

Winmostar tutorial
Quantum ESPRESSO
Spin Polarization
V8.007

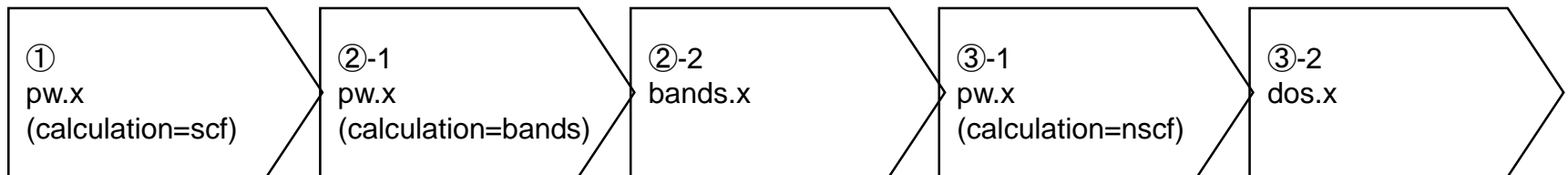
X-Ability Co., Ltd.

question@winmostar.com

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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¥Brilouin_zonew.pdf in your install directory for QE.

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 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

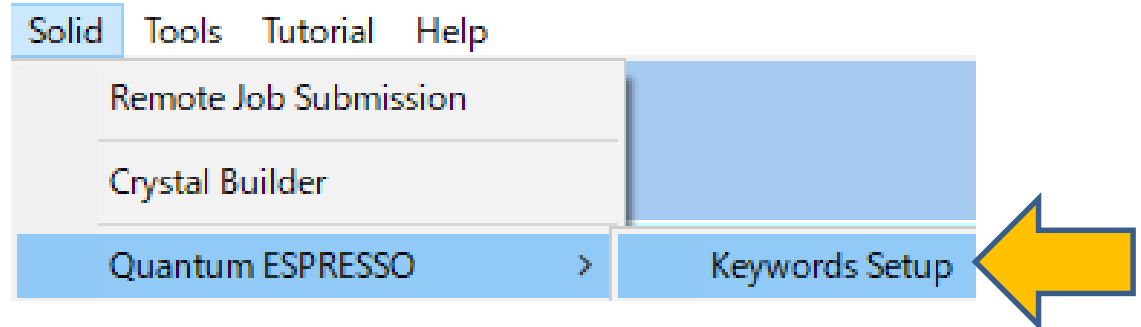
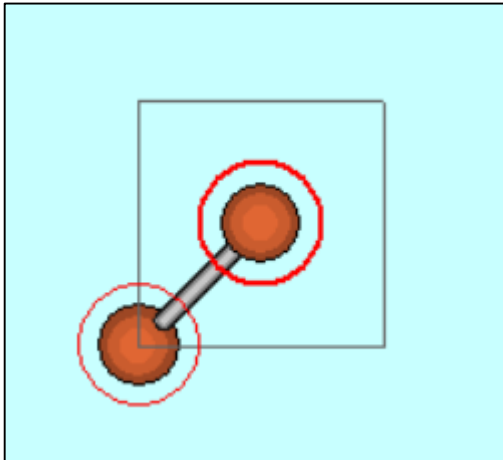
I. Creating the Model

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.

