winmostar tutorial

Quantum ESPRESSO Defect Formation Energies

V11.11.0

7 Jan. 2025 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 Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session: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.
  - Individual Training Session: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 Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. 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).)

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

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:https://qiita.com/xa_member
- 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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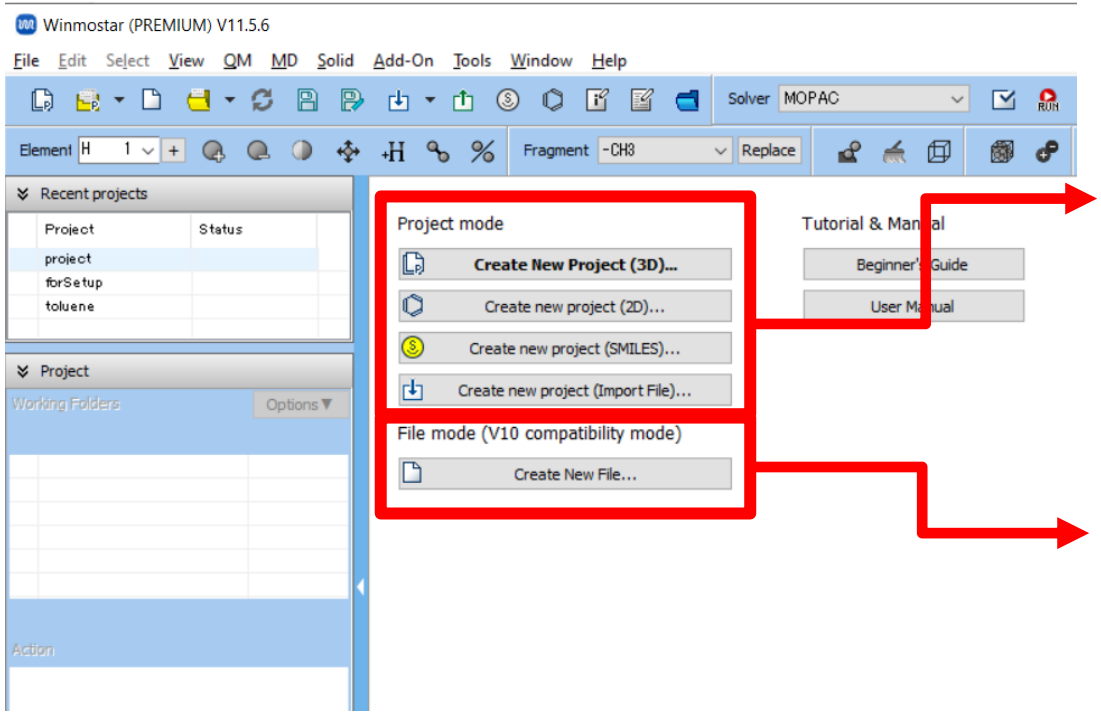
Operating Modes of Winmostar V11

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



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System (defect-free)

- Please refer to QE Basic Tutorial for the basic operation method.
- For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Structure Building'.Here, we load an existing molecular structure file.

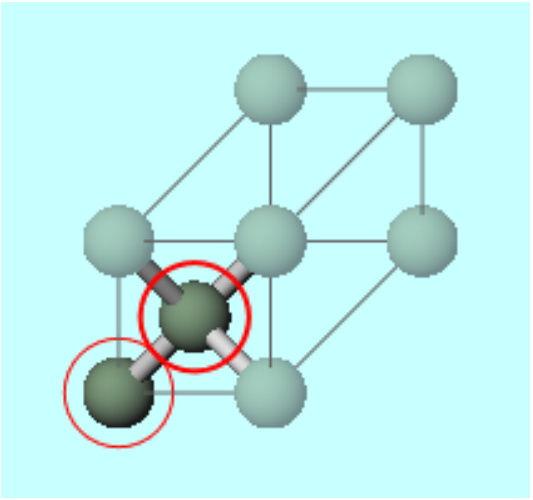
A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

