winmostar tutorial

LAMMPS Elongation Calculation (Polymer)

V11.5.6

10 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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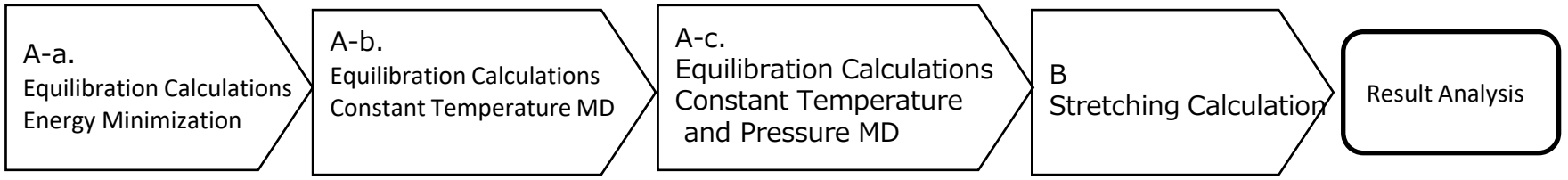
Overview

- To calculate the stretching process of a polyethylene melt and obtain the strain-stress data, follow the procedure outlined below:



Note:

- The number of steps required for equilibration may vary depending on the type of molecule and its initial density.
- The method of interaction calculation, force field, and method of charge calculation can affect the results.
- The degree of polymerization (chain length), number of molecules, stretching speed, and pressure control (Poisson's ratio) can also influence the results.
- Due to the tutorial nature of this document, a sufficient number of steps for polymer system equilibration will not be conducted here.

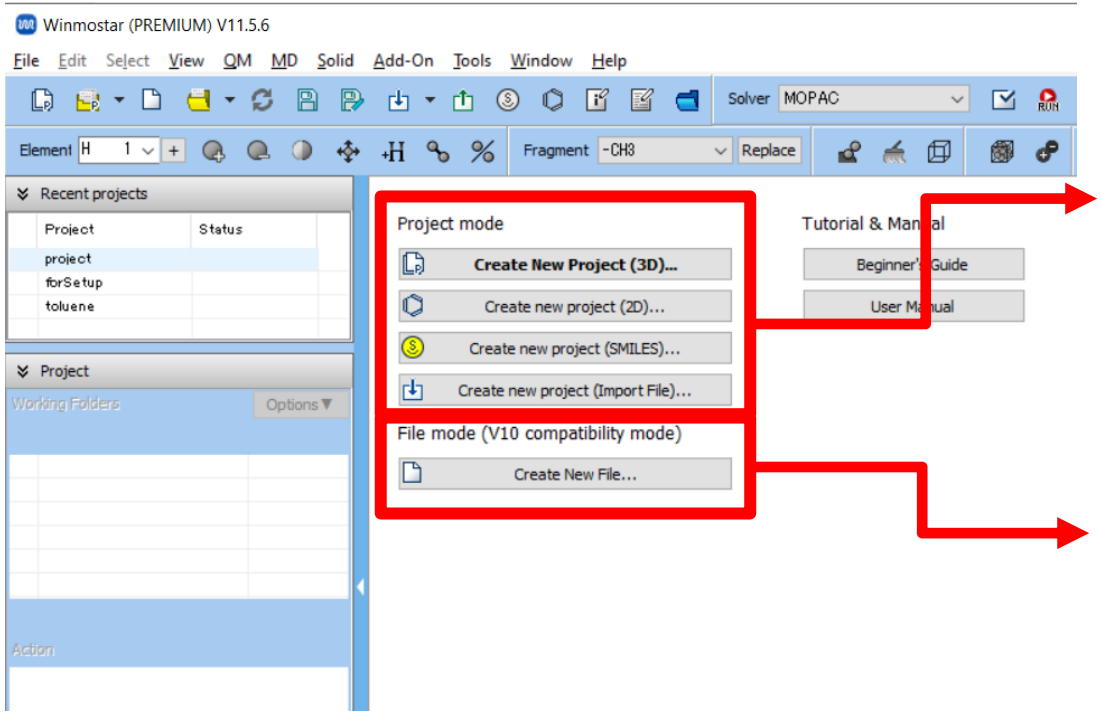
Preference of Operating Environment

- 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 the recommended version, you will need to separately install and configure the Windows version of LAMMPS.

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.

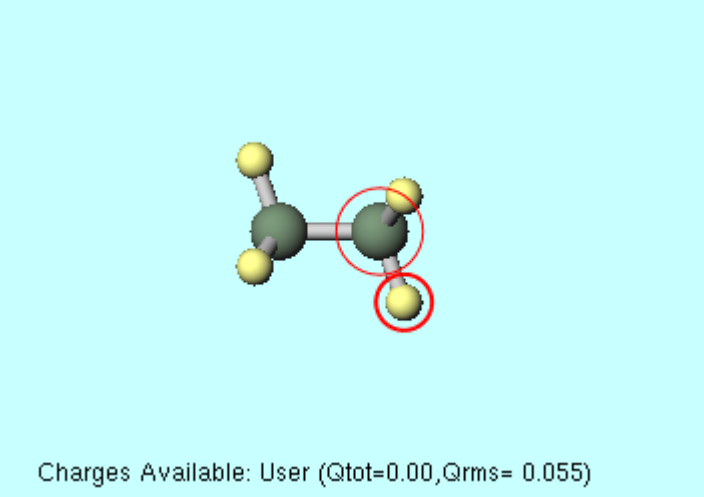
File Mode

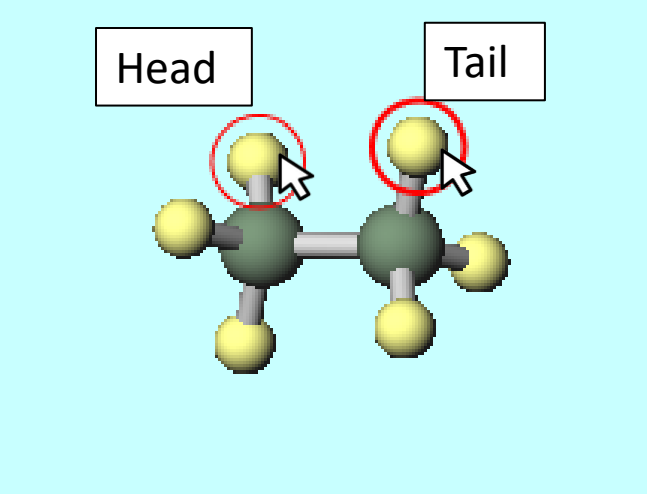
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

For basic operations, please refer to LAMMPS Basics tutorial.

