winmostar tutorial

Quantum ESPRESSO
Van der Waals Corrections

V11.6.5

6 April 2024 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 manual outlines the procedure for performing calculations on graphite crystals using the Grimme-D2 method for Van der Waals corrections.
  - The interactions between the layers of graphite are largely due to Van der Waals forces, and the use of Van der Waals corrections is expected to improve the accuracy of predicting stable structures, especially the interlayer distances.

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

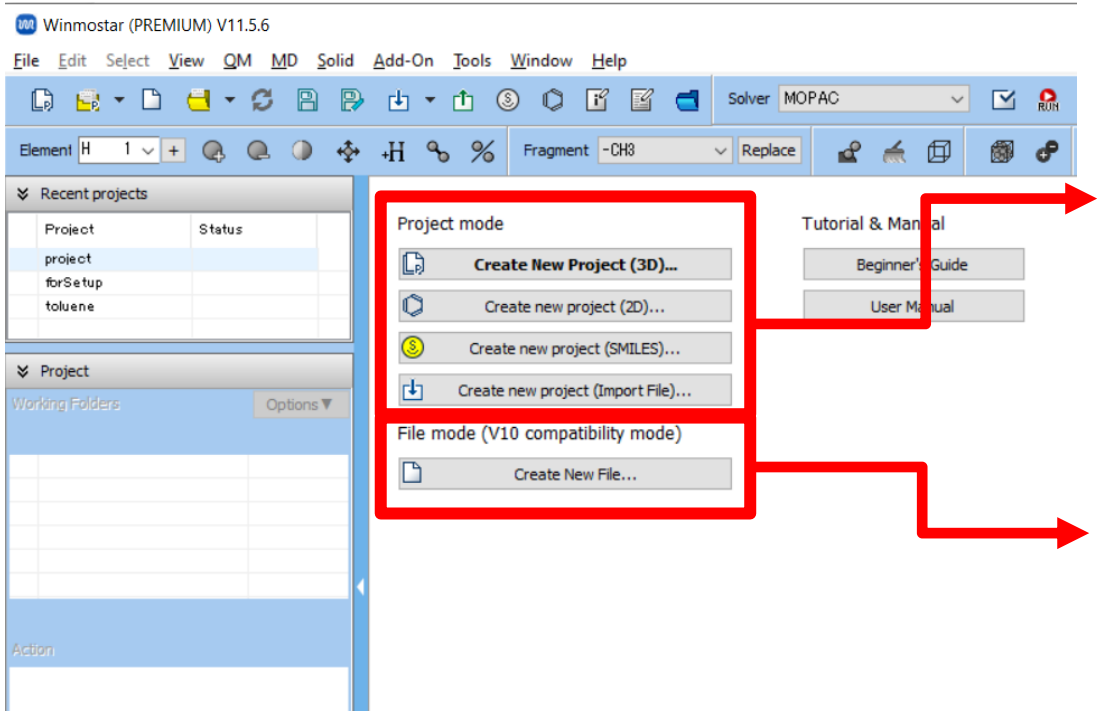
Preference of Operating Environment

- 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 the recommended one, you will need to install and configure Windows version of Quantum ESPRESSO separately.

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

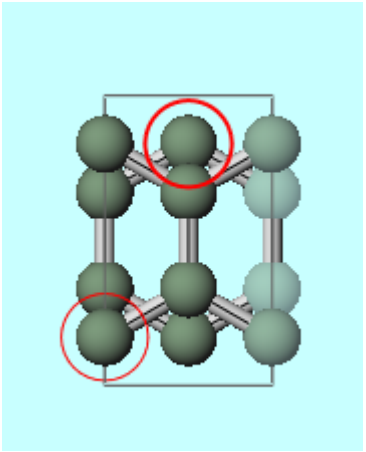
- Please refer to QE Basic Tutorial for the basic operation method.
- For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Structure Building'.