B. Enter '`diamond_defect_qe`' in **Project name** and click **Save**.

C. Click **File | Import | Sample File | dia.mol2**

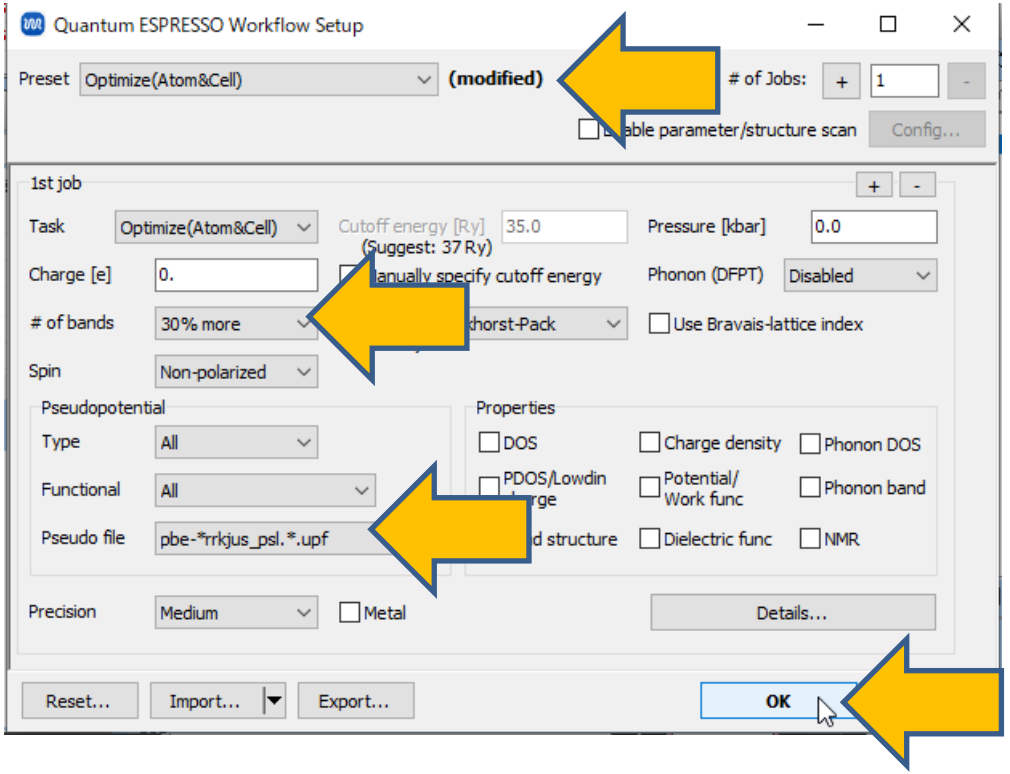
-If you wish to load a different file at this stage, use **File | Import File** instead.

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**.



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.

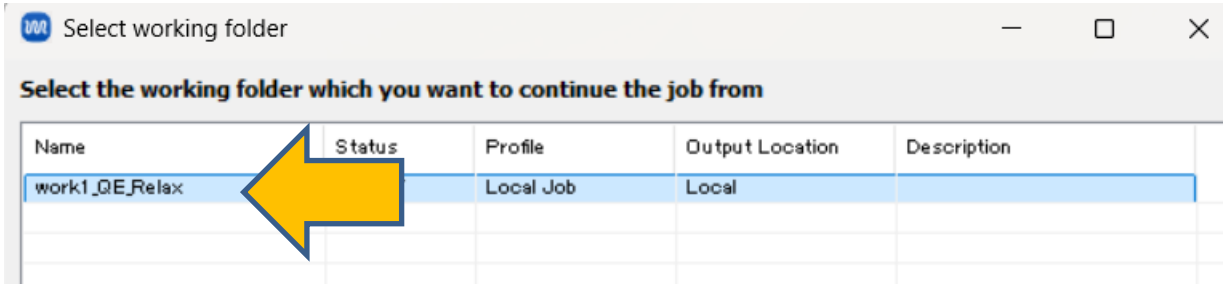
B. Click **(Workflow Setup)**, and when prompted with “Do you want to continue run?”, click **Yes**. Then select work1_QE_Relax and click **OK**. If the message “…Do you want to ignore and continue?” appears, click **Yes** to proceed.

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.

