winmostar tutorial

Quantum ESPRESSO Ferromagnetic Materials, Antiferromagnetic Materials

V11.6.5

28 February 2024 X-Ability Co., Ltd.

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About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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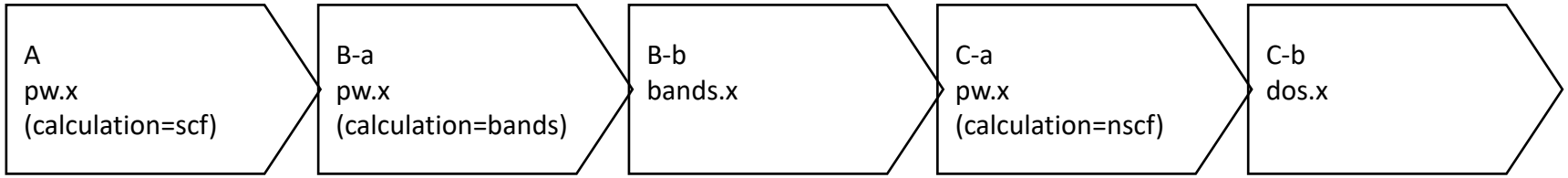
Overview

- For ferromagnetic materials, we will perform SCF calculations on Fe crystals as an example, and for antiferromagnetic materials, on NiO, followed by calculations of band structures and density of states (these tasks are run in sequence on Winmostar).



Notes:

- The choice of k-points, number of bands, type of pseudopotentials, cut-off energy, and smearing width can affect the calculation results. For this tutorial, we will use settings that reduce accuracy in order to obtain results quickly.
- The k-point path (route) needs to be set according to the crystal structure being studied. Recommended paths for each crystal structure can be set by referring to the Doc¥brillouin_zones.pdf in the Quantum ESPRESSO installation directory.

◆ For a detailed explanation of Quantum ESPRESSO's calculation methods and settings, please see the following article from our company:https://qiita.com/xa_member

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Preference of Operating Environment

- For users of Winmostar version V11.5.0 or later on a 64-bit environment, please install and configure CygwinWM version 2023/04/05 or later.
  - The CygwinWM version after 2023/04/05 includes the recommended version of 64-bit Quantum ESPRESSO.

- If the above does not apply to you or if you wish to use a version of Quantum ESPRESSO other than the recommended one, you will need to install and configure Windows version of Quantum ESPRESSO separately.

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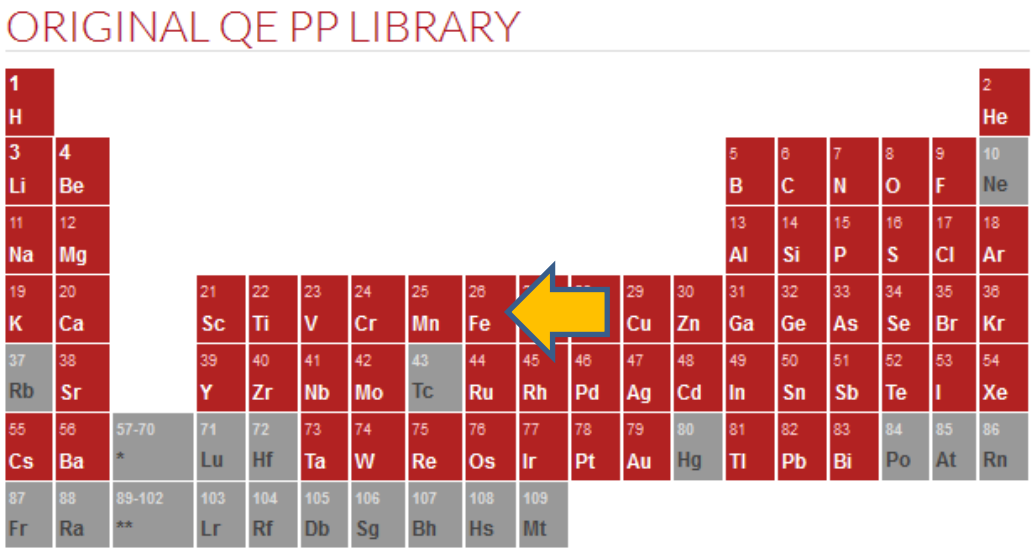
Preparing Pseudopotentials

- To conduct this tutorial, you may need to add pseudopotential files.
  Download [Fe.pbe-nd-rrkjus.UPF] from the periodic table [Fe] at the following URL:
  http://pseudopotentials.quantum-espresso.org/legacy_tables/original-qe-pp-library/
  Then, copy `Fe.pbe-nd-rrkjus.UPF` into the folder opened by clicking **Open QE pseudo directory** in **Calculate** tab of **Tools | Preference**.



Please obtain the pseudopotential files for Ni and O using **Download Pseudo Files** feature in the installation manual.

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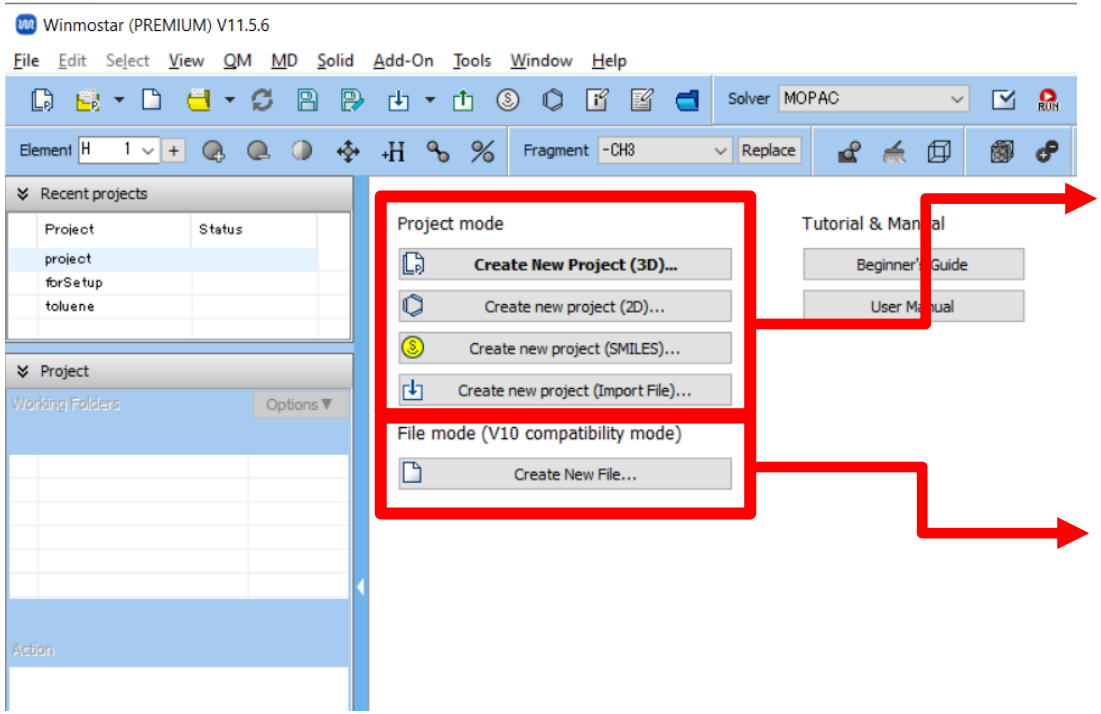
Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to Quantum ESPRESSO tutorial for version 10.



