winmostar tutorial

LAMMPS Basic

V11.5.6

19 April 2024 X-Ability Co., Ltd.

About This Document

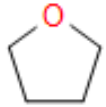
- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- If you are unable to proceed with the operations 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 from Contact. Attach files generated at the time of the issue and provide steps to reproduce the problem.
-

Overview

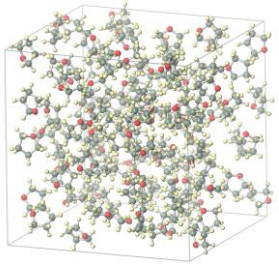
- We will obtain various thermodynamic properties, radial distribution functions, self-diffusion coefficients, specific heats, and compressibility of tetrahydrofuran (THF) liquid under room temperature and atmospheric pressure using molecular dynamics calculations with Lammps (employing GAFF and AM1-BCC charges). For equilibration, we will perform energy minimization, constant temperature MD, and constant temperature-pressure MD. Following this, the main calculation will again be executed under constant temperature and pressure conditions using MD.

Procedure Overview:

A. System Modeling
(A)Creation of a single molecule.
(B)Assignment of charges.
(C)Creation of the liquid phase.



THE Molecule



B. Execution of Calculations
(A)Assignment of the force field.
(B)Equilibration calculations.
(Energy minimization→
Constant temperature MD→
Constant temperature and pressure MD)
(C)Main calculation.
(constant temperature and pressure MD)

C. Result Analysis
Various thermodynamic properties.
Radial distribution functions.
Self-diffusion coefficients.
Specific heat and compressibility.

Note:

- The number of steps and molecules will vary depending on the type of system, the physical properties you want to calculate, and the desired level of accuracy.
- The choice of force field and type of charges significantly affects the results of the calculations.

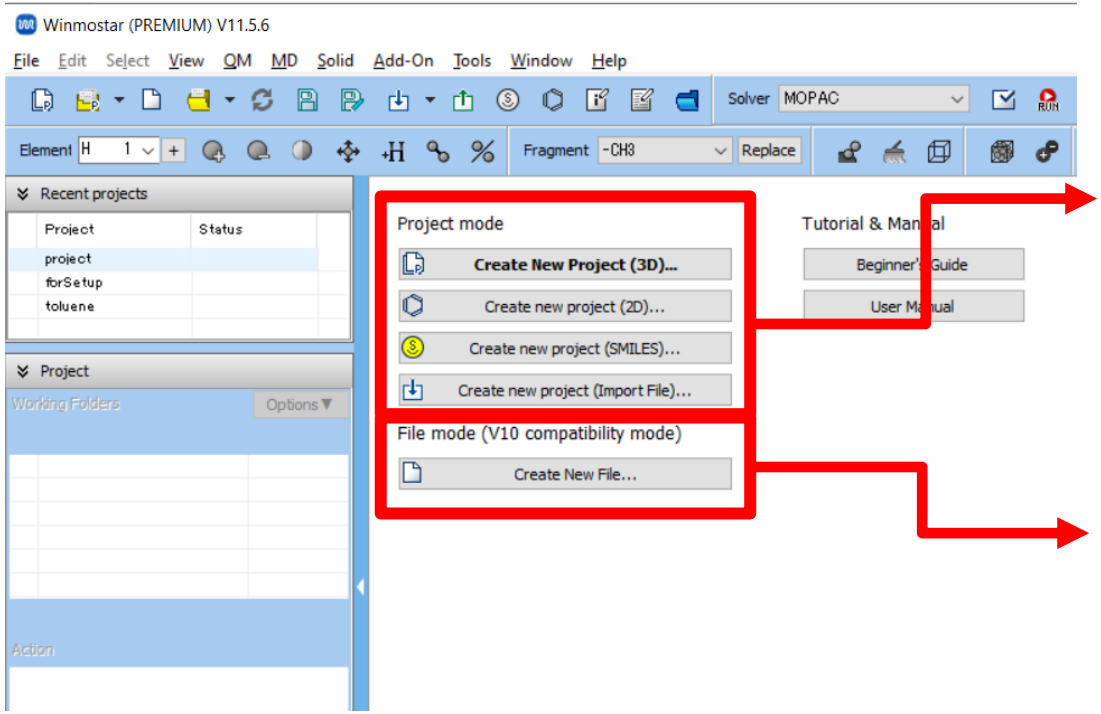
Operating environment settings

- Users operating on a 64-bit system and utilizing Winmostar version V11.5.0 or later are required to install and configure CygwinWM version dated 2023/04/05 or later.
  - CygwinWM release on or after 2023/04/05 includes recommended version of 64-bit LAMMPS bundled within.

- If your setup does not meet above criteria, or if you wish to use a different version of LAMMPS than recommended one, a separate installation and environment setup for Windows version of LAMMPS will be necessary.

Operating Modes of Winmostar V11

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



Project Mode New Features in V11

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

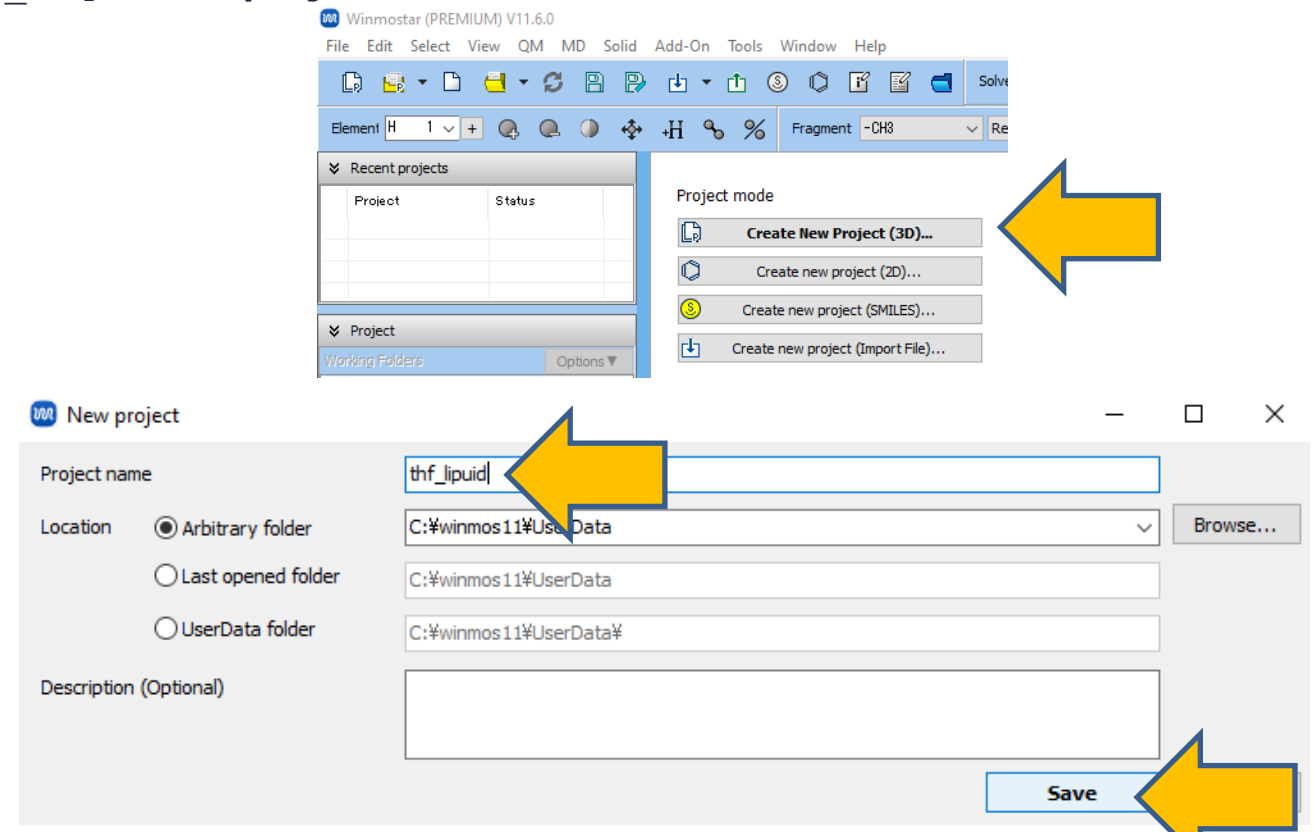
File Mode

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

I. System modeling (A) Creation of one molecule

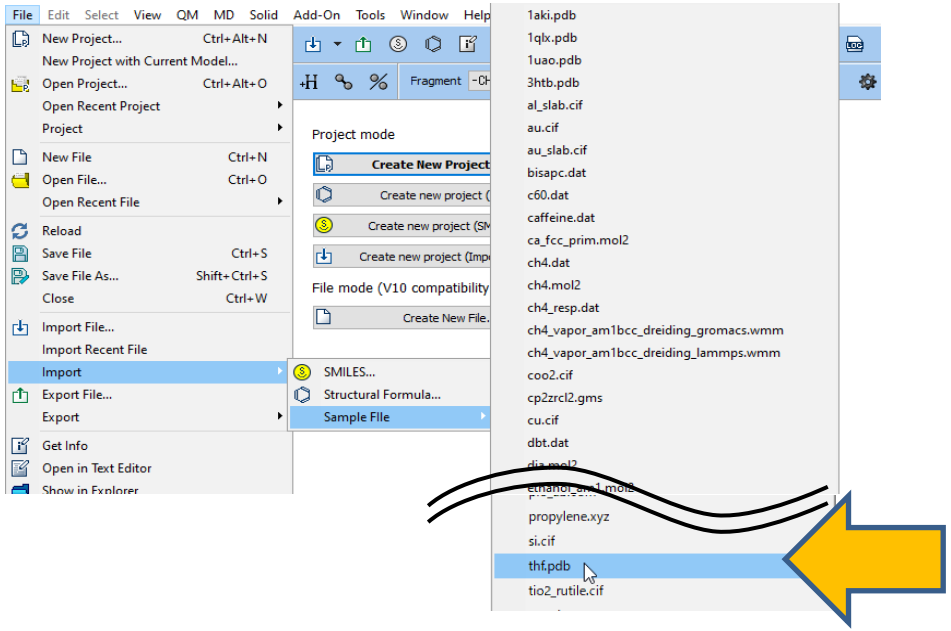
(A) Launch Winmostar and click on "**Create New Project (3D)**." (If already running, click "**File | Close**" first.)

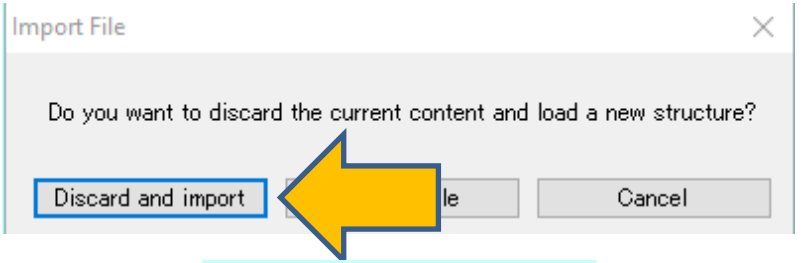
(B) Enter "`thf_liquid`" as **project name** and click "**Save**".