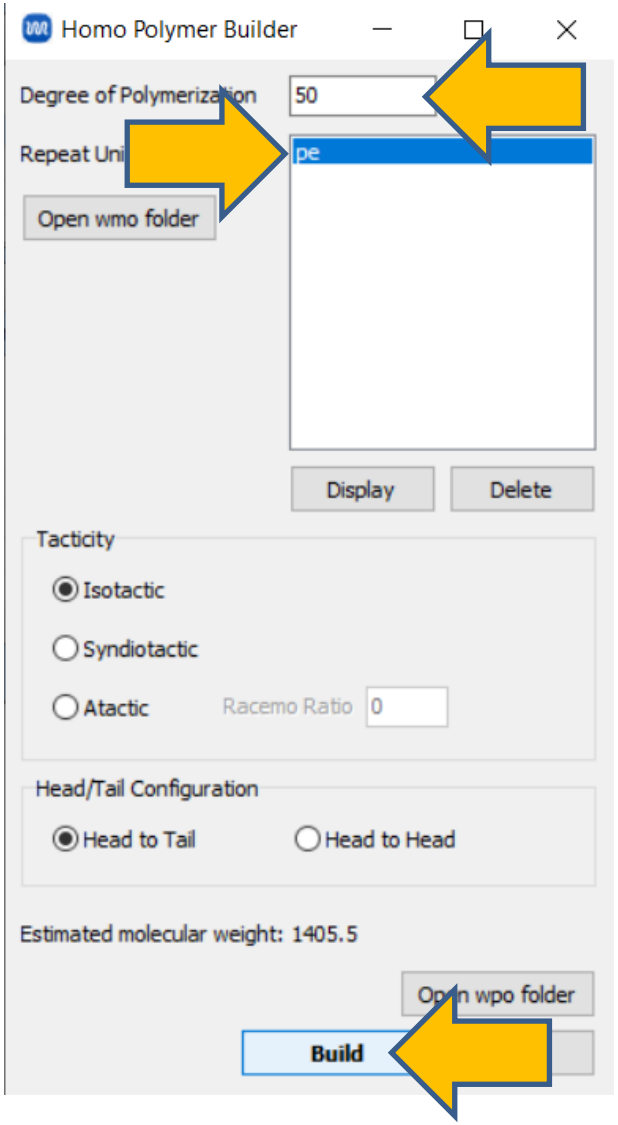
A. Click **File | New Project**, enter 'pe_elong' in **Project name**, and click **Save**.
B. Create the repeating unit of polyethylene (ethane, C2H6).
C. Click **Assign Charges Automatically** and then click **OK**.
D. Once the message 'Successfully assigned charges' appears, click **OK**.
E. Continuously click on two locations (Head and Tail) where the repeating unit will bond with the next one during polymerization.





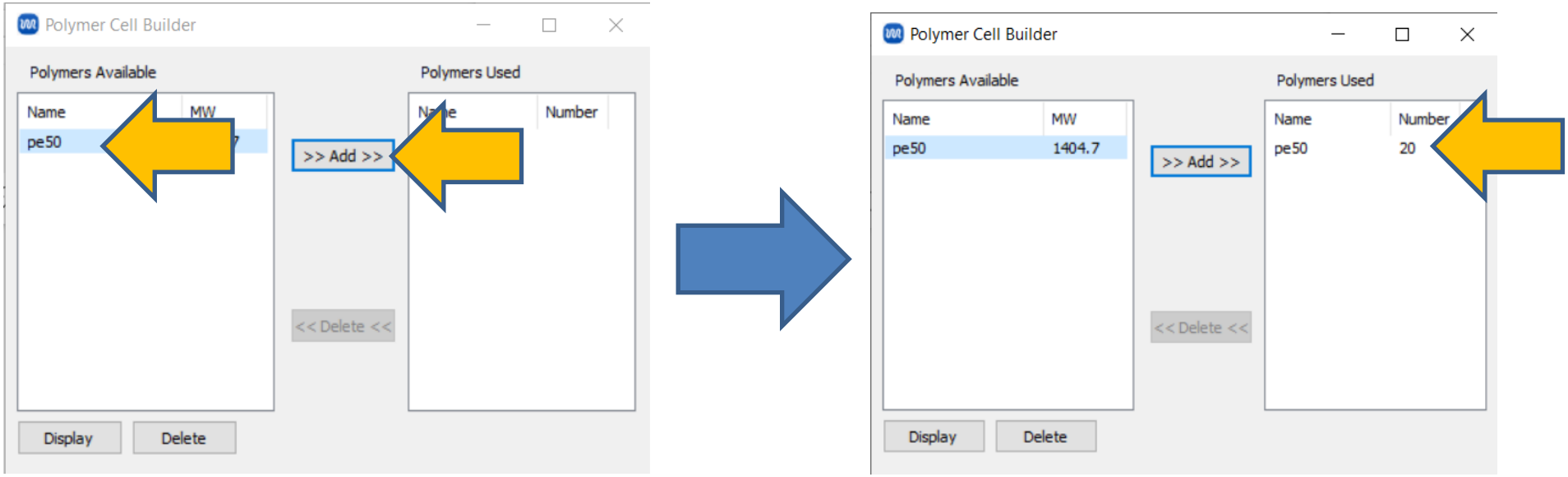
A. Modeling of the System

A. Click **MD | Polymer | Register Repeat Unit** and click **OK**.
B. Enter 'pe' for **Repeat Unit name** and click **OK**.
C. Once '…pe.wmo saved successfully.' appears, click **OK**.
D. Click **MD | Polymer | Homo Polymer Builder** and set as follows:
   – Change **Degree of Polymerization** to '50'.
   – Select 'pe' as **Repeat Unit**.
E. Click **Build**, enter 'pe50' in **Enter polymer name**, and click **OK**.
F. Once '…pe50.wpo saved successfully.' appears, click **OK**.
G. Click **Close** to exit **Homo Polymer Builder** window.