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

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A. Modeling of the System（Fe)

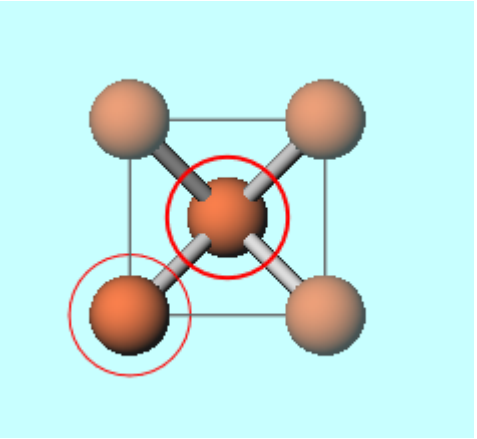
- Please refer to QE Basic Tutorial for the basic operation method.
- For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Methods for Creating Initial Structures'.

A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

B. Enter '`fe_scf`' in **Project name** and click **Save**.

C. Click **File | Import | Sample File | fe.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

D. In **Import File** dialog, click **Discard and import**.



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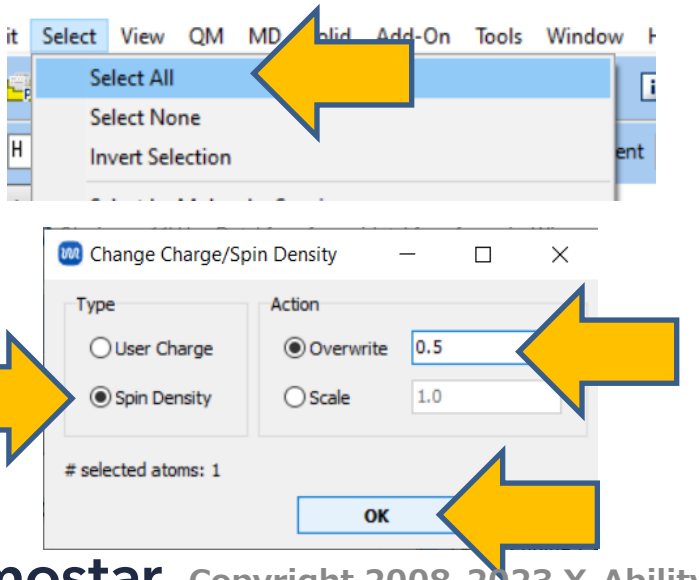
A. Modeling of the System（Fe)

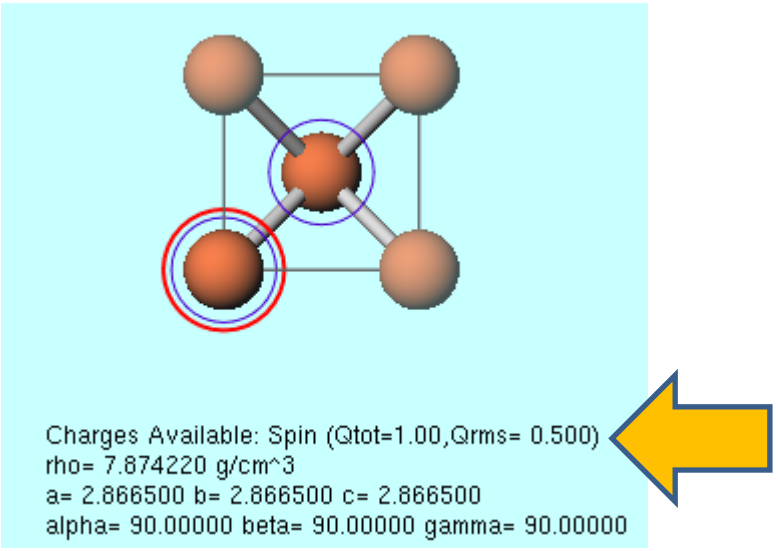
A. Click **Select | Select All**.

B. Click **Edit | Change Atom Property | Charges/Spin Density**.

C. Change **Type** to **Spin Density**, and in **Action** section, enter '0.5' next to **Overwrite** and click **OK**. This value will be interpreted as starting_magnetization when running QE through Winmostar.

D. Confirm that 'Charges Available: Spin (Rtot=1.00, Qrms...' is displayed below Viewport, indicating that Spin Density has been set.





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B. Execution of Calculation（Fe）

A. Select **Quantum ESPRESSO** from Toolbar's **Solver** and click  **(Workflow Setup)**.

B. To reduce computation time, click **Yes** when asked if you want to convert to a primitive cell. The converted structure will appear in Viewport. Click **OK** when 'Successfully converted lattice' is displayed.

C. In **Quantum ESPRESSO Workflow Setup** window, make the following changes:
   - Change **# of bands** to **50% more**
   - Change **Spin** to **Polarized**
   - Check **Use Bravais-lattice index**
   - Change **Pseudo file** to **pz-nd-rrkjus.upf**
   - Check **Properties** for **DOS**, **PDOS/Lowdin charge**, **Band structure**, and **Charge density**
   - Check **Metal**

D. Click **OK**, adjust settings as needed in **Job Setting** window, and then click **Run**.

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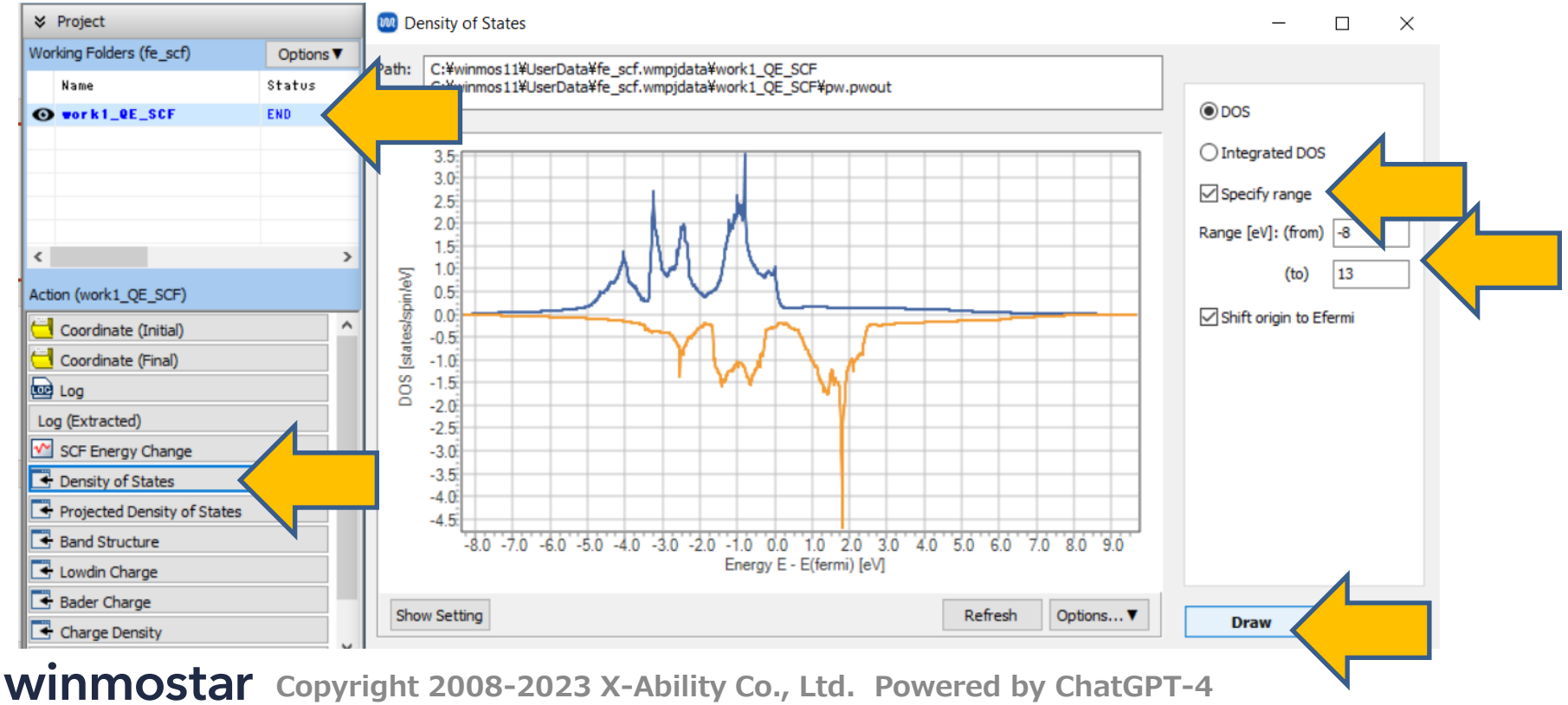
C. Analysis of Results（Fe） Density of States

A. After **the status** of **work1_QE_SCF** in **Working Folders** changes to **END(blue)**, click work1_QE_SCF in **Woriking Folders**, then click **Density of States** under **Action**.

