

## Winmostar tutorial Quantum ESPRESSO Spin Polarization V7.025

#### X-Ability Co,. Ltd.

question@winmostar.com

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#### Contents

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



#### **Environment setting**

1. See Quantum ESPRESSO install manual <u>https://winmostar.com/en/QE\_install\_manual\_en\_win.pdf</u>

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/

| PSEUDOPOTENTIALS<br>Admin PP Database     | Standard Solid State Pseudopotentials (SSSP), a collection of the best verified pseudopotentials,<br>maintained by THEOS and MARVEL, can be found, together with tests, on the Materials Cloud<br>(materials cloud orn)   |
|---|---|
| More about pseudopotentials               | (matchalocodd.org).   |
| Naming convention for the pseudopotential | PAW datasets for rare earths can be found on the web page of VLab at University of Minnesota.   |
| PSLibrary                                 | More information about pseudopotentials in general, the naming convention adopted for   |
| Unified Pseudopotential Format            | databases, can be found via the links of the menu at the left.  |
| Click                                     | results in published work, we cannot give any warranty whatsoever that they fit your actual needs.<br>(last updated April 7, 2016)           ANY FUNCTIONAL         ANY TYPE         Apply Filter           RY         OTHER OPTIONS         Provide the second se |
|   | 5 8 7 8 9 10  |
|   |   |
|   | N AI SI P S CI Ar   |
|   | 16 25 28 27 22 29 30 31 32 33 34 35 38  |
|   | N         Cu         Zi         Ga         Ge         As         Se         Bit         N           31         41         43         44         45         44         47         48         49         50         51         52         53         54   |
|   | Rb Sr ) 🖌 Nb lo Tc Ru Rh P Ag Cd In Sn Sb Te I Xe   |
|   | 55 56 57-70 7 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86<br>Ce Ba III HI Ta W Pa Oe Ir Dt Au Ha TI Dh Bù Do At Pa   |
|   |   |





#### 1. Click File | Open.

#### 2. Open fe.cif in the sample directory. (C:\u00e4winmos7\u00e4samples\u00e4fe.cif)

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

I.

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.

| Solid Tools Tutorial Help |                |
|---------------------------|----------------|
| Remote Job Submission     |                |
| Crystal Builder           |                |
| Quantum ESPRESSO >        | Keywords Setup |
|                           |                |
|                           |                |



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

| •   | Quantum ESP                             | RESSO Setup                          |            | _ 🗆 ×                           |                            |
|---|---|--------------------------------------|------------|---------------------------------|----------------------------|
| Output Directory<br>Preset<br>Basic Advance Dynam | Create<br>5CF<br>ics Options Attributes | PI PI                                | 1          | Basic Advance Sp<br>Calculation | in Phonon Epsilon Dynamics |
| Calculation                                       | SCF 🗸                                   | Total Charge [e]                     | 0.         | ✓ Automatically set             | # of bands                 |
| ✓ Automatically Set # of                          | Bands                                   | No Symmetry                          |            | # of Bands                      | 8                          |
| # of Bands  | 8<br>Gamma                              | Determine DOS                        | 50         | K Points                        | Automatic                  |
|   | ^                                       | Cell Dynamics                        | nor        |                                 | 888111                     |
|   | ~                                       | Ion Dynamics                         | nor        |                                 |                            |
|   | < >                                     | Electron Dynamics                    | nor        |                                 | < >                        |
|   |   | <ul> <li>Automatically De</li> </ul> | tect ibrav |                                 |                            |
|   |   |                                      | Set        | : Cancel                        |                            |



- 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.

