winmostar tutorial

LAMMPS
Melting Point Calculation

V11.6.5

19 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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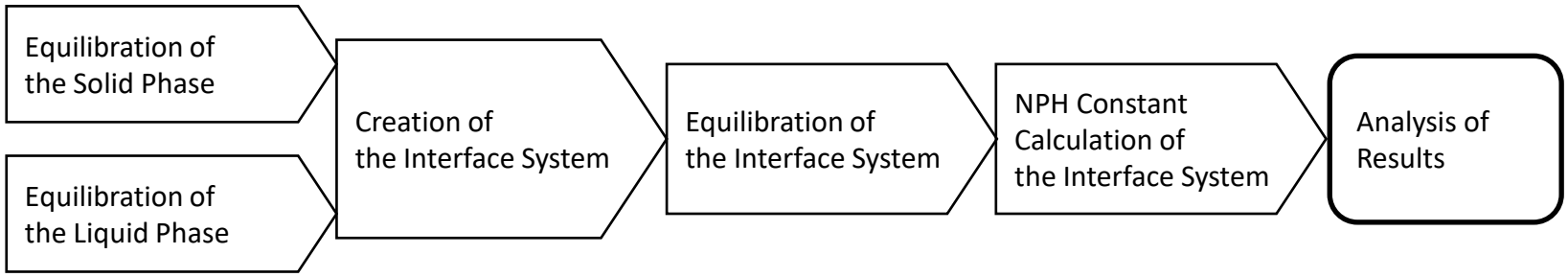
Overview・Note

- The melting point of a Si crystal at 1 atm is calculated from the NPH constant calculation of the solid-liquid interface system. In this method, if the final temperature of the NPH constant calculation matches the temperature at equilibrium, that temparature can be considered as the melting point.

S. Yoo, X. C. Zeng and J. R. Morris, J. Chem. Phys., 120, 3, (2004), 1654-1656.



Note:

- The number of steps required for equilibration may vary from this example depending on the type of molecule and initial density.
- The calculation method of interaction and the force field greatly affect the calculation results.
- The system size (number of repeats of the solid phase), initial temperature, and differences in the contact surface also affect the results.
- In this calculation, since the final temperature (around 2500 K) differs from the temperature at equilibrium (2300 K), ideally, all steps should be repeated using the final temperature.

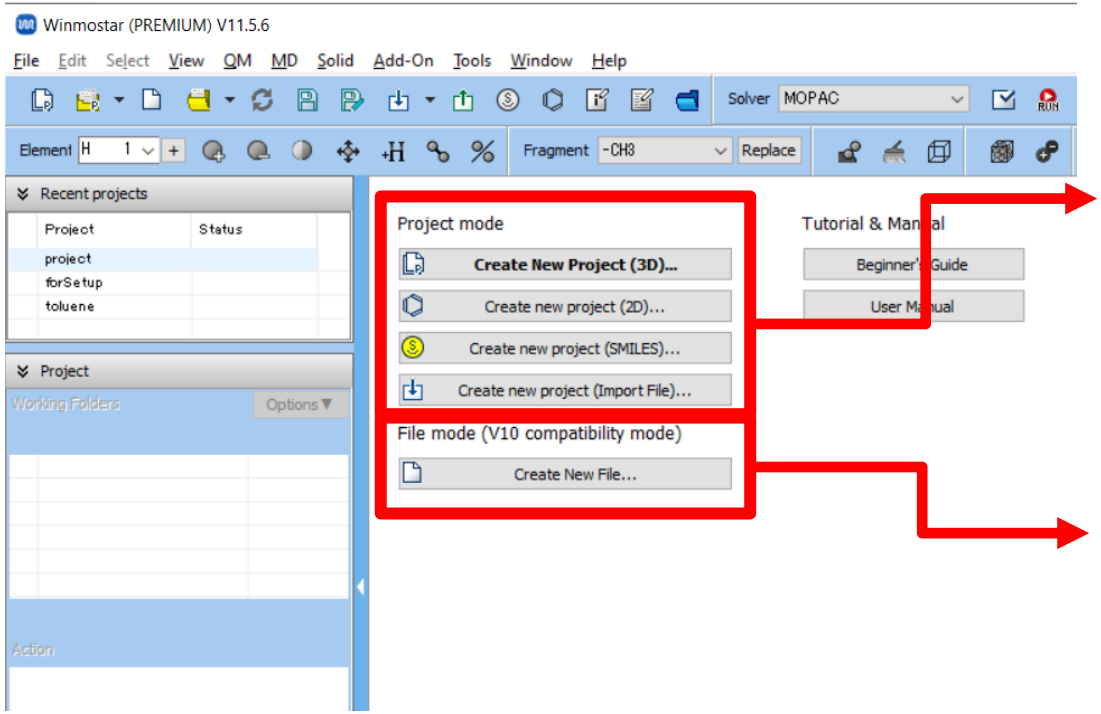
Preference of Operating Environment

- 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（Solid Phase）

For basic operations, please refer to LAMMPS Basics tutorial.

