winmostar tutorial

LAMMPS/Gromacs Interfacial Tension

V11.5.6

13 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

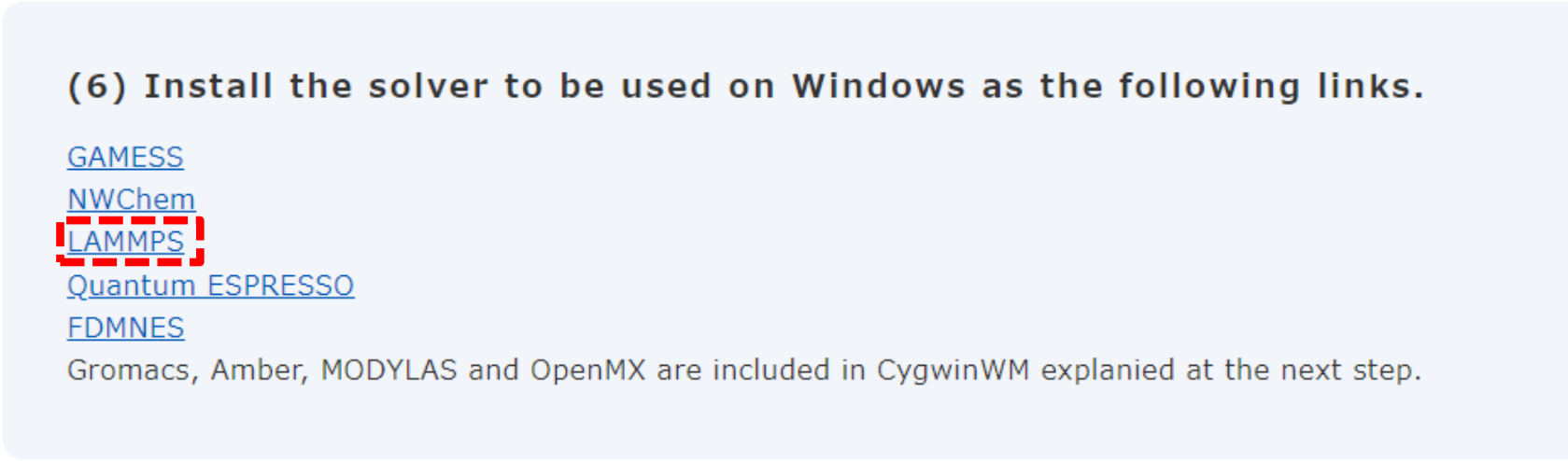
- To calculate the density distribution, equilibrium density, and interfacial tension of a water-benzene liquid-liquid interface at 300 K, follow these steps:
    A. Creation of the liquid phase for component 1
    B. Equilibration calculation for component 1's liquid phase (Energy minimization → NVT MD → NPT MD)
    C. Creation of the liquid phase for component 2
    D. Equilibration calculation for component 2's liquid phase (Energy minimization → NVT MD → NPT(z) MD)
    E. Creation of the liquid-liquid interface system
    F. Equilibration calculation for the liquid-liquid interface system (Energy minimization → NVT MD → NPT(z) MD)
    G. Main calculation for the liquid-liquid interface system (NPT(z) MD)

Notes:

- The calculations in this tutorial are performed with relatively few molecules for short execution times.
- 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 reliability of the results, especially for the convergence of interfacial tension values.
- The type of force field and calculation conditions for interactions significantly affect the results.