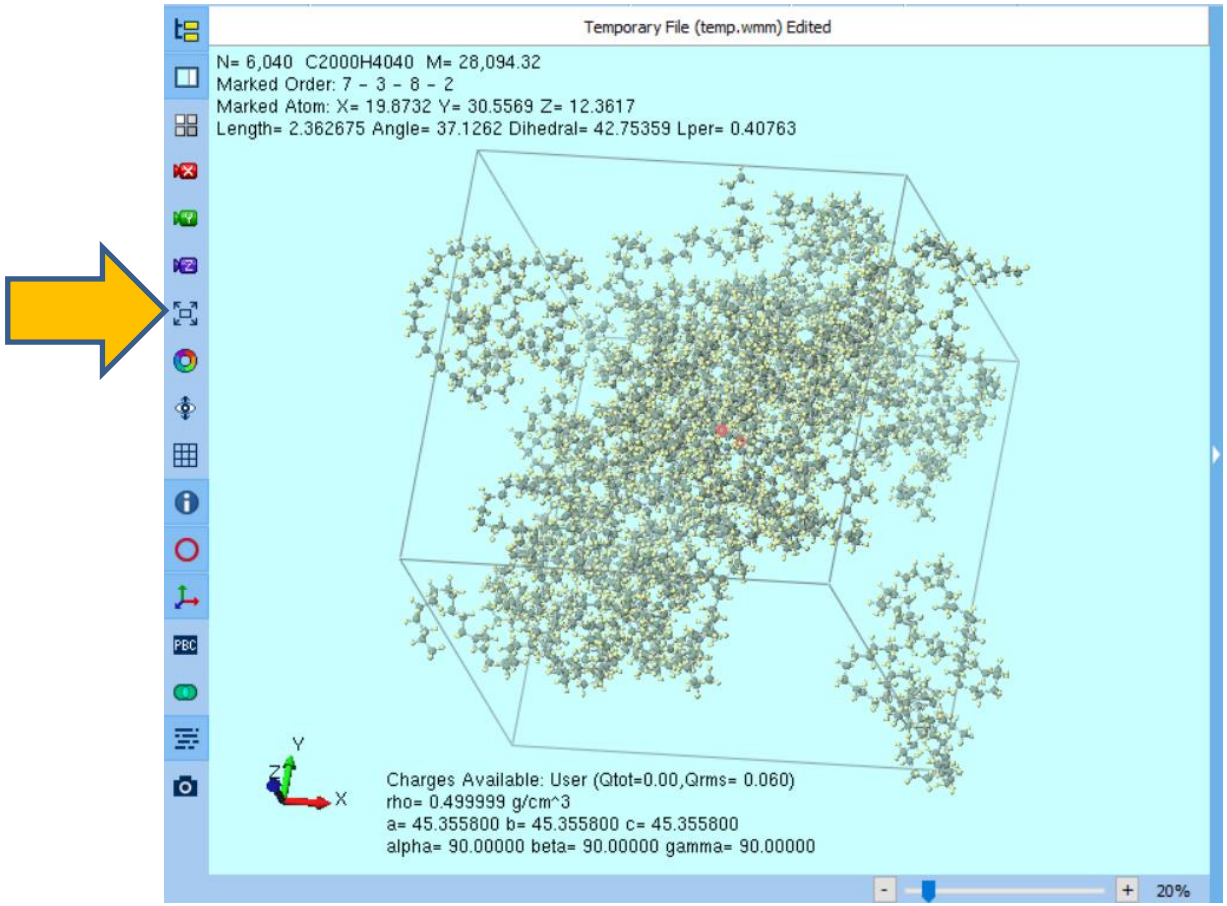
A. Modeling of the System

A. Click **MD | Polymer | Polymer Cell Builder**.
B. Select **pe50** from **Polymers Available** and click **Add**.
C. Enter '20' in **Enter Value** and click **OK**.
D. Confirm that 'pe50 20' is displayed under **Polymers Used** and click **Build**.
E. A black window appears, and after a few seconds of processing to build the polymer, 'Successfully generated polymer system.' will be displayed, then click **OK**.
F. Click **Close** to exit **Polymer Cell Builder** window.



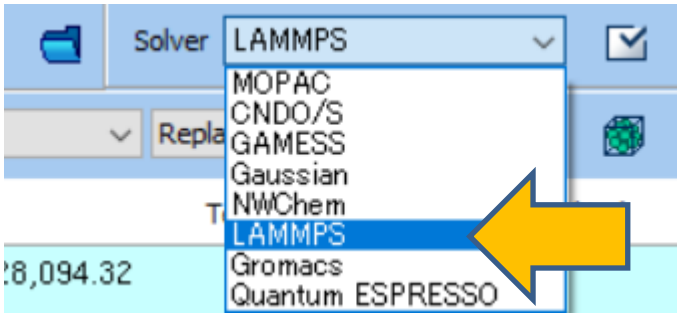
A. Modeling of the System

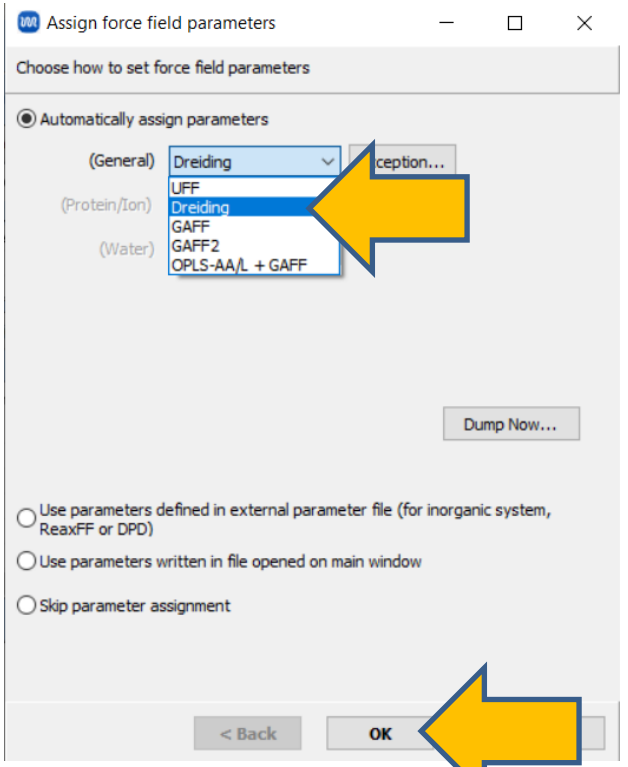
A. Click  **Fit to Window** to view the entire system.



