winmostar tutorial

LAMMPS
Calculation of Coefficient of Thermal Expansion

V11.6.5

26 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

- This tutorial introduces how to calculate the linear expansion coefficient of the Si crystal (1,0,0) surface at 1,000 K, with calculations performed at temperatures ranging from 800 K to 1200 K.

Note

- The number of steps required for equilibration may vary depending on the type of material and initial density.
- The calculation method, type of force field, size of the supercell, and the rate of temperature increase can all influence the results.
- It is recommended to perform fitting using various graphing and analysis software.

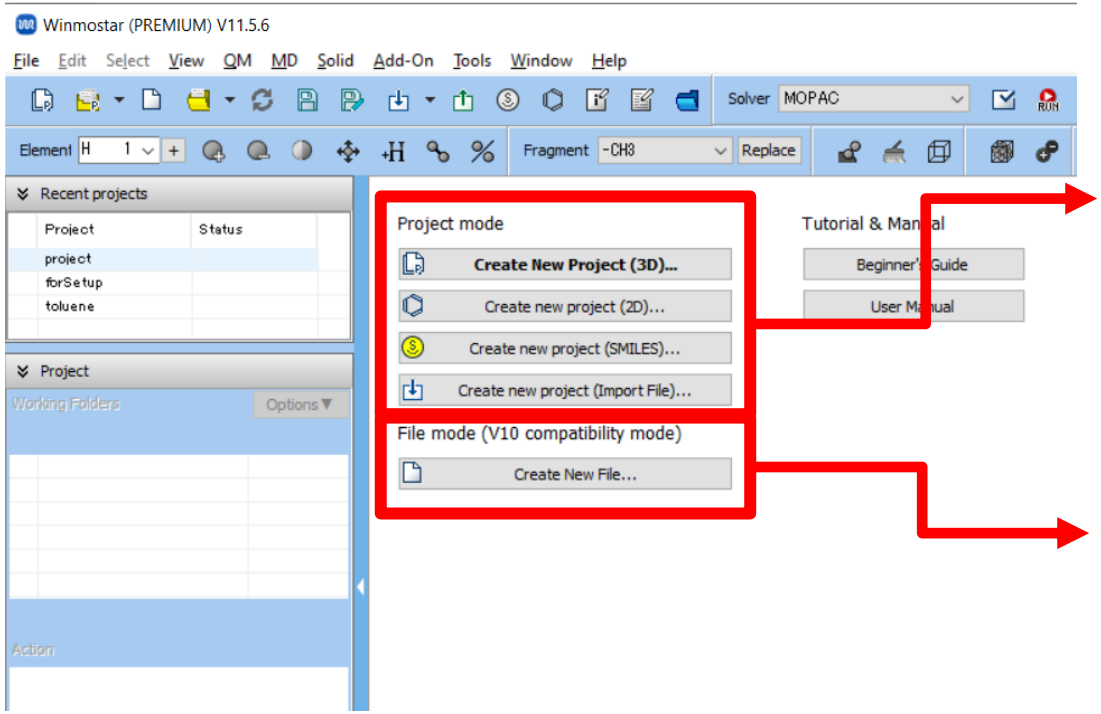
Preference of Operating Environment

- 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

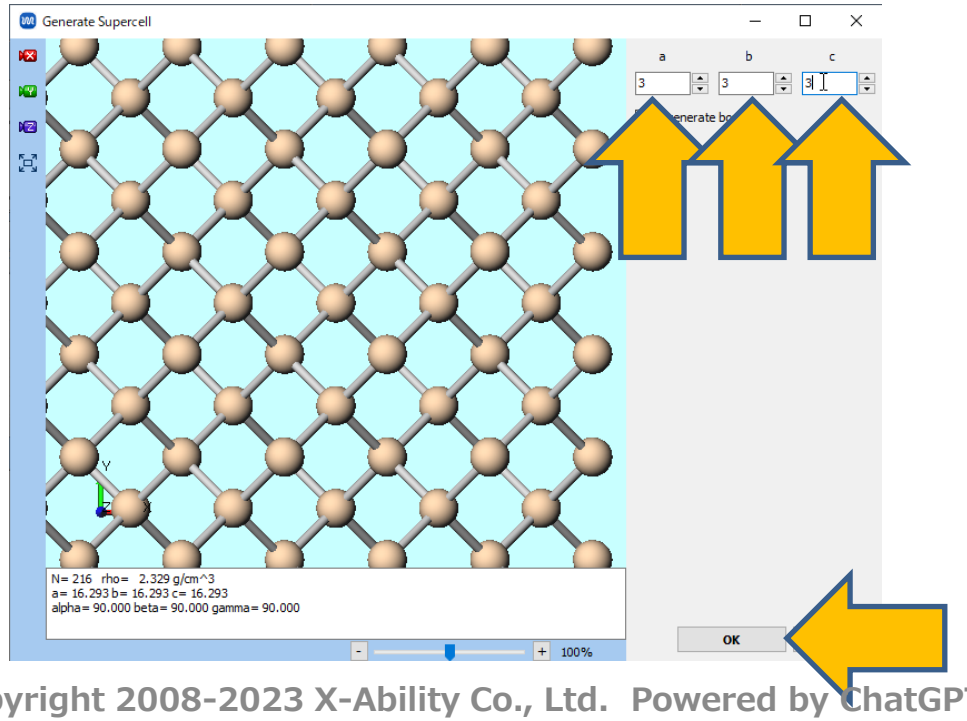
For basic operations, please refer to LAMMPS Basics tutorial.

A. Click **File | New Project**, enter '`si_exp`' in **Project name**, and click **Save**.

B. Click **File | Import | Sample Files | si.cif**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

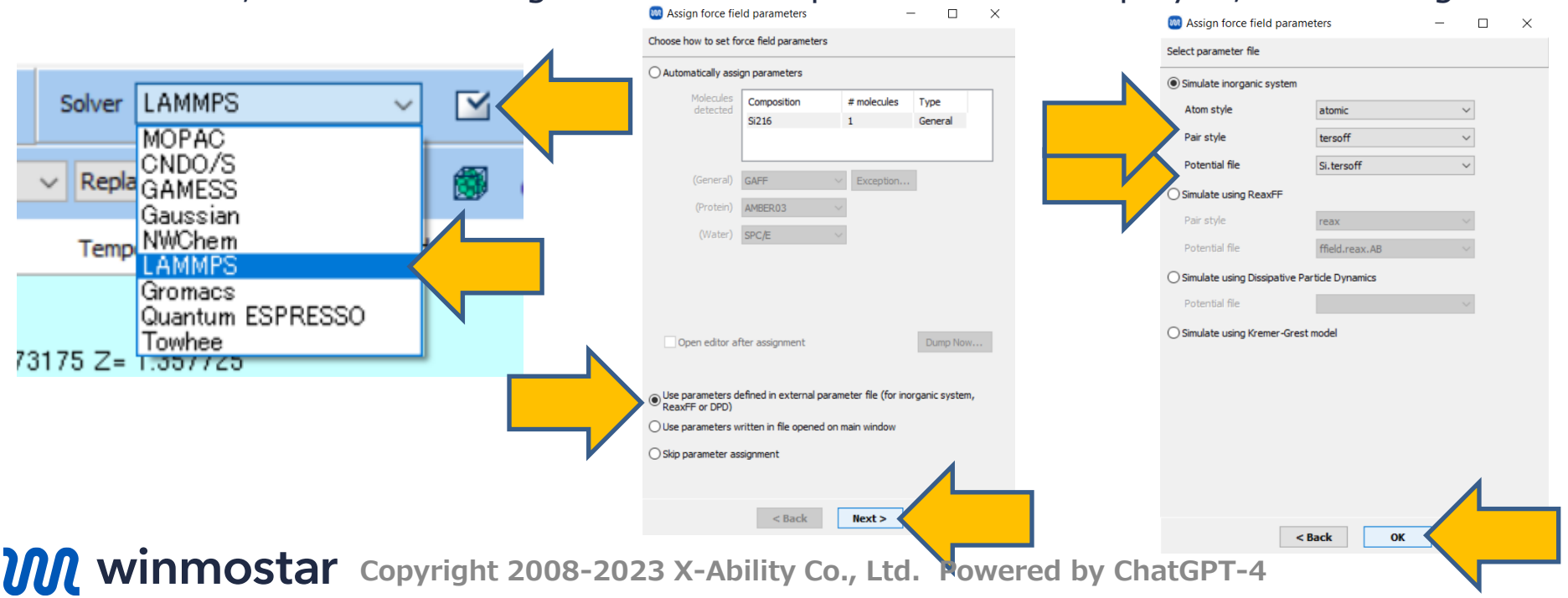
C. In **Import File** dialog, click on **Discard and Import**.

