winmostar tutorial

LAMMPS
Systems with Solid Walls

V11.6.5

29 March 2024

X-Ability Co., Ltd.

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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 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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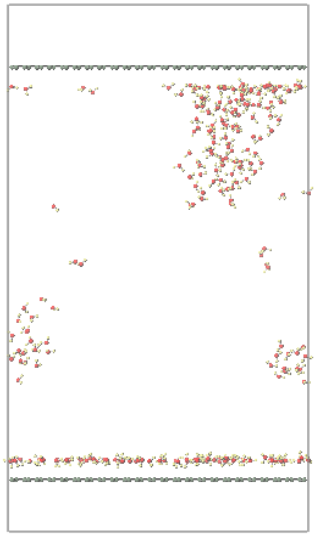
Overview

- This tutorial outlines the procedure for observing the behavior of water in a region sandwiched between two graphene sheets, as an example of a system containing solid walls and fluid (gas or liquid).



Note:

- The number of steps required for equilibration depends on the type of material targeted and its initial density.
- The method of interaction calculation, the type of force field, and the size of the supercell also affect the results.
- Note that the temperature inside the system near the solid walls may locally decrease because the coordinates of the solid walls are completely fixed.

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Preference of Operating Environment

- If you are using Winmostar V11.5.0 or later and are on a 64-bit environment, please install and configure CygwinWM version 2023/04/05 or later.
  - The CygwinWM version 2023/04/05 and later includes the recommended version of 64-bit LAMMPS.

- If the above does not apply to you, or if you wish to use a version of LAMMPS other than the recommended version, you will need to separately install and configure the Windows version of LAMMPS.

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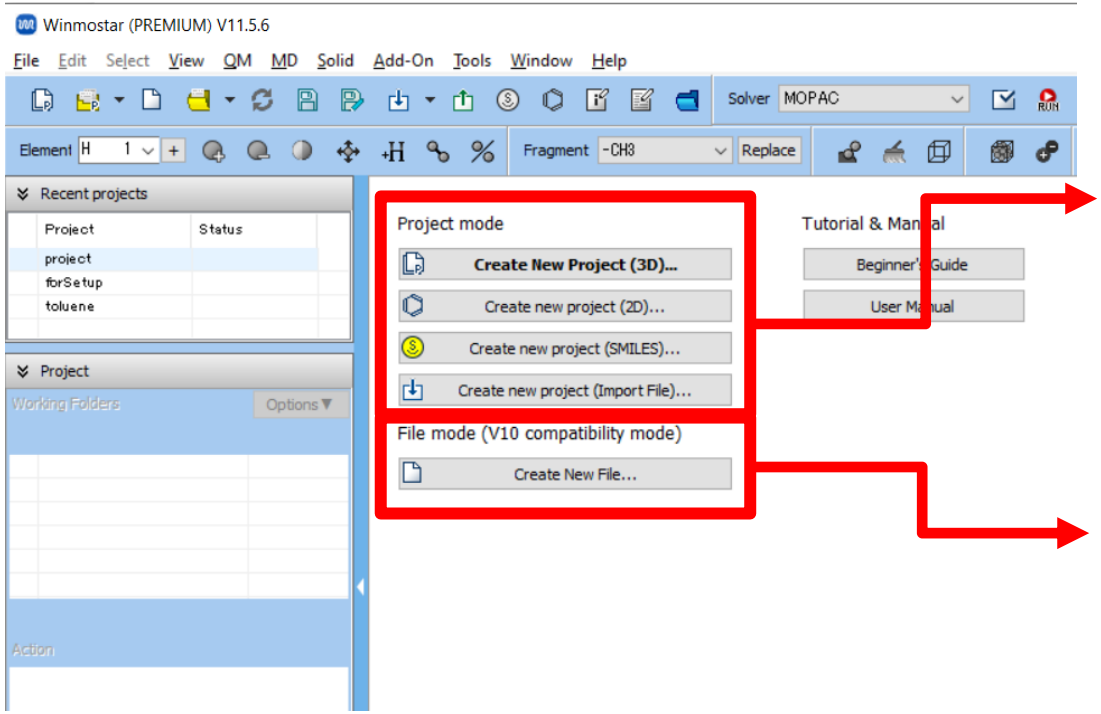
Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to 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.

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A. Modeling of the System

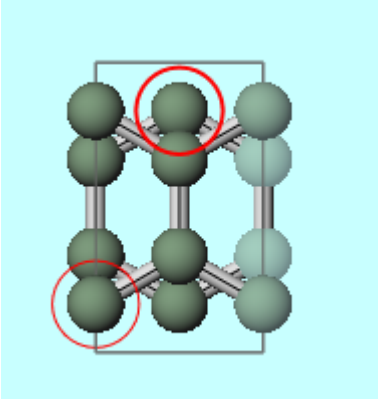
For basic operations, please refer to LAMMPS Basics tutorial.

A. Click **File | New Project**, enter 'gwg' in **Project name**, and click **Save**.

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

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

C. Click **Discard and import** in **Import File** dialog.



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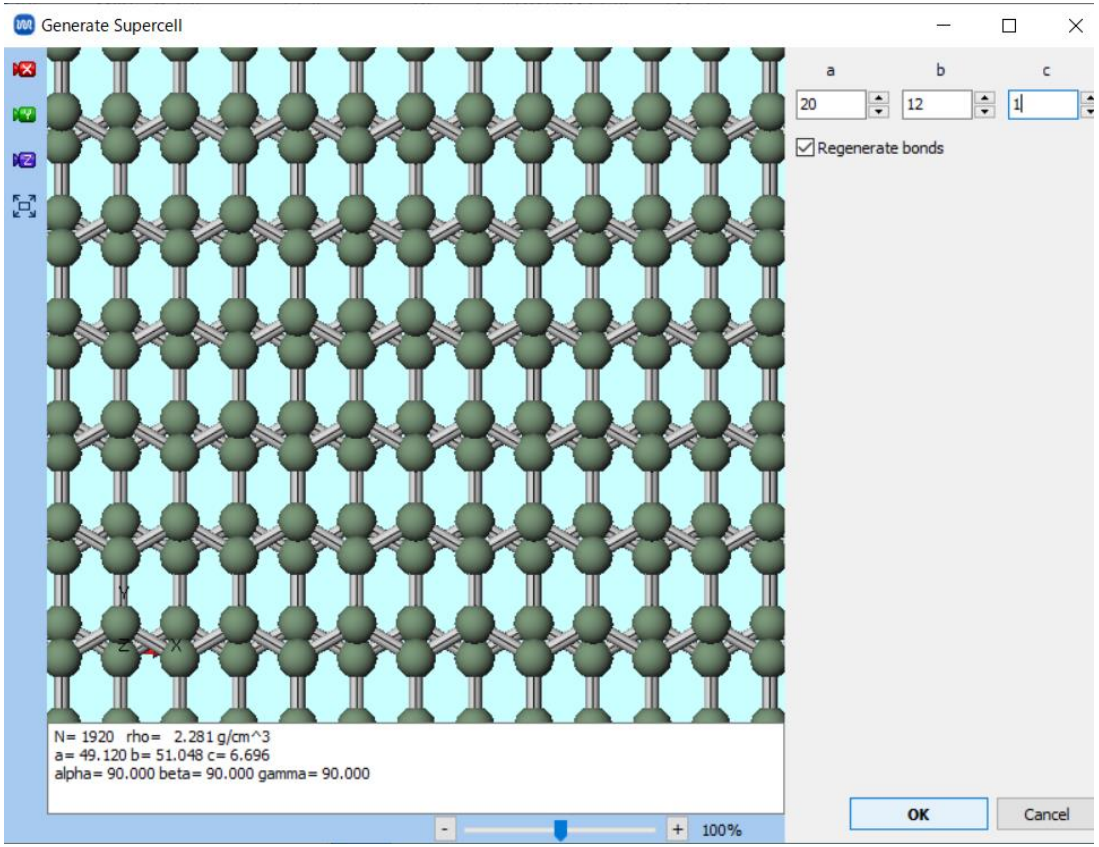
A. Modeling of the System