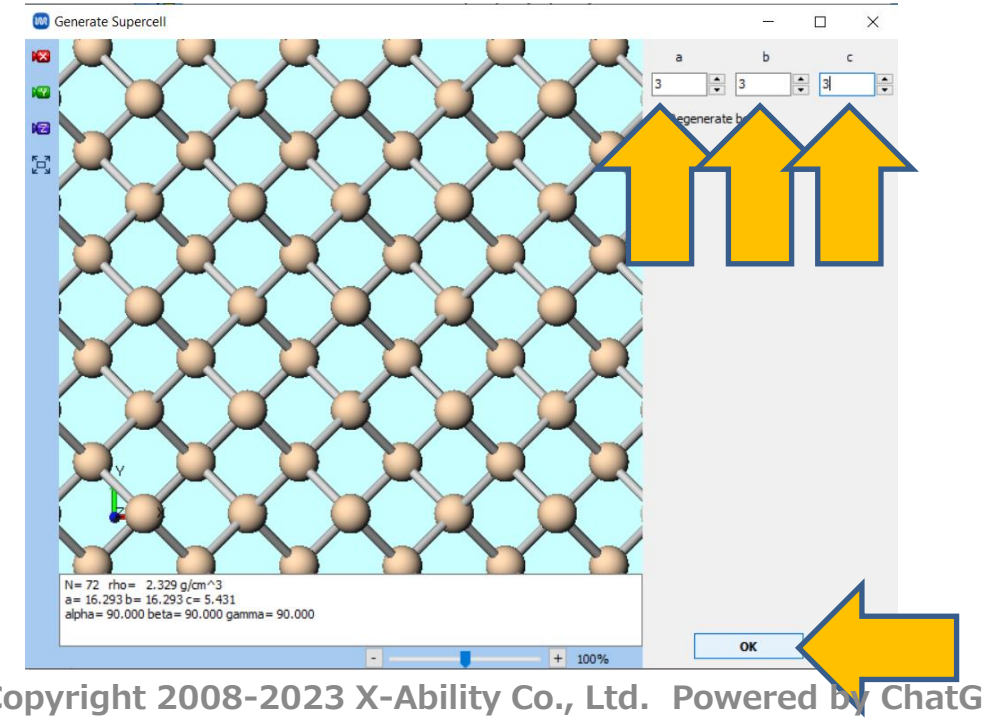
A. Click **File | New Project**, enter '`si_sle`' in **Project name**, and click **Save**.

B. Click **File | Import | Samples File | si.cif**.

   - If you wish to load a different file at this stage, use **File | Import File** instead.

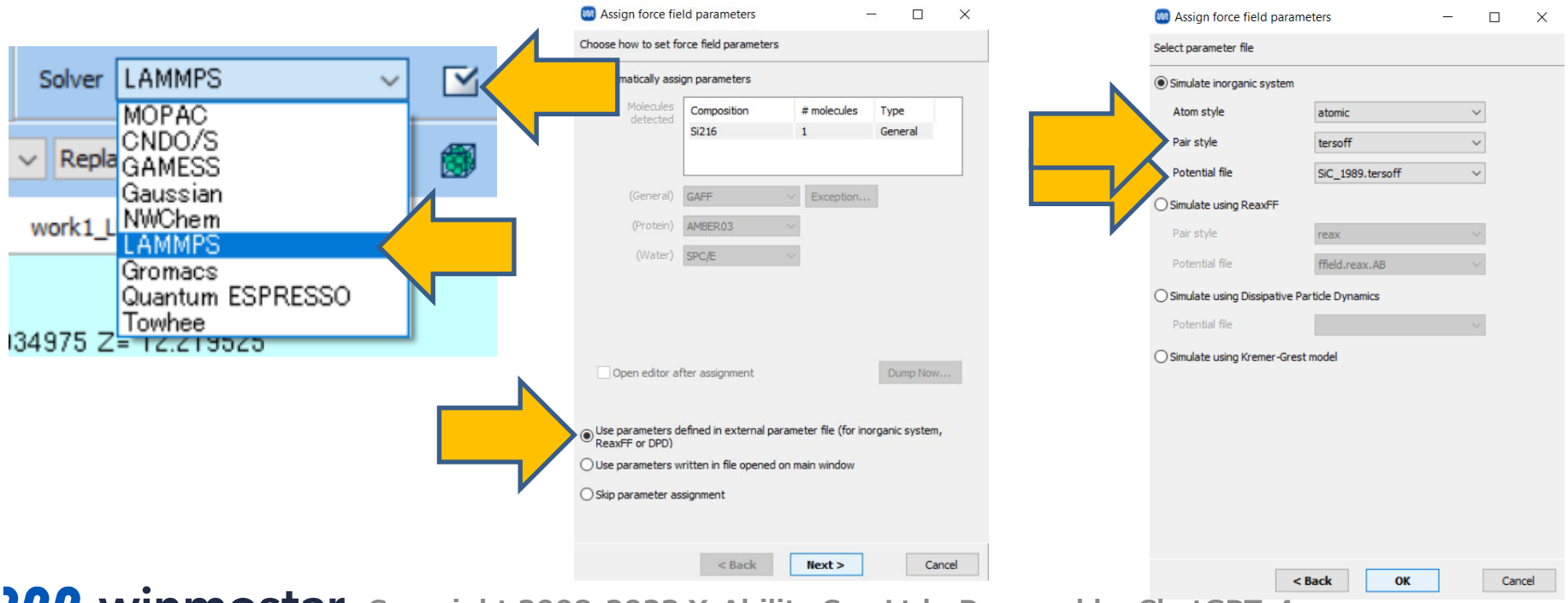
C. In **Import File** dialog, click **Discard and import**.

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



A. Modeling of the System（Solid Phase)

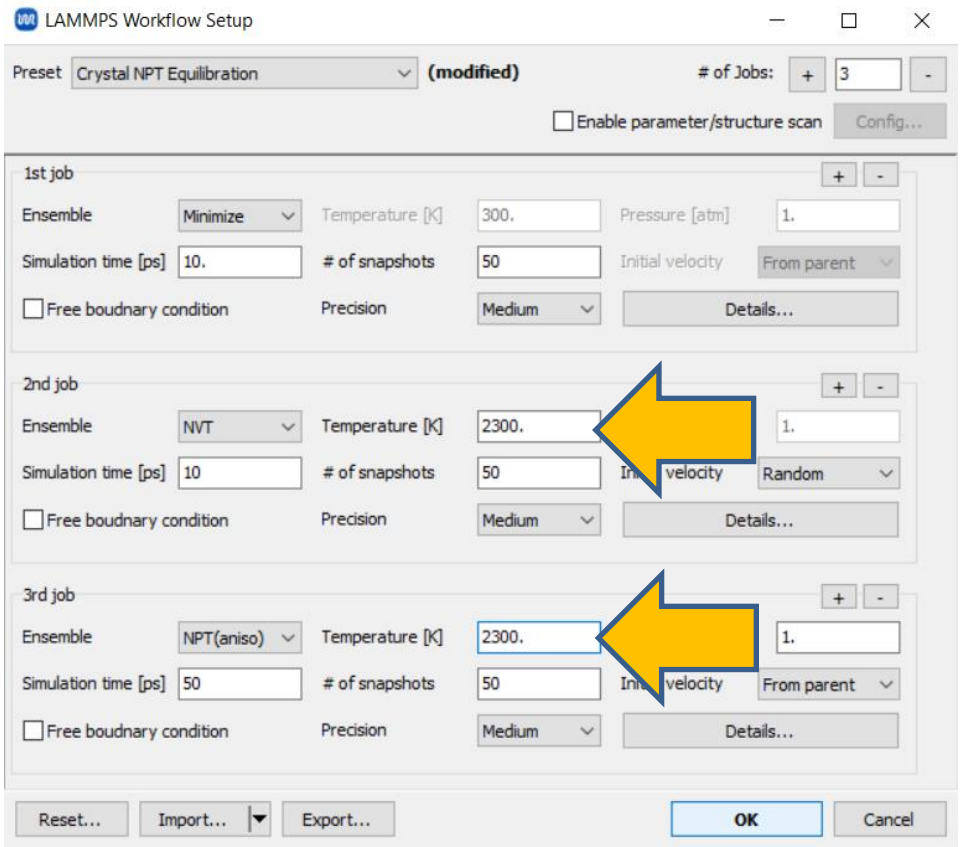
A. Select **LAMMPS** from **Solver**, and open **(Workflow Setup**).
B. If prompted 'Some molecules do not have charges. Do you want to assign charges now?' click **No**.
C. Choose **Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** and click **Next**.
D. Change **Pair Style** to 'tersoff' and **Potential File** to 'SiC_1989.tersoff'.
E. Click **OK**, and when 'Assigned force field parameters' is displayed, click **OK**.



