winmostar tutorial

Gromacs Calculation of Solubility/Chi/DPD Parameters

V11.6.5

30 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 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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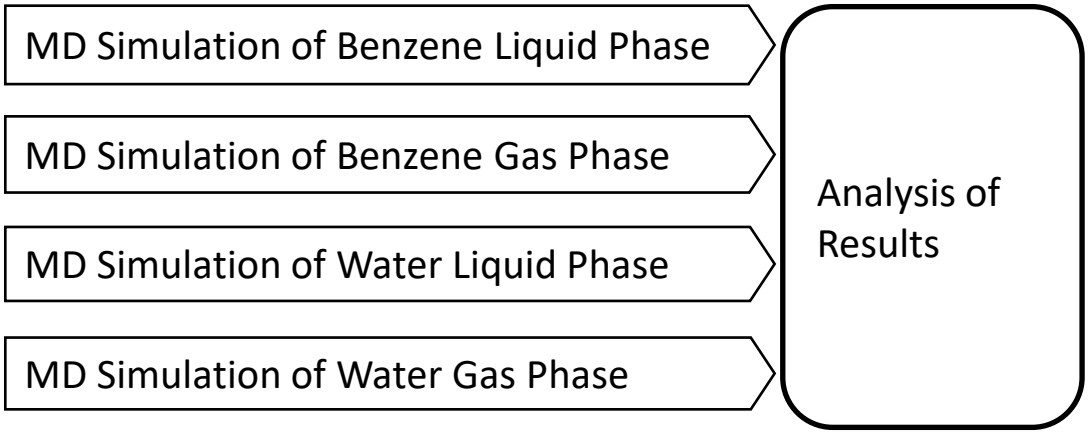
Overview

- In this tutorial, we calculate the cohesive energy of benzene (component A) and water (component B), the Hildebrand solubility parameters for both components, the Flory-Huggins parameter (χ) between water and benzene, and the DPD A_{ij} parameter.



Note :

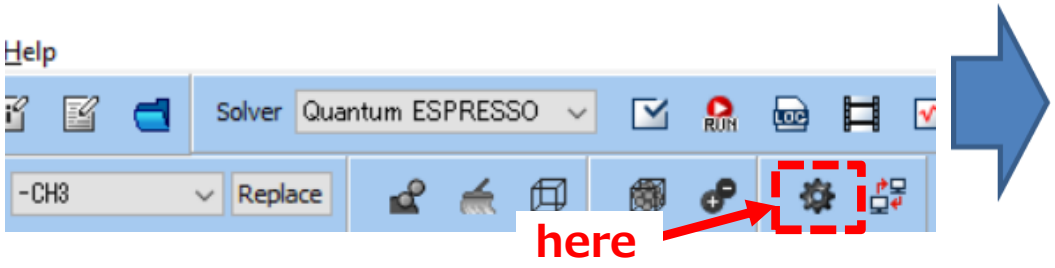
- The number of steps required for equilibration varies with the type of molecule and initial density.
- Larger step counts in the 'main calculation' lead to better reproducibility and more reliable results.
- The type of force field and interaction calculation conditions significantly affect the calculation results.
- Although the calculation of water vapor phase is not necessary when using a rigid water model, it is currently required by Winmostar™ for the energy file, so the calculation will be performed.

Operating Environment Settings

- To use this feature, it is necessary to set up Cygwin.
- https://winmostar.com/en/installation/ Set up Cygwin by following the configuration steps outlined in the installation instructions.

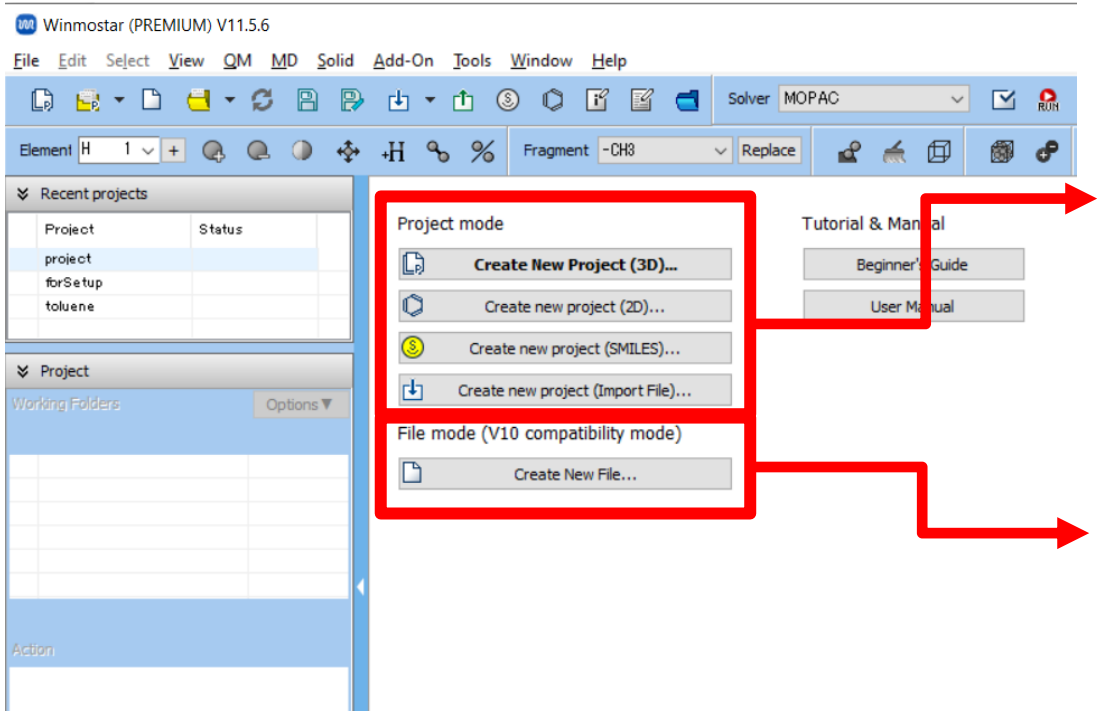
(7) Install Cygwin environment for Winmostar. ← here

- By default, it is installed directly under C:, but you can install it in a location of your choice by changing the 'Program Path' > 'Cygwin' in Winmostar Preference.



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 LAMMPS Tutorial for V10.