A. Click **Solid | Generate Supercell**.
B. Change **a**, **b**, **c** to '20', '12', '1' respectively, and click **OK**.
C. Click **(Export File)** and save the file with the name '`graphene.cif`'.



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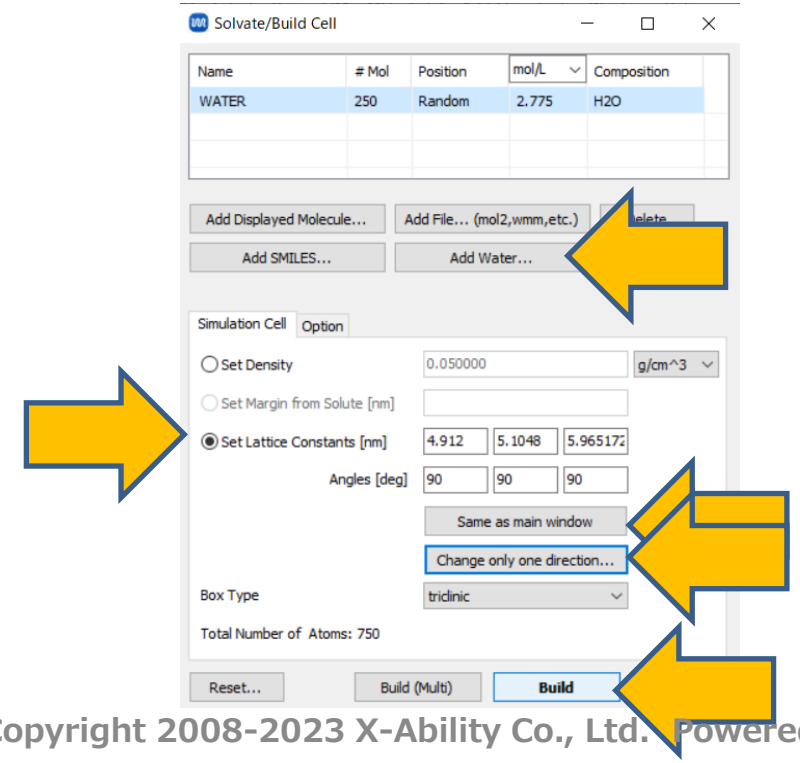
A. Modeling of the System

A. Click  **(Solvate/Build Cell)**.
B. Click **Add Water**, enter '**250**', and click **OK**.
C. Check **Set Lattice Constants** and click **Same as main window**.
D. Click **Change only one direction**, keep **Select direction** as it is and click **OK**, enter '0.05' in **Enter density**, and click **OK**.
E. Click **Build**, and when 'The system has been successfully built.' is displayed, click **OK**.



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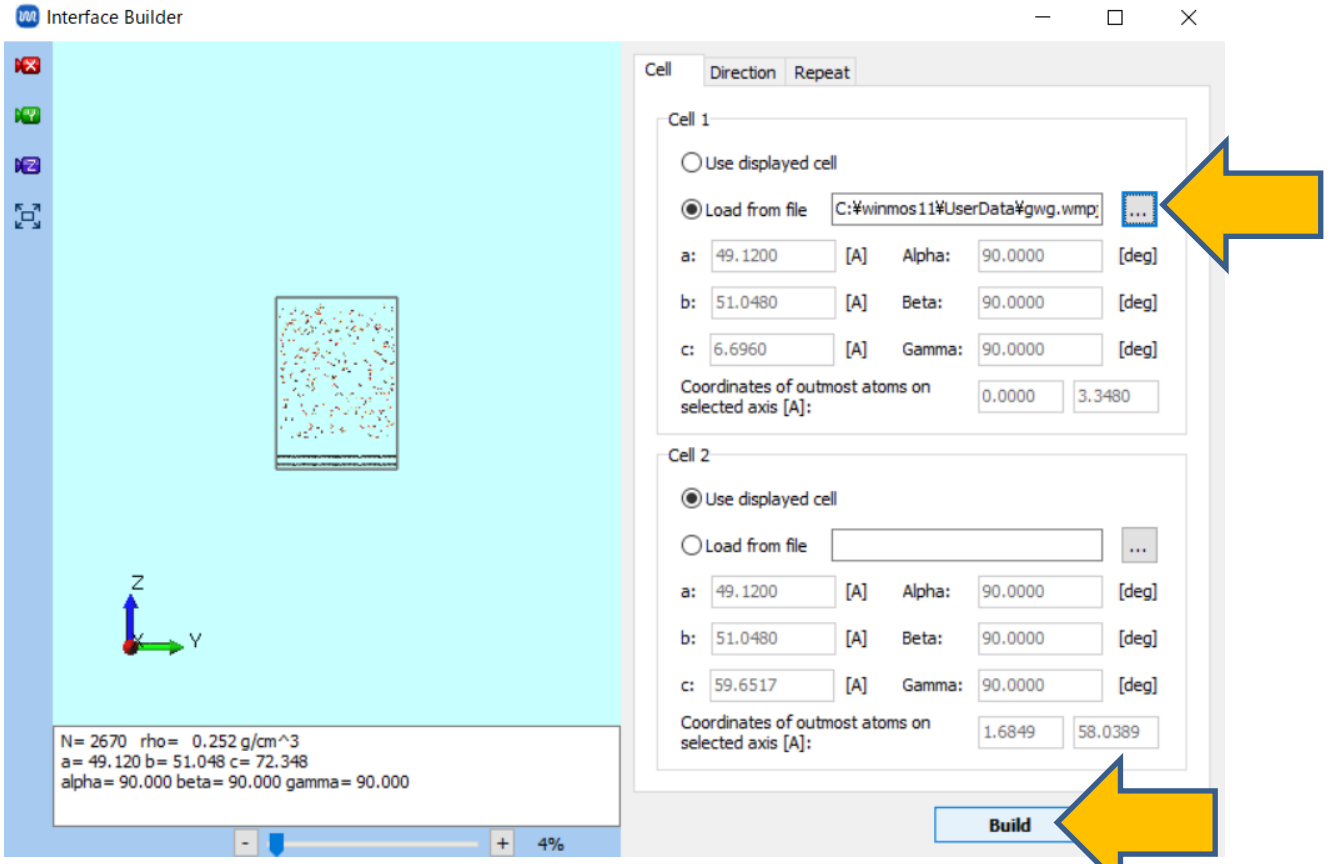
A. Modeling of the System

