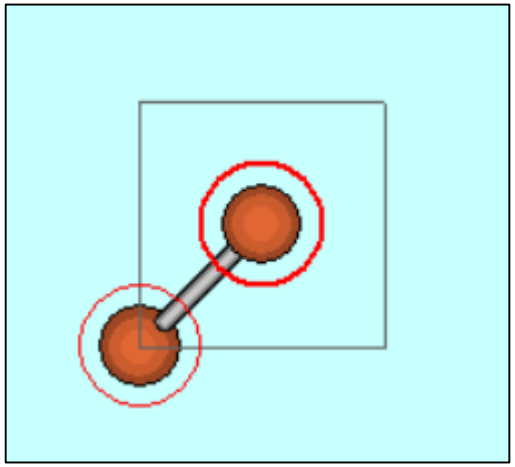
I. SCF calculation

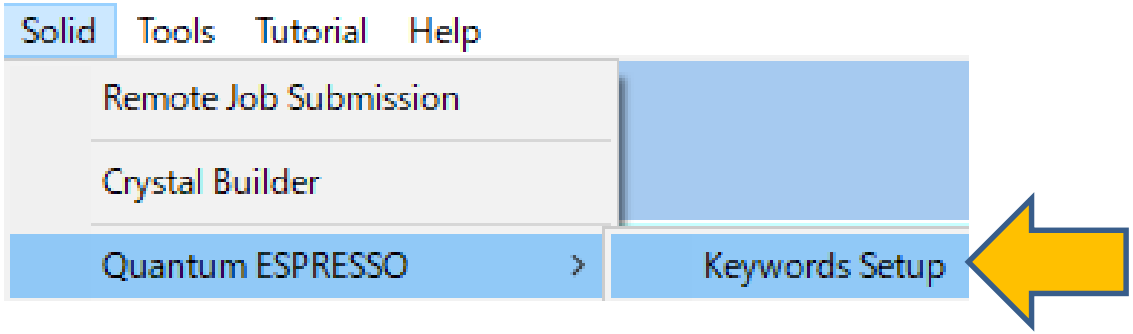
1. Click **File | Open**.
2. Open **fe.cif** in the sample directory. (C:¥winmos7¥samples¥fe.cif)

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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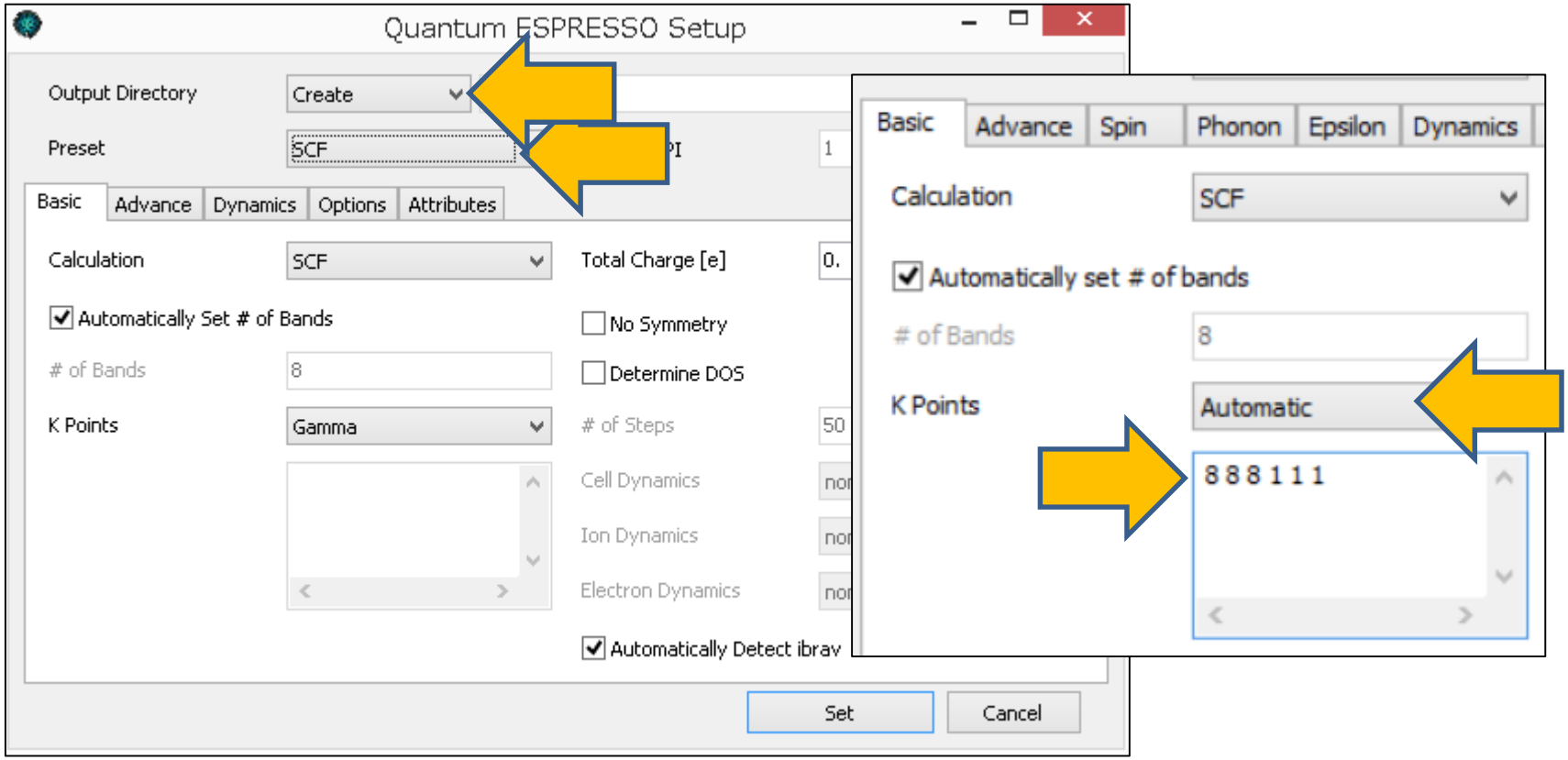
I. SCF calculation

1. Set **Output Directory** to **Create**, **Preset** to **SCF**.
2. Set **K Points** to **Automatic**, ”**8 8 8 1 1 1**”(space separated) below.



