M winmostar tutorial

Quantum ESPRESSO Nudged Elastic Band Method

V11.7.6

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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 <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

• 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: <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.

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.

pslibrary

Ready-to-use pseudopotentials from the PSlibrary

The naming convention can be found here.



Please refer to <u>QE Basic Tutorial</u> for the basic operation method.

Please refer to <u>Molecular adsorption model tutorial</u> 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. 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. 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. Click A Modify Selected Group | Delete, then click Delete.

✓ Replace	? 羔 🗇 🚳 📌 🛱	
porary File (temp	Rotate Around Axis (2 Marked Atoms)	
	Rotate Around Axis (3 Marked Atoms)	
	Rotate Around Marked Atom (Mouse)	
I= 180 Lper= 0	Rotate (Numerical)	
	Rotate by Aligning Marked Atoms	XYZ
	Translate (Mouse)	
	Translate (Numerical)	0000
	Quick Optimization	0000 5561
	Connect Between Adjacent Atoms	5561
	Cut (X)	2781
	Сору	8342 0000
	Paste (V)	0000
	Replicate	5561
	Delete	2781
	Change Optimization Flags of Group	8342
	Change Optimization Flags of Group (Z-Matrix)	
	Change Charges of Group	
	Average Charges of Group	

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



- 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



- 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 d (Modify Selected Group) | Change Optimization Flags of Group and then click Fix.
- D. Click Select | Select None.

	6	9		Y 39
			Replace with Fragment Shift+Ctrl+RightClick	Zr 40
		Delete Atom	Nb 41	
			Change Element (Shift: E5)	Mo 42
4	3	-	Change Element (Shirt+F5)	Tc 43
			Change Element to	Ru 44
	(🦱		Optimization Flags	Rh 45
	×2-		Charge/Spin Density (Q)	Pd 46
			Occupancy	Ag 47
		+H	Add Hydrogen to Maked Atom (Auto)	Cd 48
	7		Ŭ	In 49





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**.

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			Ena	able parameter/struct	ture scan Config
1st job					+ -
Task Op	timize(Atom) 🗸 🗸	Cutoff energy [(Suggest: 33	Ry] 50.0 8 Ry)	Pressure [kbar]	0.0
Charge [e]	0.	Manually spe	ecify cutoff energy	Phonon (DFPT)	Disabled \checkmark
# of bands	Default \lor	K points (4x4x1) Mor	nkhorst-Pack ~	Use Bravais-lat	tice index
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Туре	All 🗸		DOS	Charge density	Phonon DOS
Functional	All	\sim	PDOS/Lowdin charge	Potential/ Work func	Phonon band
Pseudo file	pbe-*rrkjus_psl.*.upf	· ~	Band structure	Dielectric func	NMR
Precision	Medium ~	☑ Metal		Deta	ails
Reset	Import 🖛 E	xport		ОК	Cancel

C. Modeling of the System (Final State)

- A. Even if the calculation of the initial state is in progress, return to Main window, rightclick 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**.

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Preset Optimize	e(Atom)	~	(modified)	# of Jo	bs: +	1	-
				Enable parame	eter scan	Confi	g
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Charge [e]	0.	Manually sp	ecify cutoff energy	Phonon (DFPT)	Disabled	~	
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Spin	Non-polarized \sim						
Pseudopotent	tial		Properties				
Туре	All 🗸		DOS	Charge density	Phon	on DOS	
Functional	All ~		PDOS/Lowdin charge	Potential/ Work func	Phon	on band	
Pseudo file	pbe-*rrkjus_psl.*.upt	· · ·	Band structure	Dielectric func			
Precision	Extra-low \checkmark	🗹 Metal		Det	ails]
Reset	Import	xport		O	K D	Can	cel

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.

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AST_IMAGE	C:¥winmos11¥UserData¥cu_ag.wmpjdata¥work2_QE_Relax¥pw.pwout				[Display	
				Visualize	e Initial I	Path	
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			THE ACT T	MACE.	1		Sel
			at LAST_1	TAGE	-		90
VEB configurati	on		arcasi_u	TAGE			00
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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.





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.)
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- 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.