B. If you want to change the horizontal axis of the graph, check **Specify range**, appropriately change **Range (from)** and **(to)**, then click **Draw**.



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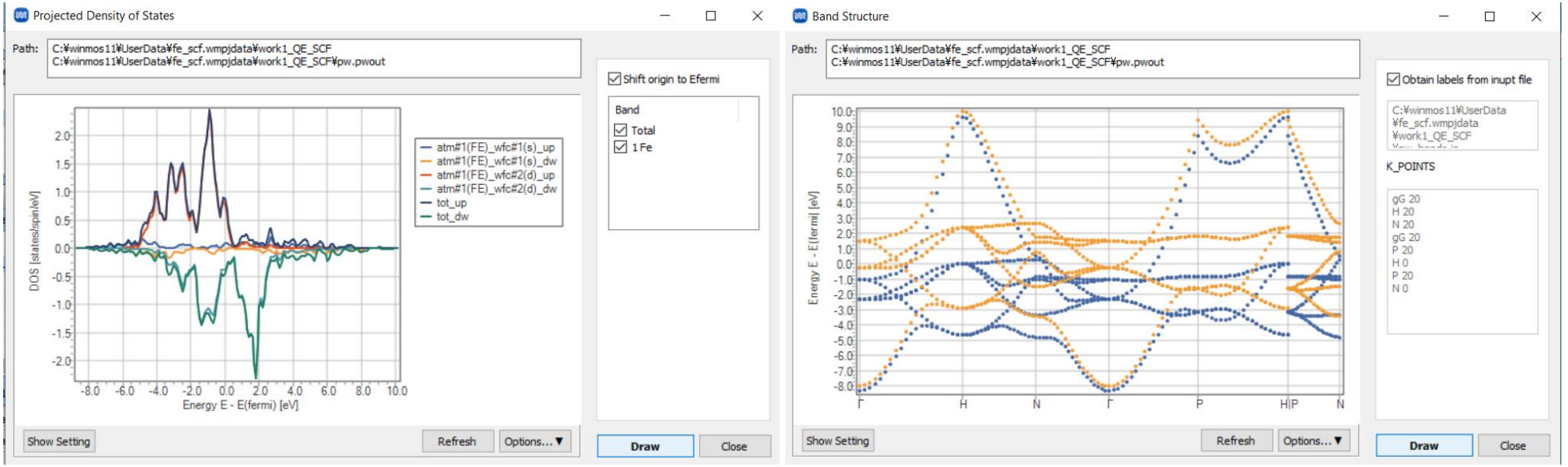
C. Analysis of Results（Fe）
Projected Density of States, Band Structure

A. After **the status** of **work1_QE_SCF** in **Working Folders** changes to **END(blue)**, click work1_QE_SCF in **Woriking Folders**, then click **Projected Density of States** or **Band Structure** under **Action**.



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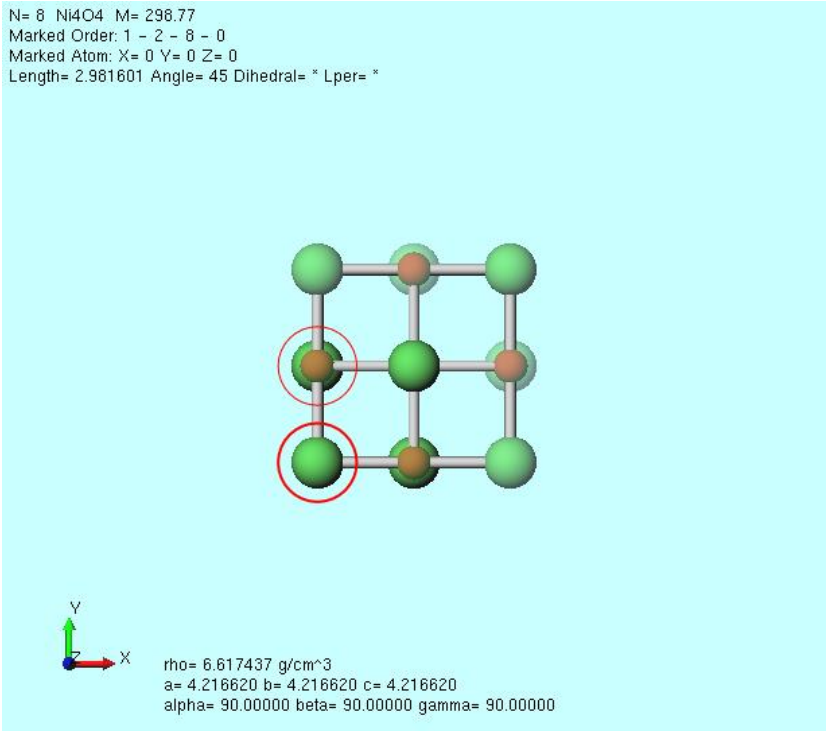
D. Modeling of the System（NiO）

A. Click **File | Close**, and then click **Create New Project (3D)**.
B. Enter '`nio_sc`' in **Project name** and click **Save**.
C. Click **File | Import | Sample File | nio.cif**.
    - If you wish to load a different file at this stage, use **File | Import File** instead.
D. In **Import File** dialog, click **Discard and import**.