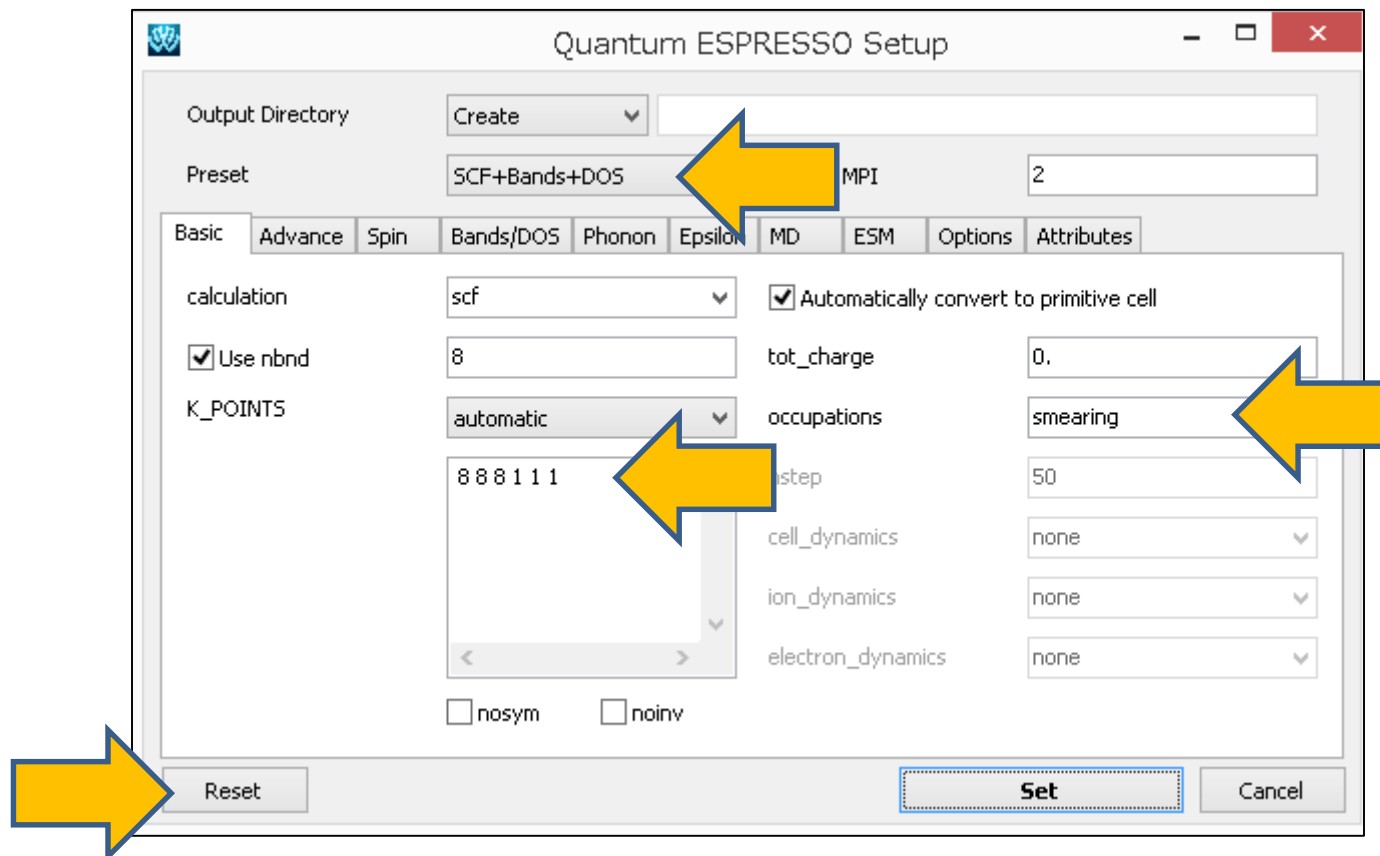
To make Fe unit cell
Crystal system: Cubic
Space group : Im-3m (229)
Lattice constants : a=2.8665 Å
Asymmetric unit: Fe (0.0 0.0 0.0)