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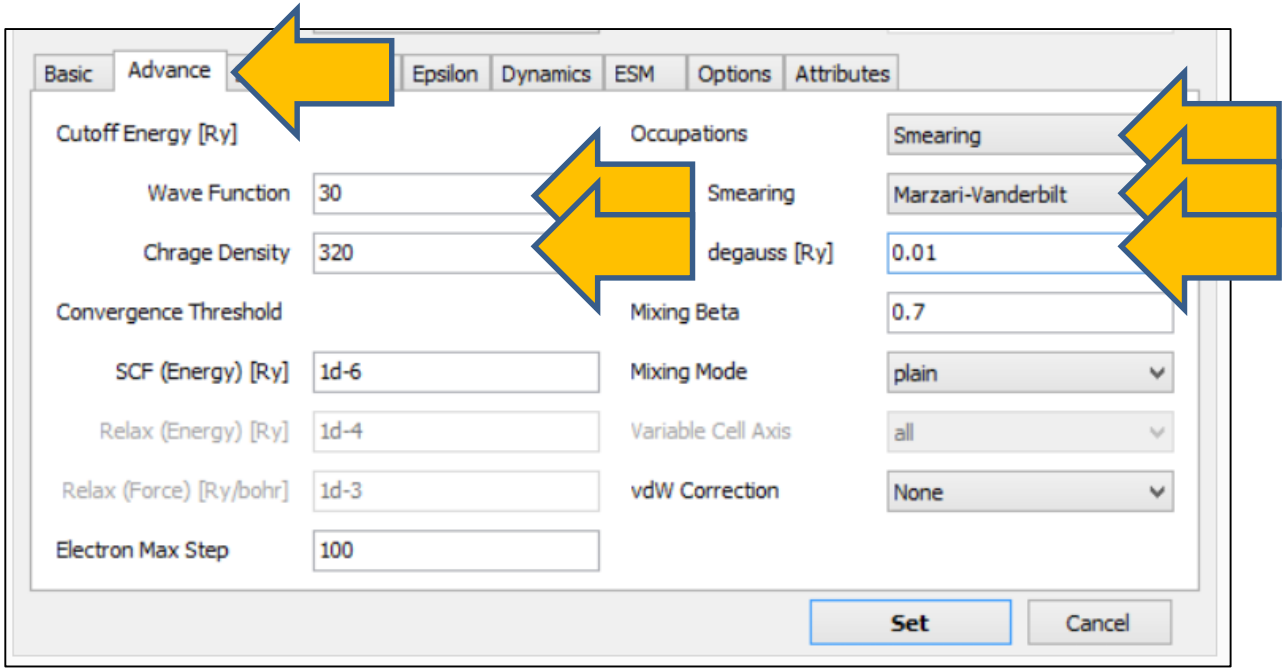
I. SCF calculation

1. Click On **Advance** tab.
2. Under **Cutoff Energy**, set **Wave Function** to **30**, **Charge Density** to **320**.
3. Set **Occupations** to **Smearing**, **Smearing** to **Marzari-Vanderbilt**, **degauss** to **0.01**.



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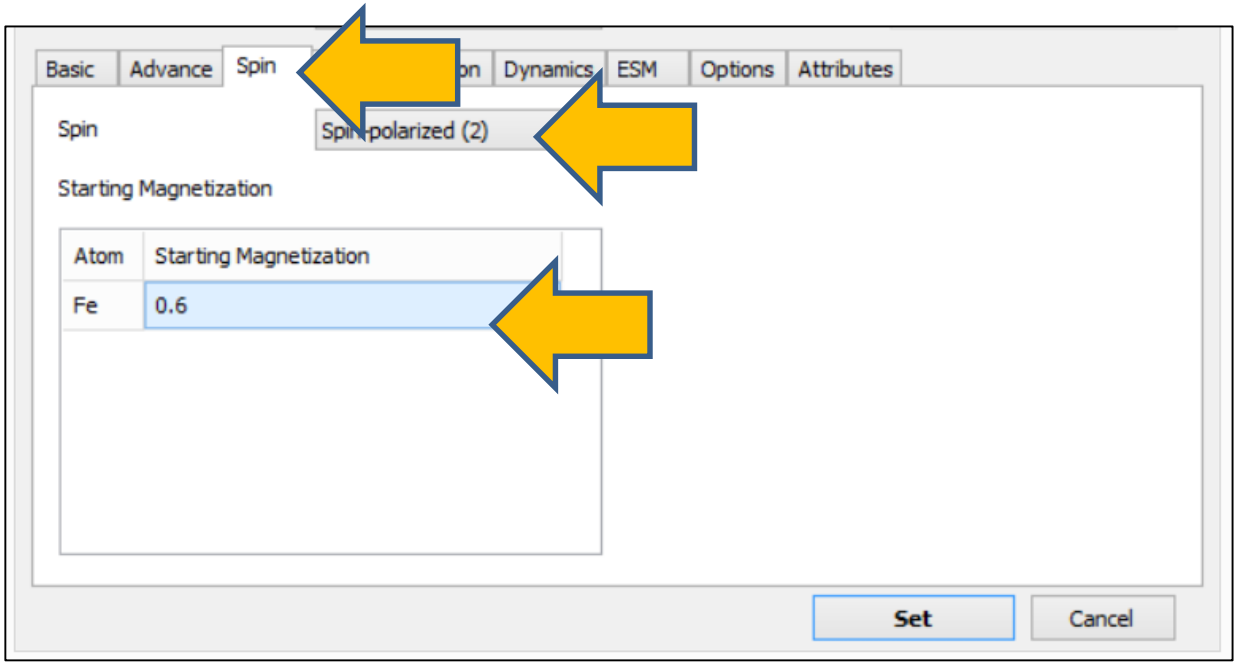
I. SCF calculation