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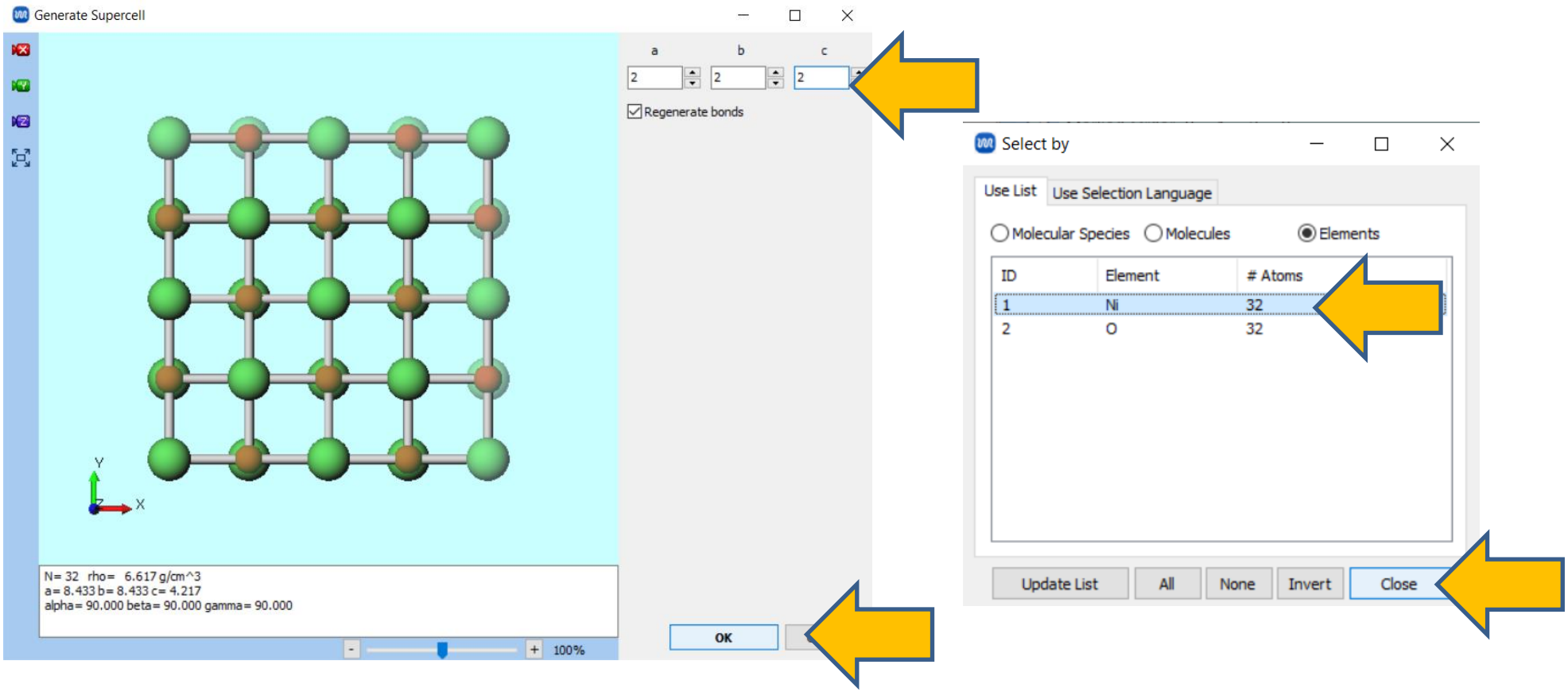
D. Modeling of the System（NiO）

A. Click **Solid | Generate Supercell**, set **a, b, c** each to '2' and click **OK**.
B. Click **Select | Select by Elements**, click on the row for 'Ni' and click **Close**.



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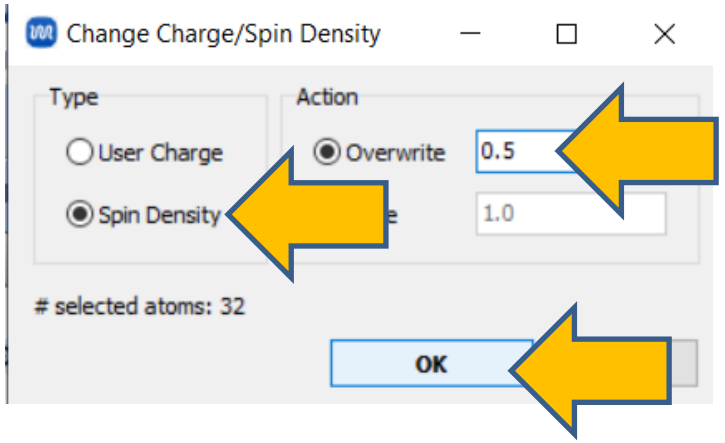
D. Modeling of the System（NiO）

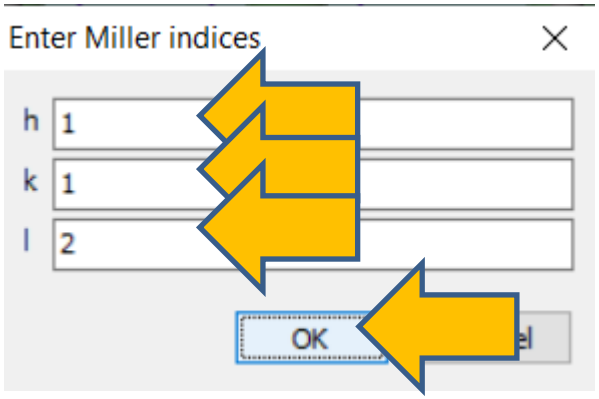
A. Click **Edit | Change Atom Property | Charge/Spin Density**, check **Spin Density**, enter '0.5' next to **Overwrite**, and click **OK**.

B. Click **Align View to X-Axis**.

C. Click **View | Align View | Arbitrary Plane**, change **h, k, l** each to '1', '1', '2', and click **OK**.

D. Click **Select | Select None**.





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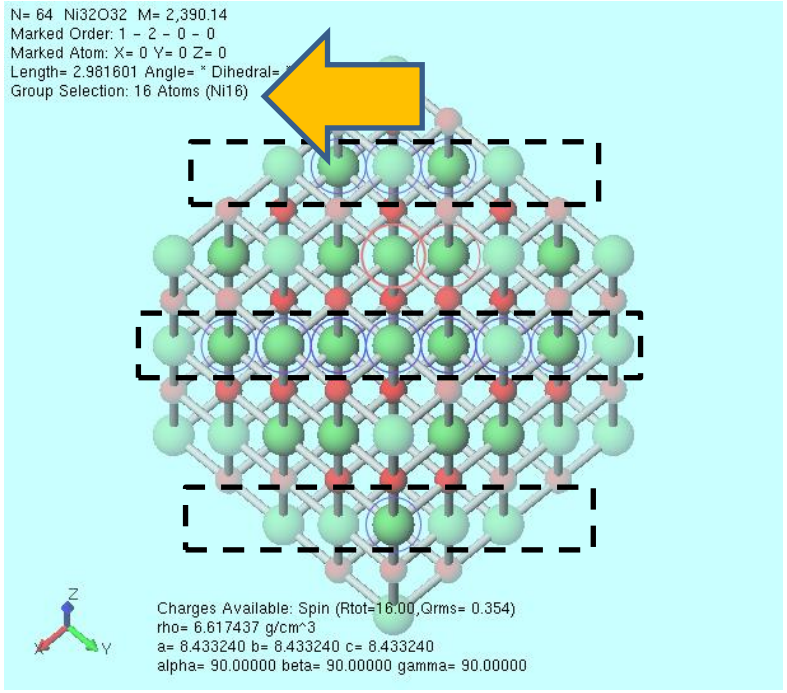
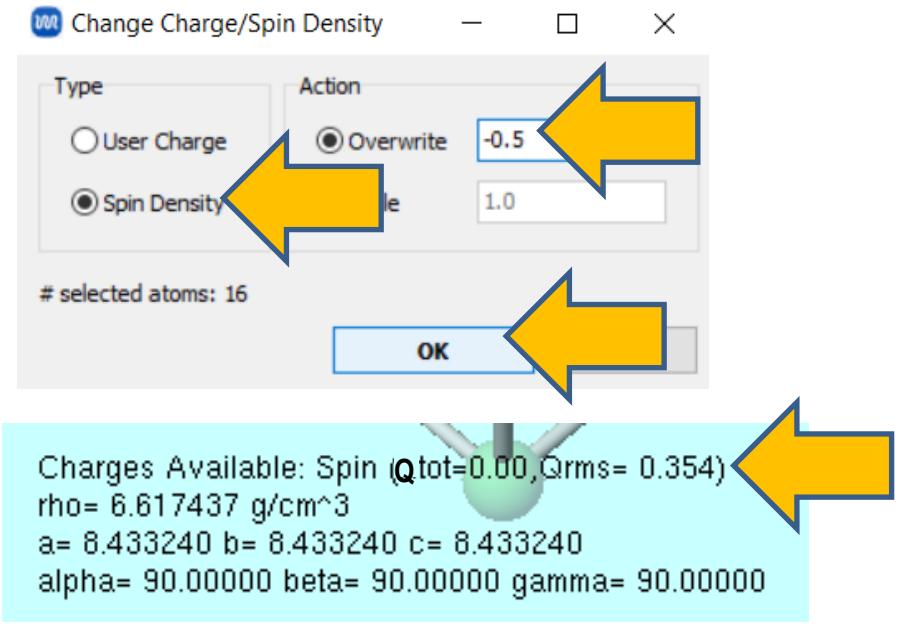
D. Modeling of the System（NiO）

A. As shown in the figure below, consecutively select three areas by Ctrl+dragging to form rectangles, and ensure 'Group Selection: 16 Atoms' is displayed at the top left of Viewport.

