M winmostar tutorial

Quantum ESPRESSO Basic

V11.5.6

6 December, 2023

X-Ability Co., Ltd.

About This Document

- 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>
- 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 from <u>Contact</u>. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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Overview

• We will obtain the band structure, density of states, partial density of states, and electron density of Si crystals through first-principles calculations using Quantum ESPRESSO.

Procedure Overview:



Operating Environment Settings

- Users utilizing Winmostar V11.5.0 or later in a 64-bit environment are advised to install and configure <u>the CygwinWM version dated 2023/04/05 or later</u>.
 - The CygwinWM version released after 2023/04/05 includes the recommended 64-bit version of 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 separately <u>install and</u> <u>configure the Windows version of Quantum ESPRESSO</u>.

Operating Modes of Winmostar V11

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

Winmostar (PREMIUM) V11.5.6 File Edit Select View QM MD Solid Add-On Tools Window Help 📴 • 🗅 🚽 • 💋 🖻 🖻 🖕 🖕 • 🏦 🔘 🛈 🗹 🗹 📹 ソルバ Quantum ESPRESSO 🗸 **Project Mode New Features in V11** H 1 V + 💽 🔍 🕼 🚸 🕂 💊 % フラਗ਼メント -CH3 Replace 🖌 🥌 🗊 **F** 元素 Users can manage jobs without having to ℅ Recent projects Project mode Tutorial & Maual Project Status manage individual files. Create New Project (3D)... Beginner Guide We generally recommend using this mode. Create new project (2D)... User N anual Create new project (SMILES)... Project File Mode гłл Create new project (Import File).. Options V Status File mode (V10 compatibility mode) Users explicitly create and manage Name Create New File... individual files. The operational procedure is the same as from V10 and earlier versions.

A. System Modeling

- A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File** | **Close**.
- B. Enter 'si_scf' for **Project name** and click **Save**.

	winmostar (PREMIUM) V11.5.6			
	<u>File E</u> dit Se <u>l</u> ect	<u>View QM MD S</u> olid	d <u>A</u> dd-On <u>T</u> ools <u>W</u> indow <u>H</u> elp	
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			Create New Project (3D)	
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			Create new project (SMILES)	
	Working Folders	Options 🔻	Create new project (Import File)	
			File mode (V10 compatibility mode)	
			Create New File	
Mew project			X	
Project name		si_scfl		
Location Arbitr	ary folder	C:#winmos11	browse	
OLast o	pened folder	C:¥winmos11¥UserDat	ata	
OUserD	ata folder	C:¥winmos11¥UserDat	ata¥	
Description (Optional)				
			Save	

A. System Modeling

For details on creating an initial structure, please refer to <u>Winmostar User Manual: 5.</u> <u>Methods for Creating Initial Structures</u>. In this section, we will load an existing molecular structure file.

- A. Click File | Import | Sample File | si.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. Verify that the desired molecule appears in Viewport.



- A. Select Quantum ESPRESSO from Toolbar's Solver.
- B. Click Workflow Setup.
- C. To reduce computation time, click **Yes** when asked if you want to convert to a primitive cell. The converted structure will appear in Viewport. Click **OK** when you see the message 'Successfully converted lattice'.



- A. To output the band structure of the valence band, change **# of bands** to **50% more**.
- B. Check **DOS**, **PDOS/Lowdin charge**, **Band structure**, and **Charge Density** in **Properties**.
- C. As it is necessary for outputting the band structure in Winmostar, check **Use Bravaislattice index**.

🥺 Quantum ES	🛛 Quantum ESPRESSO Workflow Setup - 🗆 🗙				
Preset SCF		v (modified)	# of Jo	bs: + 1	-
			Enable parameter/struc	ture scan Co	onfig
1st job				+	-
Task Ene	rgy ~ Cutoff	energy [Ry] 35.0	Pressure [kbar]	0.0	
Charge [e]	0. Mar	nually specify cutoff ener	gy Phonon (DFPT)	Disabled	~
# of bands	50% more	Monkhorst-Pack	∨ ✓ Use Bravais-la	ttice index	В
Spin	Non-polarized	<u> </u>			
Pseudopotent	ial C	Properties			
Туре	USPP V	Dos	Charge density	Phonon DC	S
Functional	PBE ~ G	GA PDOS/Low charge	din Potential/ Work func	Phonon bar	nd
Pseudo file	pbe-*rrkjus_psl.*.upf	✓ Band strue	ture Dielectric func	NMR	

