winmostar tutorial

LAMMPS/Gromacs Vapor Pressure and Surface Tension

V11.5.6

6 February 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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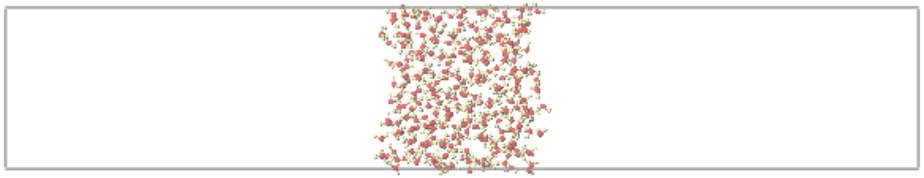
Overview

- Calculate the vapor-liquid equilibrium system of water at 300 K and determine the vapor pressure, equilibrium densities, and surface tension using the following steps:
  A. Creation of the liquid phase
  B. Equilibration calculations for the liquid phase (Energy minimization calculation → Constant temperature MD calculation)
  C. Creation of the vapor-liquid equilibrium system
  D. Equilibration calculations for the vapor-liquid equilibrium system (Energy minimization calculation → Constant temperature MD calculation)
  E. Main calculations for the vapor-liquid equilibrium system (Constant temperature MD calculation)

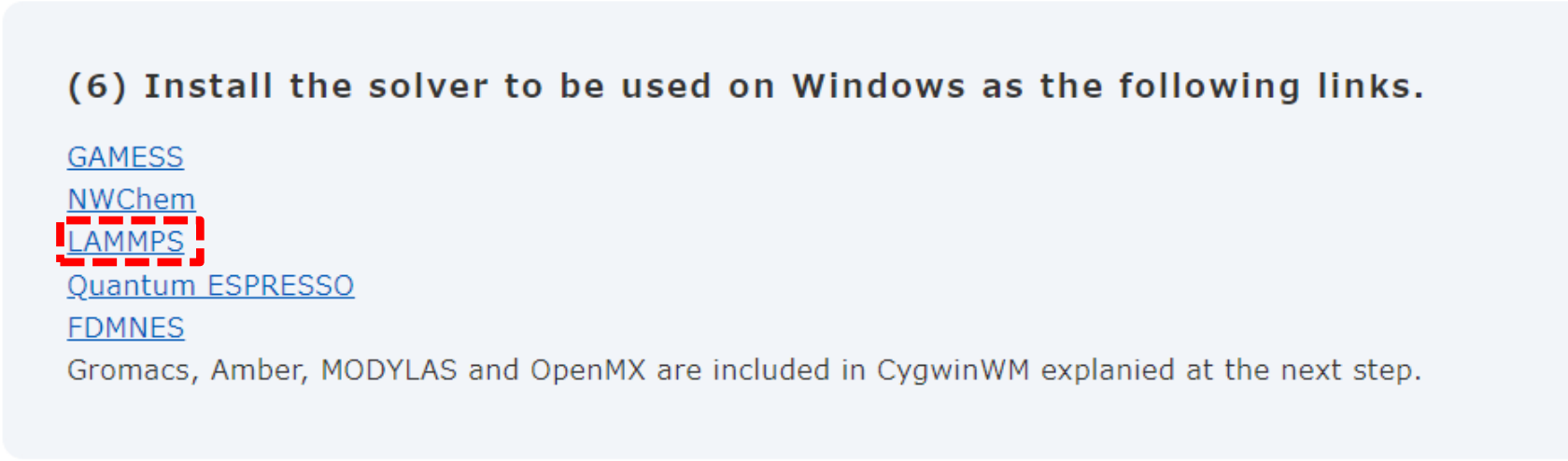


Notes:

- The number of steps required for equilibration varies depending on the type of molecules and initial density.
- The larger the number of steps in the "main calculation," the better the reproducibility and the higher the reliability of the results obtained. Especially, the convergence of the surface tension values is slow.
- The type of force field and the conditions for calculating interactions significantly affect the calculation results.

