winmostar tutorial

# LAMMPS/Gromacs Electrolyte Systems

V11.5.6

7 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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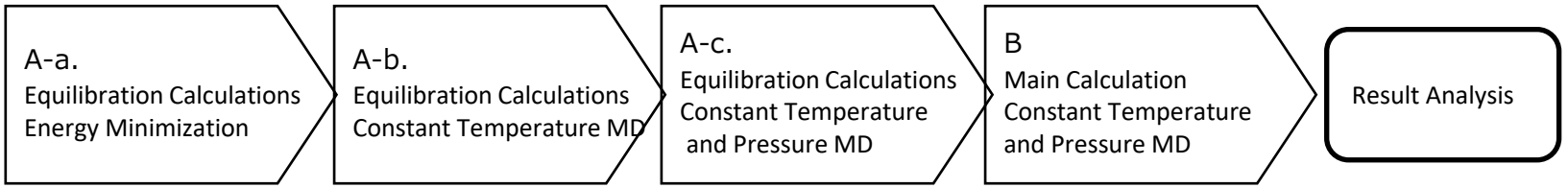
# Overview

- Perform MD simulations of a propylene carbonate (PC) solution of LiBF4, which is used as an electrolyte for lithium-ion batteries, and calculate the self-diffusion coefficients of each component.

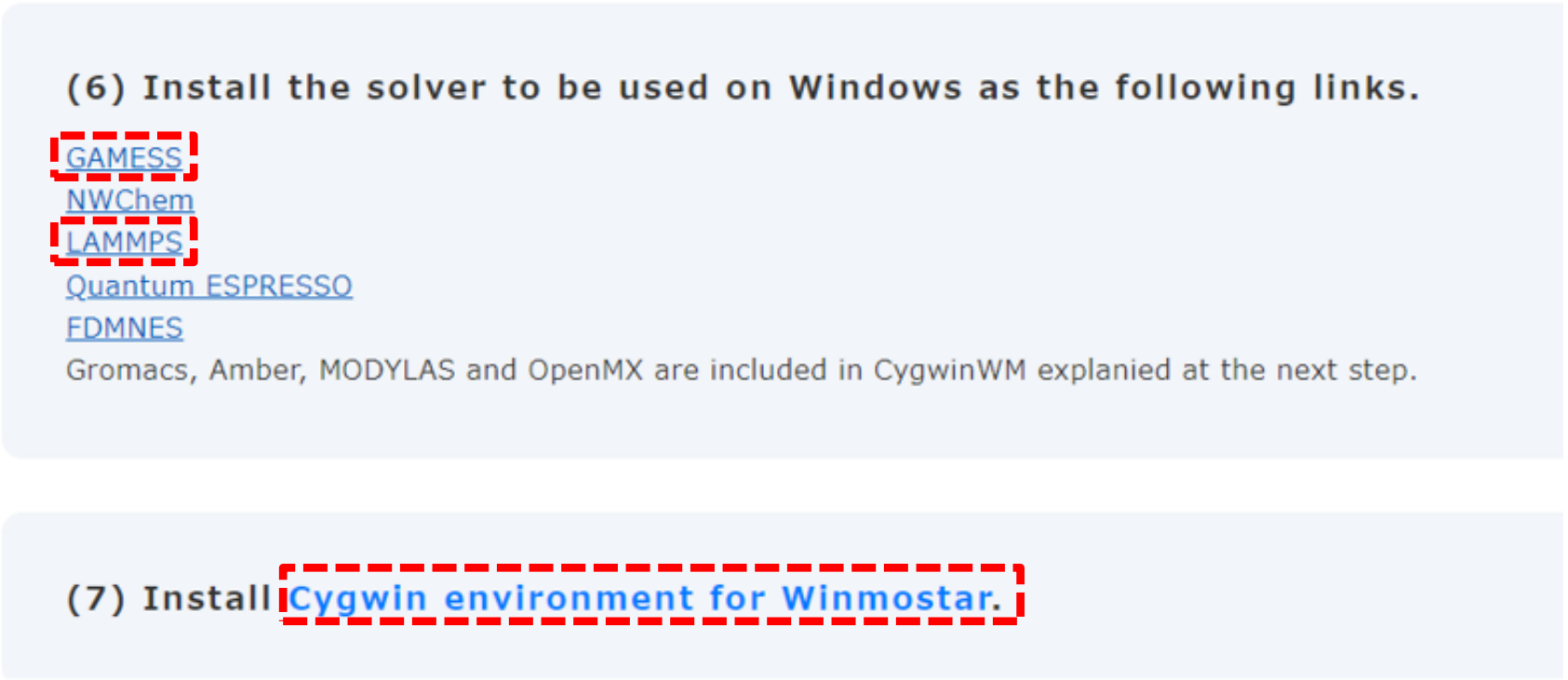



Note:

- In MD simulations of ionic solutions, it may be necessary to empirically tune force fields and charges to reproduce ionic conductivities obtained from experiments. For example, calculating PF6- ions with the Dreiding force field may result in equilibrium structures significantly deviating from experimental values, requiring caution. In such cases, refer to Force field auto-editing tutorial.
- To shorten the tutorial duration, the number of molecules is reduced, and the number of steps for equilibration calculations is set lower. Quantum chemical calculations for structure optimization before assigning charges to molecules are also omitted.
- The number of steps required for equilibration varies depending on the type of molecule and initial density.
- Larger 'production run' step numbers improve reproducibility and yield more reliable results.

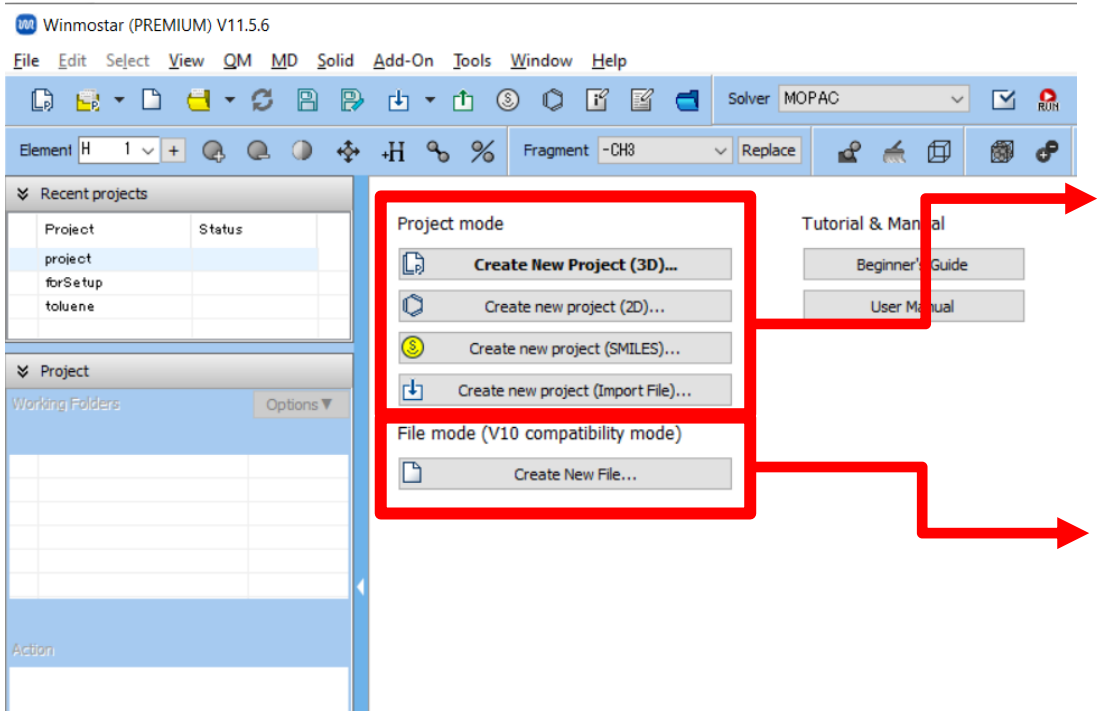
# Preference of Operating Environment

- To use this feature, the setup of Cygwin and GAMESS is required. For using LAMMPS, the setup of LAMMPS is necessary.
- **https://winmostar.com/en/installation/** The installation method for GAMESS, LAMMPS and Cygwin on Windows.