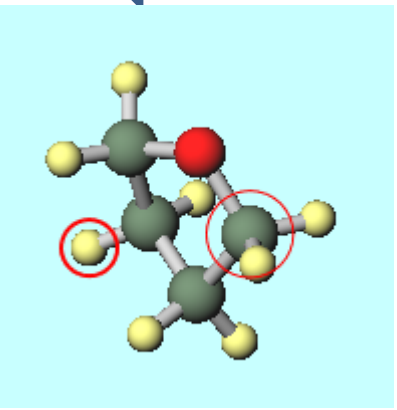


I. System modeling (A) Creation of one molecule

For details on how to create the initial structure, please refer to **Winmostar V11 Tutorial Modeling Molecule Organic Molecule**
Here, we will load an existing molecular structure file.
(A) **Click File | Import | Samples File | thf.pdb.**
-If you wish to load a specific file, use "**File" | "Import File**" at this step instead.
(B) **In "Import File" dialog,** select **"Discard and import".**
(C) Ensure the target molecule appears in "Viewport".





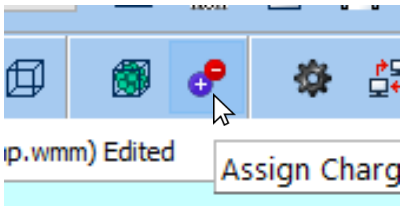


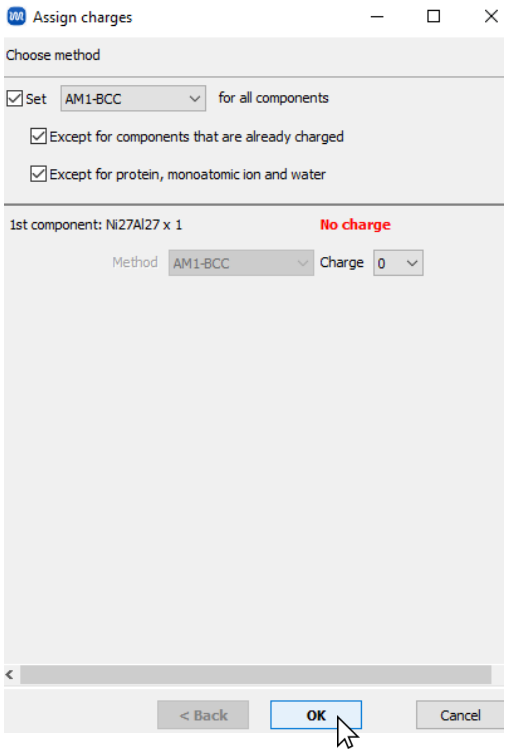
I. System modeling (B) Charge assignment

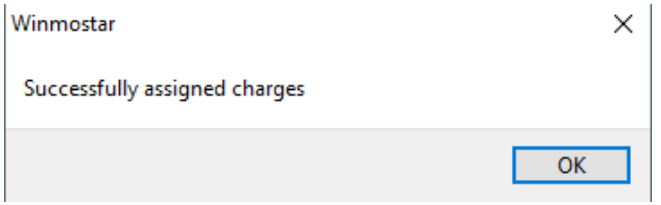
(A) **Click "Assign Charges".**

(B) Click **OK** in **Assign Charges** window.

(C) After several appearances of a black window, click "OK" when the message "successfully assigned charges" is displayed.





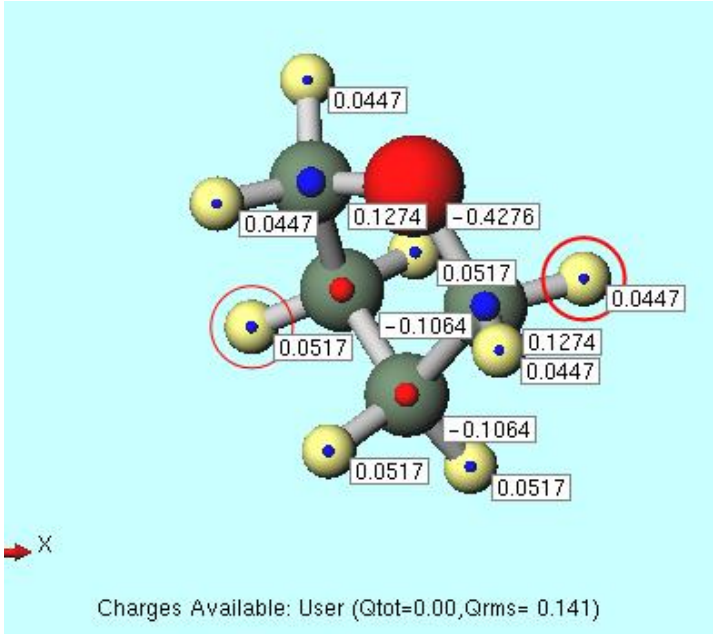


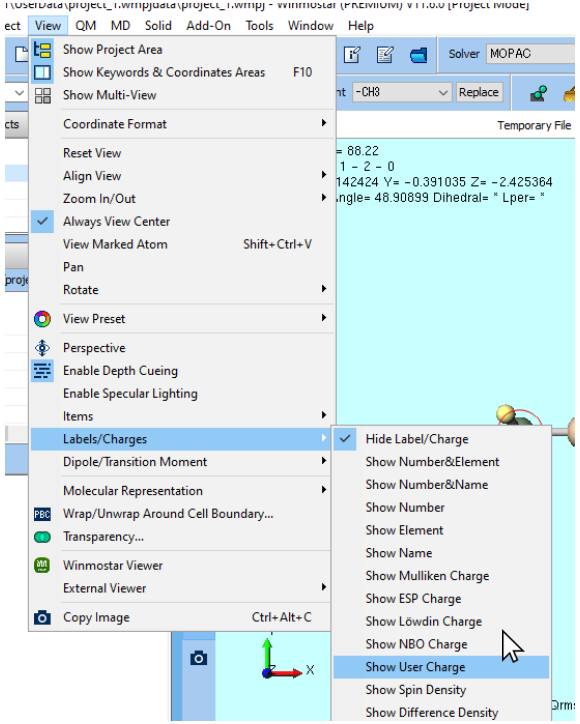
I. System modeling (B) Charge assignment

(A) Ensure "Charges Available: User (Qtot=0.00, Qrms=0.141)" appears below Viewport, confirming a total charge of zero and that non-zero User charges are assigned to individual atoms.

(B) To graphically display charges, select "**View | Labels/Charges | ShowUser Charges**".

(C) To undo action (B),click "**View | Labels/Charges | Hide Labels/Charges**".

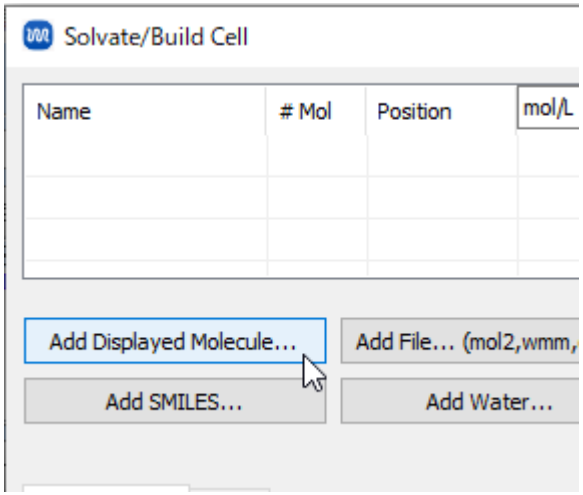


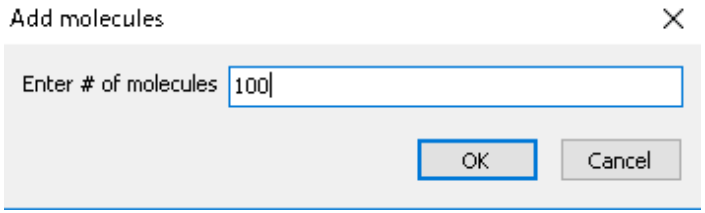


I. System modeling (C) Creation of liquid phase

(A) Click **Solvent/Build Cell** button.

(B) Click "**Add Displayed Molecule...**" button, and in dialog that appears, enter "**100**" and click "**OK**" button.

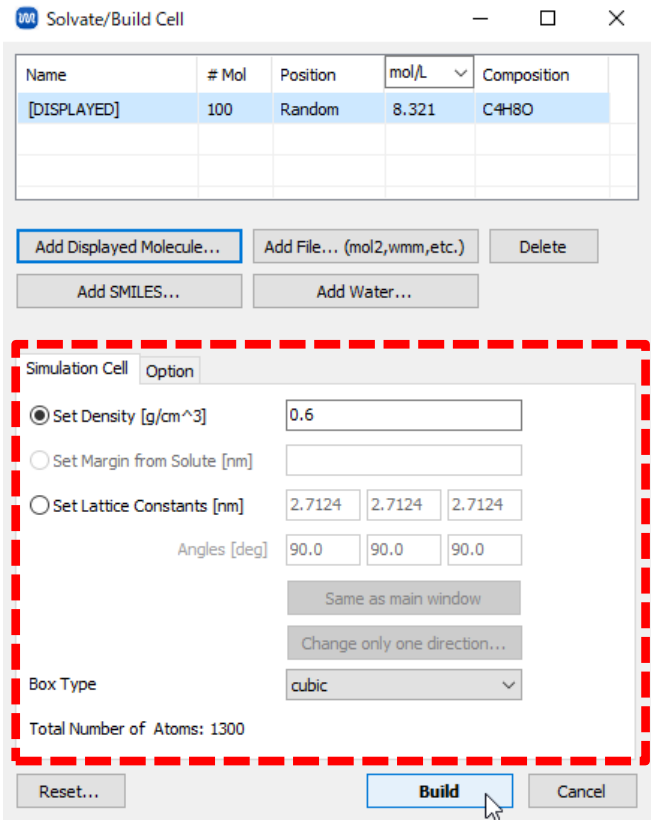


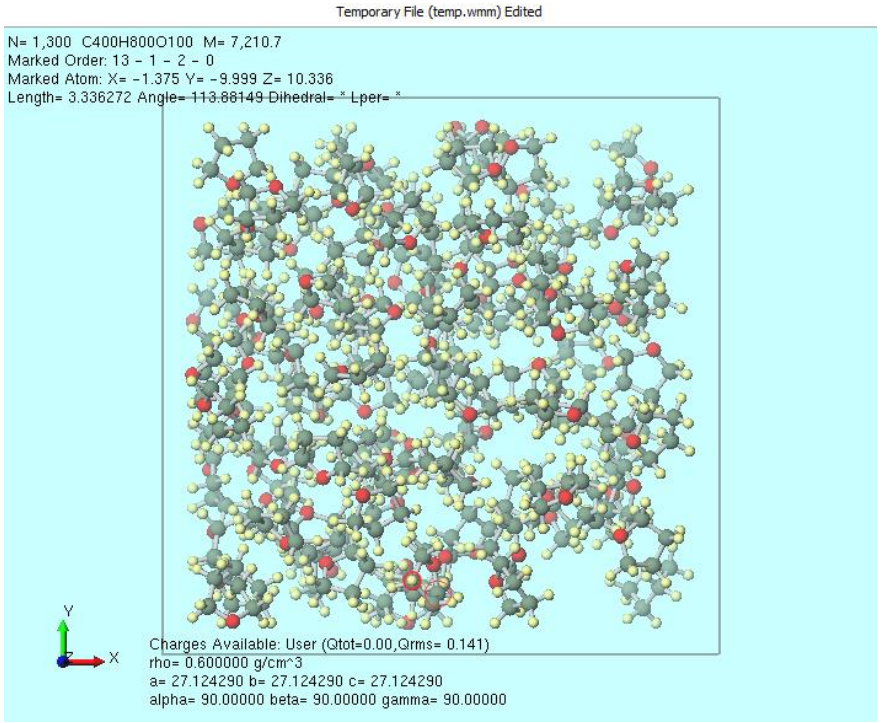


I. System modeling (C) Creation of liquid phase

(A) Confirm settings in '**Simulation Cell**' (document proceeds without making specific changes).