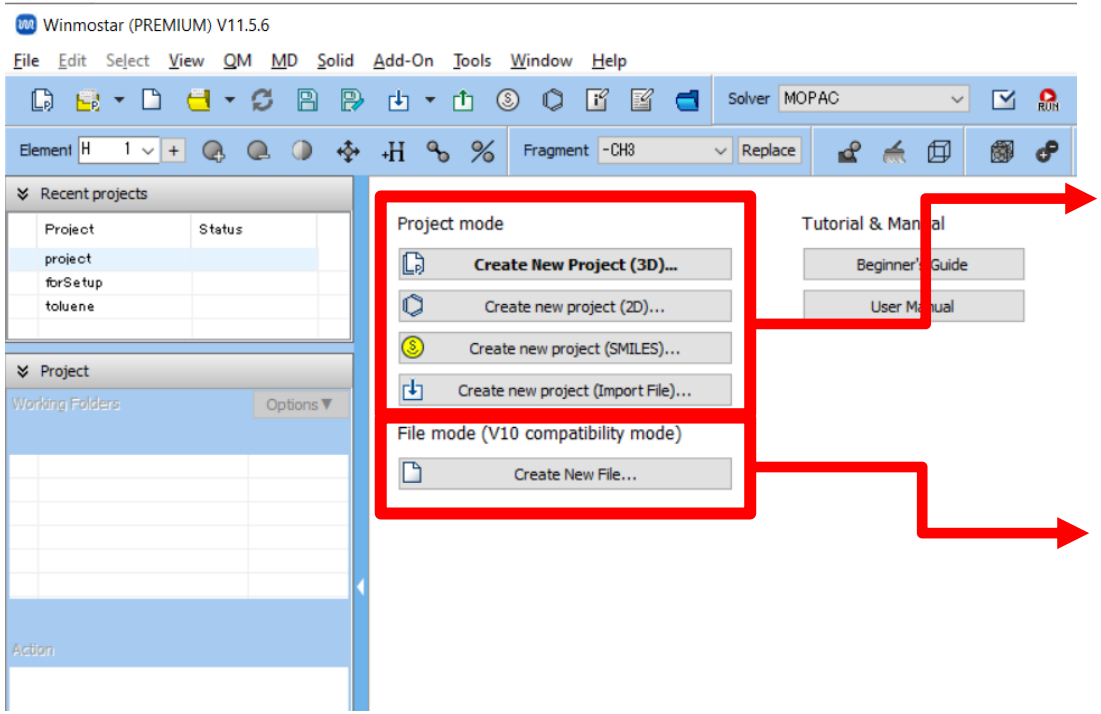
Preference of Operating Environment

- To use this feature, Cygwin setup is required. To use LAMMPS, LAMMPS setup is necessary. Follow the setup instructions for LAMMPS and Cygwin for Windows available at:
- https://winmostar.com/en/installation/ The installation method for LAMMPS and Cygwin on Windows.



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.

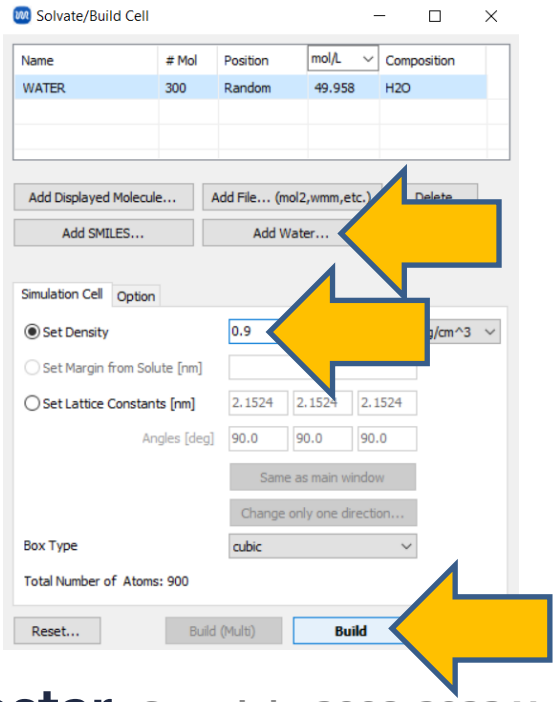
A. Modeling of the System (Liquid Phase)