B. Click **Edit | Change Atom Property | Charge/Spin Density**, check **Spin Density**, enter '-0.5' next to **Overwrite**, and click **OK**.

C. Confirm that 'Charges Available: Spin (Qtot=0,⋯)' is displayed below Viewport.





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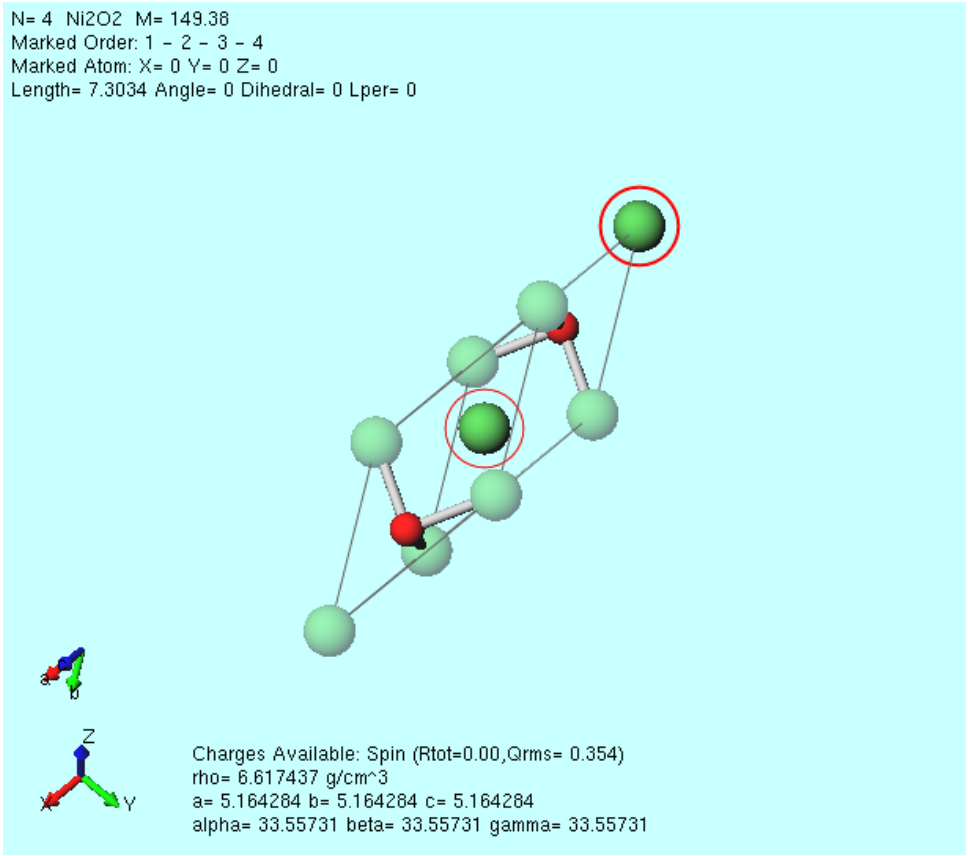
D. Modeling of the System（NiO）

A. Click **Solid | Convert Lattice**, check **Spin Density**, and when 'Do you want to convert to primitive cell' appears, click **Yes**.



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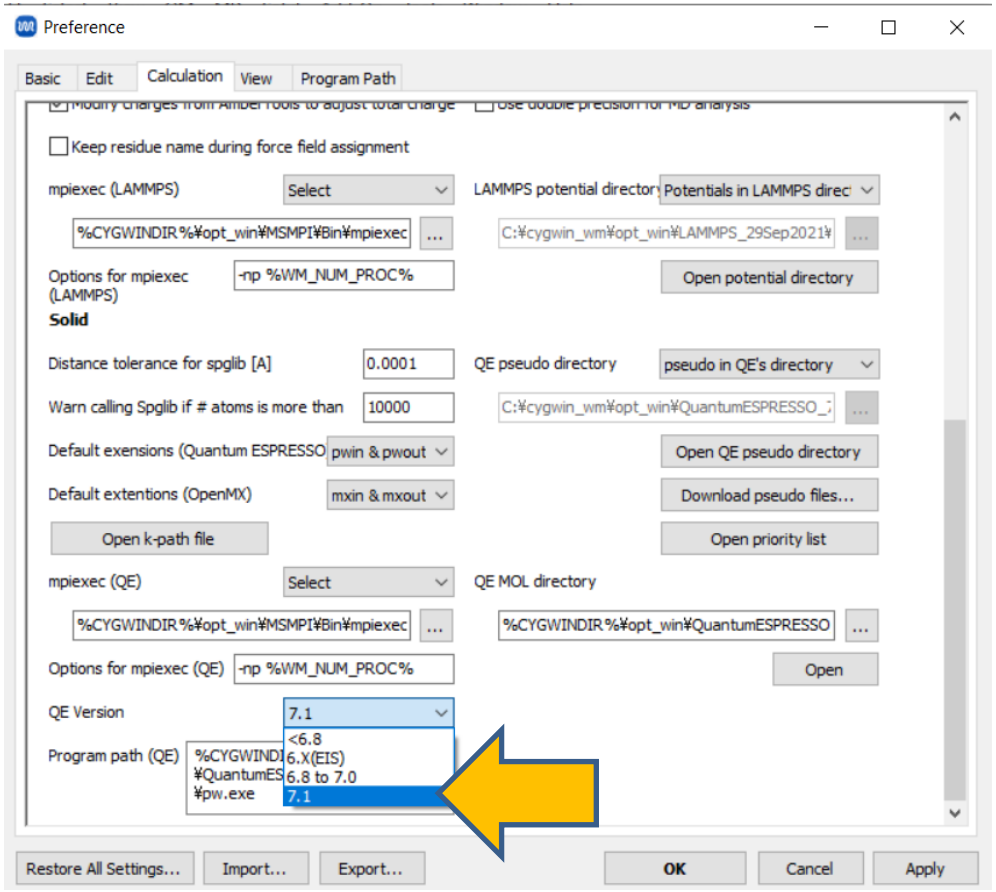
E. Execution of Calculation （NiO）

A. Click **(Preferences)** and, in **Calculation tab**, set **QE Version** appropriately, then click **OK**. (For QE 5.2.1, select '<6.8'; for QE 7.1 included with CygwinWM, select '7.1').