1. Click **Spin** tab.
2. Set **Spin** to **Spin-polarized (2)**.
3. Set **Starting Magnetization** of **Fe** atom to **0.6**.



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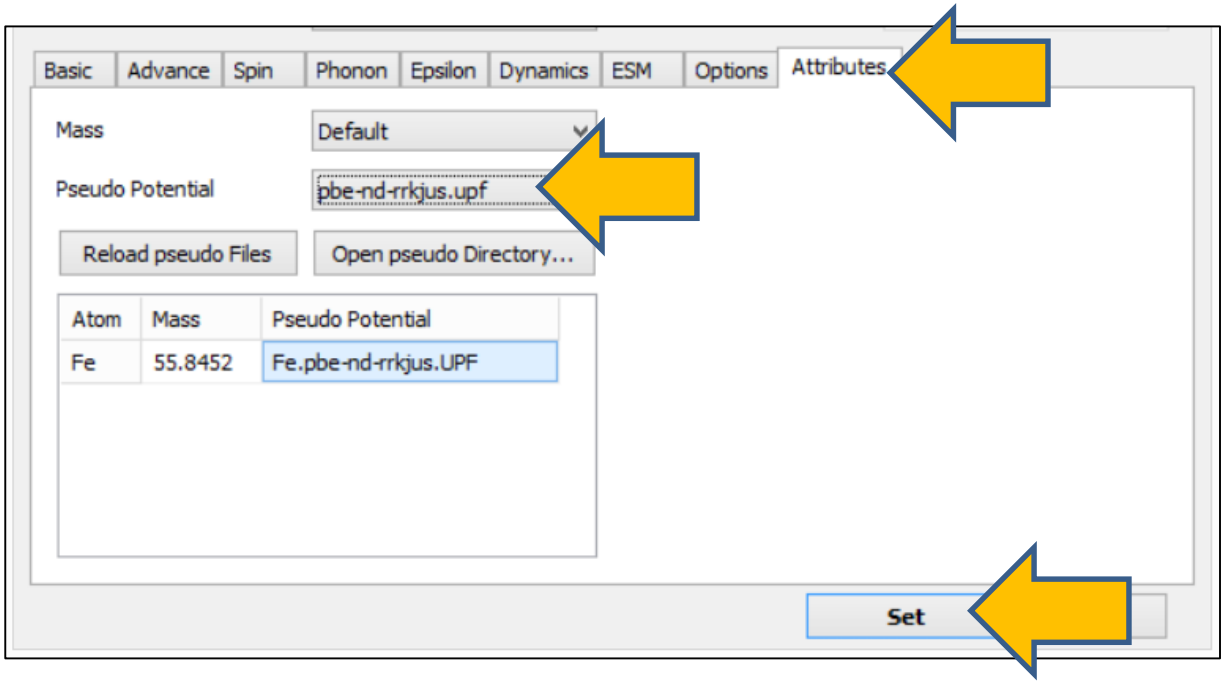
I. SCF calculation

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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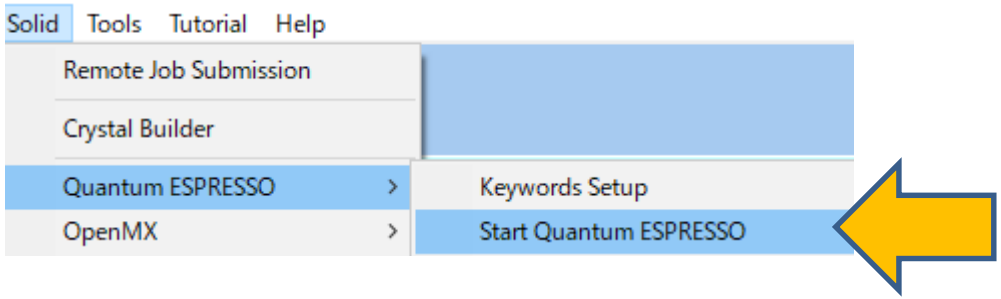
I. SCF calculation

