winmostar tutorial

Quantum ESPRESSO
Born-Oppenheimer MD

V11.6.5

3 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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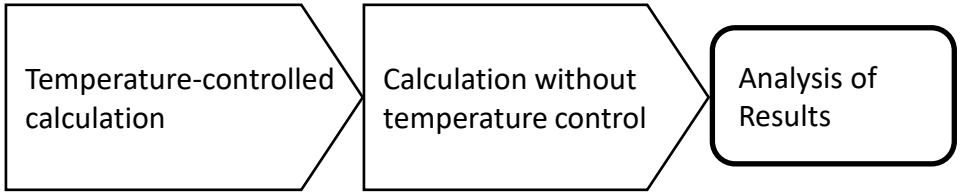
Overview

- Perform a brief Born-Oppenheimer (BO) MD calculation for methane molecules. Start by conducting the calculation at 300 K under temperature control, then proceed to perform the calculation without temperature control. Visualize energy temperature and animations.



Notes:

- The number of bands, type of pseudopotential, and cutoff energy affect the calculation results. This tutorial utilizes settings with reduced precision to obtain results quickly.
- The size of the system also influences the calculation results.
- By allowing sufficient equilibration time and conducting long-duration calculations, highly reproducible data can be obtained.

◆ For detailed information on the calculation method and settings in Quantum ESPRESSO, please refer to our article at https://qiita.com/xa_member

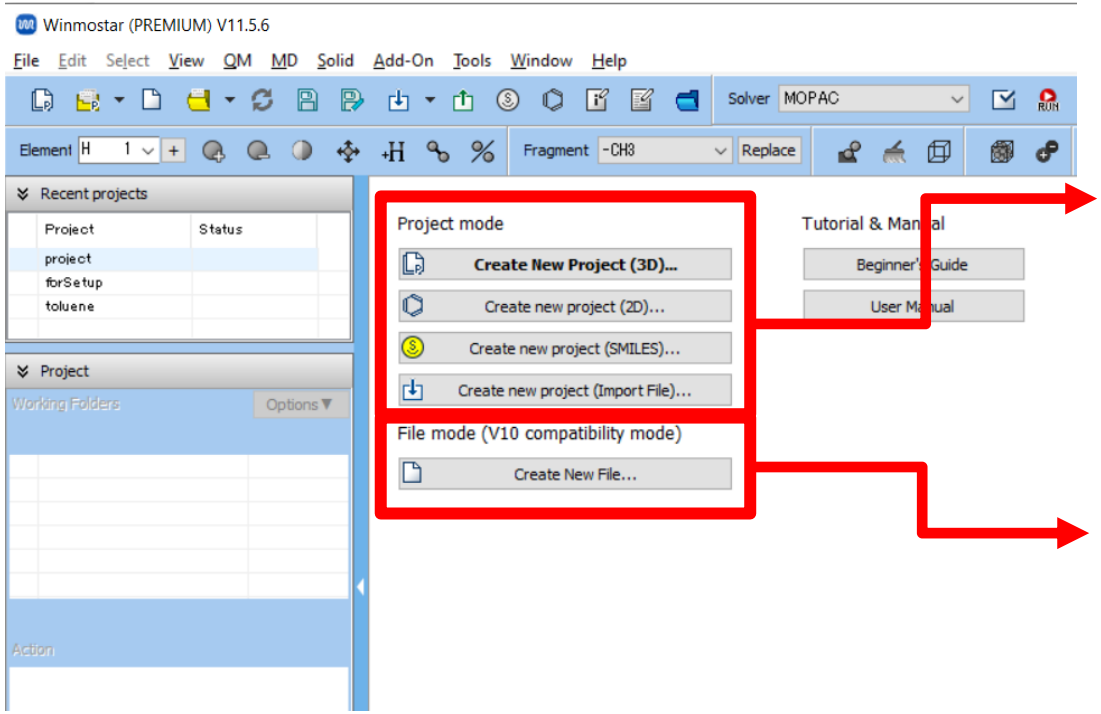
Preference of Operating Environment

- 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.
For operations in File Mode, please refer to [Quantum ESPRESSO tutorial for version 10].