B. Execution of Calculation（Solid Phase)

A. Chane **Preset** to 'Crystal NPT Equilibration' and adjust **Temperature** for **2nd job** and **3rd job** to '2300'.

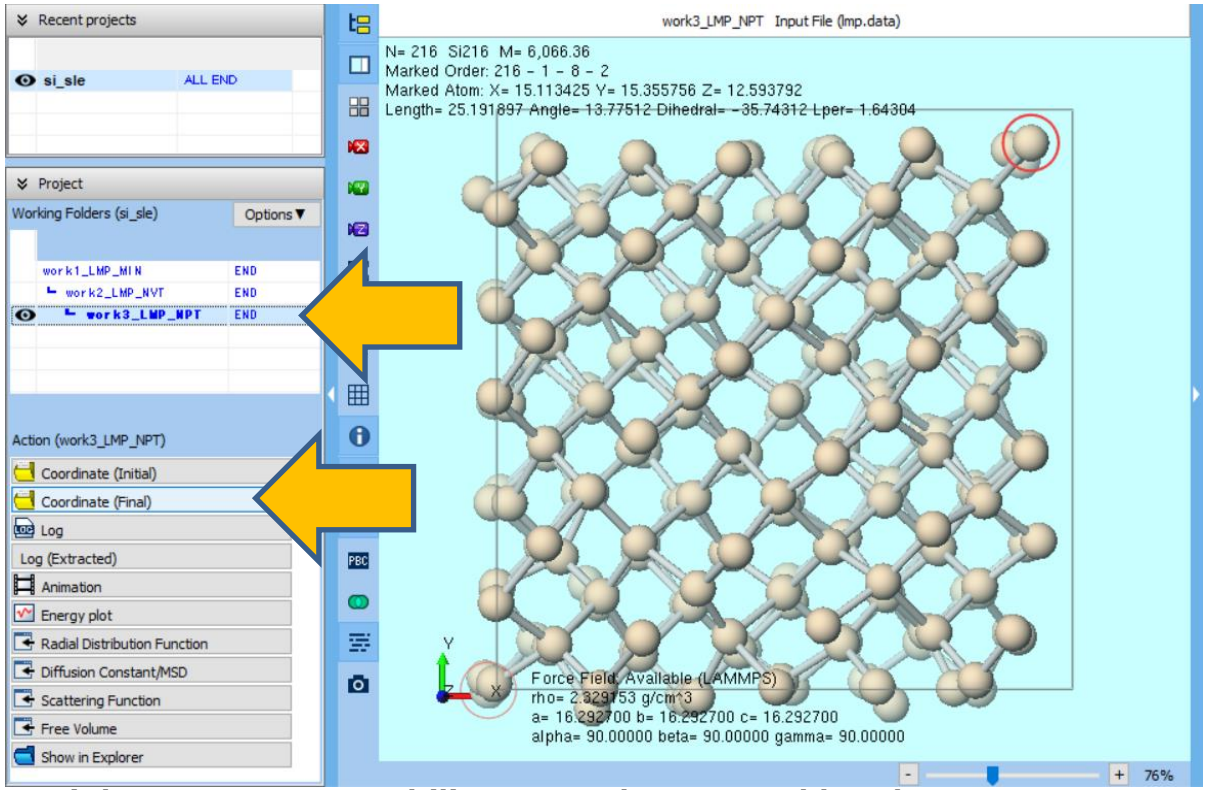
B. Click **OK**, then make any necessary adjustments in **Job Setting** window before clicking **Run**.



C. Post-Processing (Solid Phase)

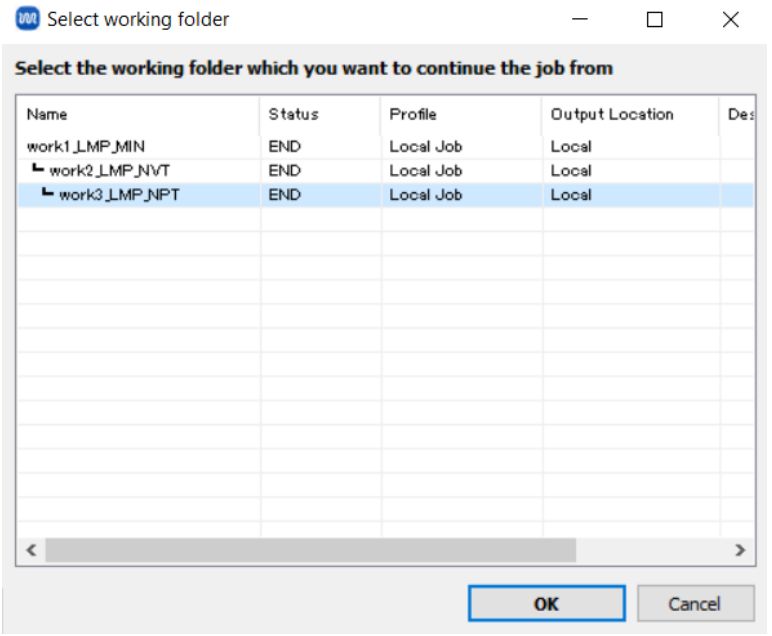
A. Once **the status** of **the work folders** from work1_LMP_MIN to work3_LMP_NPT changes to **END** or **END(-)**, click on 'work3_LMP_NPT' in **Working Folders** and then click **Coordinate(Final)** under **Action**.

