winmostar tutorial

Quantum ESPRESSO
DFT+U & Equilibrium Potentials

V11.6.5

10 April 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 manual, we calculate the equilibrium potential E_{eq} for LiCoO2 using the following method with the Hubbard U parameter in DFT+U calculations.

$$E_{eq} \sim E_0(CoO_2) + E_0(Li) - E_0(LiCoO_2)$$ (E_0represents the total energy of each substance.)

Note :

- In this manual,CoO_2 and $LiCoO_2$ are calculated as non-magnetic materials, but in reality, calculations as antiferromagnetic or ferromagnetic materials may be necessary, requiring the search for a reasonable spin structure in the case of antiferromagnetism.
- The procedure for calculating the equilibrium potential introduced in this book includes approximations.

Reference URL:
https://mmnakayama.jimdofree.com/study/%E7%AC%AC%E4%B8%80%E5%8E%9F%E7%90%86%E8%A8%88%E7%AE%97%EF%BC%92/

- Please use QE series 6 for structural optimization calculations with Hubbard U, as errors may occur with QE series 5.
- The choice of k-points, number of bands, type of pseudopotential, cutoff energy, and smearing width can impact the calculation results. In this tutorial, settings with reduced accuracy are used to obtain results more quickly.

◆ 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

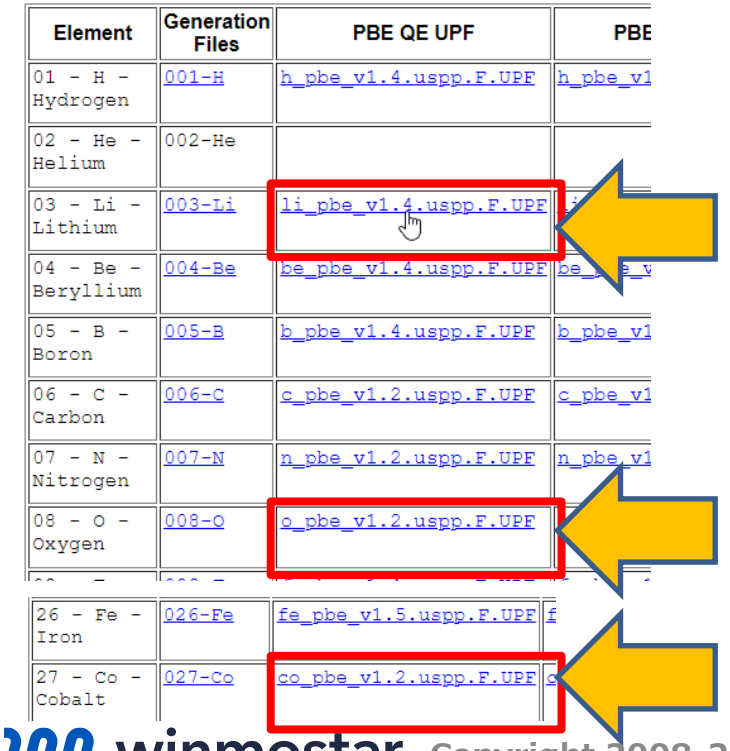
- For users of Winmostar version V11.5.0 or later on a 64-bit environment, please install and configure CygwinWM version 2023/04/05 or later.
  - The CygwinWM version after 2023/04/05 includes the recommended version of 64-bit Quantum ESPRESSO.