A. Click **MD | Interface Builder**.
B. Click ... button for **Cell 1** and select `graphene.cif` saved in step 7.
C. Click **Build**, and when 'Successfully generated.' is displayed, click **OK**.



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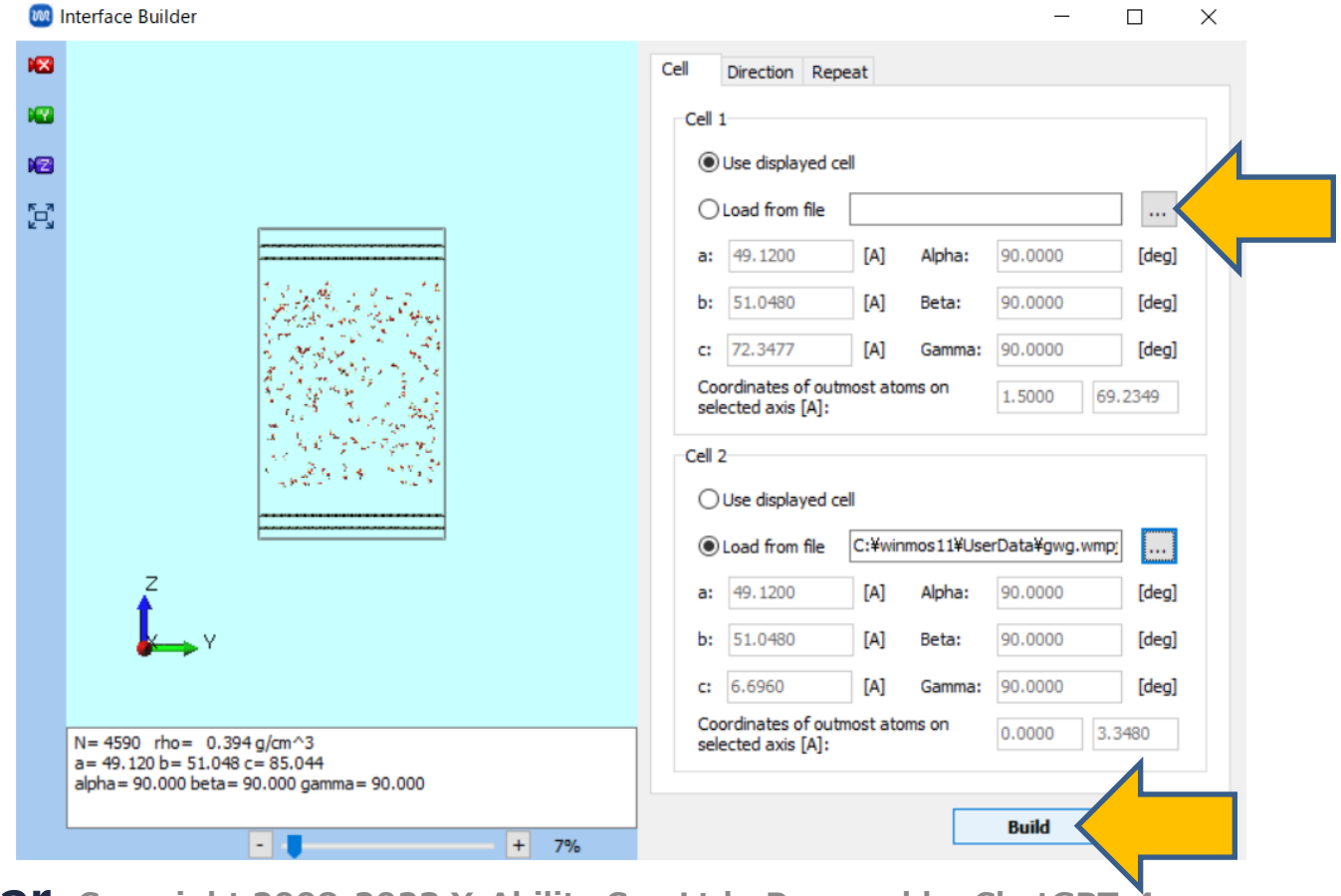
A. Modeling of the System

A. Click **MD | Interface Builder**.
B. Click ... button for **Cell 2** and select `graphene.cif` saved in step 7.
C. Click **Build**, and when 'Successfully generated.' is displayed, click **OK**.



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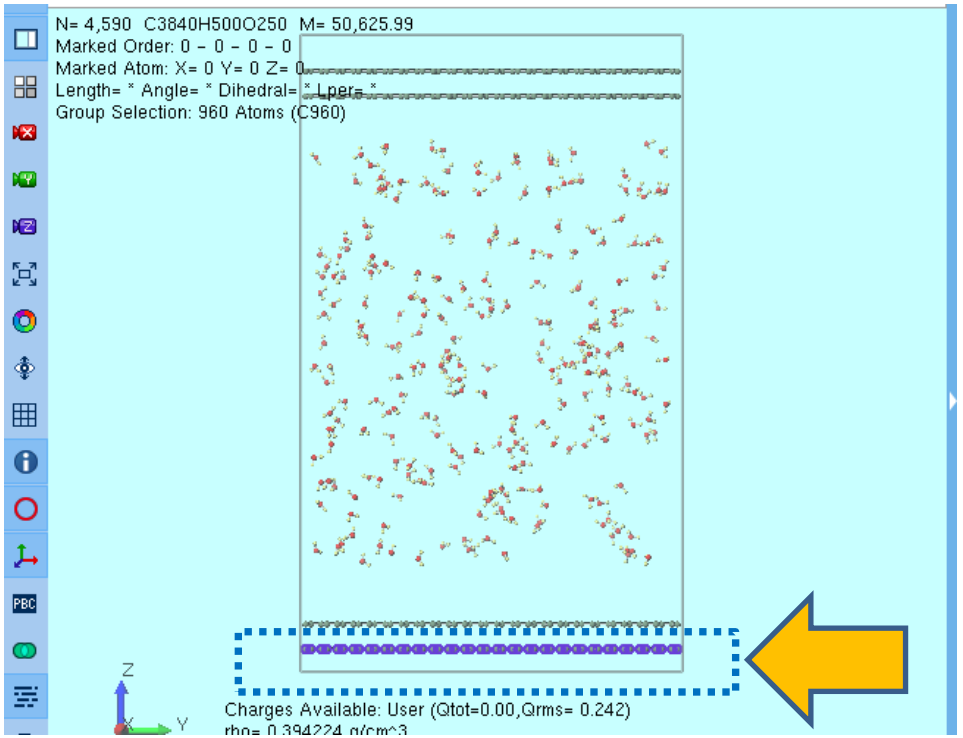
A. Modeling of the System