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



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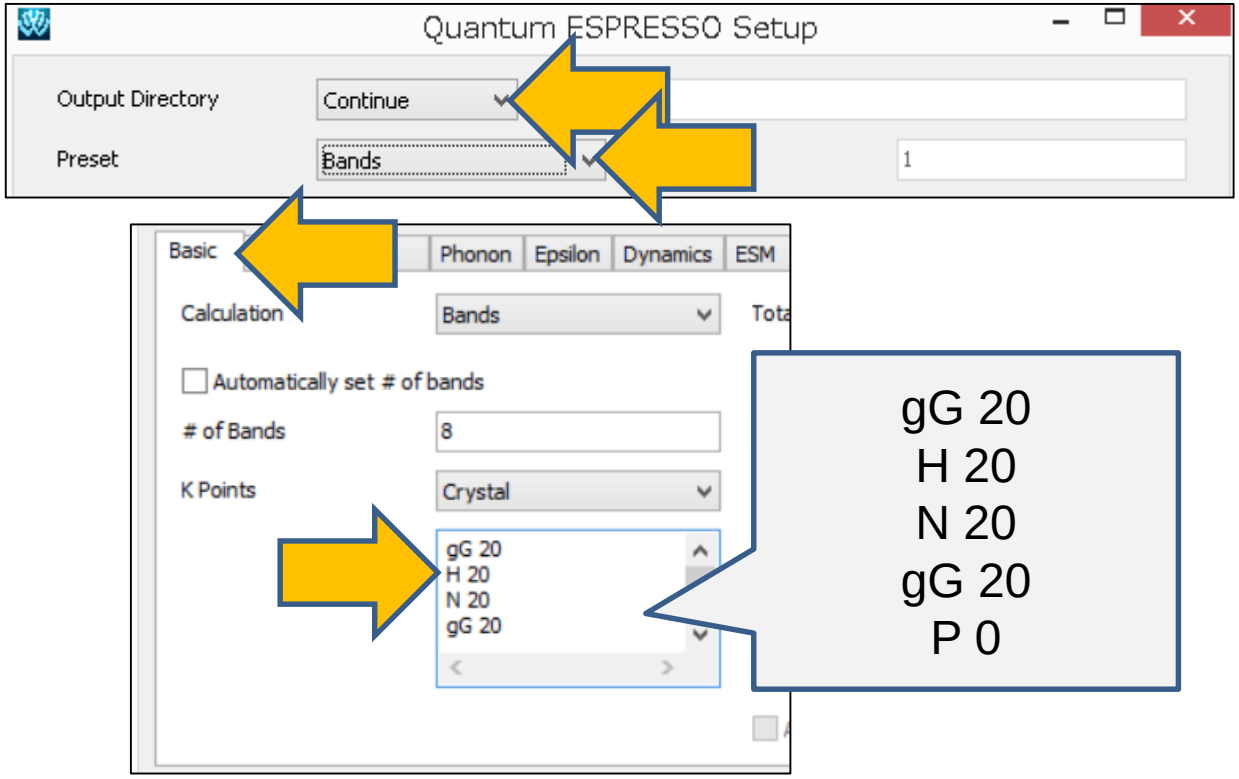
II. Bands calculation

1. After the calculation, click **Solid** | **Quantum ESPRESSO** | **Keywords Setup**.
2. Set **Output Directory** to **Continue**, **Preset** to **Bands**.
3. On **Basic** tab, set **K Points** as shown below.



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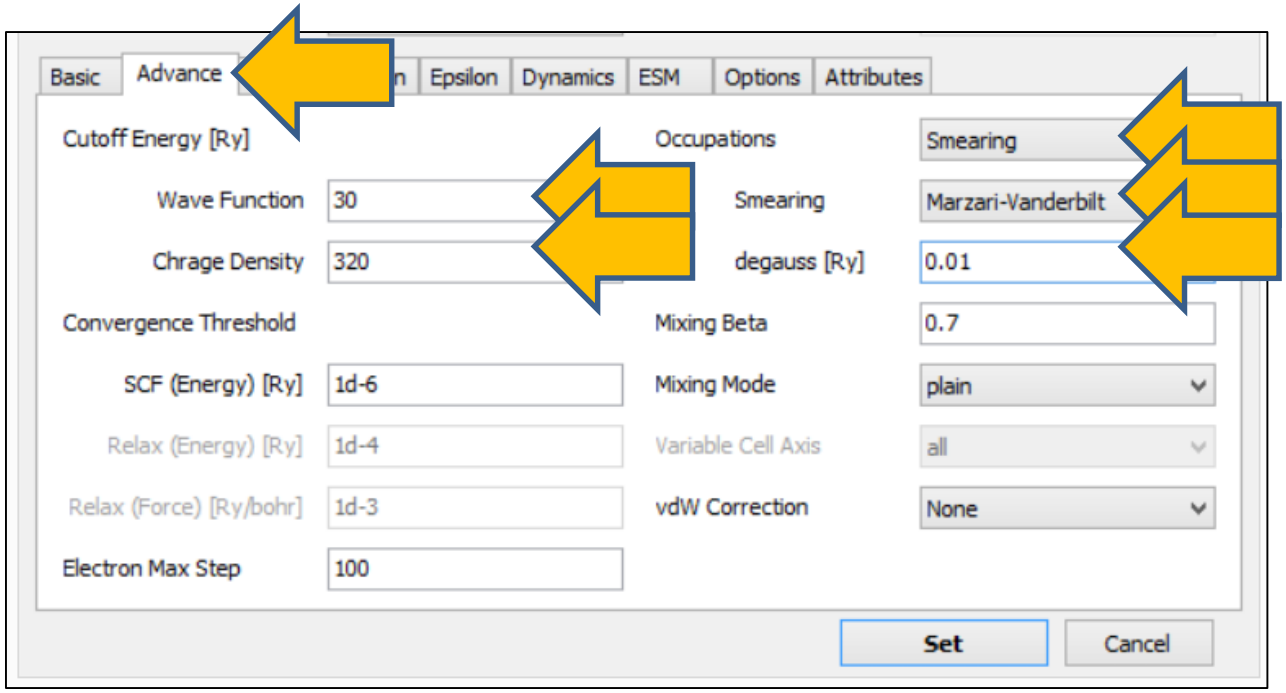
II. Bands calculation

1. Click **Advance** tab.
2. On **Cutoff Energy**, set **Wave Function** to **30**, **Charge Density** to **320**.
3. Set **Occupations** to **Smearing**, **Smearing** to **Marzari-Vanderbilt**, **degauss** to **0.01**.



