

# Winmostar tutorial

## Quantum ESPRESSO

### Spin Polarization

V7.025

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# Contents

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

# Environment setting

1. See Quantum ESPRESSO install manual

[https://winmostar.com/en/QE\\_install\\_manual\\_en\\_win.pdf](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 ESPRESSO installation directory.  
Then reopen Winmostar.

<http://www.quantum-espresso.org/pseudopotentials/>

**PSEUDOPOTENTIALS**

Admin PP Database  
More about pseudopotentials  
Naming convention for the pseudopotential  
PSLibrary  
Unified Pseudopotential Format

*Standard Solid State Pseudopotentials (SSSP), a collection of the best verified pseudopotentials, maintained by THEOS and MARVEL, can be found, together with tests, on the Materials Cloud (materialscloud.org).*

*PAW datasets for rare earths can be found on the web page of VLab at University of Minnesota.*

More information about **pseudopotentials in general**, the **naming convention** adopted for pseudopotential files, the **Unified Pseudopotential Format**, and on other pseudopotential databases, can be found via the links of the menu at the left.

*Important Note: although most of these pseudopotentials were published or used with satisfactory results in published work, we cannot give any warranty whatsoever that they fit your actual needs.*

(last updated April 7, 2016)

ANY FUNCTIONAL  ANY TYPE  Apply Filter

OTHER OPTIONS

**Click Fe.**

**Fe.pbe-nd-rrkjus.UPF**

Pseudopotential type: ULTRASOFT  
Method: Rappe Rabe Kaxiras Joannopoulos  
Functional type:  
Nonlinear core  
scalar relativistic

**Click Fe.pbe-nd-rrkjus.UPF.**

Origin: Original QE PP library  
Author: Andrea Dal Corso  
Generated by Andrea Dal Corso code (rrkj3)  
Uploaded by Erica Vidal  
Classification controlled by Paolo Giannozzi

Fe.pbe-nd-rrkjus.UPF

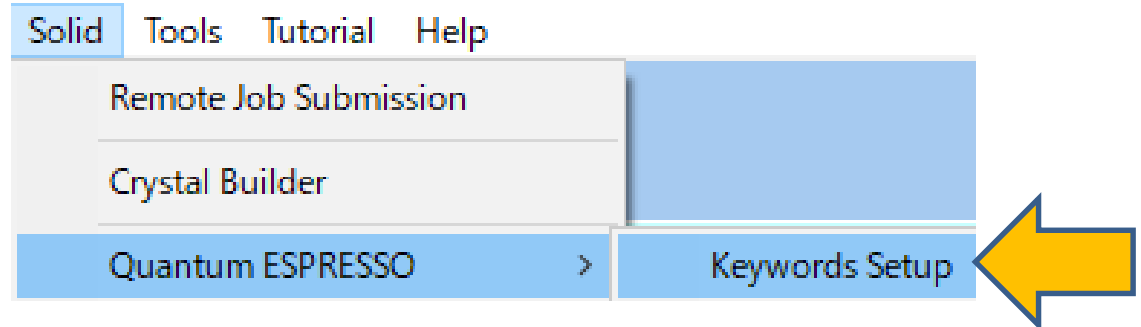
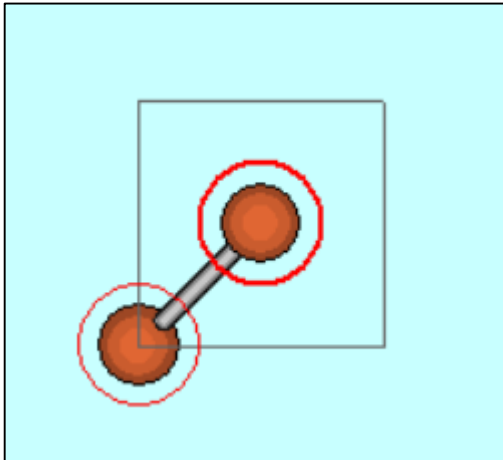
# I. SCF calculation

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.