Project Mode New Features in V11

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

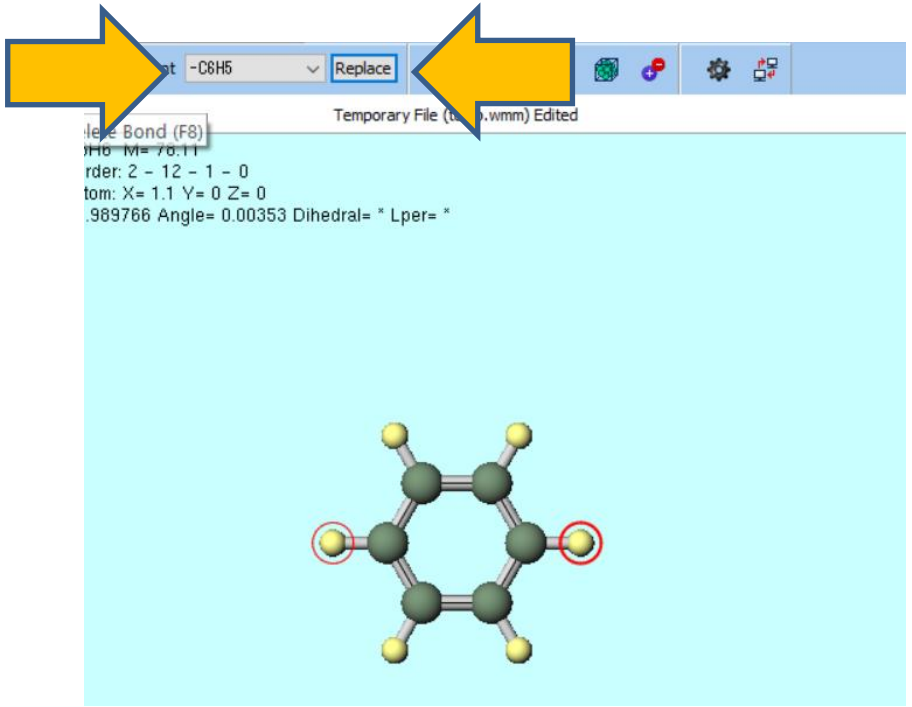
File Mode

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 A Liquid Phase)

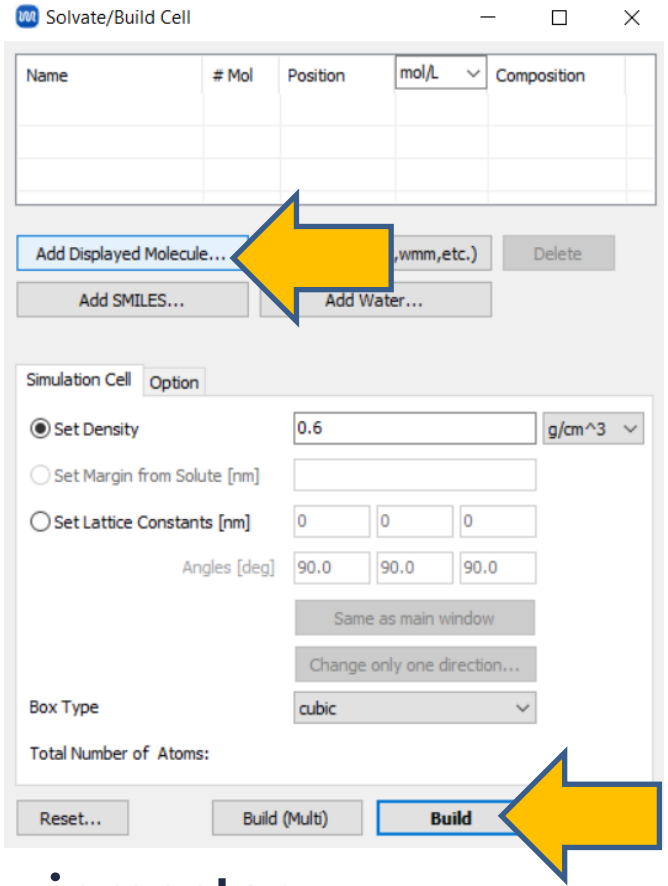
For basic operations, please refer to Gromacs Basics tutorial.

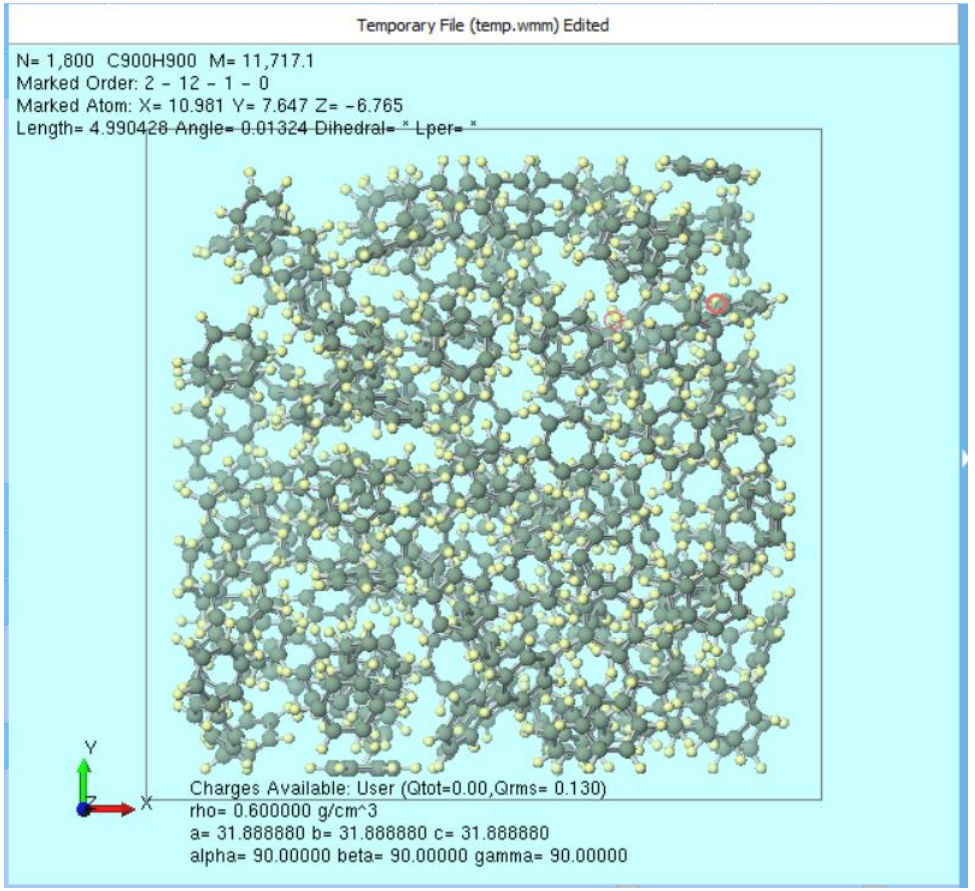
A. Click **File | New Project**, enter '`solub_param`' in **Project name**, and click **Save**.
B. Select '-C6H5' from **Fragment** and click **Replace** to create benzene.
C. Click  **Assign Charges Automatically** and then click **OK**.
D. Click  **Export File** and save as '`benzene_am1bcc.mol2`'.