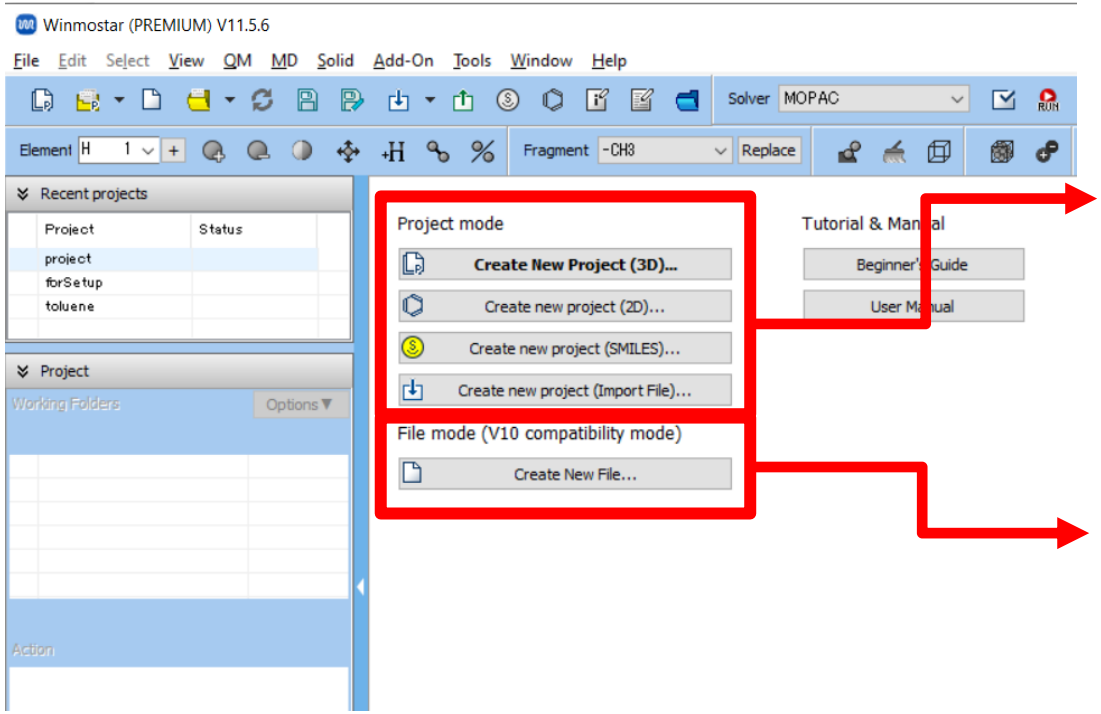
Preference of Operating Environment

- 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.

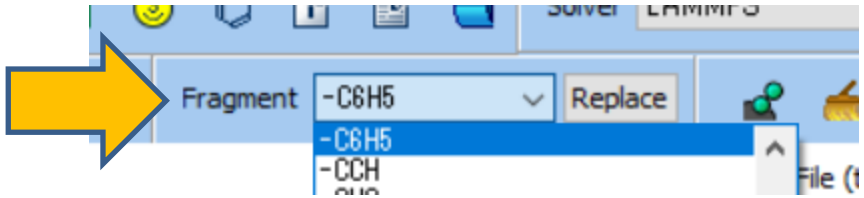
File Mode

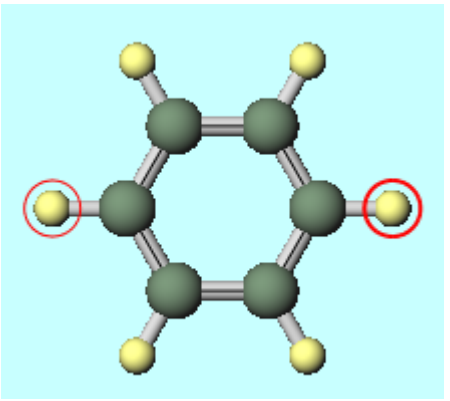
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System（Component 1）

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

A. Click **File | New Project**, enter '`water_benzene_ift`' in **Project name**, and click **Save**.
B. Change toolbar's **Fragment** to '-C6H5' and click **Replace** to confirm that benzene has been created.
C. Click  **Assign Charges Automatically** and then click **OK**. If the message 'Successfully assigned charges' appears, click **OK**.
D. Click  **Solvate/Build Cell**, then click **Add Displayed Molecule**. When prompted with **Enter # of molecules**, enter '100' and click **OK**.
E. Click **Build**. If the message 'The system has been successfully built.' appears, click **OK**.





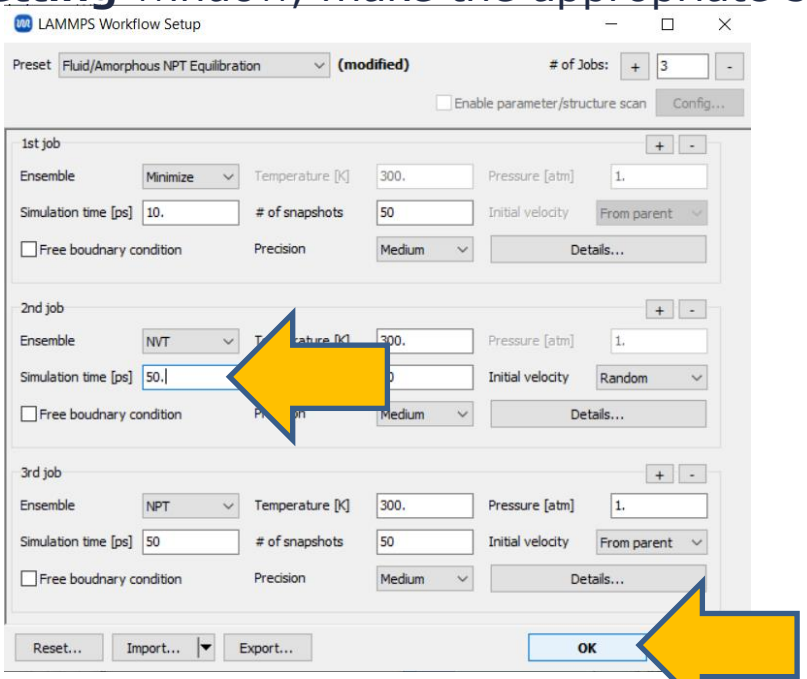
B. Execution of Calculations (Equilibration Calculation of Component 1)

A. Select 'LAMMPS' or 'Gromacs' as **Solver**, and click **(Workflow Setup)**, then click **OK**. If the message 'Assigned force field parameters' appears, click **OK**.