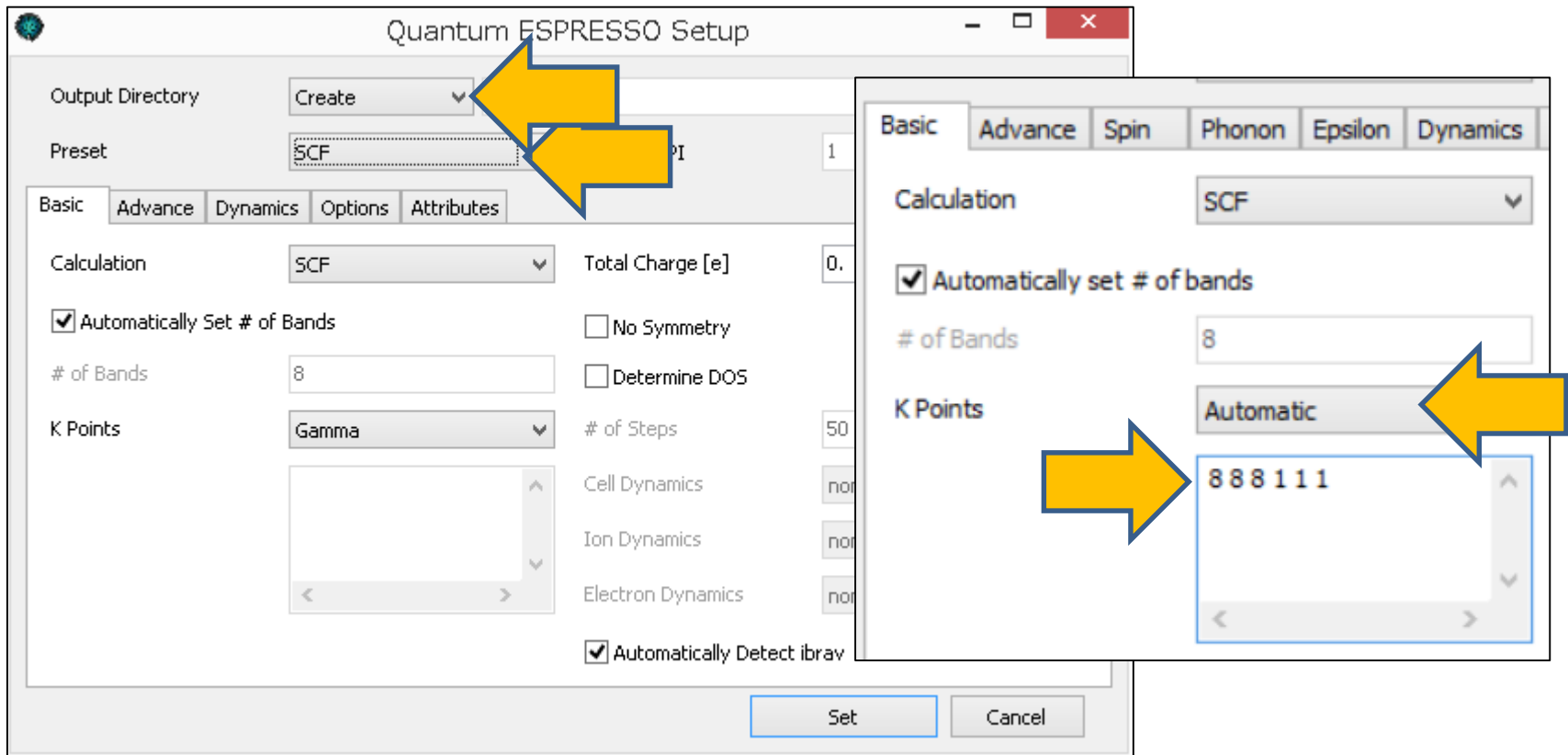
To make Fe unit cell  
Crystal system: Cubic  
Space group : Im-3m (229)  
Lattice constants : a=2.8665 Å  
Asymmetric unit: Fe (0.0 0.0 0.0)