A. Modeling of the System (Component A Liquid Phase)

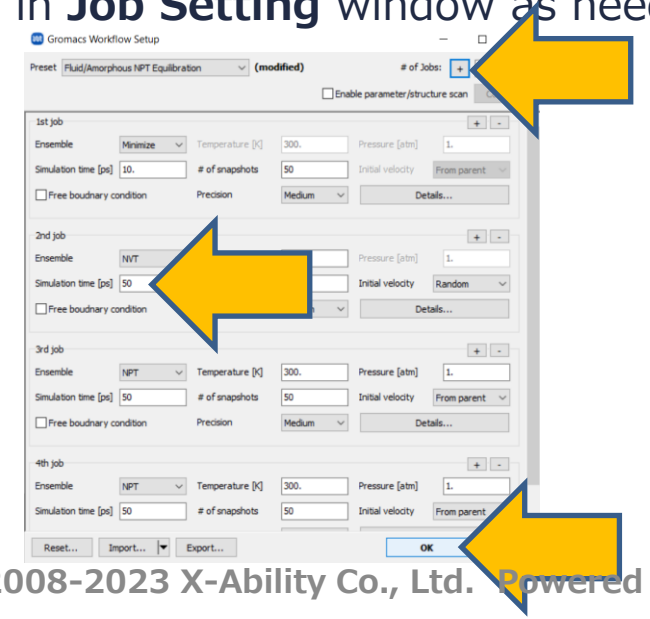
A. Click  **Solvate/Build Cell**.
B. Click **Add Displayed Molecule**, enter '**150**', and click **OK**.
C. Click **Build**.





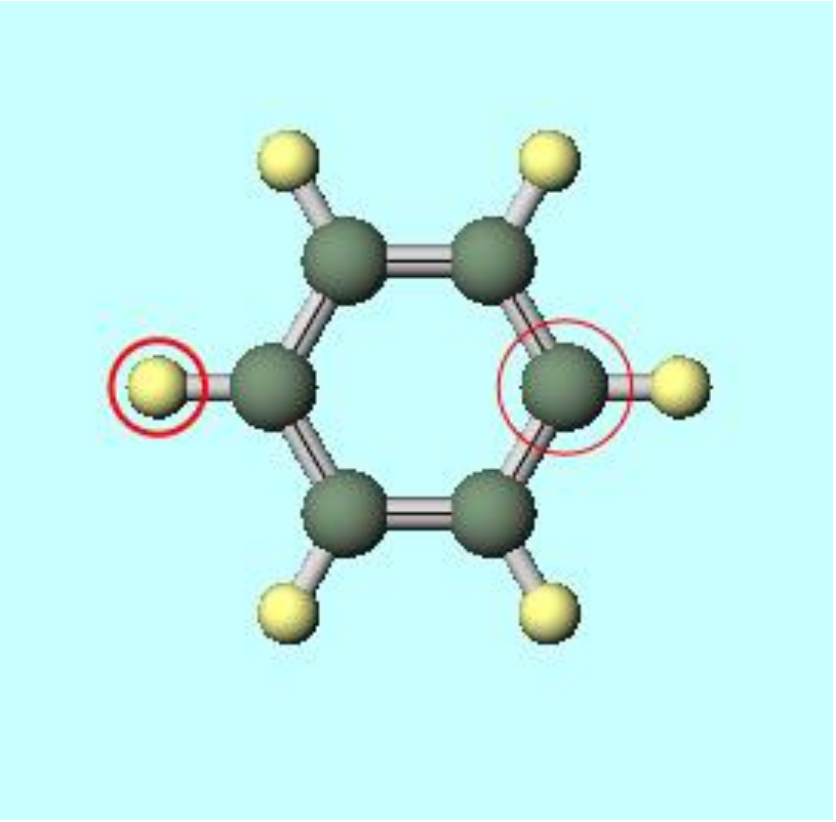
B. Execution of Calculation (Component A Liquid Phase)

A. Select **Gromacs** from **Solver**, and open **(Workflow Setup)**.
B. Click **OK**, and if 'Assigned force field parameters' is displayed, click **OK** again.
C. Change **Simulation time** of **2nd job** to '50'.
D. Adjust **Simulation time**, **Temperature**, **Pressure** as needed (no changes needed for this tutorial).
E. If you want to finish the calculation quickly by reducing computational accuracy, change **Precision** of **all jobs** from **1st** to **3rd** to 'Low'.
F. Click **+** next to **# of jobs** once.
G. Click **OK**, adjust settings in **Job Setting** window as needed, and then click **Run**.



C. Modeling of the System (Component A Vapor Phase)

A. Click **Import File** and select `benzene_am1bcc.mol2` saved in P. 6.
B. In **Import File** dialog, click **Discard and import**.



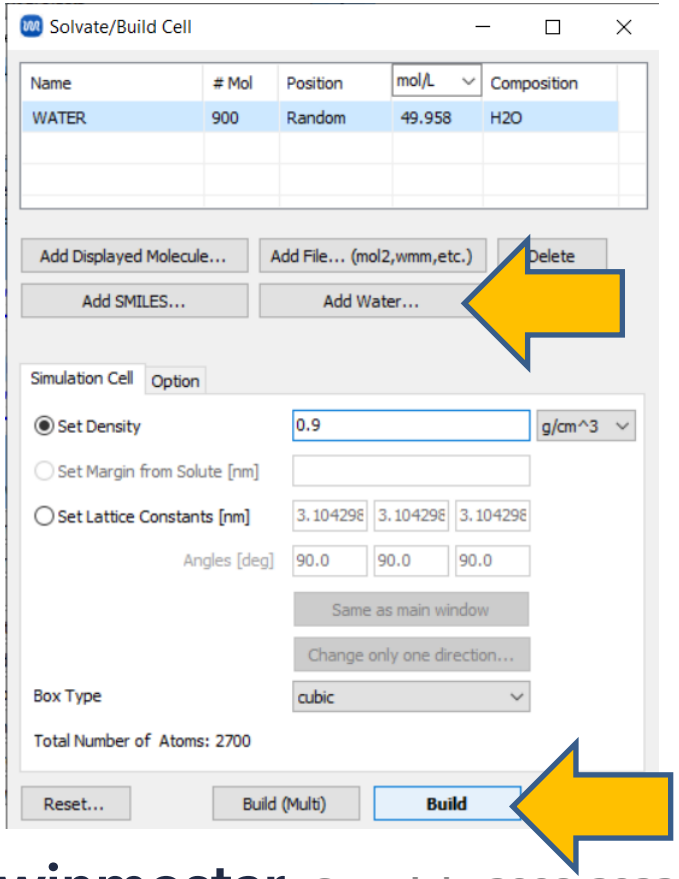
D. Execution of Calculation (Component A Vapor Phase)