Project Mode New Features in V11

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

File Mode

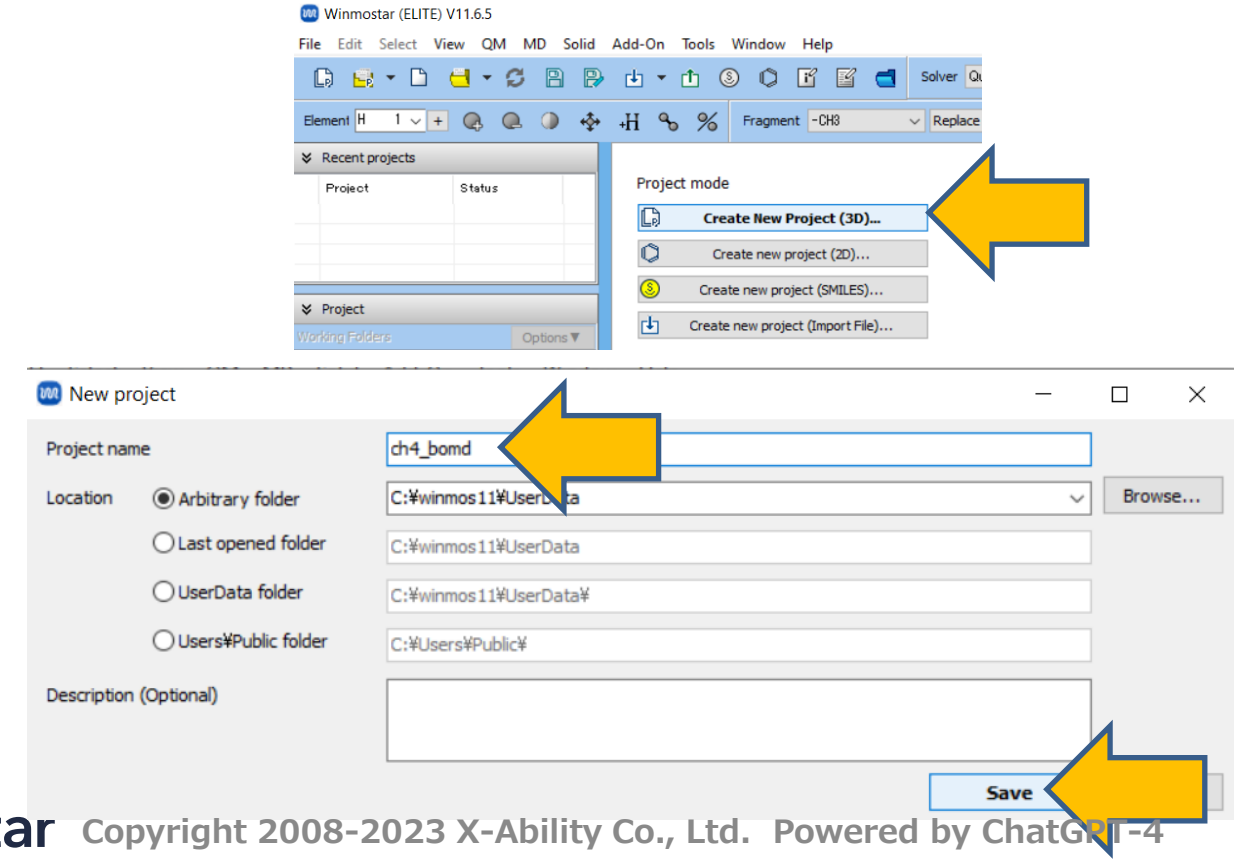
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

Please refer to QE Basic Tutorial for the basic operation method.