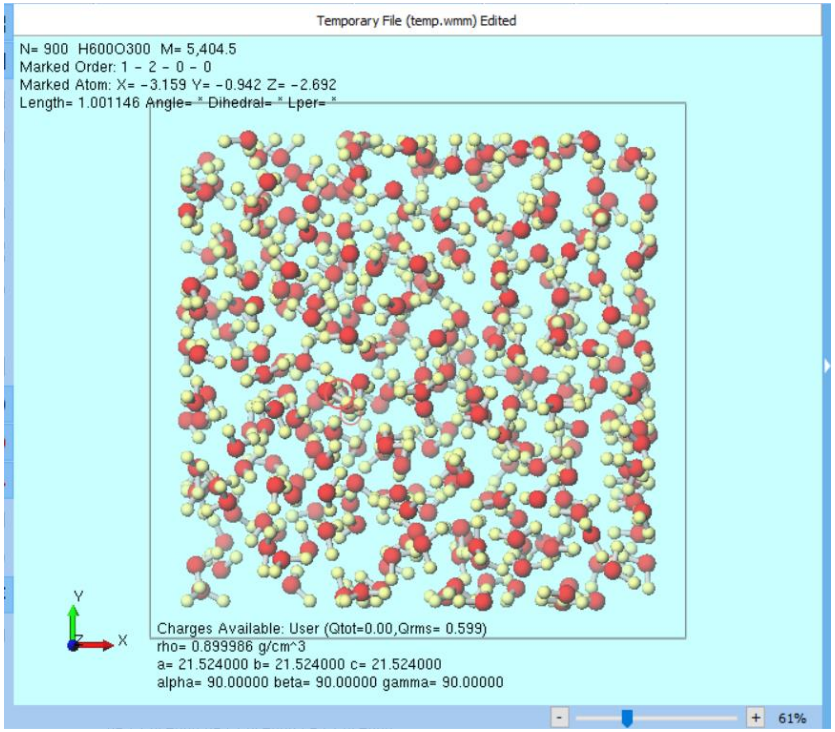
Refer to LAMMPS Basics Tutorial or Gromacs Basics Tutorial for basic operation methods.

A. Click **File | New Project**, enter "water_vle" as **Project name**, and click **Save**.

B. Click  **Solvate/Build Cell**, click **Add Water**, when "**Enter # of molecules**" appears, enter "300" and click **OK**.

C. Enter "0.9" in **Set Density** and click **Build**. When "The system has been successfully built" appears, click **OK**.





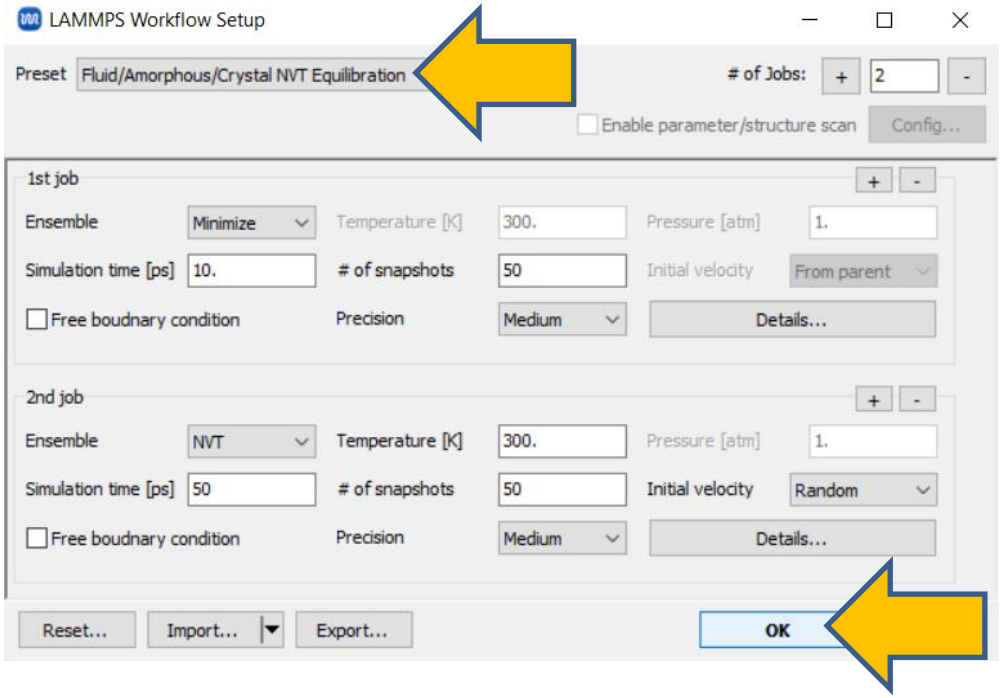
B. Execution of Calculations (Equilibration of the Liquid Phase)

A. Select "LAMMPS" or "Gromacs" from **Solver**, click **(Workflow Setup)**, and click **OK**. Click **OK** when "Assigned force field parameters" appears.