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



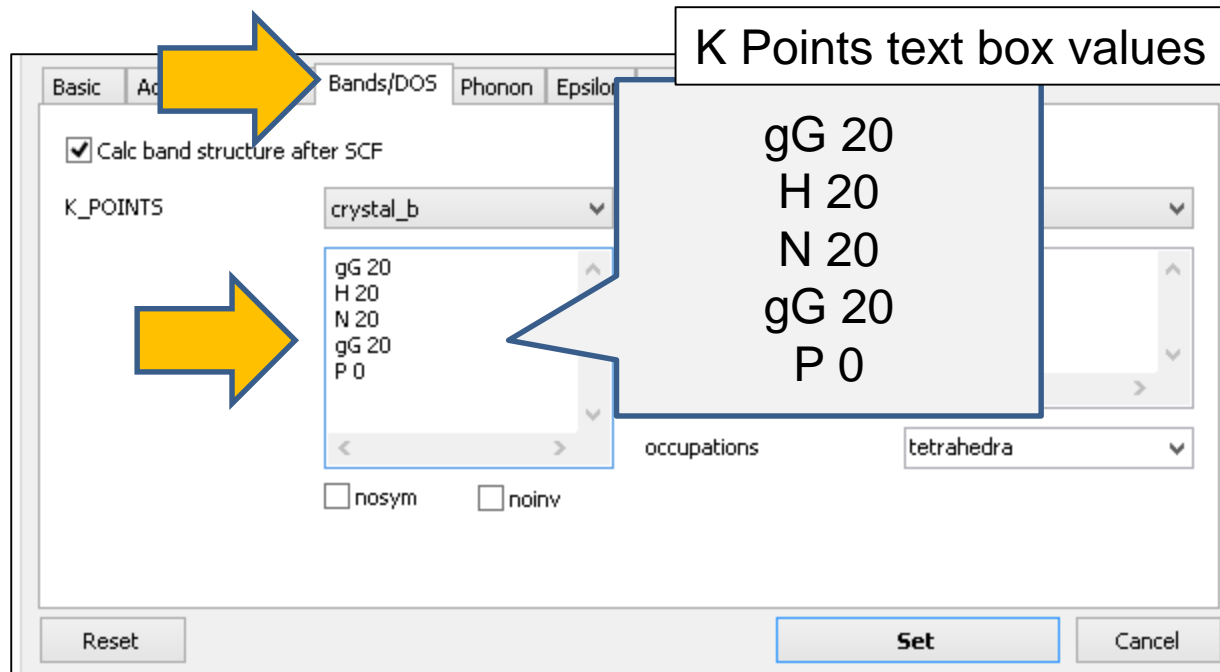
II. QE Calculation

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**.



