winmostar tutorial

Quantum ESPRESSO
Work Function & Surface Energy

V11.6.5

28 February 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

・In this tutorial, we calculate the work function of Pt using the difference between the potential energy of new quantum levels (bulk and slab) generated through the calculation and the Fermi energy in a surface (slab) model where the Pt(111) surface is exposed to vacuum. This difference corresponds to the work function. Furthermore, the surface energy ***σ*** per surface atom is calculated by dividing the difference between the total energy ***E*****slab** of the slab model and the total energy ***E*****bulk** of the monocrystalline (bulk) model (multiplied by the ratio ***N*** of the number of atoms in the slab to the bulk models) by the number of surface atoms ***N*****surface** in the slab model.

$$\sigma = \frac{1}{N_{surface}}\left(E_{\text{slab}} - NE_{\text{bulk}}\right)$$

– To preserve symmetry during the structure optimization process, the optimization is performed on the primitive cell.
– The exchange-correlation potential energy becomes zero in vacuum, so the vacuum level is obtained from the value of the Kohn-Sham effective potential energy minus the exchange-correlation potential energy.
– References: N. E. Singh-Miller and N. Marzari, Phys. Rev. B 80, 235407 (2009)

Note:
・The choice of k-points, number of bands, type of pseudopotential, cutoff energy, and smearing width affect the calculation results.
・The size of the slab model and the vacuum layer also affects the calculation results.
◆ 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

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.

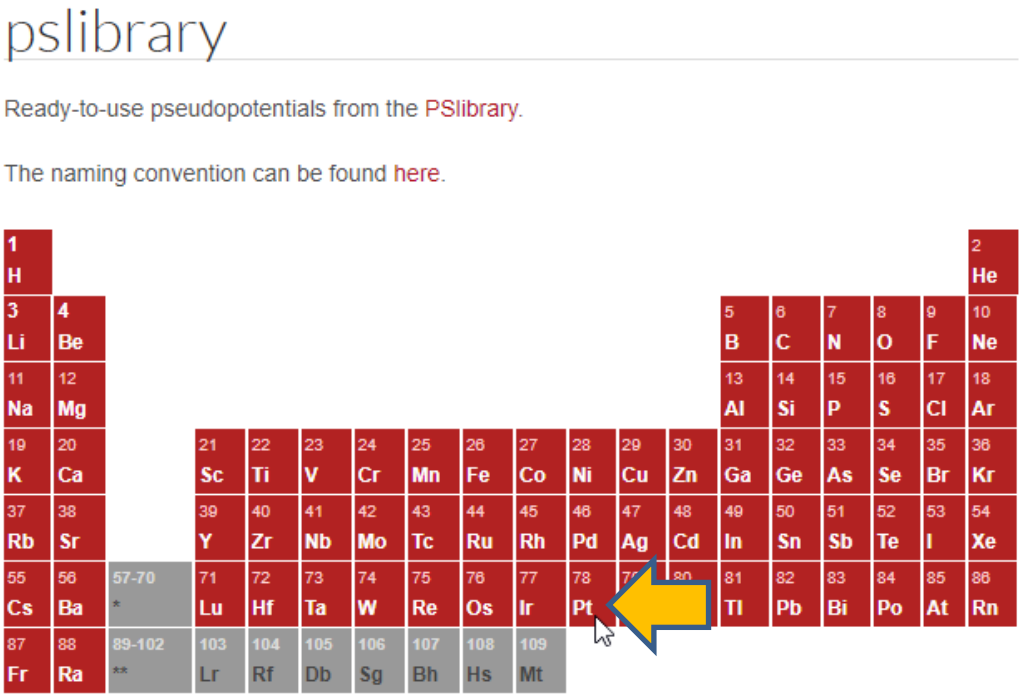
Preparing Pseudopotentials

- To conduct this tutorial, you may need to add pseudopotential files.