# 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

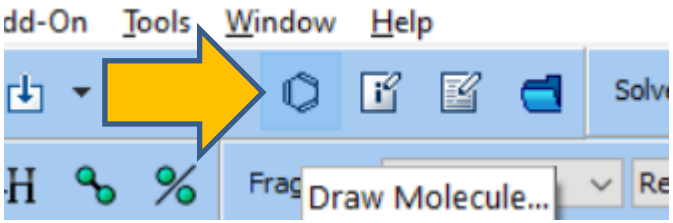
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

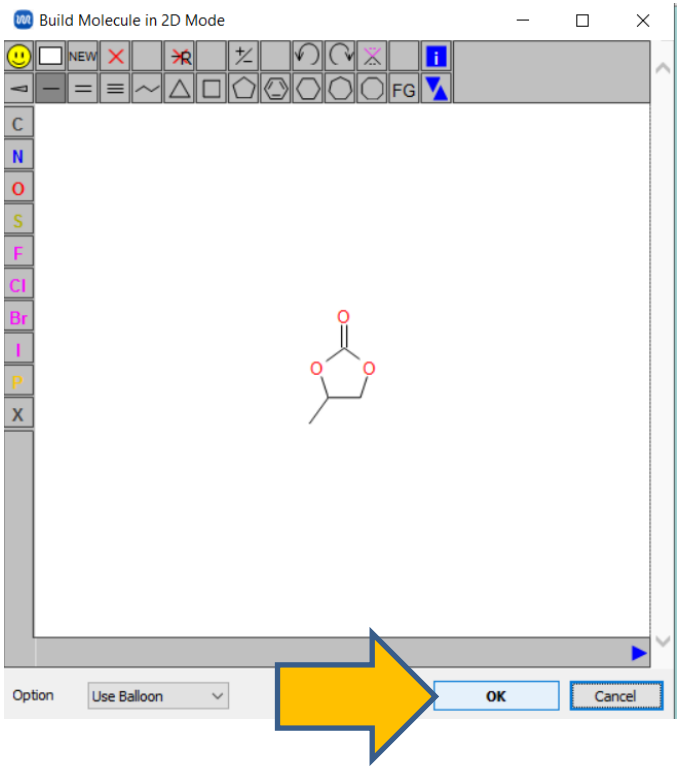
# A. Modeling of the System (PC)

Refer to LAMMPS Basics Tutorial or Gromacs Basics Tutorial for basic operation methods.