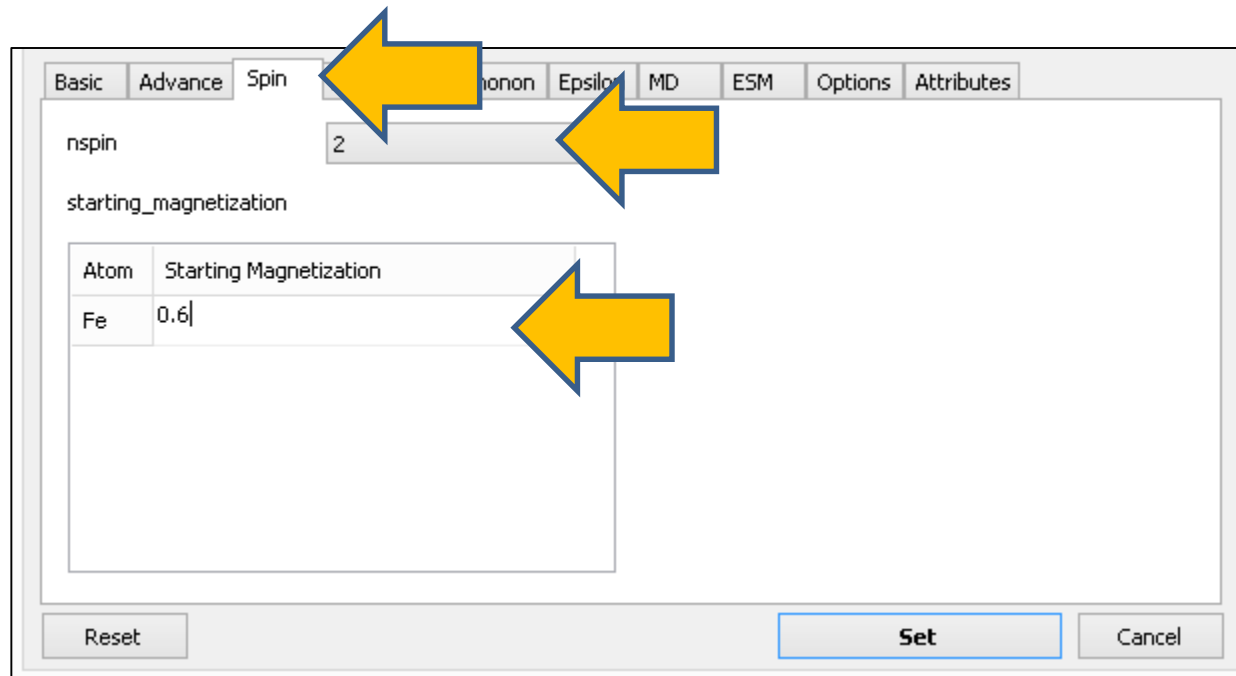
II. QE Calculation

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



II. QE Calculation

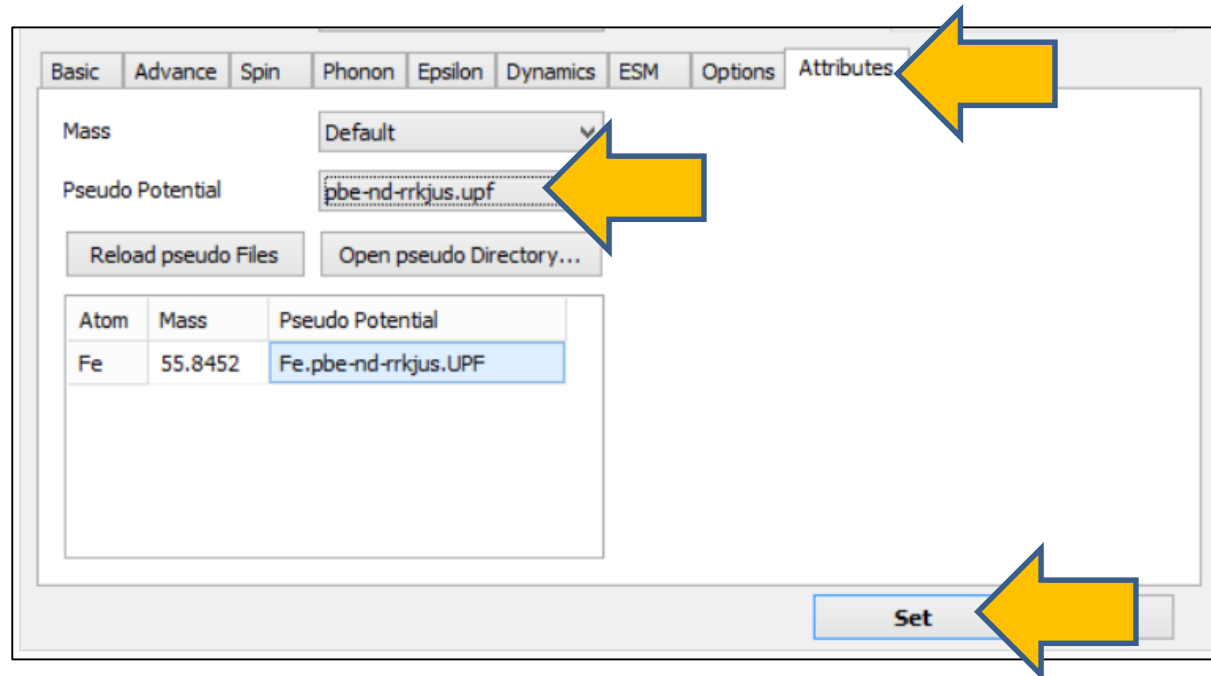
1. Click **Spin** tab.
2. Set **nspin** to 2.
3. Set **Starting Magnetization** of Fe atom to **0.6**.



II. QE Calculation

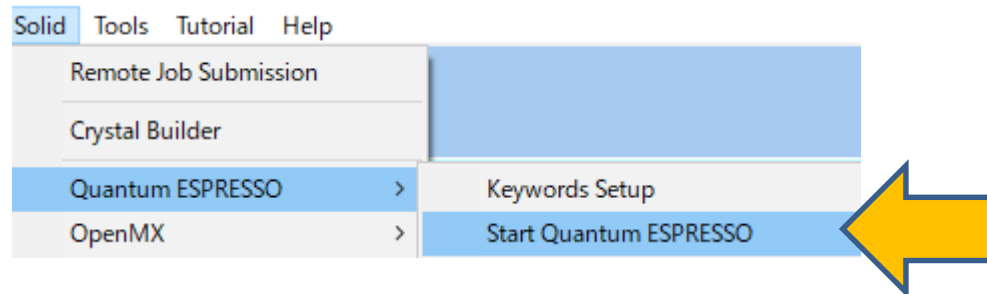
1. On **Attributes** tab, set **Pseudo Potential** to **pbe-nd-rrkjus.upf**.
2. Click **Set**.

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**.