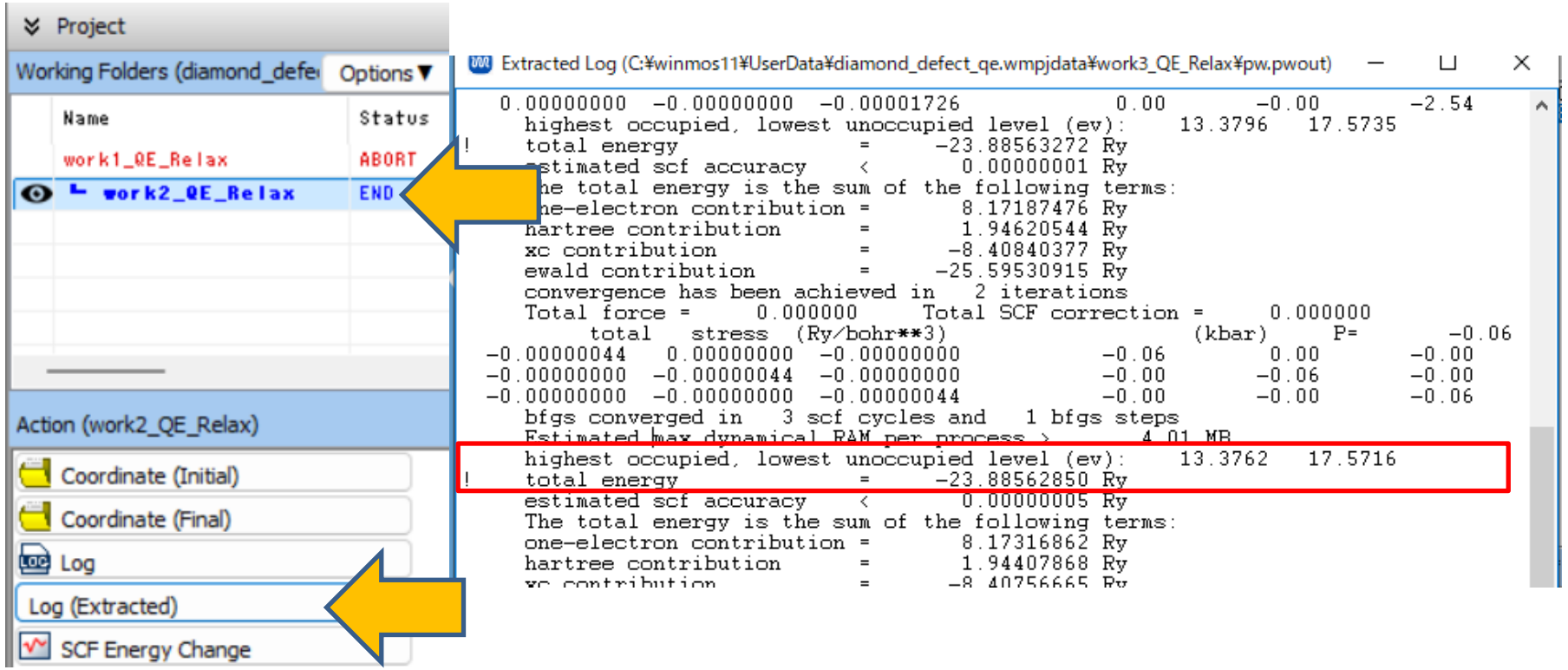
F. After adjusting the settings as needed in the **Job Setting** window, click **Run**.



C. Analysis of Results (defect-free)

A. Once the **Status** of work3_QE_SCF changes to **END**, click **Log (Extracted)** from the **Action** menu.

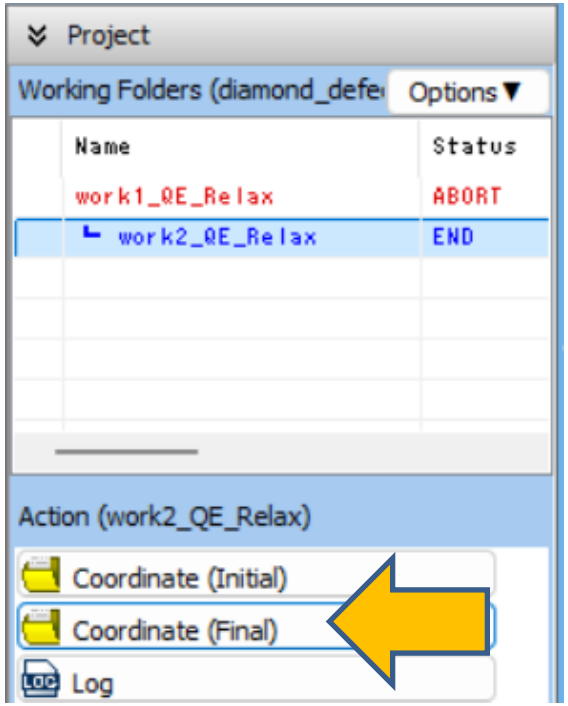
B. Once the log is displayed, scroll down to the bottom and locate the line that starts with '! Total energy'. Note the total energy value shown on this line. Also, check the line above that reads 'highest occupied, lowest unoccupied level (ev):', and record the values for the valence band maximum and conduction band minimum.