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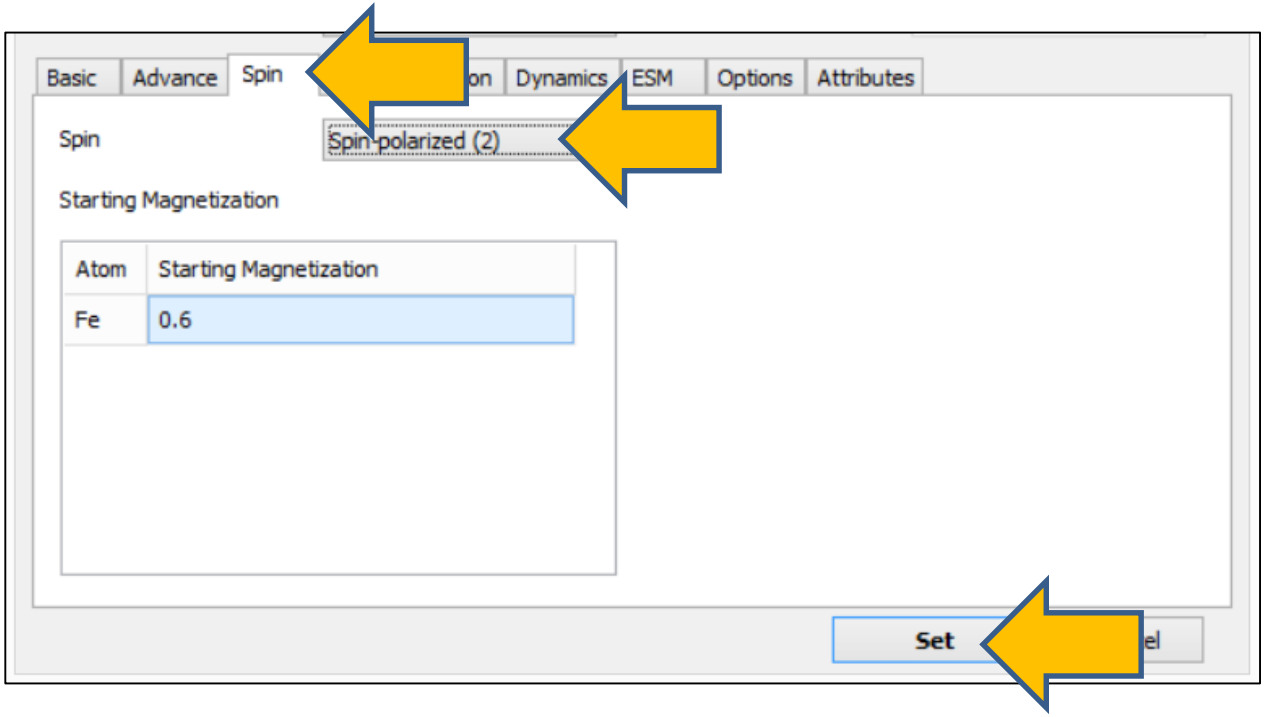
II. Bands calculation

1. On **Spin** tab, set **Spin** to **Spin-polarized (2)**.
2. Click **Set**.



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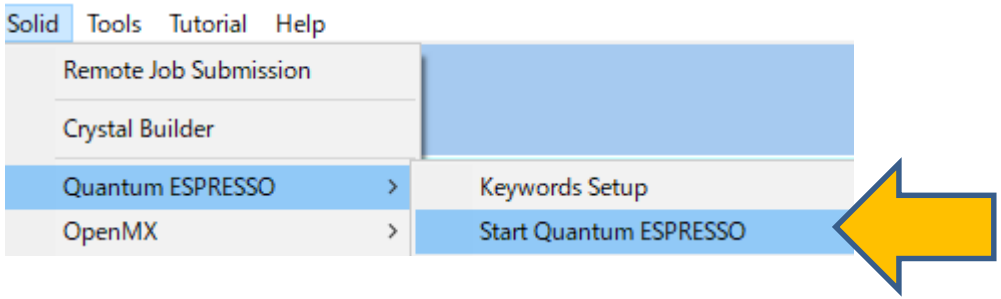
II. Bands calculation