(B)"Click "**Build"** and a black terminal window appears for a few seconds; upon successful processing, a message ″**The system has been successfully built**' will display. A system with 100 THF molecules aligned at 0.6 g/cm³ will appear. System size and density are indicated at the bottom of 'Viewport'"



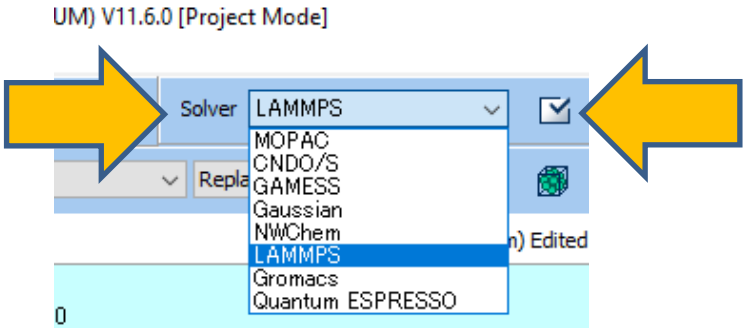


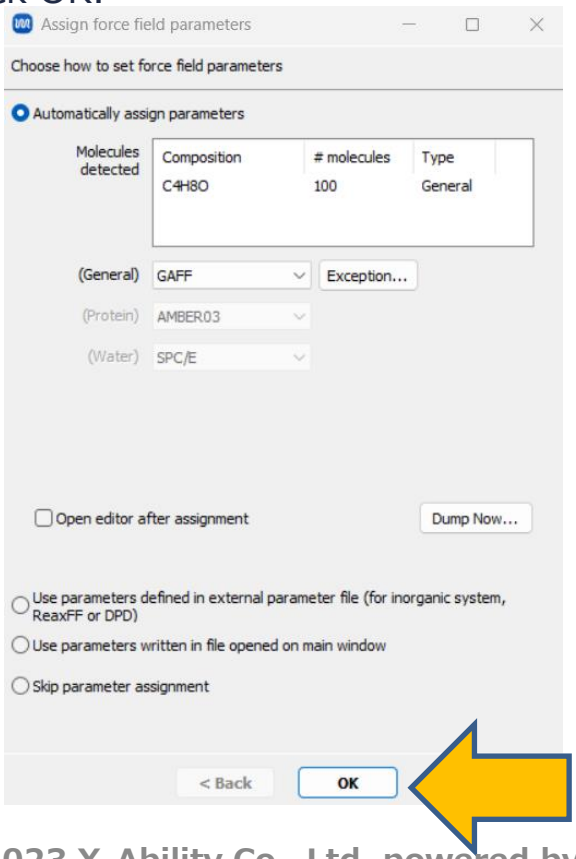
II. Execution of calculation (A) Force field assignment

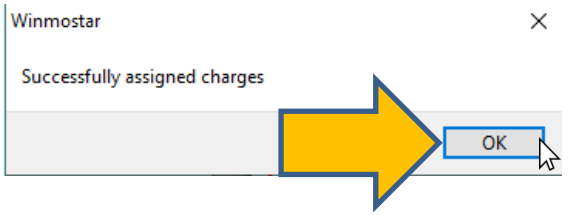
(A) Select "**LAMMPS**" from "**Solver**" on toolbar.

(B) Click on(**Workflow Setup**).

(C) When Assign force field parameters window opens, click OK at the bottom right. A black terminal window will appear for a few seconds. Once the processing is successful and the message 'Assigned force field parameters' is displayed, click OK.



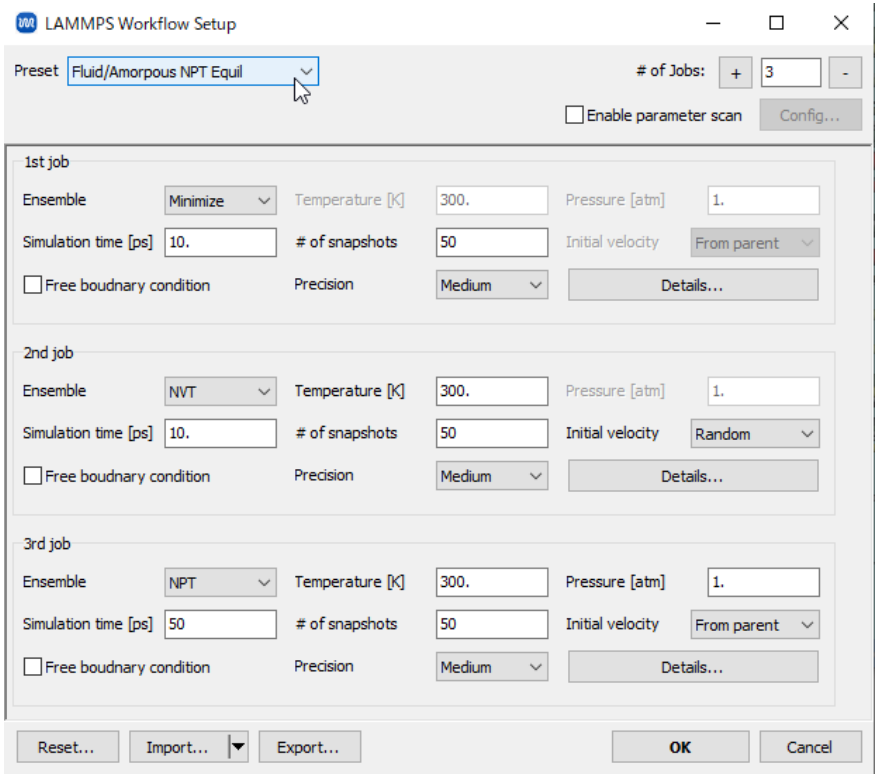




II. Execution of calculation (B) Equilibration calculation

(A) In "**LAMMPS Workflow Setup**" window, check the flow of the calculation. No changes are made to the settings here. With this configuration, a total of three jobs - energy minimization (**Minimize**), constant temperature MD (**NVT**), and constant temperature-pressure MD (**NPT**) - will be executed consecutively.

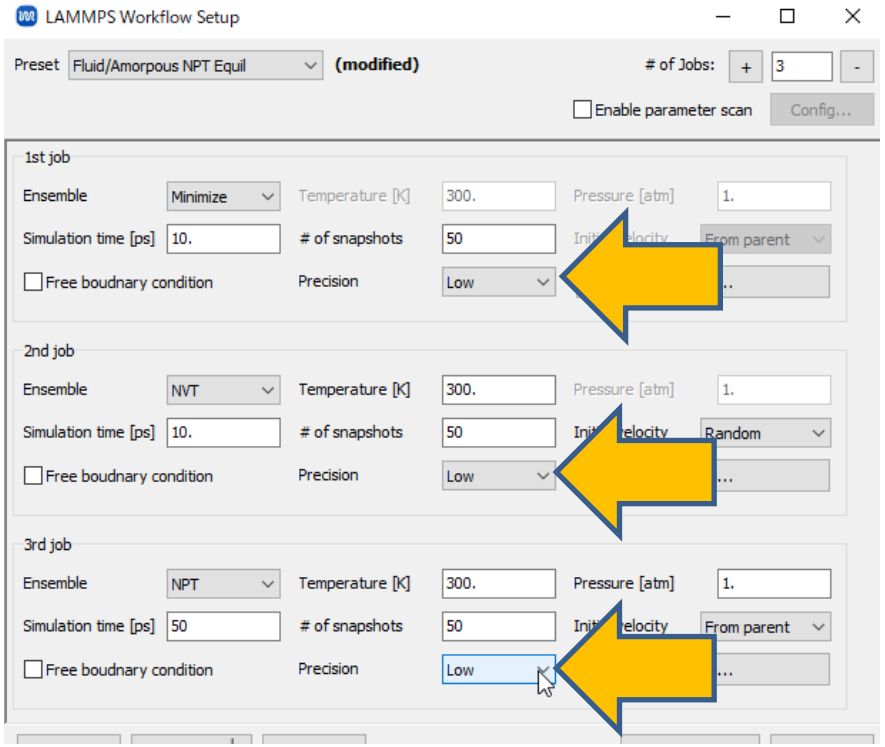
(B) If you want to change "**simulation time**", "**temperature**", or "**pressure**" for each calculation, modify the relevant parts. (Not necessary for this guide.)



II. Execution of calculation (B) Equilibration calculation

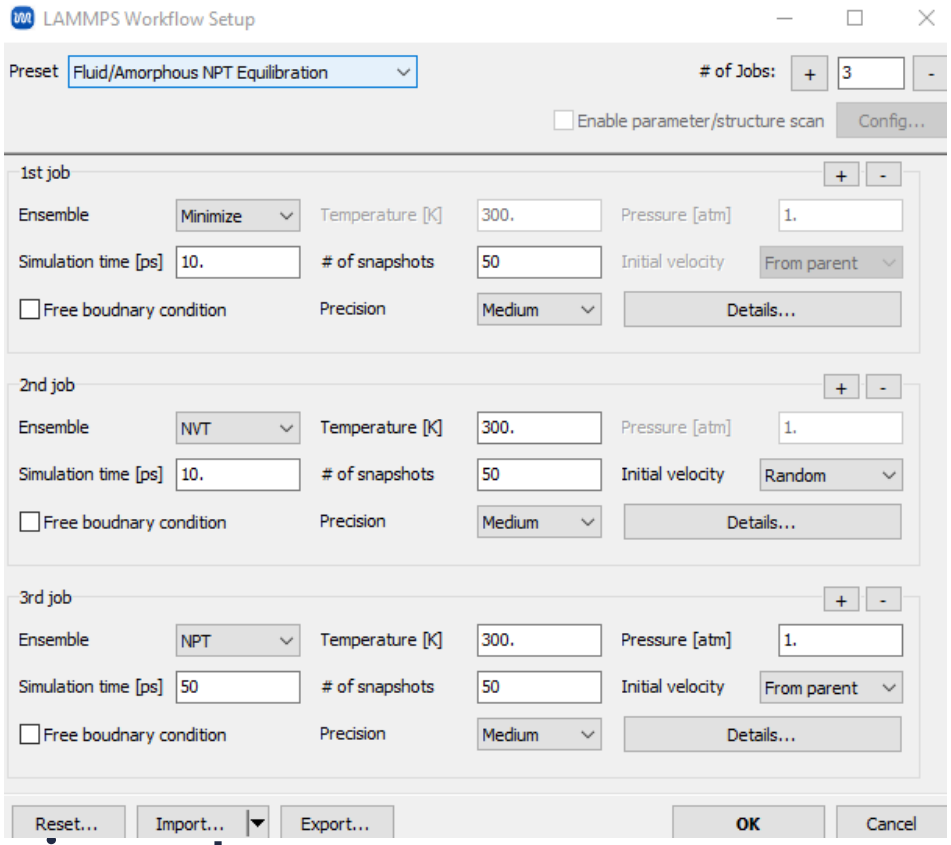
(A) To reduce calculation accuracy to speed up the computation, set **Precision** to 'Low' for **1st job**, **2nd job**, and **3rd job**. If not, proceed to the next page.