B. Execution of Calculation

A. Select 'LAMMPS' from **Solver**, and click **(Workflow Setup)**.
B. Change **Automatically assign parameters (General)** to **Dreiding** and click **OK** at the bottom right.
C. After processing for a few seconds, click **OK** when 'Assigned force field parameters' is displayed.



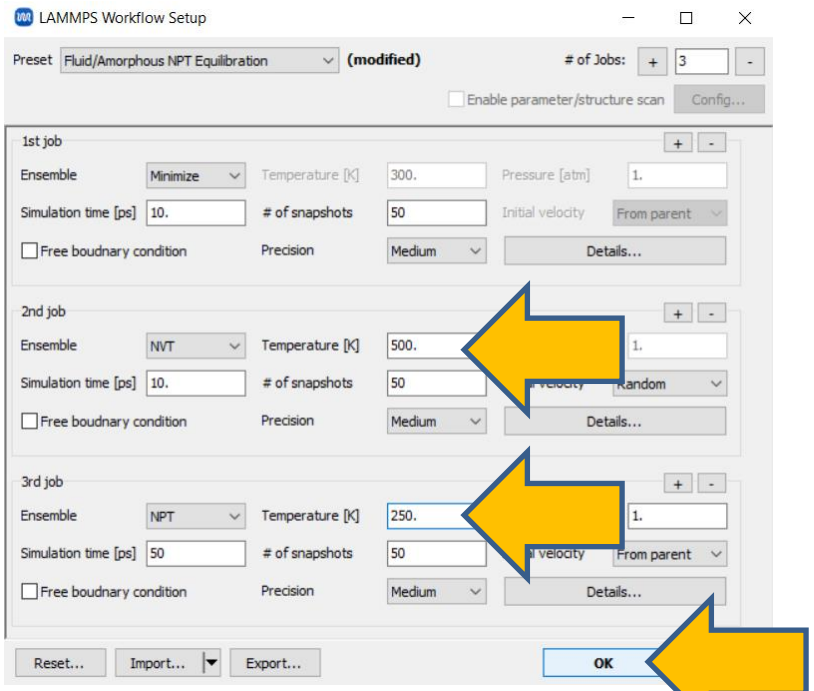


B. Execution of Calculation

A. In **LAMMPS Workflow Setup** window, make the following changes:
   - Change **Temperature** of **2nd job** to '500'.
   - Change **Temperature** of **3rd job** to '250'.

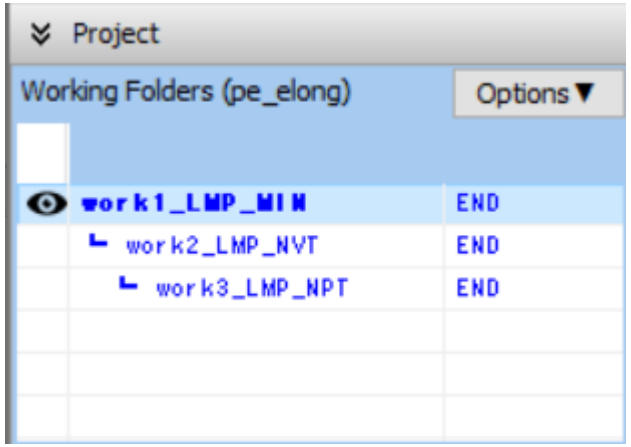
B. If you want to reduce the computational accuracy to finish the calculation faster, change **Precision** of **1st job**, **2nd job**, and **3rd job** to 'Low'.

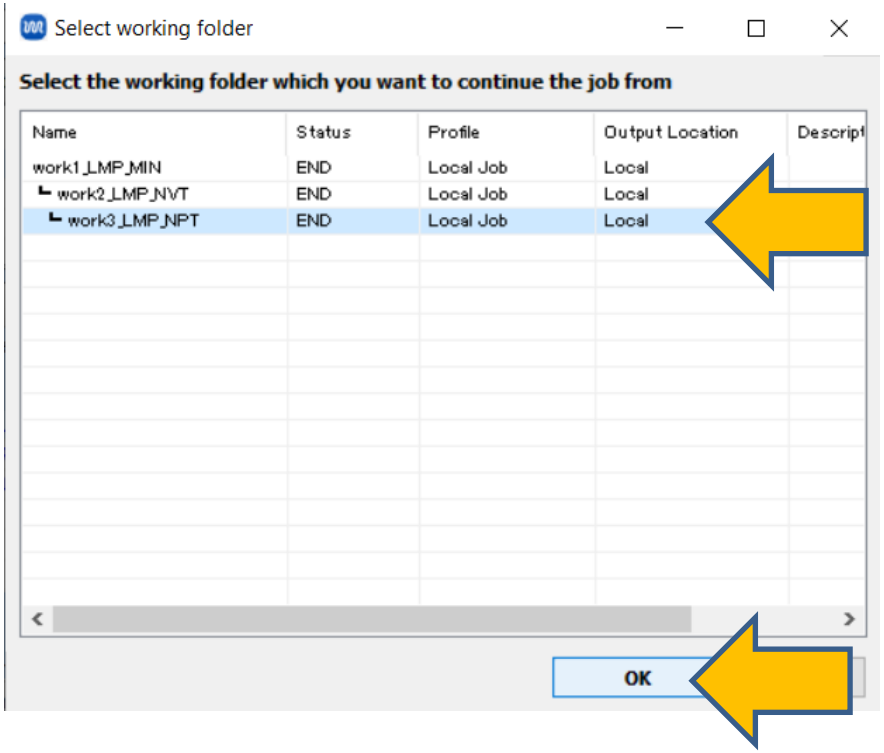
C. Click **OK**, then in **Job Setting** window, adjust the settings as needed before clicking **Run**.