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

B. Enter '`ch4_bomd`' in **Project name** and click **Save**



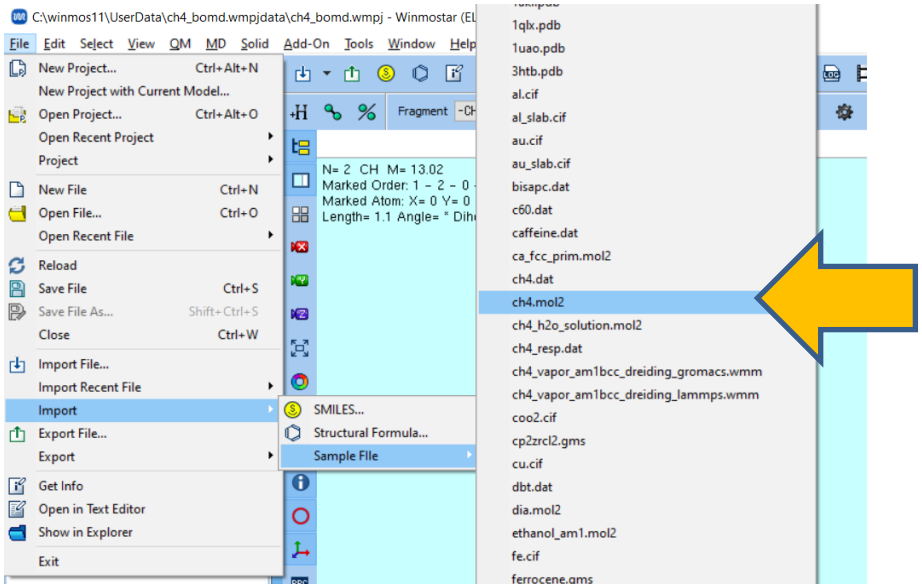
A. Modeling of the System

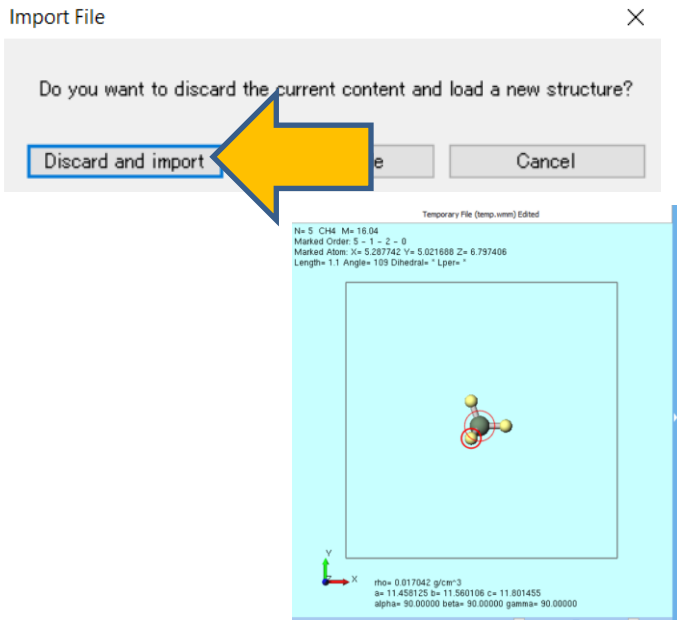
For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Methods for Creating Initial Structures'.Here, we load an existing molecular structure file.

A. Click **File | Import | Sample File | ch4.mol2**.
   - 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**.

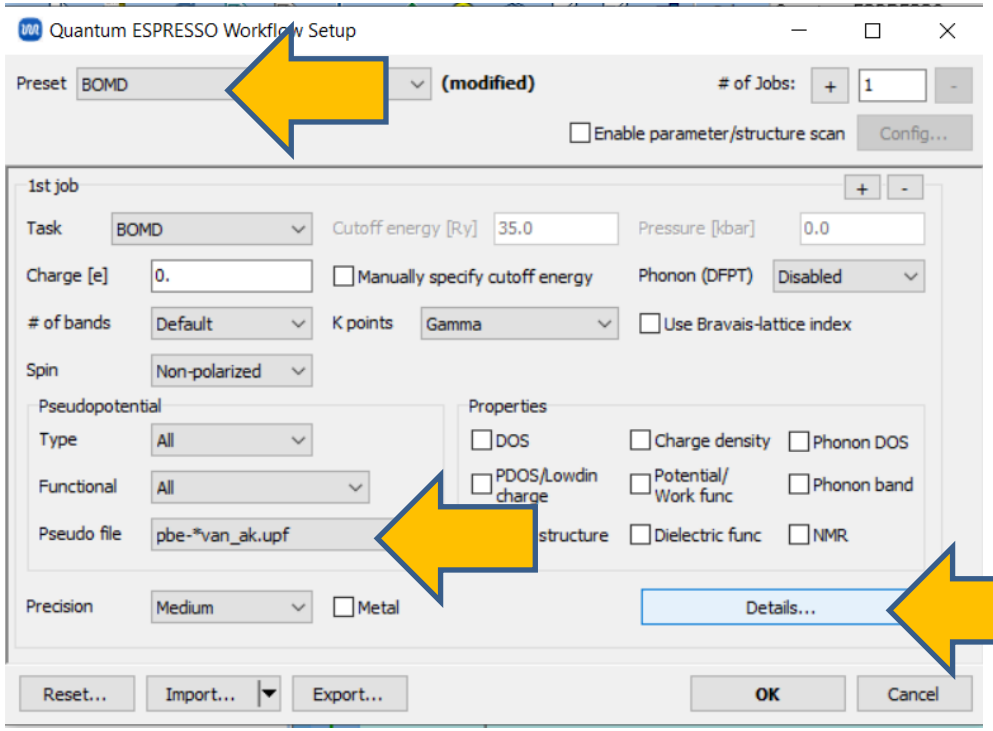
C. Confirm that the desired structure appears in Viewport.