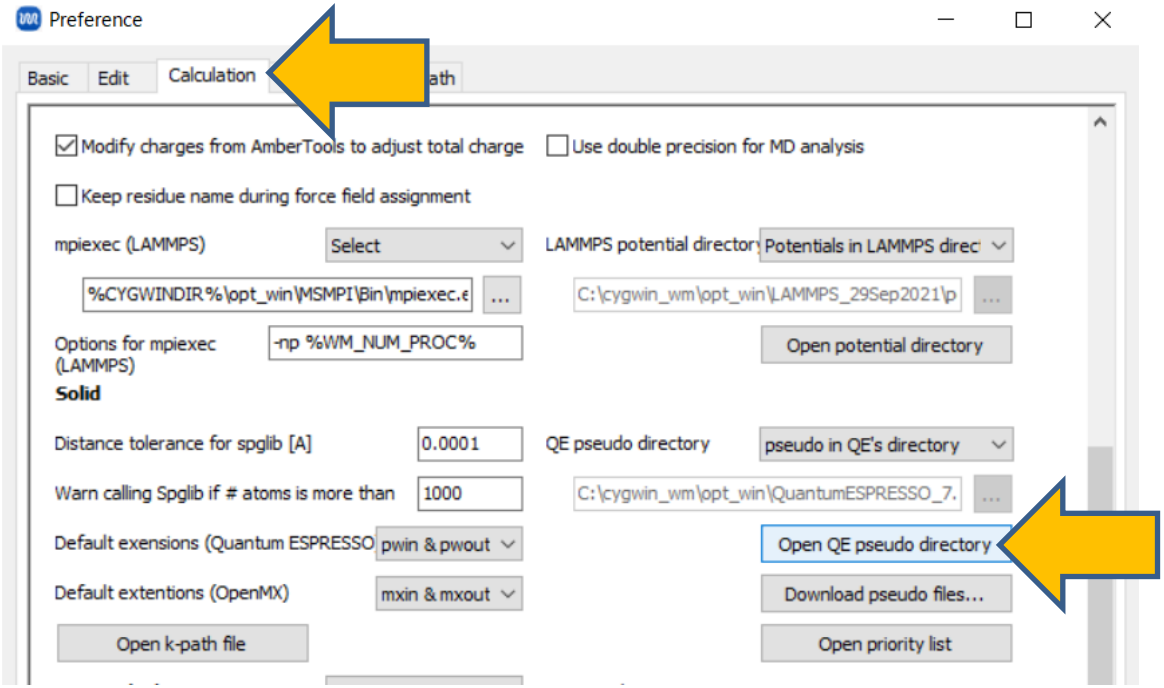
- If the above does not apply to you or if you wish to use a version of Quantum ESPRESSO other than the recommended one, you will need to install and configure Windows version of Quantum ESPRESSO separately.

Preference of Operating Environment

- li_pbe_v1.4.uspp.F.UPF
- o_pbe_v1.2.uspp.F.UPF
- co_pbe_v1.2.uspp.F.UPF

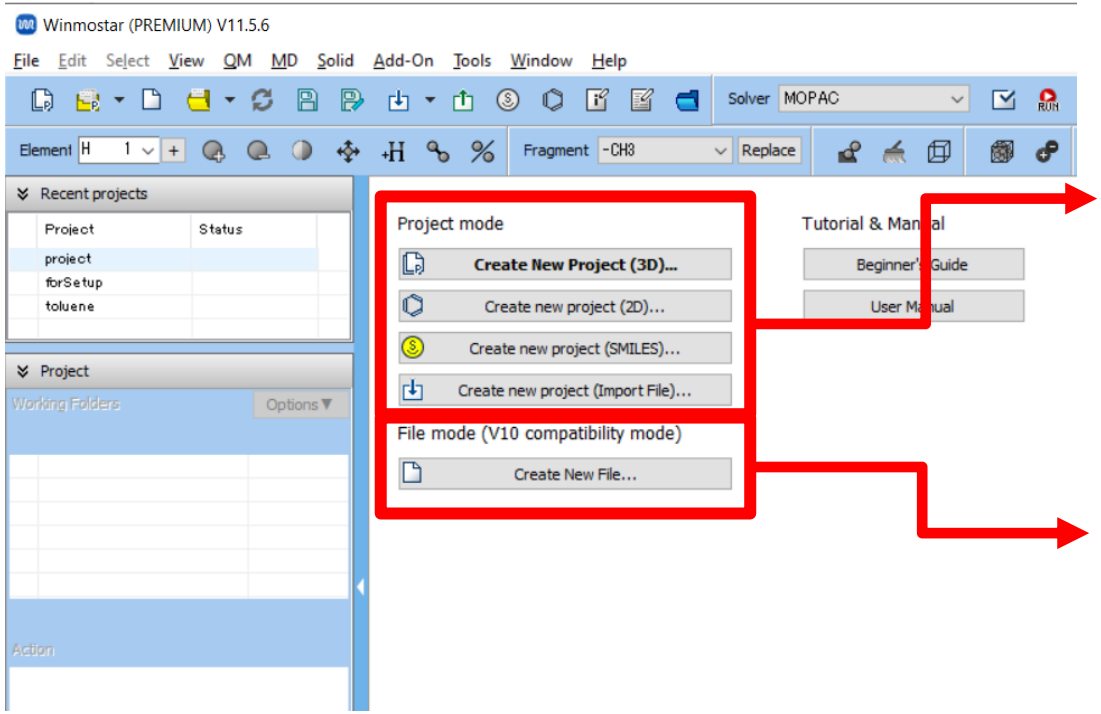
Obtain the above three from the following URLs, and copy them into the folder opened by clicking **Tools | Preference | Calculation | Solid | Open QE pseudo directory**.
https://www.physics.rutgers.edu/gbrv/





Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.



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（LiCoO2）

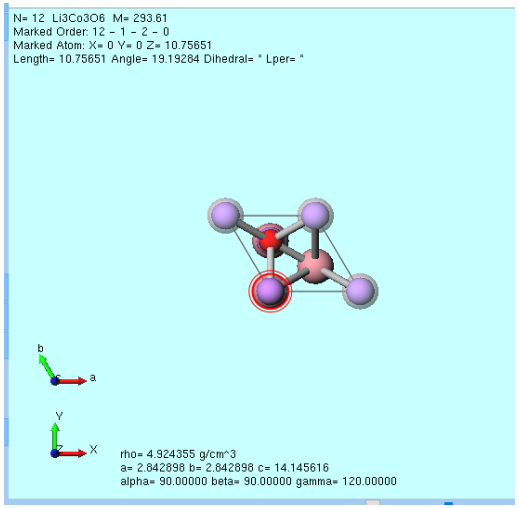
- Please refer to QE Basic Tutorial for the basic operation method.
- For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Structure Building'.

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

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

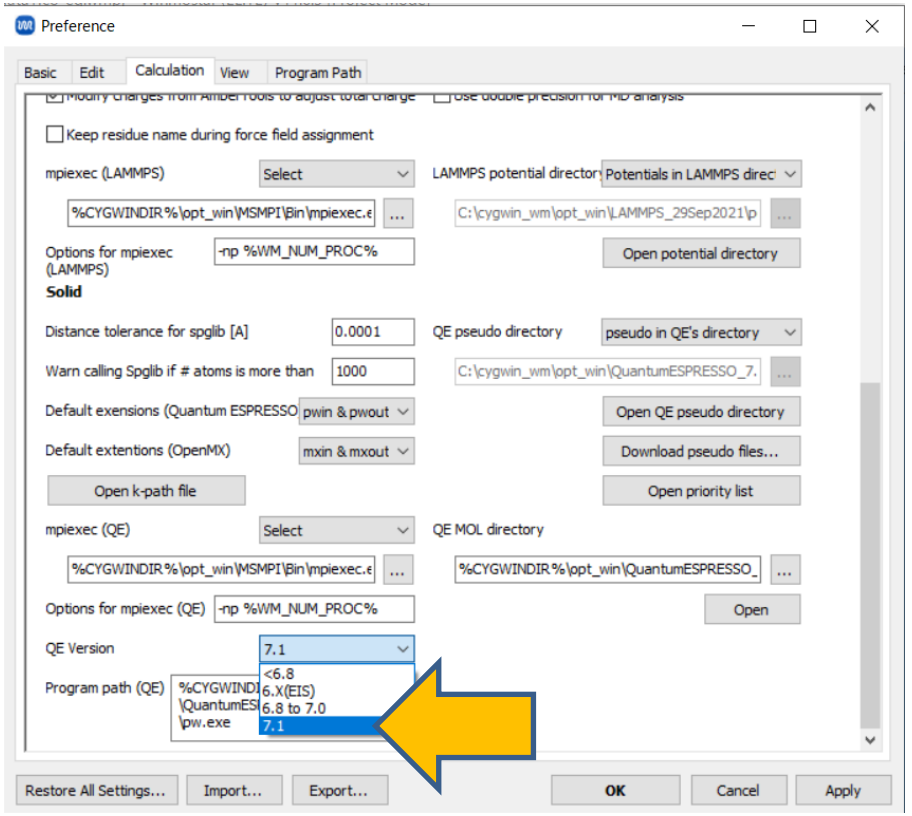
C. Click **File | Import | Sample File | licoo2.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

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



B. Execution of Calculation（LiCoO2）

A. The setting keywords for Hubbard U calculations depend on the version of QE, so click **(Preference)**, set the appropriate **QE Version you are using** in **Calculation** tab, and click **OK**. (For QE 5.2.1, select '<6.8', and for QE 7.1 included with CygwinWM, select '7.1').