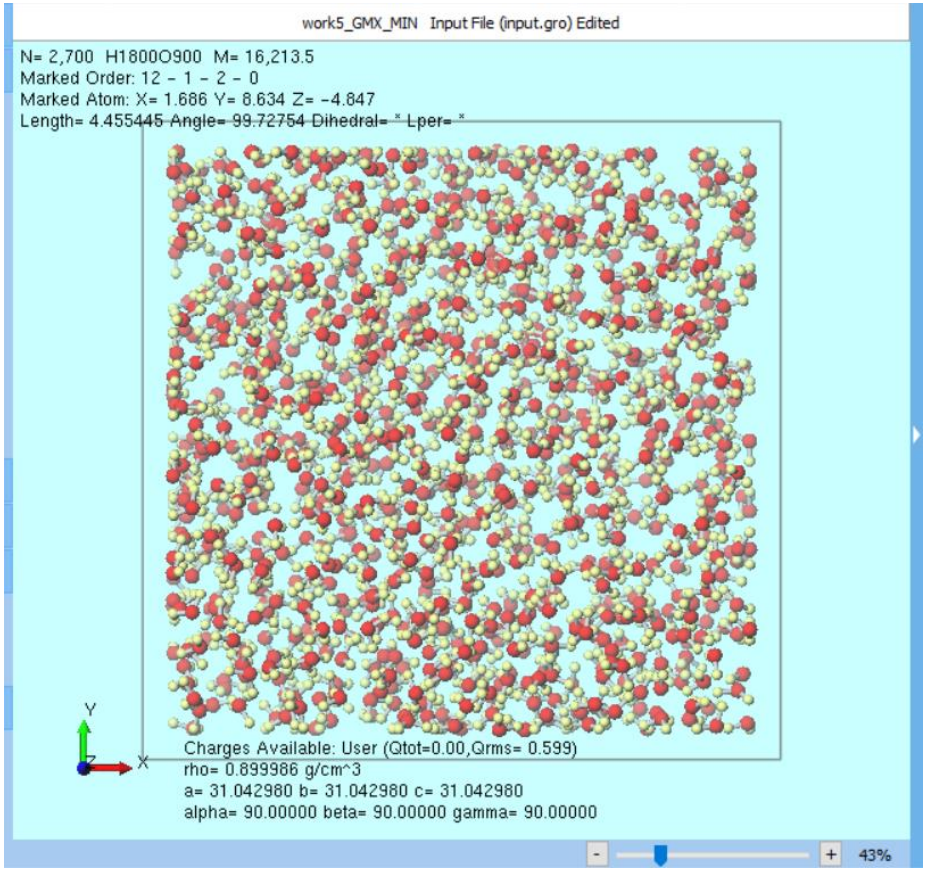
A. Open **(Workflow Setup)**.
B. Click **No** when prompted 'Do you want to continue from previous run?'.
C. Click **OK** when 'Create Cell' is displayed.
D. Click **OK** in **Assign force field parameters** window, and then click **OK** again when 'Assigned force field parameters' is displayed.
E. Change **Preset** to 'Isolated system NVT Equilibration'.
F. Change **Simulation time**, **Temperature**, **Pressure** as needed (no changes are needed for this tutorial).
G. If you want to speed up the calculation by lowering the calculation accuracy, change **Precision** of **1st** and **2nd jobs** to 'Low'.
H. Click **+** next to **# of jobs** once.
I. Change **Initial velocity** of **3rd job** to 'From Parent'.
J. Click **OK**, then adjust settings as needed in **Job Setting** window and click **Run**.

Proceed to 'IX. Result Analysis' if only the solubility parameter of component A is needed.

E. Modeling of the System (Component B Liquid Phase)

A. Click **Solvate/Build Cell**.
B. Click **Add Water**, enter '**900**', and click **OK**.
C. Enter '**0.9**' in **Set Density**, and click **Build**.





F. Execution of Calculation (Component B Liquid Phase)

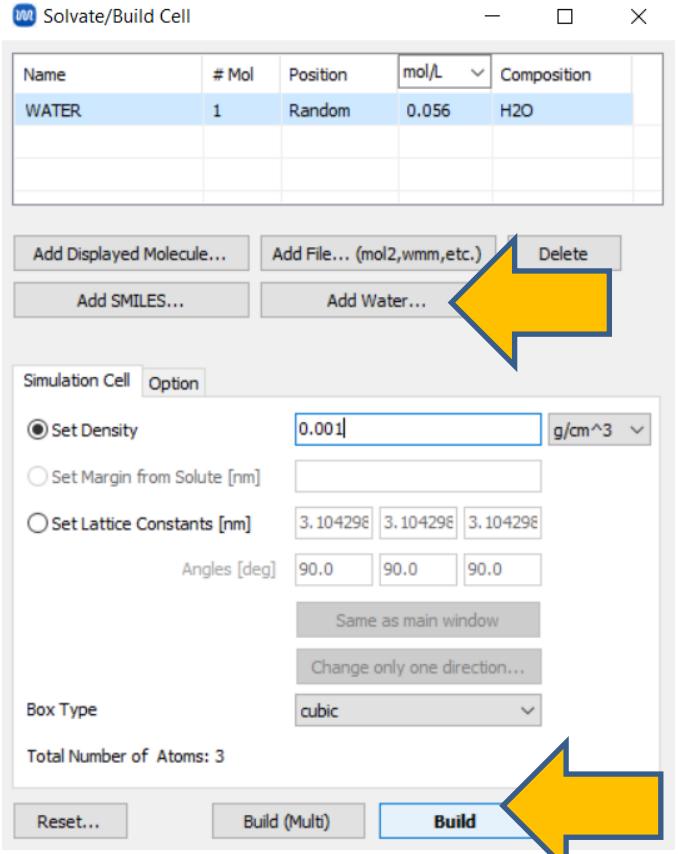
A. Open  **(Workflow Setup)**.
B. If prompted 'Do you want to continue from previous run?', click **No**.
C. Click **OK**, and when 'Assigned force field parameters' is displayed, click **OK**.
D. Change **Preset** to 'Fluid/Amorphous NPT Equilibration'.
E. Change **Simulation time** of **2nd job** to '50'.
F. Adjust **Simulation time**, **Temperature**, **Pressure** as needed (no changes are needed for this tutorial).
G. If you want to shorten the calculation time, change **Precision** of **all jobs** from **1st** to **3rd** to 'Low'.
H. Click **+** next to **# of jobs** once.
I. Click **OK**, adjust the settings in **Job Setting** window as needed, and then click **Run**.