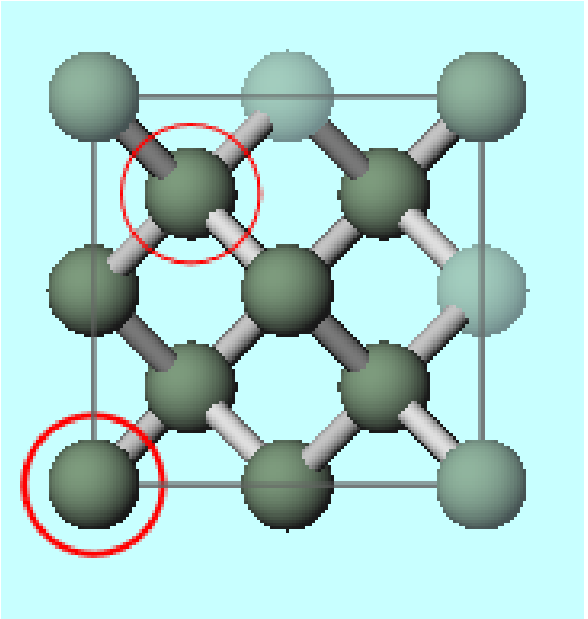


D. Modeling of the System (defective model)

A. Finally, in the Action menu of the successfully completed work2_QE_Relax, click Coordinate (Final).

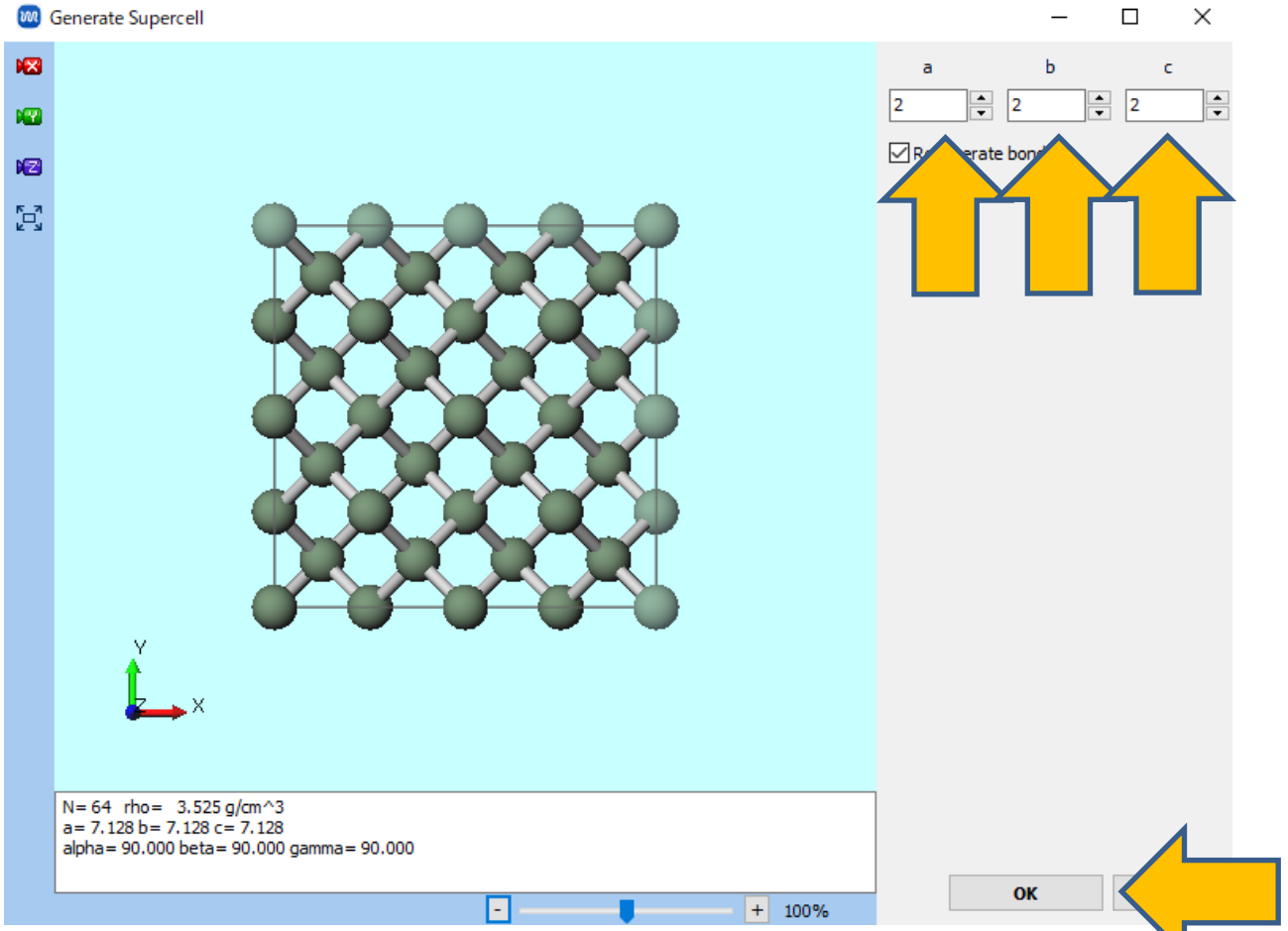
B. Click **Solid | Convert Lattice** to revert back to the conventional cell. If you see the message 'You are not allowed to save in format of the file…', click **Yes**.