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



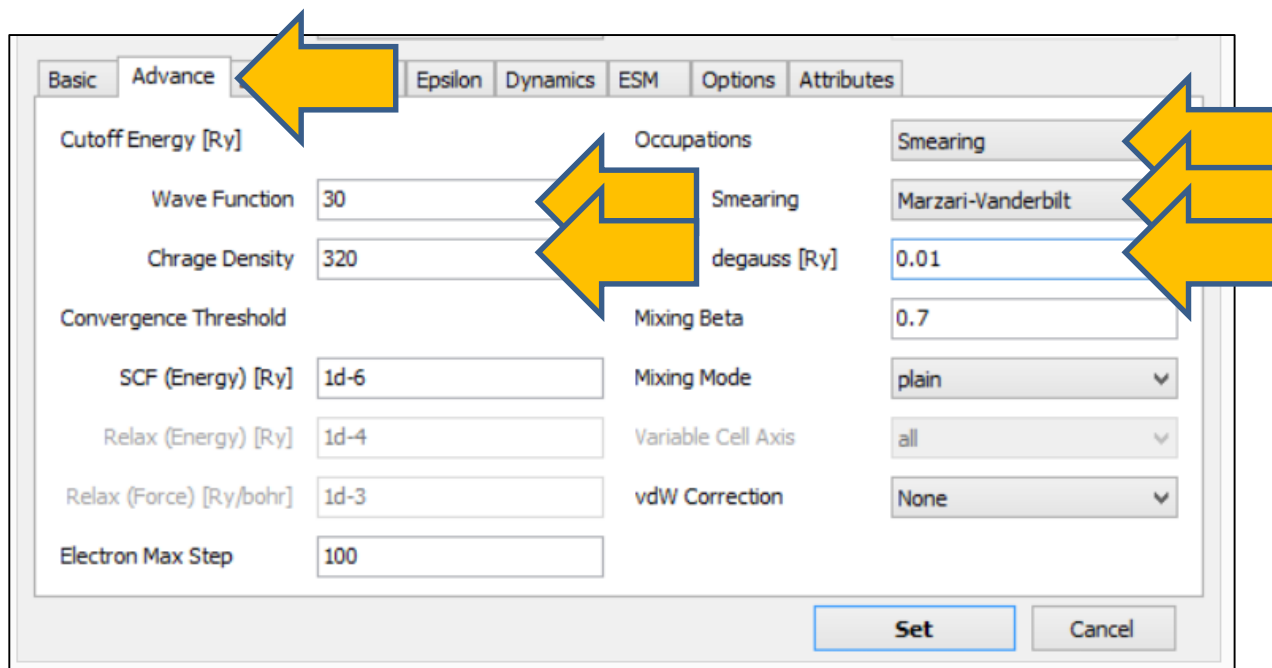
# I. SCF calculation

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



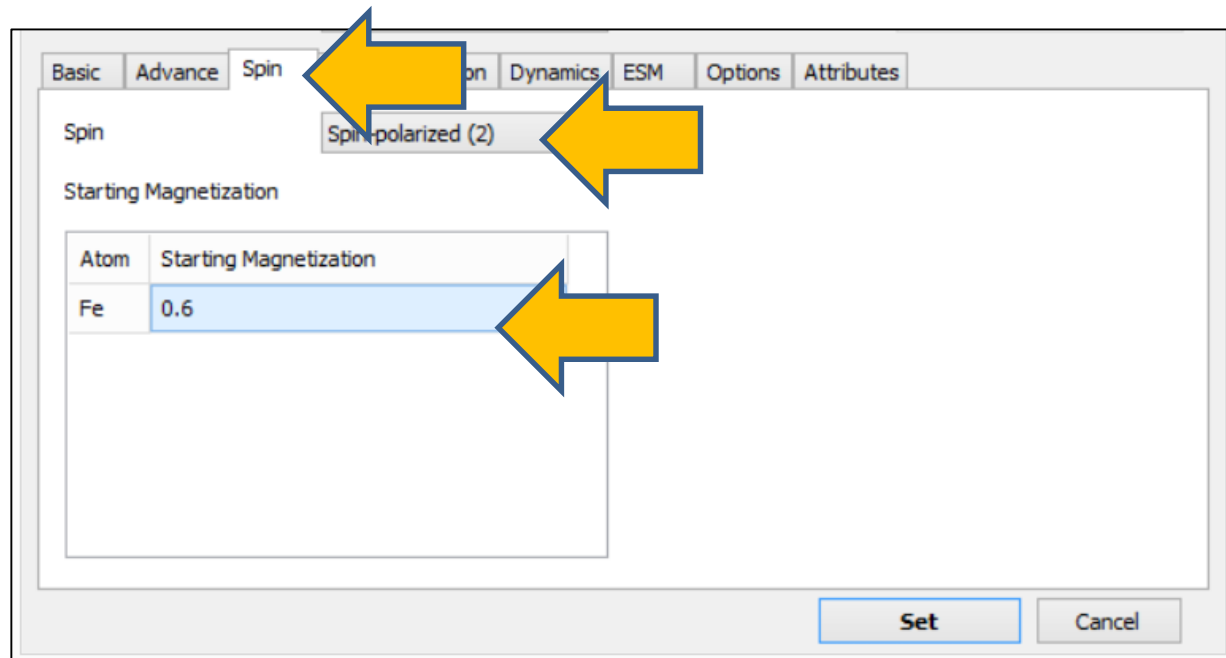
# I. SCF calculation

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**.



# I. SCF calculation

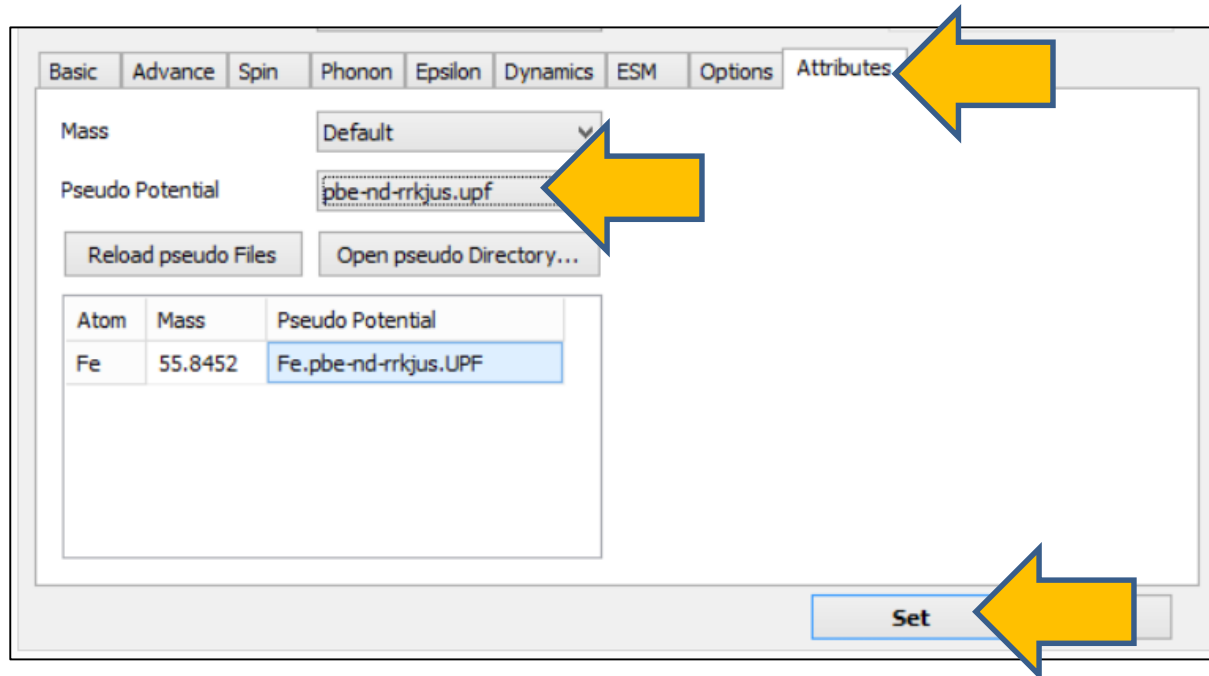
1. Click **Spin** tab.
2. Set **Spin** to **Spin-polarized (2)**.
3. Set **Starting Magnetization** of **Fe** atom to **0.6**.