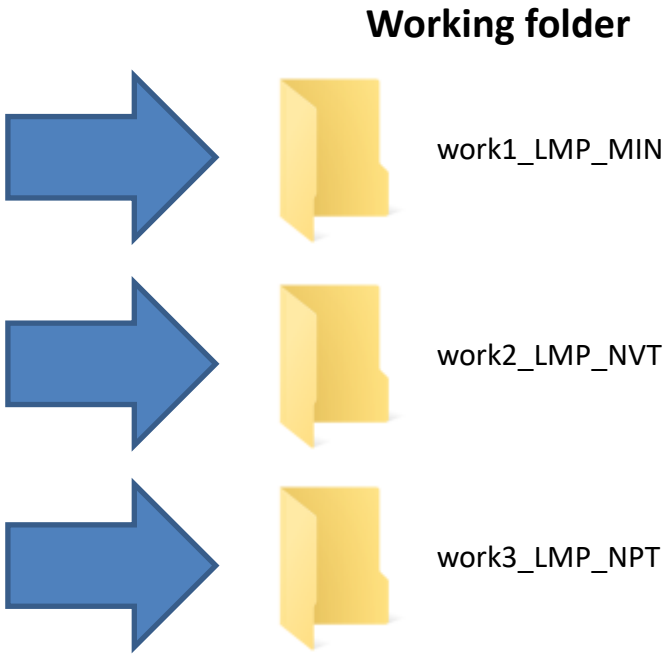
Note: Without reducing the calculation precision, it might take several hours to half a day, depending on the machine specifications. However, lowering the precision can shorten this to just a few minutes. Be aware that reducing precision may decrease the stability of the calculations.



Supplementary calculation flow

Following the execution of Minimize calculation (A), NVT calculation (B) proceeds. Atomic coordinates and velocity information transfer automatically between sequentially executed calculations, ensuring final structure from (A) aligns with initial structure for (B). After NVT calculation (B), NPT calculation (C) initiates. Calculations occur within distinct working folders.



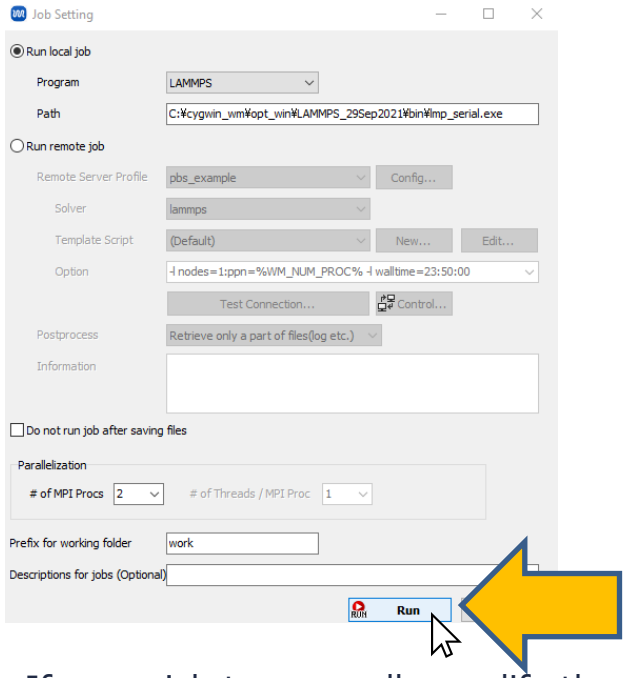


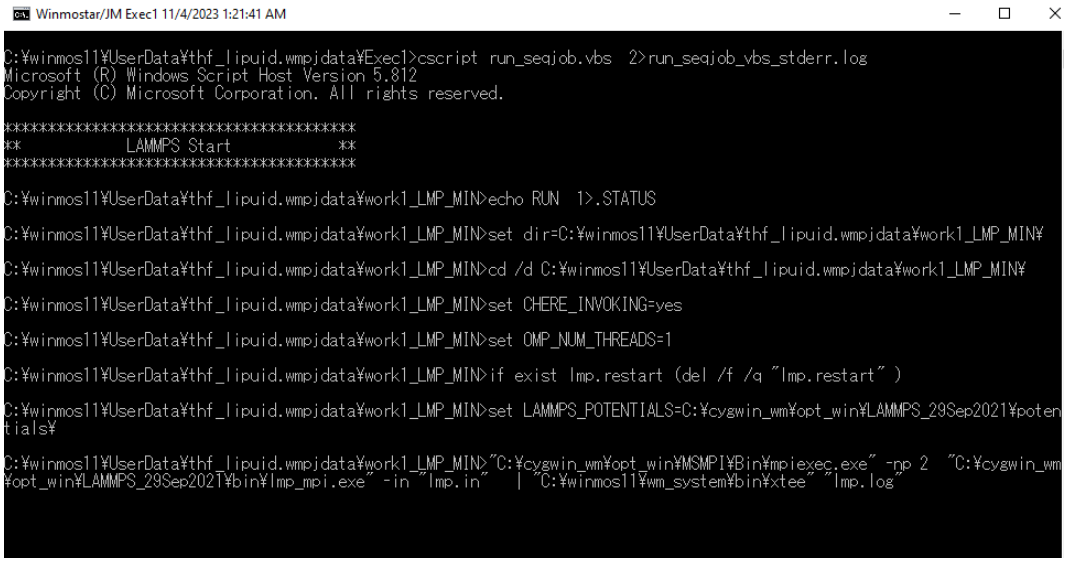
II. Execution of calculation (B) Equilibration calculation

(Proceed to designated section first for remote job submission.)

(A) Click "**OK**" in "**LAMMPS Workflow Setup**" window at the bottom right.

(B) Click "**Run**" in "**Job Settings**" window. "**Winmostar Job Manager**" initiates in the background, and a black console window, as shown in the figure to the right, appears, marking the start of the calculation.



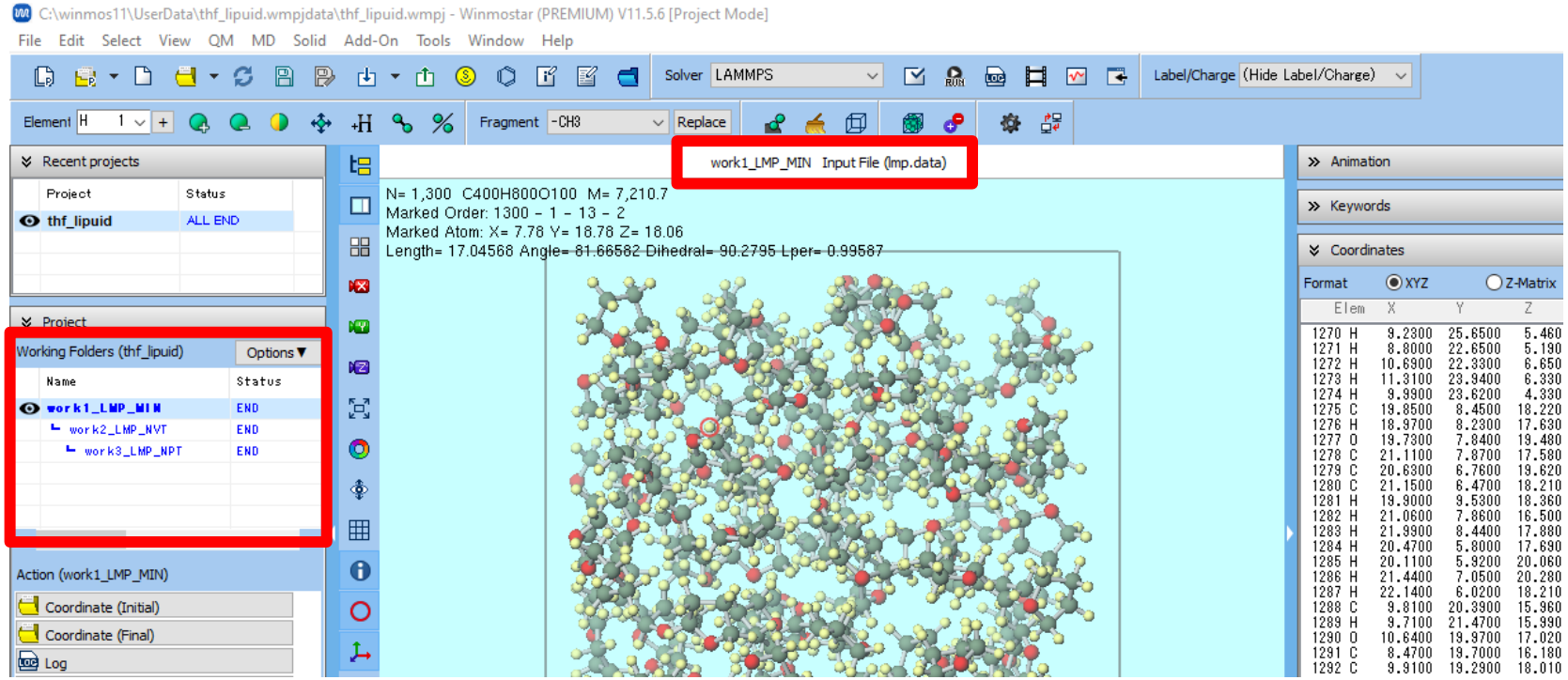


Note: If you wish to manually modify the input file or copy it to a remote server for use, check "**Do not run jobafter saving files**" in "**Job Settings**" window before clicking "**Run**". If you decide to execute the calculation after saving, click **"File" | "Project" | "Selected Working Folder" | "Run"**.

II. Execution of calculation (B) Equilibration calculation

(A) Upon return to main window(calculations may still be running), even while calculations proceed, **project area** presents a tree-like representation of the three working folders corresponding to each job from **LAMMPS Workflow Setup** window.