B. Change **Preset** to "Fluid/Amorphous/Crystal NVT Equilibrium".

C. If you want to finish the calculation quickly by reducing the calculation accuracy, change **Precision** of both **1st job** and **2nd job** to "Low".

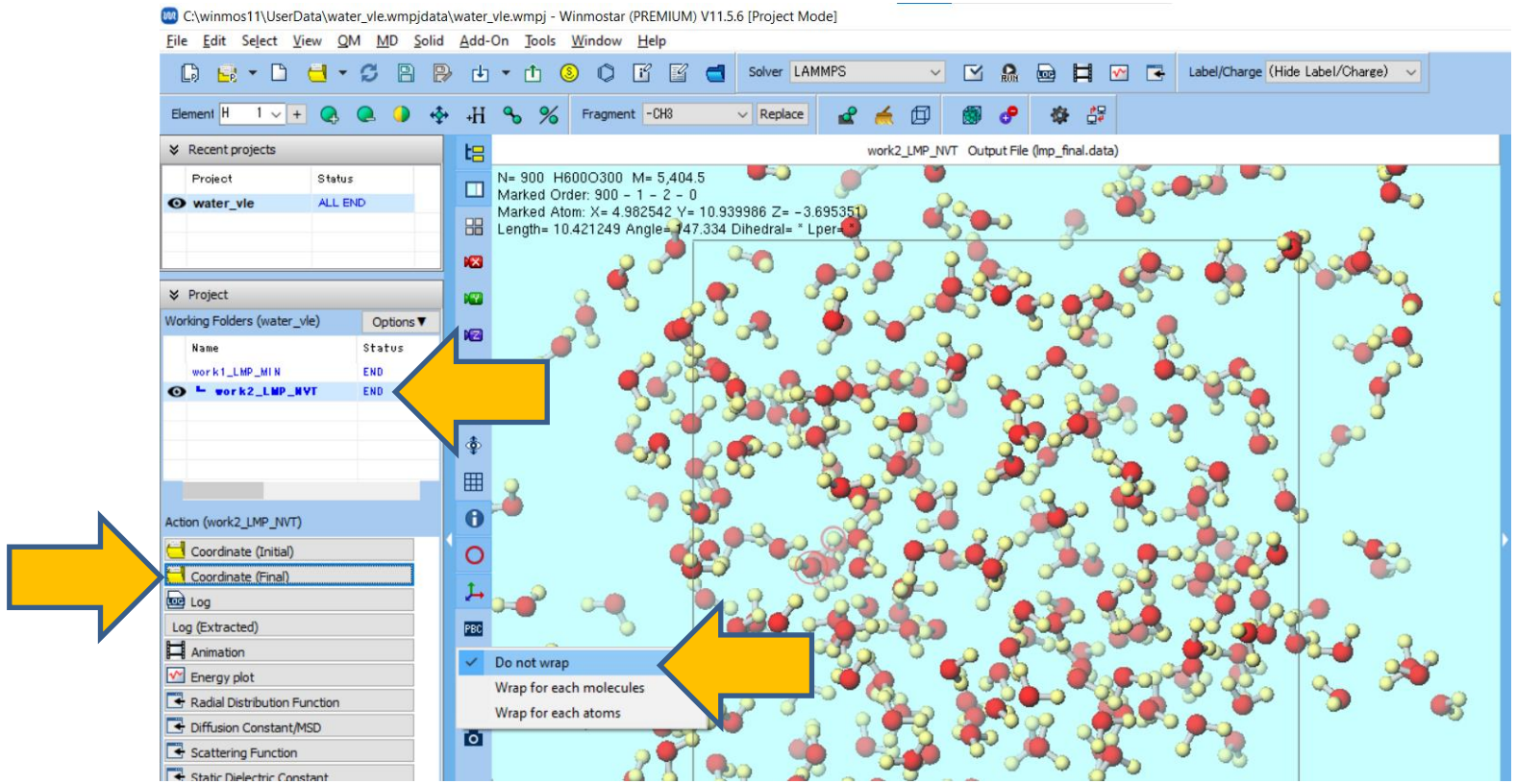
D. Click **OK**, then in **Job Setting** window, make appropriate settings and click **Run**.