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



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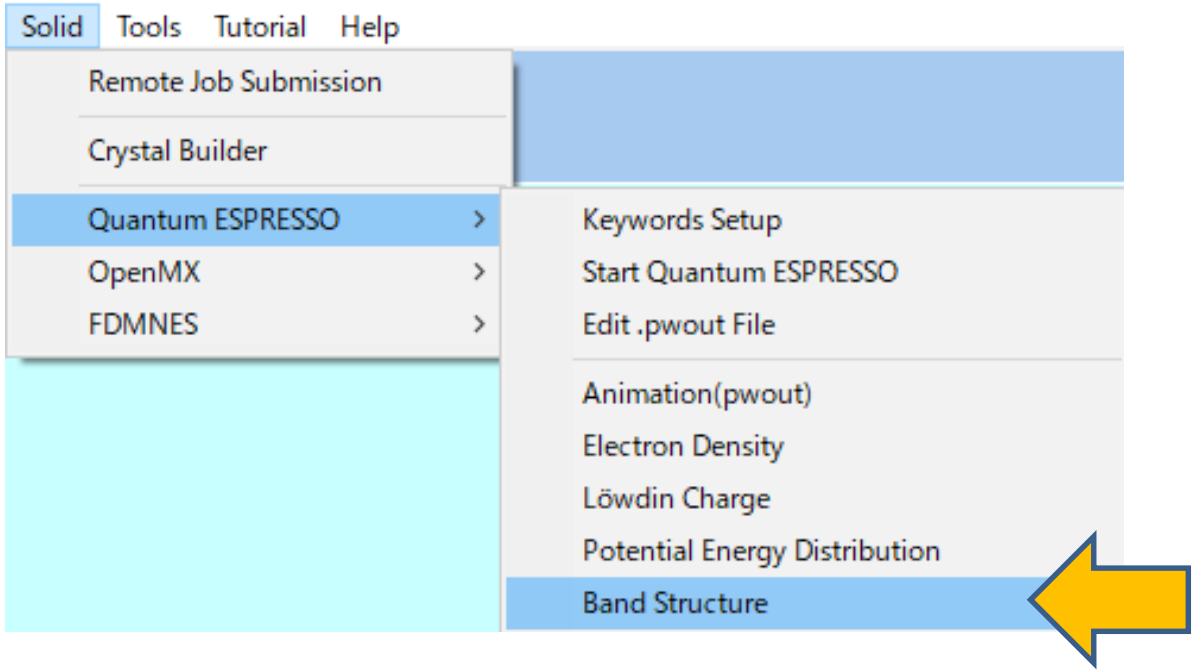
II. Bands calculation

1. Click **Solid** | **Quantum ESPRESSO** | **Band Structure**.
2. Select the output directory, **fe_scf_qe_data**, then click **OK**.
3. Select the output file of SCF calculation, **fe_scf.pwout**.



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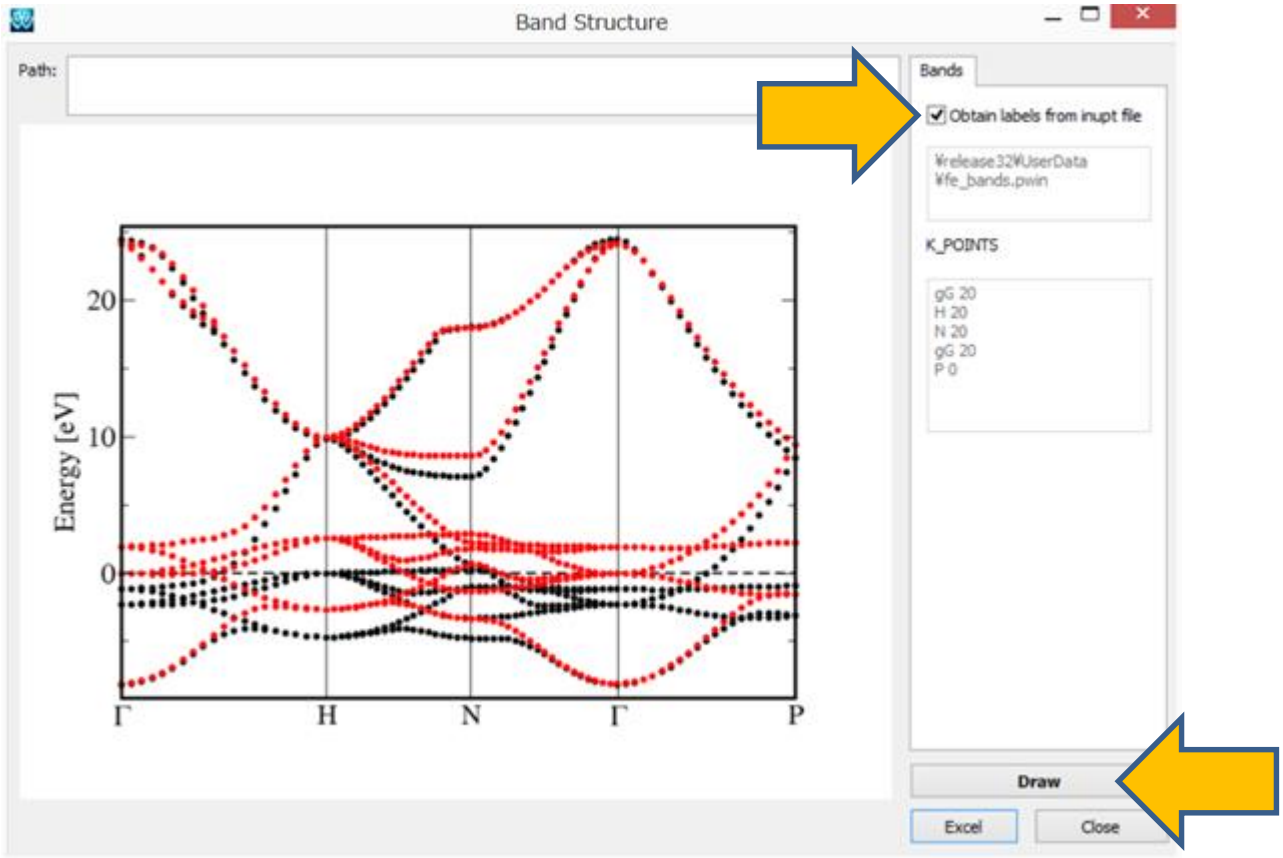
II. Bands calculation

1. Check **obtain labels from input file**.
2. Select the input file, **fe_bands.pwin**.
3. Click **Draw** to draw the band structures of up and down spin.