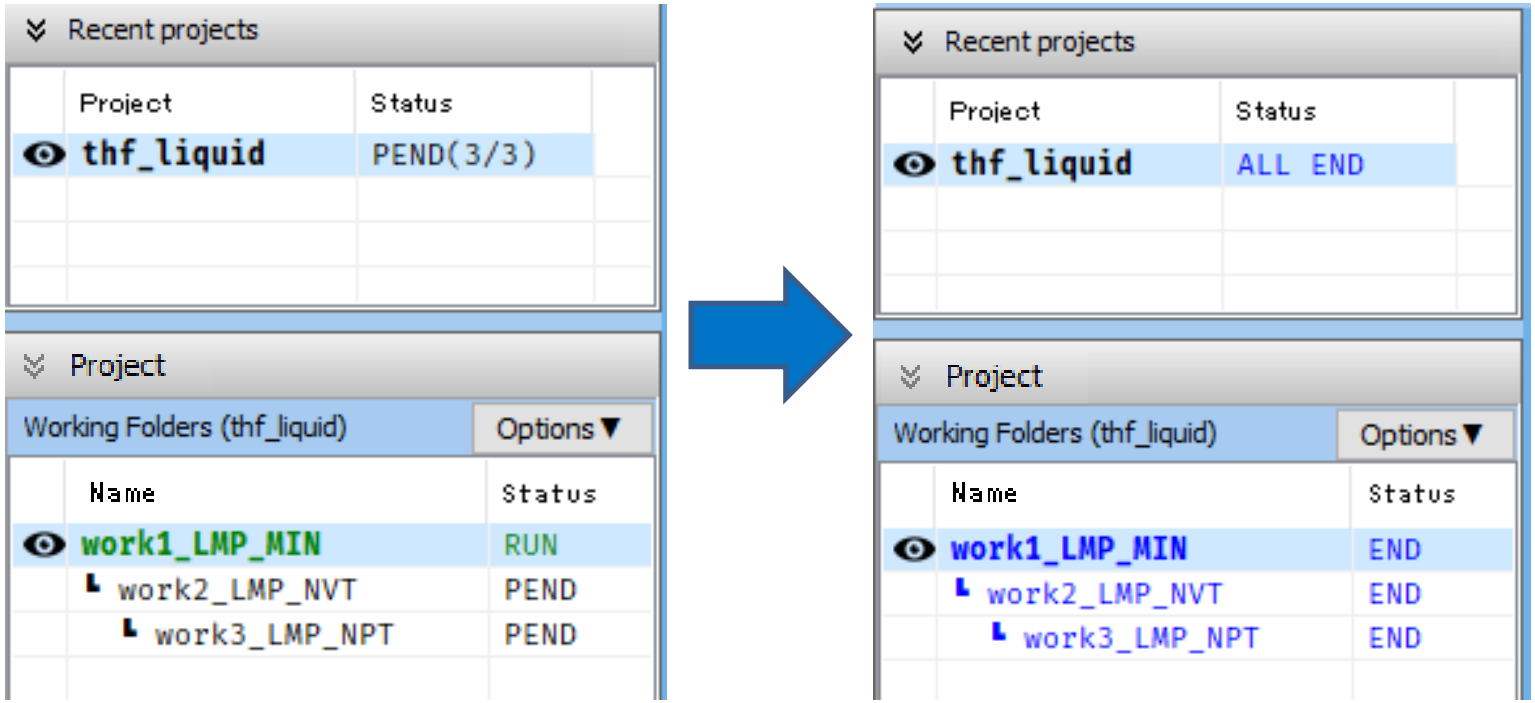
(B) In "**Viewport**", input file from the first working folder (work1_LMP_MIN) opens automatically. Confirmation of this can be found at the top of "**Viewport**".



II. Execution of calculation (B) Equilibration calculation

(A)Monitor changes in **status** for each working folder in **Project Area** they will switch from **PEND (black)** to **RUN (green)**, then to **END (blue)**.

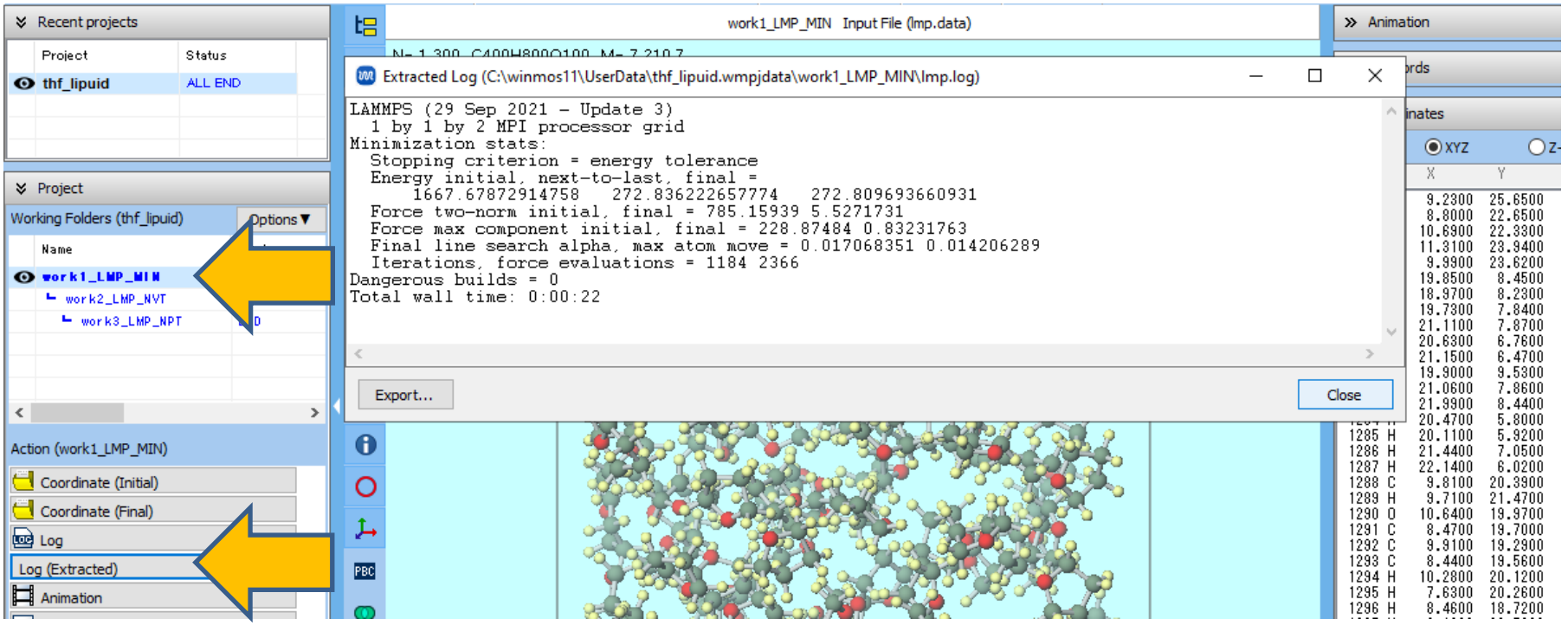
(B) Continue until every working folder shows an **END (blue)** status. Concurrently, **status** for **recently utilized project** "thf_liquid" will also change to ALL **END (blue)**.



II. Execution of calculation (B) Equilibration calculation

(A) If you wish to view the primary contents of each computation log, select the appropriate **working folder** for the calculation within **Project Area** by clicking on it, then click on "**Action"|" Log (Extracted)**". (This function is exclusively available in the Professional Premium version.)

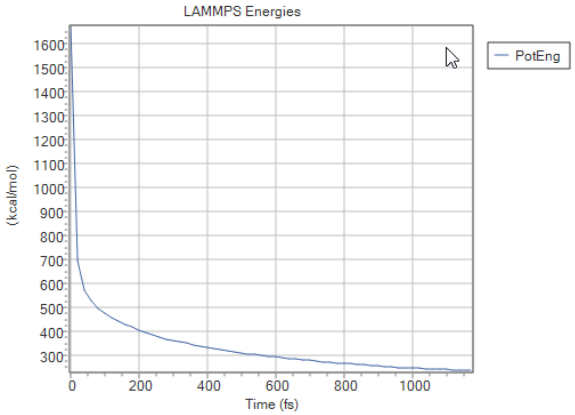
(B) To view complete log, click on **Log**.



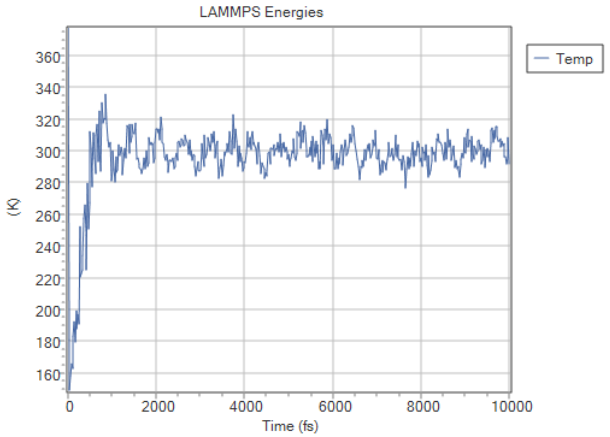
Supplement: Confirmation of Convergence of Thermodynamic Quantities in Equilibration Calculations

To ensure that the temperature, potential energy, pressure, and density have stabilized during the equilibration calculation, it's necessary to confirm convergence as directed on page 24. If convergence has not been achieved,
you should perform additional calculations with adjusted conditions as needed, following the procedures on pages 21-22, until convergence is attained.

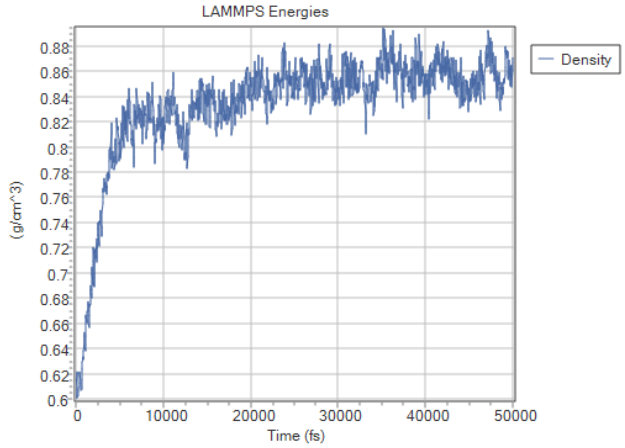
Example:



work1_LMP_MIN
(Minimize)
PotEng (potential energy)



work2_LMP_NVT
(constant temperature MD)
Temp



work3_LMP_NPT
(Constant temperature/pressure MD)
Density

*Please note that density convergence may be slow.