  Download [Pt.pbe-n-rrkjus_psl.0.1.UPF] from the periodic table [Pt] at the following URL:

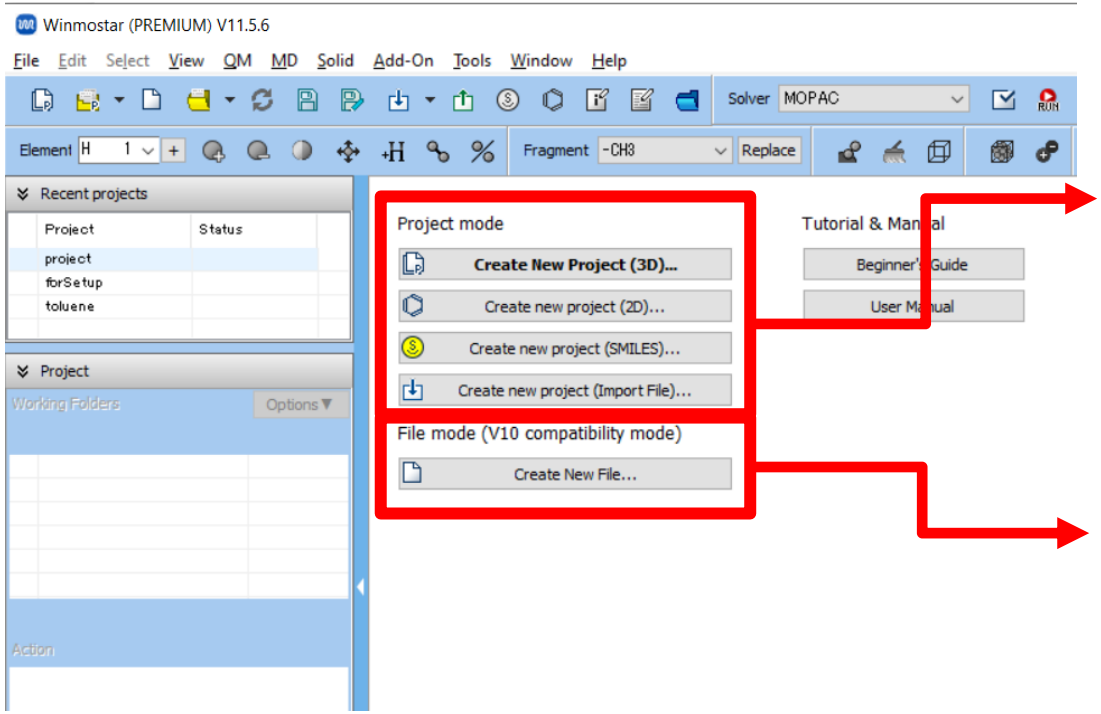
  http://pseudopotentials.quantum-espresso.org/legacy_tables

  Then, copy `Pt.pbe-n-rrkjus_psl.0.1.UPF` into the folder opened by clicking **Open QE pseudo directory** in **Calculate** tab of **Tools | Preference**.



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.

A. Modeling of the System (Optimization of Bulk Crystal Structure)

Please refer to QE Basics Tutorial for basic operation methods.

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

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

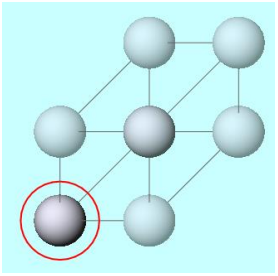
For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Methods for Creating Initial Structures'. Here, we will load an existing molecular structure file.