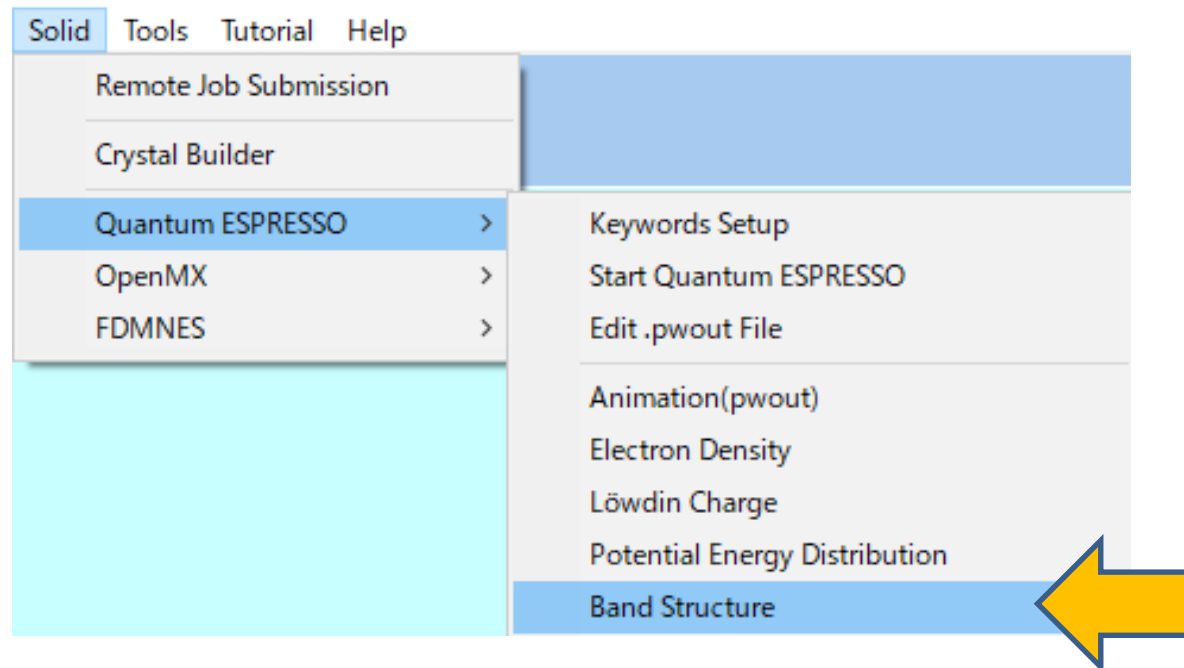
II. QE Calculation

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



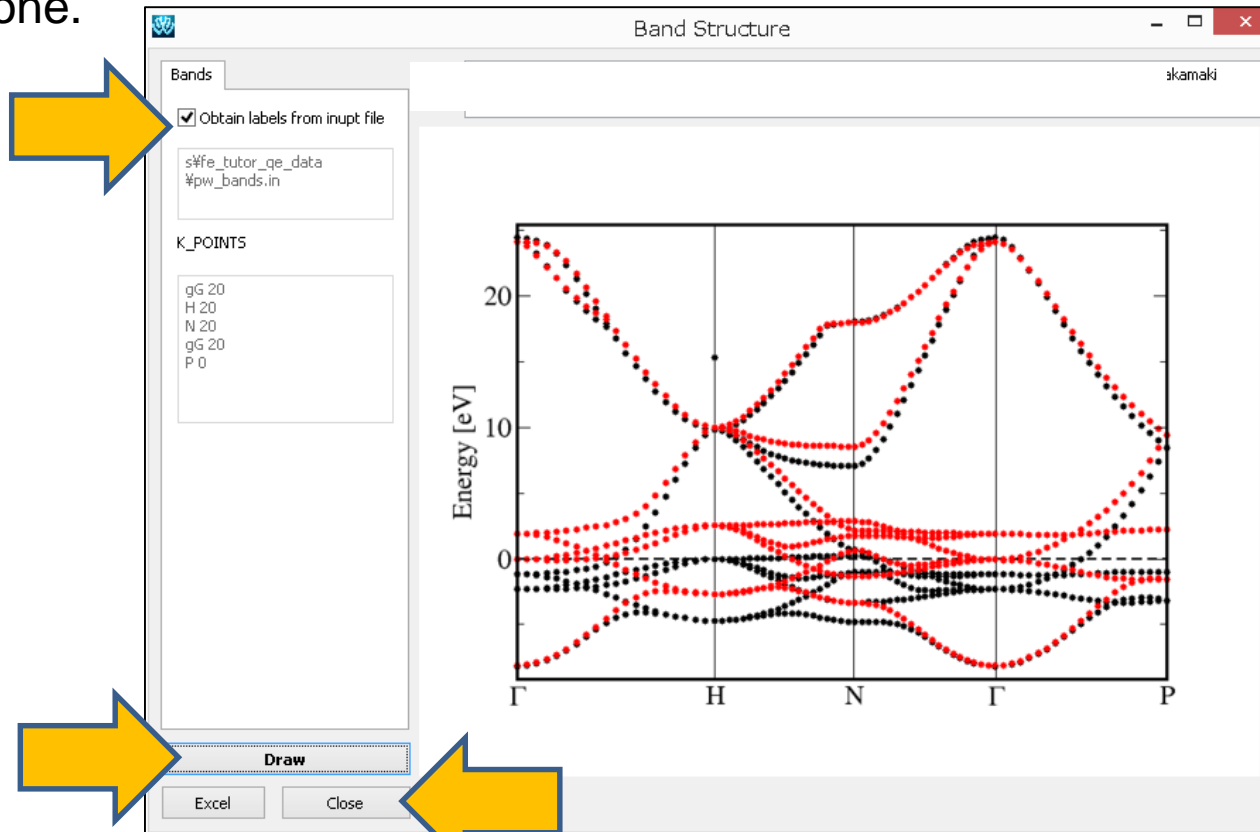
III. Analysis

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