II. Execution of calculation (C) Main calculation

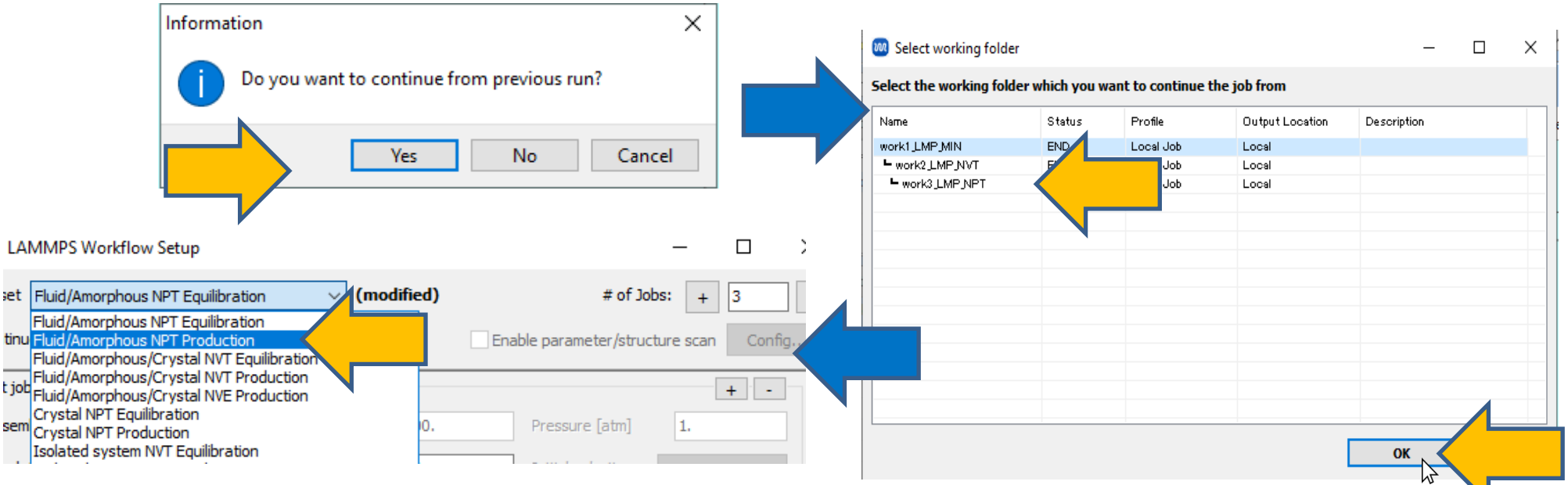
(A) After the status of continuation source working folder (in this case work3_LMP_NPT) changes to END (blue), click (**Workflow Settings**).

(B) In **information** dialog, click "**Yes**".

(C) **"Select working folder"** by choosing the source working folder (work3_LMP_NPT) and then click **"OK".**

(D) Select "Fluid/Amorphous NPT Production" from **presets**.

(E)To expedite the calculation process by reducing computational precision, change "**Precision**" setting to "Low".



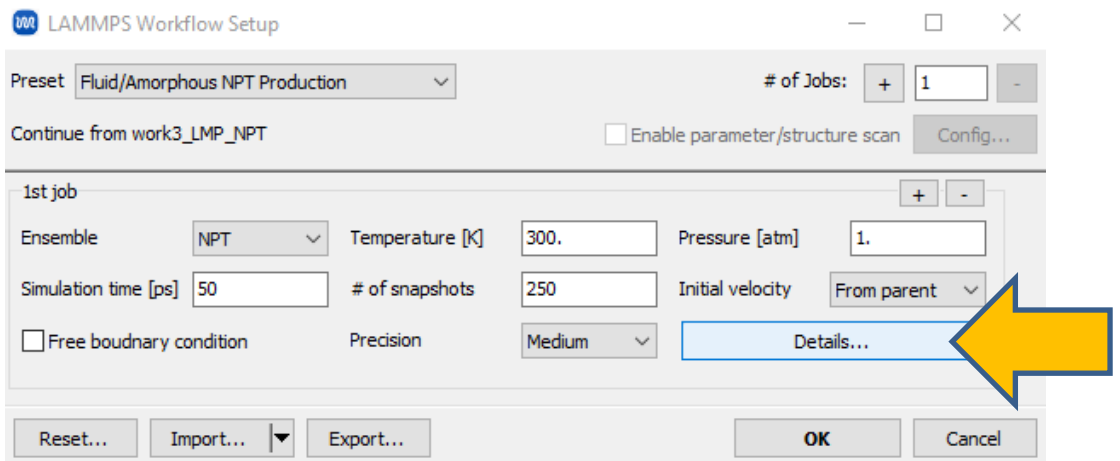
II. Execution of Calculation: (C)Main Calculation

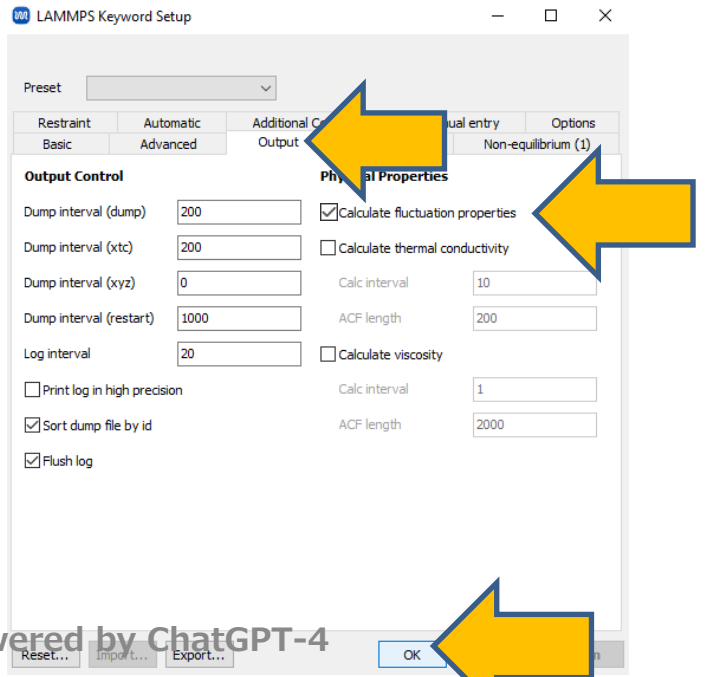
(A)Click on "**Details**" for "**1st job**", then in "**LAMMPS Keyword Setup**" under **Output** tab, check "**Calculate fluctuation properties**" option before clicking "**OK**" (This feature is not available in the Professional Economy or Student editions).

– Following the steps on pages 26 and 27, the isobaric heat capacity and isothermal compressibility will be output as '**Cpm**' and '**betat**', respectively.

Note: The method used here for calculating the heat capacity does not include quantum effects, which leads to the calculated values being higher than the experimental values (refer to J. Chem. Theory Comput., 2012, 8, 61-74, among others). Also, please be aware that these values typically require a larger number of steps to converge properly.

(B) Click '**OK**', and in **job settings** window, click '**OK**'.



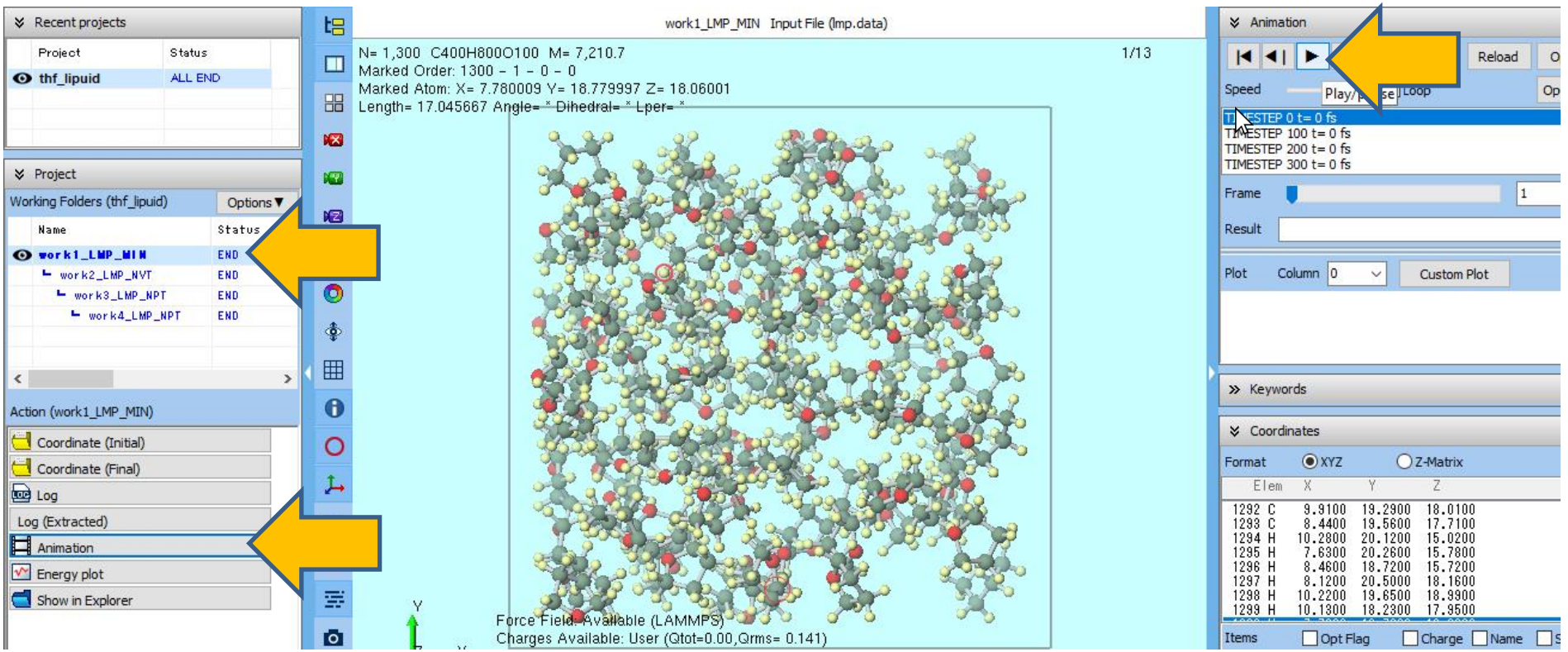


III.Result Analysis: Animation

Beyond this point, you may skip any analysis items that do not require verification.

(A) In "**project area**", click on the target **working folder** (here, we will use "work1_LMP_MIN").