D. Click **Solid | Generate Supercell**, change **a**, **b**, **c** all to '3', and click **OK**.



B. Execution of Calculation（Equilibration）

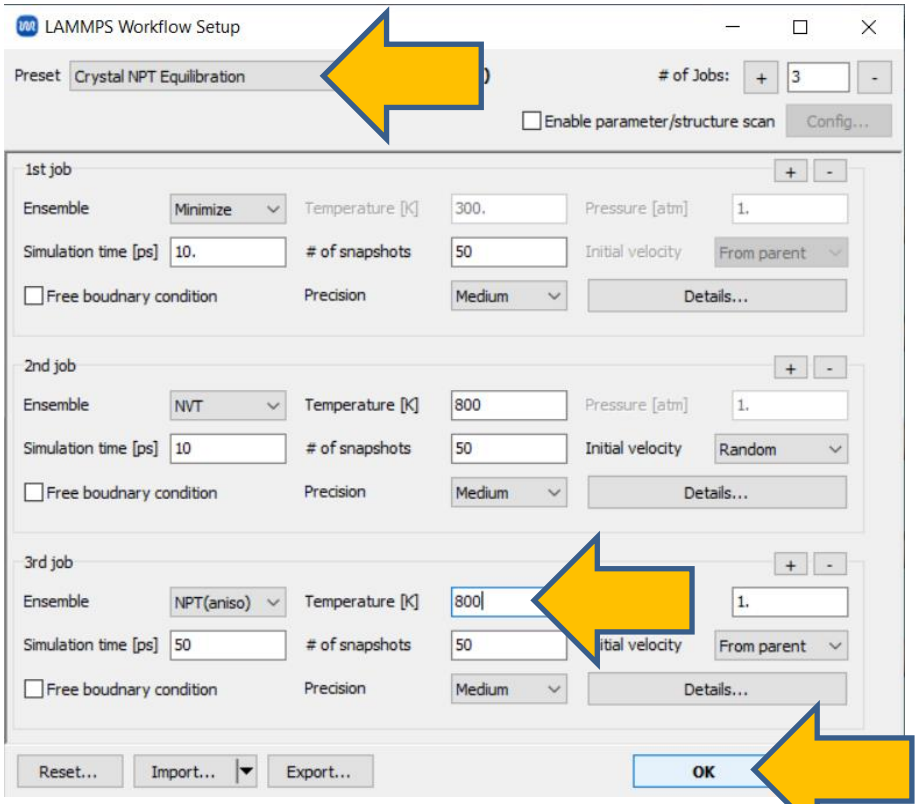
A. Select **LAMMPS** from **Solver** and open **(Workflow Setup)**.
B. If prompted 'Some molecules do not have charges. Do you want to assign charges now?', click **No**.
C. Choose **Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** and click **Next**.
D. Change **Pair Style** to 'tersoff' and **Potential File** to 'Si.tersoff'.
E. Click **OK**, and when 'Assigned force field parameters' is displayed, click **OK** again.



