# M winmostar tutorial Quantum ESPRESSO Effective Screening Medium (ESM) Method

V11.9.5

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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**

- This tutorial demonstrates an Effective Screening Medium (ESM) calculation using an aluminum monolayer (slab) as an electrode. The boundary condition representing a vacuum–slab–metal system (bc3) is applied.
- ※Because of the implementation of ESM in Quantum ESPRESSO, the boundary of the input supercell is internally mapped to the center of the simulation cell. This is illustrated in the figure below.



Using the PBE functional and ultrasoft pseudopotentials, we first perform a constant-N calculation (with no applied bias), followed by a constant- $\mu$  calculation with an applied voltage of 0.5 V. These calculations allow us to analyze the electronic structure and charge distribution of the Al slab under bias. We also confirm that a potential difference of approximately 0.5 V appears between the slab and the virtual electrode (metal).

Note:

- constant-*N calculation* constant-*µ calculation* Analysis of w/o applied voltage Applied voltage: 0.5 V results
- The choice of k-points, type of pseudopotential, and cutoff energy 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.

# **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 (constant-N calculation)

- Please refer to <u>QE Basic Tutorial</u> for the basic operation method.
- A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.
- B. Enter 'al\_esm' in **Project name** and click **Save**.

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### A. Modeling of the System (constant-N calculation)

- For detailed instructions on creating the initial structure, please refer to <u>Winmostar User Manual section 5, 'Methods for Creating Initial Structures'</u>.
- A. Click File | Import | Sample File | al\_slab.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.



- A. Select **Quantum ESPRESSO** from **Solver** in Toolbar and click **└ (Workflow Setup)**. If asked whether to convert to a primitive cell, click **No**.
- B. Change the **K points** setting to **Monkhorst-Pack (Slab)**, enable the **Metal** option, and select **pbe-\*rrkjus\_psl.\*.upf** in **Pseudo file**.
- C. Click Details

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- A. Select the **ESM** tab, enable the **assume\_isolated = 'esm'** setting, and change the **esm\_bc** parameter to **bc3**.
- B. Click **OK**
- C. Click **OK**, then make appropriate settings in **Job Setting** window before clicking **Run**.

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esm_w bc3	
Citation	
M. Otani and O. Sugino, PRB 73, 115407, (2006).	
N. Bonnet, T. Monshita, O. Sugino and M. Otani, PRL 109, 266101, (2012).	
Reset Import Export OK un	

### C. Modeling of the System (constant- $\mu$ calculation)

- A. Click Select | Select All.
- B. Click **a** (Modify Selected Group) | Change Optimization Flags of Group and then click Fix.
  - In the charge optimization calculation, the structure optimization routine is reused. By assigning fixed optimization flags to all atoms, the atomic positions are held fixed while only the charges are optimized.



A. The keyword settings required for constant- $\mu$  calculations vary depending on the version of Quantum ESPRESSO being used. To ensure compatibility, click **Preference**, open the **Calculation** tab, and select the correct **QE version**. Then click **OK** to apply the setting.

(For Winmostar V11.5.0 or later with the default QE path, select "7.1" to use the bundled QE 7.1 via CygwinWM. If you are using QE 5.2.1, select "<6.8".)

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- A. After the status of Working Folders work1\_QE\_SCF changes to END (blue), Click (Workflow Setup) in Toolbar. If asked 'Do you want to continue from previous run?', click No.
- B. If asked to convert to a primitive cell, click No.
- C. Change **Preset** to 'Optimize(Atom)', The settings for the constant-N calculation will be reset.
- D. Set K points to Monkhorst-Pack (Slab), and check the Metal option.
- E. Click Details.

Enable parameter/structure s         1st job         Task       Optimize(Atom)       Cutoff energy [Ry]       50.0       Pressure [kbar]       0.         Charge [e]       0.       Manually specify cutoff energy       Phon (DFPT)       Disab         # of bands       Default       K points (4x4x1)       Monkhorst-Pack(Slab)       Properties         Spin       Non-polarized       Properties       ODS       Charge density       P         Type       All       POOS/Lowdin       Potential/ Work func       P         Pseudo file       obe-*trkius psl * unf       Band structure       Dielectric func       D	an Config
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Precision Medium V Metal Details	$\langle \_$

- A. Select the **ESM** tab, enable the **assume\_isolated = 'esm'** setting, and change the **esm\_bc** parameter to **bc3**.
- B. Check the **lfcopt** option, then click **Enter Relative Potential**.
- C. You will be prompted to select the output file used as the Relative Potential. Open the log file from the constant-N calculation folder (e.g., work1\_QE\_SCF¥pw.pwout). Then, enter **0.5** as the Relative Potential and click **OK**. When the message "The reference Fermi energy…" appears, click "**OK**". Finally, note down the value assigned to **fcp\_mu** (e.g., "-0.27062") using a text editor such as Notepad.