# I. SCF calculation

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

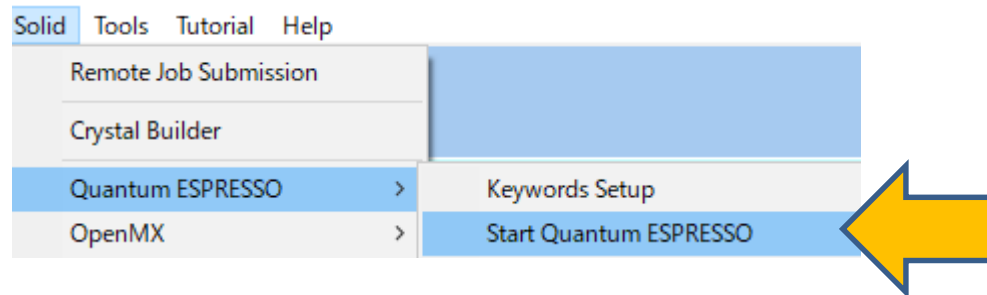
If "pbe-nd-rrkjus.upf" is not found, follow the instructions in Page 3 to save the pseudo file in pseudo folder. Then click **Reload pseudo Files**.





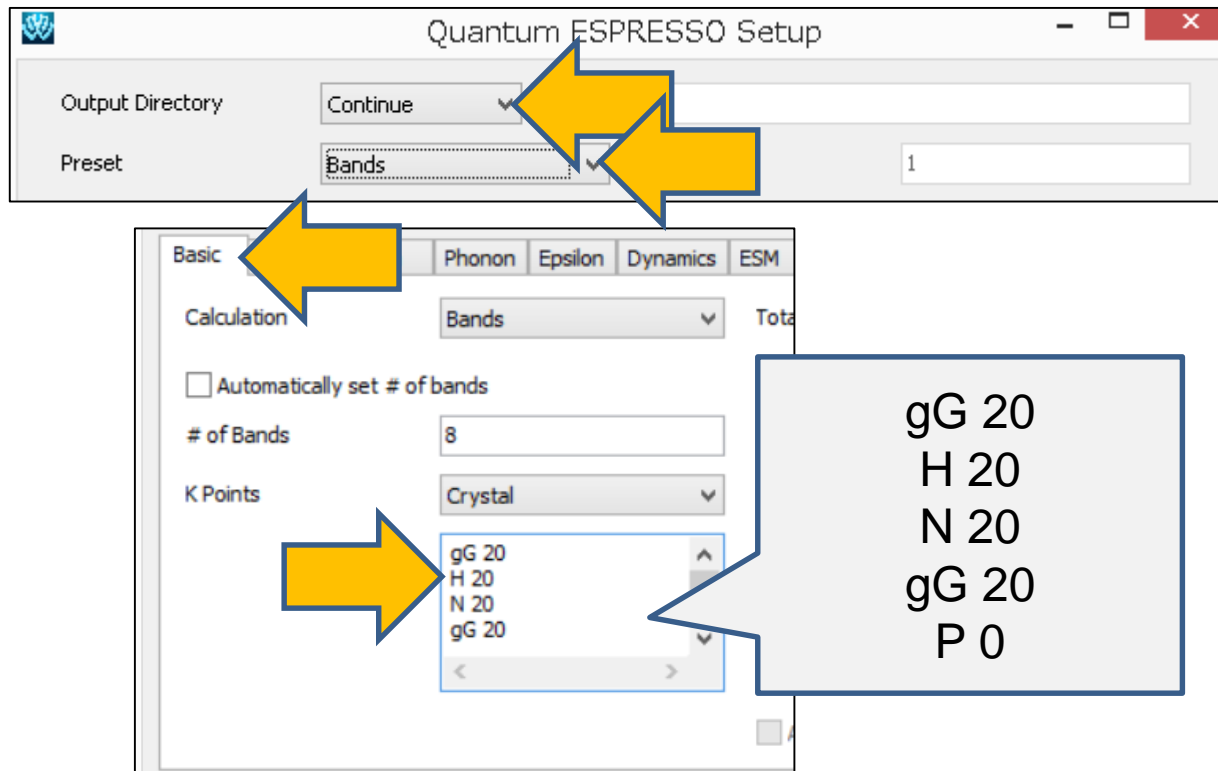
# I. SCF calculation

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. Save as **fe\_scf.pwin**.