B. Execution of Calculation

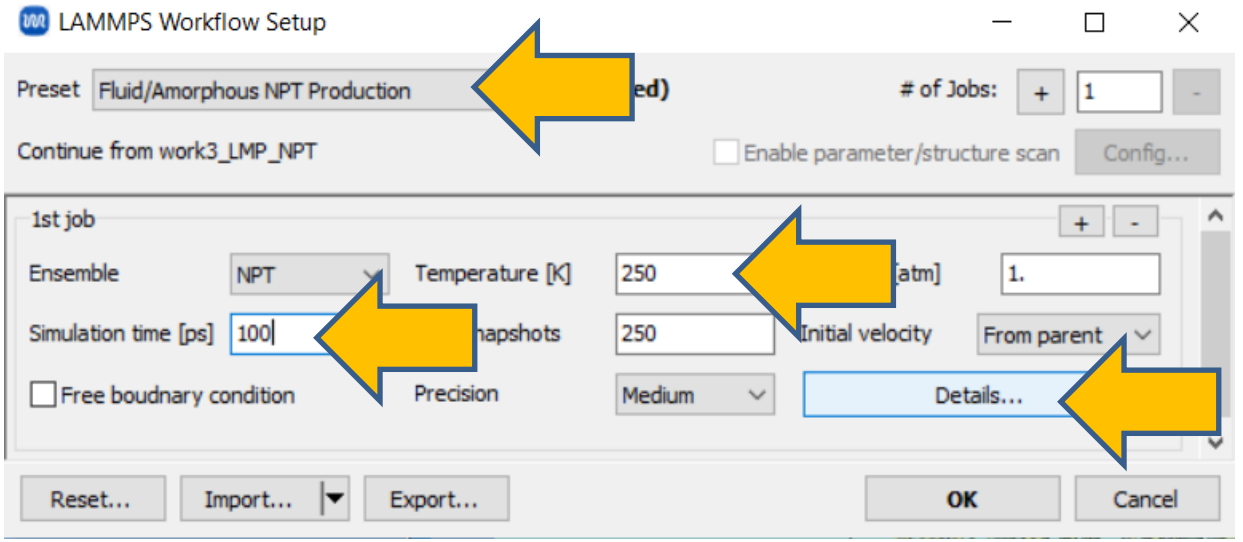
A. Once **the status** of the three work folders from work1_LMP_MIN to work3_LMP_NPT changes to **END** or **END(-)**, click **(Workflow Setup)** again.
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.
C. Select work3_LMP_NPT and click **OK**.





B. Execution of Calculation

A. Change **Preset** to 'Fluid/Amorphous NPT Production.'
B. Modify the settings as follows:
   - Change **Temperature** of **1st job** to '250.'
   - Change **Simulation time** of **1st job** to '100.'
C. If you want to decrease the calculation accuracy to finish the computation faster, change **Precision** of **1st job** to 'Low.'
D. Click **Details…**.



B. Execution of Calculation

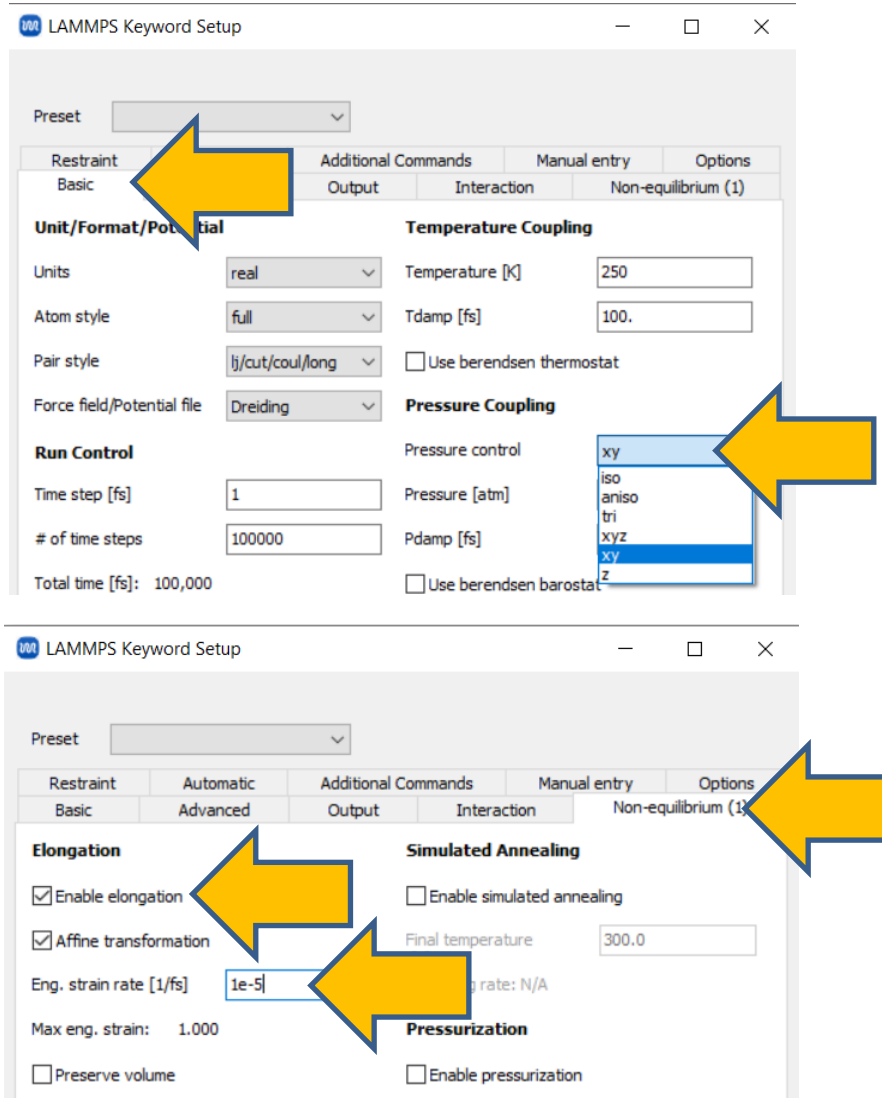
A. In **LAMMPS Keyword Setup** window, change **Pressure control** in **Basic** tab to 'xy'.