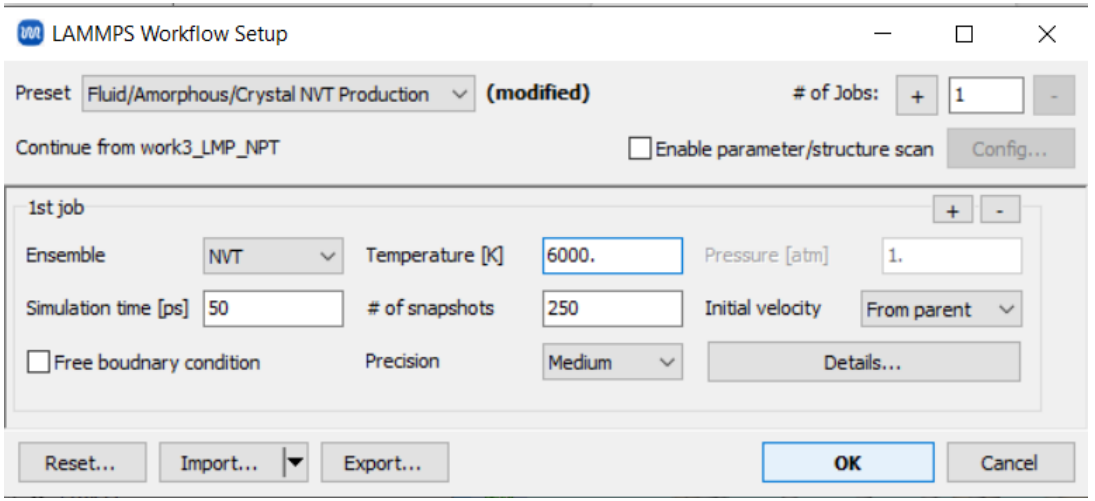
B. Click  **(Export File)** and save the file under `si_sle.wmpjdata` folder one level up with the file name '`si_solid.cif`'.



D. Execution of Calculation（Liquid Phase）

A. Click again **(Workflow Setup)**.
B. If prompted 'Do you want to continue from previous run?', click **Yes**.
C. Select work3_LMP_NPT and click **OK**.
D. Change **Preset** to 'Fluid/Amorphous/Crystal NVT Production' and **Temperature** to '6000'.
E. Click **OK**, then adjust settings in **Job Setting** window as necessary and click **Run**.



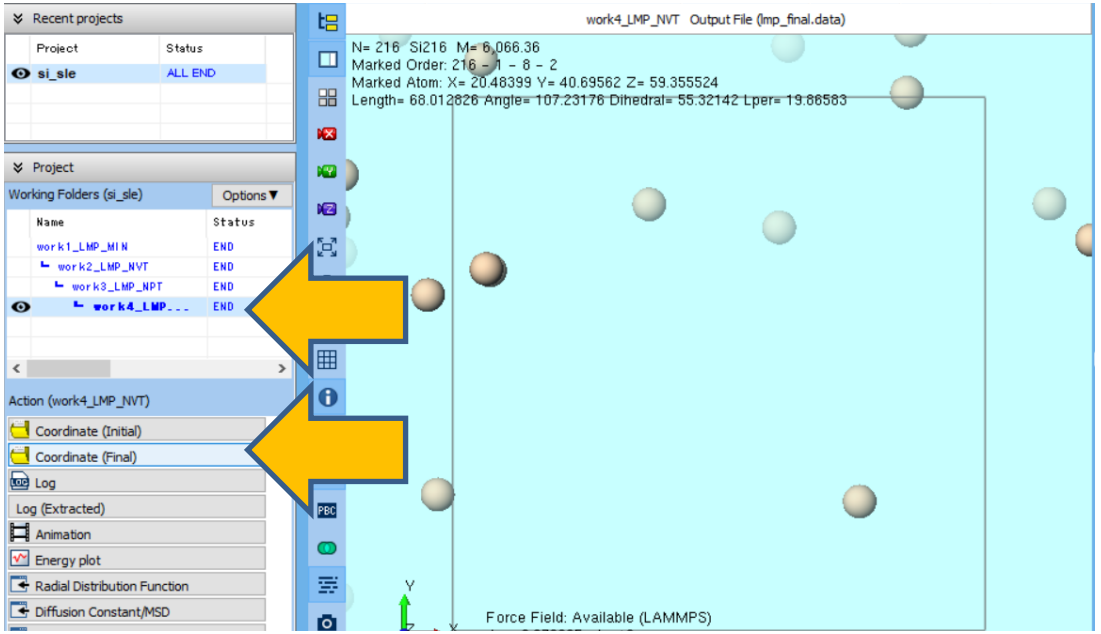


E. Post-Processing（Liquid Phase）

A. Once **the status** of **the work folder** for work4_LMP_NVT changes to **END** or **END(-)**, click 'work4_LMP_NVT' in **Working Folders** and then click **Coordinate(Final)** under **Action**.

