winmostar tutorial

Quantum ESPRESSO
Nudged Elastic Band Method

V11.7.6

19 June 2024 X-Ability Co., Ltd.

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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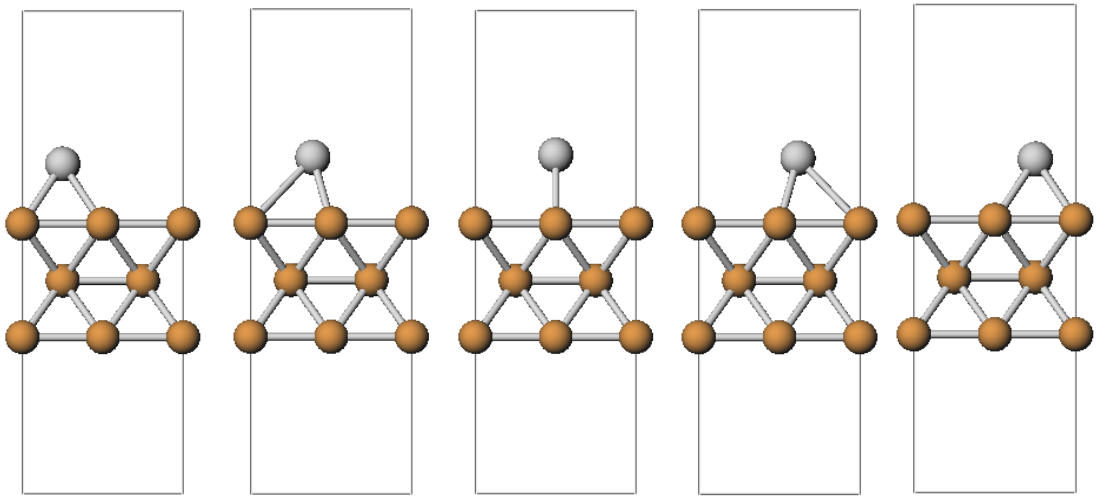
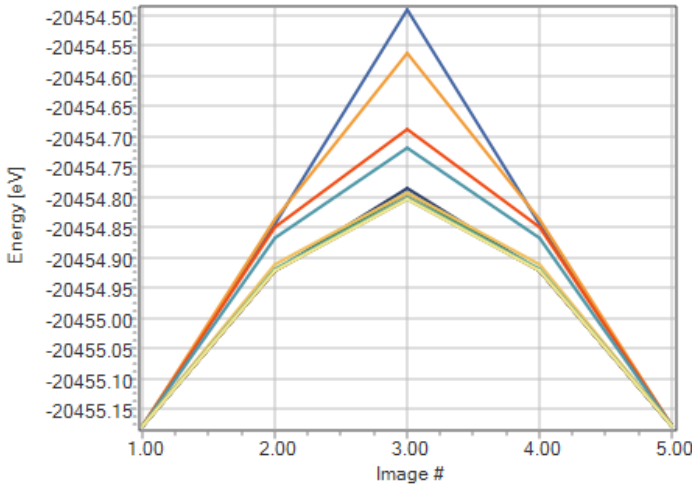
Overview

- We use the NEB (Nudged Elastic Band) method to calculate the energy barrier associated with the migration of an Ag atom between hollow sites on the Cu(100) surface. The transition process is modeled using five images along the reaction path.





Note:

- This tutorial is designed to quickly grasp the overall flow, hence it omits the relaxation of the slab's surface structure and sets the system size small. The NEB calculation will not be converged but will run for a specified number of iterations only.
- Similarly, the accuracy of electronic state calculations and structural optimization calculations is reduced.
- For a detailed explanation of Quantum ESPRESSO's calculation methods and settings, please see the following article: https://qiita.com/xa_member

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.

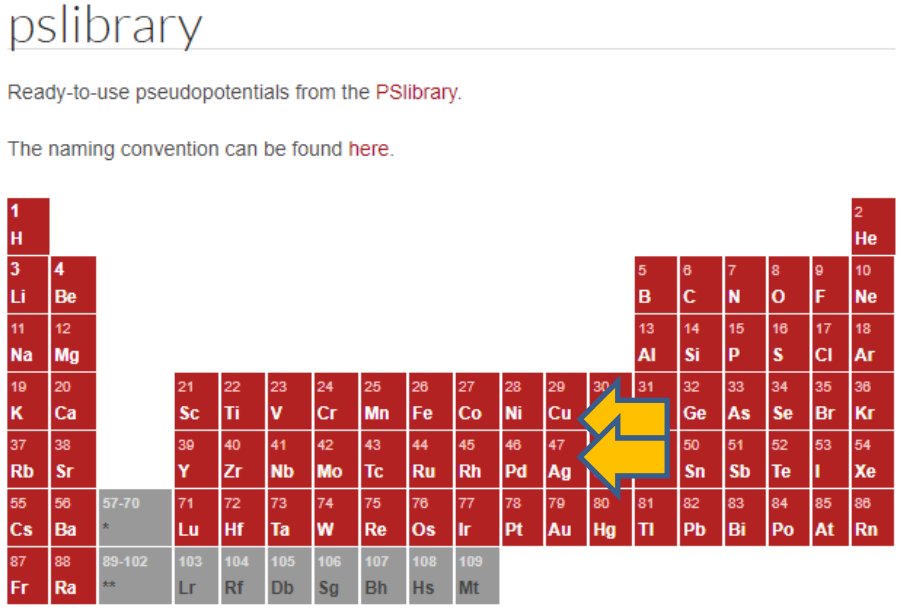
- If the above does not apply to you or if you wish to use a version of Quantum ESPRESSO other than the recommended one, you will need to install and configure Windows version of Quantum ESPRESSO separately.

Preparing Pseudopotentials

- For the implementation of this tutorial, it may be necessary to add pseudopotential files.
- Download the pseudopotential files from the following URL.

  http://pseudopotentials.quantum-espresso.org/legacy_tables

  Save [Cu.pbe-dn-rrkjus_psl.0.2.UPF] from [Cu] and [Ag.pbe-dn-rrkjus_psl.0.1.UPF] from [Ag] on the periodic table displayed on the link, into the pseudo folder under the Quantum ESPRESSO installation directory, and then restart Winmostar.