B. Execution of Calculation（Equilibration）

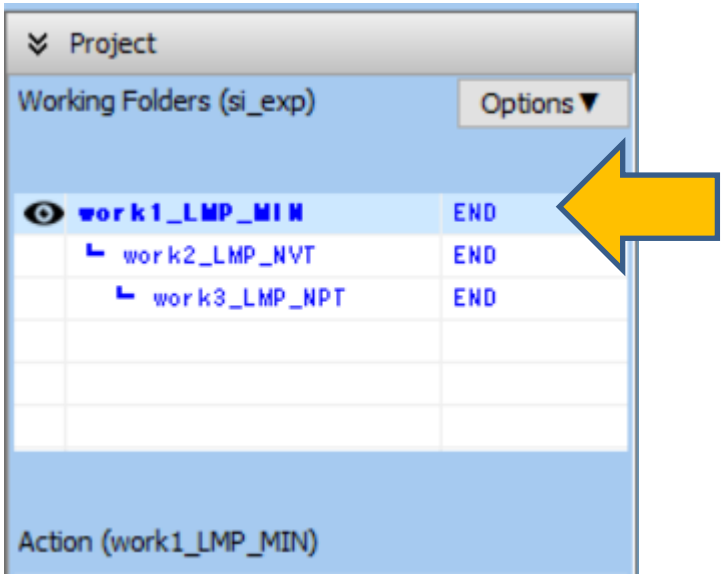
A. Change **Preset** to 'Crystal NPT Equilibration' and adjust **Temperature** for **2nd** and **3rd jobs** to '800'.

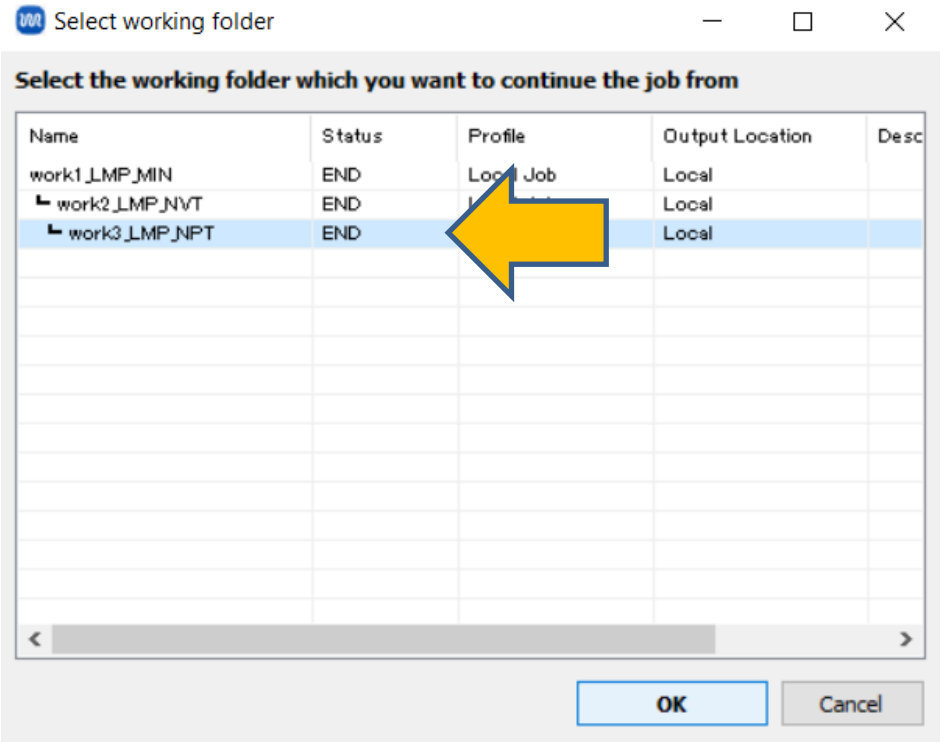
B. Click **OK**, then adjust settings as appropriate in **Job Setting** window before clicking **Run**.