A. Click **(Align View to X-Axis)** and then click **(Fit to Window)**.
B. Ctrl+drag to rectangle-select the lower one of the two graphene layers below. If atoms are hard to see, shift+drag to pan the view.
C. Click **(Modify Selected Group) | Delete**, and when asked 'Do you want to delete or leave group?' click **Delete**.



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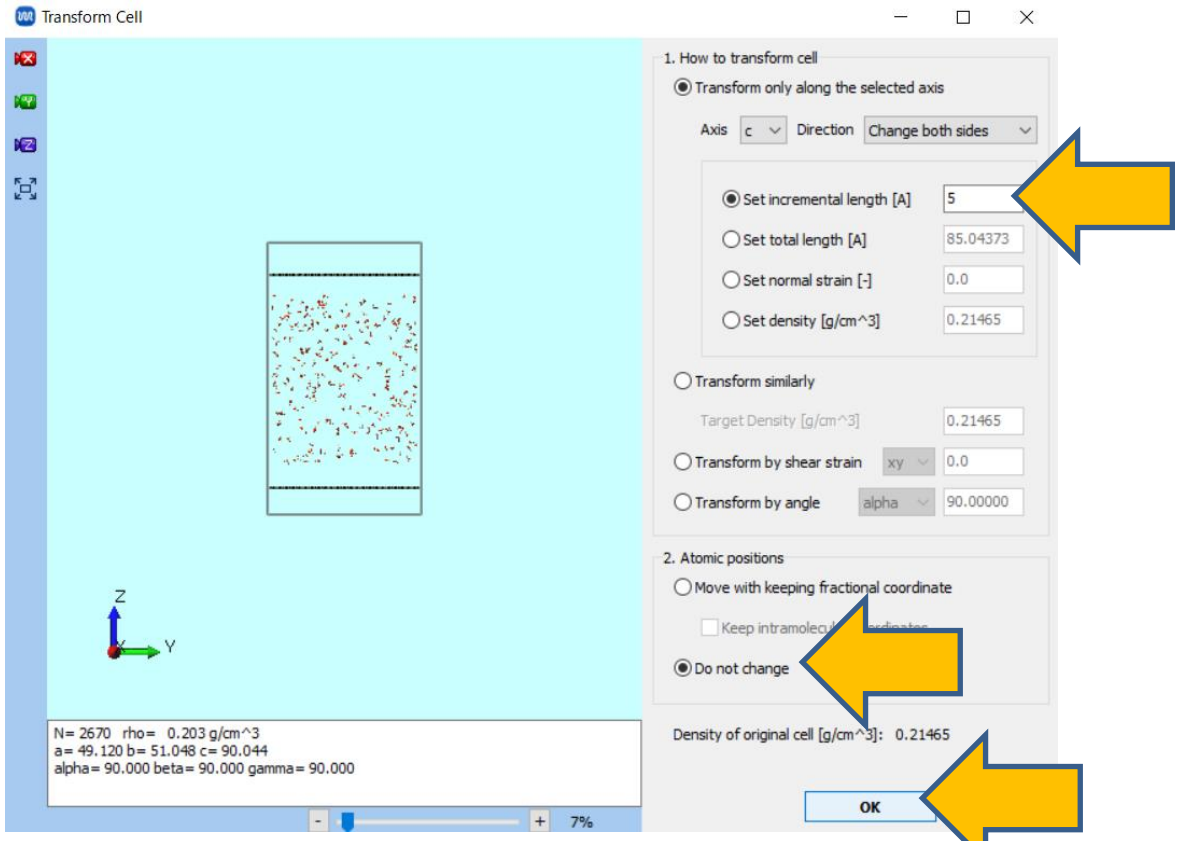
A. Modeling of the System

A. Similarly, delete the upper one of the two graphene layers above.
B. Click  **(Create/Edit Cell) | Transform Cell**.
C. Change **Set incremental length** to '5', check **Do not change** under **Atomic positions**, and click **OK**.



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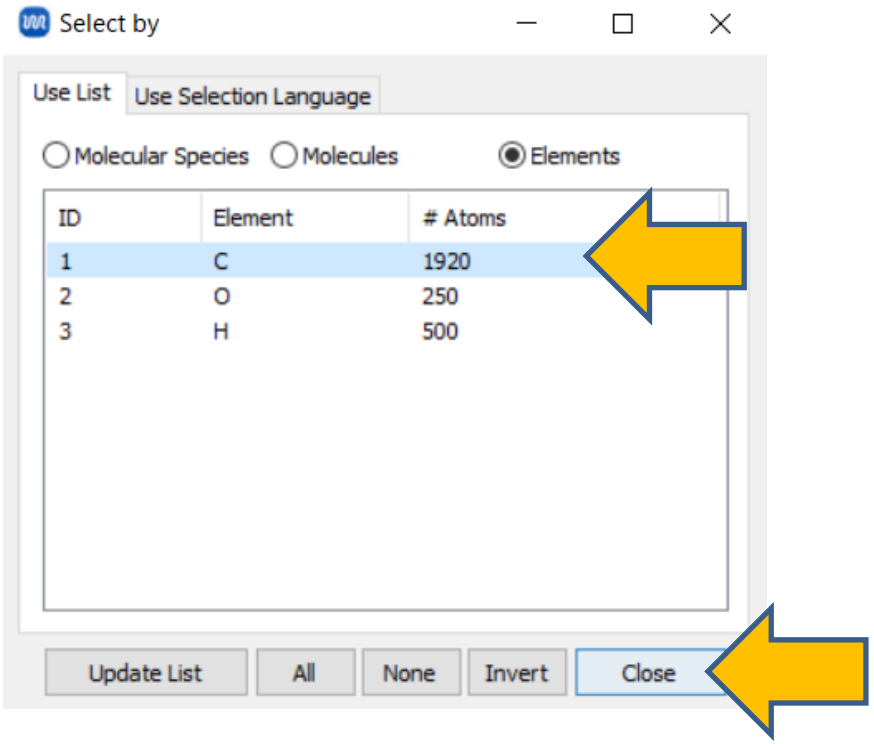
A. Modeling of the System

A. Click **Select | Select by Elements**.
B. Click on the row labeled '1 C 1920' and click **Close**.
C. Click **Select | Register Selected Group**, enter '**graphene**' as **Group name**, and click **OK**.