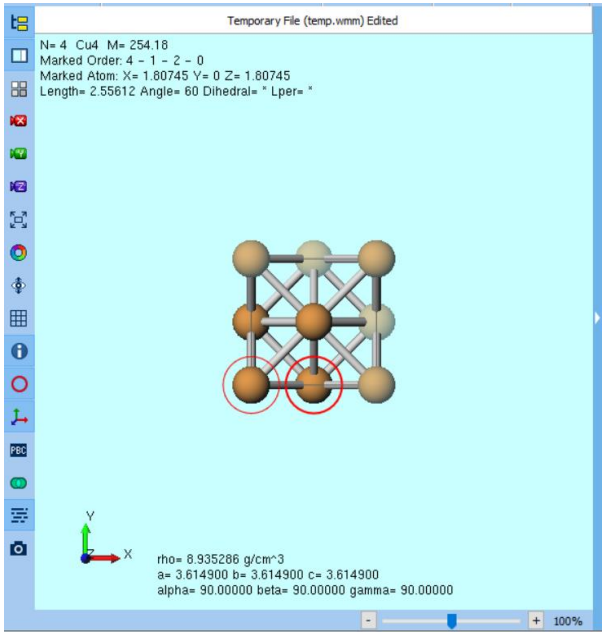


A. Modeling of the System (Initial State)

Please refer to QE Basic Tutorial for the basic operation method.

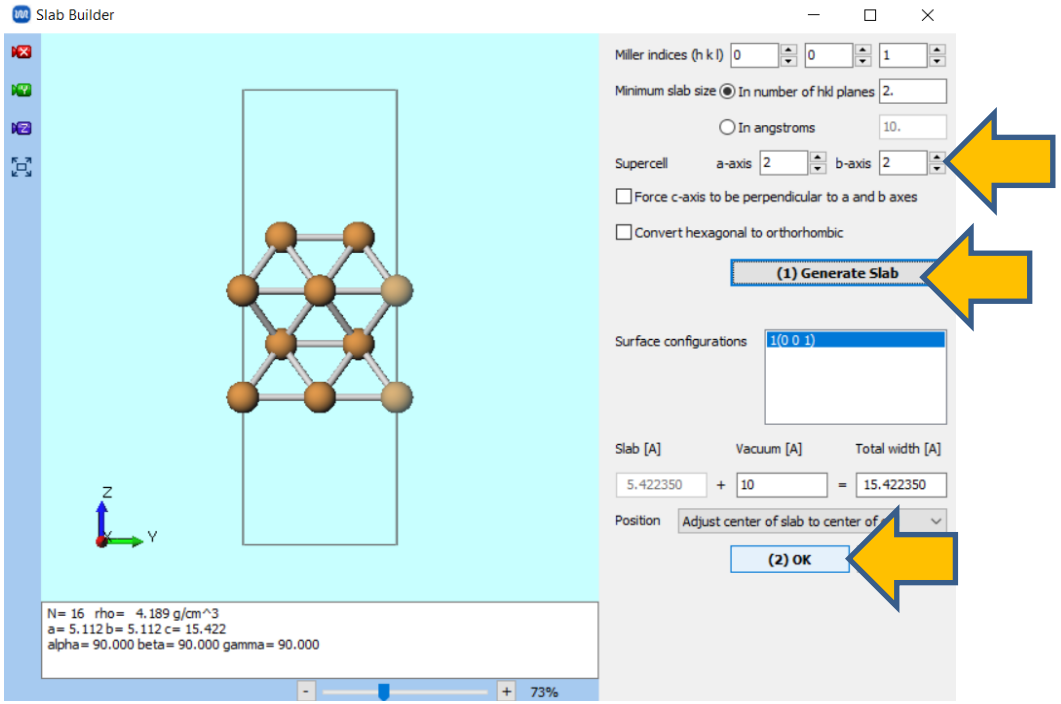
Please refer to Molecular adsorption model tutorial for the method of creating atomic and molecular adsorption models.

A. Click **File | New Project**, enter '`cu_ag`' as **Project name**, and click **Save**.
B. Click **File | Import | Samples File | cu.cif** and click **Discard and import**.
   - If you want to load a different file, use **File | Import File** at this stage instead.



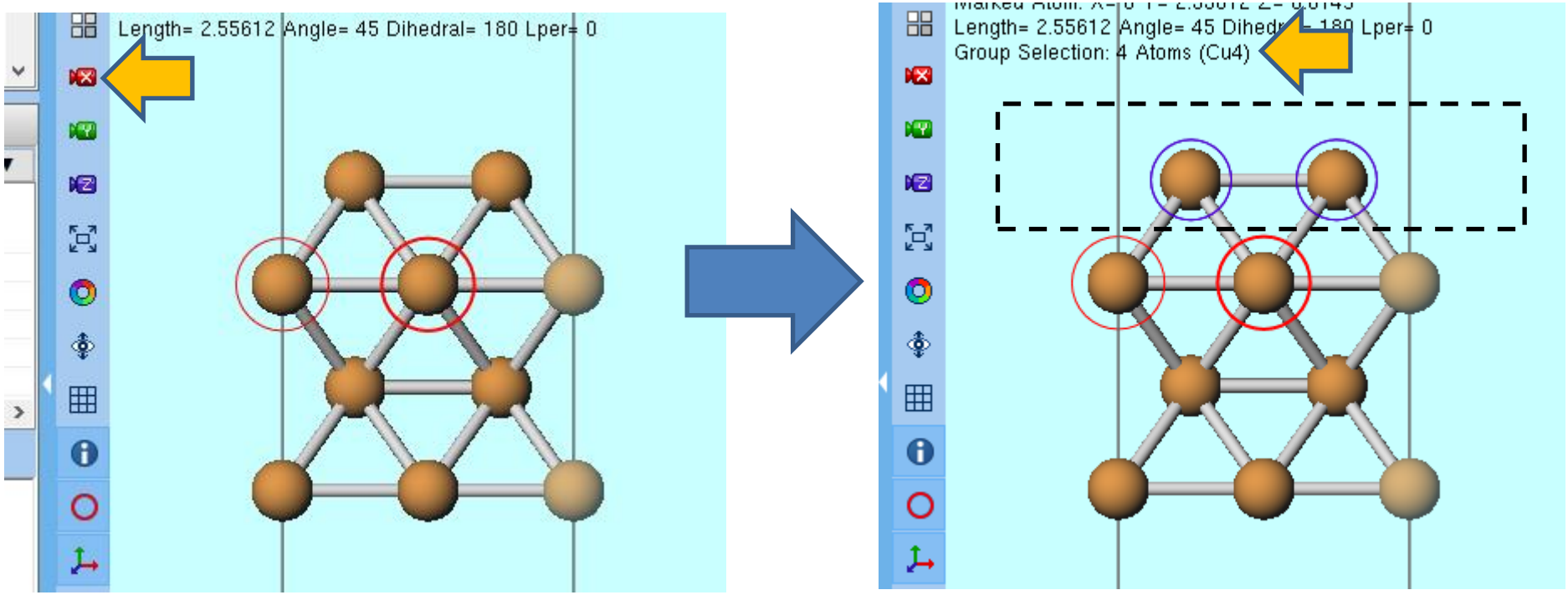
A. Modeling of the System (Initial State)

A. Click **Solid | Slab Builder**.
B. Change **a-axis** and **b-axis** of **Supercell** to '2' and click **(1) Generate Slab**.
   – Ideally, **a-axis** and **b-axis** should be larger values.
C. Click **(2) OK**.
D. Click **OK** when 'Successfully generated slab' is displayed.