B. Change **Simulation time** for **2nd job** to '50' (as it takes time for the pressure to stabilize).

C. If you wish to reduce the calculation accuracy to finish the calculation faster, change **Precision** of **1st job**, **2nd job**, and **3rd job** to 'Low.'

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



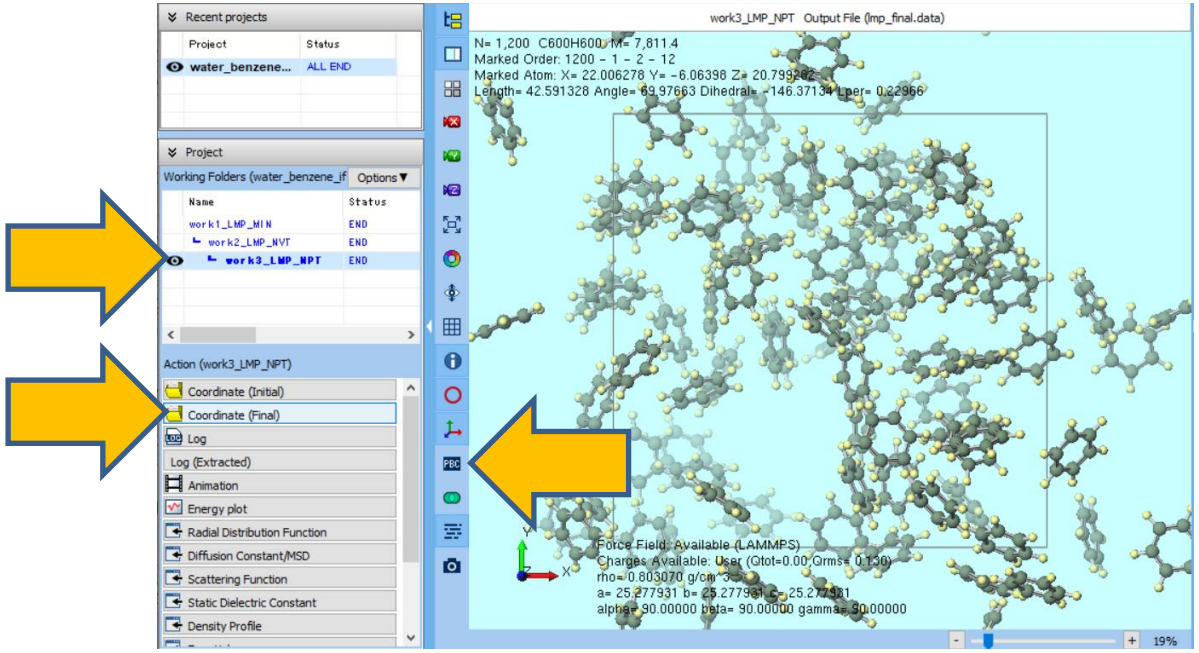
B. Execution of Calculations (Equilibration Calculation of Component 1)

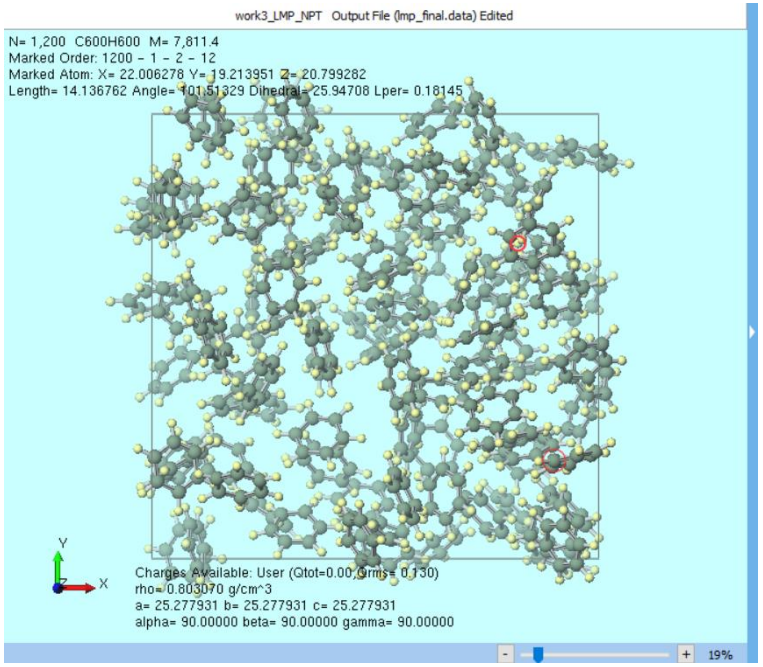
A. Once **the status** of work folders work1 to work3 changes to **END** or **END(-)**, click on work3 in **Working Folders**, then click **Coordinate (Final)** under **Action** to display the final structure from the NPT calculation.