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

B. Click **(Draw Molecule)** in Toolbar, create a molecule as shown in the diagram below, and click **OK**.

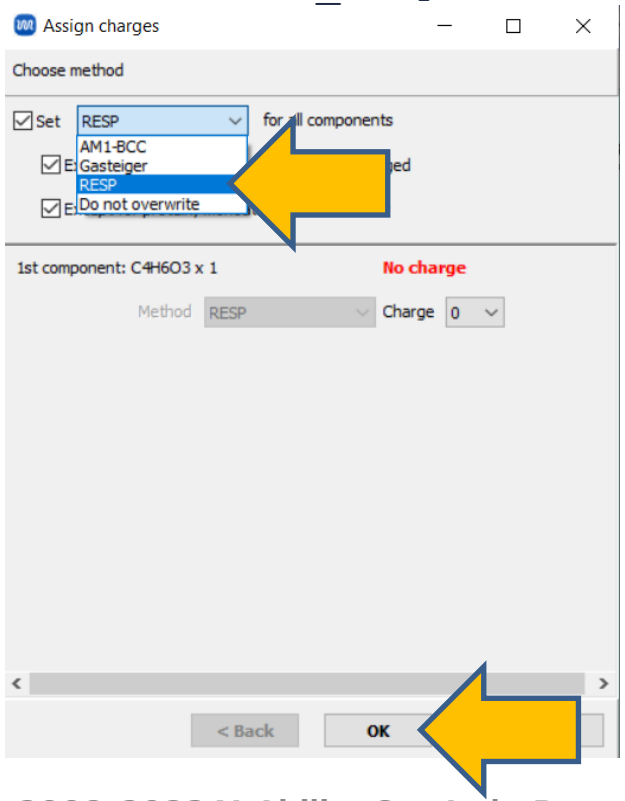


# A. Modeling of the System (PC)

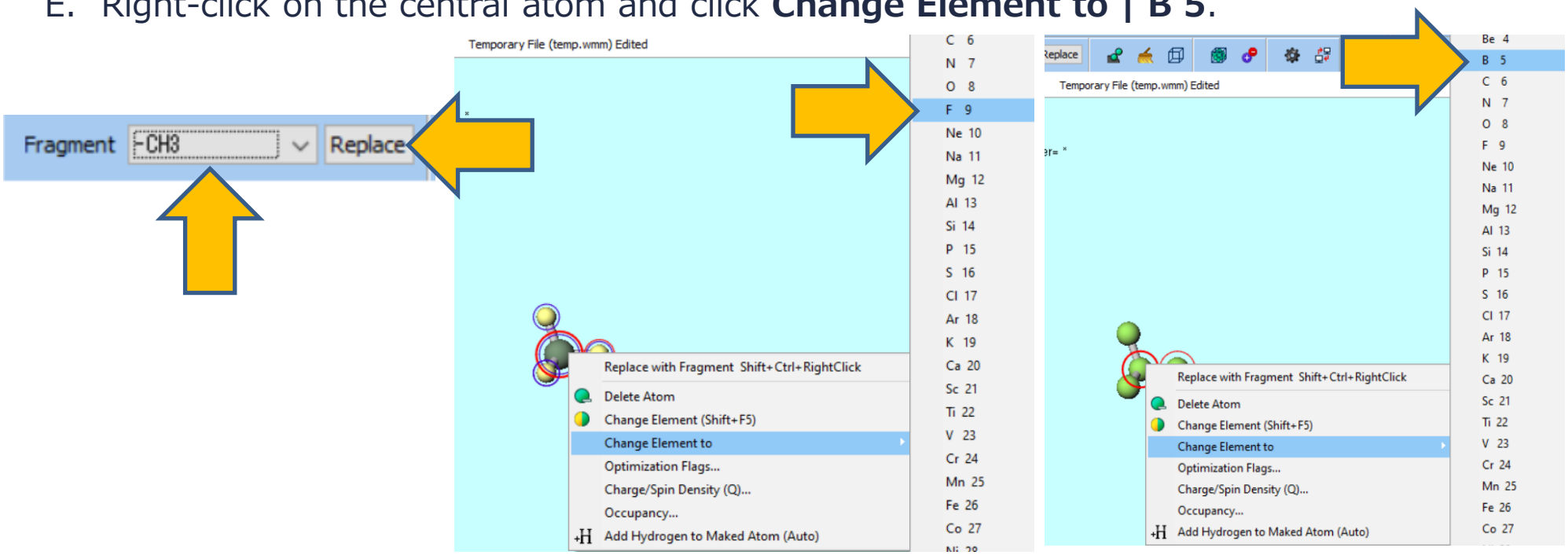
A. Click **Assign Charges Automatically**, change 'Set' to 'RESP', and click **OK**. If a message saying 'Successfully assigned charges' appears, click **OK**.
   – If necessary, perform structural optimization calculations using GAMESS before assigning charges.

B. Click **Export File** and save as '`PC_resp.mol2`'.



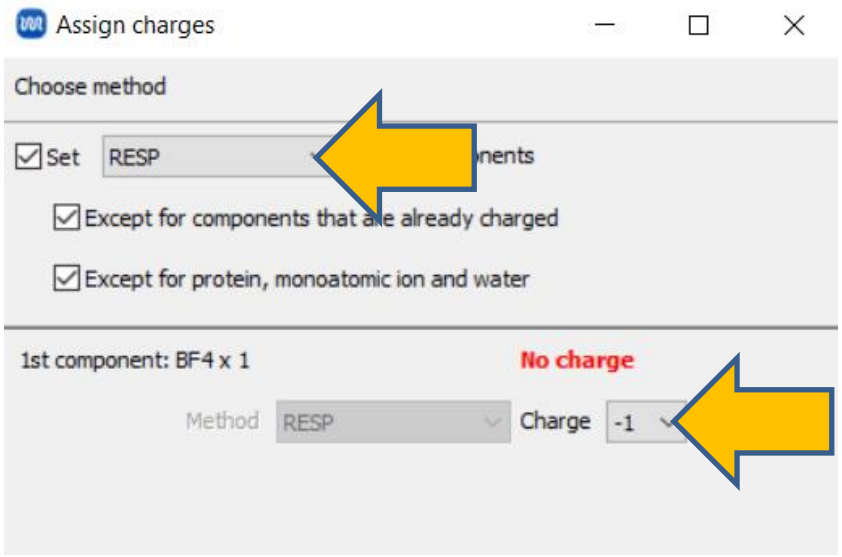
# A. Modeling of the System ($BF_4^-$)

A. Click **Edit | Reset Structure**, select **Fragment** '-CH3' and click **Replace** to create methane.
B. Shift-click on methane to select it as a group.
C. Right-click on any atom and click **Change Element to | F 9**.
D. Click on an empty space to deselect the group selection.
E. Right-click on the central atom and click **Change Element to | B 5**.