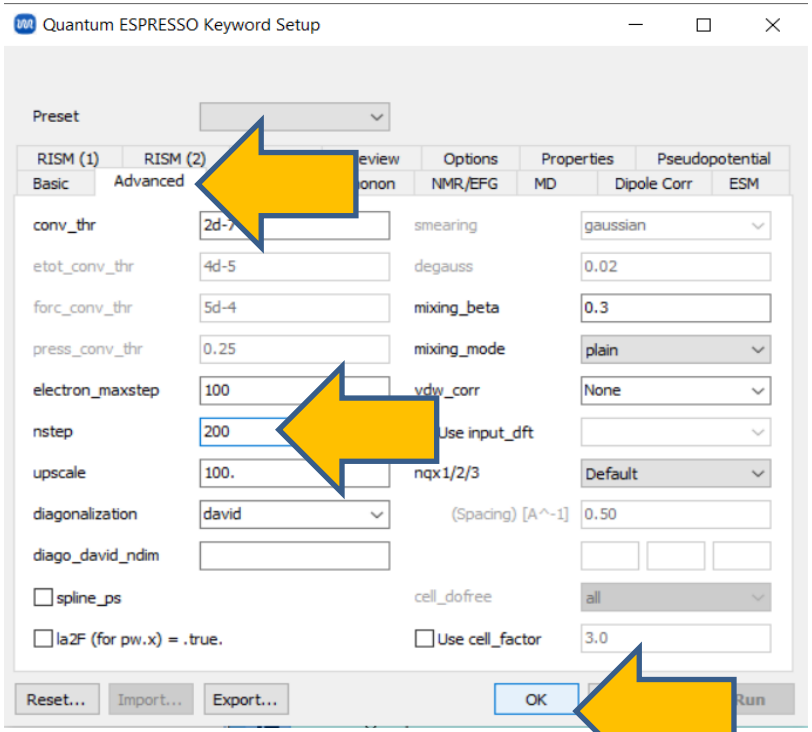




B. Execution of Calculation

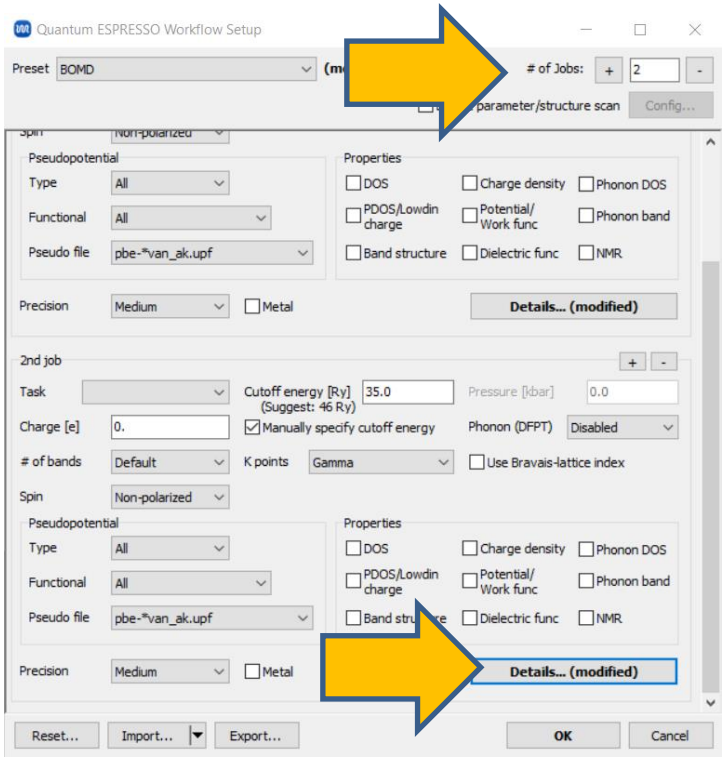
A. Select **Quantum ESPRESSO** from **Solver**, and then click **(Workflow Setup)**.
B. If 'Current cell can be converted to primitive cell....Do you want to convert?' message appears, click **No**.
C. Select **BOMD** in **Preset**, then select **pbe-*van_ak.upf** in **Pseudo file**.
D. Click **Details**.
E. Change **nstep** to '200' in **Advanced** tab, then click **OK**.