B. Click PBC **(Wrap Around Cell Boundary)** and then click on **Do not wrap**.

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

D. Click **Export File** and save as '`benzene_eq.mol2`'.





C. Modeling of the System（Component 2）

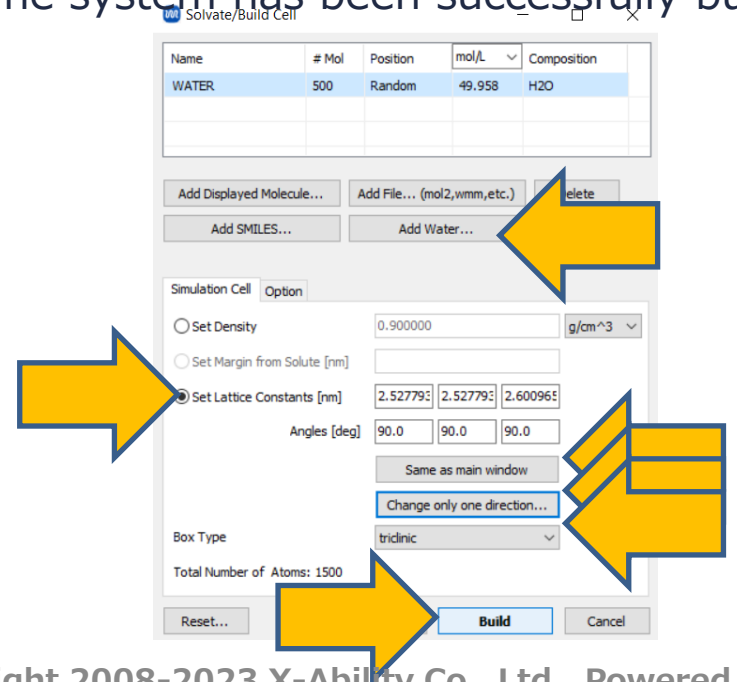
A. Click  **Solvate/Build Cell**, then click **Add Water**. When prompted with **Enter # of molecules**, type '500' and click **OK**.

B. Select **Set Lattice Constants** and click **Same as main window**.

C. Change **Box Type** to **Triclinic**.

D. Click on **Change only one direction**, and when '**Select direction**' appears, click **OK**. When 'Enter density' appears, type '0.9' and click **OK**.

E. Click **Build**. When 'The system has been successfully built.' appears, click **OK**.



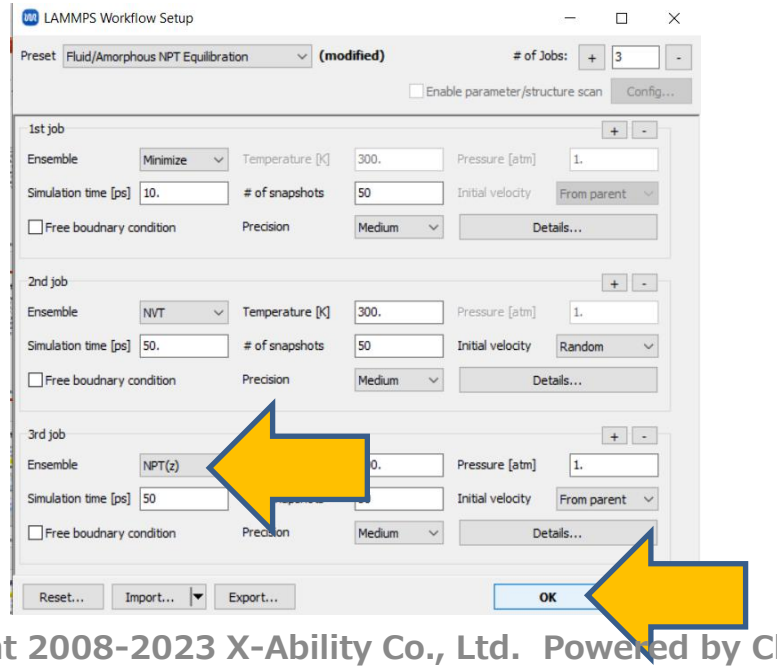
D. Execution of Calculations (Equilibration Calculation of Component 2)

A. Click **(Workflow Setup)**. If prompted with 'Do you want to continue from previous run?', click **No**. When Assign force field parameters window appears, click **OK**. Once 'Assigned force field parameters' is displayed, click **OK** again.

B. Change **Ensemble** for **3rd job** to **NPT(z)**.

C. If you wish to expedite the calculation by reducing accuracy, set **Precision** for **1st job**, **2nd job**, and **3rd job** to 'Low' and **Simulation time** to '10'.