| isic Advance            | E    | Epsilon | Dynamics | ESM    | Options      | Attributes |                  |    |
|-------------------------|------|---------|----------|--------|--------------|------------|------------------|----|
| Cutoff Energy [Ry]      |      |         |          | Occup  | pations      |            | Smearing         |    |
| Wave Function           | 30   |         |          |        | Smearin      | g          | Marzari-Vanderbi | lt |
| Chrage Density          | 320  |         |          |        | degauss      | s [Ry]     | 0.01             |    |
| Convergence Threshold   |      |         |          | Mixing | g Beta       |            | 0.7              |    |
| SCF (Energy) [Ry]       | 1d-6 |         |          | Mixing | g Mode       |            | plain            | ~  |
| Relax (Energy) [Ry]     | 1d-4 |         |          | Varial | ole Cell Axi | s          | all              | ~  |
| Relax (Force) [Ry/bohr] | 1d-3 |         |          | vdW    | Correction   |            | None             | ~  |
| lectron Max Step        | 100  |         |          |        |              |            |                  |    |
|                         |      |         |          |        |              |            |                  |    |



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

| Basic A  | dvance Spir   | n <b>(</b>  | on            | Dynamics | ESM | Options | Attributes |     |        |
|----------|---------------|-------------|---------------|----------|-----|---------|------------|-----|--------|
| Spin     |               | Spin        | polarized (2) |          |     |         |            |     |        |
| Starting | Magnetizatior | ı           |               |          |     |         |            |     |        |
| Atom     | Starting Ma   | gnetization |               |          |     |         |            |     |        |
| Fe       | 0.6           |             |               | $\sim$   |     |         |            |     |        |
|          |               |             |               |          |     |         |            |     |        |
|          |               |             |               |          |     |         |            |     |        |
|          |               |             |               |          |     |         |            |     |        |
|          |               |             |               |          |     |         |            |     |        |
|          |               |             |               |          |     |         |            |     |        |
|          |               |             |               |          |     |         |            | iat | Cancel |



- 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**.

| Basic  | Advance     | Spin  | Phonon     | Epsilon   | Dynamics | ESM | Options | Attributes |  |
|--------|-------------|-------|------------|-----------|----------|-----|---------|------------|--|
| Mass   |             |       | Default    |           | ×        | 1   |         |            |  |
| Pseudo | o Potential |       | pbe-nd-    | rkjus.upf |          |     |         |            |  |
| Rele   | oad pseudo  | Files | Open p     | seudo Dir | ectory   |     |         |            |  |
| Atom   | Mass        | Ps    | eudo Poter | ntial     |          |     |         |            |  |
| Fe     | 55.845      | 2 Fe  | .pbe-nd-rr | kjus.UPF  |          |     |         |            |  |
|        |             |       |            |           |          |     |         |            |  |
|        |             |       |            |           |          |     |         |            |  |
|        |             |       |            |           |          |     |         |            |  |
|        |             |       |            |           |          |     |         |            |  |
|        |             |       |            |           |          |     |         | Set        |  |



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

| Solid | d Tools Tutorial Help |   |                        |  |
|-------|-----------------------|---|------------------------|--|
|       | Remote Job Submission |   |                        |  |
|       | Crystal Builder       |   |                        |  |
|       | Quantum ESPRESSO      | > | Keywords Setup         |  |
|       | OpenMX                | > | Start Quantum ESPRESSO |  |
|       |                       |   |                        |  |



- 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.





- 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.

| Basic Advance           | n Epsilon | Dynamics | ESM    | Options       | Attributes |              |         |   |
|-------------------------|-----------|----------|--------|---------------|------------|--------------|---------|---|
| Cutoff Energy [Ry]      |           |          | Occup  | ations        | [          | Smearing     |         |   |
| Wave Function           | 30        |          |        | Smearin       | g          | Marzari-Vand | lerbilt |   |
| Chrage Density          | 320       |          |        | degauss       | [Ry]       | 0.01         |         |   |
| Convergence Threshold   |           |          | Mixing | Beta          | [          | 0.7          |         |   |
| SCF (Energy) [Ry]       | 1d-6      |          | Mixing | Mode          | [          | plain        |         | ¥ |
| Relax (Energy) [Ry]     | 1d-4      |          | Variab | ole Cell Axis | s          | all          |         | V |
| Relax (Force) [Ry/bohr] | 1d-3      |          | vdW (  | Correction    | [          | None         |         | ۷ |
| Electron Max Step       | 100       |          |        |               |            |              |         |   |