🚳 Quantum ESPRESSO Keyword Setup – 🗆 🗙	
Preset	Enter Relative Potential X Relative Potential [V]: 0.5 OK Cancel
esm_w 0.0	Winmostar ×
Citation M. Otani and O. Sugino, PRB 73, 115407, (2006).	The reference Fermi energy, relative potential and target Fermi energy (fcp_mu) would be set to -4.182 eV, 0.500 V and -3.682 eV (-0.2706 Ry), respectively.
N. DOI IIICL, T. POINSI ILA, O. Sugino and P. Olarii, FRE 109, 200101, (2012).	ОК
Reset Import Export OK Cancel Run	

A. Click **OK** to close the **Quantum ESPRESSO Keyword Setup** window. Then, click **OK** in the **Quantum ESPRESSO Workflow Setup** window. In the **Job Setting** window, configure the settings as needed and click **Run** to start the calculation.

Preset Optimize(Atom) v (modified) # of Jobs: + 1
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Spin Non-polarized V
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Pseudo file pbe-*rrkjus_psl.*.upf  Band structure Dielectric func NMR
Precision Medium V Metal Details (modified)
Reset Import 💌 Export OK

Since the target Fermi energy (**fcp\_mu**) is written in Rydberg units in the input file but output in electron volts (eV) in the log file, it is important to check and note the value in eV here.

#### A. Click Tools | Unit Converter

B. Set the physical quantity to **Energy**, change the left unit to **Ry** and the right unit to **eV**, then paste the previously copied **fcp\_mu** value into the left input field. The value shown on the right represents the target Fermi energy for the constant-µ calculation.

🚳 Winmostar Unit Conve	rter	_		×
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Ry ~	]	eV		~
				Close

- A. After the status of work2\_QE\_Relax changes to END (blue), In the Working Folders section, click work2\_QE\_Relax, then go to the Action menu and select Animation.
- B. Change the **Column** setting in the **Animation** control area to "9" to display a graph of the Fermi energy variation. Confirm that the value asymptotically approaches the result obtained in the previous step.



A. Change the **Column** setting in the **Animation** control area to "7" to display a graph of the charge variation.



A. In the **Working Folders** section, click **work2\_QE\_Relax**, then go to the **Action** menu and select either **Log** (full log file) or **Log (Extracted)** (summary view). Check the final values such as the total energy and Fermi energy for the Al slab from the log output.

¥ Project	Extracted Log (C:\winmos11\UserData\al_esm2.wmpjdata\work2_QE_Relax\pw.pwout)
➢ Project          Working Folders (al_esm2)       Options ▼         Name       Status         work1_QE_SCF       END         Image: The state of the state	<pre>Extracted Log (C:\winmos11\UserData\al_esm2.wmpjdata\work2_QE_Relax\pw.pwout) hartree contribution = 314.05513635 Ry xc contribution = -9.48666057 Ry ewald contribution = 302.52606339 Ry pot.stat. contrib. (-muN) = -0.00000000 Ry mvergence has been achieved in 22 iterations le Fermi energy is -3.7668 ev ttal energy = -19.82211181 Ry estimated scf accuracy &lt; 0.00000010 Ry smearing contrib. (-TS) = -0.01528305 Ry internal energy E=F+TS = -19.80682877 Ry The total energy is F=E-TS. E is the sum of the following terms: one-electron contribution = -627.27046697 Ry hartree contribution = -627.27046697 Ry hartree contribution = -627.27046697 Ry kartree contribution = -9.48911794 Ry ewald contribution = -9.48911794 Ry ewald contribution = -9.48911794 Ry ewald contribution = -3.6815 ev total energy is -3.6815 ev total energy = -19.82211715 Ry estimated scf accuracy &lt; 8.9E-10 Ry estimated scf accuracy &lt; 0.1529592 Ry</pre>
Coordinate (Final)  Log Log (Extracted)  SCF Energy Change  Animation  Charge/Energy Profile  Show in Explorer	<pre>smearing contrib. (-TS) = -0.01529592 Ry internal energy E=F+TS = -19.80682123 Ry The total energy is F=E-TS. E is the sum of the following terms: one-electron contribution = -627.34237450 Ry hartree contribution = 314.49654698 Ry xc contribution = 302.52606339 Ry pot.stat. contrib. (-muN) = 0.00262420 Ry convergence has been achieved in 21 iterations bfgs converged in 3 scf cycles and 2 bfgs steps Final grand-energy = -19.8221171480 Ry PWSCF : 3m30.97s CPU 3m45.08s WALL This run was terminated on: 11:43: 0 20Apr2025</pre>

- A. In the **Working Folders**, click **work2\_QE\_Relax**, then select **Charge/Energy Profile** from the "Action" menu.
- B. In the **Terms** section, check only **Tot chg** (charge) and **Avg v\_hart+v\_loc** (potential), then click **Draw**.
  - Note that in this graph, z = 0 (the position of the slab) is centered.



- A. To plot the difference in charge or potential between the constant-N and constant-µ calculations, check **Select another esm1 file and plot difference**, then select the wm.esm1 file from the constant-N calculation folder (e.g., work1\_QE\_SCF¥wm.esm1).
- B. Click Draw.



# 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.