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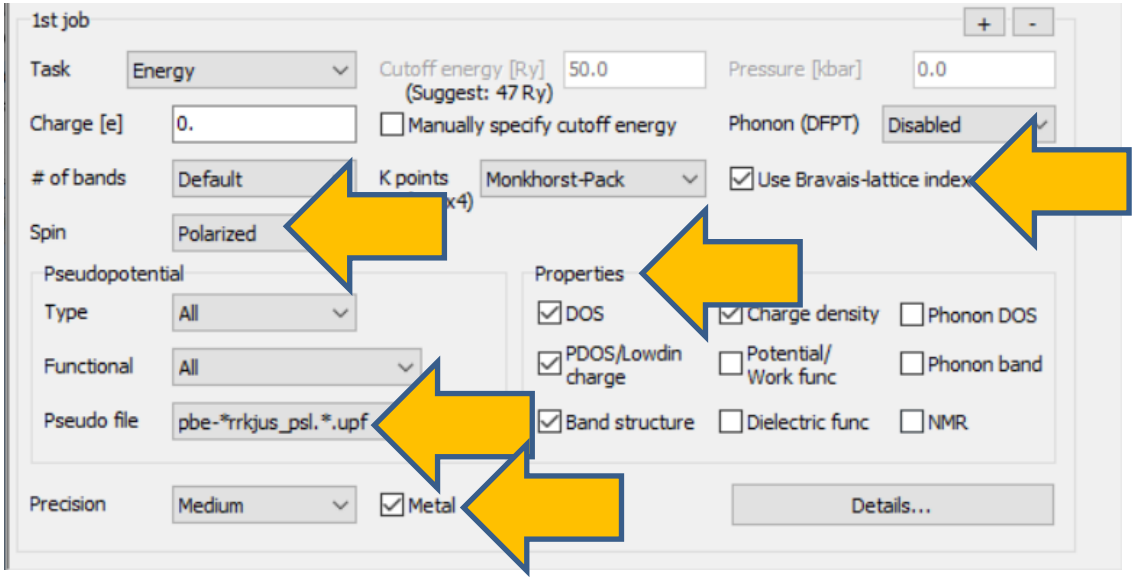
E. Execution of Calculation （NiO）

A. Select **Quantum ESPRESSO** from Toolbar's **Solver** and click **(Workflow Setup)**.
B. In **Quantum ESPRESSO Workflow Setup** window, make the following changes:
   - Change **Spin** to **Polarized**
   - Check **Use Bravais-lattice index**
   - Change **Pseudo file** to **pbe-*rrkjus_psl.*.upf**
   - Check **Properties** for **DOS**, **PDOS/Lowdin charge**, **Band structure**, and **Charge density**
   - Check **Metal**



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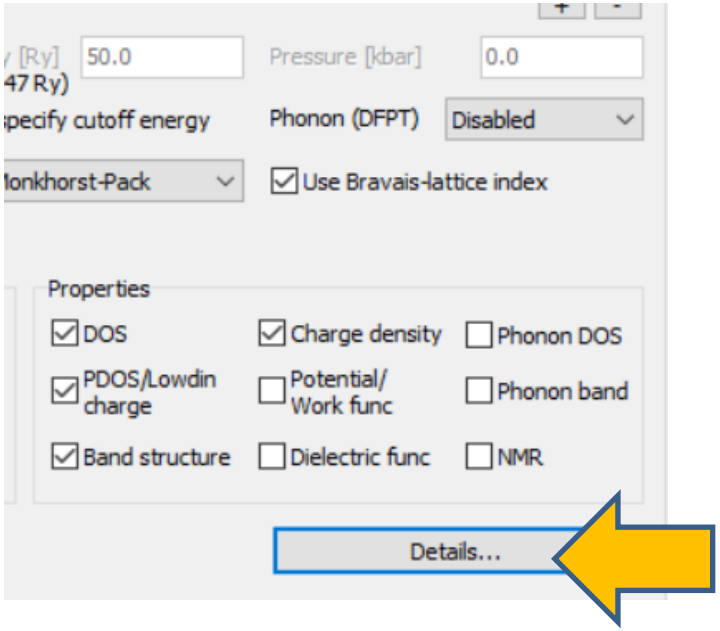
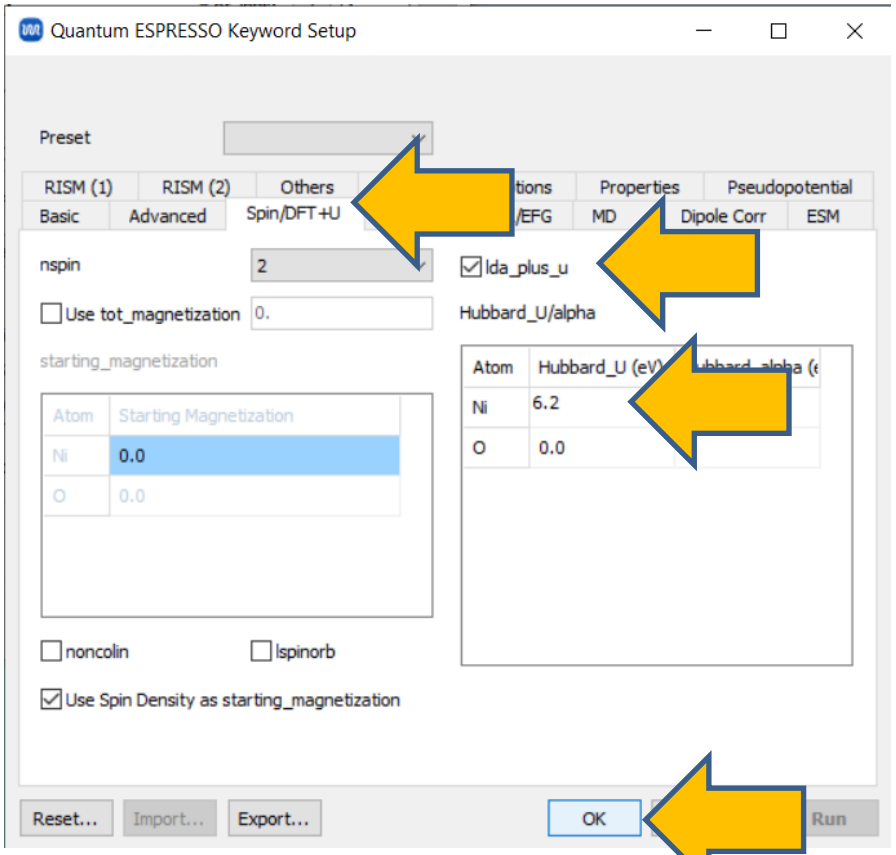
E. Execution of Calculation （NiO）

A. Click **Details**, and in **Spin/DFT+U** tab, check **lda_plus_u** and change **Hubbard_U** for **Ni** to '6.2' (referring to the value from Materials Project). Click **OK**.