C. Click **File | Import | Sample File | pt.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**.

E. Click **Solid | Convert Lattice** and if asked '…Do you want to convert to primitive cell?', click **Yes**.

F. Click **OK** when 'Successfully converted lattice.' is displayed. (The structure shown below will appear)

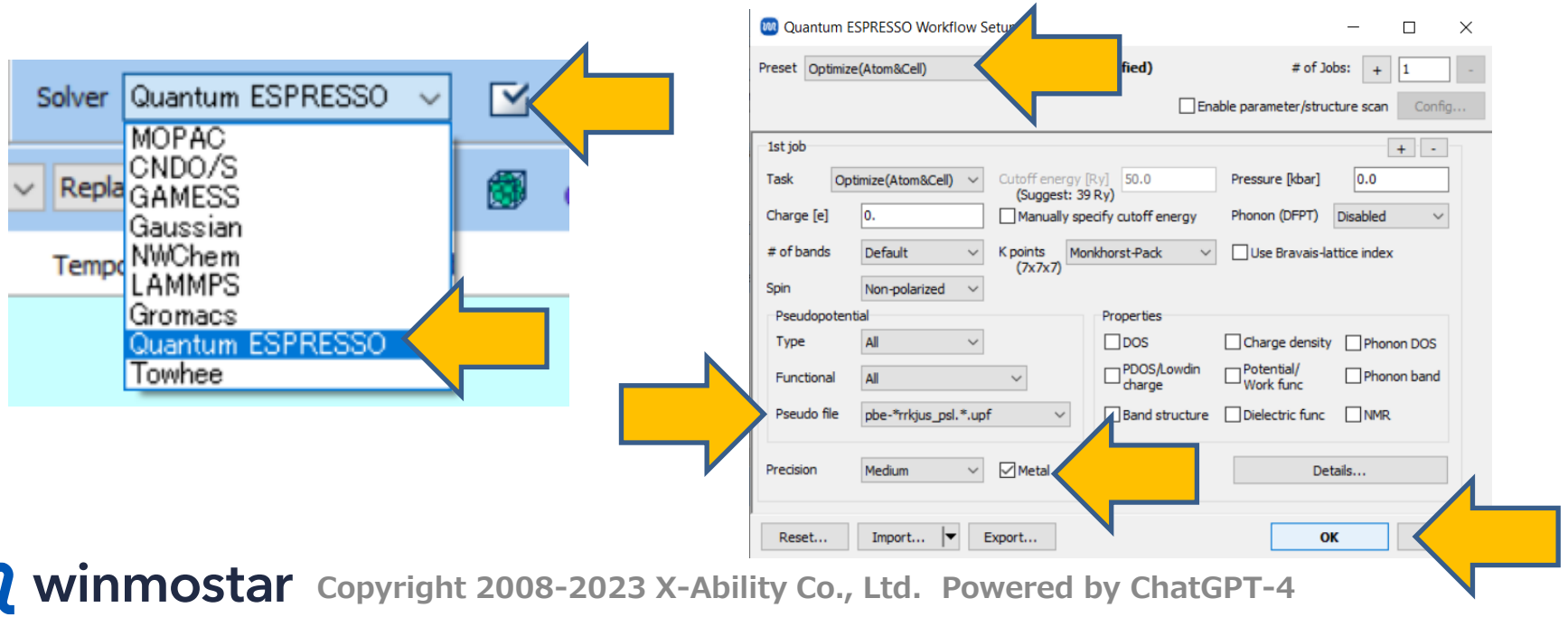


B. Execution of Calculation (Optimization of Bulk Crystal Structure)

A. Select **Quantum ESPRESSO** from **Solver**, and click **(Workflow Setup)**.

B. Change **Preset** to **Optimize (Atom & Cell)**, check **Metal**, and change **Pseudo file** to **pbe-*rrkjus_psl.*.upf**.
   - If **pbe-*rrkjus_psl.*.upf** is not available, refer to Quantum ESPRESSO for Windows Installation Manual to obtain the pseudopotential file.
   - For higher accuracy, set **Precision** to 'High' or higher, or adjust the settings appropriately in **Details**.

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



C. Modeling of the System (Optimization of Slab Model Structure)

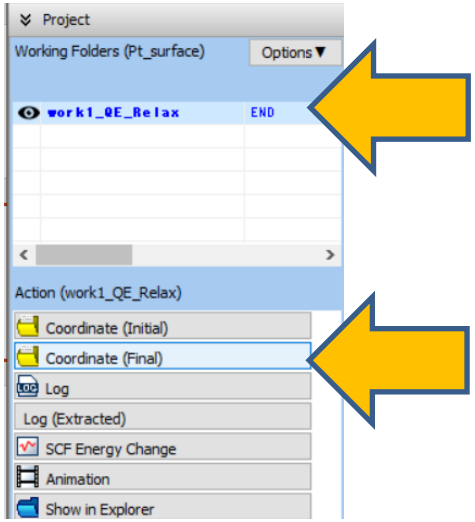
Please refer to Slab Model Tutorial for the method of creating a slab model.