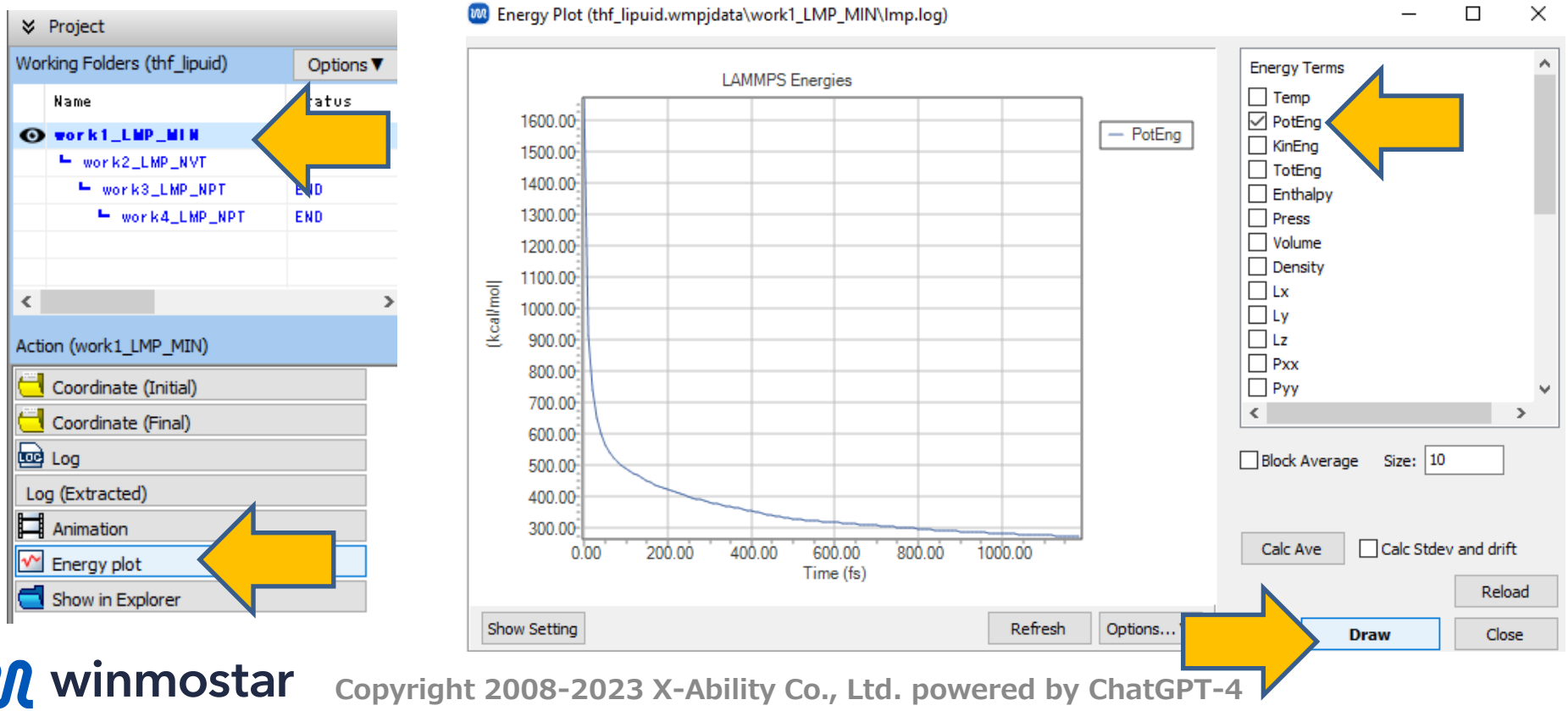
(B) Click on "**Animation**" in "**action**" to bring up "**animation Panel**" on the right side of main window. Pressing ▶ play button will display the calculation process as an animation.



III.Result Analysis: Time Evolution of Energy and Related Parameters - Average Value

(A) In **project area**, click on target **working folder** (in this example, "work1_LMP_MIN").

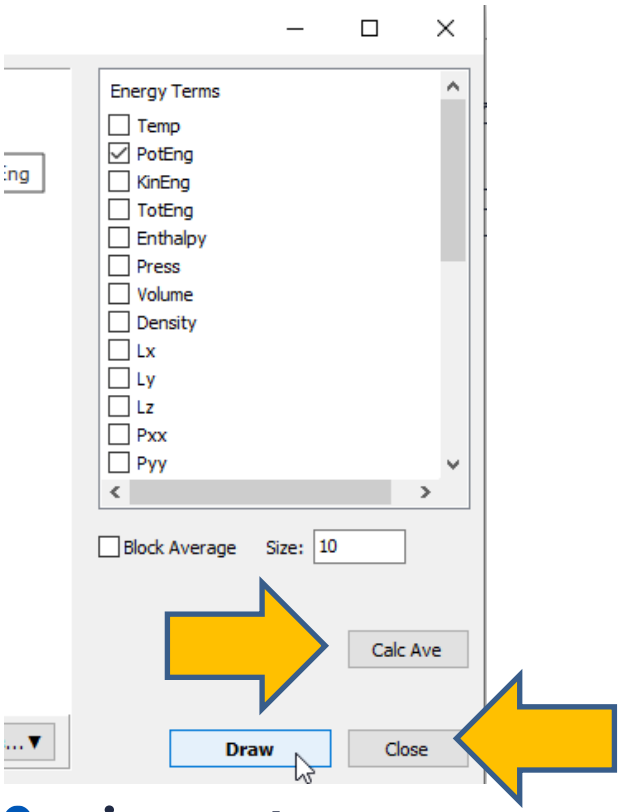
(B) In "**action**", click on "**Energy plot**" to bring up "**Energy Plot** window".In "**Energy Terms**" section, check the boxes for the physical quantities you want to visualize (in this case, select "PotEng" for potential energy), and then click on "**Draw**" to see the graph of how it changes over time.



III.Result Analysis: Time Evolution of Energy and Related Parameters - Average Value

(A) To check the average values, click "**Calc Ave**". A text file will open displaying the average values and standard errors of various physical quantities. Please note that the average values are physically meaningless unless they are from a calculation that has reached a certain level of equilibration (in this manual, corresponding to "work4_LMP_NPT").

(B) After verificatio, click '**Close**' to close '**Energy Plot**' window.



energy_ave.log - Notepad

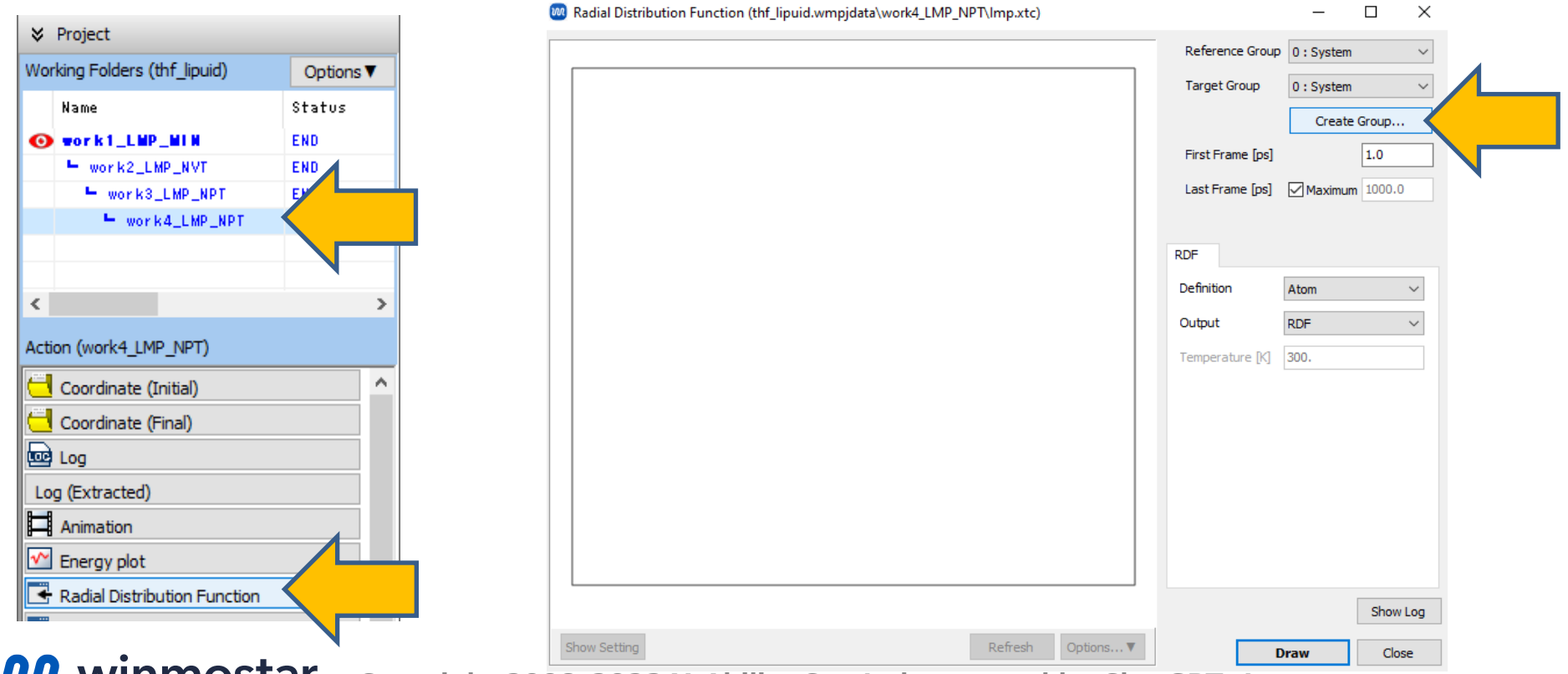
File Edit Format View Help

# data	Average	Standard error
Temp (K)	0.000000000000000	0.000000000000000
PotEng (kcal/mol)	348.391234500000190	25.170539185458522
KinEng (kcal/mol)	0.000000000000000	0.000000000000000
TotEng (kcal/mol)	348.391234500000190	25.170539185458522
Enthalpy (kcal/mol)	200.348655016666660	75.040080094477274
Press (atm)	-508.685721616666620	177.661581027747230
Volume (A^3)	19955.435000000032000	3.75728835565913E-012
Density (g/cm^3)	0.599994420000001	1.00330423315483E-016
Lx (A)	27.124000000000019	2.75192018236753E-015
Ly (A)	27.124000000000019	2.75192018236753E-015
Lz (A)	27.124000000000019	2.75192018236753E-015
Pxx (atm)	-442.197806500000060	193.586135260033090
Pyy (atm)	-575.517229166666430	177.392421571822880
Pzz (atm)	-508.342117750000060	163.033870593444320
Pxy (atm)	18.319507023333341	25.137684096462102
Pxz (atm)	36.623633150833344	25.843877134202525
Pyz (atm)	8.364973538333332	7.240932608347771
GamNsurf (mN/m)	0.141650473333337	7.561892847632891
E_pair (kcal/mol)	-767.631870333333250	18.741399290349107
E_vdwl (kcal/mol)	-683.738154999999870	15.727903153816989
E_coul (kcal/mol)	1250.749386666666400	2.543026348188388
E_long (kcal/mol)	-1334.643090000000000	0.864374295300429
E_tail (kcal/mol)	0.000000000000000	0.000000000000000
E_mol (kcal/mol)	1116.023103333333300	6.839636803403122
E_bond (kcal/mol)	6.380519678333332	2.113790221979792
E_angle (kcal/mol)	334.106627500000060	5.739981166836300
E_dihed (kcal/mol)	775.535956500000000	1.240163455143242
E_impro (kcal/mol)	0.000000000000000	0.000000000000000

III.Result Analysis: Radial Distribution Function

(A) In **project area**, click on target **working folder** (here, let's assume it's "work4_LMP_NPT").

(B) Click on **Radial Distribution Function** in "**action**" menu, and "**Radial Distribution Function**" window will appear. Here, to obtain the radial distribution function between specific atoms rather than between all atoms, click on "**Create Group**".