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

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

C. Click **File | Import | Sample File | graphite.cif**.
   - 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**.

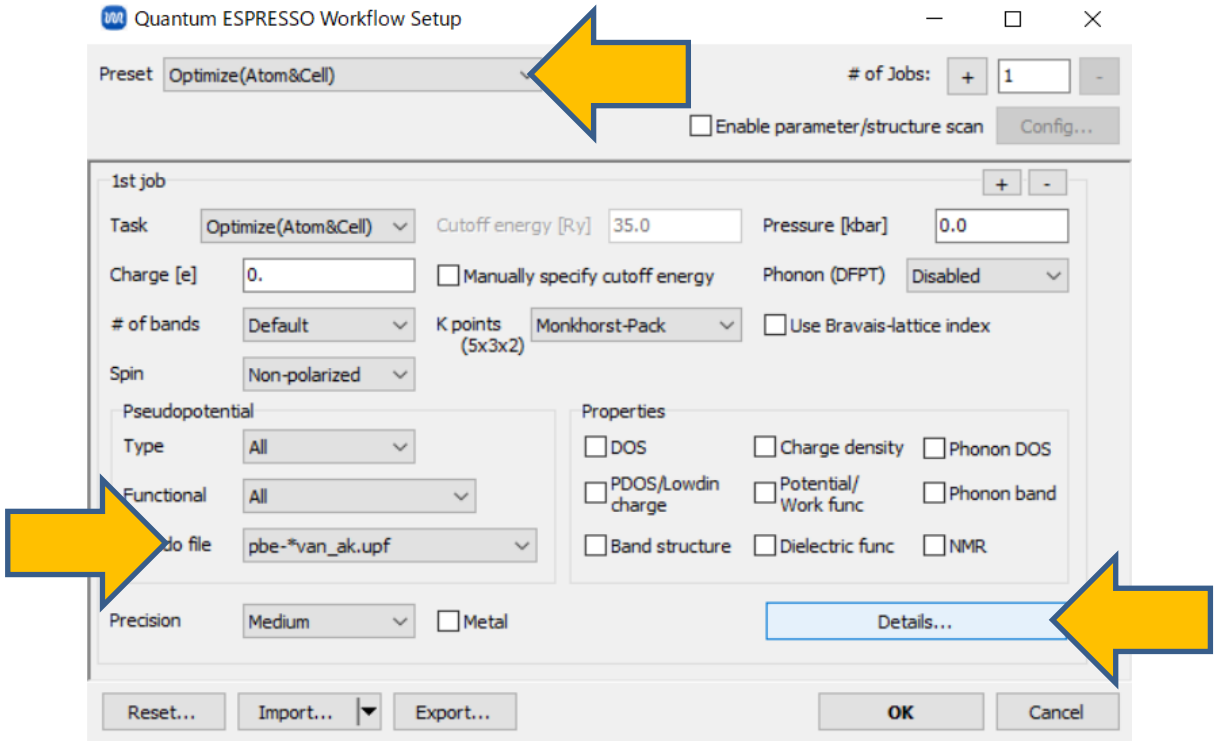


B. Execution of Calculation

A. Select **Quantum ESPRESSO** from **Solver** in Toolbar and click **(Workflow Setup)**. If asked whether to convert to a primitive cell, click **No**.

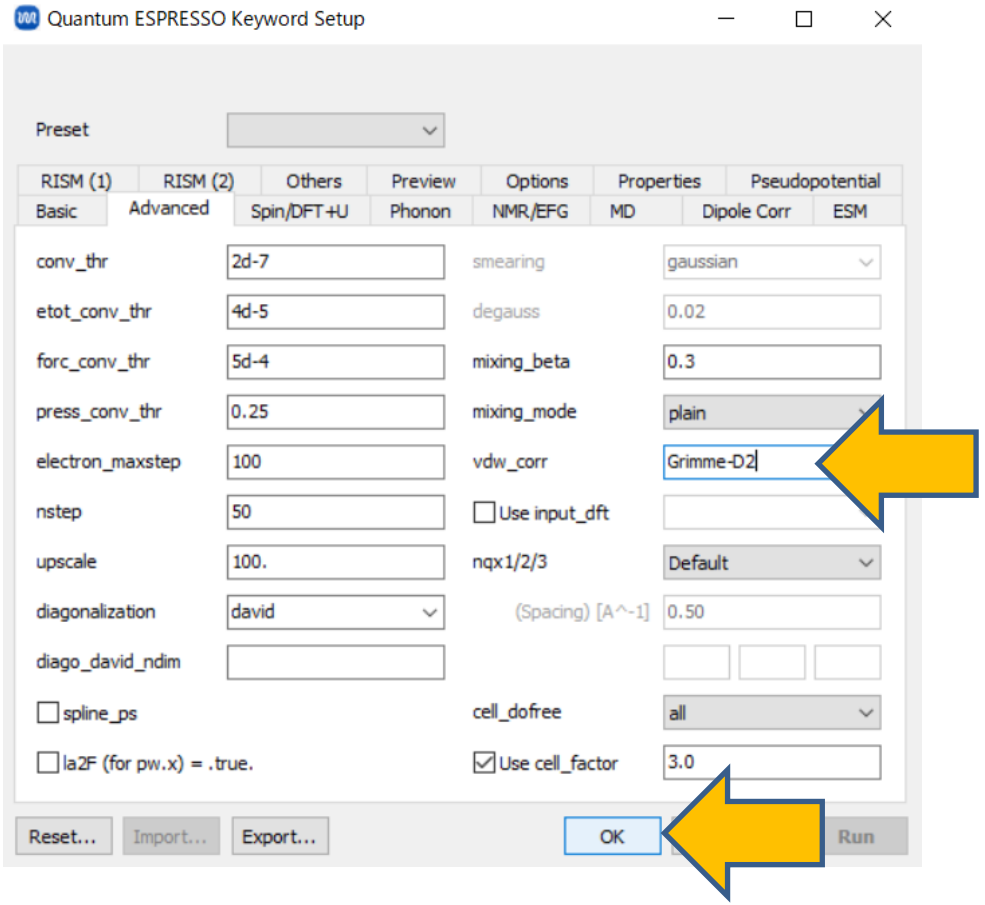
B. Change **Preset** to 'Optimize (Atom & Cell)' and **Pseudo file** to 'pbe-*van_ak.upf'.