- A. Change **Pseudopotential Type** to '**USPP**', **Functional** to '**PBE**', and **Pseudo file** to '**pbe-n-van.upf**'.
 - The choices for 'Pseudo file' are narrowed down based on Type and Functional selections. If you can infer the type of pseudopotential and functional from the notation of Pseudo file, please select Pseudo file directly.
 - If you want to add pseudopotential files, please refer to Quantum ESPRESSO Installation Manual for <u>installation instructions</u>.
- B. Adjust computational conditions as necessary. (Not required in this manual)

	🥺 Quantum E	SPRESSO Workflow S	etup			- 🗆	×
	Preset SCF		~ (modified)	# of Job	os: + 1	-
				Ena	ble parameter/struct	ture scan Config	
	1st job					+ -	
	Task Ene	rgy 🗸	Cutoff energy [[Ry] 35.0	Pressure [kbar]	0.0	
	Charge [e]	0.	Manually spe	ecify cutoff energy	Phonon (DFPT)	Disabled \lor	
	# of bands	50% more 🗸 🗸	K points (3x3x3) Mor	nkhorst-Pack ~	🗹 Use Bravais-lat	ttice index	
	Spin	Non-polarized \sim					
	Pseudopotent	ial		Properties			
/	Туре	USPP ~		DOS	Charge density	Phonon DOS	
	Functional	PBE	∽ GGA	PDOS/Lowdin charge	Potential/ Work func	Phonon band	
	Pseudo file	pbe-n-van.upf	~	Band structure	Dielectric func	NMR	

Supplement: Adjusting the Number of k-Points

To adjust the number of divisions in the Brillouin Zone using the Monkhorst-Pack method, follow these steps.

- A. For rough adjustments: Change **Precision**. (The number of divisions will be displayed under **K points**.)
- B. For finer adjustments: Click **Details**, go to **Basic** tab, change **K_POINTS** to 'automatic (by Spacing)', and adjust the value in **(Spacing)**.
- C. For specific inputs: Click **Details**, go **Basic** tab, change **K_POINTS** to 'automatic', and adjust the values in the input fields located two lines below.



Supplement: If the Pseudopotential Files for Each Element are Not Available

If you do not have the necessary pseudopotential files for all elements in the substance you wish to calculate, perform one of the following operations.

- A. Obtain the appropriate pseudopotential files, click **Tools** | **Preference** | **Calculation** | **Open QE pseudo directory**, and copy the files into the opened folder.
- B. If the appropriate pseudopotential files are available but not recognized due to slight differences in names, click **Tools** | **Preference** | **Calculation** | **Open priority list**, and add items in a recognizable format. You can use an asterisk (*) as a wildcard.
- C. In **Quantum ESPRESSO Workflow Setup** window, click **Details**, go to **Pseudopotential** tab, and individually select the **File** for each element.

Quantum ESPRESSO Workflow Setup	- 🗆 ×	Basic Advanced Spin/DFT+U Phonon MD Dipole Corr ESM RISM (1)	
Preset SCF v (modified)	# of Jobs: + 1	RISM (2) Other Preview Options Properties Pseudopotential	
Eashie a		Mass Default v pseudo Directory pseudo in QE's directo v	
		Pseudopotential (Type) All 🗸	
1st job	+ -	(Functional) All V Open Pseudo Directory	
Task Energy Cutoff energy [Ry] (Suggest: 44 Ry)	essure [kbar] 0.0	(File) (Manual) V Download Pseudo Files	
Charge [e] 0. Manually specify cutoff energy Pho	onon (DFPT) Disabled ~	Reload Pseudo Files Open Priority List	
# of bands 50% more V K points Monkhorst-Pack V	Use Bravais-lattice index	Onen Pseudo Files	
Spin Non-polarized V		Mara Ela	
Pseudopotential Properties		Ni 58.693 Ni PRE TM 2ni.LIPE NCPR	
Type USPP V DOS 0	Charge density Phonon DOS		
Functional PBE V GGA	Potential/ Phonon band Work func	O.blyp-mt.UPF O.phe-kinaw.LPF	
Pseudo file pbe-*rrkjus_psl.*.upf V Band structure		O.pbe-rrkjus-gipaw-dc.UPF O.pbe-rrkjus-IPF	
		O,pbe-tm-gipaw.UPF O,pbe-yan_ak.UPF	
Precision Medium ~ Metal	Details	O.pz-kjpaw.UPF O.pz-rrkius.UPF	
		Reset Import O.pz-van ak.UPF OK Cancel Cancel O PBE TM.UPF	
Reset Import 💌 Export	OK Cance	0_PBE_USPP.UPF (Undefined) 2.981601 b= 2.981601 c= 2.981601 c= 0.0000 kpts = 0.00000 kpts = 0.00000 games	

Supplement: Editing the Path of the Band Structure

To edit the path of the band structure, follow these steps (not required in this manual).