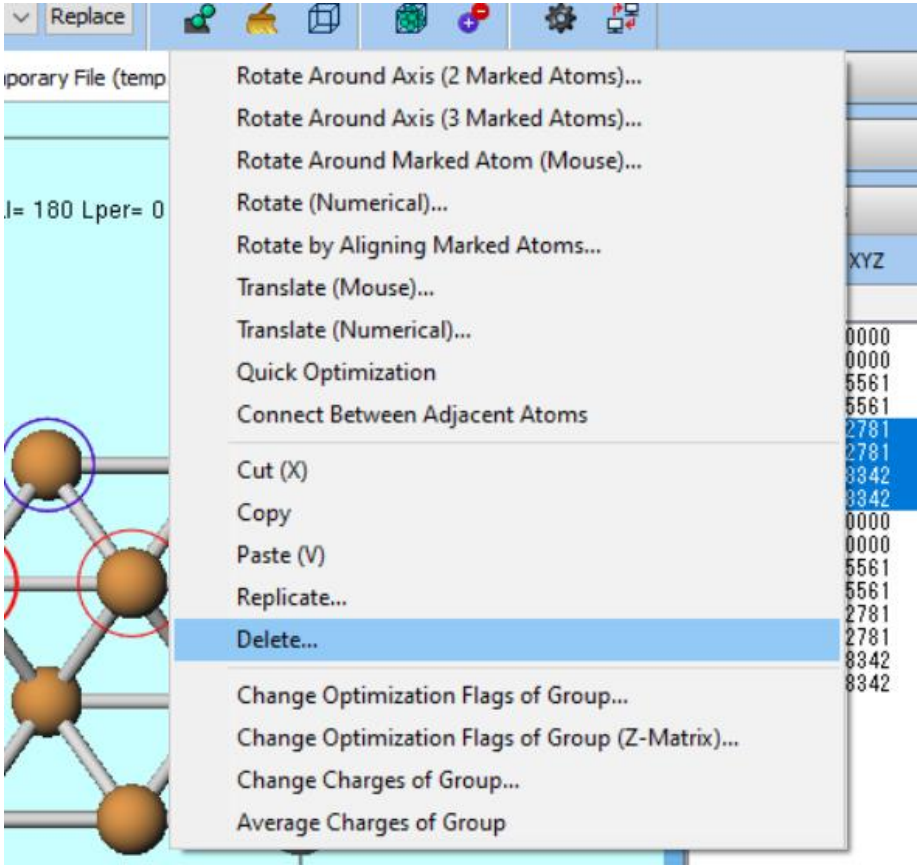
A. Modeling of the System (Initial State)

A. Click **Align View to X-axis**.
B. Use Ctrl+drag to rectangularly select the top layer of the slab.
C. Confirm that 'Group Selection: 4 Atoms (Cu4)' is displayed at the top of Viewport.



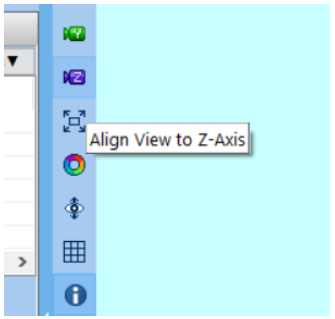
A. Modeling of the System (Initial State)

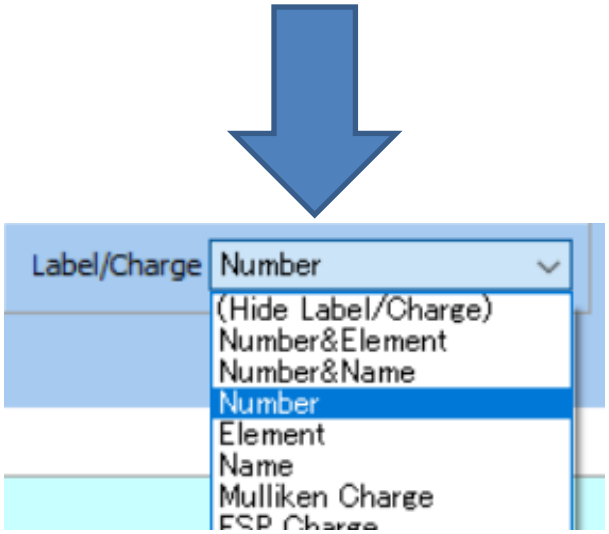
A. Click  **Modify Selected Group** | **Delete**, then click **Delete**.