B. Click **OK**, adjust settings as needed in **Job Setting** window, and then click **Run**.





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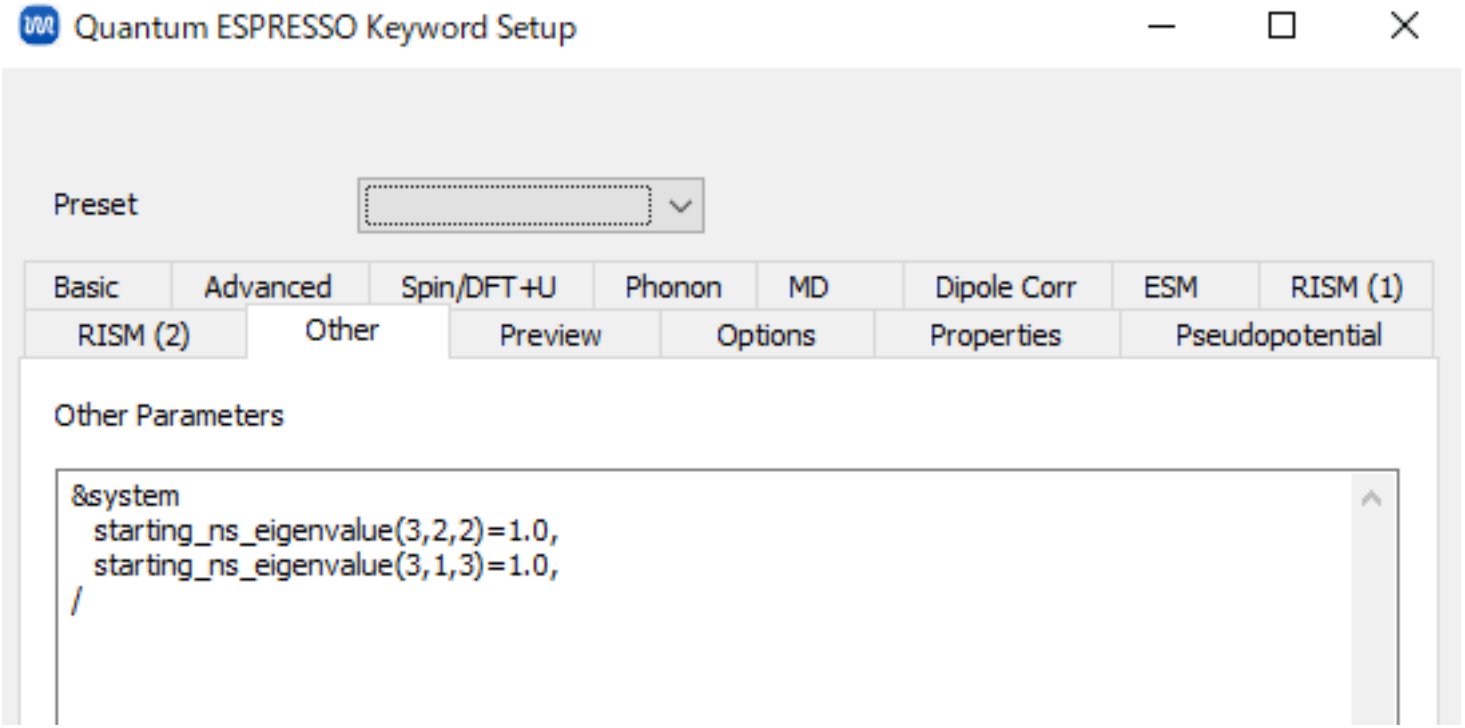
Supplement: Adjusting Initial Values

In some cases, it might be necessary to set starting_ns_eigenvalue and adjust its initial value. In such cases, input as shown below in **Other** tab of **Details…**. The first and second indices of starting_ns_eigenvalue (m, ispin) should be set according to the system, and the third index (ityp) should be determined after running a calculation (since the same element can have different typs if starting_magnetization differs).



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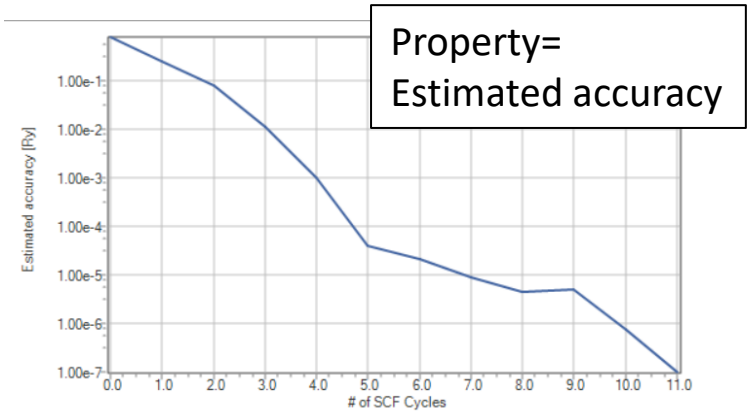
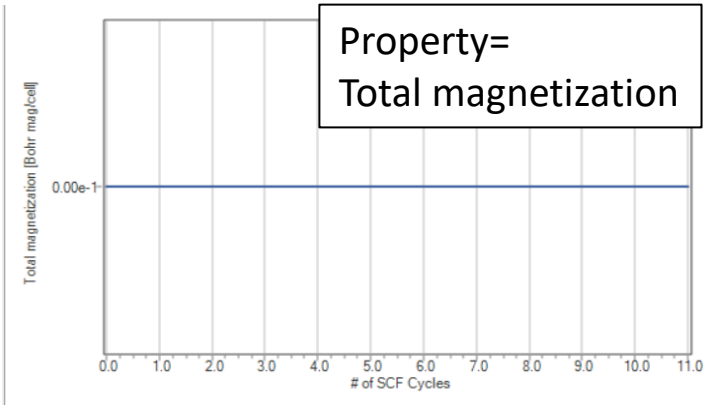
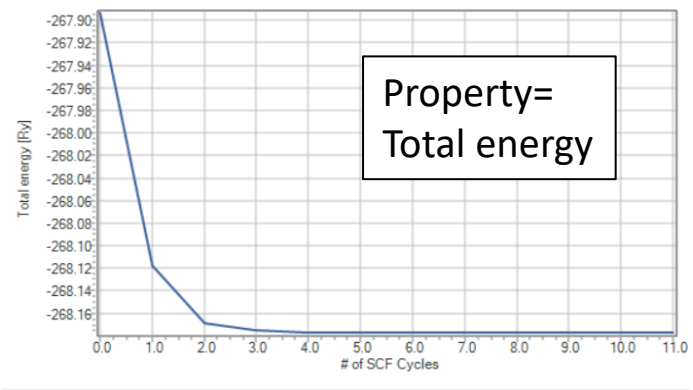
F. Analysis of Results（NiO） SCF Energy Change

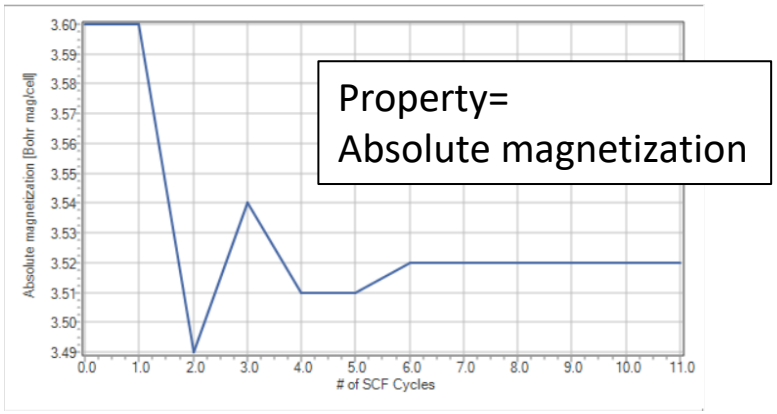
A. Click work1_QE_SCF in **Working folders** and then click **SCF Energy Change** under **Action**.