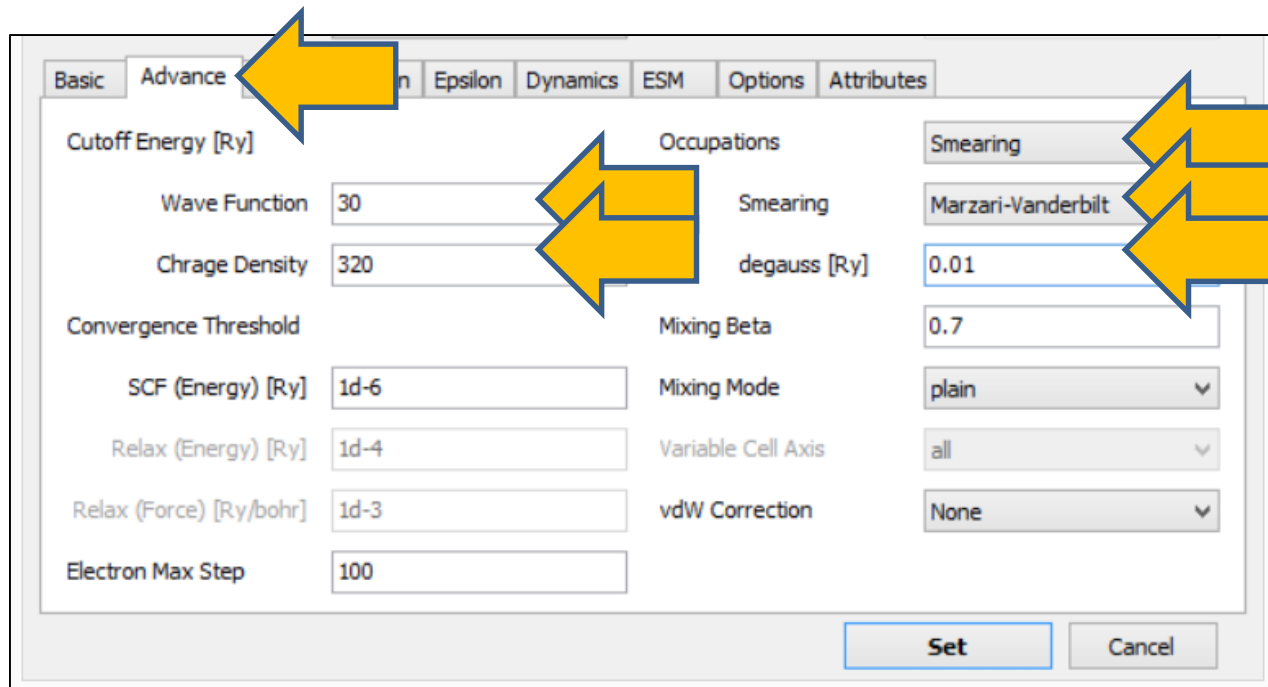
## II. Bands calculation

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.



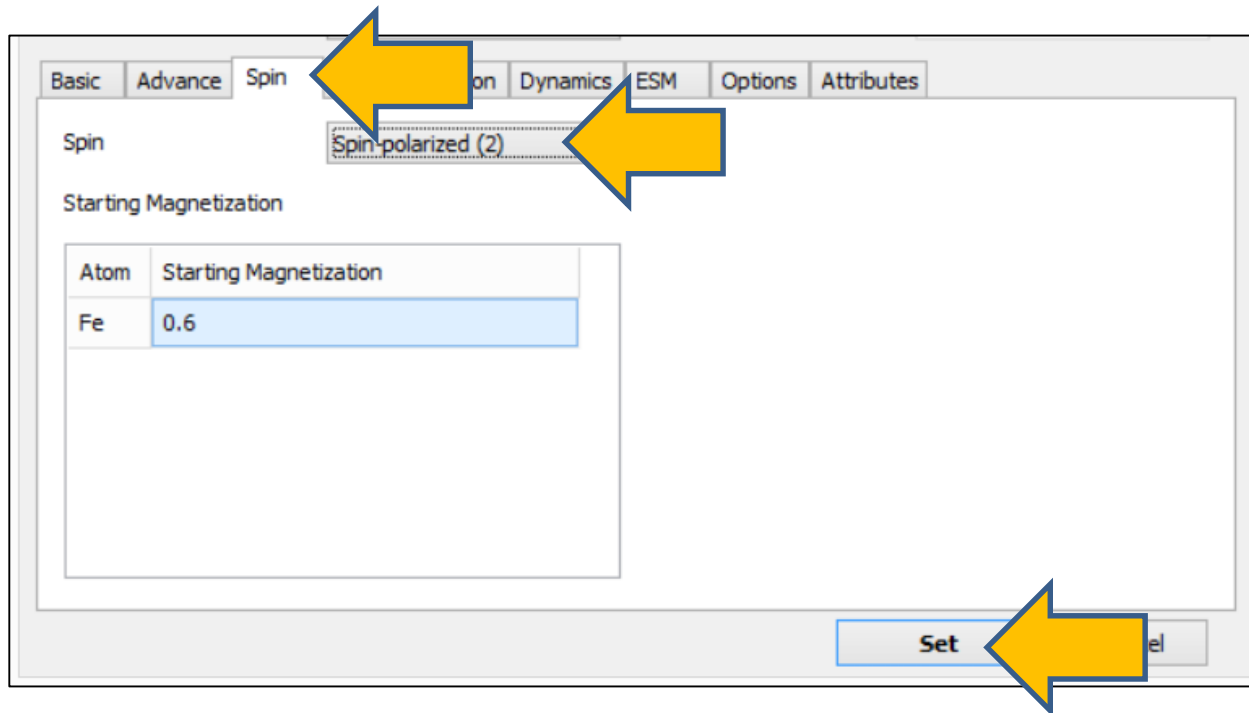
## II. Bands calculation

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**.



