M winmostar tutorial

LAMMPS Systems with Solid Walls

V11.6.5

29 March 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 <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 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.

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 <u>the recommended version</u>, you will need to separately <u>install and configure the</u> <u>Windows version of LAMMPS</u>.

Operating Modes of Winmostar V11

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



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 <u>Winmostar User Manual section 5</u>, '<u>Methods for Creating Initial Structures</u>'.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.



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



- 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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M winmostar	Copyright 20	008-2023	X-/	bility	Со.,	Ltd.	powered k	y ChatG	יד- 4

- 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. Click MD | Interface Builder.

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- 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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	+ 7%	Build	
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- 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**.



- 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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		 ○ Transform similarly Target Density [g/cm^3] 0.21465 ○ Transform by shear strain xy 0.0 ○ Transform by angle alpha ○ 90.00000
Z Y		2. Atomic positions Move with keeping fractional coordinate Keep intramolecy Do not change
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- 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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- A. Select **LAMMPS** from **Solver** and click **Markov (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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- 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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- 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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- 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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/ winn	nosta	ar Copyri	iaht 2008	3-2023 X-	-Ability (Co., Ltd. P	Reset Import	Export	СК	Cancel	Run Run

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.



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

- 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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