C. Execution of Calculation（Main Calculation）

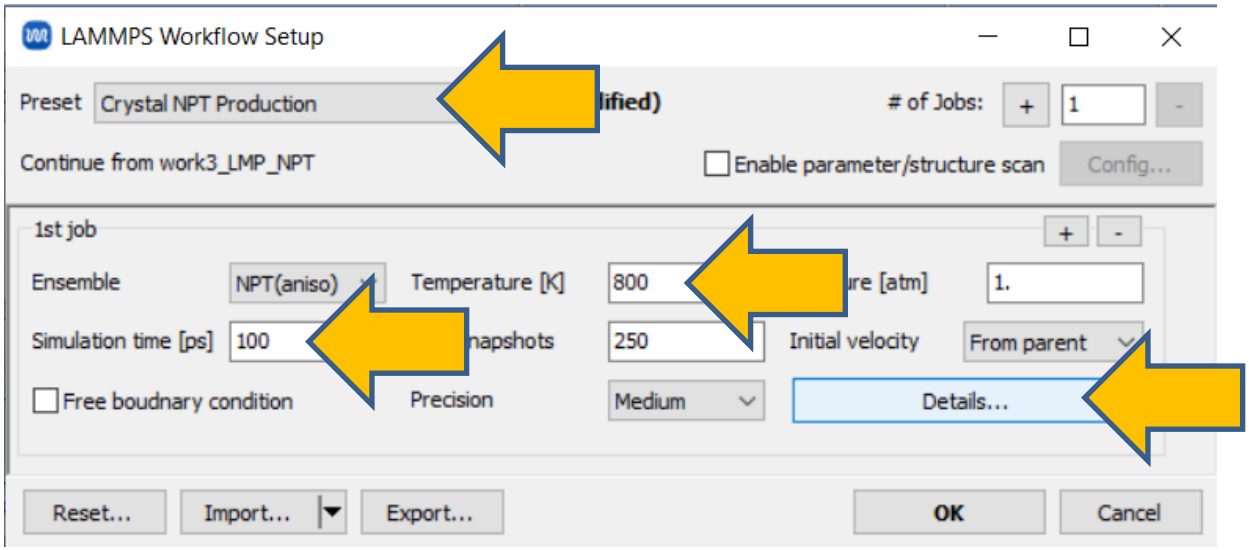
A. Once **the status** of the three **work folders** from work1_LMP_MIN to work3_LMP_NPT changes to **END** **END(-)**, click **(Workflow Setup)**.
B. If prompted 'Do you want to continue from previous run?' click **Yes**.
C. Select work3_LMP_NPT and click **OK**.





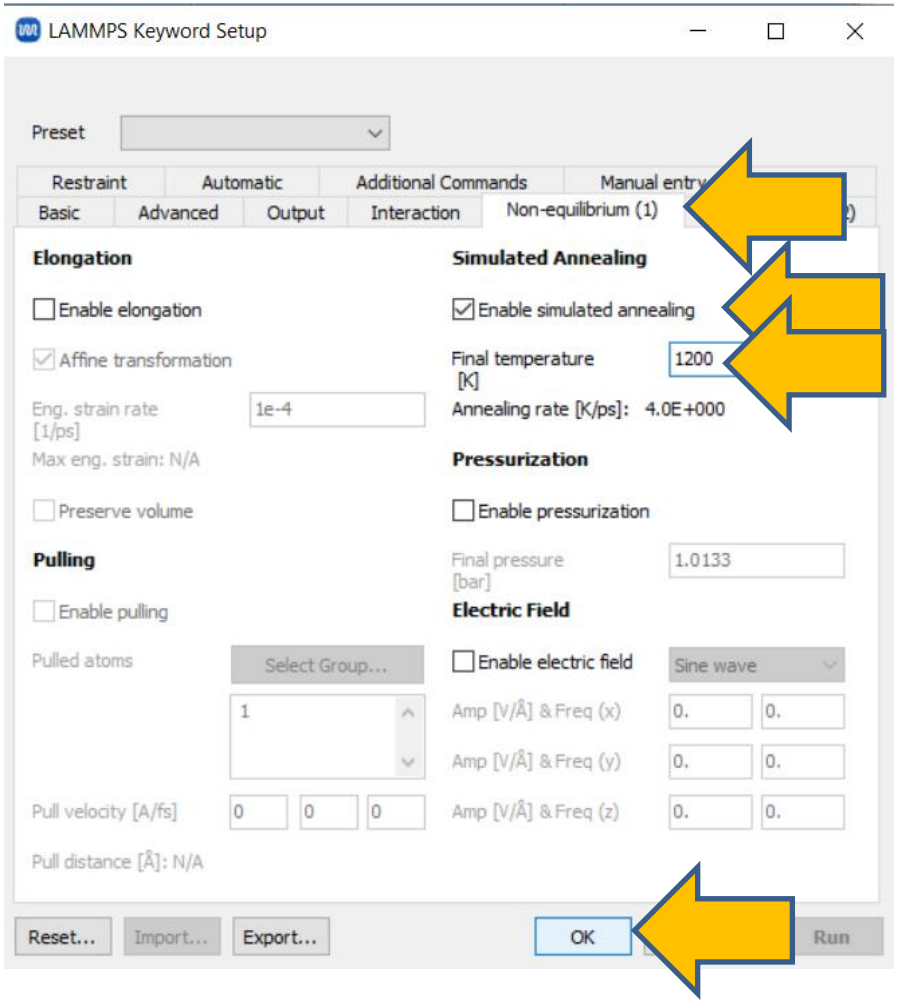
C. Execution of Calculation（Main Calculation）