D. Click **OK**, then in **Job Setting** window, adjust settings as needed and click **Run**.

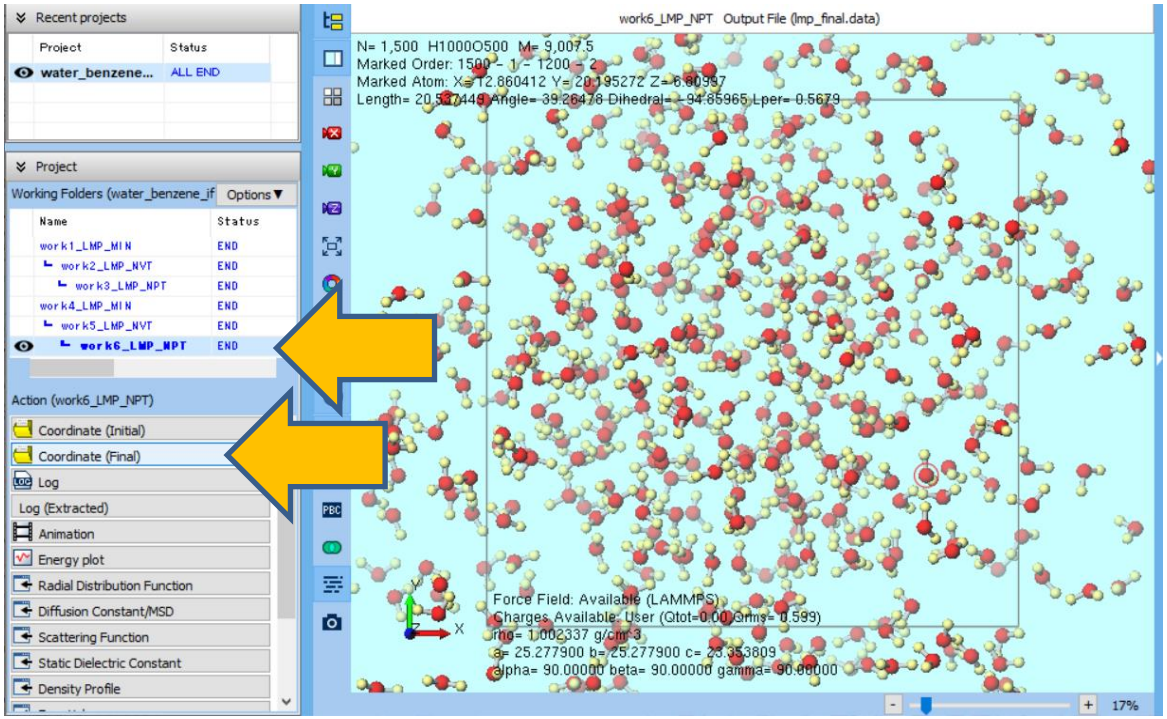


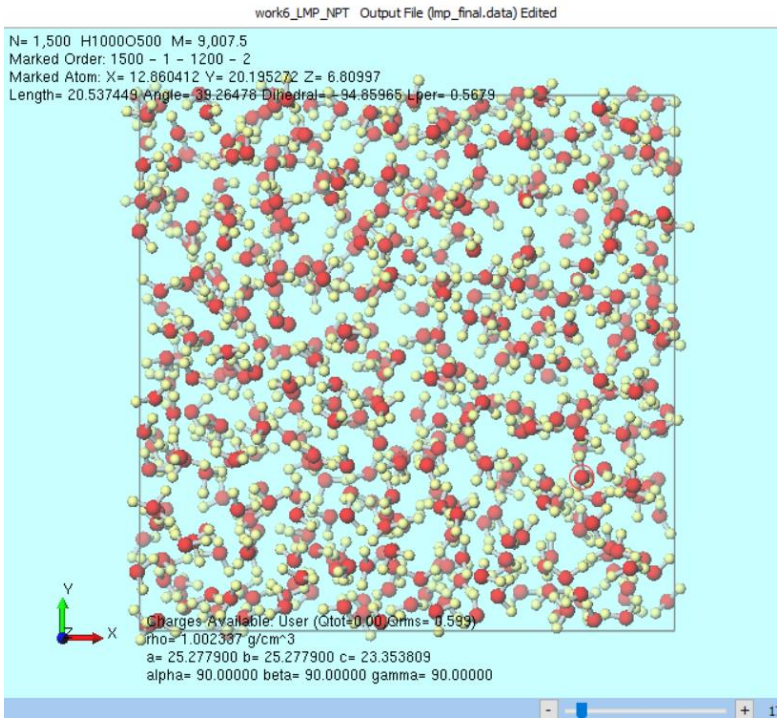
D. Execution of Calculations (Equilibration Calculation of Component 2)

A. Once **the status** of work folders work4 to work6 changes to **END** or **END(-)**, click on work6 in **Working Folders**, then click **Coordinate (Final)** under **Action** to display the final structure from the NPT calculation.