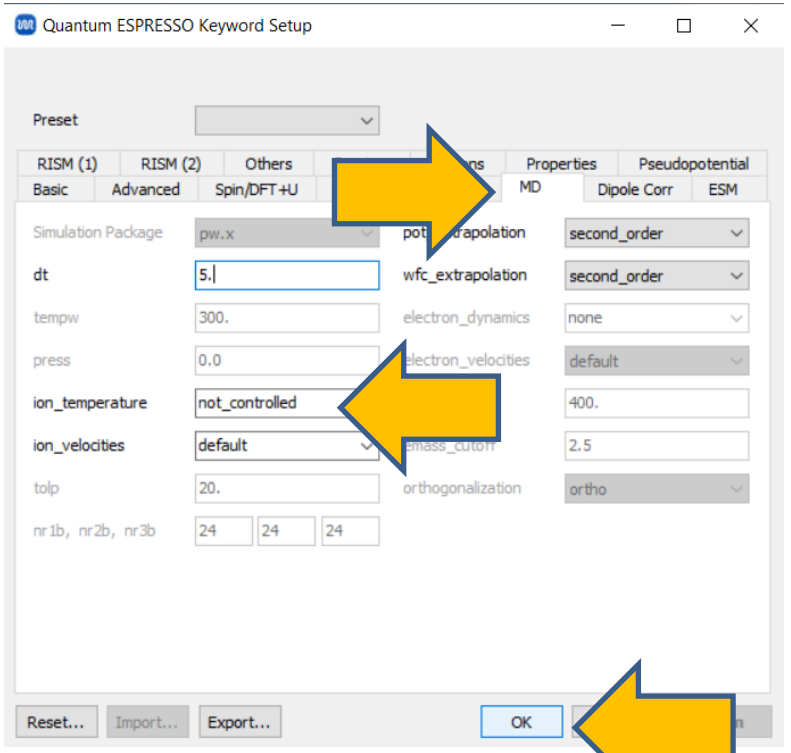




B. Execution of Calculation

A. Click **+** next to **# of Jobs** once.
B. Scroll down in the window and click **Details... (modified)** for **2nd job**.
C. Change **ion_temperature** to 'not_controlled' under **MD** tab, then click **OK**.
D. Click **OK** in **Quantum ESPRESSO Workflow Setup** window, then after setting **Job Setting** as needed, click **Run**.





