## **M** 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 <u>Beginner's Guide</u>.
- For those who wish to explore the details of each feature, please refer to <u>Winmostar User Manual.</u>
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - <u>Winmostar Introductory Training Session</u>: This guide only introduces the operation methods of the Basic Tutorial.
  - <u>Winmostar Basic Training Session</u>: 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.
  - <u>Individual Training Session</u>: 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 <u>Frequently asked questions</u>.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using <u>Contact page</u>. 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.

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

- In this manual,CoO<sub>2</sub> and LiCoO<sub>2</sub> 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: <u>https://qiita.com/xa\_member</u>

## **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 <u>the recommended one</u>, you will need to install and configure <u>Windows version of Quantum ESPRESSO</u> 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/

Element	Generation Files	PBE QE UPF	PBE	Preference — [
01 - H - Hydrogen	<u>001-н</u>	h_pbe_v1.4.uspp.F.UPF	h_pbe_v1	Basic Edit Calculation ath
02 - He - Helium	002-не			Modify charges from AmberTools to adjust total charge Use double precision for MD analysis
03 - Li - Lithium	<u>003-Li</u>	li_pbe_v1.4.uspp.F.UPF		Keep residue name during force field assignment
04 - Be - Beryllium	<u>004-Be</u>	be_pbe_v1.4.uspp.F.UPF		%CYGWINDIR%\opt_win\MSMPI\Bin\mpiexec.e        C:\cygwin_wm\opt_win\LAMMPS_29Sep2021\p
05 - B - Boron	<u>005-B</u>	b_pbe_v1.4.uspp.F.UPF	b_pbe_v1	Options for mpiexec -np %WM_NUM_PROC% Open potential directory
06 - C - Carbon	<u>006-C</u>	c_pbe_v1.2.uspp.F.UPF	<u>c_pbe_v1</u>	Solid
07 - N - Nitrogen	<u>007-n</u>	n_pbe_v1.2.uspp.F.UPF	<u>n_pbe, v1</u>	Distance tolerance for spglib [A] 0.0001 QE pseudo directory pseudo in QE's directory Ware calling Spglib if # atoms is more than 1000 C:\currently win\out win\out to the spglib SSO 7
08 - 0 - Oxygen	008-0	o_pbe_v1.2.uspp.F.UPF	K	Default exensions (Quantum ESPRESSO pwin & pwout ~ Open QE pseudo directory
26 - Fe -	026-Fe	fe_pbe_v1.5.uspp.F.UPF		Default extentions (OpenMX) mxin & mxout ~ Download pseudo files
27 - Co -	027-Co	co_pbe_v1.2.uspp.F.UPF		Open k-path file Open priority list

## **Operating Modes of Winmostar V11**

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



# A. Modeling of the System (LiCoO2)

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

A CONTRACT OF A	M.I.
000 Preference	- 🗆 X
Basic Edit Calculation View Program Path	
Privary charges from Amber tools to adjust total charge	
Keep residue name during force field assignment	
mpiexec (LAMMPS) Select $\checkmark$	LAMMPS potential director Potentials in LAMMPS direct $$
%CYGWINDIR%\opt_win\MSMPI\Bin\mpiexec.e	C:\cygwin_wm\opt_win\LAMMPS_29Sep2021\p
Options for mpiexec -np %WM_NUM_PROC%	Open potential directory
Solid	
Distance tolerance for spglib [A] 0.0001	QE pseudo directory $\qquad$ pseudo in QE's directory $\qquad \checkmark$
Warn calling Spglib if # atoms is more than 1000	C:\cygwin_wm\opt_win\QuantumESPRESSO_7.
Default exensions (Quantum ESPRESSO pwin & pwout $\sim$	Open QE pseudo directory
Default extentions (OpenMX) mxin & mxout ~	Download pseudo files
Open k-path file	Open priority list
mpiexec (QE) Select ~	QE MOL directory
%CYGWINDIR%\opt_win\MSMPI\Bin\mpiexec.e	%CYGWINDIR%\opt_win\QuantumESPRESSO
Options for mpiexec (QE) -np %WM_NUM_PROC%	Open
QE Version 7.1 ~	
Program path (QE) %CYGWINDI 6.X(EIS) \QuantumES(6.8 to 7.0	
pw.exe 7.1	×
Restore All Settings Import Export	OK Cancel Apply

## **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 **Ida\_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**.

Uliantum ENPRENSICI Worktlow Setup	
Preset SCF (modified) # of Jobs: + 1 -	Preset
1st job     +     -       Tack     Energy (Rv)     50.0     Pressure (khar)     0.0	20 Others Preview Options Properties Pseud Spin/DFT+U Phonon NMR/EFG MD pole Corr 1 Vida nius u
Charge [e] 0. Manually specify cutoff energy Phonon (DFPT) Disabled V	Use tot_magnetization 0. Hubbard_U/alpha
# of bands Default  V K points (4x4x4) Monkhorst-Padk  Use Bravais-lattice index Spin	starting_magnetization     Atom     Hubbard_U (eV)     Hubfard_al       Atom     Starting Magnetization     Li     0.0
Pseudopotential  Type All   DOS  Charge density  Phonon DOS	i         0.0         Co         3.32           Co         0.0         0         0.0
Functional All PDOS/Lowdin Potential/ Phonon band	o 0.0
do file pbe_v*.uspp.f.upf   Band structure Dielectric func NMR	
Precision Medium V Metal Details	Use Spin Density as starting_magnetization
Reset Import V Export	

### 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 **Ida\_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 =  $\cdots$ ' (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  $E_{eq} \sim E_0(\text{CoO}_2) + E_0(\text{LiCoO}_2)$ . You can convert values from Ry to eV using **Tools | Unit Converter**.

							-	-		
Working Folders (lco_eq)	Options ▼	Extracted Log (C:¥winmos11¥UserData¥lco_eq.wmpjdata¥work1_QE_SCF¥pw.pwout)	- 🗆	×		A	В	С		
Name	5	Program PWSCF v.7.1 starts on 10Apr2024 at 8:58: 7		~	1	LiCoO2	-377.5814148	Ry		
workl_QE_SCF	$\boldsymbol{\langle}$	Parallel version (MPI), running on 1 processors Estimated max dynamical RAM per process > 150.87 MB			2	CoO2	-362.810352	Ry		
work2_QE_SCF work3_QE_SCF	END	he Fermi energy is 10.4312.ev ! total energy = -377.58146892 Ry			3	Li	-14.47288966	Ry		
5		estimated sci accuracy = -0.0000000 Ry smearing contrib. (-TS) = -0.0000000 Ry internal energy E=F+TS = -377 58146892 Ry			4	CoO2+Li-LiCoO2	0.29817314	Ry		
Action (work1_QE_SCF)		The total energy is F=E-TS. E is the sum of the following terms: one-electron contribution = -266.09993920 Ry hartree contribution = 148.72161269 Ry xc contribution = -50.77502440 Ry				🚾 Winmostar Unit Converter 🛛 — 🗆 🗙				
Coordinate (Initial)		Hubbard energy = 0.12546638 Ry			E	nergy		~		
Log (Extracted)		PWSCF : 1m19.17s CPU 1m22.31s WALL This run was terminated on: 8:59:29 10Apr2024		~	0.	29817314	= 4.0568522404	Ţ		
SCF Energy Change		<		>	R	y ~	eV	~		
Show in Explorer			Clos	e			[	Close		

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