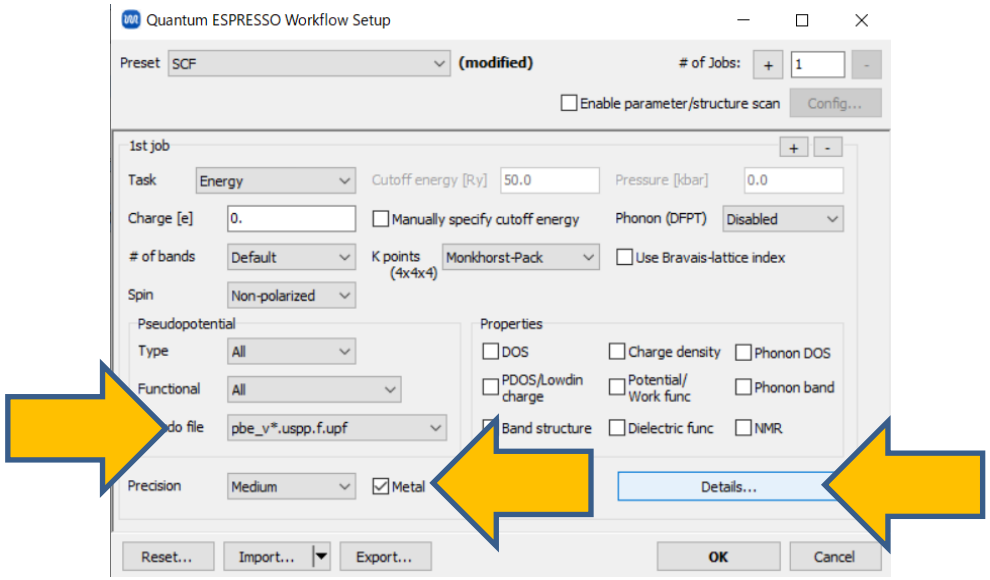
B. Execution of Calculation（LiCoO2）

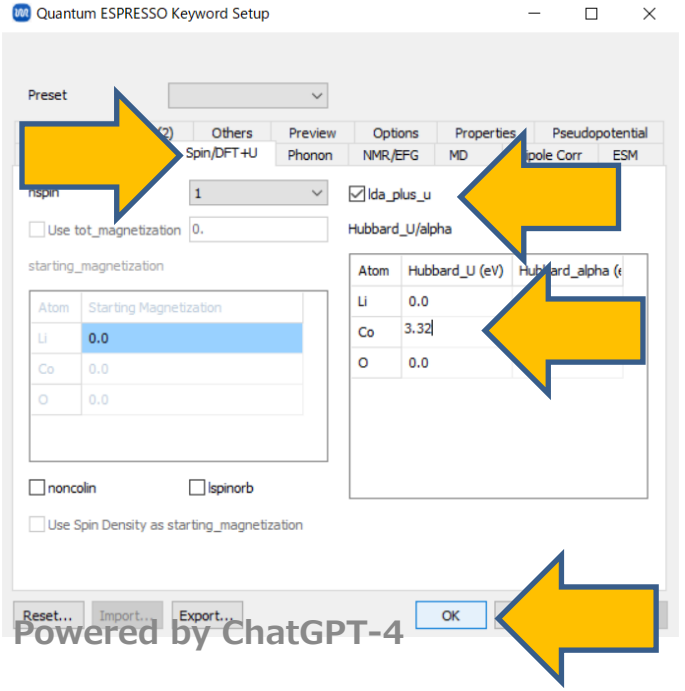
A. Select **Quantum ESPRESSO** from **Solver** in Toolbar and click **(Workflow Setup)**. Click **Yes** when asked if you want to convert to a primitive cell. Click **OK** when 'Successfully converted lattice.' is displayed.