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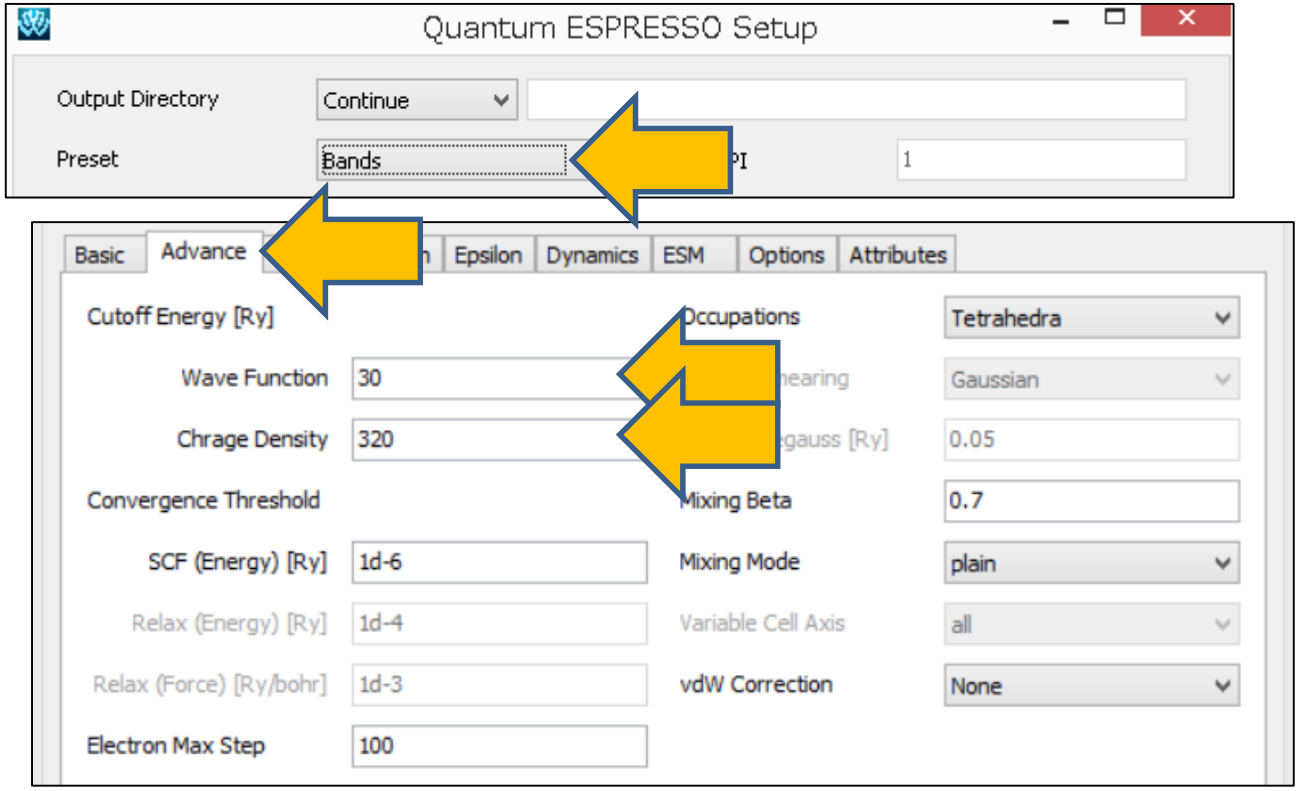
III. DOS calculation

1. Click **Solid** | **Quantum ESPRESSO** | **Keywords Setup**.
2. Set **Preset** to **DOS**.
3. On **Advance** tab, set **Wave Function** to **30**, **Charge Density** to **320**.



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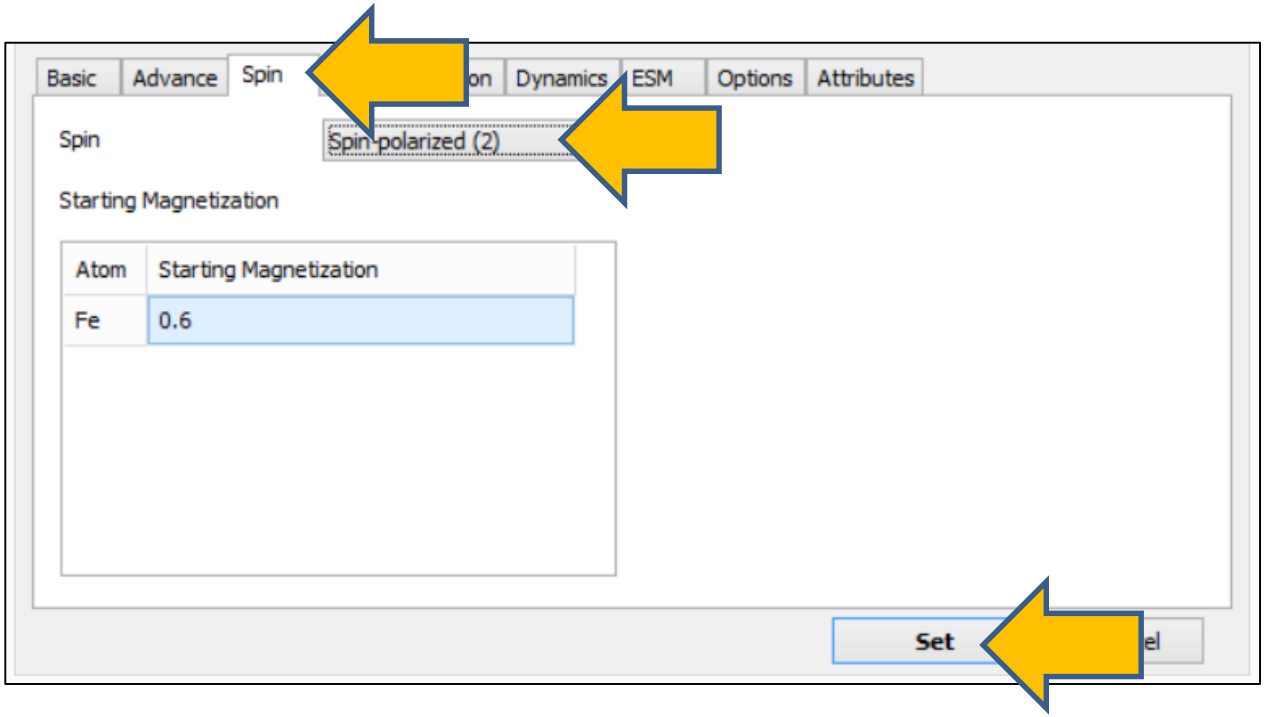
III. DOS calculation