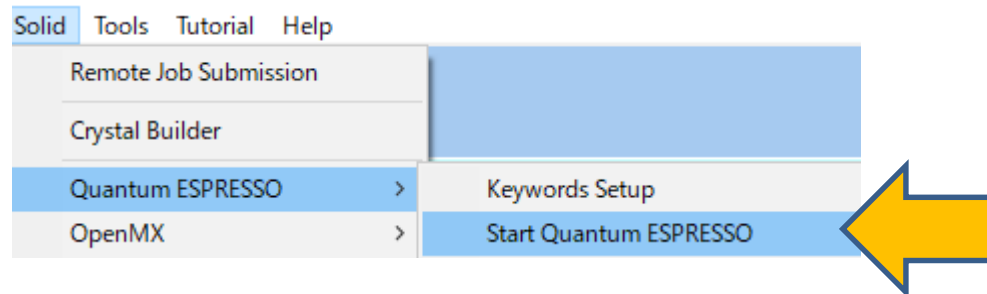
## II. Bands calculation

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



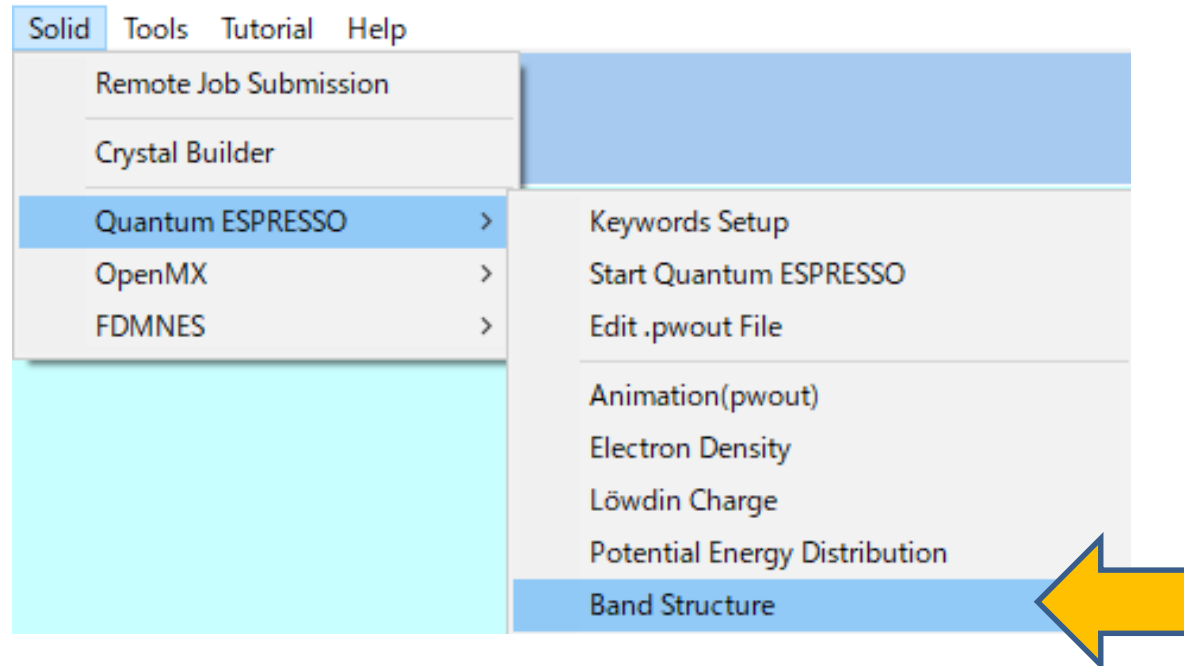
## II. Bands calculation

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. Save as **fe\_bands.pwin**.



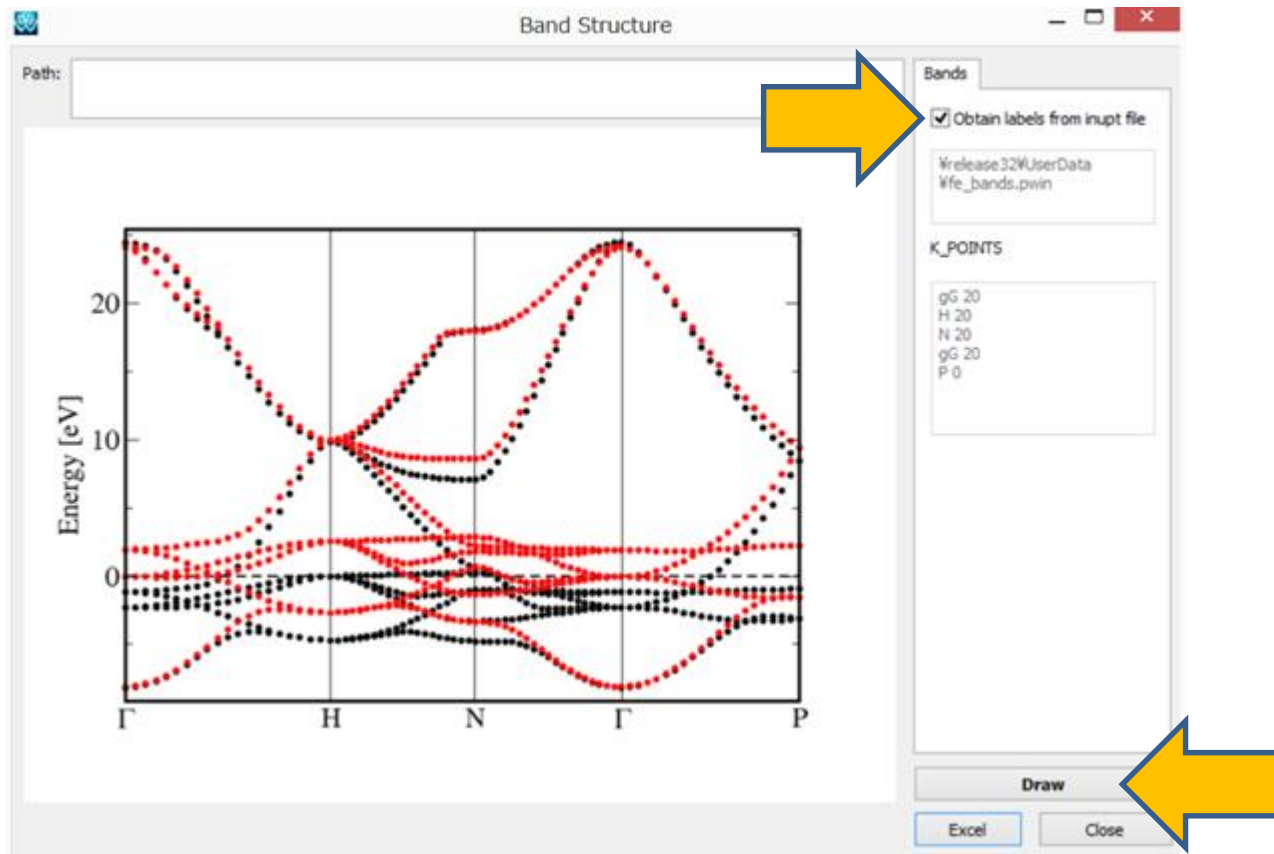
## II. Bands calculation

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**.