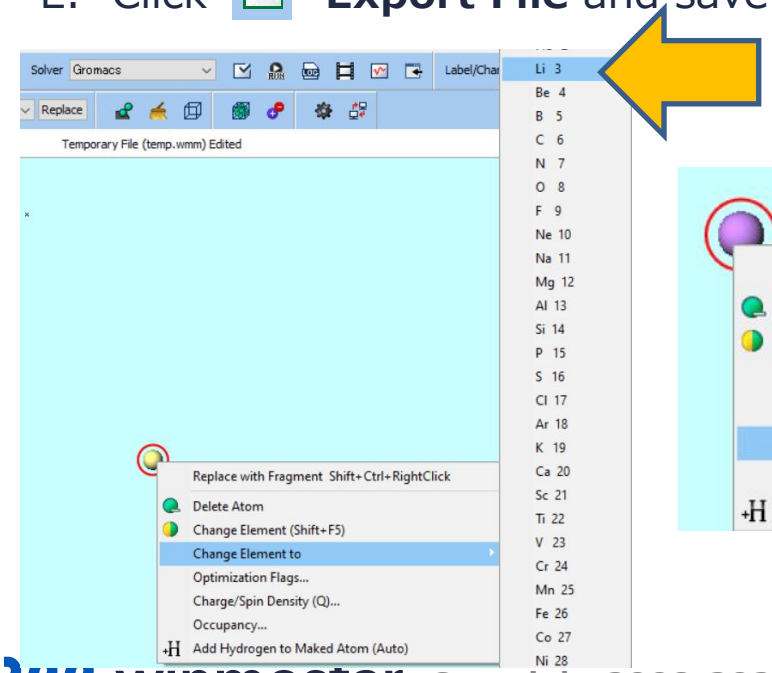
# A. Modeling of the System ($BF_4^-$)

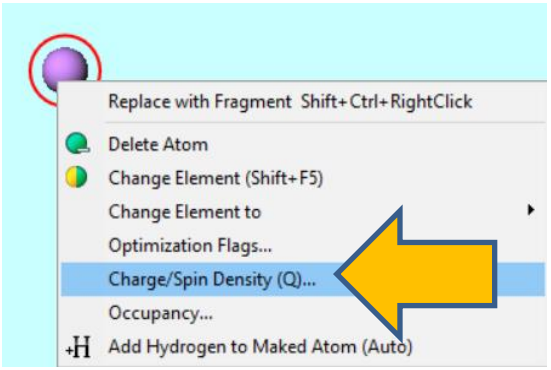
A. Click **Quick Optimization**.
B. Click **Assign Charges Automatically**, change 'Set' to 'RESP' and modify **Charge** of **1st component** to '-1' then click **OK**. Click **OK** again when 'Successfully assigned charges' is displayed.
C. Click **Export File** and save as '`BF4_resp.mol2`'.
   – If you wish to change the absolute value of the ion charge (for example, making the total charge of BF4- to -0.75), first follow the above steps to assign the charges. Then click Select | Select All, click Edit | Change Atom Property | Charge/Spin Density, check Scale, enter the scaling factor to the right, and click OK.

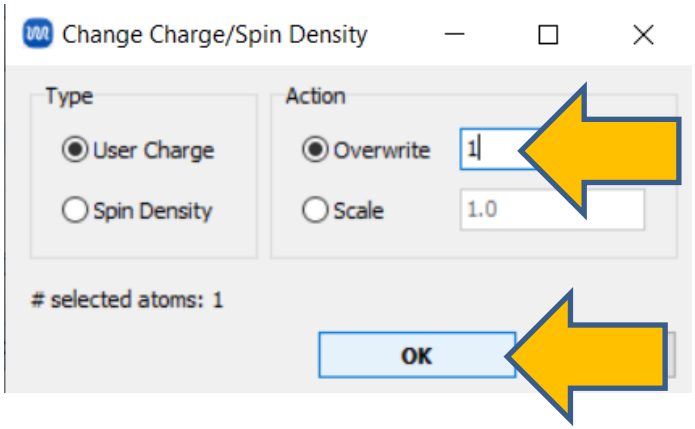


# A. Modeling of the System（$Li^+$）

A. Click **Edit | Reset Structure**, then click **Delete Atom**. Click **Yes** when asked 'Are you sure…'.
B. Right-click an atom and click **Change Element to | Li 3**.
C. Right-click the atom again and click **Change/Spin Density**.
D. Enter '1' next to **Overwrite** and click **OK**.
   – If you wish to change the absolute value of the ion charge, enter that value.
E. Click **Export File** and save as '`Li.mol2`'.