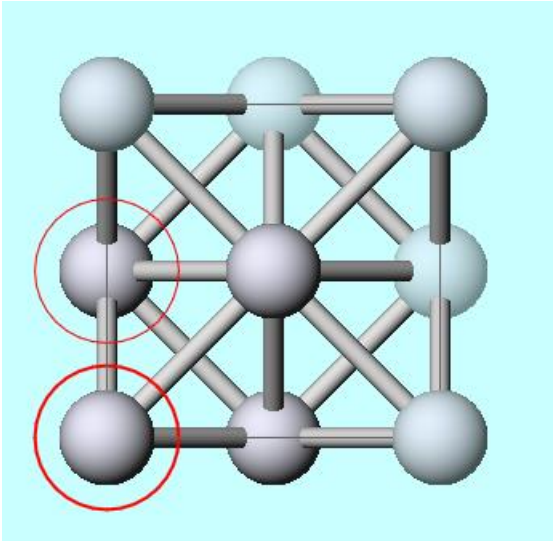
A. After **the status** of work1_QE_Relax in **Working Folders** changes to **END(blue)**, click work1_QE_Relax in **Working Folders**, then click **Coordinate (Final)** under **Action** to display the structure after optimization.

B. Click **Solid | Convert Lattice**, and if asked '…Do you want to change to an output-ready format (wmm) and continue?', click **Yes**.

C. If asked '…Do you want to convert to conventional cell?', click **Yes**.

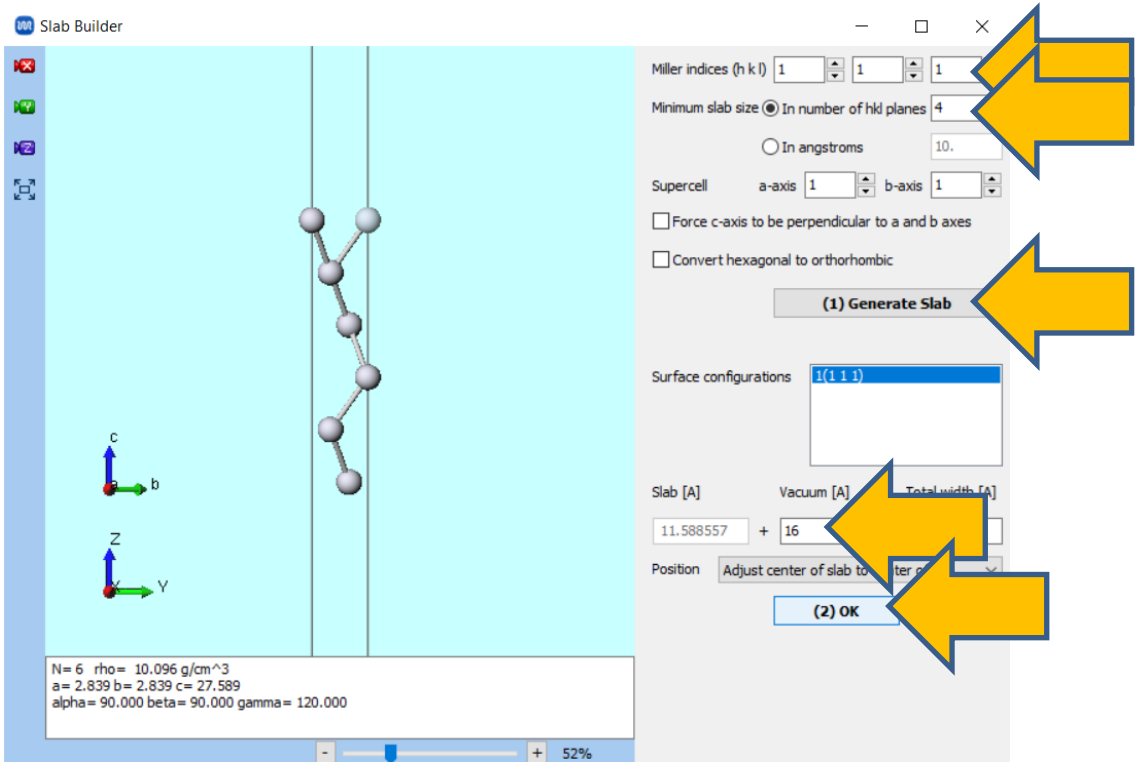
D. Click **OK** when 'Successfully converted lattice.' is displayed, and the structure on the bottom right will appear.