A. Change **Preset** to 'Crystal NPT Production'.
B. Modify the settings as follows:
    A. Change **Temperature** in **1st job** to '800'.
    B. Change **Simulation time** in **1st job** to '100'.
C. If you wish to decrease the computational precision to finish calculations faster, change **Precision** in **1st job** to 'Low' and **Simulation time** to '50'.
D. Click **Details…**.



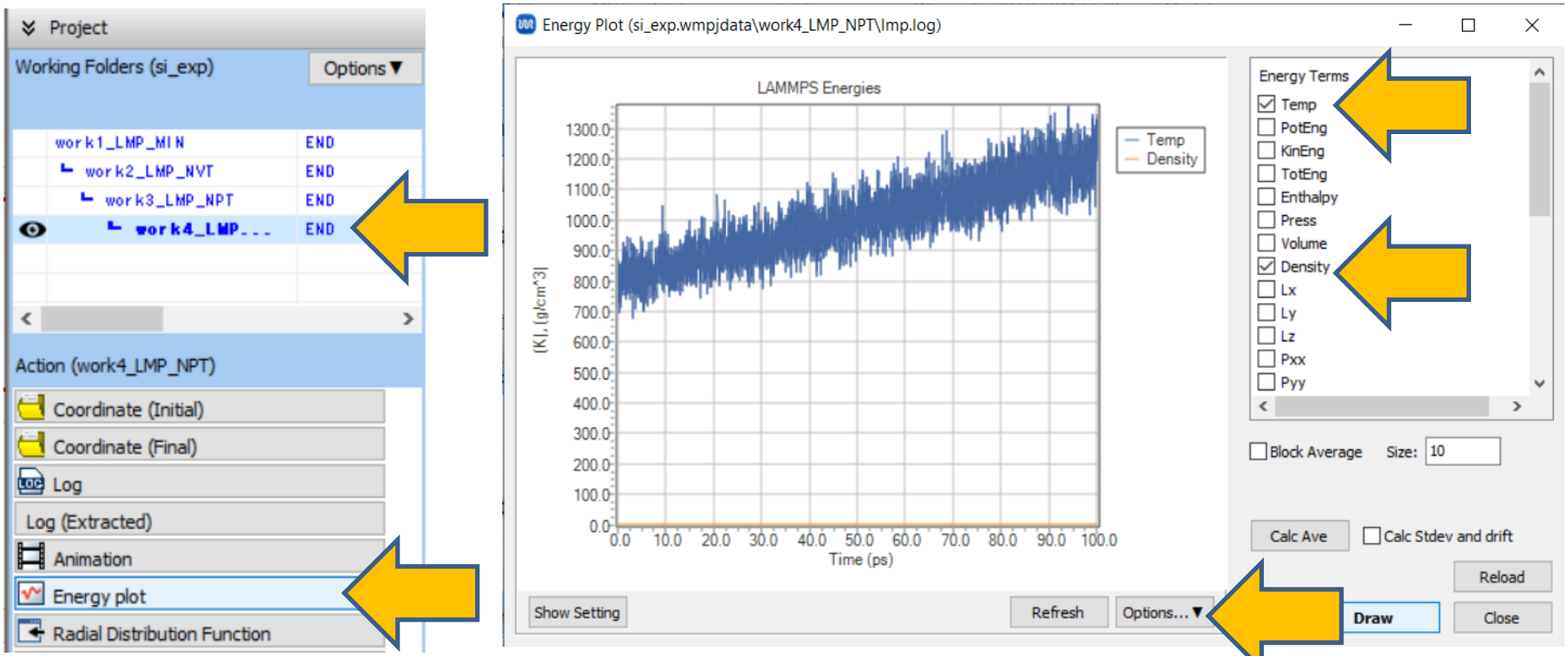
C. Execution of Calculation（Main Calculation）