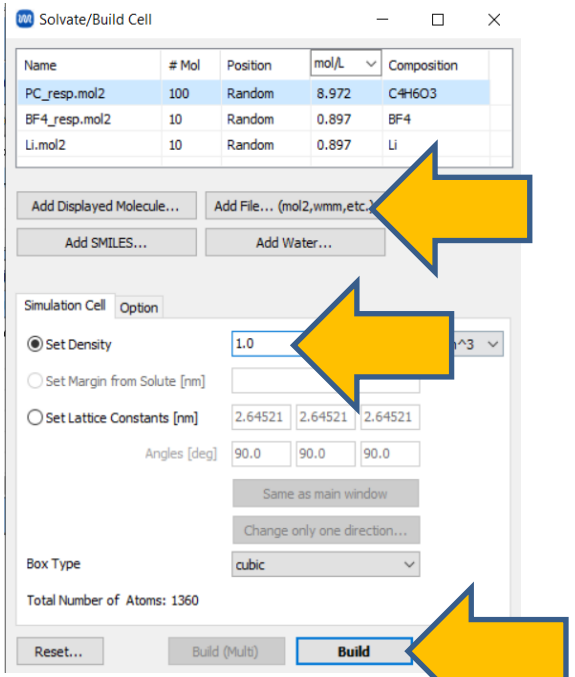
# A. Modeling of the System (Creating the Liquid Phase)

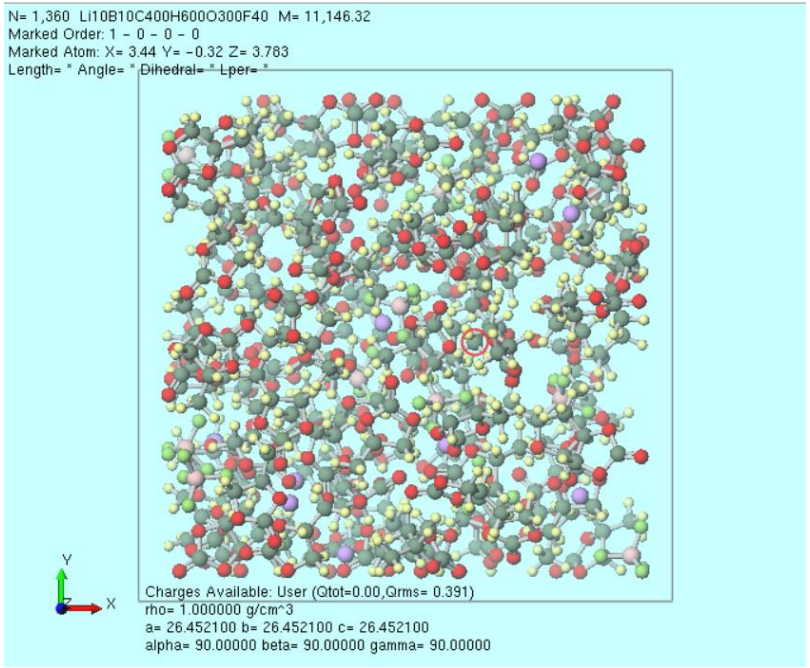
A. Click **Solvate/Build Cell**.

B. Click **Add File…(mol2,wmm,etc.)** and select `PC_resp.mol2` saved in P. 7, enter '100' for **Enter # of molecules**, and click **OK**.