C. Modeling of the System (Optimization of Slab Model Structure)

A. Click **Solid | Slab Builder**.
B. Set **Miller indices** to '1', '1', '1', and change **Minimum slab size | In number of hkl planes** to '4', then click **(1) Generate Slab**.
C. Change **Vacuum** to '16', then click **(2) OK**.
D. Click **OK** when 'Successfully generated slab.' is displayed.



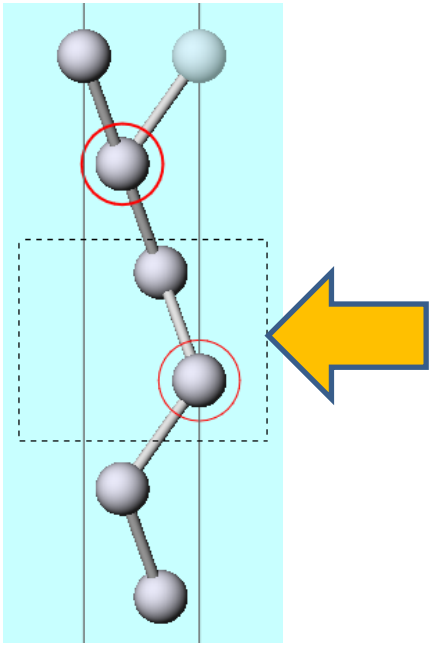
C. Modeling of the System (Optimization of Slab Model Structure)

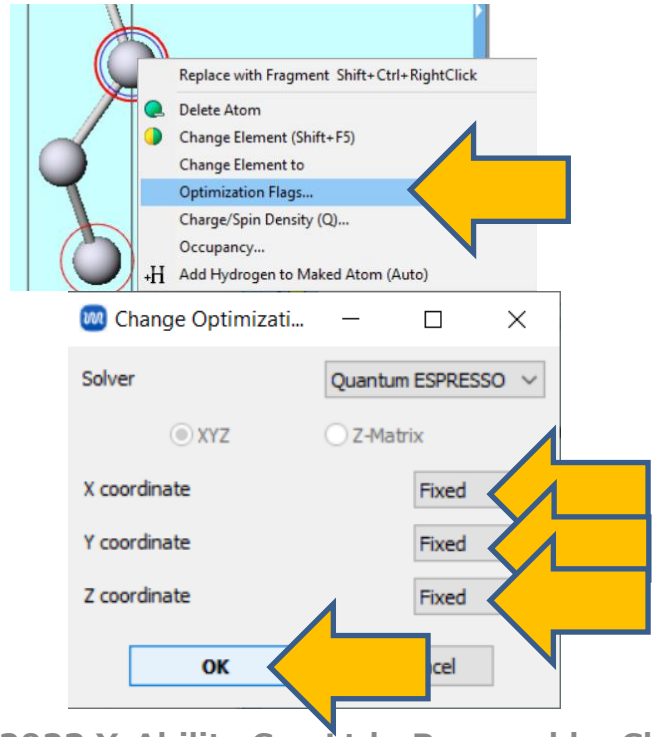
A. Click Toolbar's **Align View to X-Axis**.

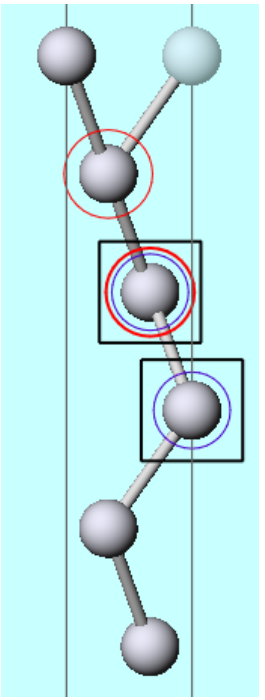
B. While holding down the **Ctrl key**, drag the mouse to **group select** the atoms corresponding to the middle two layers.

C. Right-click on the selected atoms and click **Optimization Flags**.

D. In the Change Optimization Flags window, select **Fixed** for the **X**, **Y**, and **Z** coordinates, then click **OK** button.