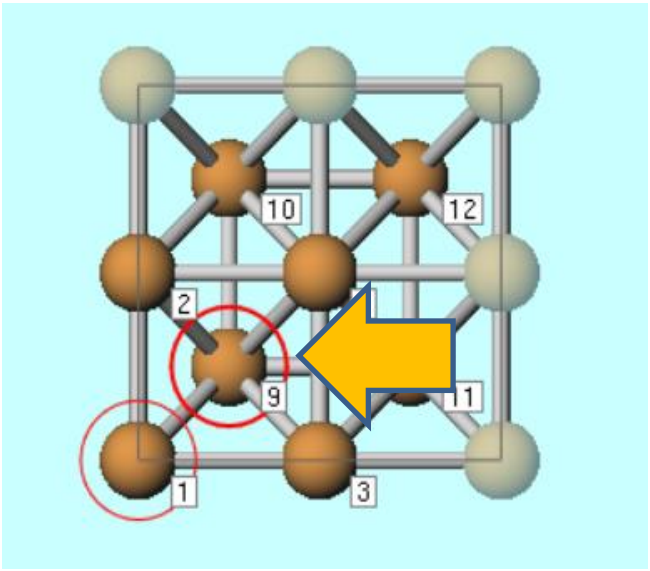


A. Modeling of the System (Initial State)

A. Click **Align View to Z-Axis**.
B. Select 'Number' from Toolbar's **Label/Charge**.
C. Click on the atom labeled '9.'







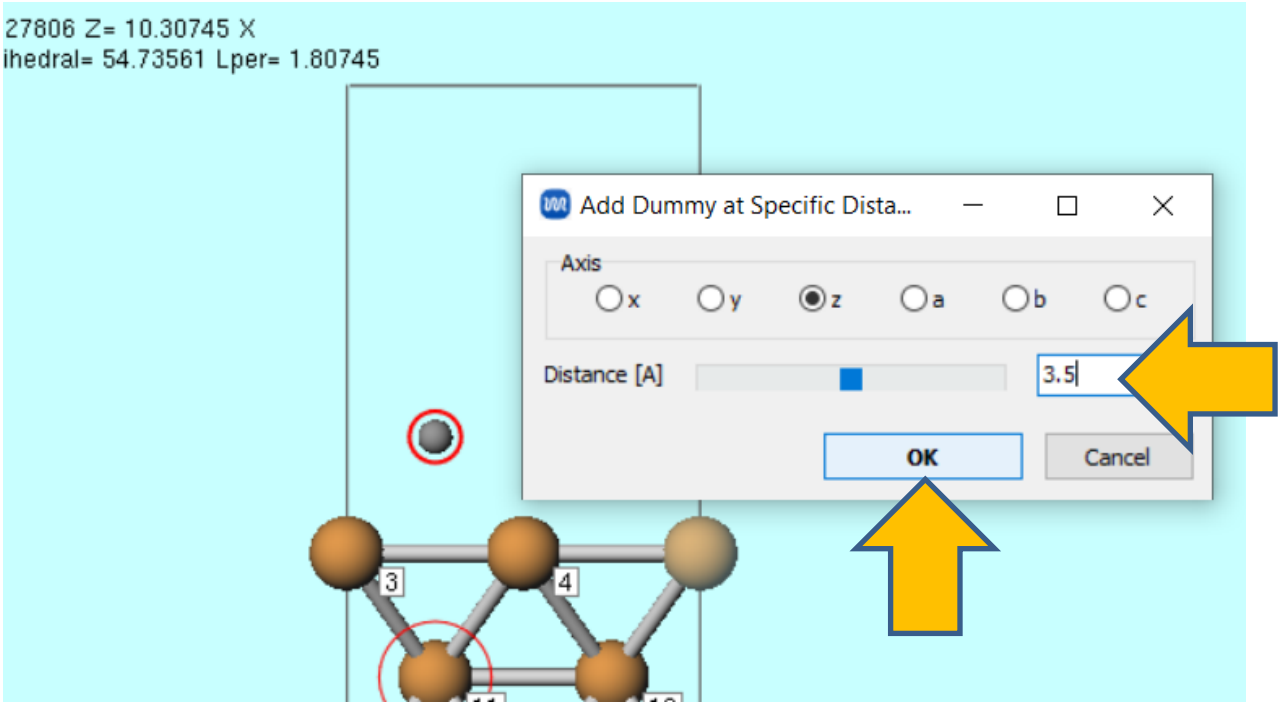
A. Modeling of the System (Initial State)

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

B. Click **Edit | Add Atom | Add Dummy Atom at Specific Distance from Marked Atom**.

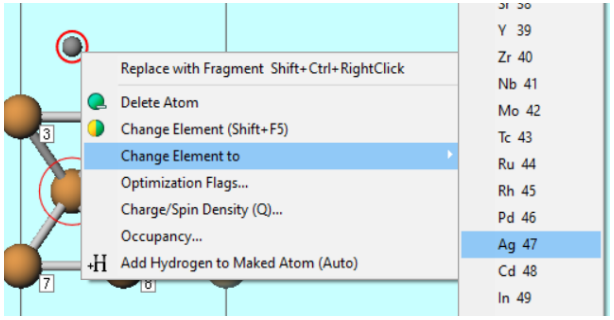
C. Enter '3.5' in **Distance** and click **OK**.

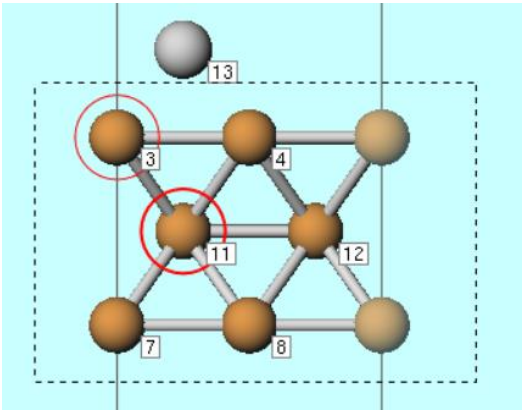
※If you want to adsorb any molecule, use **MD | Replace Molecules** afterwards. (Not required for this tutorial)

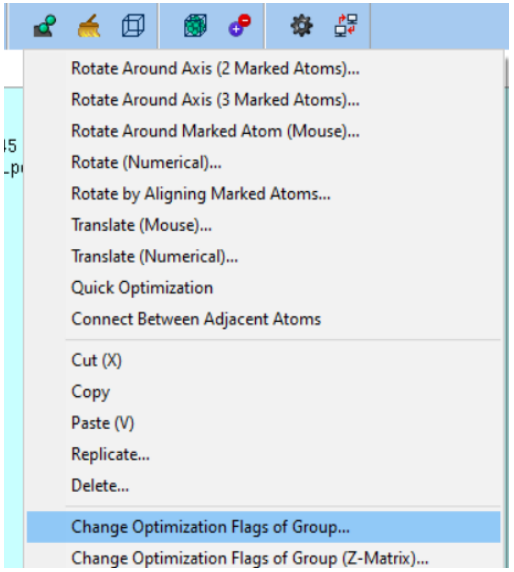


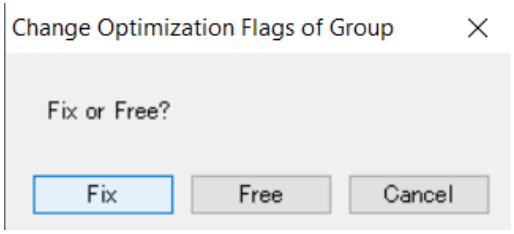
A. Modeling of the System (Initial State)

A. Right-click on the atom shown in the figure below (dummy atom) and click **Change Element to | Ag 47**.
B. Select the all 3 layers of Cu slab using Ctrl+Drag to make a rectangular selection.
C. Click  **(Modify Selected Group) | Change Optimization Flags of Group** and then click **Fix**.
D. Click **Select | Select None**.