- A. Click **Details**, and in the opened **Quantum ESPRESSO Keywords Setup** window, click **Properties** tab. Then click the line for **Band structure plot** in **Properties**.
- B. Uncheck **Set default k-path** and edit the path in the field to its right. The format follows the Quantum ESPRESSO K_POINTS syntax. Labels for special points can be found in the doc¥Brillouin_zones.pdf in the Quantum ESPRESSO installation folder.
- C. After editing, click **OK**. 🚾 Quantum ESPRESSO Keywords Setup X Quantum ESPRESSO Workflow Setup X Preset \sim # of Jobs: + 1 Preset SCF (modified) Spin/DFT+U MD Dipole Corr Basic Advanced Phonon RISM (2) Preview Properties Α Othe Options Enable parameter/structure scan Config. Properties Values 1st job + crystal_b Band structure plot Α Cutoff energy [Ry] 35.0 0.0 False Task Energy DOS plot (Suggest: 44 Ry) PDOS plot/Lowdin charge False Charge [e] Manually specify cutoff energy Phonon (DFPT) Disabled Fermi surface Dielectric function # of bands 50% more K points Monkhorst-Pack Use Bravais-lattice index (3x3x3) Charge density Spin Potential/work function Non-polarized Phonon band Pseudopotential Properties Phonon DOS DOS Type USPP ✓ Charge density Phonon DOS K POINTS gG 20 Potential/ PDOS/Lowdin X 20 Phonon band Functional ✓ GGA В PRF Set default k-path Work func W 20 B K 20 Band structure Dielectric func Pseudo file pbe-*rrkius psl.*.upf NMR gG 20 L 20 Α U 20 Precision Medium Metal Details. W 20 L 20 < Reset... Import... Export... OK Cancel OK Reset... Import... Export...

Supplement: Calculating Properties for Past Jobs Post-Hoc

To calculate properties such as the density of states for previously completed SCF or structure optimization calculations, follow these steps (not required in this manual).

- A.
 ☐ Click Workflow Setup, and when prompted 'Do you want to continue from previous run?', click Yes. Then select the working folder of the completed SCF or structure optimization calculation and click OK.
- B. Change **Task** to 'NSCF', and in **Properties**, check the items you want to calculate.
- C. Click **OK**, and then click **Run** in **Job Setting** window.

W Quantum ESPRESSO Workflow Se	etup	- 🗆 X
Preset SCF	✓ (modified)	# of Jobs: + 1 -
	En	able parameter/structure scan Config
1st job		+ -
Task NSCF	energy [Ry] 35.0 ggest: 44 Ry)	Pressure [kbar] 0.0
Charge [e] 0.	Manually specify cutoff energy	Phonon (DFPT) Disabled \checkmark
# of bands Default ~	K points (3x. 3) Monkhorst-Pack ~	Use Bravais-lattice index
Spin Non-polarized		
Pseudopotential	Properties	
Type All	Dos	Charge density Phonon DOS
Functional All	✓ PDOS/Lowdin charge	Potential/ Phonon band Work func
Pseudo file pbe-*rrkjus_psl.*.upf	Band structure	Dielectric func
Precision Medium ~	Metal	Details
Reset Import 🔽 E	xport	OK Cancel

(If working with remote jobs, please proceed here first.)

- A. Click **OK** at the bottom right of **Quantum ESPRESSO Workflow Setup** window.
- B. Click **Run** in **Job Setting** window. **Winmostar Job Manager** will start in the background, and a black console window, as shown in the right figure, will appear, indicating the start of the calculation.

Job Setting	– 🗆 ×		
Run local job		Com Winmostar/JM Exec 1 2022/02/02 17:36:25	- 🗆 ×
Program	Quantum ESPRESSO V	isym = 21 inv. 180 deg rotation - cart. axis [0,1,1]	^
Path	C:\cygwin_wm\cygwin\cyg		
O Run remote job		cryst. $s(21) - 1 - 1 - 0 - 1$	
Remote Server Profile	pbs_example V Config		
Solver	quantumespresso 🗸	cart. s(21) = (1.0000000 0.0000000 0.0000000) (0.0000000 0.0000000 -1.0000000)	
Template Script	(Default) V New Edit	(0.0000000 -1.0000000 0.0000000)	
Option	-I nodes=1:ppn=%WM_NUM_PROC% -I walltime=23:50:00		
	Test Connection	isym = 22 inv. 180 deg rotation - cart. axis [0,1,-1]	
Postprocess	Retrieve only a part of files(log etc.)	cryst. s(22) = $\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$	
Information		(ľ i o č)	
		cart. s(22) = (1.0000000 0.0000000 0.0000000)	
Do not run job after savir	ng files		
Parallelization			
# of MPI Procs 1	♥ # of Threads / MPI Proc 1 ♥	isym = 23 inv. 90 deg rotation - cart. axis [-1,0,0]	
Prefix for working folder	work	cryst. s(23) = (0 0 -1)	
Descriptions for jobs (Option	hal)		
	Run		~