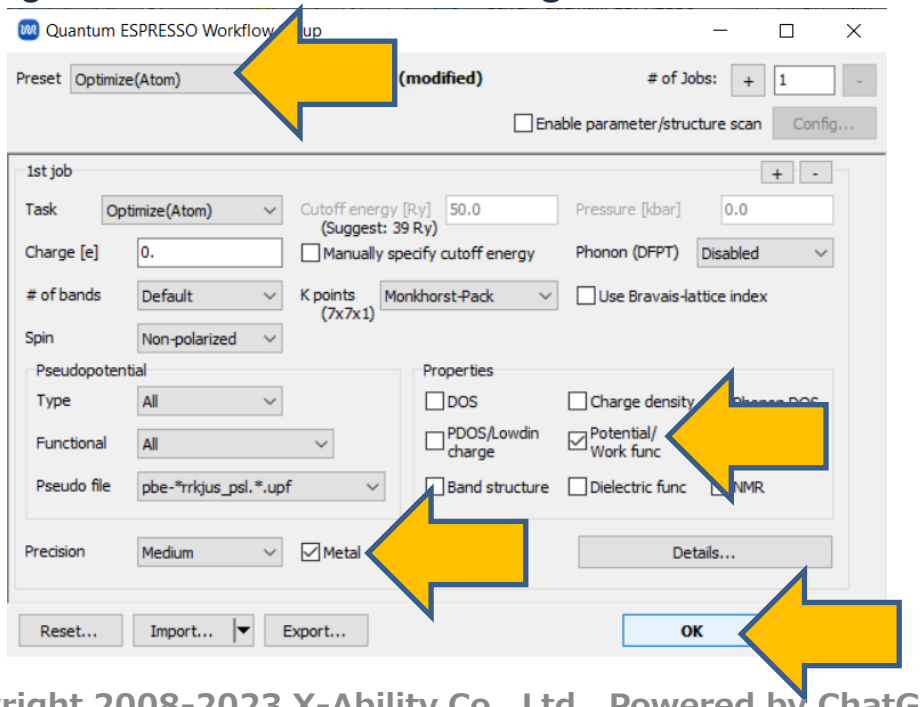


D. Execution of Calculation （Optimization of Slab Model Structure）

A. Click  **(Workflow Setup)**, and if asked 'Do you want to continue from previous run?', click **No**. If 'For the current project...' appears, click **Close**.

B. Change **Preset** to **Optimize(Atom)** and check **Metal** and **Potential/Work func** in **Properties**.
   - For higher accuracy, set **Precision** to 'High' or higher, or adjust the settings appropriately in **Details**.

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

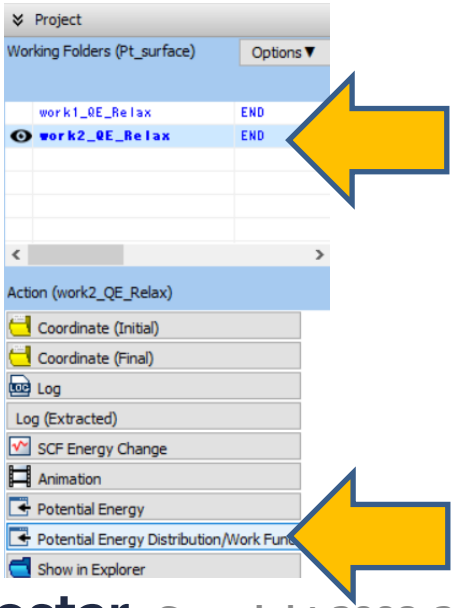


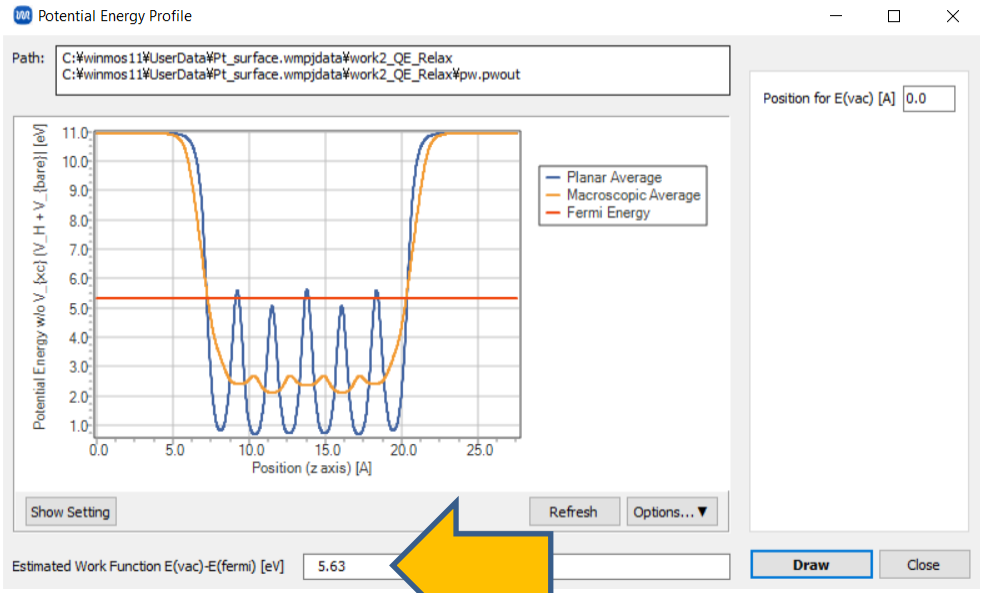
E. Analysis of Results (Work Function)