B. Check **Metal** and select **Pseudo file** 'pbe_v*.uspp.f.upf'. If not available, follow the steps outlined in P.5.

C. Click **Details**, go to **Spin/DFT+U** tab, check **lda_plus_u**, enter '3.32' for **Hubbard_U** of **Co**, and click **OK**.

D. Click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.





C. Modeling of the System
Execution of Calculation（CoO2）

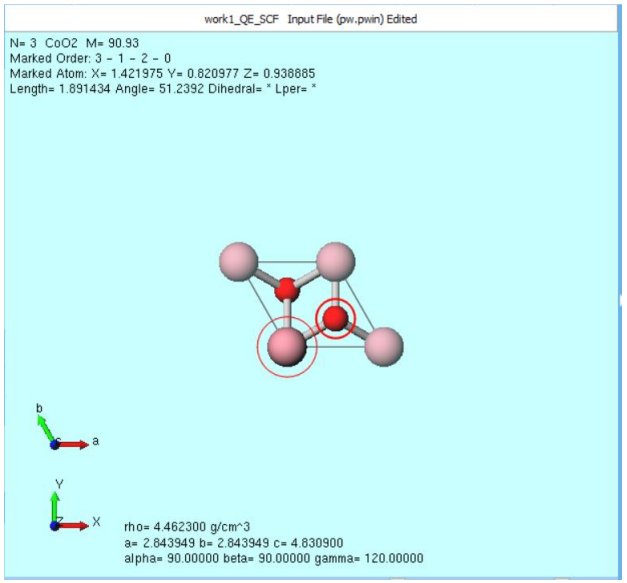
A. Click **File | Import | Sample file | coo2.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

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

C. Click **(Workflow Setup)**. If asked 'Do you want to continue from previous run?', click **No**.

D. Click **Details**, enter '3.32' for **Hubbard_U** of **Co** in **Spin/DFT+U** tab, and click **OK**.

E. Click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.



D. Modeling of the System
Execution of Calculation（Li)

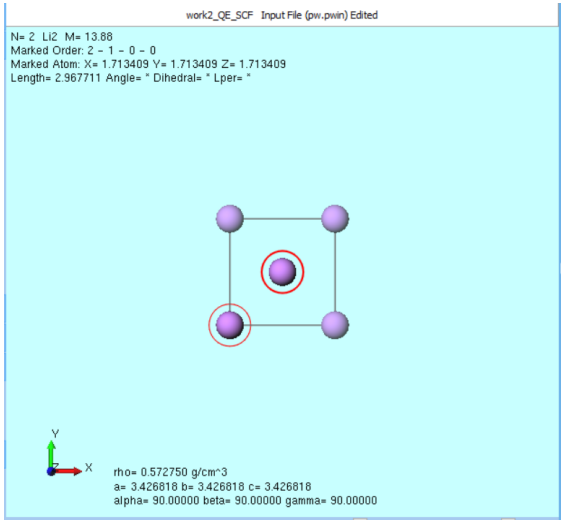
A. Click **File | Import | Sample file | li.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

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

C. Click  **(Workflow Setup)**. If asked 'Do you want to continue from previous run?', click **No**. Click **Yes** when asked if you want to convert to a primitive cell. Click **OK** when 'Successfully converted lattice.' is displayed.