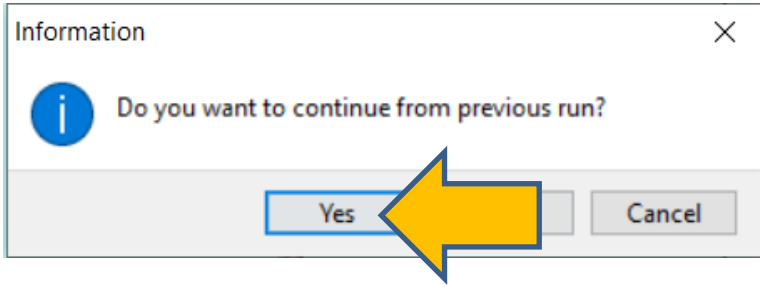
Supplement: Continuing the Calculation

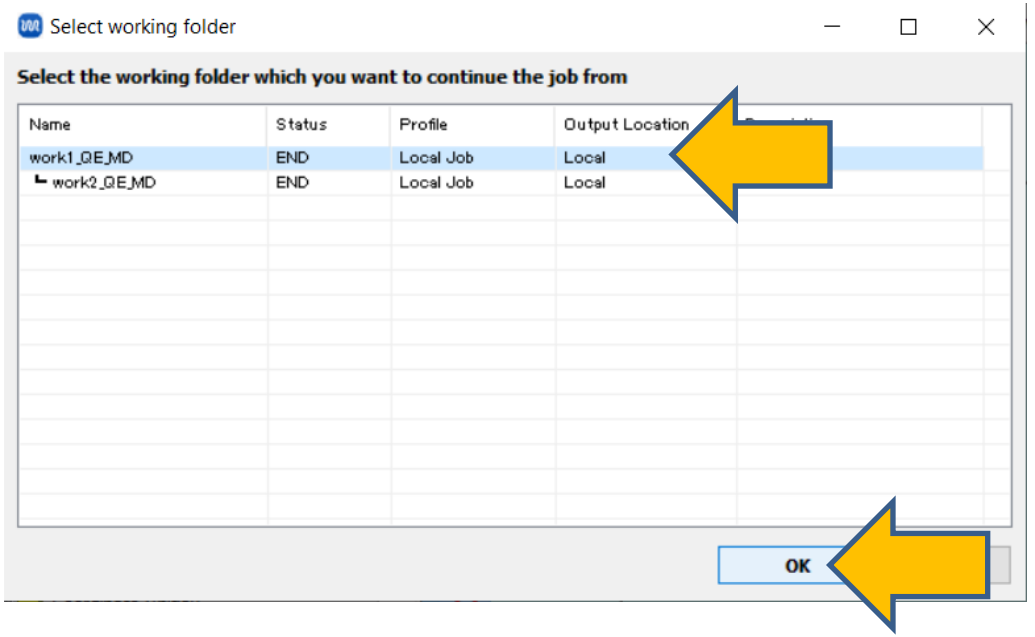
To start a BOMD calculation by inheriting the final state from a previously completed BOMD calculation, follow these steps:

A. Click **(Workflow Setup)**.

B. When prompted with 'Do you want to continue from previous run?' click **Yes**.

C. Select the original working folder for continuation and click **OK**, then set up the calculation conditions similar to the initial job.