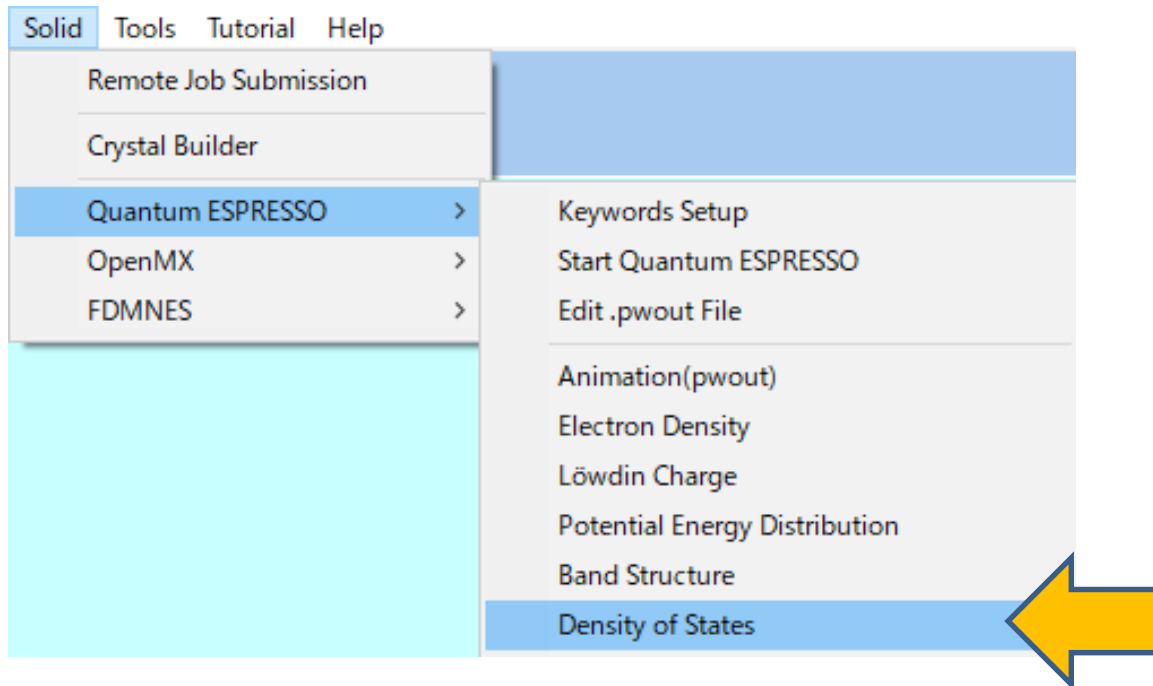
III. Analysis

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.



III. Analysis

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



III. Analysis

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