C. Follow the same steps to add 10 molecules of `BF4_resp.mol2` and 10 molecules of `Li.mol2`.

D. Change the value of **Set Density** to '1.0' and click **Build**.



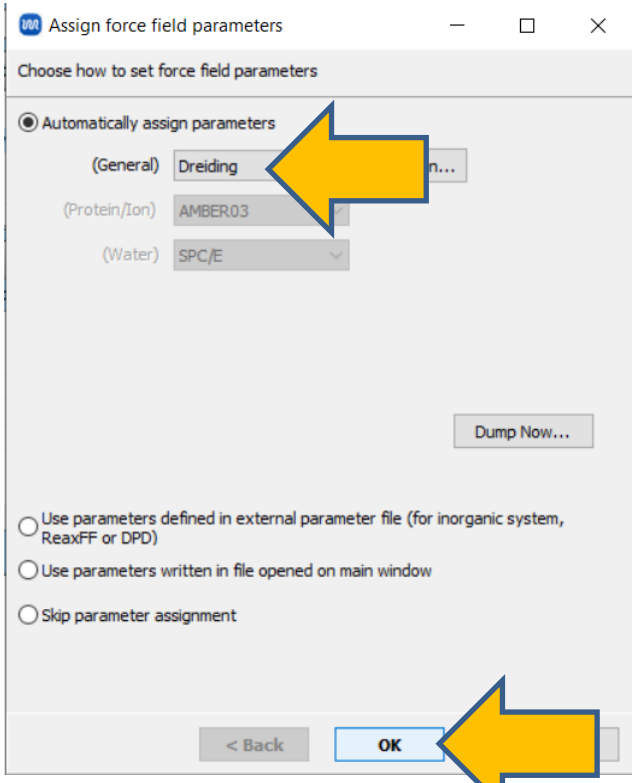



# B. Execution of Calculation (Equilibration)

A. Select 'LAMMPS' or 'Gromacs' as **Solver**, and click **(Workflow Setup)**. Then change (**General**) to 'Dreiding' and click **OK**.

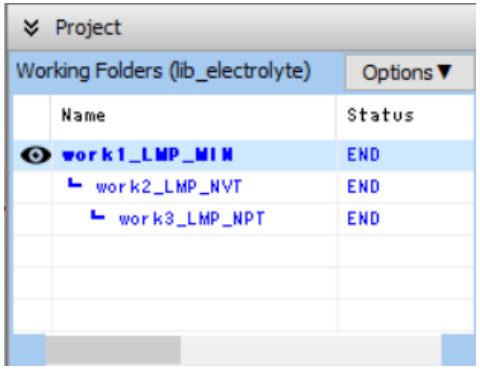
B. If you want to decrease the calculation precision to finish the computation faster, change **Precision** to 'Low' for **1st job**, **2nd job**, and **3rd job**.

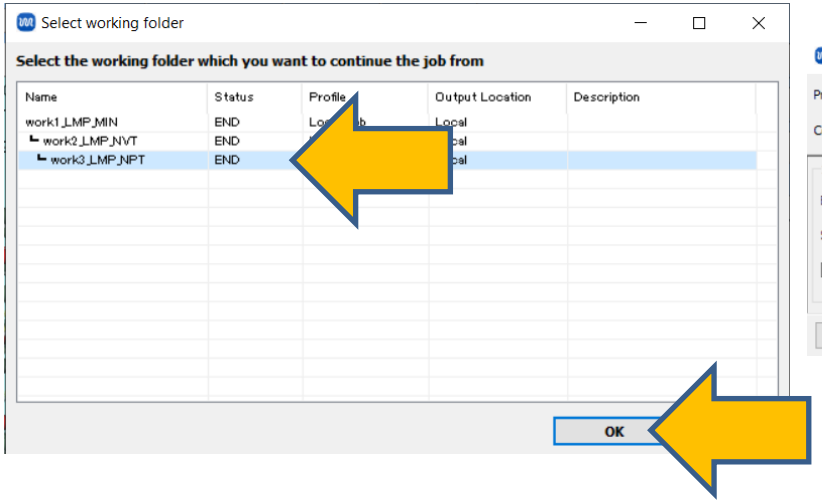
C. Click **OK**, then in **Job Setting** window, adjust the settings as needed and click **Run**.

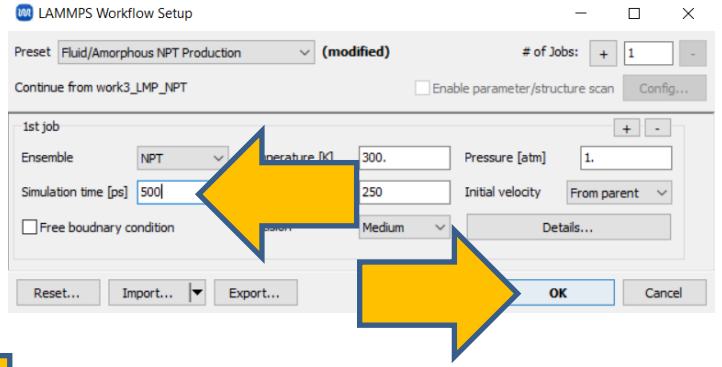


# C. Execution of Calculation (Main Calculation)

A. Once **the status** of work3 folder changes to **END** or **END(-)**, click **(Workflow Setup)**.
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.
C. Select work3_LMP_NPT or work3_GMX_NPT and click **OK**.
D. Change **Preset** to 'Fluid/Amorphous NPT Production.'
E. Modify **Simulation time** to '500' and click **OK**.
F. To expedite the calculation by reducing precision, set **Precision** to 'Low' and **Simulation time** to '50.'
G. After appropriately adjusting settings in **Job Setting** window, click **Run**.