C. Click **Details**.



B. Execution of Calculation

A. Navigate to **Advanced** tab and change **vdw_corr** to 'Grimme-D3', then click **OK**.
B. Click **OK**, then make the appropriate settings in **Job Setting** window before clicking **Run**.

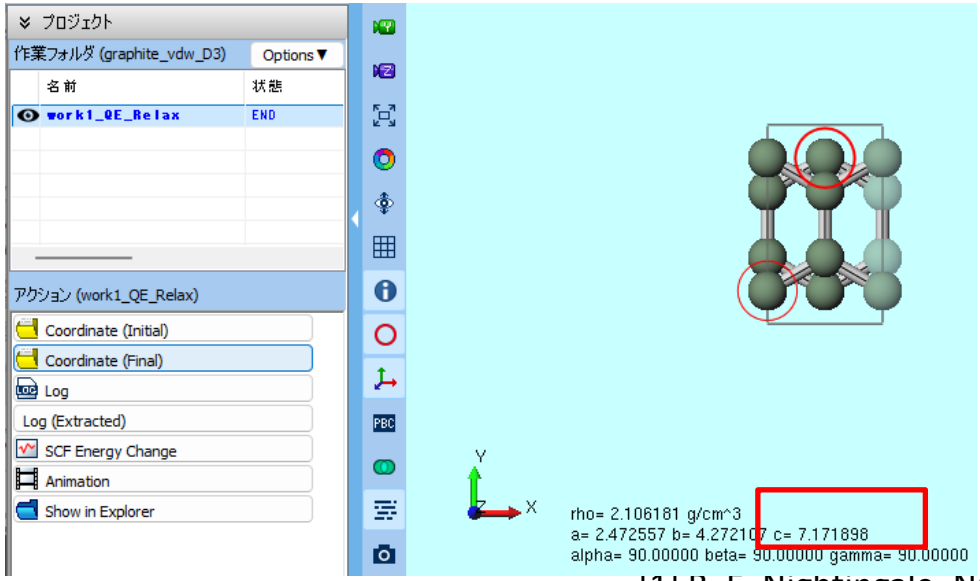


C. Result Analysis Lattice Constant

A. After **the status** of **work1_QE_SCF** in **Working Folders** changes to **END (blue)**, click work1_QE_SCF in **Working Folders** and select **Coordinate (Final)** from **Action**.

B. Obtain the lattice constant (twice the interlayer distance) from the value of 'c=' below Viewport.

   – Although the k-points and cutoff energy are not adjusted in this manual, making these values only reference, the calculations in this book showed that including Van der Waals corrections brings the values closer to the experimental value (around 6.70 Å[1]) compared to the values without Van der Waals corrections.



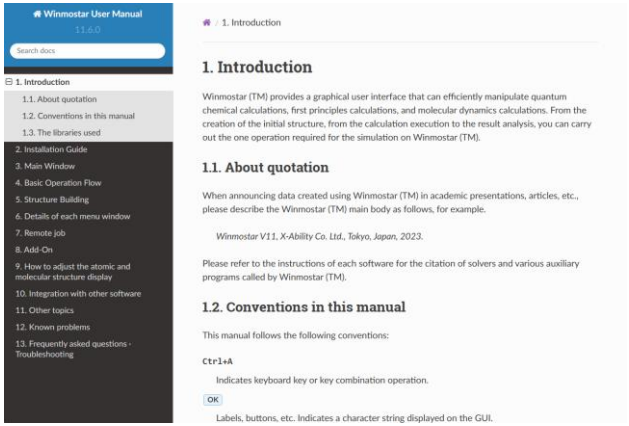
Without Van der Waals Corrections

rho= 1.980480 g/cm^3
a= 2.473064 b= 4.273358 c= 7.623306
alpha= 90.00000 beta= 90.00000 gamma= 90.00000

[1] R. E. Nightingale, Nuclear Graphite, Academic Press, New York, (1962).etc

Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



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Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact page, detailing the steps to reproduce the issue and attaching any generated files at that time.