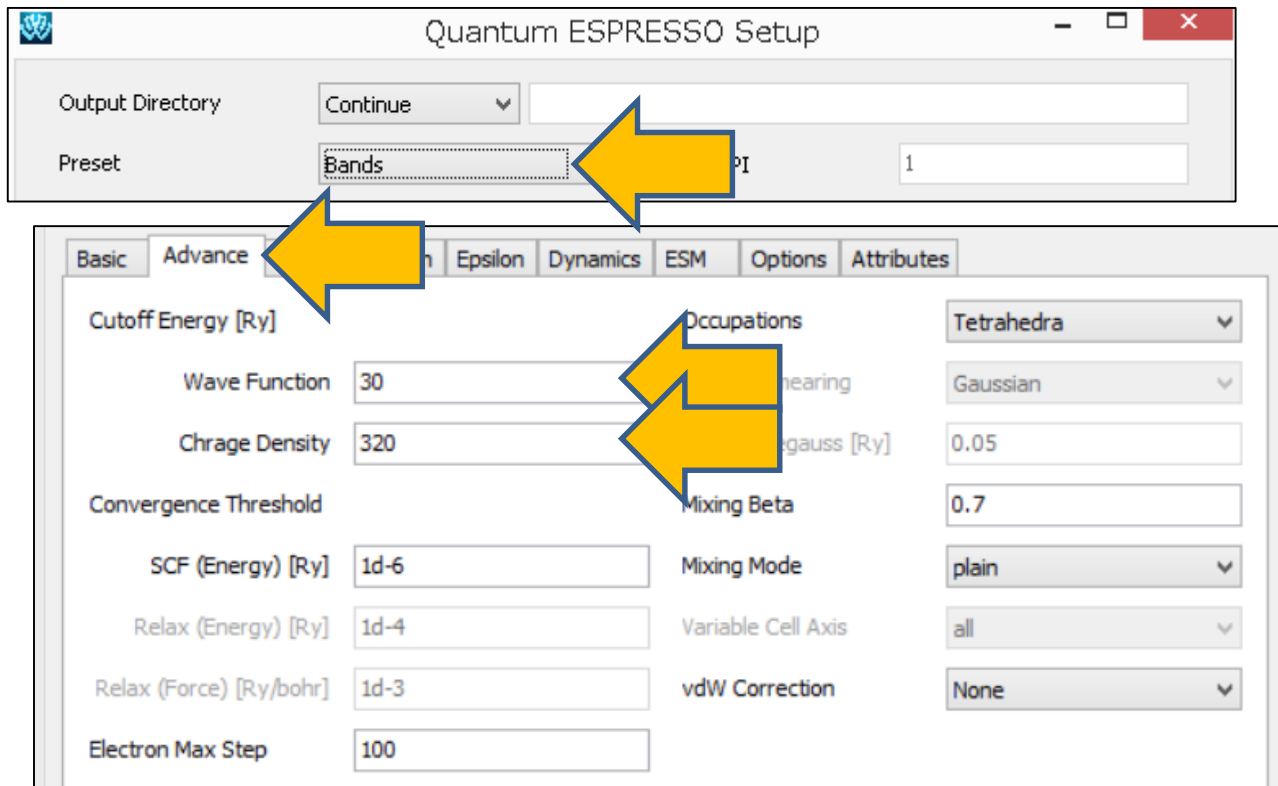
## II. Bands calculation

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.