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

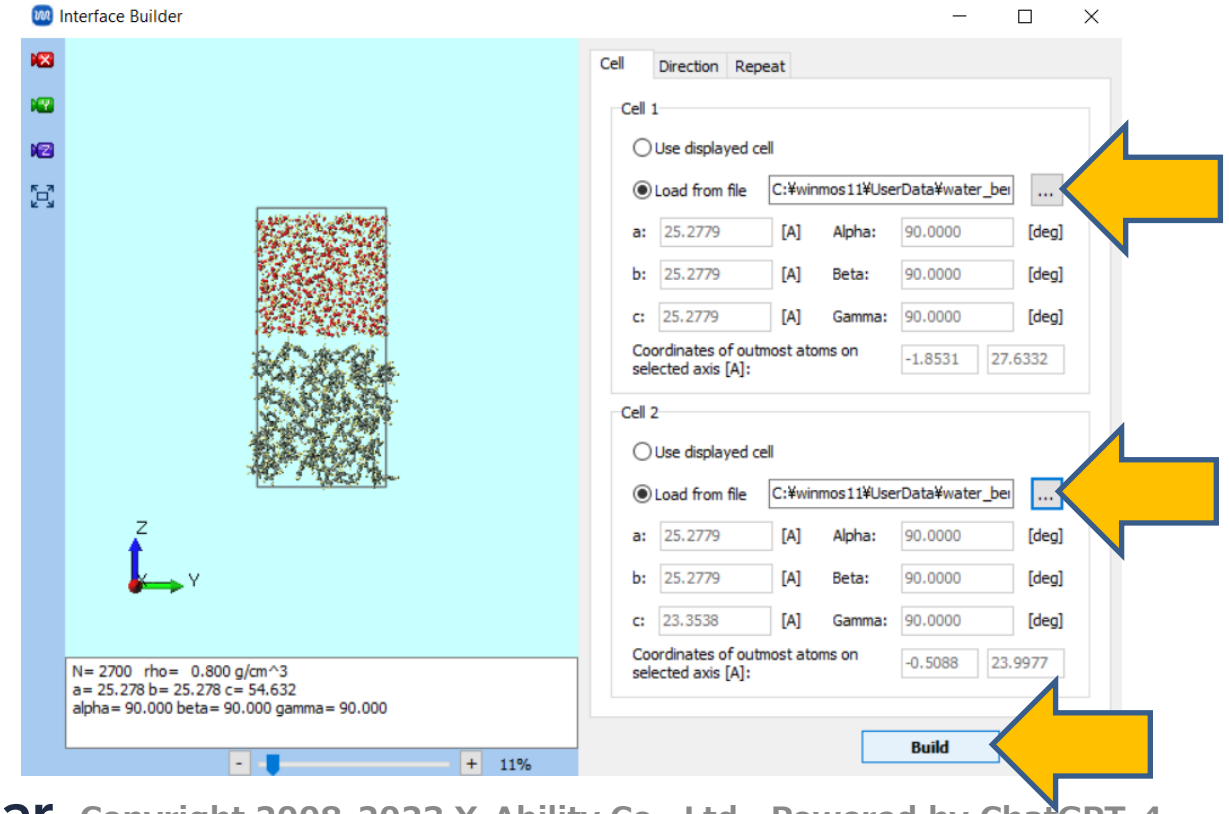
C. Click  **Export File** and save as '`water_eq.mol2`'.





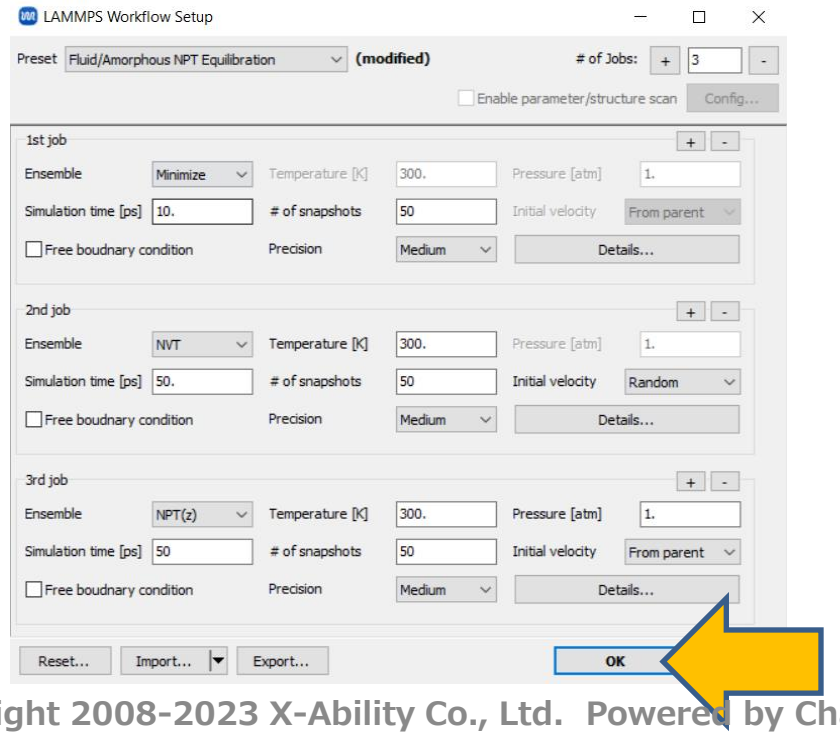
E. Modeling of the System (Liquid-Liquid Interface)

A. Click on **MD | Interface Builder**.
B. For **Cell 1**, click ... button and select benzene_eq.mol2 saved in P.8.
C. For **Cell 2**, click ... button and select water_eq.mol2 saved in P.11.
D. Click **Build**. Click **OK** when 'Successfully generated' is displayed.