III.Result Analysis: Radial Distribution Function

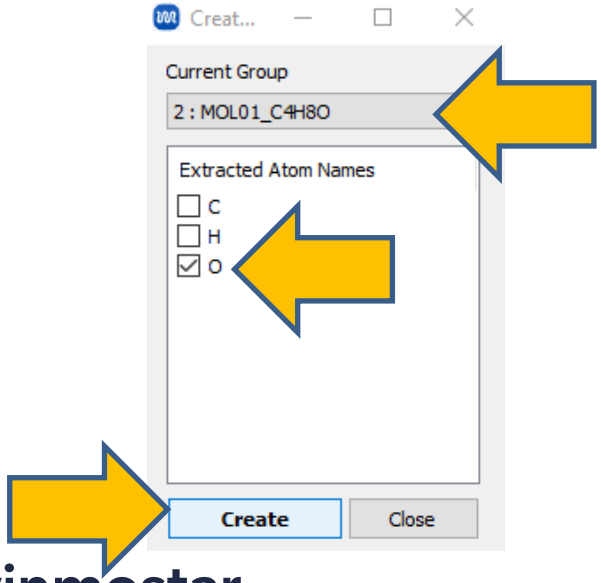
(A) In "**Create Group**" window, under "**Current Group**", select "**2: MOL01_C4H8O**"(which refers to THF in this instance). For "**Extracted Atom Names**", choose "**O**".

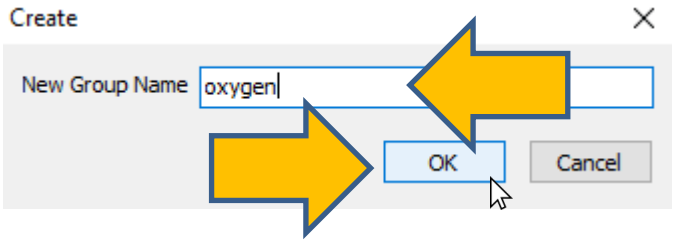
(B) Enter "**oxygen**" in "**New Group Name**" field and then click "**Create**".

- By checking "**View | Labels/Charges | Show Name**" in main window beforehand, you can view the Atom Name for each atom in Viewport.

- Furthermore, by clicking "**MD | LAMMPS | Analysis | Radial Distribution Function**" and selecting a previously created .ndx file, you can make more detailed adjustments to the analysis target group. You can create an .ndx file from **selection menu** in main window. (For more details, refer to the user manual.).

(C) Once terminal window appears and the process is complete, click "**Close**".

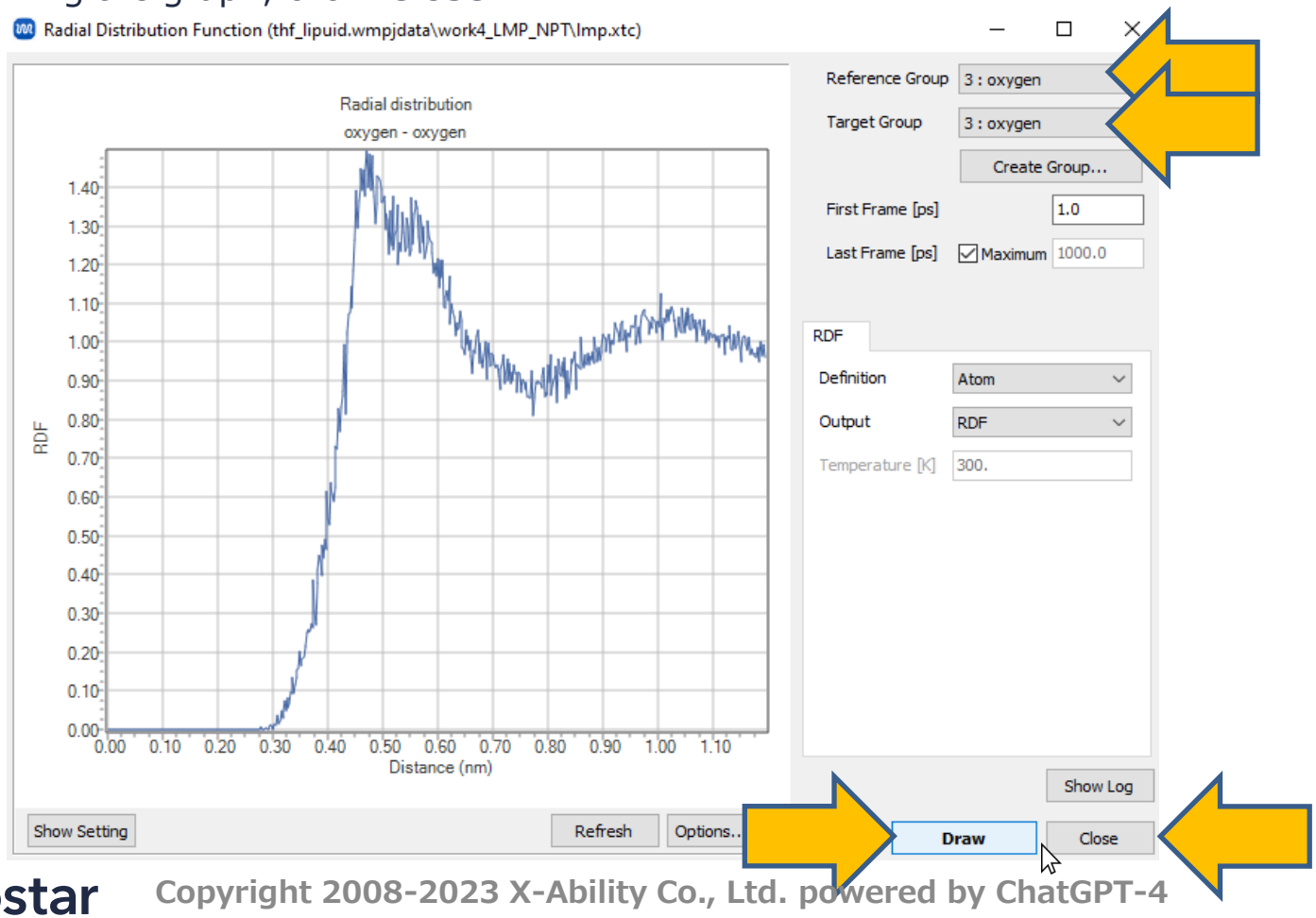




III.Result Analysis: Radial Distribution Function

(A) Select “**oxygen”** group you just created for both “**Reference Group”** and “**Target Group**”. When you press '**Draw**' button, the radial distribution function between oxygen-oxygen will be displayed.

(B) After reviewing the graph, click "**Close"**



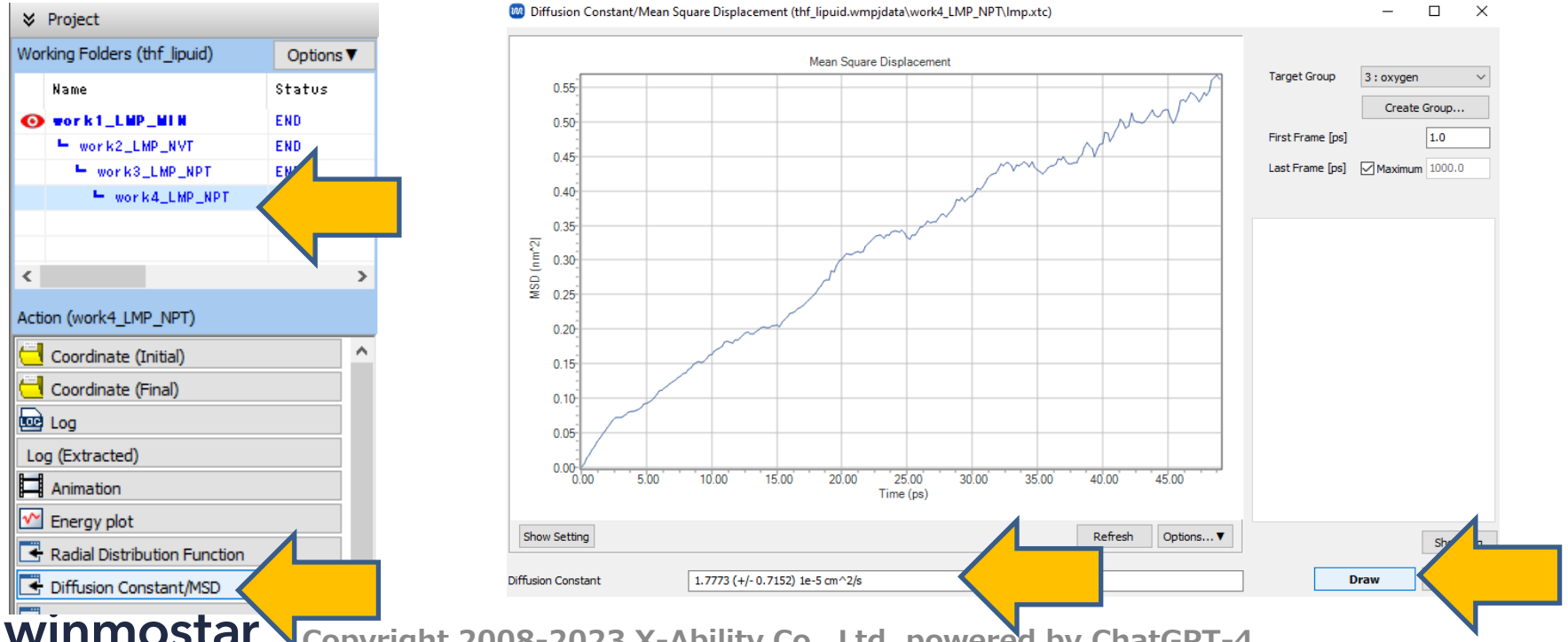
III.Result Analysis: Self-Diffusion Coefficient

(A) In "**project area**", select target "**working folder**" (in this example, "work4_LMP_NPT") by clicking on it.

(B) Within "**Action**", click on "**Diffusion Constant/MSD**".

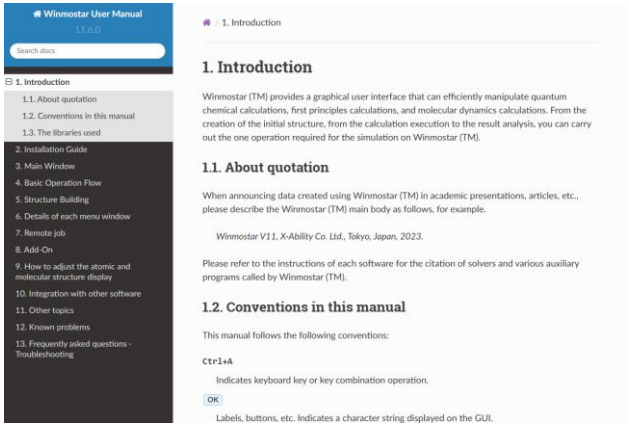
"**Diffusion Constant/Mean Square Displacement**" window will appear. When you click "**Draw**", a graph of the mean square displacement and the self-diffusion coefficient (**Diffusion Constant**) will be displayed.

Note: Ideally, the self-diffusion coefficient should be determined from NVT calculations. However, for simplicity in this guide, it is derived from NPT calculations. (Refer to J. Chem. Phys. 153, 021101 (2020), among others).



Troubleshooting and Additional Resources

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



Winmostar User Manual

- If you are unable to proceed as instructed in this guide, please first refer Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact, detailing the steps to reproduce the issue and attaching any generated files at that time.