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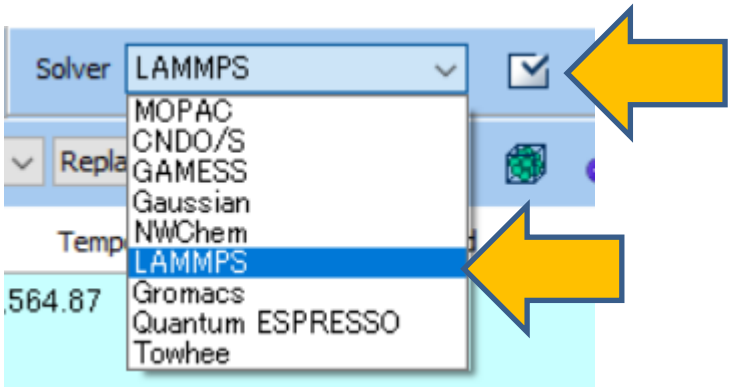
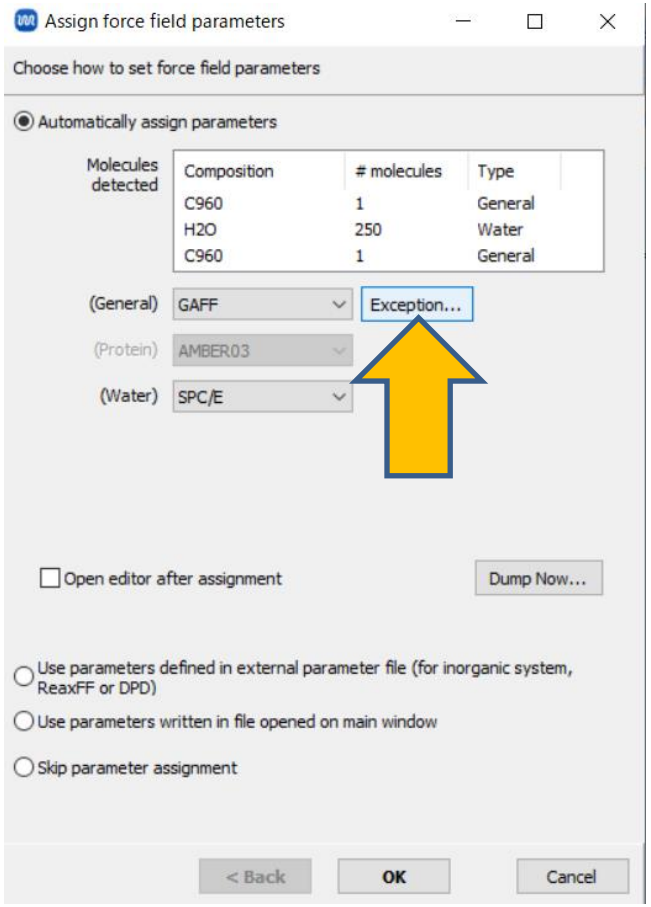
B. Execution of Calculation

A. Select **LAMMPS** from **Solver** and click **(Keyword Setup)**.
B. If prompted with '**Some molecules do not have charges. Do you want to assign charges now?**', click **No**.
C. Click **Exception**.





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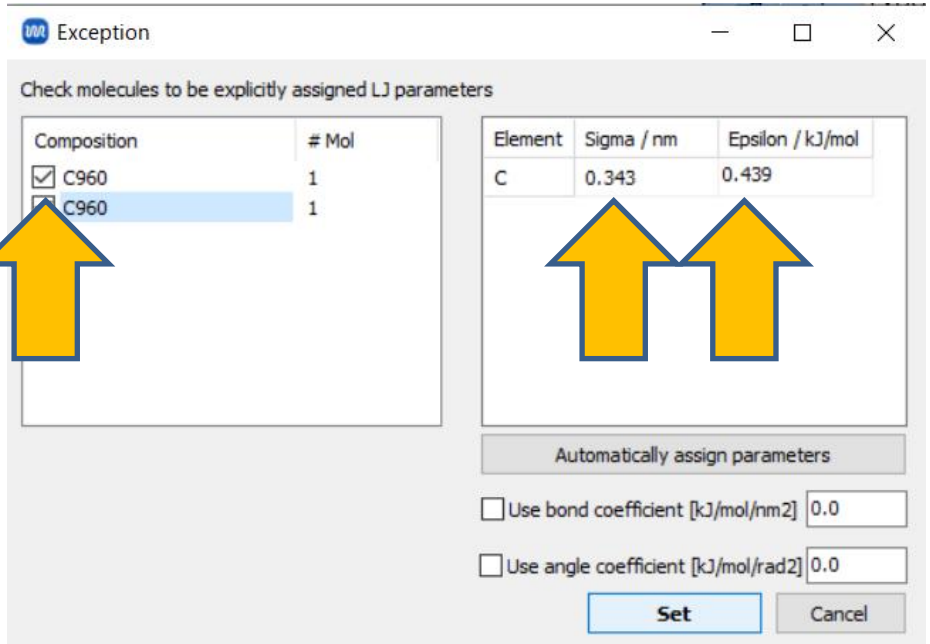
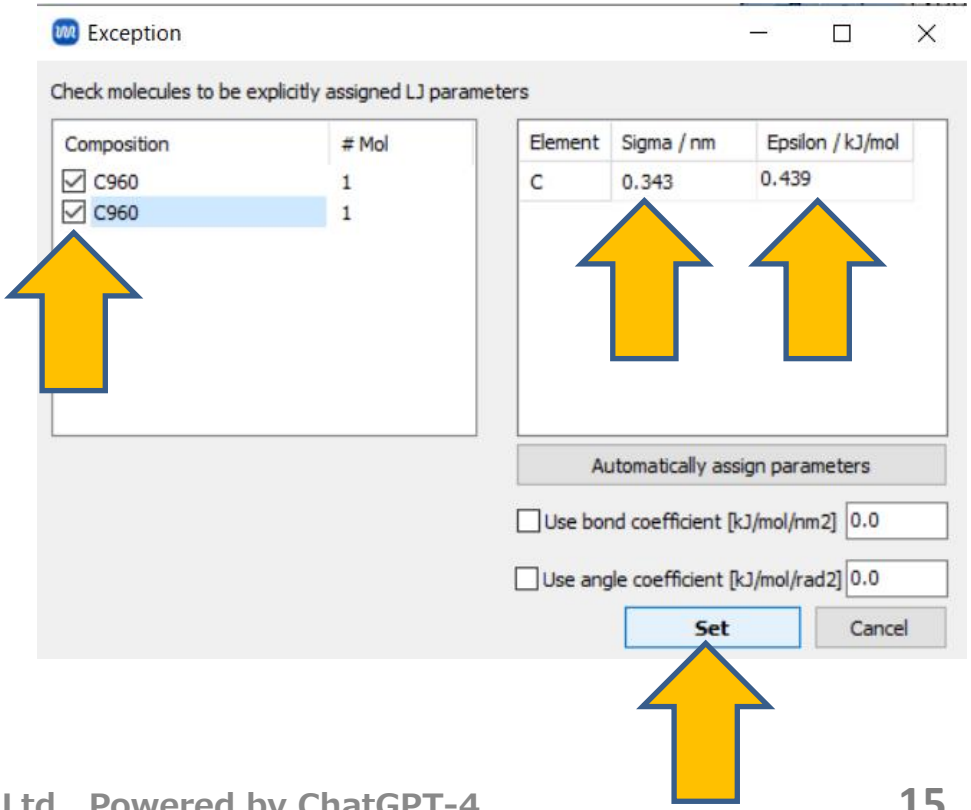
B. Execution of Calculation