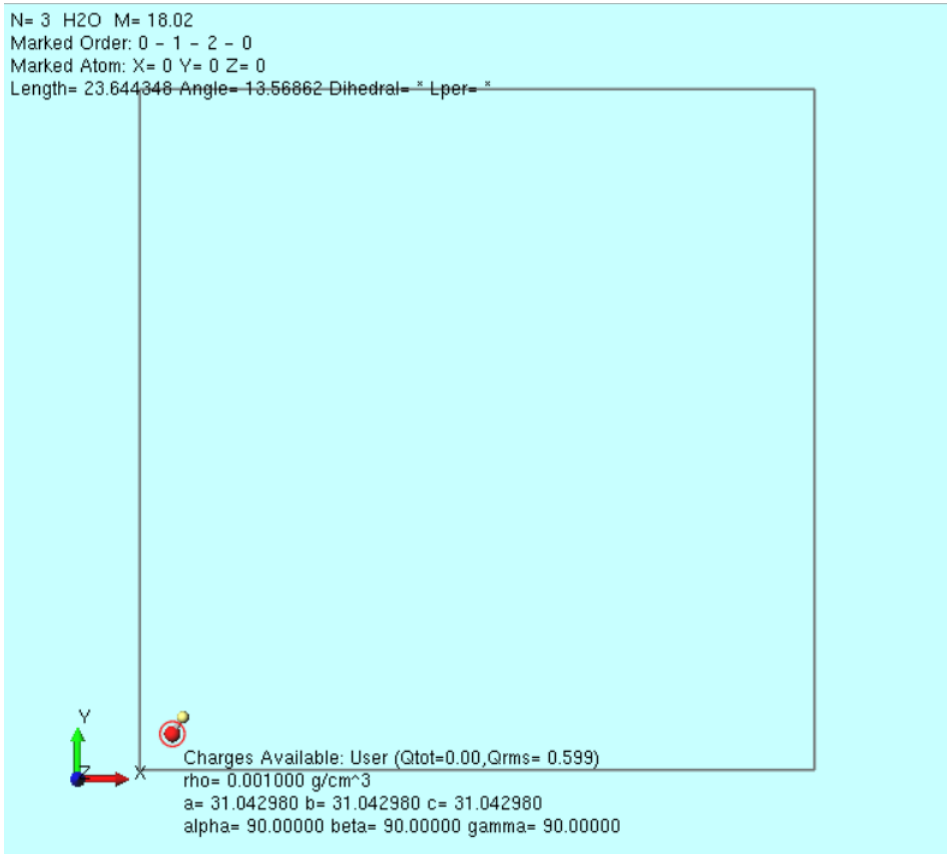
G. Execution of Calculation (Component B Vapor Phase)

A. Click  **Solvate/Build Cell**.

B. Click **Add Water**, enter '**1**', and click **OK**.

C. Enter '**0.001**' in **Set Density**, and click **Build**.



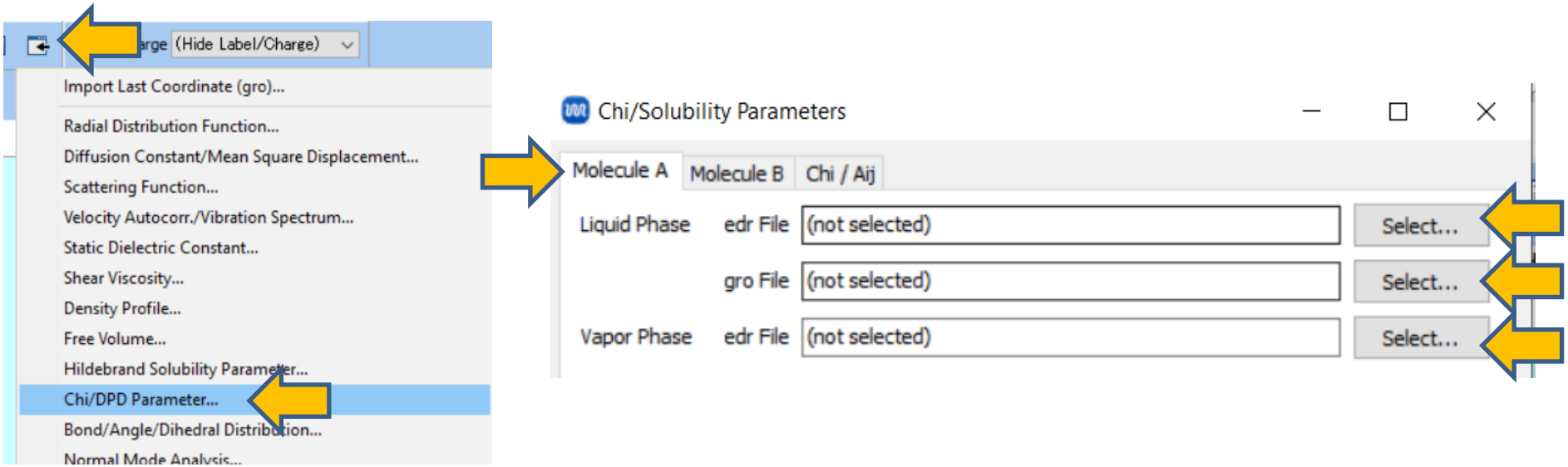


G. Execution of Calculation (Component B Vapor Phase)

A. Open **(Workflow Setup)**.
B. If prompted 'Do you want to continue from previous run?', click **No**.
C. Click **OK**, and when 'Assigned force field parameters' is displayed, click **OK**.
D. Change **Preset** to 'Isolated system NVT Equilibration'.
E. Adjust **Simulation time**, **Temperature**, **Pressure** as needed (no changes are needed for this tutorial).
F. If you want to shorten the calculation time, change **Precision** of **1st** and **2nd jobs** to 'Low'.
G. Click **+** next to **# of jobs** once.
H. Change **Initial velocity** of **3rd job** to 'From Parent'.
I. Click **OK**, adjust the settings in **Job Setting** window as needed, and then click **Run**.