C. Modeling of the System (Vapor-Liquid Equilibrium System)

A. Once **the status** of the work1 and work2 folders changes to **END** or **END(-)**, click on the work2 folder in Working Folders, then click on **Coordinate (Final)** under **Action** to display the final structure from the NVT calculation.

B. Click PBC **(Wrap Around Cell Boundary)** and select **Do not wrap**.



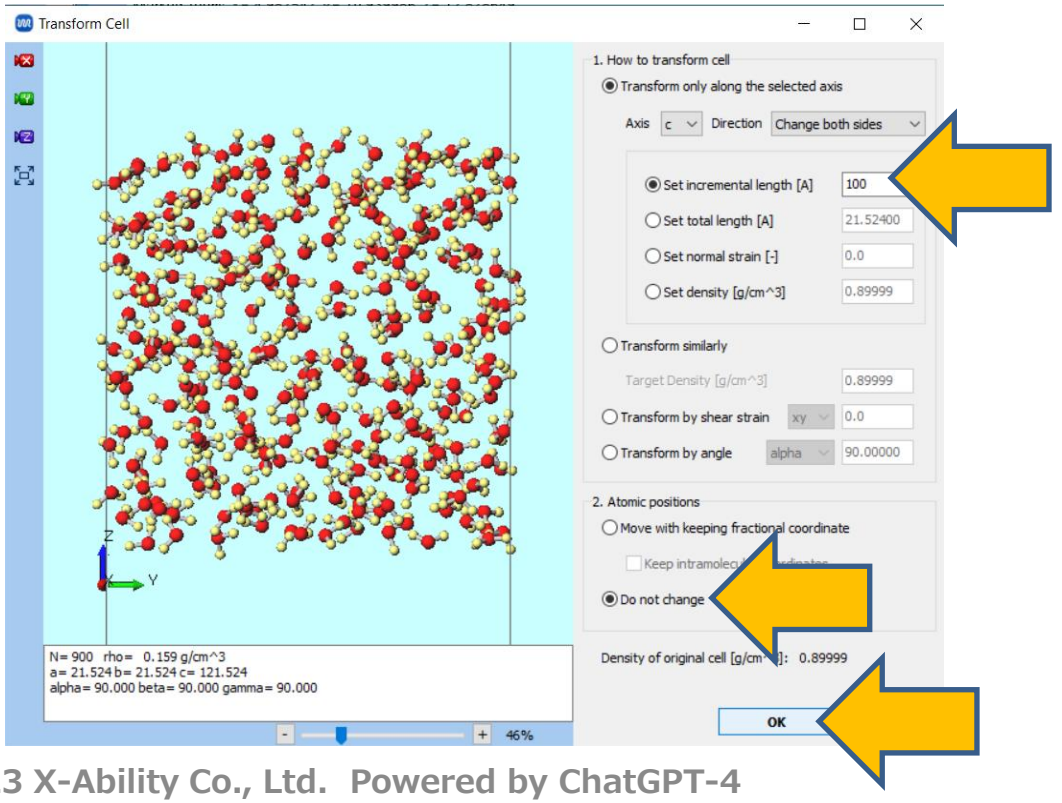
C. Modeling of the System (Vapor-Liquid Equilibrium System)

A. Click **Edit | Wrap/Unwrap Around Cell Boundary** and then click **OK**.

B. Click **Create/Edit Cell | Transform Cell**.

C. Change the value of **Set incremental length** to "100", check **Do not change** under **Atomic positions**, and then click **OK**.