D. Click **Details**, uncheck **lda_plus_u** in **Spin/DFT+U** tab, and click **OK**.

E. Click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.



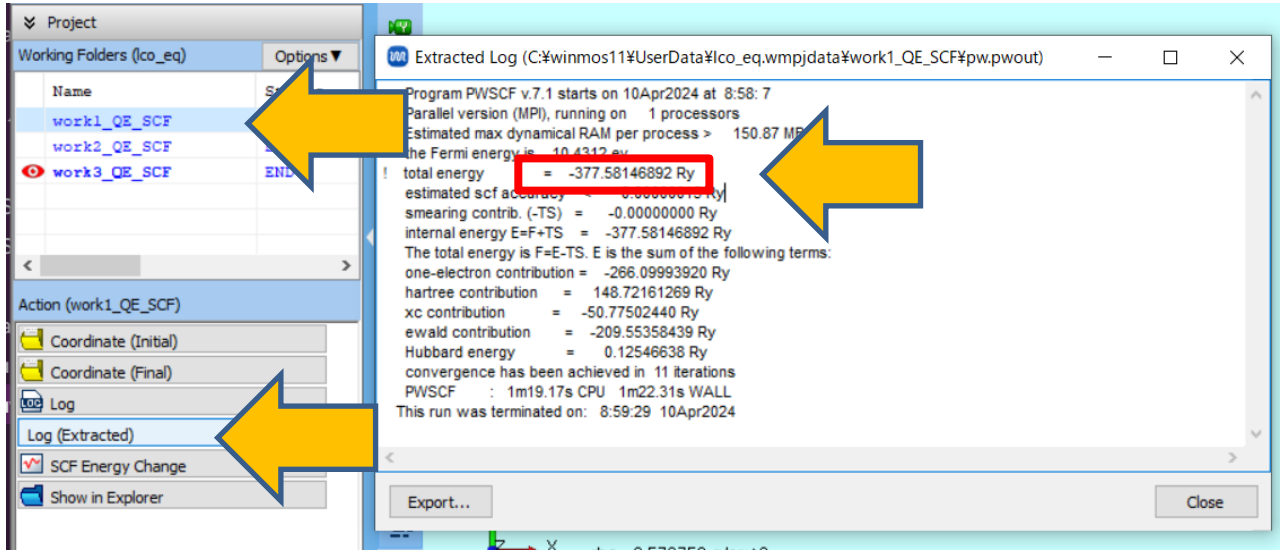
E. Result Analysis

A. Once **the status** of work1_QE_SCF (LiCoO2) changes to END, click 'work1_QE_SCF' in Project display area's **Working Folders**, and click **Log (Extracted)** in **Action**.

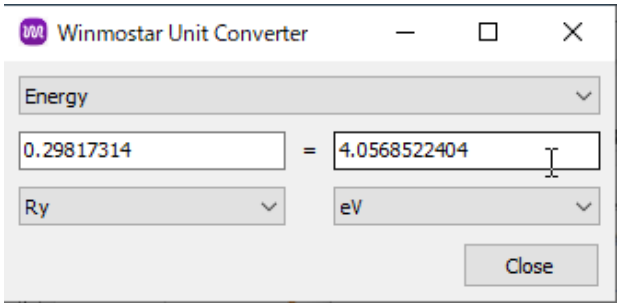
B. In **Extracted Log** window, copy the value from the line '! total energy = ⋯' (in the example below, '-377.58141482') and paste it into Excel or Notepad.

C. Do the same for work2 (CoO2) and work3 (Li) to obtain total energy values.

D. Calculate the value of $E_{eq} \sim E_0(CoO_2) + E_0(Li) - E_0(LiCoO_2)$. You can convert values from Ry to eV using **Tools | Unit Converter**.

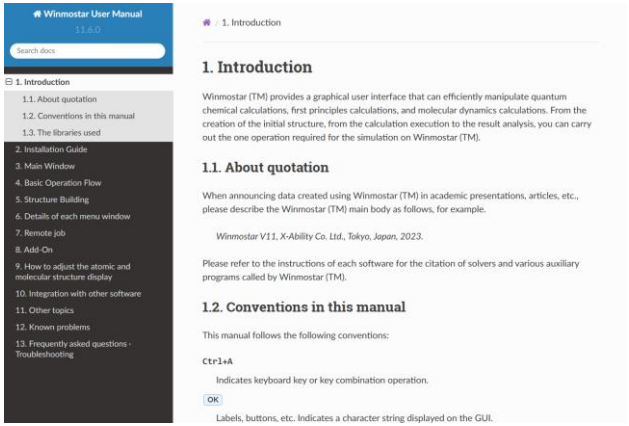


	A	B	C
1	LiCoO2	-377.5814148	Ry
2	CoO2	-362.810352	Ry
3	Li	-14.47288966	Ry
4	CoO2+Li-LiCoO2	0.29817314	Ry



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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