Supplement: If you want to modify the input files yourself or copy them to a remote server for use, check **Do not run job after saving files** in **Job Setting** window and click **Run**. To run the calculation after saving, click **File** | **Project** | **Selected Woking Folder** | **Run**.

- A. Upon returning to the main window (it's fine even if a calculation is running), Project Area will show the working folder for the job set up in Quantum ESPRESSO Workflow Setup window.
- B. In Viewport, the input file from the first working folder (work1_QE_SCF) will automatically open. You can also confirm this at the top of **Viewport**.



- A. Based on the progress of the calculation, the status of each working folder in Working
 Folders section of Project Area changes from PEND (black) → RUN
 (green) → END (blue).
- B. Wait until the status of all work folders changes to END (blue). During this time, the status of the recently used project 'si_scf' will also change to ALL END (blue).

≈	Recent projects			*	Recent projects		
\square	Project	Status			Project	Status	
0	si_scf	RUN(1)		O	si_scf	ALL EN	D
*	Project			*	Project		
Wor	king Folders (si_scf)		Options ▼	Wor	king Folders (si_scf)		Options ▼
					Name		Status
0	work1_QE_SCF		RUN	O	work1_QE_SCF		END
				_			

- A. If you want to view the main contents of each calculation's log, select the relevant calculation's working folder in **Working Folders section of Project Area**, then click **Log(Extracted)** under **Action**. (This feature is exclusive to the Professional Premium Edition.)
- B. If you wish to view the complete log, click Log.



C. Result Analysis SCF Energy Change

From here on, you may skip any analysis items that are not of interest.

- A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').
- B. When you click **SCF Energy Change** in **Action**, **SCF Energy Change** window will open, displaying the plot of Estimated accuracy from the Quantum ESPRESSO log.
- C. After reviewing, click Close.



C. Result Analysis Density of States

- A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').
- B. When you click **Density of States** in **Action**, **Density of States** window will open, displaying the plot of the density of states..
- C. After reviewing, click **Close**.



C. Result Analysis Partial Density of States

- A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').
- B. When you click **Projected Density of States** in **Action**, **Projected Density of States** window will open, displaying the plot of the partial density of states.
- C. After reviewing, click **Close**.



C. Result Analysis Band Structure

- A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').
- B. When you click **Band Structure** in **Action**, **Band Structure** window will open, displaying the plot of the band structure.
- C. After reviewing, click **Close**.



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C. Result Analysis Electron Density

- A. In **Working Folders section of Project Area**, click the relevant working folder (here, we will use 'work1_QE_SCF').
- B. When you click Charge Density in Action, after automatic processing for a few seconds, Winmostar Viewer will start and the electron density will be displayed in 3D. If you want to change the settings of the isosurface, modify Isosurface Value in Cube Plot window and click Draw.



Supplement: Visualization of Electron Density Using Programs Other Than Winmostar

It is possible to visualize the electron density using other programs like VESTA.

- A. By checking the box for tools | Preference | Basic |
 Use external program to view cube file and selecting the executable file of VESTA in Program path | Cube Viewer, VESTA will open as per the procedure on page 23.
- B. Click **Show in Explorer** under **Action**, and explicitly open the

'pp_density_comp.cube' file in the working folder with VESTA or a similar program.

Preference	- 🗆 X	Action (work1_QE_SCF)
Basic Edit Calculation View Program Path		Coordinate (Initial)
Language Cocale Japanese English	Use old functions adopted up to V8 for unzip Use old format adopted up to V9 when saving xyz file Write Lattice Vectors in xyz and txy file	Coordinate (Final) Log Log (Extracted) SCF Energy Change
License code : DA610807C1A1EE98728E3D0C1E1B5506D4260441937 036213958D6FDD1F4871DAE87C27039FD94555530A60	☐ Write residue number in xyz and txy file ☐ Keep project area when opening file	Density of States Projected Density of States Band Structure
7EFB01C3C5C087988863D06103	Number of recent used files/projects 30	Lowdin Charge Charge Density
PAC BUILESS -		Show in Explorer

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