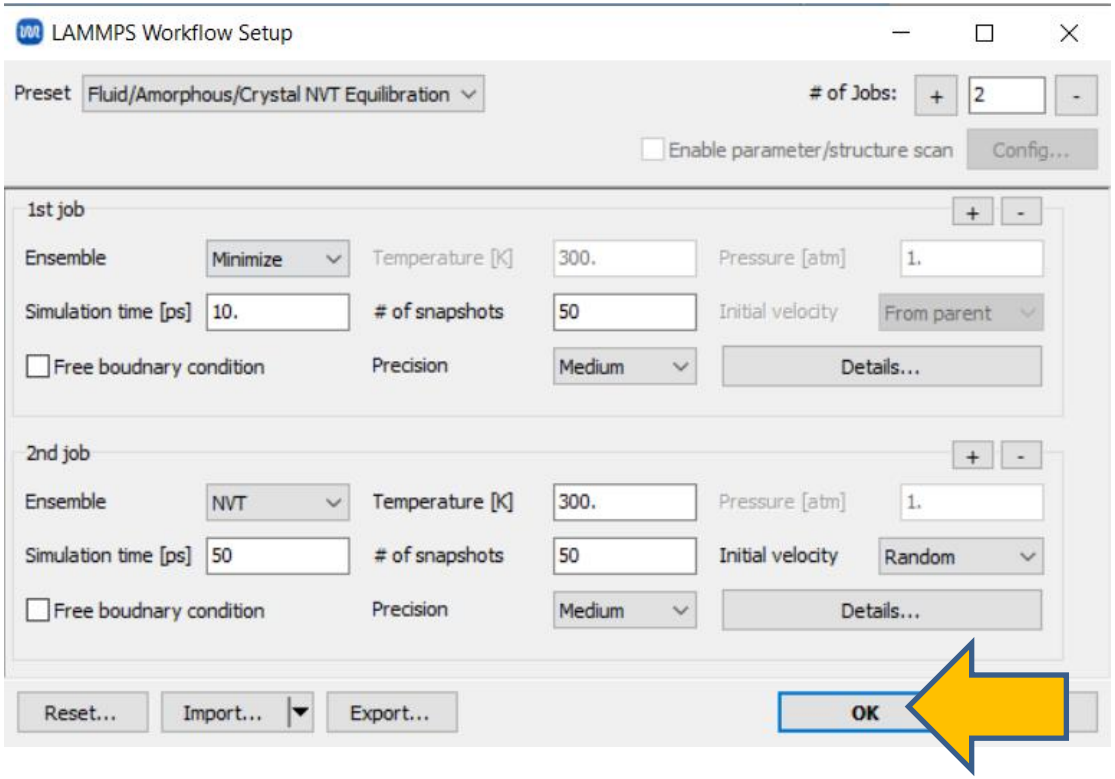
D. Click **(Align view to X-axis)**, and then click **(Fit to Window)**.



D. Execution of Calculation (Equilibration Calculation for Vapor-Liquid Equilibrium System)

A. Click **(Workflow Settings)**. If you see a message asking, "Do you want to continue from previous run?" click **No**. Click **OK** in **Assign force field parameters** window.

B. In **LAMMPS** or **Gromacs Workflow Setup** window, click **OK**, then in **Job Setting** window, make appropriate settings before clicking **Run**.



E. Execution of Calculation (Main Calculation for Vapor-Liquid Equilibrium System)

A. Once **the status** of work3 and work4 folders changes to **END** or **ID(-)**, click **(Workflow Settings)**.

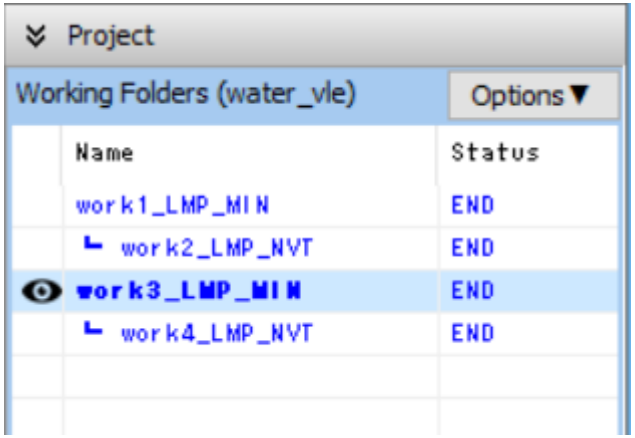
B. If the prompt "Do you want to continue from previous run?" appears, click **Yes**.