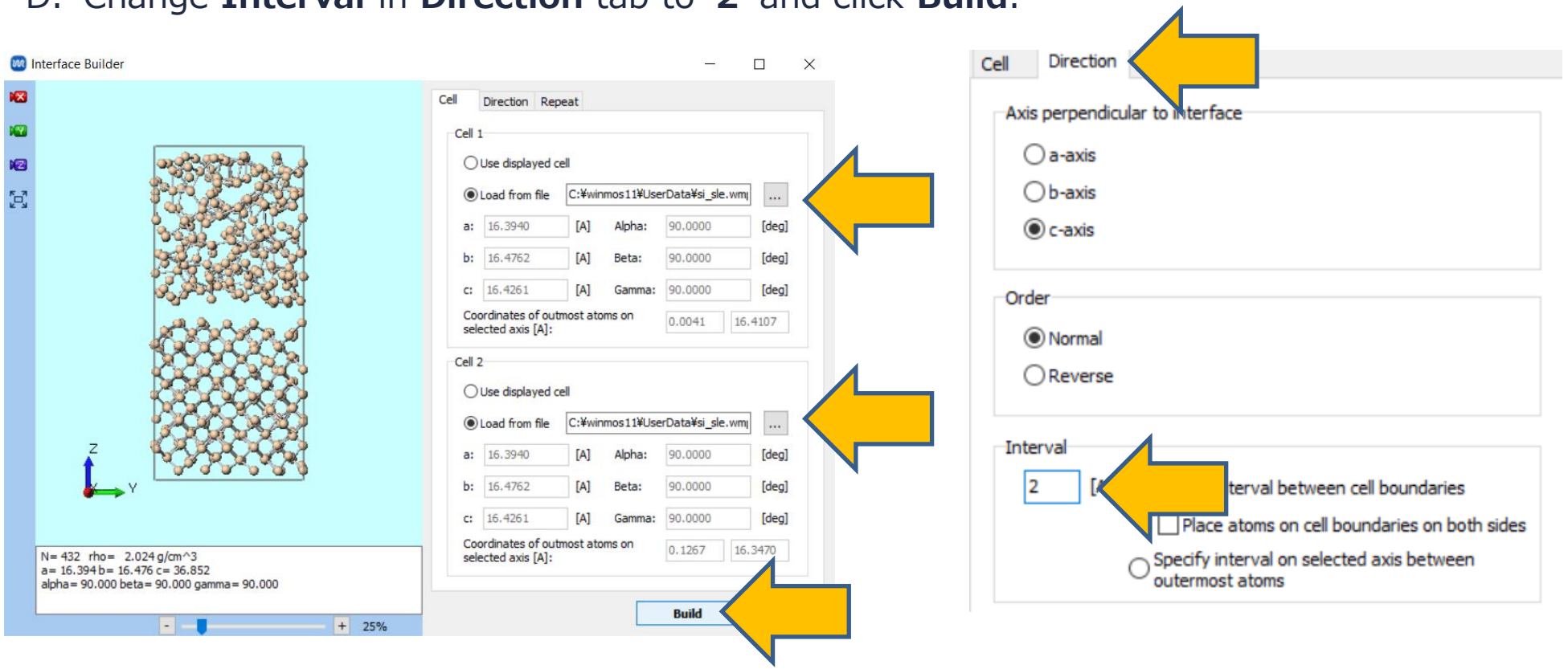
B. Click **(Export File)**, and save it under `si_sle.wmpjdata` folder with the file name '`si_liquid.cif`'.

※Atoms may appear outside the simulation cell, but when saved and loaded in CIF format with Winmostar, atoms are repositioned inside the simulation cell, so there is no problem.



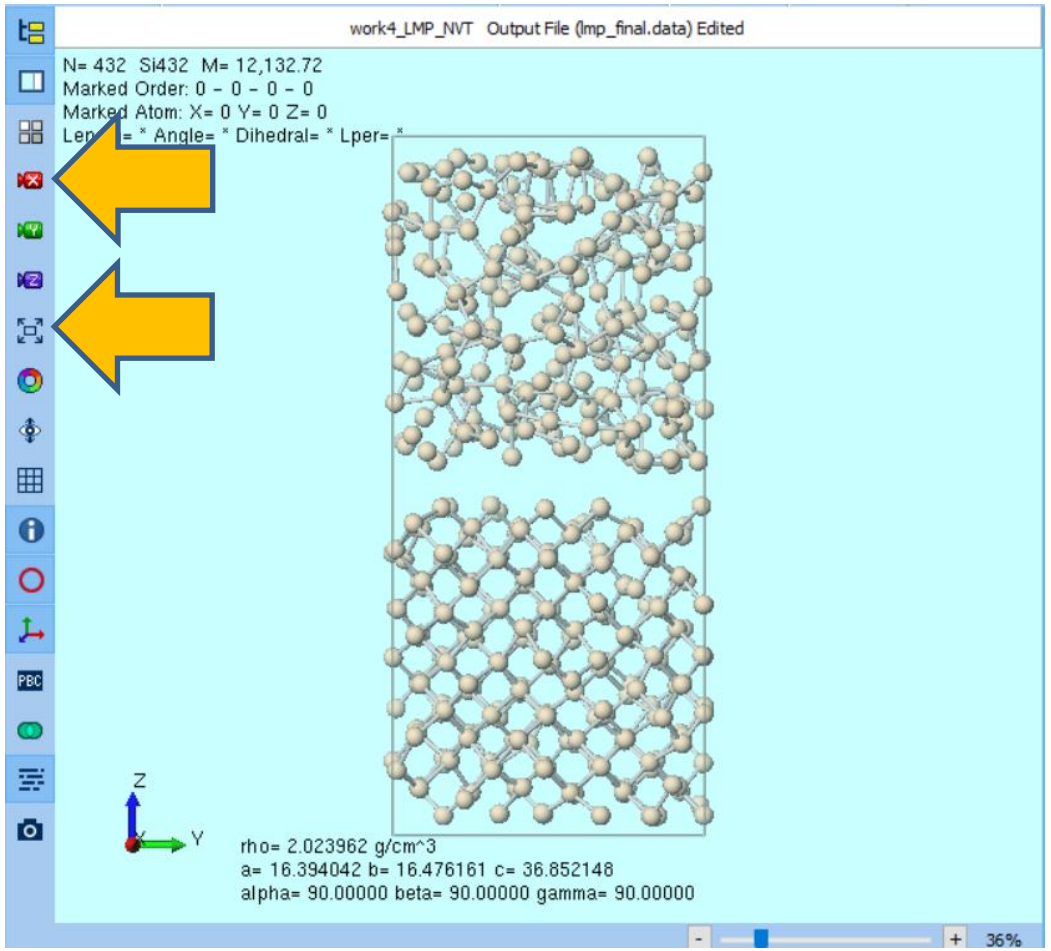
F. Modeling of the System（Interface System）

A. Click **MD** | **Interface Builder**.
B. Click **...** button for **Cell 1** and select `si_solid.cif` exported on P. 8.
C. Click **...** button for **Cell 2** and select `si_liquid.cif` exported on P. 10.
D. Change **Interval** in **Direction** tab to '**2**' and click **Build**.