A. Check the first **C960** in the list on the left, and enter '**0.343**' for **Sigma** and '**0.439**' for **Epsilon** on the right (this tutorial uses UFF parameters).

B. Similarly, check the second **C960**, and enter '**0.343**' and '**0.439**' in the fields on the right.

C. Click **Set**.





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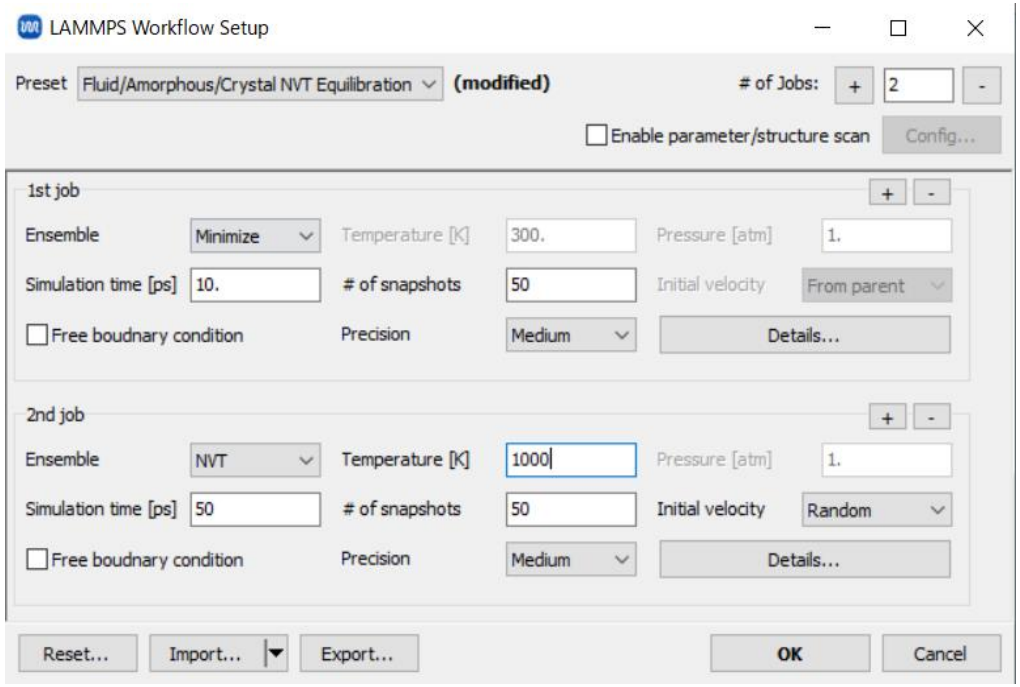
B. Execution of Calculation

A. Once you return to **Assign force field parameters** window, click **OK**.
B. When '**Assign force field parameters**' is displayed, click **OK**.
C. Change **Preset** to 'Fluid/Amorphous/Crystal NVT Equilibration.'
D. Change **Temperature** of **2nd job** to '1000.'
E. If you want to reduce the calculation accuracy to finish the calculation quicker, change **Precision** of **2nd job** to 'Low.'



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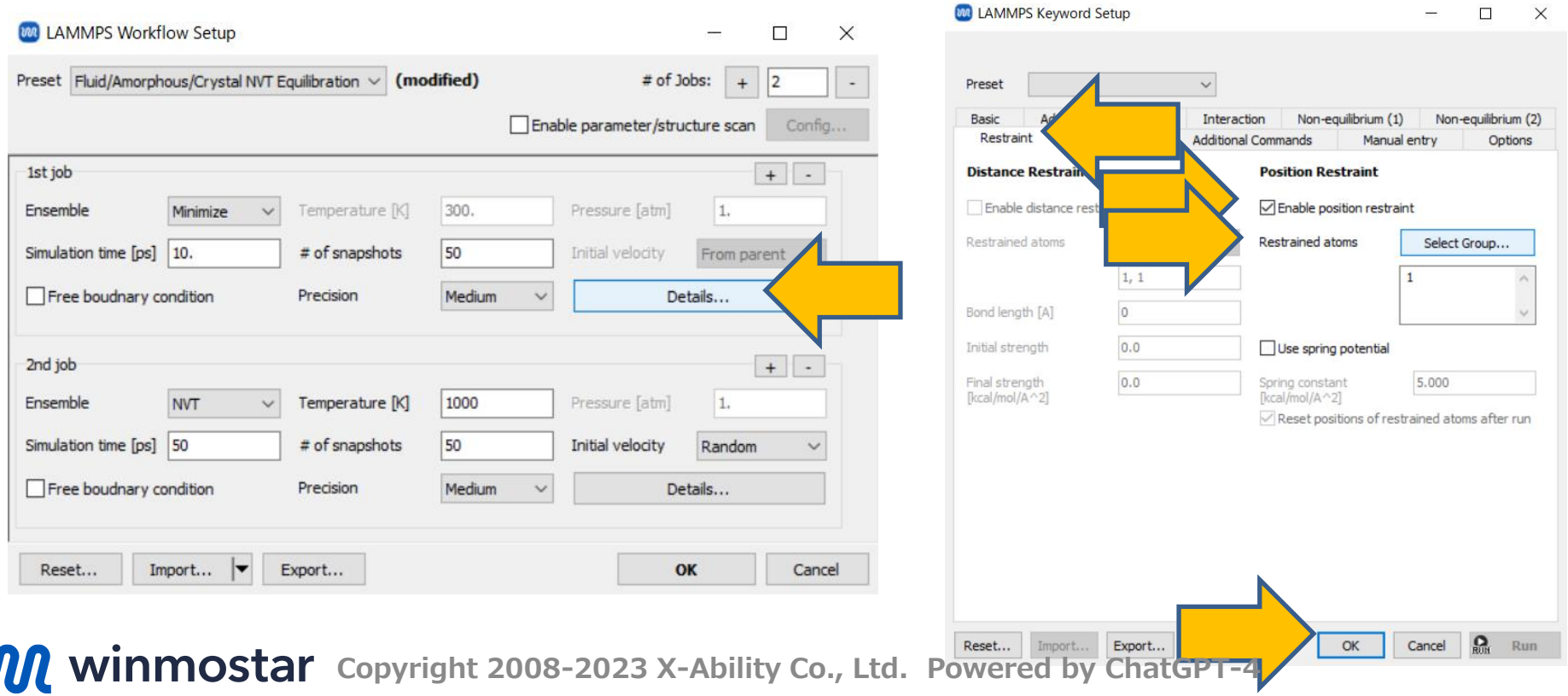
B. Execution of Calculation