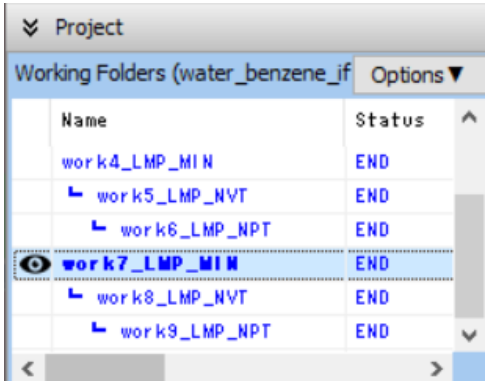
F. Execution of Calculations（Liquid-Liquid Interface）

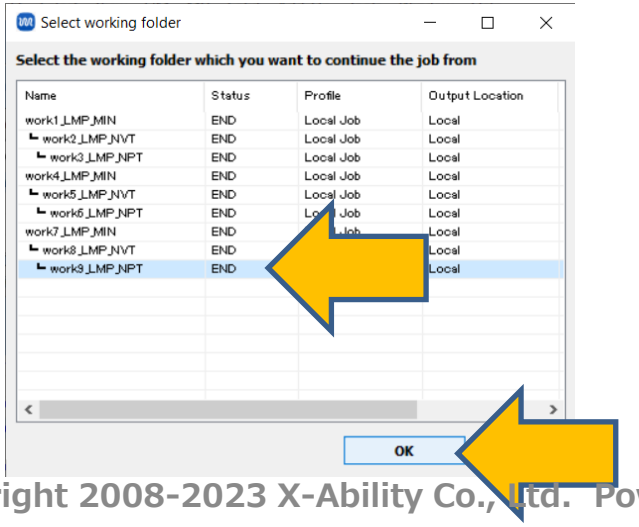
A. Click **(Workflow Setup)**.
B. If prompted with 'Do you want to continue from previous run?', click **No**.
C. Click **OK** in **Assign force field parameters** window. Once 'Assigned force field parameters' is displayed, click **OK** again.
D. Click **OK** in **LAMMPS** or **Gromacs Workflow Setup** window.
E. In **Job Setting** window, adjust settings as necessary and then click **Run**.

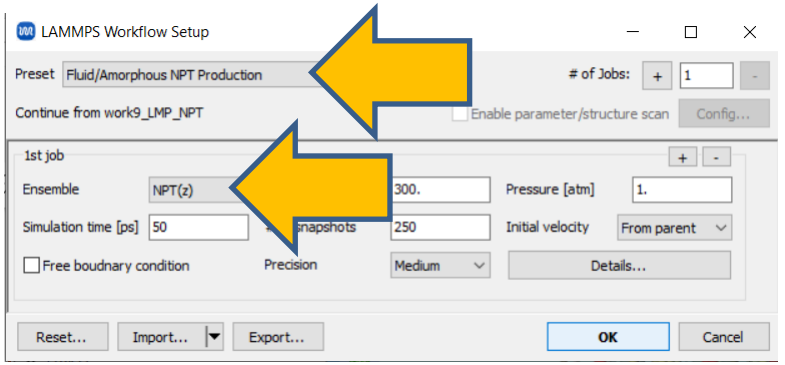


G. Execution of Calculations (Main Calculation for Liquid-Liquid Interface)

A. Once **the status** of work9 folder changes to **END** or **END(-)**, click **(Workflow Setup)**.
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.
C. Select work9_LMP_NPT or work9_GMX_NPT and click **OK**.
D. Change **Preset** to 'Fluid/Amorphous NPT Production'.
   - Adjust **Simulation time** as needed since calculating interfacial tension requires relatively long computations.
E. Change **Ensemble** to **NPT(z)**.
F. If you wish to expedite the calculation, change **Precision** to 'Low'.
G. Click **OK**, adjust settings as needed in **Job Setting** window, and then click **Run**.



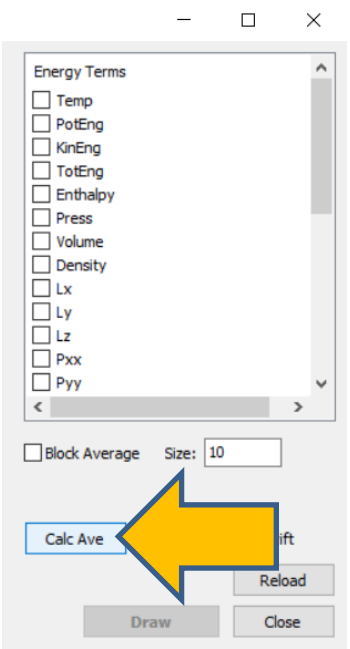




H. Analysis of Results

A. Once **the status** of work10 folder changes to **END** or **END(-)**, click work10_LMP_NPT or work10_GMX_NPT, then click **Energy plot** under **Action** and click **Calc Ave**. If prompted with 'Enter the first frame to read,' click **OK**.