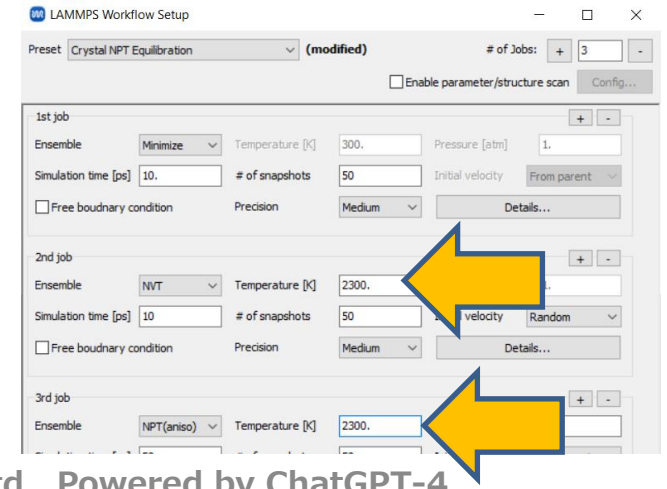
F. Modeling of the System（Interface System）

A. Click **(Align View to X-Axis)**.
B. Click **(Fit to Window)**.



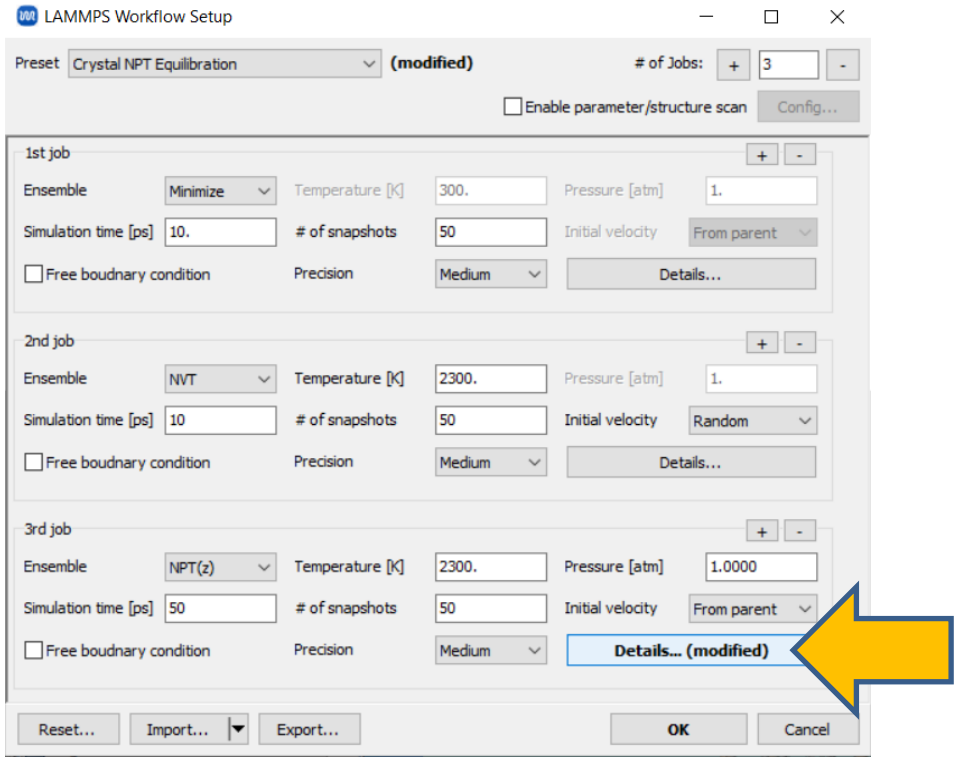
G. Execution of Calculation（Interface System）

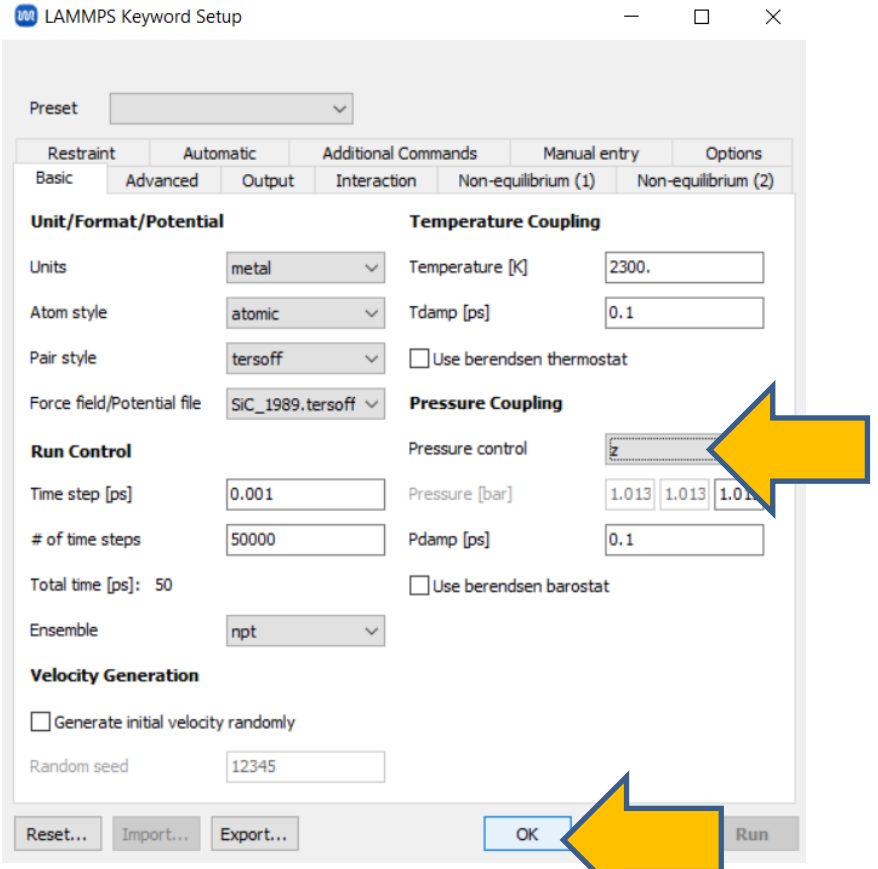
A. Click again **(Workflow Setup)**.
B. If prompted 'Do you want to continue from previous run?', click **No**.
C. If prompted 'Some molecules do not have charges. Do you want to assign charges now？', click **No**.
D. If prompted 'Indices are not sorted by molecules. Do you want to sort？', click **Yes**.
E. Select **Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** and click **Next**.
F. Change **Pair Style** to 'tersoff' and **Potential File** to 'SiC_1989.tersoff'.
G. Click **OK** and, when 'Assigned force field parameters' is displayed, click **OK**.
H. Change **Preset** to 'Crystal NPT Equilibration' and change **Temperature** for **2nd and 3rd job** to '2300'.