B. Move to **Non-equilibrium(1)** tab and modify the settings as follows:
   - Check **Enable elongation**.
   - Change **Eng. Strain Rate** to '1e-5.'

C. Click **OK** to close **LAMMPS Keyword Setup** window.

D. Click **OK** in **LAMMPS Workflow Setup** window.

E. In **Job Setting** window, modify the settings as needed and click Run.



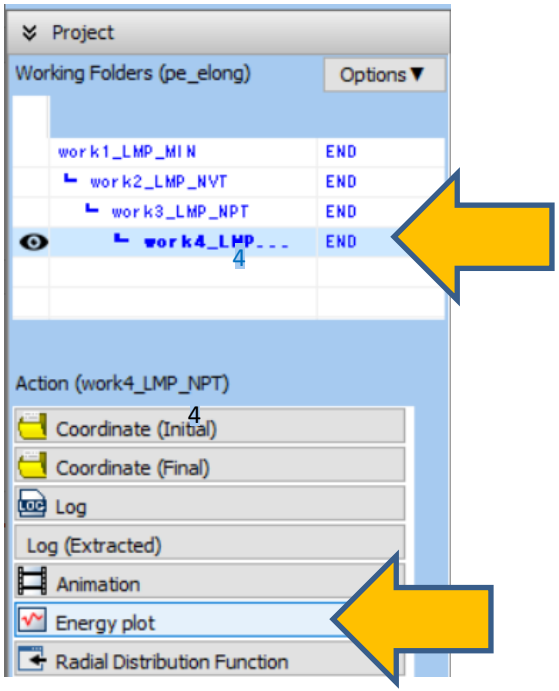
C. Analysis of Results

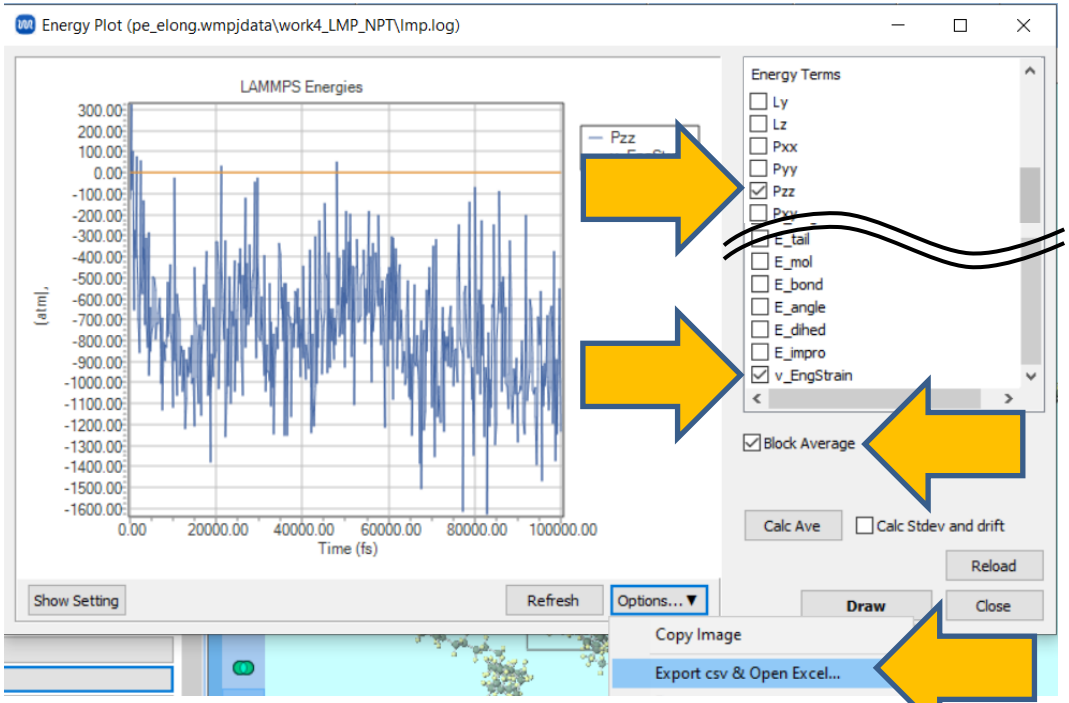
A. Once **the status** of 'work4_LMP_NPT' changes to either **END** or **END(-)**, click on 'work4_LMP_NPT' and then click **Energy plot** under **Action**.