B. For LAMMPS, read the product of the number of interfaces (2) and the interfacial tension as **GamNsurf** (in mN/m). For Gromacs, read it as **#SurfSurfTen** (in bar*nm). After reading, click **Close**. If you wish to convert units, use **Tools | Unit Converter**.



For the case of LAMMPS

Pxz (atm)	7.7151239299120278		11.857266877573670
GamNsurf (mN/m)	67.069032977688845		10.027778359600330
E_pair (kcal/mol)	-5507.0880264294240000		0.7112984857794630

For the case of Gromacs

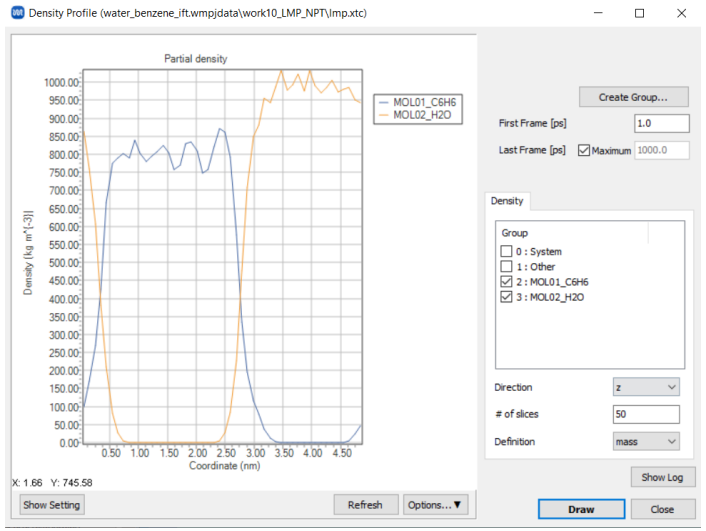
Pres-ZX	-2.78973	27	596.871	-18.0433	(bar)
Pres-ZY	14.0067	13	620.482	73.1588	(bar)
Pres-ZZ	0.27705	13	1064.72	27.0455	(bar)
#Surf*SurfTen	624.889	210	5993.7	858.899	(bar nm)
Box-Vel-YY	0	0	0	0	(nm/ps)

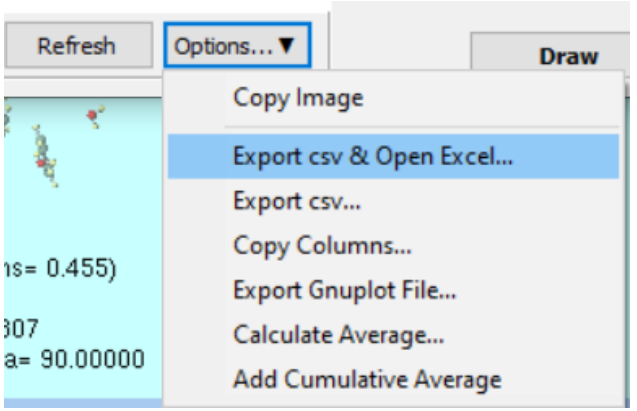
VI.結果解析

A. For remote jobs, first click on **Receive all remote output files** for work10 to obtain the output files.

B. Click **Density Profile** in **Action** for work10. Ensure that for LAMMPS in **Group**, 'MOL01_C6H6' and 'MOL02_H2O' are checked, and for Gromacs, 'MOL01' and 'Water' are selected, then click **Draw** to display the density distribution along the z-axis.

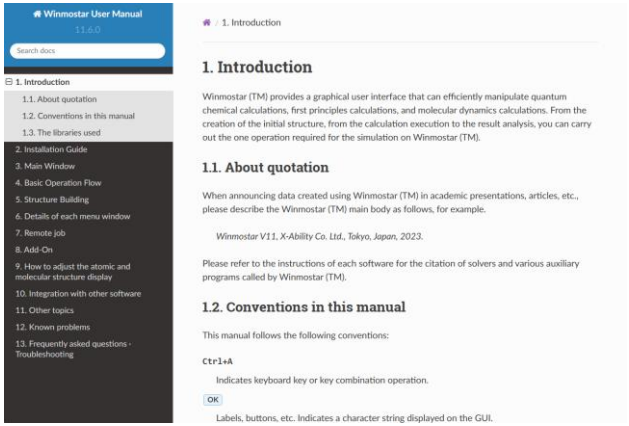
C. To obtain the equilibrium density of each phase, click on **Options | Export csv & Open Excel** in the bottom right of the graph to generate a csv file. Then, use various graphing software to fit the data to an appropriate function as needed. You can also use **Options | Calculate Average** to calculate the sectional average 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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