M winmostar tutorial

Quantum ESPRESSO Defect Formation Energies

V11.11.0

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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 requires Winmostar V11 Professional Elite Edition.
- In this tutorial, we calculate the defect formation energy of various charge states for a point defect in diamond. We begin by performing structural optimization on the pristine model (defect-free) to obtain the total energy per atom (μ), the valence band maximum (*E*_V), and the conduction band minimum. Next, using a defective supercell containing *N* atoms, we calculate the total energy *E*_d(*q*) for different charge states *q*. Finally, we use these values to plot the defect formation energy *E*_f(*q*) as a function of the Fermi level μ_e for each charge state. (Reference : *Phys. Rev. B*, 71, 035206 (2005).)

 $E_{\rm f}(q) = E_{\rm d}(q) - N\mu + q(E_{\rm V} + \mu_{\rm e})$

Note :

- 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>
- The calculated defect formation energy can be affected by the supercell size and whether structural optimization is performed for the defective structure. Depending on the purpose of the study, it may be necessary to compute correction terms to account for finite-size effects in such calculations.

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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 (defect-free)

- 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</u> <u>User Manual section 5, 'Structure Building</u>'.Here, we load an existing molecular structure file.
- A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.
- B. Enter 'diamond_defect_qe' in Project name and click Save.
- C. Click File | Import | Sample File | dia.mol2

-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 (defect-free)

- A. Select Quantum ESPRESSO from Solver in Toolbar and click 🗹 (Workflow Setup).
- B. Set **Preset** to 'Optimize (Atom & Cell)', then change the **Pseudo file** to pbe-*rrkjus_psl*.upf and set **# of bands** to "30% more".
- C. Click **OK** in **Quantum ESPRESSO Workflow Setup** window, then make appropriate settings in **Job Setting** window before clicking **Run**.

Preset Optimize	e(Atom&Cell)	~ (m	odified)	# of Jol	os: + 1	
				ble parameter/struc	ture scan Conf	ıg
1st job					+ -	h
Task Opt	timize(Atom&Cell) 🗸 🗸	Cutoff energy [R: (Suggest: 37 F	() 35.0	Pressure [kbar]	0.0	
Charge [e]	0.	lanually spec	ify cutoff energy	Phonon (DFPT)	Disabled ~	
# of bands	30% more		horst-Pack 🗸 🗸 🗸	Use Bravais-lat	ttice index	
Spin	Non-polarized \sim					
Pseudopoten	tial		Properties			
Туре	All 🗸		DOS	Charge density	Phonon DOS	
Functional	All		PDOS/Lowdin	Potential/ Work func	Phonon band	
Pseudo file	pbe-*rrkjus_psl.*.upf		d structure	Dielectric func	NMR	
Precision	Medium \vee	Metal		Det	ails	
Reset	Import 🖛 E	xport		OK		

B. Execution of Calculation (defect-free)

Note: If the calculation terminates abnormally, please repeat the following process until the calculation successfully ends.

- A. The work1_QE_Relax calculation terminates abnormally (**status:ABORT**) because it fails to satisfy all convergence criteria for energy, forces, and pressure. Therefore, the structural optimization will be executed again.
- B. Click **⊆** (Workflow Setup), and when prompted with "Do you want to continue run?", click Yes. Then select work1_QE_Relax and click OK. If the message "…Do you want to ignore and continue?" appears, click Yes to proceed.
- C. After adjusting the settings as needed in the **Job Setting** window, click **Run**.
- D. The work2_QE_Relax calculation terminates abnormally too (**status:ABORT**) because it fails to satisfy all convergence criteria for energy, forces, and pressure. Therefore, the structural optimization will be executed again.
- E. Click **⊆** (Workflow Setup), and when prompted with "Do you want to continue run?", click Yes. Then select work2_QE_Relax and click OK. If the message "…Do you want to ignore and continue?" appears, click Yes to proceed.
- F. After adjusting the settings as needed in the **Job Setting** window, click **Run**.