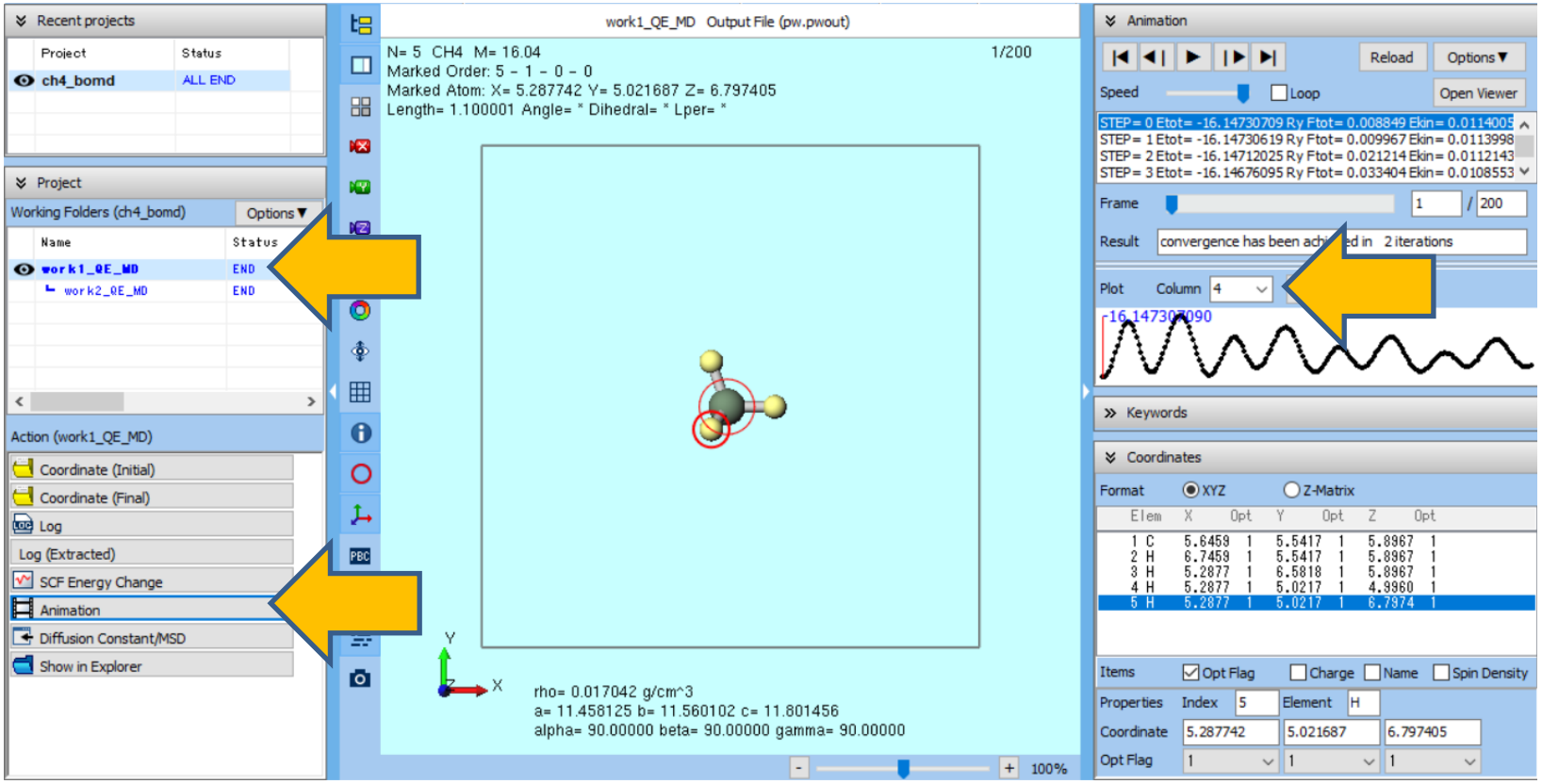




C. Result Analysis (Animation, Energy)

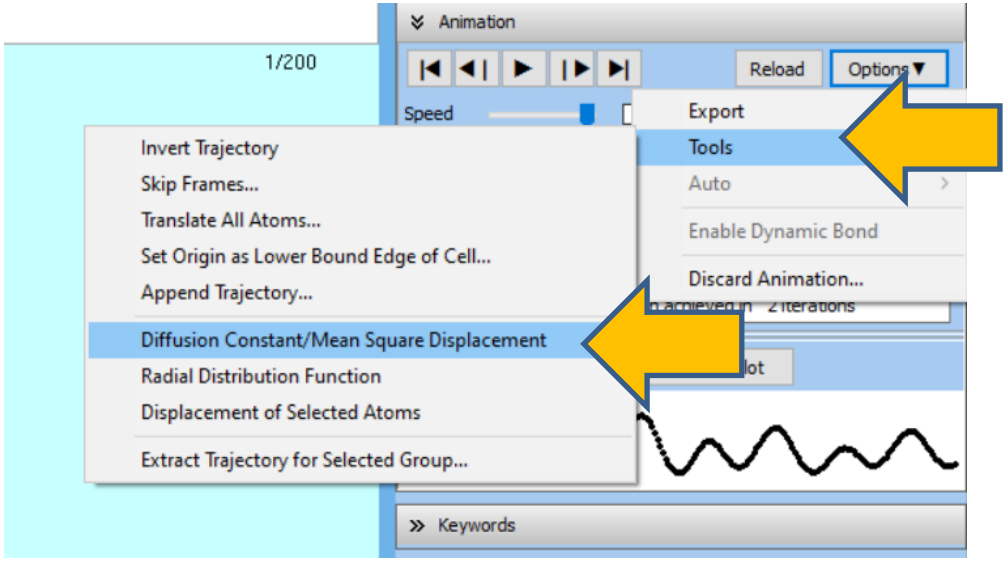
A. After **the status** of **work1_QE_MD** in **Working Folders** changes to **END (blue)** , click on work1_QE_MD in **Working Folders** and select **Animation** from **Action**.

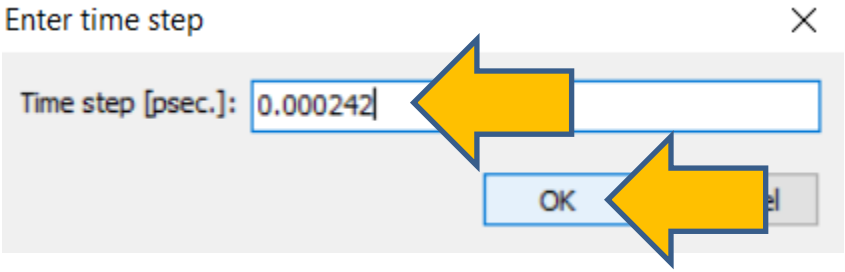
B. In **Animation Panel**, select the items you wish to graph in **Column**. (4 for Potential Energy, 9 for Kinetic Energy, 12 for Temperature, 15 for Total Energy).