A. Click **Details** for **1st job**, check **Enable position restraint** in **Restraint** tab, and click **Select Group** button under **Restrained atoms**.
B. Select '**graphene**' as **Group name** and click **OK**.
C. Click **OK** in **LAMMPS Keyword Setup** window.
D. Also click **Details** for **2nd job** and set it up in the same way as steps A to C.



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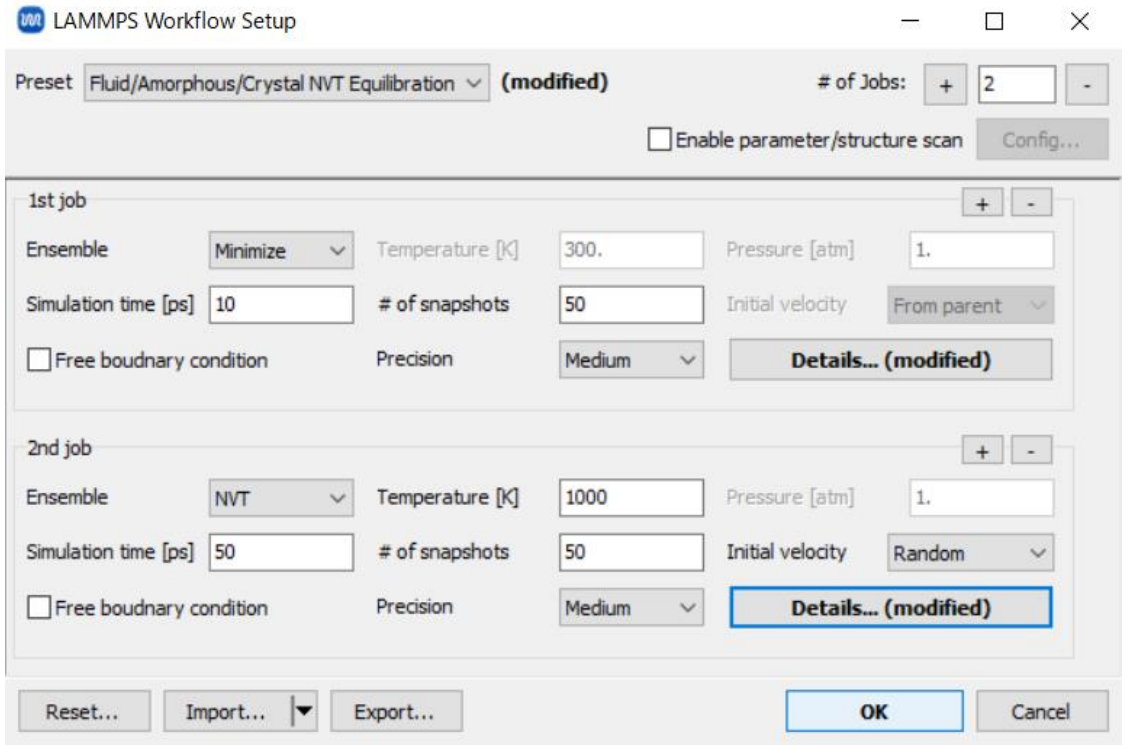
B. Execution of Calculation

A. Click **OK** in **LAMMPS Workflow Setup** window, set as appropriate in **Job Setting** window, and then click **Run**.

Note that if you want to graph the temperature change in **2nd job** using **Energy Plot**, select **TempFree** instead of **Temp** to graph the temperature of only the unrestrained atoms.