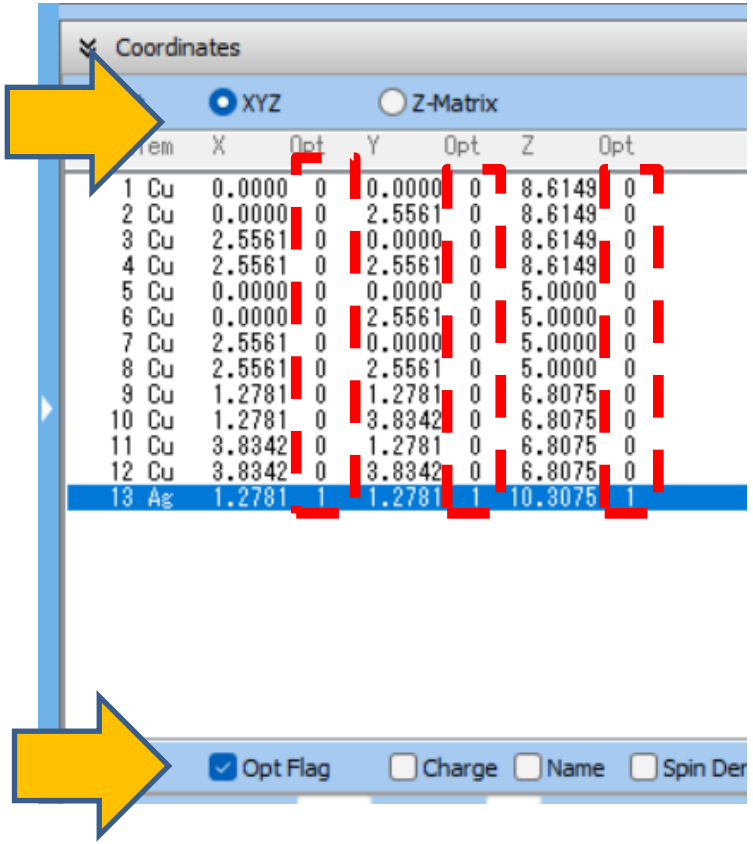






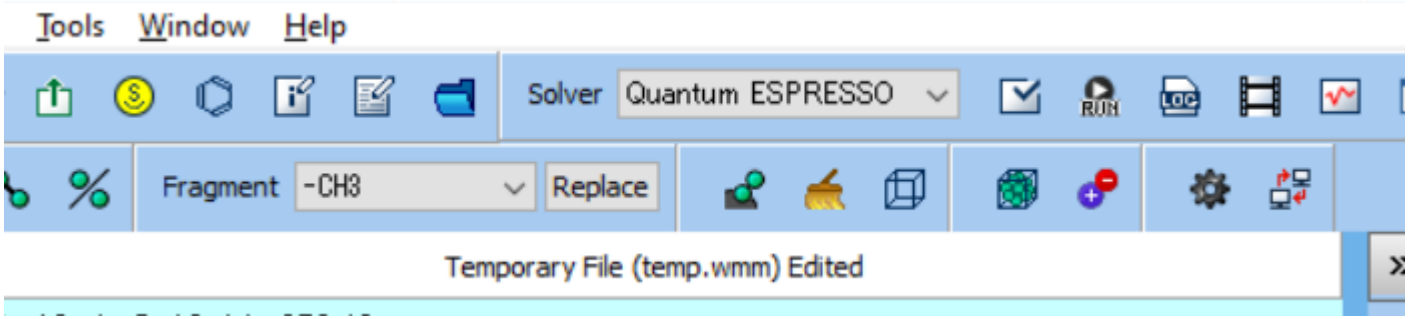
A. Modeling of the System (Initial State)

A. Check **XYZ** in **Format** of **Coordinate Viewer** and check **Opt Flag** in **Items**. Confirm that only XYZ component of the 13th atom (Ag) is marked as '1', and all others are '0'.



B. Execution of Calculation(Initial State)

A. Select **Quantum ESPRESSO** as **Solver**.
B. Click **Workflow Setup**.

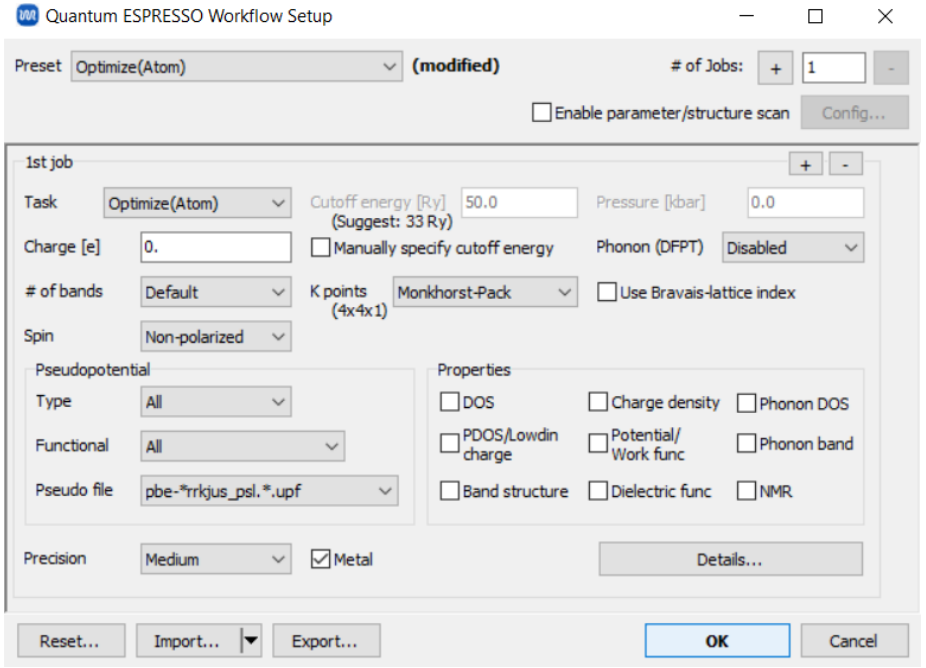


B. Execution of Calculation(Initial State)

A. Change **Preset** to 'Optimize(Atom)', switch **Pseudo file** to 'pbe-rrkjus_psl..upf', and check the box for **Metal**.
   - If 'pbe-rrkjus_psl..upf' is not available as an option for **Pseudo file**, obtain the pseudopotential file following the instructions in section P.5.

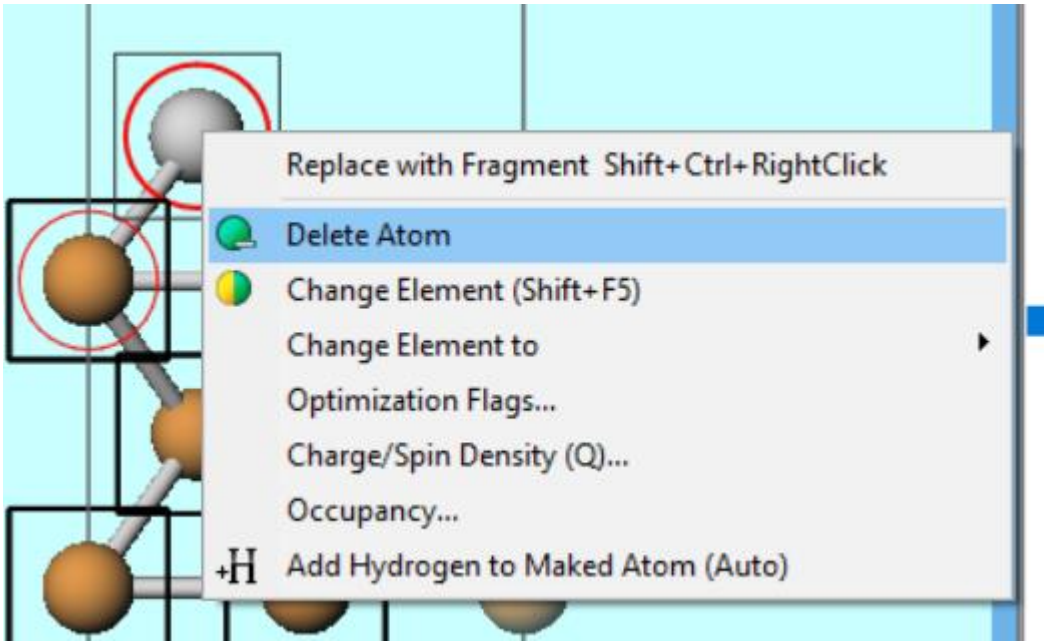
B. To decrease the computation time at the expense of accuracy, change **Precision** to 'Extra-low' and **K points** to 'Gamma'.