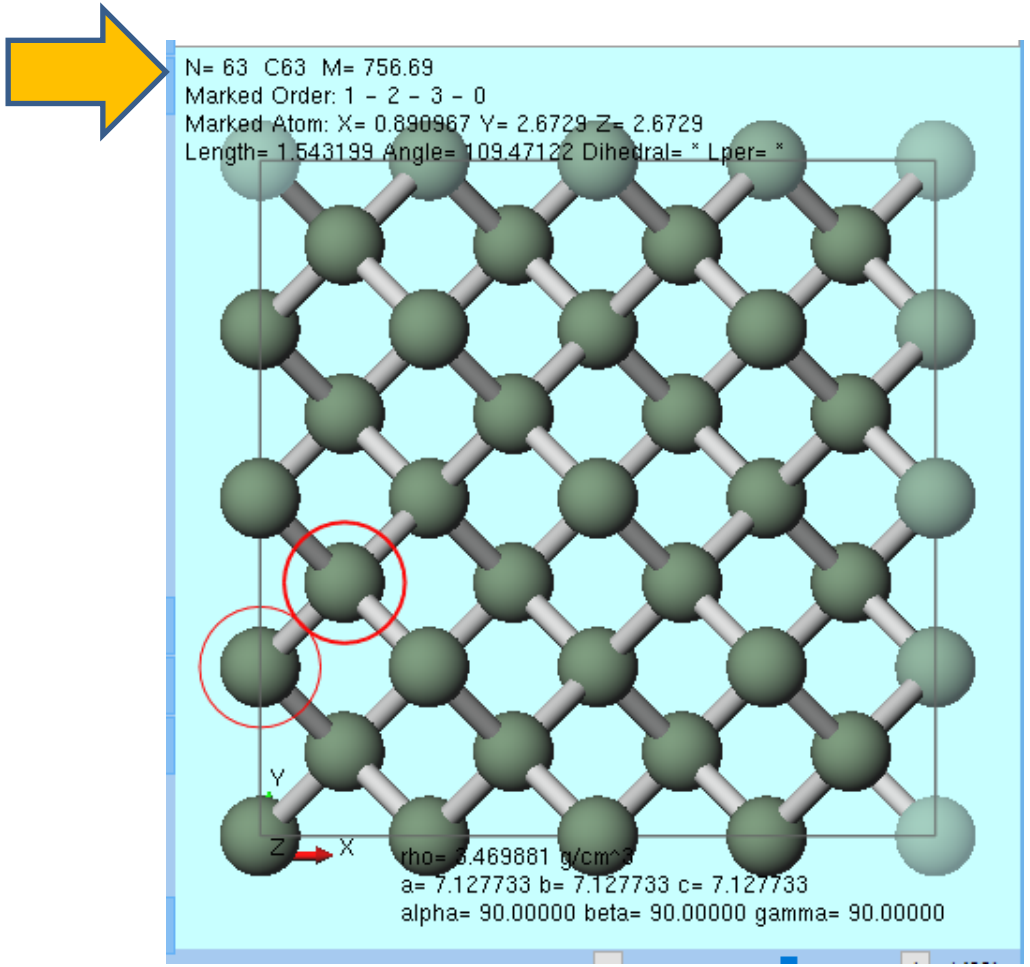
D. Modeling of the System (defective model)

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).