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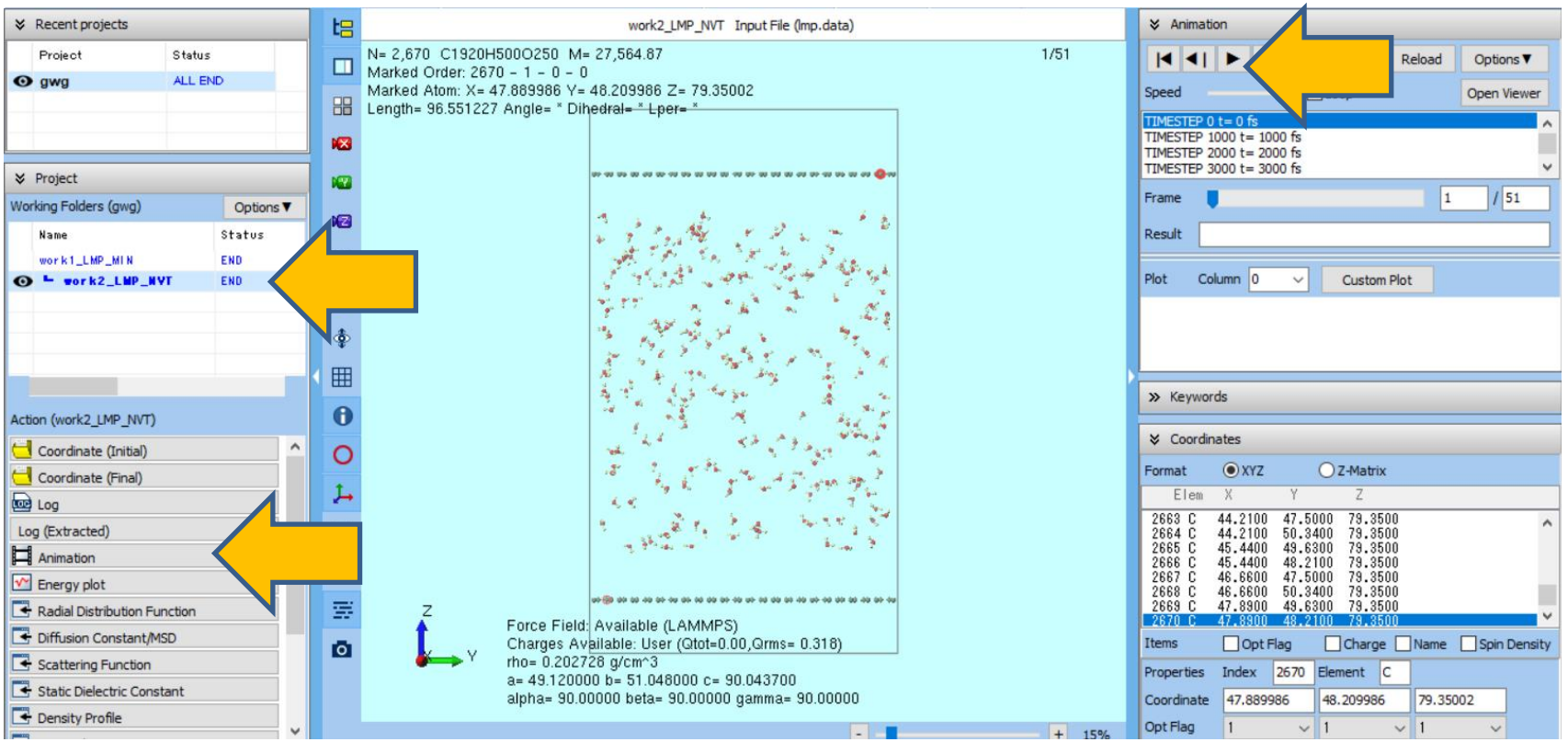
C. Analysis of Results

A. Once **the status** of **the work folder** work2_LMP_NVT changes to **END** or **END(-)** , click on 'work2_LMP_NVT' and then click **Animation** in **Action**.

B. Click **(Align View to X-Axis)** and **(Fit to Window)**.

C. In **Animation** area, click **(Play/Pause)** to observe the movement of the molecules.



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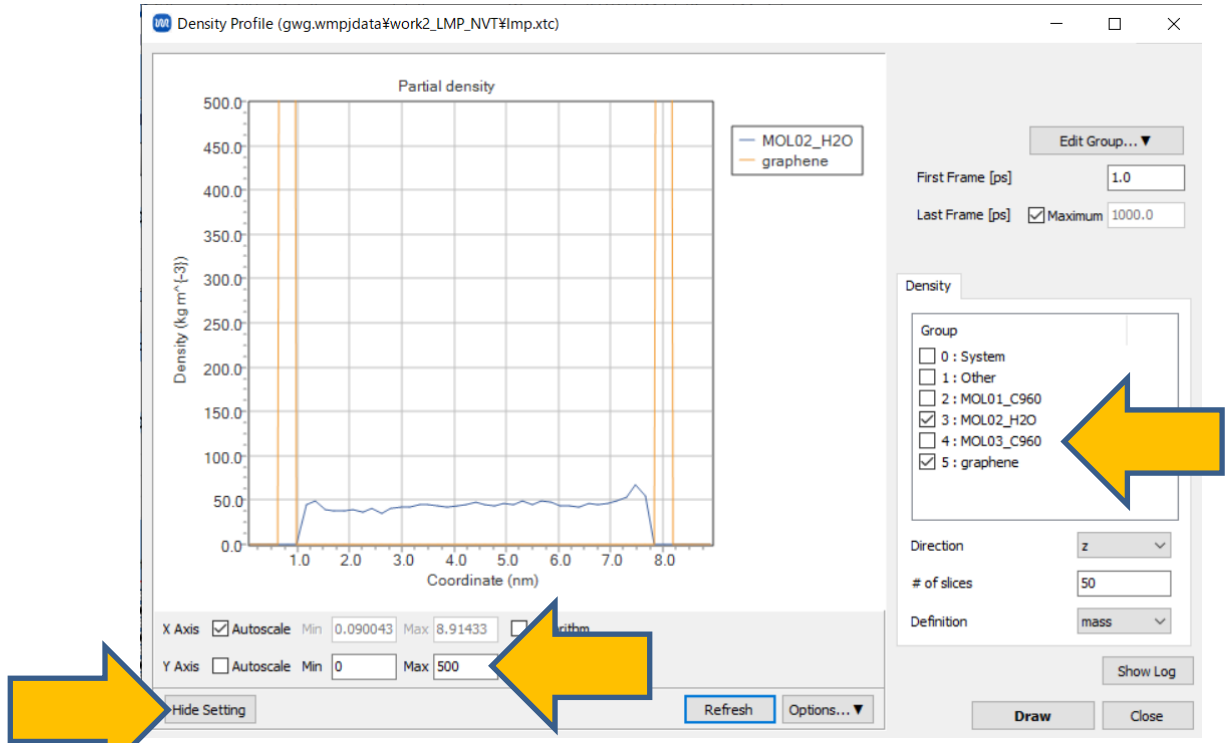
C. Analysis of Results

A. Click on 'work2_LMP_NVT' in **Working Folders**, then click **Density Profile** in **Action**.
B. Ensure '**3: MOL02_H2O**' and '**5: graphene**' are checked in **Group**, then click **Draw**.
C. By clicking **Show Setting** below the graph, uncheck **Autoscale** in **Y Axis**, and change **Max** to '500', you can observe the density distribution of water. (Note that it is not in a steady state).



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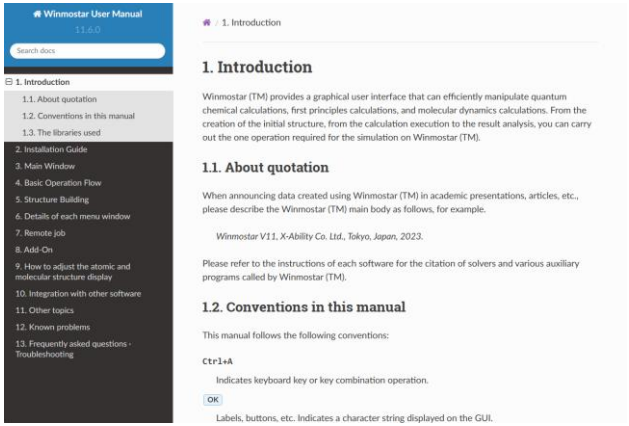
Finally

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



Winmostar User Manual

Scenes from Winmostar Training Session

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