1. On **Spin** tab, select **Spin** to **Spin-polarized (2)**.
2. Click **Set**.



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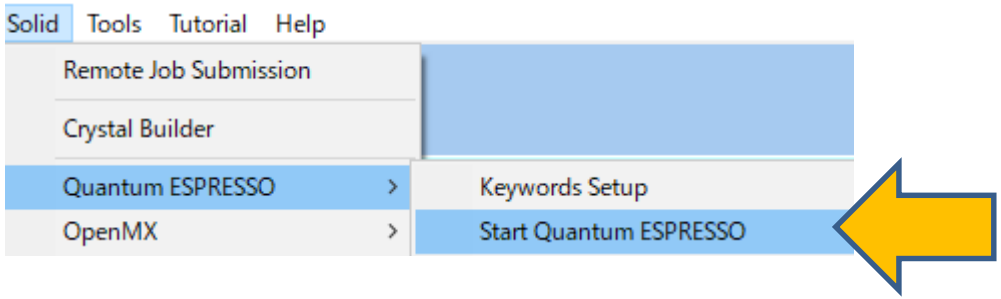
III. DOS calculation

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



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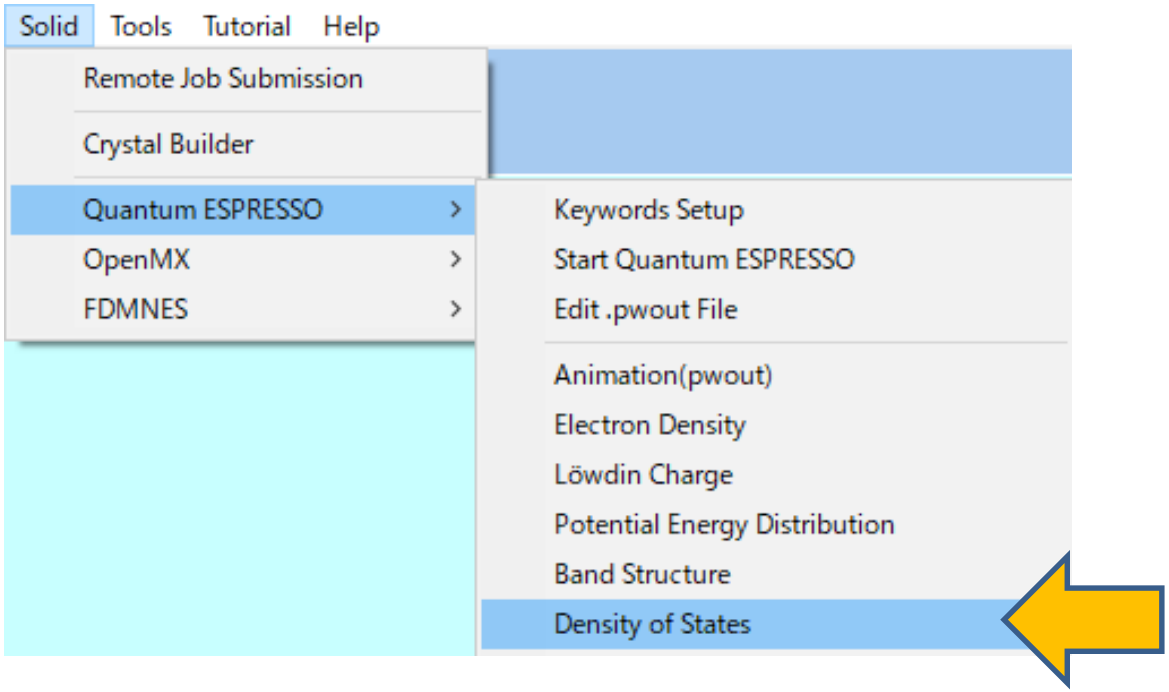
III. DOS calculation

1. Click **Solid** | **Quantum ESPRESSO** | **Band Structure**.
2. Select the output directory, **fe_scf_qe_data**, then click **OK**.
3. Select the output file of SCF calculation, **fe_scf.pwout**, then click **OK**.



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III. DOS calculation

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