G. Execution of Calculation（Interface System）

A. Click **Details** for **3rd job**, change **Pressure control** to 'z', and click **OK**.
B. Click **OK**, then adjust settings as needed in **Job Setting** window and click **Run**.



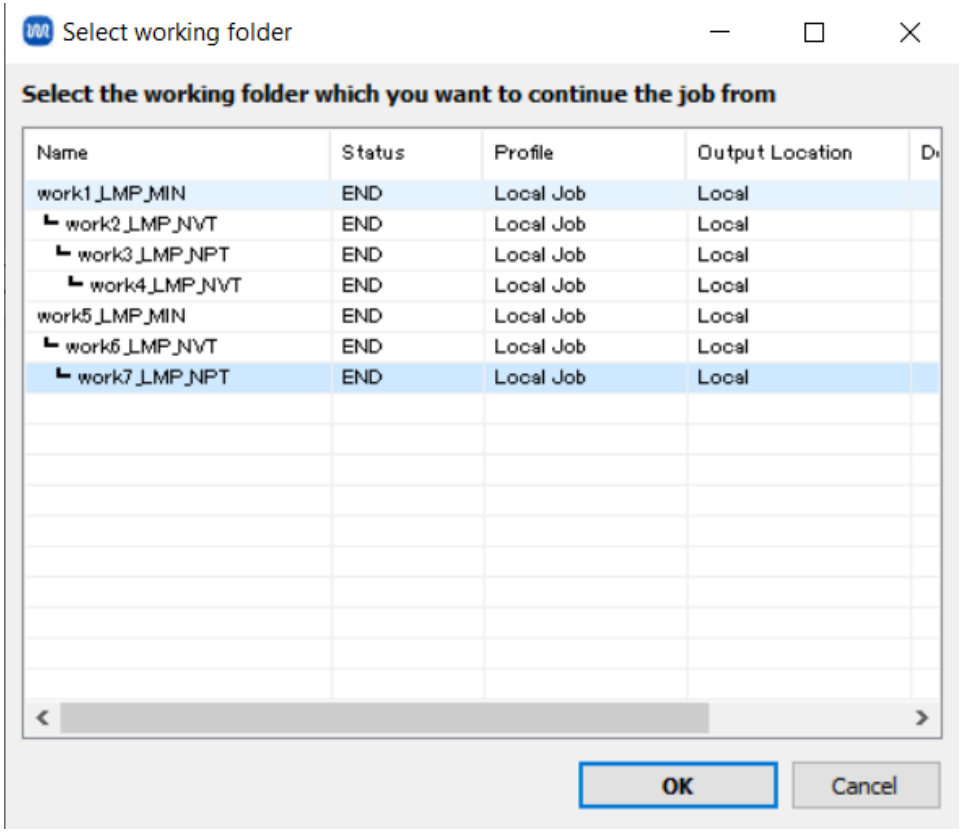


G. Execution of Calculation（Interface System）

A. Once **the status** of **the work folders** from work5_LMP_MIN to work7_LMP_NPT changes to **END** or **END(-)**, click again **(Workflow Setup)**.

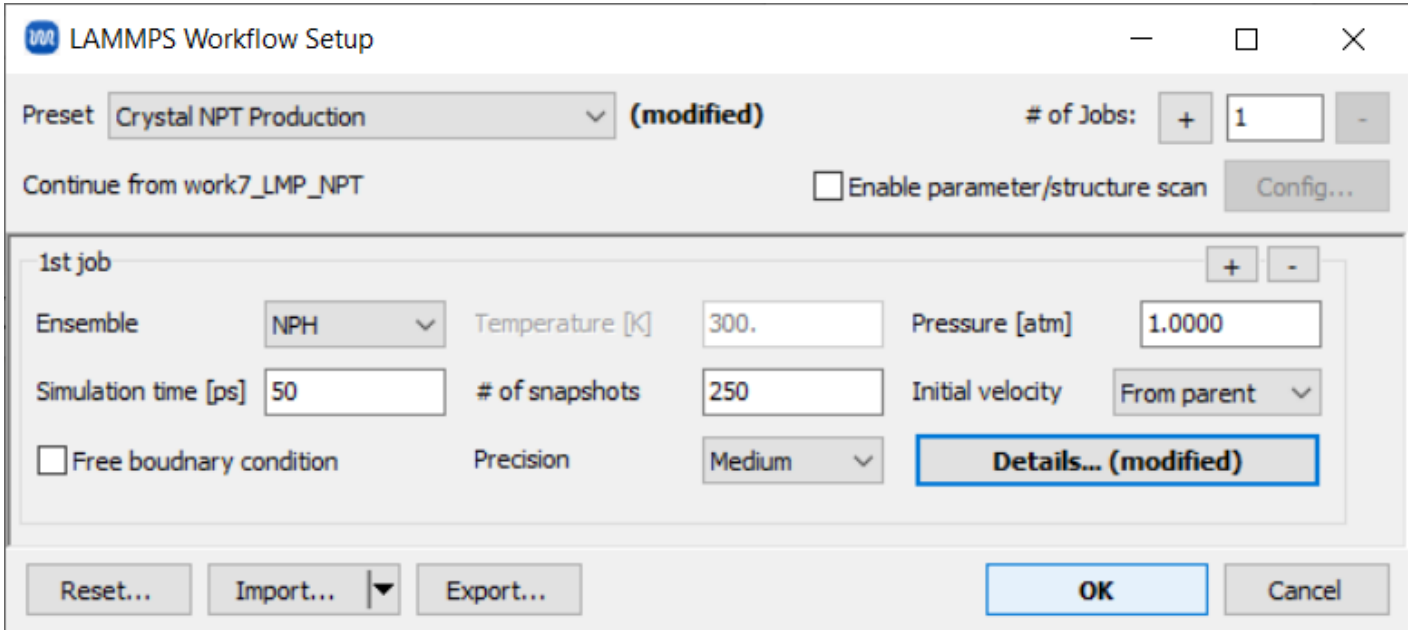
B. If prompted 'Do you want to continue previous run?', click **Yes**.