A. In **LAMMPS Keyword Setup** window, go to **Non-equilibrium(1)** tab and make the following changes:
   A. Check **Enable simulated annealing.**
   B. Change **Final temperature** to '1200'.
B. Click **OK** to close **LAMPS Keyword Setup** window.
C. Click **OK** in **LAMMPS Workflow Setup** window.
D. Modify the settings as appropriate in **Job Setting** window and click Run.



D. Analysis of Results

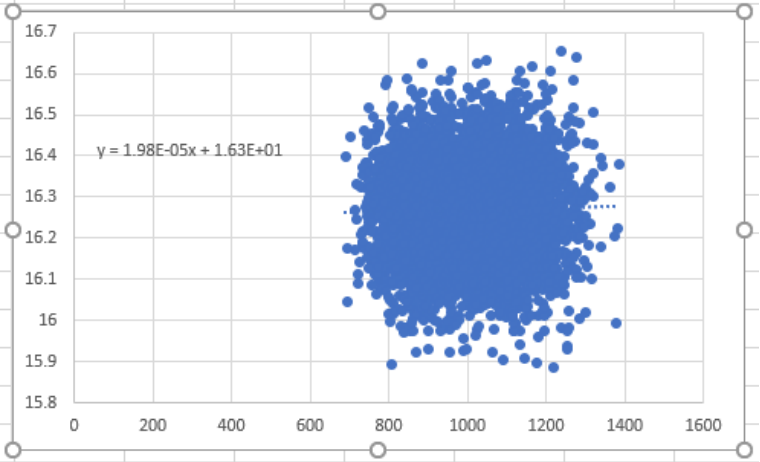
A. Once **the status** of **the work folder** work4_LMP_NPT changes to **END** or **END(-)**, click 'work4_LMP_NPT' and then click **Energy plot** in **Action**.
B. Check **Temp** and **Density** in **Energy Terms**, click **Draw**, and then click **Options | Export csv & Open Excel**.
C. Click Save in **Save as** dialog.



D. Analysis of Results

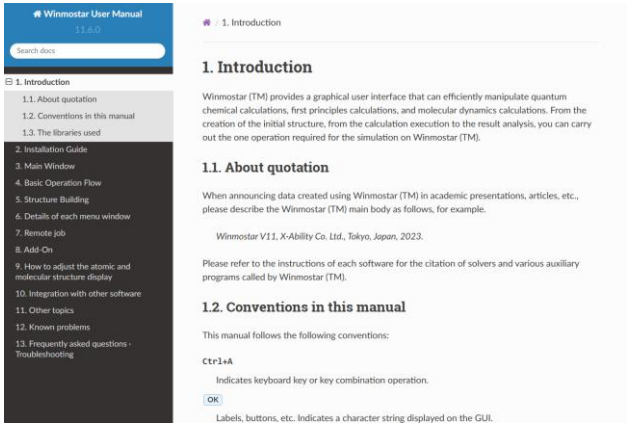
Fit the second column (temperature) and the third column (system size in the X-direction) of the generated csv file with a linear function y = a*x + b.
The expansion coefficient is given by a/(a*1000+b).
In the example below, it is calculated as 1.98e-5 / (1.98e-5 *1000+16.3) = 1.2e-6 K^{-1}.

Temp	Lx
824.2394	16.39661
799.0766	16.24357
798.2147	16.15447
797.3507	16.25704
813.2067	16.25624
791.3088	16.36967
861.6687	16.34693
784.8201	16.09104
797.8853	16.23532
809.2485	16.46295
767.0234	16.29994
796.3277	16.17976
776.7948	16.20732
781.7229	16.31405
752.4496	16.31275
713.8953	16.26681



Finally

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



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Scenes from Winmostar Training Session

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