A. After **the status** of **work2_QE_Relax** in **Working Folders** changes to **END (blue)**, click work2_QE_Relax in **Working Folders** and then click **Potential Energy Distribution/Work Function** in **Action**.

B. You can check the estimated value of the work function under **Estimated Work Function**.

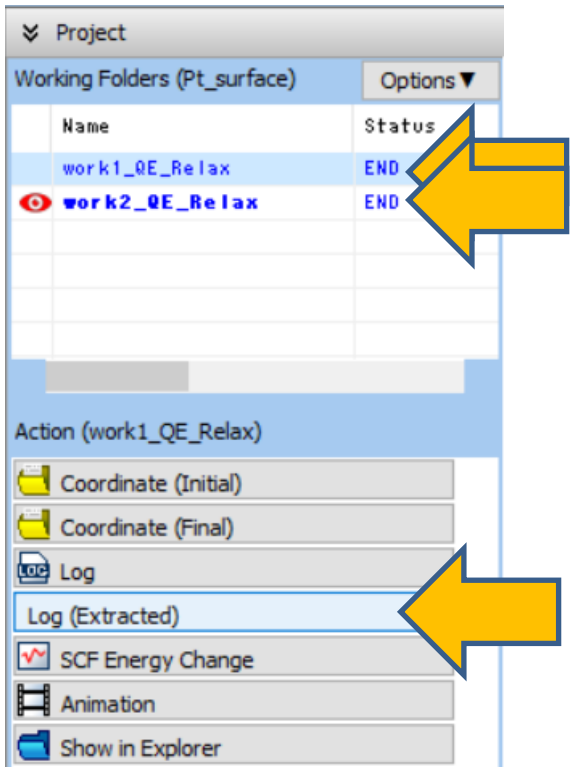
   – The **Planar Average** (blue) calculates the average potential energy within the same z-plane, while the **Macroscopic average** (orange) locally averages the Planar Average values in the z-direction. In this calculation, only the vacuum level (z→±∞) values are considered, and both averages generally coincide.