M Select working	g folder			_	×
Select the working	ng folder which you v	vant to continue	the job from		
Name	Status	Profile	Output Location	Description	
work1_QE_Relax		Local Job	Local		

C. Analysis of Results (defect-free)

- A. Once the **Status** of work3_QE_SCF changes to **END**, click **Log (Extracted)** from the **Action** menu.
- B. Once the log is displayed, scroll down to the bottom and locate the line that starts with '! Total energy'. Note the total energy value shown on this line. Also, check the line above that reads 'highest occupied, lowest unoccupied level (ev):', and record the values for the valence band maximum and conduction band minimum.

➢ Project	
Working Folders (diamond_defe Options▼	🔤 Extracted Log (C:¥winmos11¥UserData¥diamond_defect_qe.wmpjdata¥work3_QE_Relax¥pw.pwout) — 🛛 🗙
Name Status	0.00000000 -0.00000000 -0.00001726 0.00 -0.00 -2.54 highest occupied, lowest unoccupied level (ev): 13.3796 17.5735
work1_QE_Relax ABORT	stimated scf accuracy < 0.0000001 Ry
O └ work2_QE_Relax END	he total energy is the sum of the following terms:
	hartree contribution = 1.94620544 Ry xc contribution = -8.40840377 Ry ewald contribution = -25.59530915 Ry convergence has been achieved in 2 iterations
	Total force = 0.000000 Total SCF correction = 0.000000 total stress (Pu(bobr**2) (kbar) P= -0.06
	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
Action (work2_QE_Relax)	bfgs converged in 3 scf cycles and 1 bfgs steps Estimated max dynamical RAM per process > 4 01 MB
Coordinate (Initial)	highest occupied, lowest unoccupied level (ev): 13.3762 17.5716 ! total energy = -23.88562850 Ry
Coordinate (Final)	estimated sof accuracy < 0.00000005 Ry The total energy is the sum of the following terms:
E Log	one-electron contribution = 8.17316862 Ry hartree contribution = 1.94407868 Ry
Log (Extracted)	$\mathbf{v} \in \operatorname{Contribution} = -8 4 \mathrm{M/SbbbS} \mathrm{Kv}$
SCF Energy Change	

D. Modeling of the System (defective model)

- A. Finally, in the Action menu of the successfully completed work2_QE_Relax, click Coordinate (Final).
- B. Click **Solid | Convert Lattice** to revert back to the conventional cell. If you see the message 'You are not allowed to save in format of the file...', click **Yes**.

×	Project	
Wo	orking Folders (diamond_defe	Options V
	Name work1_QE_Relax work2_QE_Relax	Status ABORT END
Act	tion (work2_QE_Relax)	
	Coordinate (Initial) Coordinate (Final)	

D. Modeling of the System (defective model)

- A. Click Solid | Generate Supercell…
- B. Set the values of **a**, **b**, and **c** to "2", and then click **OK** to apply the changes.



D. Modeling of the System (defective model)

A. Click **Delete Atom**, and when prompted with "Are you sure you want to delete 1C?", click **Yes**. Then confirm that the number of atoms has been updated to 63 (N = 63).



E. Execution of Calculation (defective model)

- A. Click (Workflow Setup), and when prompted with "Do you want to continue run?", click No.
- B. Set the **Preset** to 'SCF', then enter '%WM_SCAN1%' for **Charge**, and change the **Pseudo file** to pbe-*rrkjus_psl*.upf.
- C. Click Details.

💹 Quantum I	ESPRESSO Workflow Setup	- 🗆 X
Preset SCF	(modified)	# of Jobs: + 1 -
	nat	ble parameter/structure scan Config
1st job		+ -
Task Ene	ergy Cut (ff energy [Ry] 35.0	Pressure [kbar] 0.0
Charge [e]	%WM_SCAN1% cify cutoff energy	Phonon (DFPT) Disabled ~
# of bands	Default v Ints Monkhorst-Pack v	Use Bravais-lattice index
Spin	Non-polarized ~	
Pseudopoten	tial Properties	
Туре	All ~ Dos	Charge density Phonon DOS
Functional	All PDOS/Lowdin charge	Potential/ Phonon band
Pseudo file	pbe-*rrkjus_psl.*.upf	Dielectric func NMR
Precision	Medium V Metal	Details
Reset	Import 🔽 Export	OK Cancel

E. Execution of Calculation (defective model)

• Set occupations to 'smearing', then click OK.