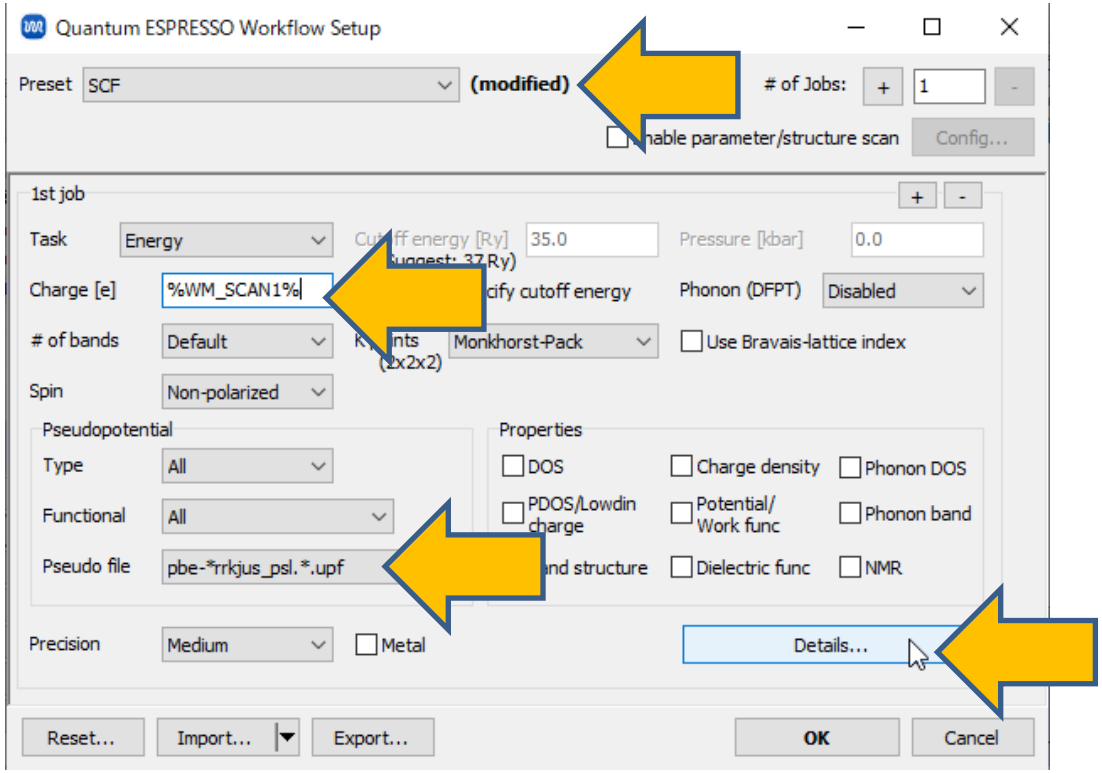


E. Execution of Calculation (defective model)

A. Click **(Workflow Setup)**, and when prompted with “Do you want to continue run?”, click **No**.

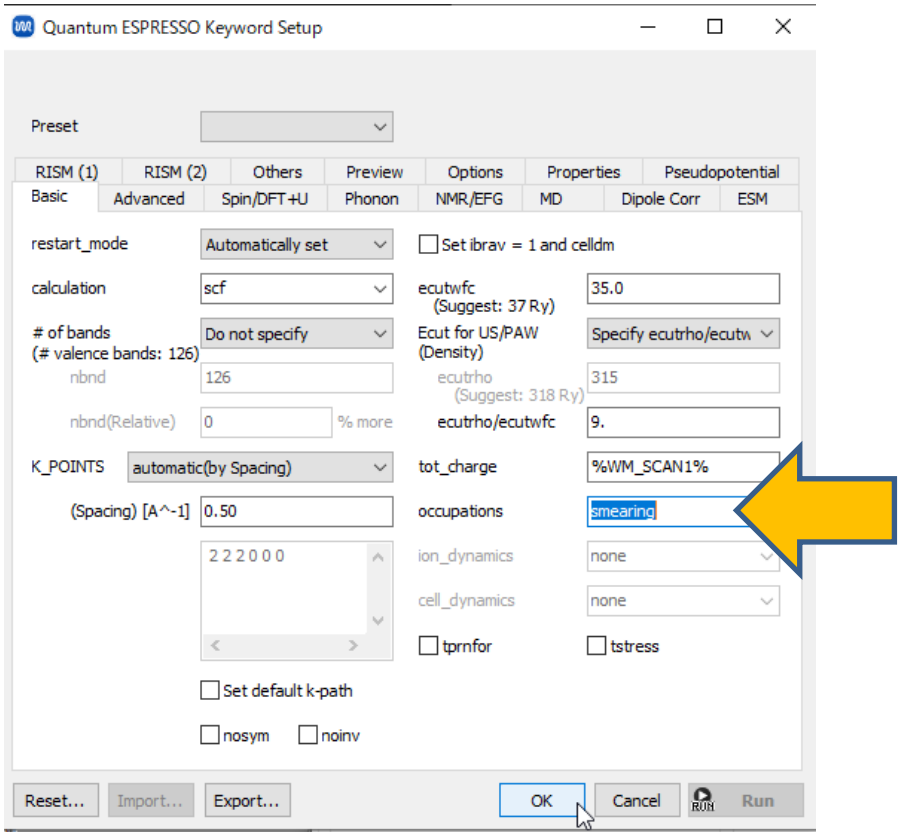
B. Set the **Preset** to ‘SCF’, then enter ‘%WM_SCAN1%’ for **Charge**, and change the **Pseudo file** to pbe-*rrkjus_psl*.upf.

C. Click **Details.**



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.)



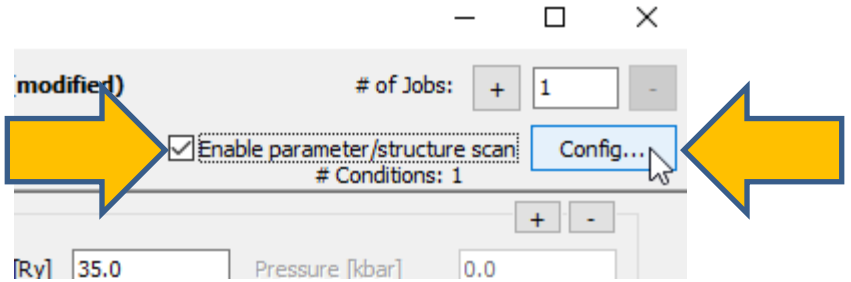
E. Execution of Calculation (defective model)