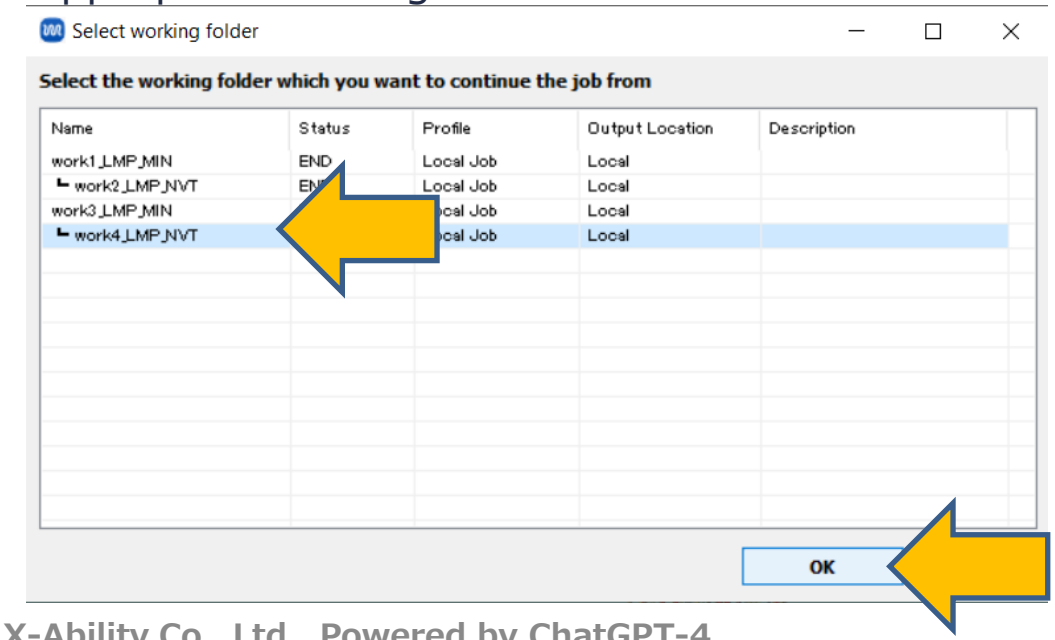
C. Select work4_LMP_NVT or work4_GMX_NVT and click **OK**.

D. Change **Preset** to "Fluid/Amorphous/Crystal NVT Production" and click **OK**.

   A. Because calculating surface tension requires relatively long simulation times, adjust the **Simulation time** as necessary.

E. In **Job Setting** window, make the appropriate settings and then click **Run**.





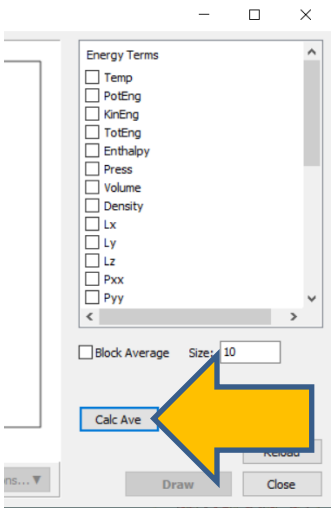
F. Analysis of Results

A. When **the status** of work5 changes to **END** or **END(-)**, click on work5_LMP_NVT or work5_GMX_NVT and then click on **Energy plot** under **Action**, and click **Calc Ave**.

B. 'Enter first frame to read' appears, click **OK**.

C. For LAMMPS, the vapor pressure is read from **Pzz** (in atm), and the product of the number of interfaces (2) and surface tension from **GamNsurf** or **v_GamNsurf** (in mN/m). For Gromacs, the vapor pressure is read from **Pres-ZZ** (in bar), and the product of the number of interfaces (2) and surface tension from **#SurfSurfTen** (in barnm). After reading, click **Close**. To convert units, use **Tools | Unit Converter**.

   – If the number of steps is insufficient, the average value of vapor pressure may become negative as shown in the figure below, but it will converge to a positive reasonable value with longer calculations.