B. Adjust **Property** as needed and observe the convergence behavior of the SCF calculation.









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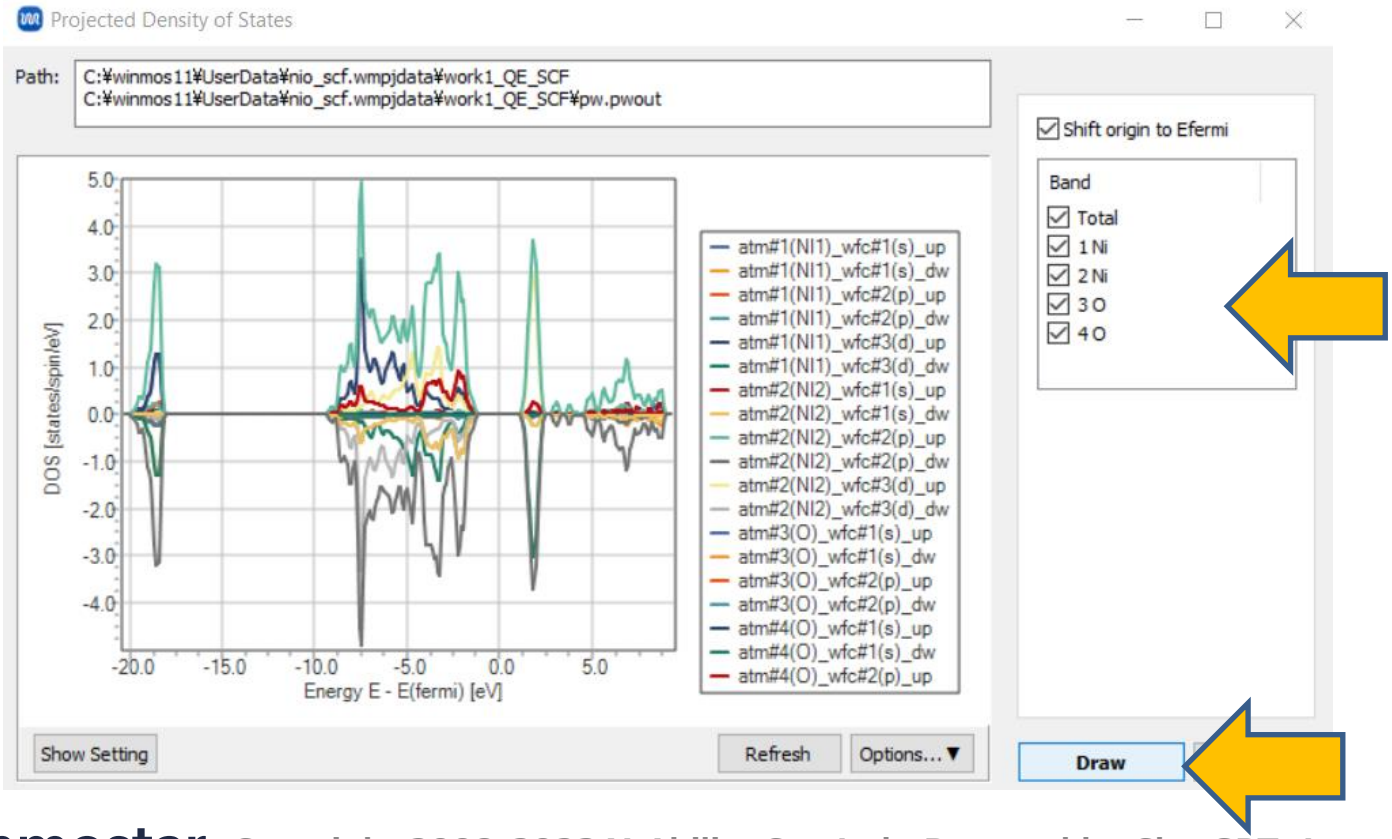
F. Analysis of Results (NiO)

Projected Density of States

A. After **the status** of **work1_QE_SCF** in **Working Folders** changes to **END(blue)**, click work1_QE_SCF in **Woriking Folders**, then click **Projected Density of States** under **Action**.

B. Adjust the checkboxes on the right side as necessary and click **Draw**.



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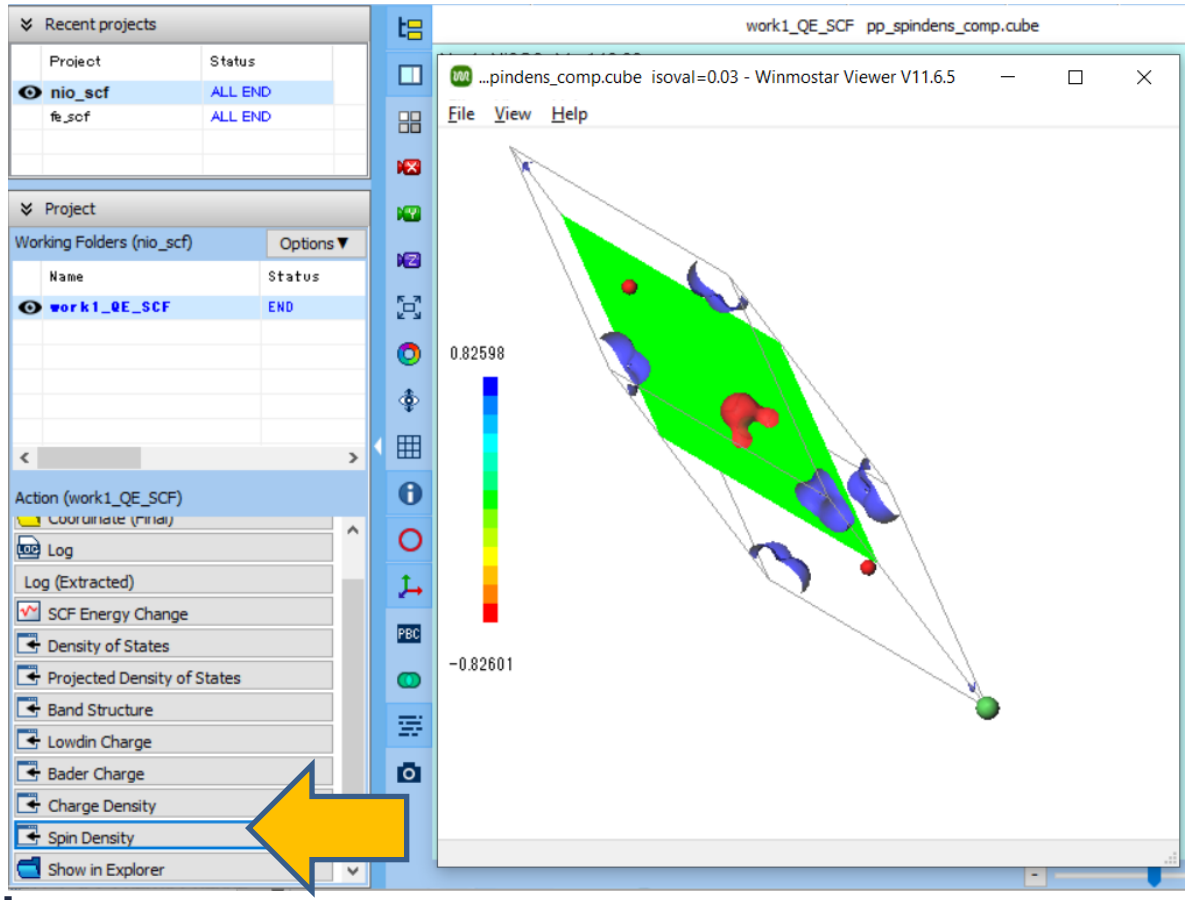
F. Analysis of Results（NiO） Spin Density

A. After **the status** of **work1_QE_SCF** in **Working Folders** changes to **END(blue)**, click work1_QE_SCF in **Woriking Folders**, then click **Spin Density** under **Action**.

B. Winmostar Viewer launches and displays the spin density.



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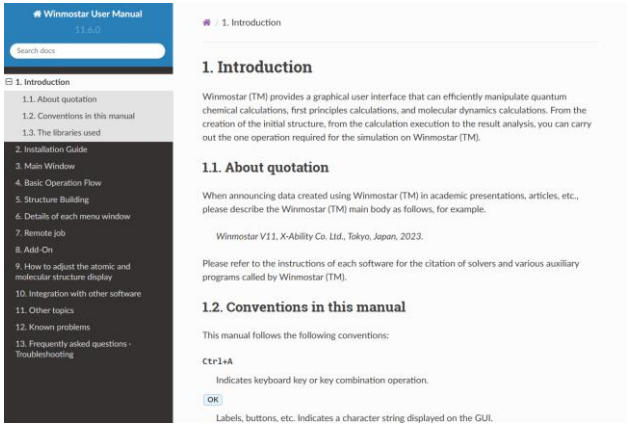
Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact page, detailing the steps to reproduce the issue and attaching any generated files at that time.

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