(Defect levels that appear within the band gap can negatively affect SCF convergence, so smearing is applied. Although the calculation conditions should be kept consistent between the defect-free and defective models, setting **Metal** in the Workflow Setup window can unintentionally change other parameters. Therefore, we apply smearing directly via the Keyword Setup window instead.)

) Quantu	m ESPRESSO) Keyword Setup					- C	X נ
Preset			~					
RISM (1)	RISM (2	2) Others	Preview	Options	Prope	erties	Pseudo	potential
Basic	Advanced	Spin/DFT+U	Phonon	NMR/EFG	MD	Dip	ole Corr	ESM
restart_m	ode	Automatically set	~	Set ibrav =	1 and ce	elldm		
calculation	ı	scf	\sim	ecutwfc (Suggest: 37	7Rv)	35.0		
# of band (# valence	s e bands: 126)	Do not specify	\sim	Ecut for US/PA (Density)	W	Specify	ecutrho/e	cutvi ~
nbno	l	126		ecutrho (Suggest:	318 Rv)	315		
nbno	l(Relative)	0	% more	ecutrho/ecu	twfc	9.		
K_POINTS	automatio	c(by Spacing)	\sim	tot_charge		%WM_	SCAN1%	
(Spa	cing) [A^-1]	0.50		occupations		smearir	g	
		222000	^	ion_dynamics		none		
				cell_dynamics		none		\sim
		<	>	tprnfor		tstre	SS	
		Set default k-p	ath					
		nosym r	noinv					
Reset	Import	Export			ок	Can	cel RUN	Run

E. Execution of Calculation (defective model)

- A. Check **Enable parameter/structure scan**, then click **Config**. (This feature is available only in the Professional edition Elite.)
- B. Click Enter Step…, then enter "-4" for Minimum value, "1" for Interval, and "7" for Number of steps.
- C. Click **OK** in the **Parameter/Structure Scan** window.
- D. Click **OK** in the **Quantum ESPRESSO Workflow Setup** window, adjust the settings as needed in the **Job Setting** window, and then click **Run**.



F. Analysis of Results (defective model)

- A. Once all jobs from work3 QE Relax to work9 QE Relax have the **status END**, click File | Project | Parameter/Structure Scan Results.
- B. Click **Draw**, then go to **Options** in the lower-right corner of the graph and select **Export csv & Open Excel**. When the save dialog appears, click **Save**.
- C. Once the CSV file opens, check the total energy (in Ry) for each charge state.



-747.3538115-748.5700222-749.7388543-750.8609651-751.9370589 -752.9675631 -753.9452054

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F. Analysis of Results (Defect Formation Energies)

From this point on, we will use external graphing tools instead of Winmostar. For each charge state q, plot the defect formation energy $E_f(q)$ as a function of μ_e using the following equation. To convert units, go to **Tools** | **Unit Converter**. Set the upper limit of the x-axis (μ_e) to the energy difference between the conduction band minimum and the valence band maximum obtained from the defect-free model on page 9. An example plot is shown on page 18.

	Definition	q = 0	q = 1	•••
$E_{\rm d}(q)$	Total energy of the defective model at charge state q (obtained on p.16)	-751.9370589 Ry = -10230.62487 eV	-752.9675631 Ry = -10244.64560 eV	
N	Number of atoms in the defective model	63	63	
μ	Total energy per atom of the defect-free model (from page 9)	-23.88562850 Ry ÷ 2 = -324.9805314 eV÷ 2	-23.88562850 Ry ÷ 2 = -324.9805314 eV÷ 2	
$E_{ m V}$	Valence band maximum of the defect- free model (highest occupied level from page 9)	13.3762 eV	13.3762 eV	

F. Analysis of Results (Defect Formation Energies)



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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