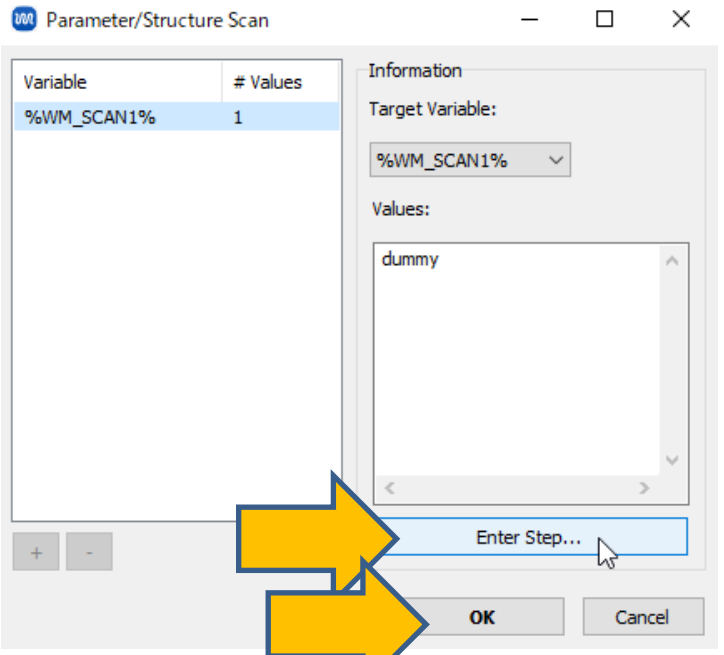
A. Check **Enable parameter/structure scan**, then click **Config**. (This feature is available only in the Professional edition Elite.)

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**.



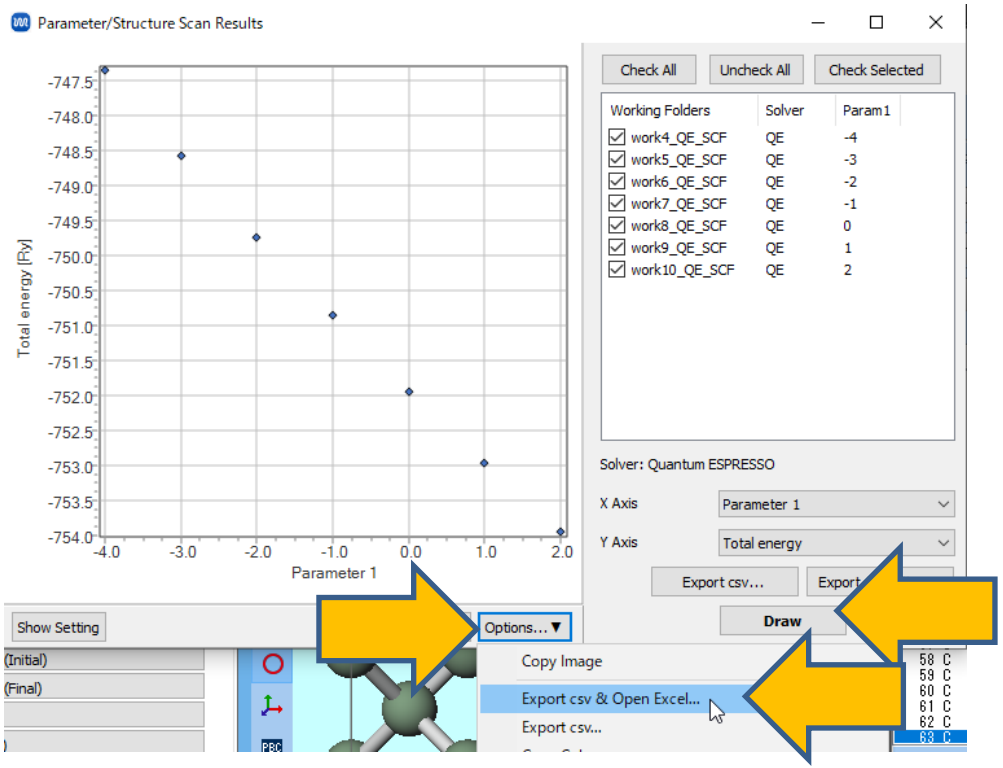


F. Analysis of Results (defective model)

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.