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

| asic A   | dvance Spin   |             | on Dyna | mics ESM | Options | Attributes |    |
|----------|---------------|-------------|---------|----------|---------|------------|----|
| Spin     |               | Spin-polari | zed (2) |          |         |            |    |
| Starting | Magnetization |             |         |          |         |            |    |
| Atom     | Starting Magn | etization   |         |          |         |            |    |
| Fe       | 0.6           |             |         |          |         |            |    |
|          |               |             |         | - I      |         |            |    |
|          |               |             |         |          |         |            |    |
|          |               |             |         |          |         |            |    |
|          |               |             |         |          |         |            |    |
|          |               |             |         |          |         |            |    |
|          |               |             |         |          |         |            |    |
|          |               |             |         |          |         | Set        | el |



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

| Solid | d Tools Tutorial Help |   |                        |           |
|-------|-----------------------|---|------------------------|-----------|
|       | Remote Job Submission |   |                        |           |
|       | Crystal Builder       |   |                        |           |
|       | Quantum ESPRESSO      | > | Keywords Setup         |           |
|       | OpenMX                | > | Start Quantum ESPRESSO | $\langle$ |
|       |                       |   |                        |           |



- 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**.





- 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.





- 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.

| 30                      | Quantum ESP       | RESSO Setup              | - 🗆 ×        |
|-------------------------|-------------------|--------------------------|--------------|
| Output Directory        | ontinue 🗸         | 1                        |              |
| Preset                  | ands              | PI 1                     |              |
| Basic Advance           | n Epsilon Dynamic | cs ESM Options Attribute | ·S           |
| Cutoff Energy [Ry]      |                   | Dccupations              | Tetrahedra 🗸 |
| Wave Function           | 30                | nearing                  | Gaussian V   |
| Chrage Density          | 320               | gauss [Ry]               | 0.05         |
| Convergence Threshold   |                   | Mixing Beta              | 0.7          |
| SCF (Energy) [Ry]       | 1d-6              | Mixing Mode              | plain 🗸      |
| Relax (Energy) [Ry]     | 1d-4              | Variable Cell Axis       | all 🗸 🗸      |
| Relax (Force) [Ry/bohr] | 1d-3              | vdW Correction           | None 🗸       |
| Electron Max Step       | 100               |                          |              |



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

| asic A   | dvance Sp    | pin           | on            | Dynamics ESM | Options | Attributes  |    |
|----------|--------------|---------------|---------------|--------------|---------|-------------|----|
| Spin     |              | Spin          | polarized (2) |              |         |             |    |
| Starting | Magnetizatio | on            |               |              |         |             |    |
| Atom     | Starting M   | lagnetizatior | ı             |              |         |             |    |
| Fe       | 0.6          |               |               |              |         |             |    |
|          |              |               |               |              |         |             |    |
|          |              |               |               |              |         |             |    |
|          |              |               |               |              |         |             |    |
|          |              |               |               |              |         |             |    |
|          |              |               |               |              |         |             |    |
|          |              |               |               |              |         | <b>C</b> -1 | -1 |
|          |              |               |               |              |         | Set         | el |



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

| Solid | d Tools Tutorial Help |   |                        |  |
|-------|-----------------------|---|------------------------|--|
|       | Remote Job Submission |   |                        |  |
|       | Crystal Builder       |   |                        |  |
|       | Quantum ESPRESSO      | > | Keywords Setup         |  |
|       | OpenMX                | > | Start Quantum ESPRESSO |  |
|       |                       |   |                        |  |



- 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**.





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