C. Select work7_LMP_NPT and click **OK**.



G. Execution of Calculation（Interface System）

A. Change **Preset** to 'Crystal NPT Production' and change **Ensemble** to 'NPH'.
B. Click **Details**, change **Pressure control** to 'z', and click **OK**.
C. Click **OK**, then adjust settings as necessary in **Job Setting** window and click **Run**.

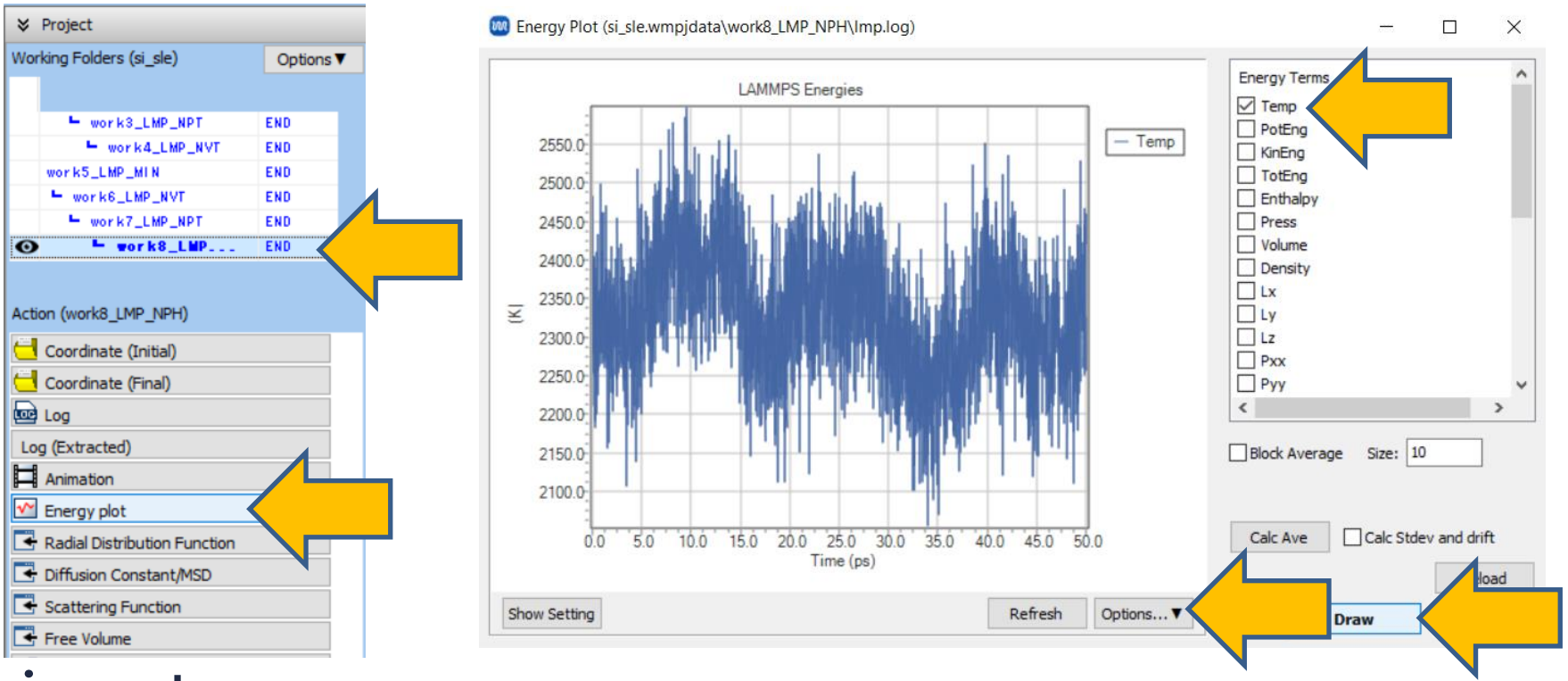


H. Analysis of Results

A. Once **the status** of **the work folder** for work8_LMP_NPH changes to **END** or **END(-)**, click on 'work8_LMP_NPH' in **Working Folders** and then click **Energy Plot** under **Action**.

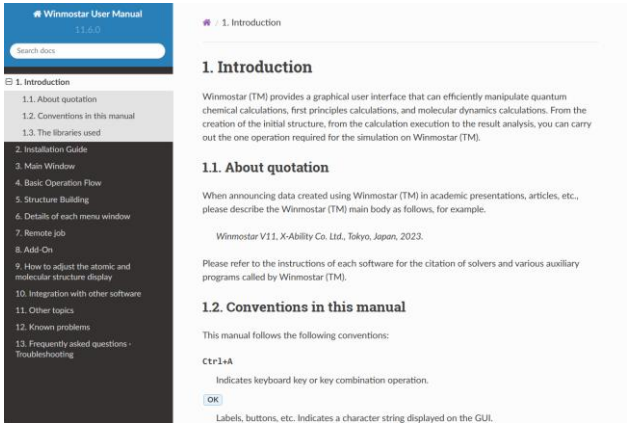
B. Check the box for **Temp**, and press **Draw** button to display the temperature change.

C. If you want to obtain the average temperature for a specific time range, use **Options | Calculate Average** below 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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