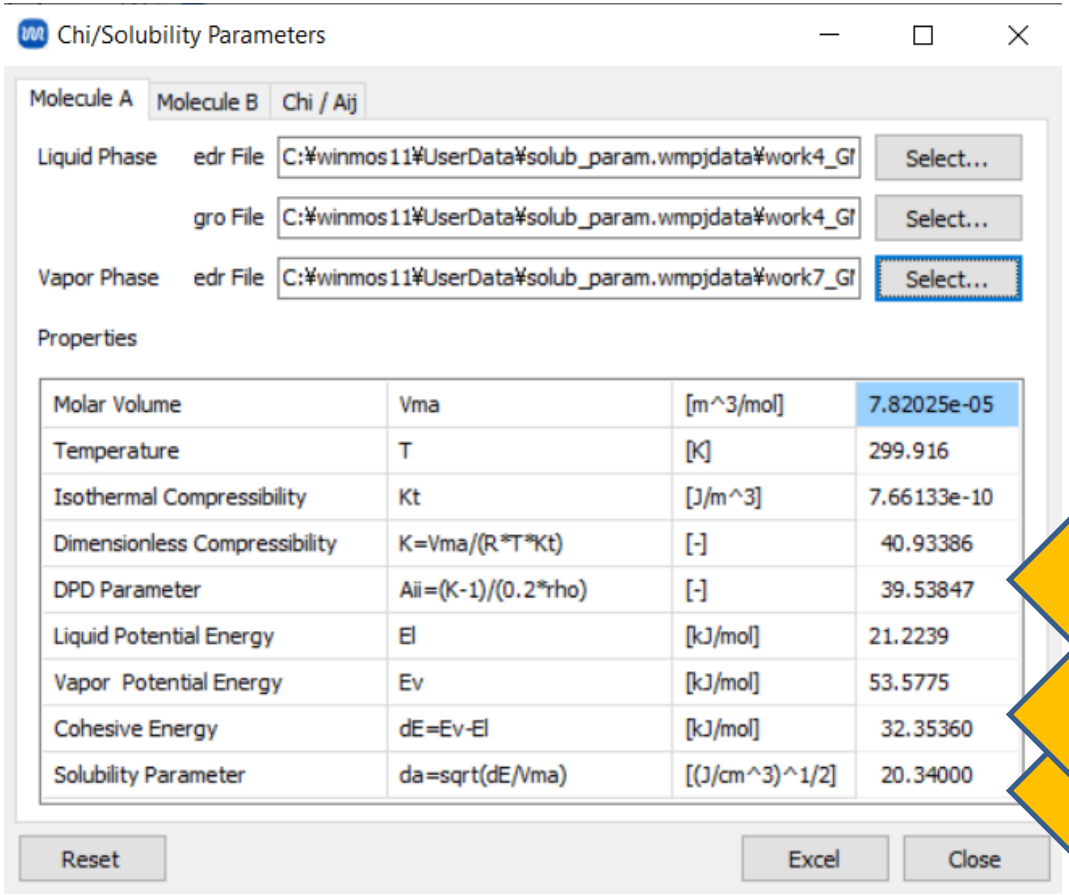
H. Analysis of Results

A. After all calculations are completed, click  **Analyses | Chi/DPD Parameter**, and then click **Molecule A tab**.
B. Click **Select** for **Liquid Phase's edr File**, and select `gmx_mdrun.edr` under `work4_GMX_NPT`.
C. Click **Select** for **Liquid Phase's gro File**, and select `gmx_mdrun.gro` under `work4_GMX_NPT`.
D. Click **Select** for **Vapor Phase's edr File**, and select `gmx_mdrun.edr` under `work7_GMX_NVT`.



H. Analysis of Results

A. The **Hildebrand solubility parameter δ** of **Molecule A** (in this case, benzene) and **DPD Parameter A_{ii}** between **Molecule As** are output at the following location. (Be careful of the units when comparing with literature values, etc.)



Intra-species DPD Parameters

Cohesive Energy

Solubility Parameter

H. Analysis of Results

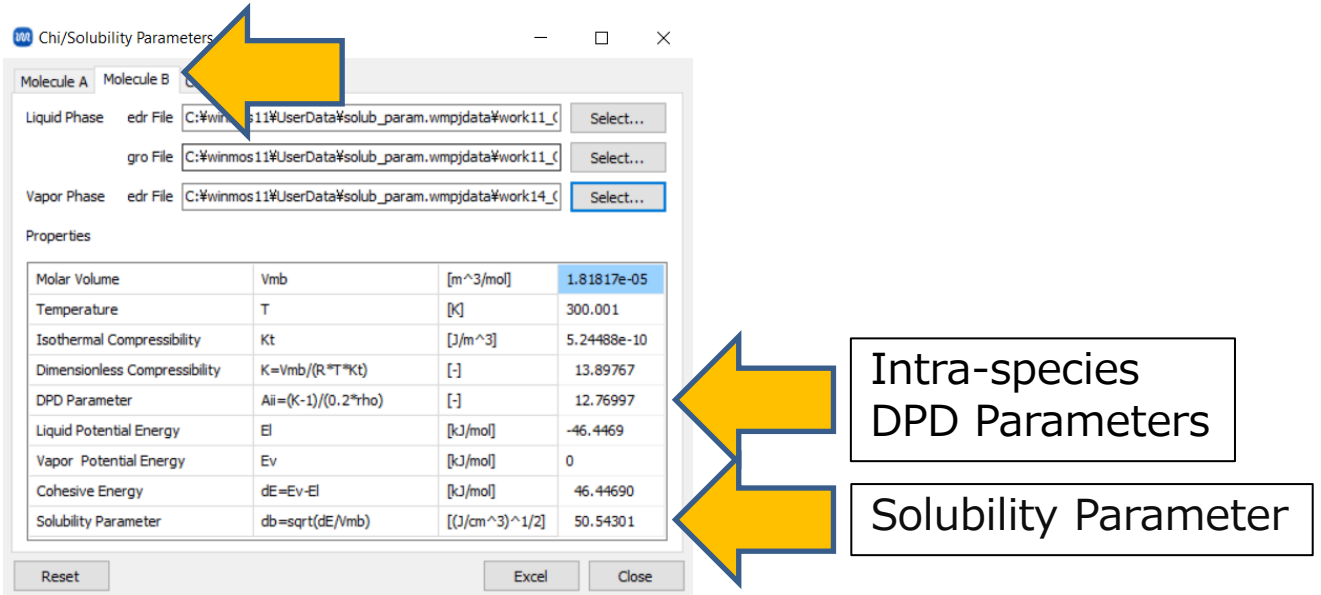
To determine the χ parameter and the DPD parameter A_{ij}:

A. Click **Molecule B tab**.

B. Click **Select** next to **Liquid Phase's edr File**, and select `gmx_mdrun.edr` under `work11_GMX_NPT`.

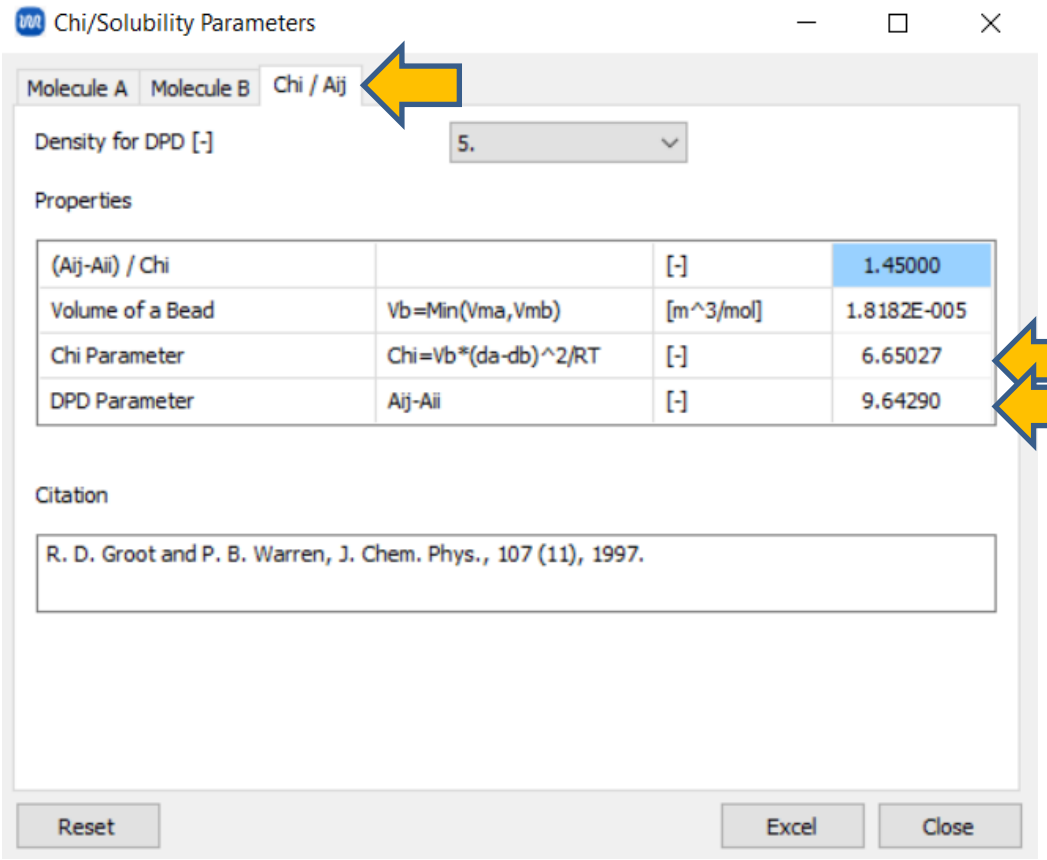
C. Click **Select** next to **Liquid Phase's gro File**, and select `gmx_mdrun.gro` under `work11_GMX_NPT`.

D. Click **Select** next to **Vapor Phase's edr File**, and select `gmx_mdrun.edr` under `work14_GMX_NVT`.



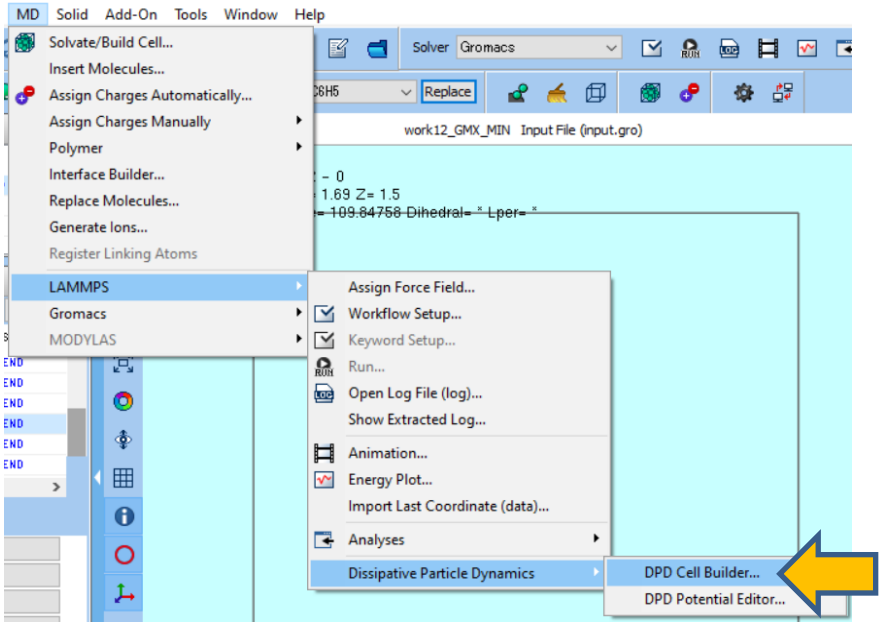
H. Analysis of Results

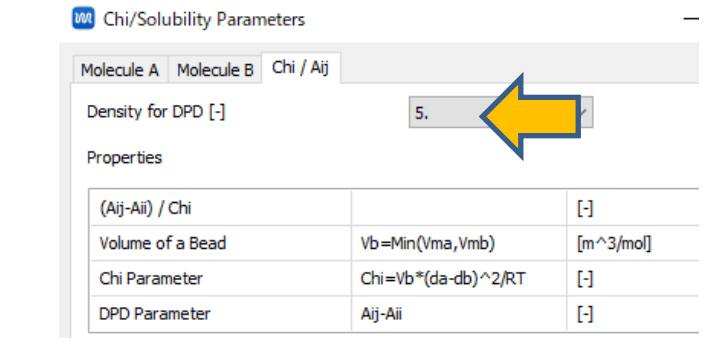
A. In **Chi/Aij tab**, **χ parameter** and **DPD parameter (A_{ij} - A_{ii})** are displayed.