## III. DOS calculation

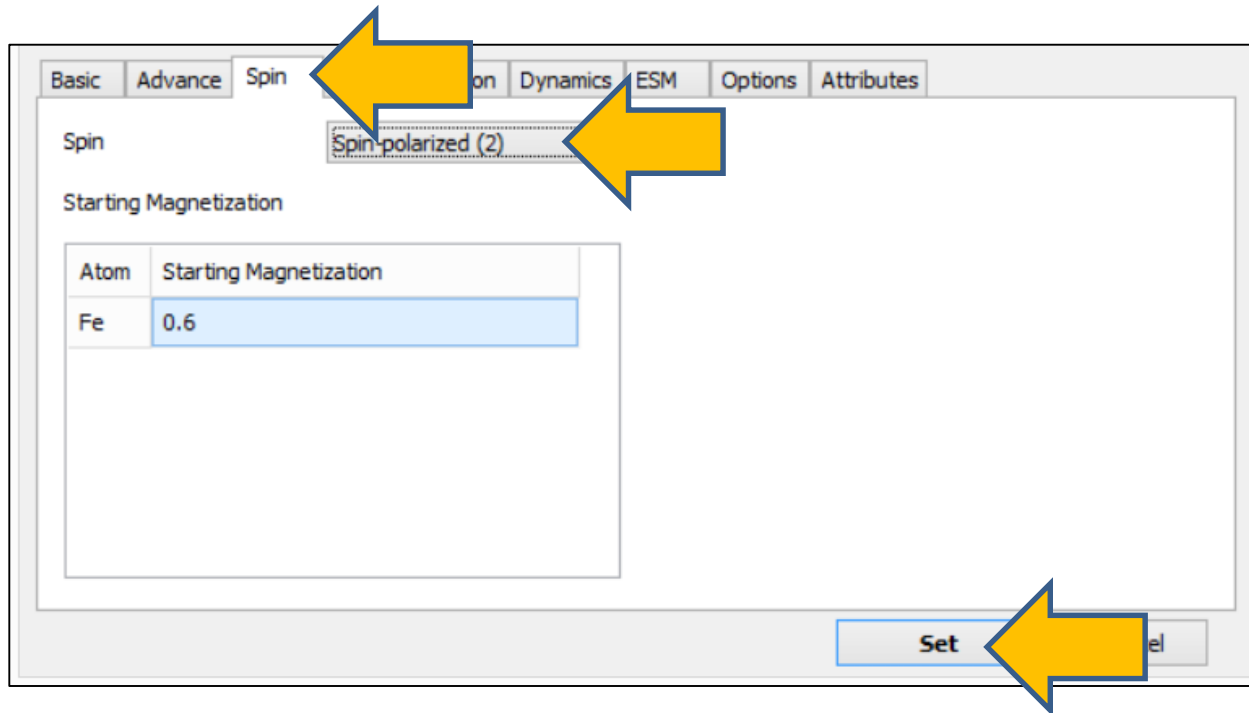
1. Click **Solid | Quantum ESPRESSO | Keywords Setup**.
2. Set **Preset** to **DOS**.
3. On **Advance** tab, set **Wave Function** to **30**, **Charge Density** to **320**.





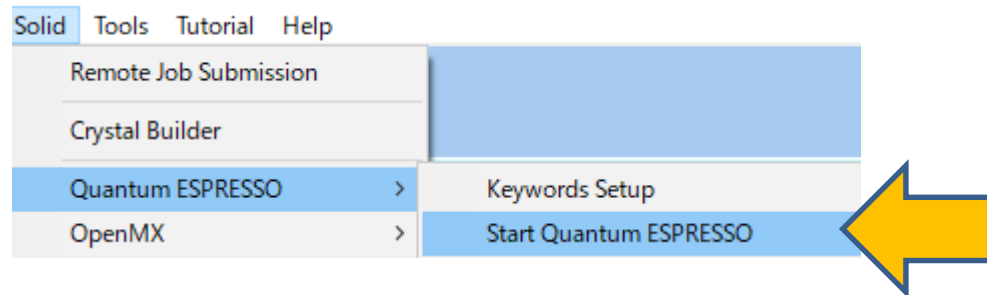
## III. DOS calculation

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



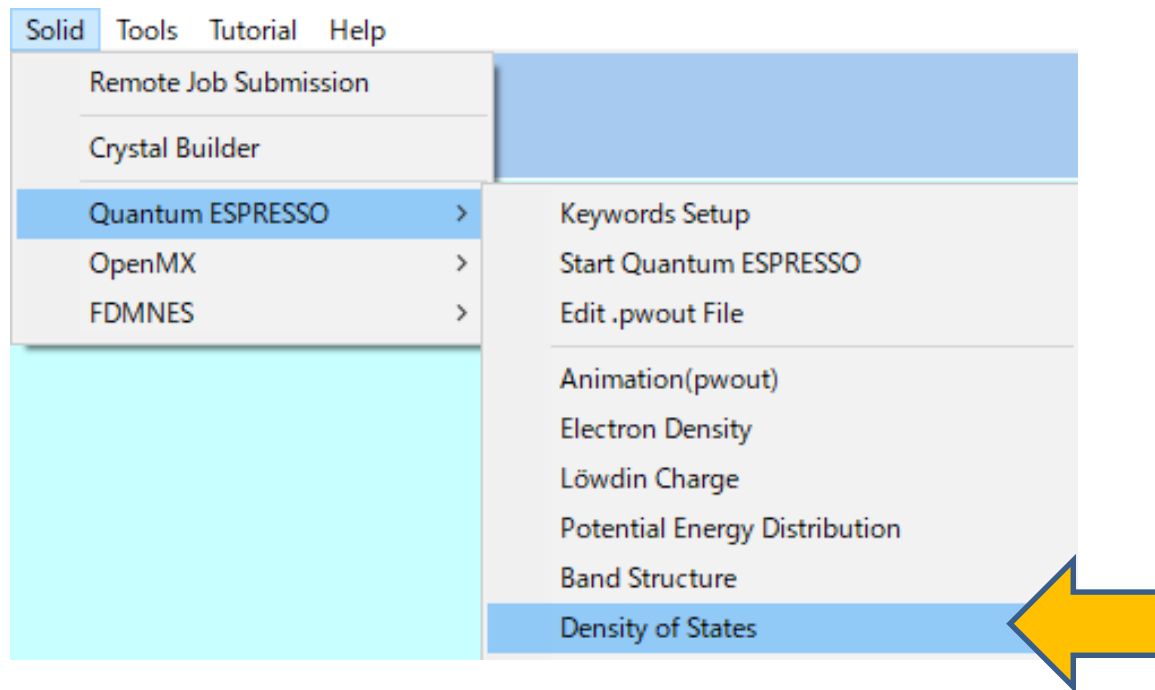
### III. DOS calculation

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. Save as **fe\_dos.pwin**.



### 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**.



### III. DOS calculation

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