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



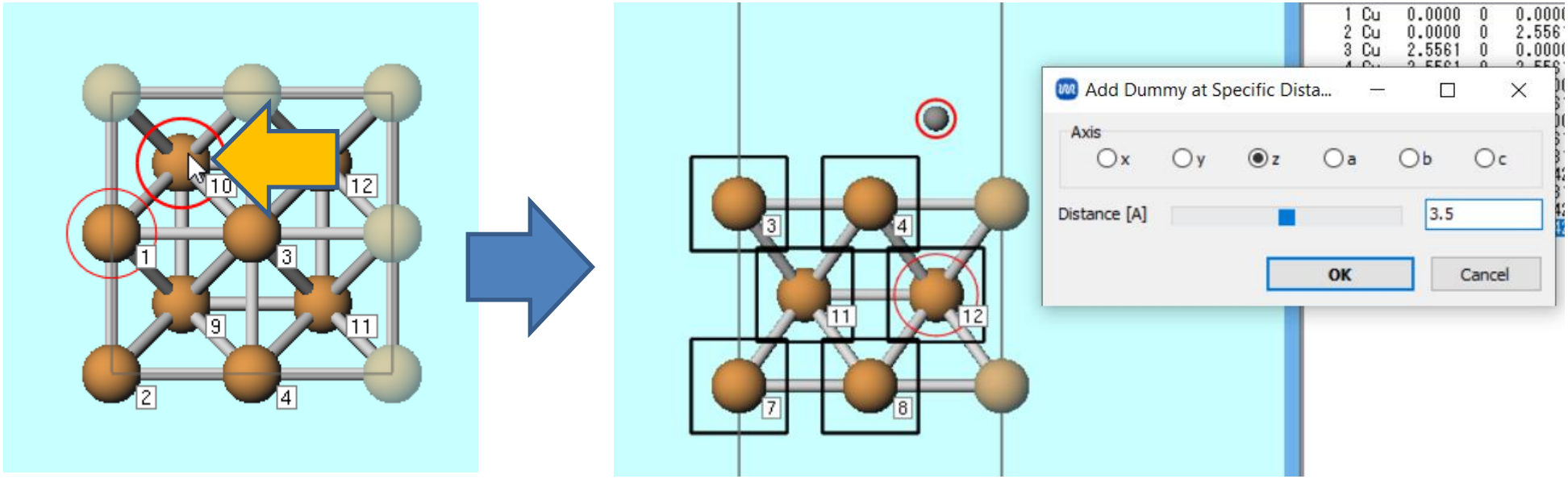
C. Modeling of the System (Final State)

A. Even if the calculation of the initial state is in progress, return to Main window, right-click on the 13th Ag atom, and click **Delete Atom**.
B. When asked 'Are you sure you want to delete 13Ag?', click **Yes**.



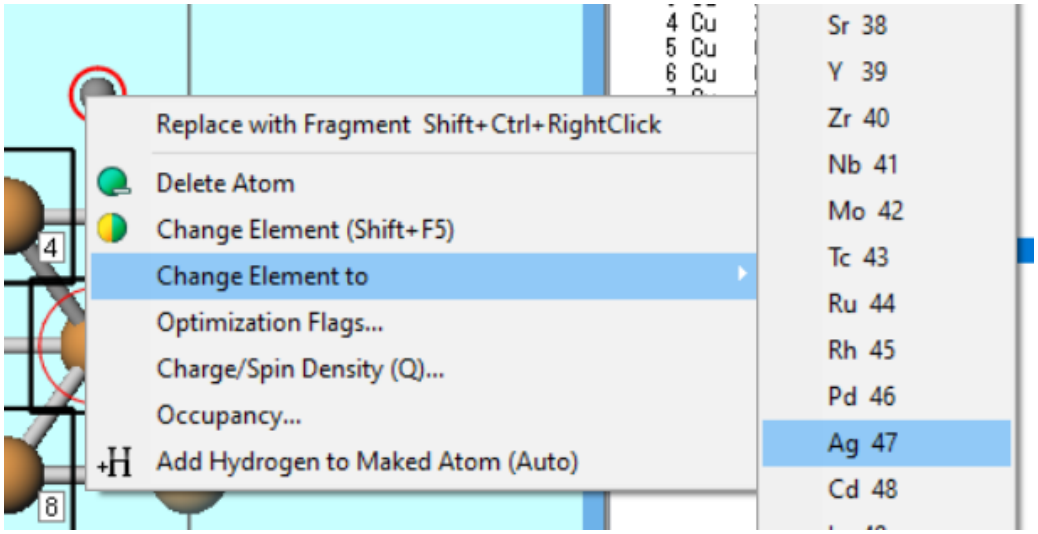
C. Modeling of the System (Final State)

A. Click  **Align View to Z-Axis**.
B. Click on the atom labeled '10'.
C. Click  **Align View to X-Axis**.
D. Click **Edit | Add Atom | Add Dummy Atom at Specific Distance from Marked Atom**.
E. Enter '3.5' in **Distance** and click **OK**.