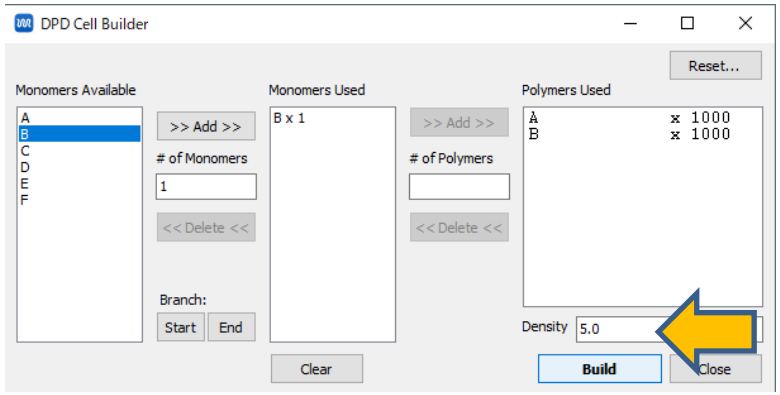


Supplementary: Setting up DPD Calculations

A. If you are not performing DPD calculations, skip this section.
B. For detailed settings for DPD calculations, refer to '**Winmostar™ LAMMPS Tutorial on Dissipative Particle Dynamics**'.
C. When creating a system in **MD | LAMMPS | Dissipative Particle Dynamics | DPD Cell Builder**,enter the value displayed in **Density for DPD** field in **Chi/Aij tab** of **Chi/Solubility Parameters** window into **Density** field.



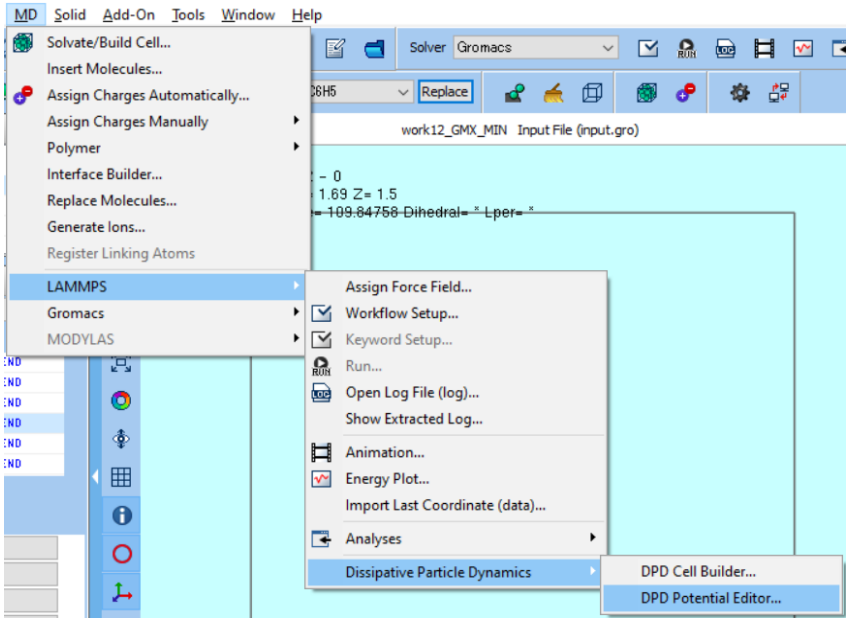


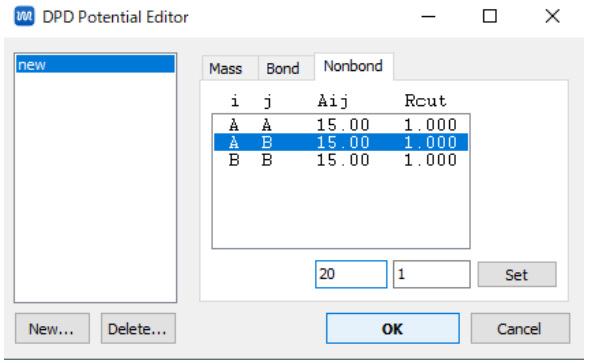


Supplementary: Setting up DPD Calculations

A. Next, in **MD | LAMMPS | Dissipative Particle Dynamics | DPD Potential Editer**, under **Nonbond tab**, for A-A and B-B interactions, specify the intraspecies DPD parameter A_{ij} obtained for MonomerA and MonomerB, respectively, in **MonomerA**, **MonomerB tabs**. However, unify the value for either component 1 or 2. For A-B interactions, input the sum of the adopted intraspecies DPD parameter and the obtained interspecies DPD parameter (A_{ij} - A_{ii}).

B. The calculation of the DPD parameters for water-benzene was referenced from the literature [A. Maiti and S. McGrother, J. Chem. Phys., 120 (3), 2004, 1594.].

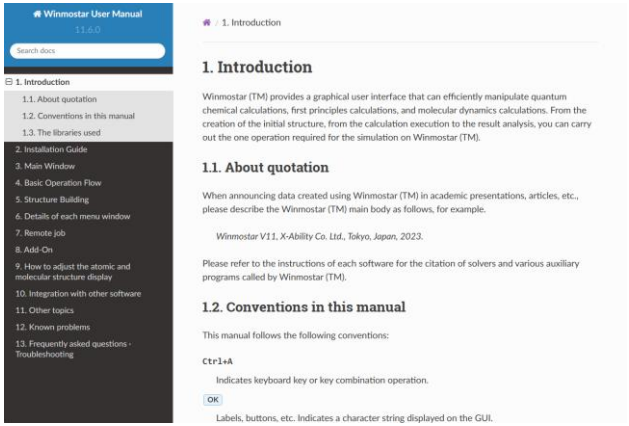




In this example, the value for the intraspecies parameter of H2O is adopted, and values are rounded to the nearest decimal point.

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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