For the case of LAMMPS

Pzz (atm)	-0.923636305017188		3.307415192654845
Pxz (atm)	-0.237060960120312		2.115183392939580
v_GamNsurf (mN/m)	121.088728953206690		4.332641883432600

For the case of Gromacs

Pres-YZ	0.542897	0.62	102.919	2.20051	(bar)
Pres-ZX	-0.0559363	1.3	99.2834	2.15514	(bar)
Pres-ZZ	2.79624	2.9	178.195	-13.9699	(bar)
#Surf*SurfTen	1196.12	71	2146.95	-299.467	(bar nm)
Xi-System	-0.56962	0.0046	0.0679523	0.0152251	(1/ps)

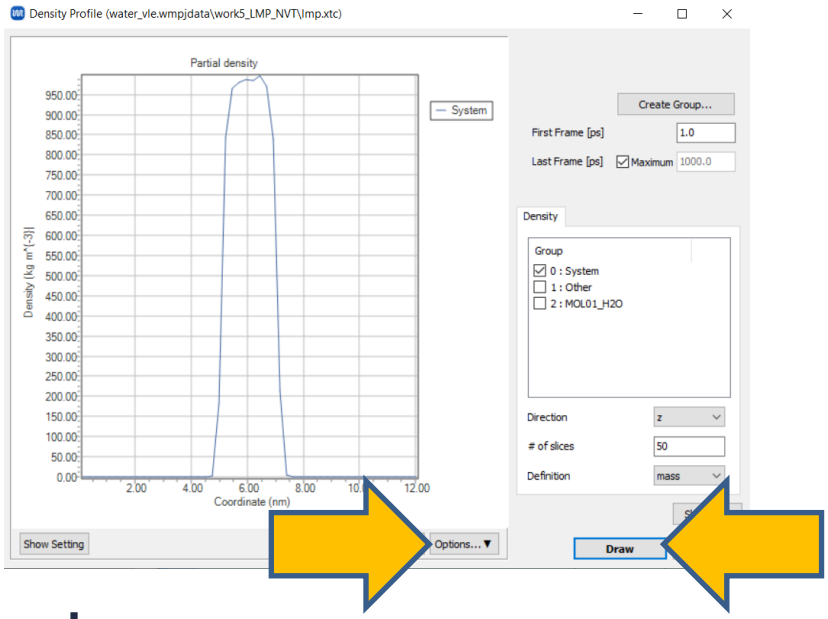
References : R. Sakamaki *et al*., J. Chem. Phys., 134, 124708 (2011).

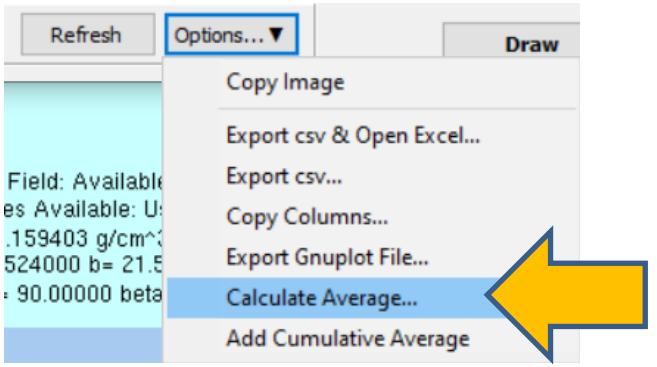
F. Analysis of Results

A. For remote jobs, first click on **Receive all remote output files** for work5 to retrieve the output files.

B. Click on **Density Profile** under **Action** for work5 and then click **Draw** to display the density distribution along the z-axis.

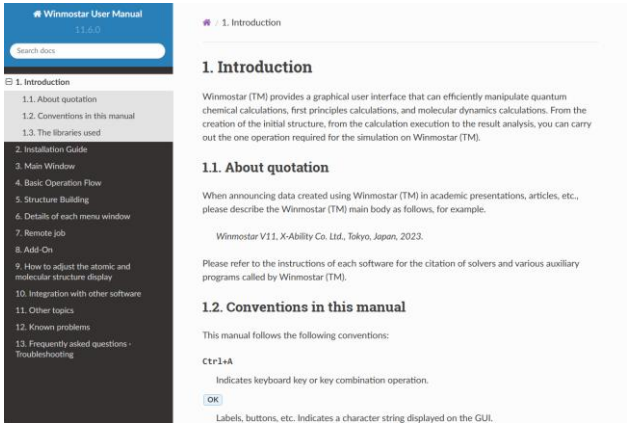
C. To obtain the equilibrium densities of the liquid and gas phases, click on **Options | Export csv & Open Excel** in the bottom right of the graph to generate a csv file and perform fitting to functions such as the tanh function using various graphing software. Alternatively, use **Options | Calculate Average** to calculate the average over a section of the graph.





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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