Parameter 1	
-4	-747.3538115
-3	-748.5700222
-2	-749.7388543
-1	-750.8609651
0	-751.9370589
1	-752.9675631
2	-753.9452054

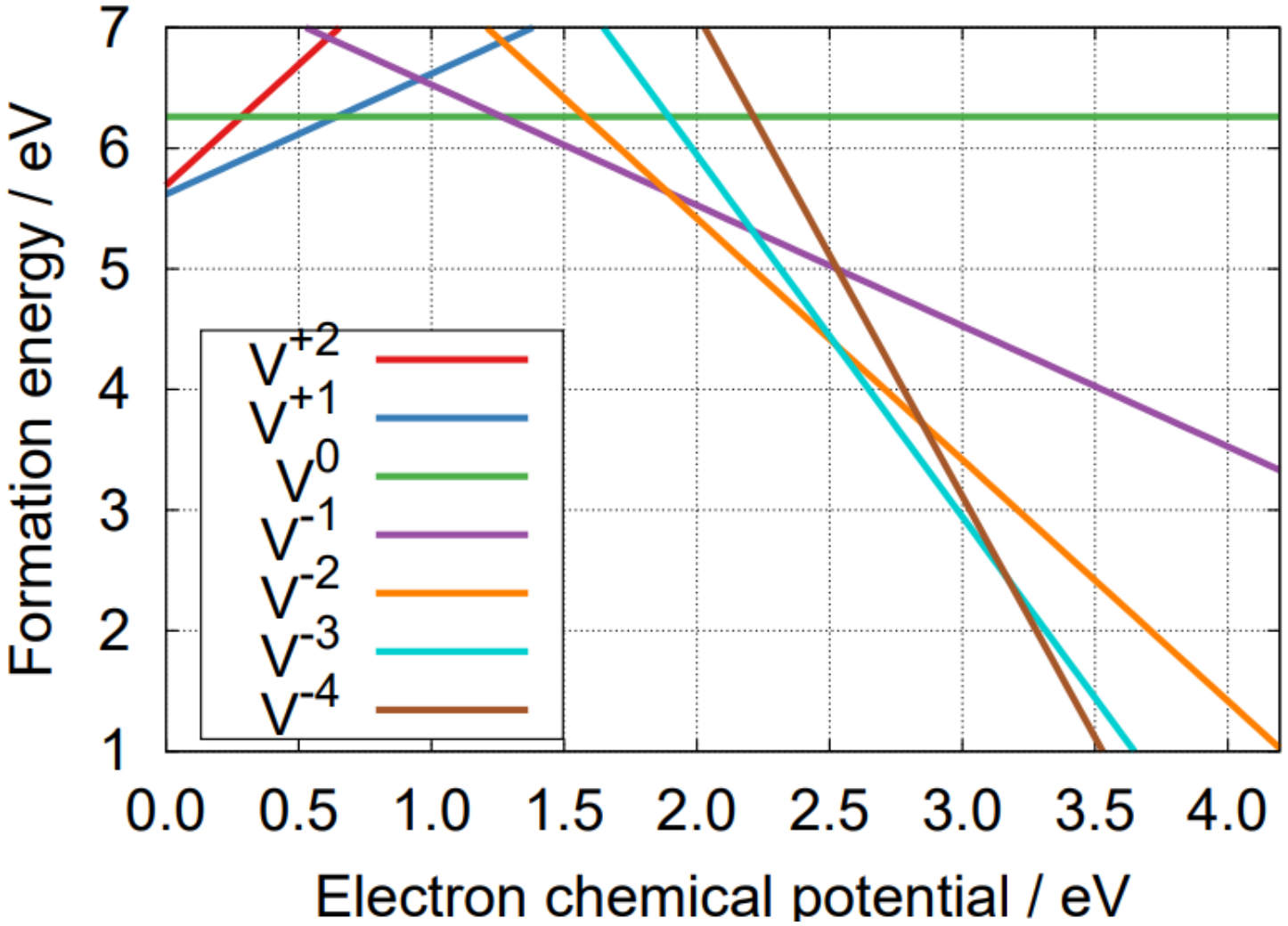
F. Analysis of Results (Defect Formation Energies)

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.

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

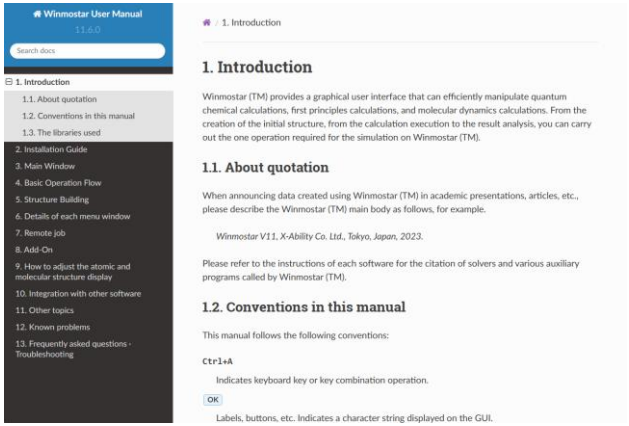
	Definition	$q = 0$	$q = 1$	...
$E_{\mathrm{d}}(q)$	Total energy of the defective model at charge state q (obtained on p.16)	-751.9370589 Ry = -10230.62487 eV	-752.9675631 Ry = -10244.64560 eV	
N	Number of atoms in the defective model	63	63	
μ	Total energy per atom of the defect-free model (from page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

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