B. In **Energy Terms**, check both **Pzz** and **EngStrei**. Also, check **Block Average** and change **Size** to 10.

C. Click **Draw**, then click **Options | Export csv & Open Excel**.

D. Click **Save** in **Save As** dialog.

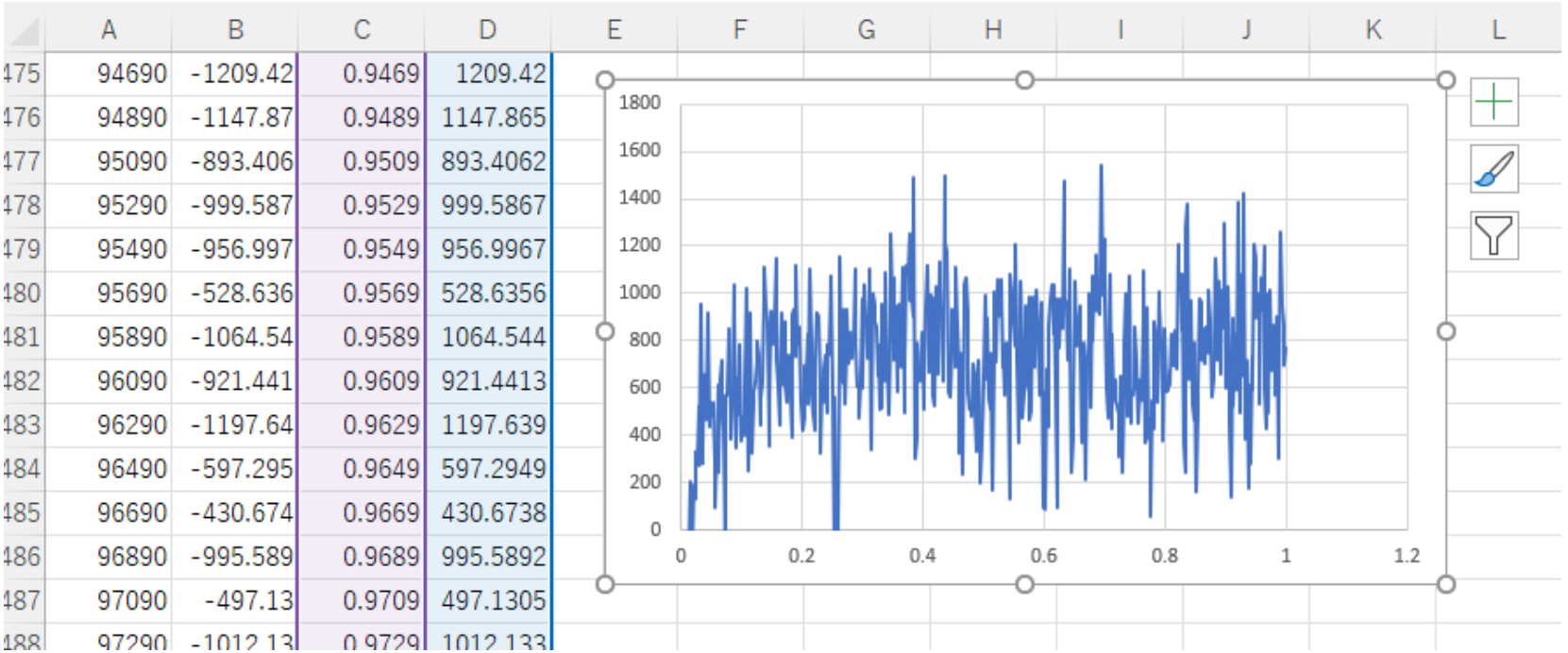




C. Analysis of Results

A. Plot the third column and the column obtained by multiplying the second column by -1 (here referred to as column D). This corresponds to the strain-stress curve (S-S curve).

(Here, the lower limit of the y-axis is set to 0 for plotting.)



	A	B	C	D
475	94690	-1209.42	0.9469	1209.42
476	94890	-1147.87	0.9489	1147.865
477	95090	-893.406	0.9509	893.4062
478	95290	-999.587	0.9529	999.5867
479	95490	-956.997	0.9549	956.9967
480	95690	-528.636	0.9569	528.6356
481	95890	-1064.54	0.9589	1064.544
482	96090	-921.441	0.9609	921.4413
483	96290	-1197.64	0.9629	1197.639
484	96490	-597.295	0.9649	597.2949
485	96690	-430.674	0.9669	430.6738
486	96890	-995.589	0.9689	995.5892
487	97090	-497.13	0.9709	497.1305
488	97290	-1012.13	0.9729	1012.133

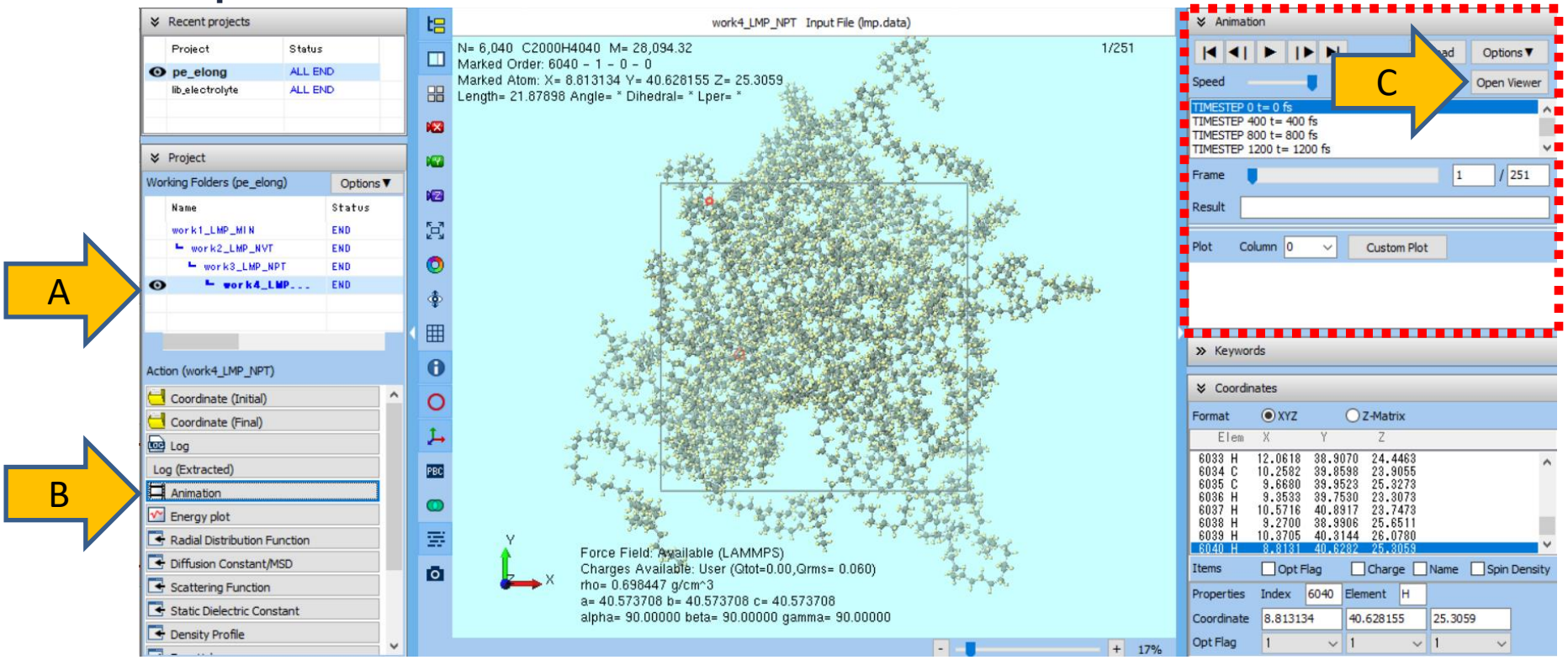
References: Hossain, D., Tschopp, M.A., Ward, D.K., Bouvard, J.L., Wang, P., Horstemeyer, M.F., Polymer, 51 (2010) 6071-6083.