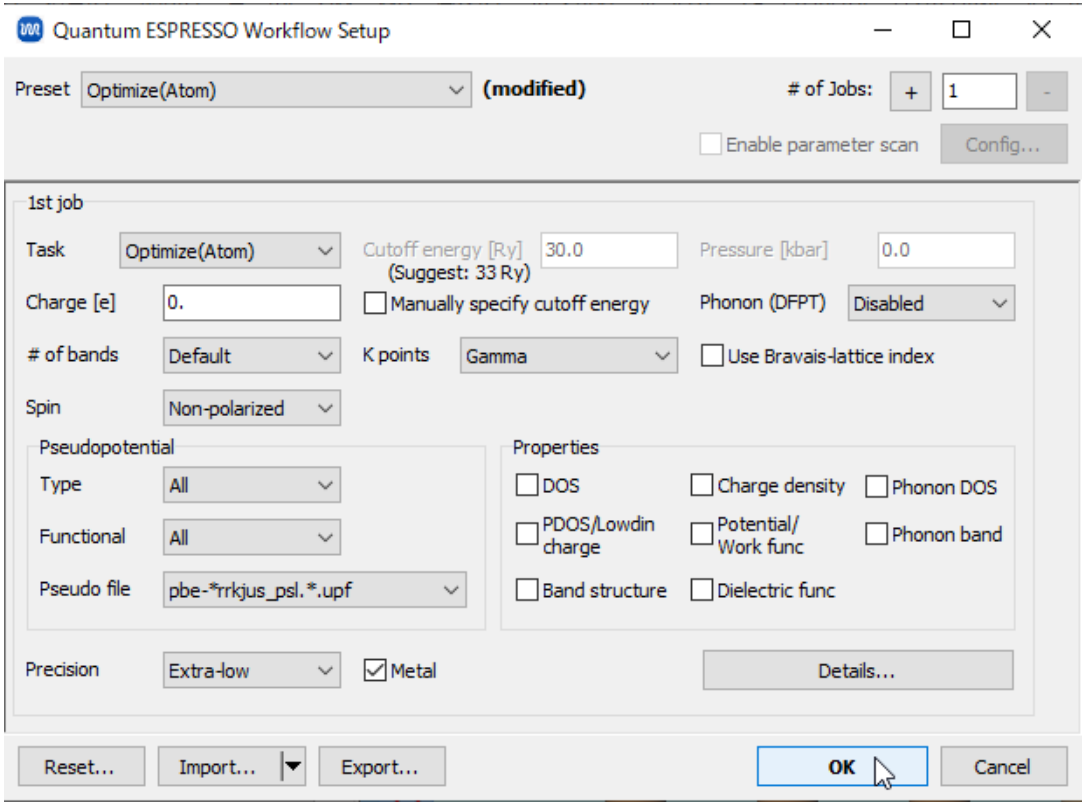
C. Modeling of the System (Final State)

A. Right-click on the atom shown below (dummy atom) and click **Change Element to | Ag 47**.



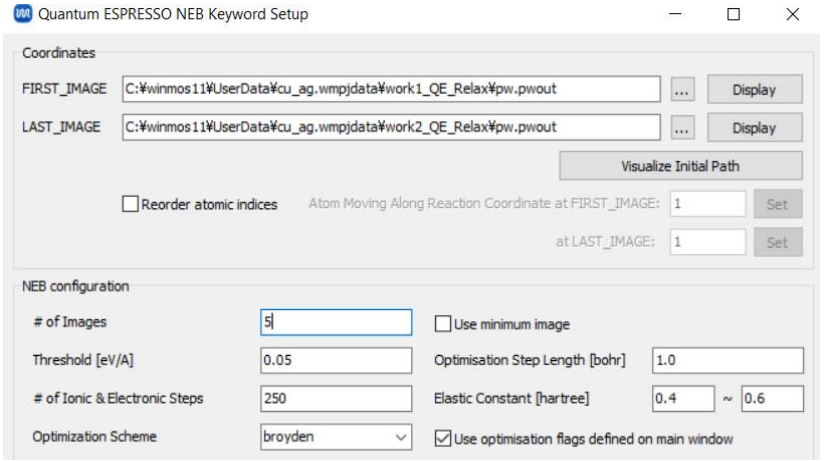
D. Execution of Calculation(Final State)

A. Click **Workflow Setup**.
B. If asked 'Do you want to continue from previous run?', click **No**.
C. Click **OK** in **Quantum ESPRESSO Workflow Setup** window, then adjust settings as needed in **Job Setting** window and click **Run**.



F. Execution of Calculation (NEB Calculation)

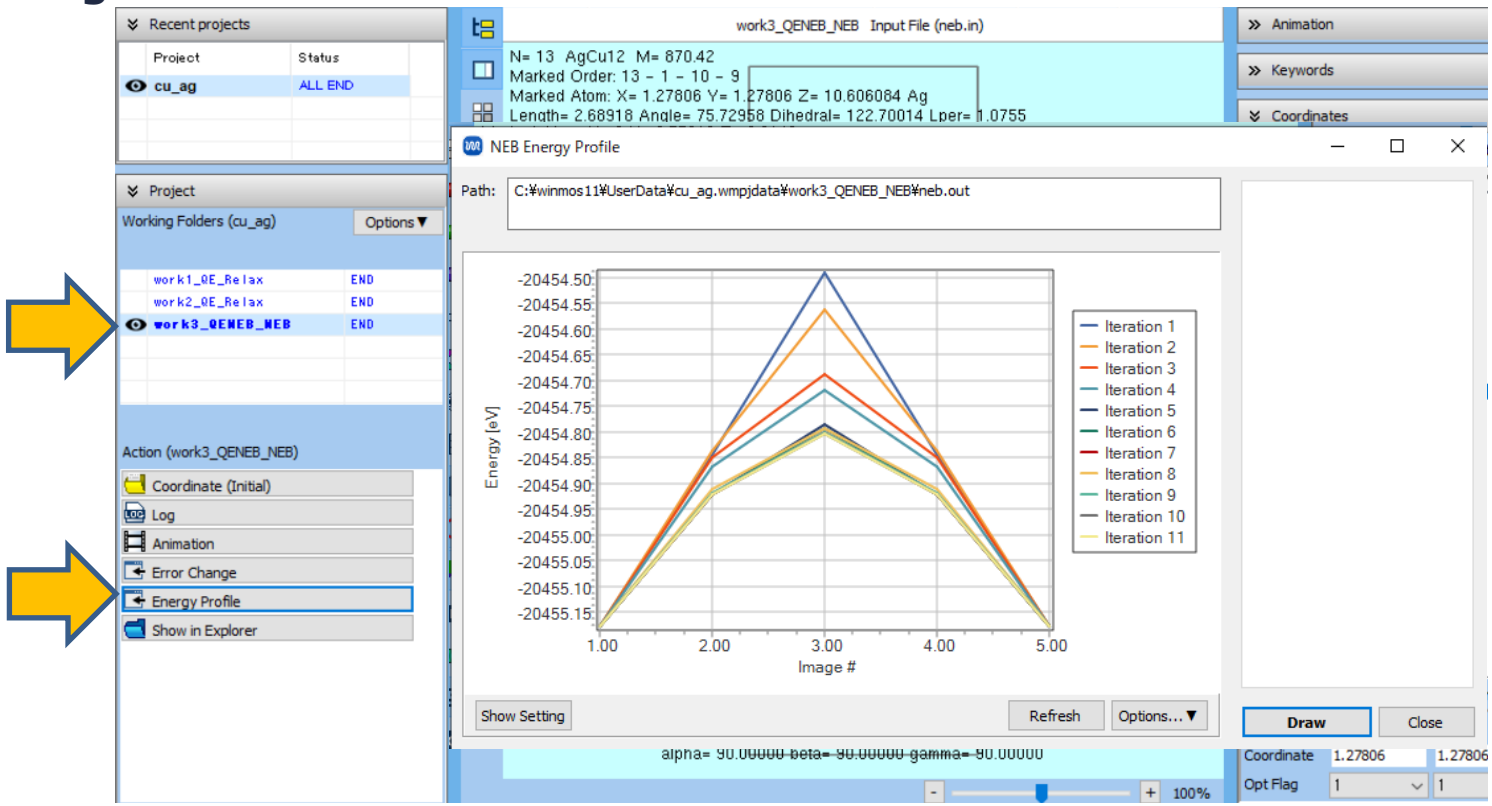
A. Once the status of the initial and final state calculations (work1, work2) changes to **END** or **END(-)**, click **Solid | Quantum ESPRESSO | Nudged Elastic Band | Workflow Setup**.
B. Click **...** button for **FIRST_IMAGE** and open `pw.pwout` from `work1_QE_Relax`.
C. Click **...** button for **LAST_IMAGE** and open `pw.pwout` from `work2_QE_Relax`.
D. Change **# of Images** to '5'.
E. If you wish to decrease the computational accuracy to finish the calculation faster, change **# of Images** to '3' and **Threshold** to '5'. Without decreasing the accuracy, it may take several hours to days.
F. Click **OK**, then click **Run** after setting the job in **Job Setting** window as appropriate.