C. Result Analysis (Self-Diffusion Coefficient)

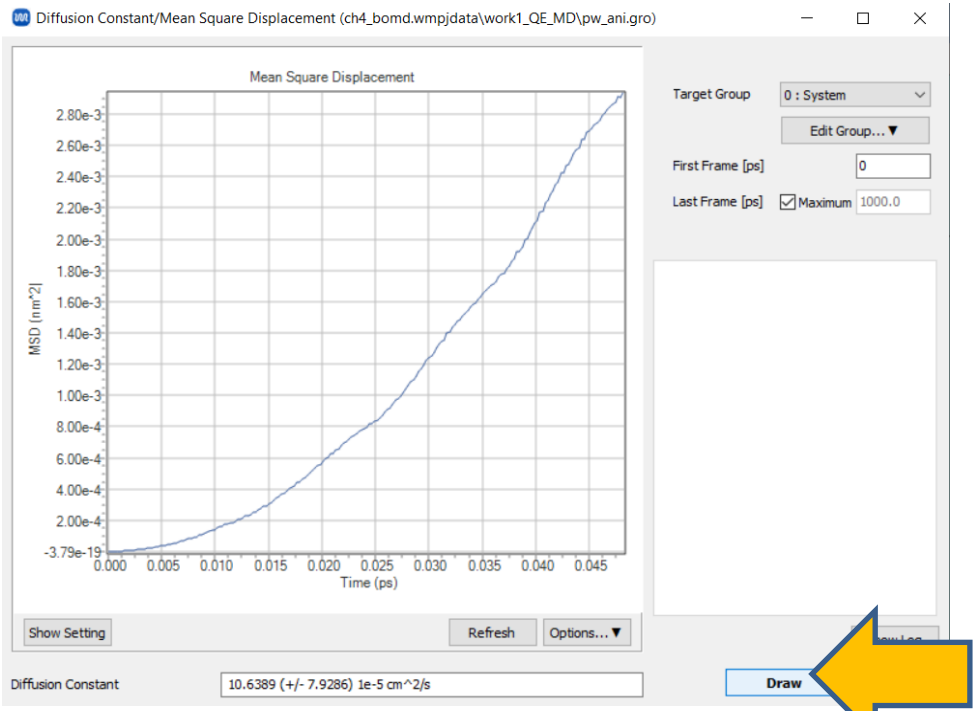
A. In **Animation Panel**,
   Click Options | Tools | Diffusion Constant/Mean Square Displacement.
B. Click **Save** in **Save as** dialog.
C. Enter time step of this calculation, '0.000242', in **Time step** field and click **OK**.
   – You can verify the time step from **Workflow Setup** > **Details** > **MD Tab** > **dt**.
   – Use **Tools | Unit Converter** for unit conversion.





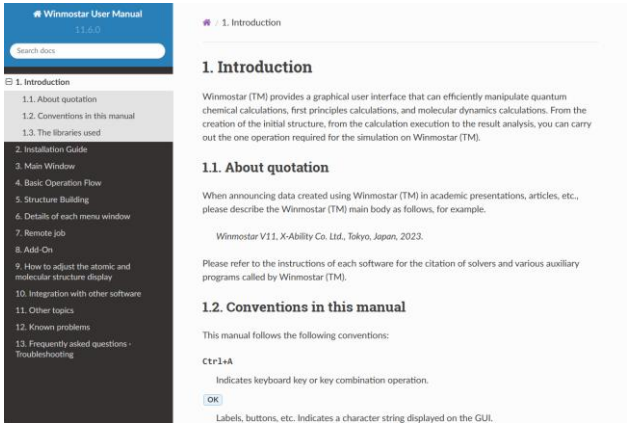
C. Result Analysis (Self-Diffusion Coefficient)

A. Clicking **Draw** will display the mean square displacement (graph) and the diffusion constant (**Diffusion Constant** below the graph).
   - For detailed usage instructions, please refer to the user manual.
   - The calculations in this document have very short step counts and are for a single molecule, so the mean square displacement and diffusion constant obtained here are not meaningful. For actual calculations, please derive them from calculations with sufficient step counts and atomic numbers.



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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