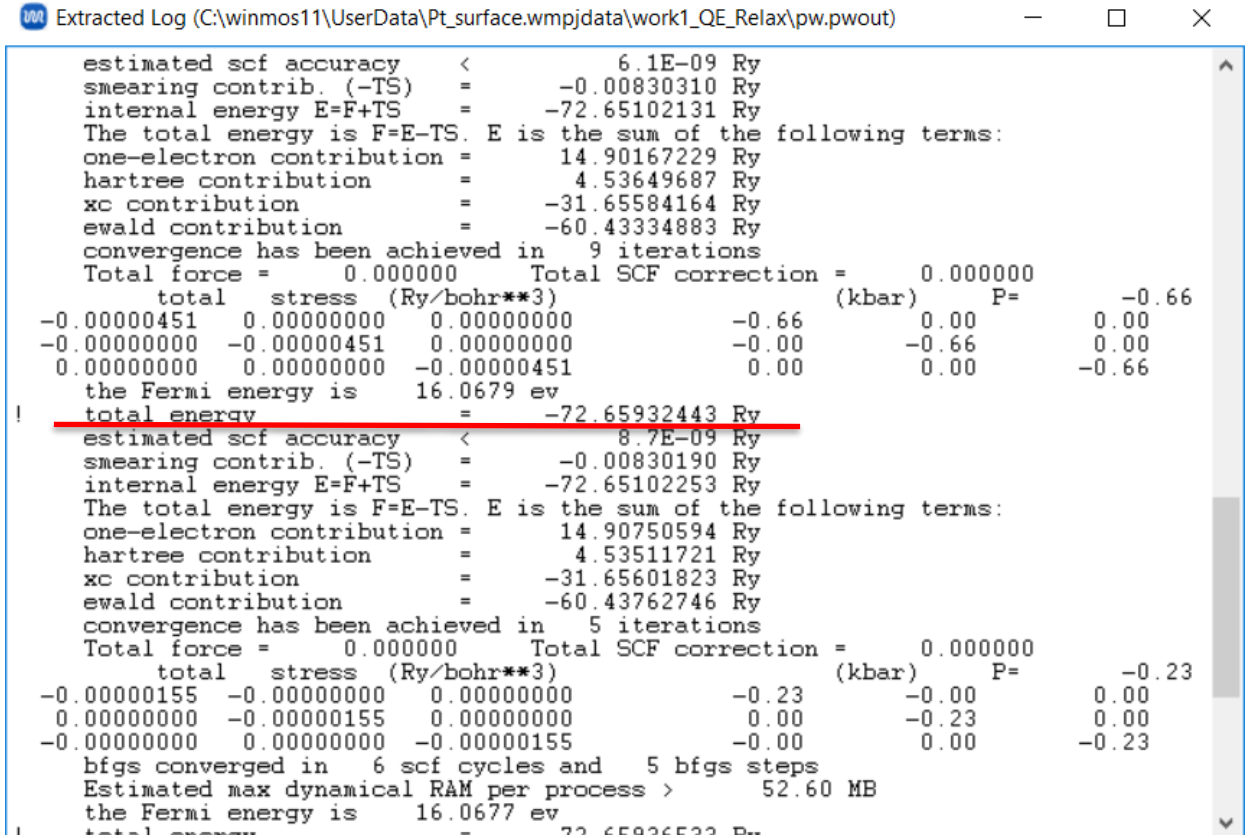




E. Analysis of Results (Surface Energy Calculation)

A. Click **Log(Extracted)** in **Action** for **work1** and **work2** in **Working Folders** (if using the Professional Economy version, click **Log**), and extract the value of **total energy** at the very end.





E. Analysis of Results (Surface Energy Calculation)

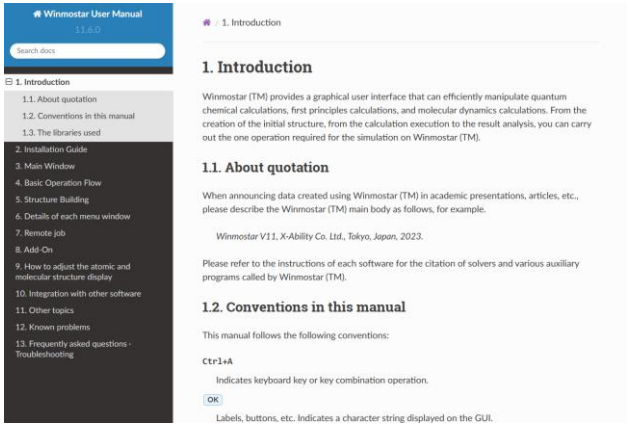
- Insert the values obtained in P.14 into the following formula to calculate the surface energy. Use **Tools | Unit Converter** for unit conversion.

$$\sigma = \frac{1}{N_{\mathrm{surface}}}\left(E_{\mathrm{slab}} - NE_{\mathrm{bulk}}\right)$$

	Meaning	In the context of this manual
E_{bulk}	Total energy of the bulk model (Value obtained from work1)	-72.676473 [Ry]
E_{slab}	Total energy of the slab model (Value obtained from work2)	-435.972734 [Ry]
N_{surface}	Number of surface atoms in the slab model	2
N	Ratio of the number of atoms in the bulk and slab models	6
σ	**Surface energy per surface atom**	**(-435.972734 - 6 * (-72.676473))/2 ≈ 0.043 [Ry/atom] ≈ 0.59 [eV/atom]**

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.)
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