G. Analysis of Results

A. To view the energy of each image at each iteration, click on 'work3_QENEB_NEB' in **Working Folders**, then click **Energy Profile** in **Action**.

B. Similarly, to observe the change in errors during the NEB calculation, click on **Error Change**' in **Action**.

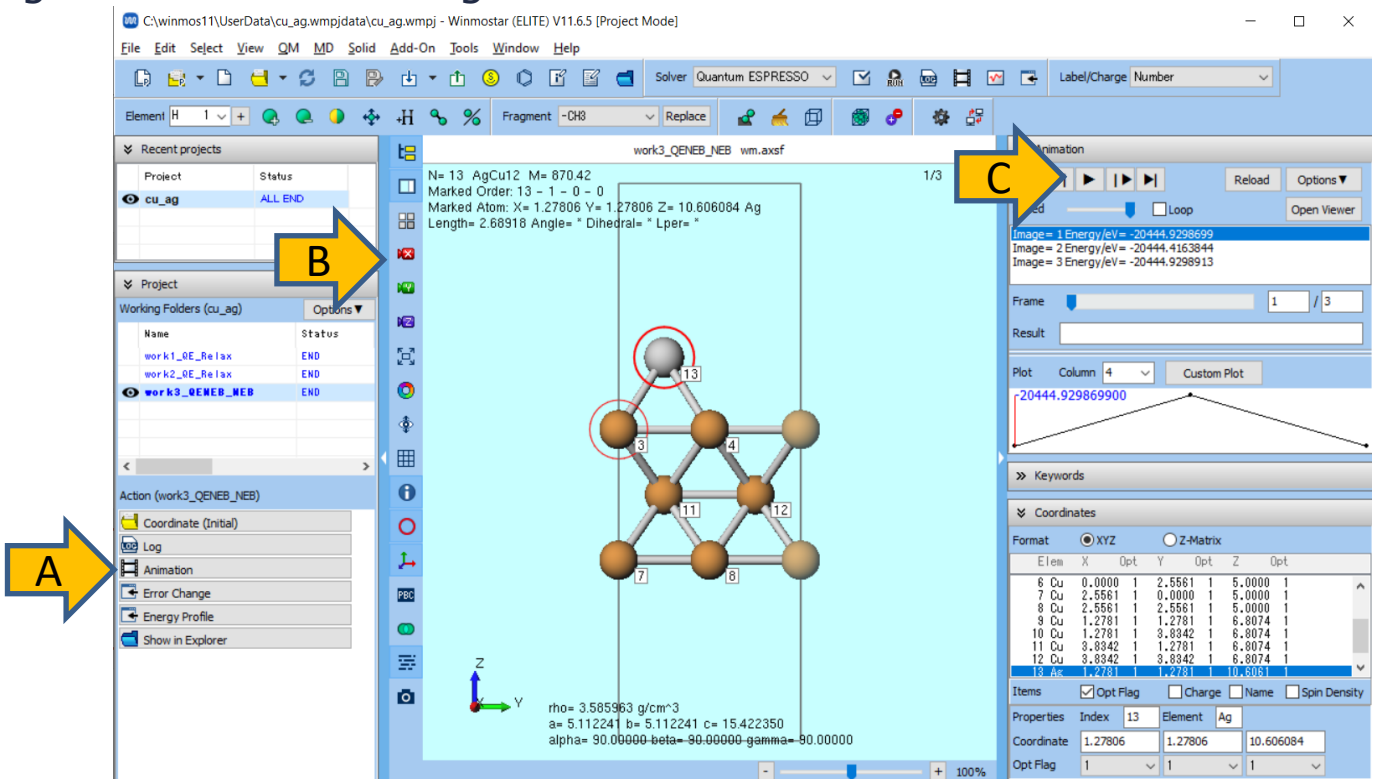


G. Analysis of Results

A. When the status of NEB calculation (work3) changes to **END** or **END(-)**, click **Animation** in **Action**.

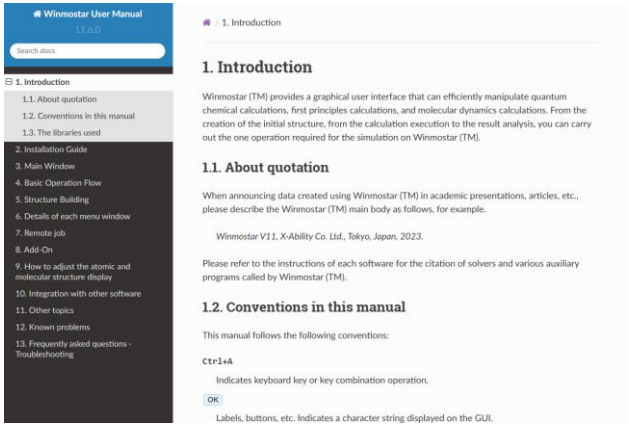
B. Click  **Align View to X-axis**.

C. In **Animation Panel**, clicking  **(Play/pause)** allows you to confirm the atomic configuration of each Image obtained in the NEB calculation eventually.



Finally

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



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Scenes from Winmostar Training Session

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