C. Analysis of Results

A. Return to Winmostar, close **Energy Plot** window by clicking **Close**.

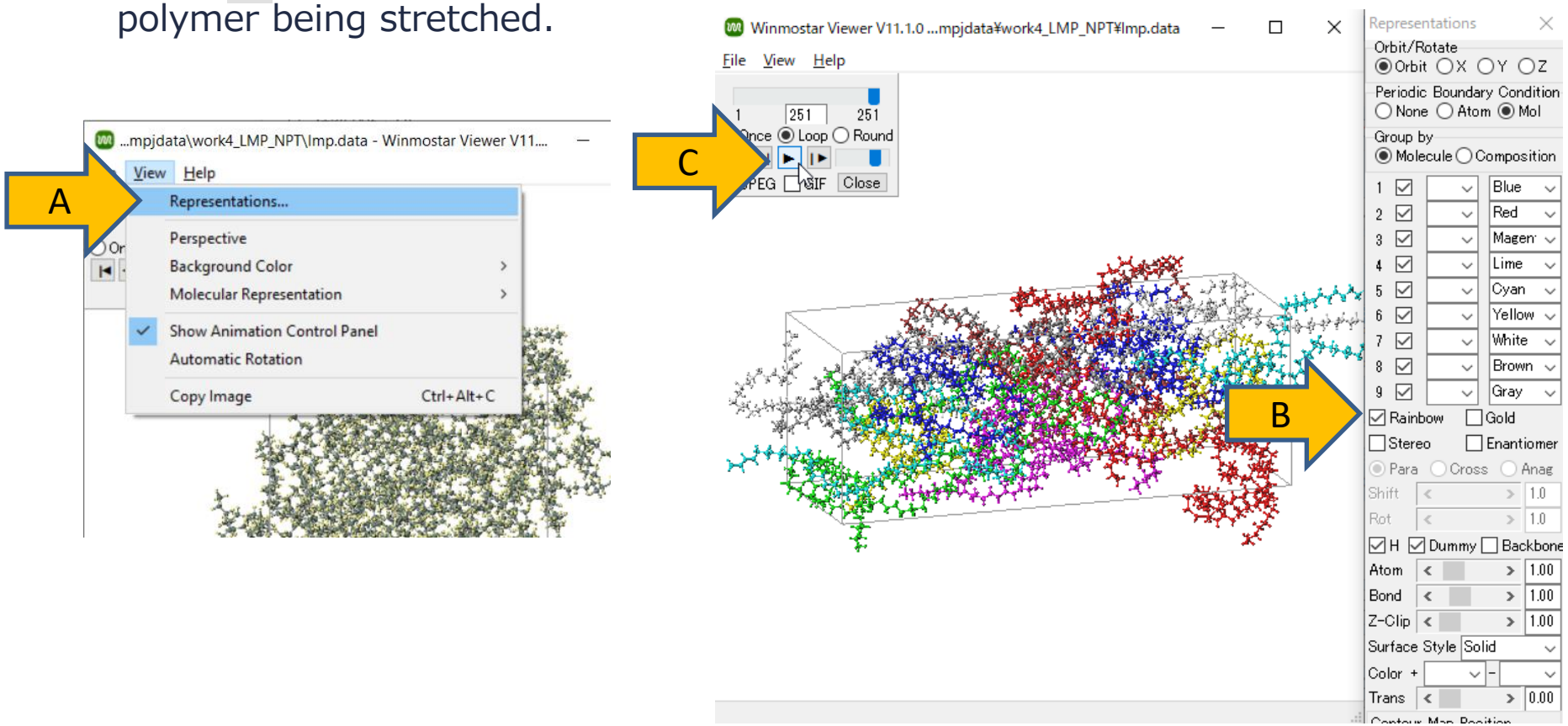
B. Click 'work4_LMP_NPT' in **Working Folders** and then click **Animation** under **Action**. After a few seconds of processing, an area to control the animation will appear.

C. Click **Open Viewer**.



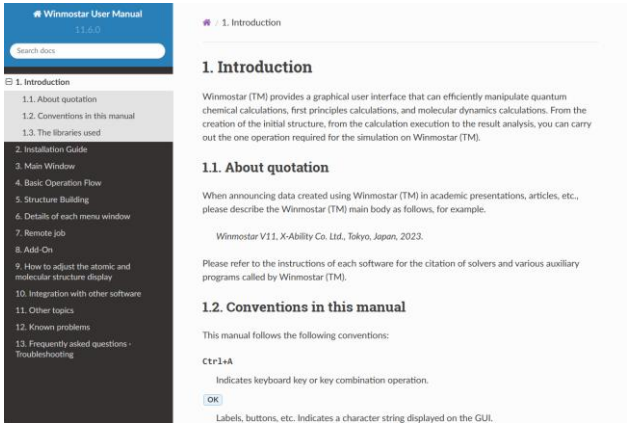
C. Analysis of Results

A. Click **View | Representations** in the launched **Winmostar Viewer**.
B. In **Representations window**, check **Rainbow**.
C. Click  button in the top left of **Winmostar Viewer** window to observe the polymer being stretched.



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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