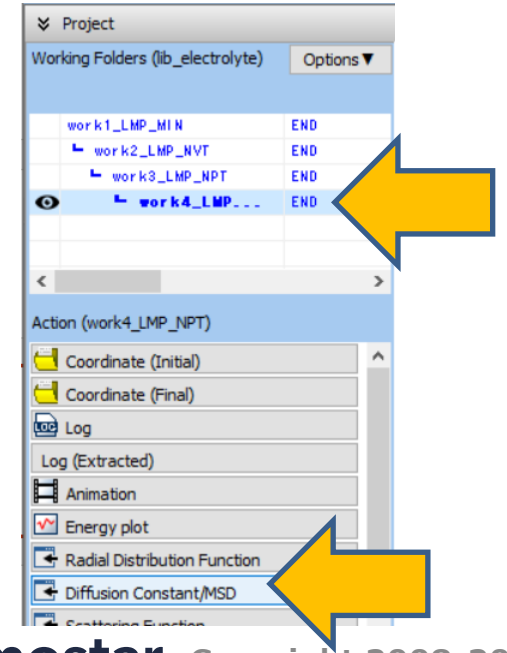



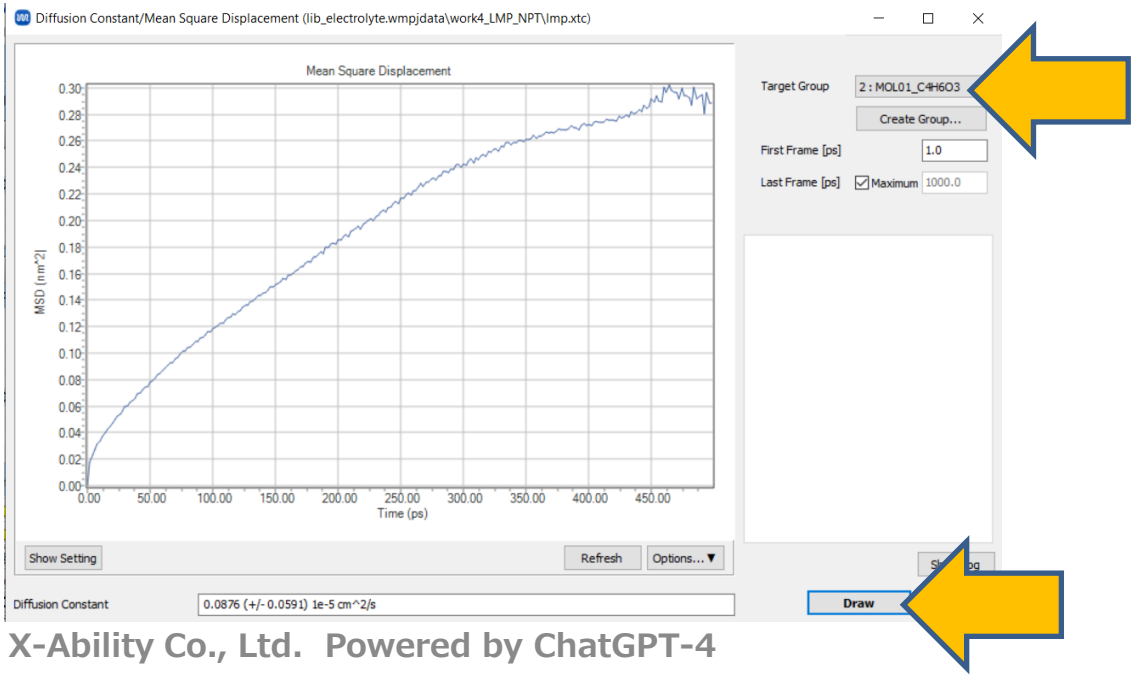



# D. Analysis of Results

A. Once **the status** of work4 folder changes to **END**, click on work4_LMP_NPT or work4_GMX_NPT, then click **Diffusion Constant/MSD** under Action. For remote jobs, click **Receive all remote output files** first to fetch the output files.

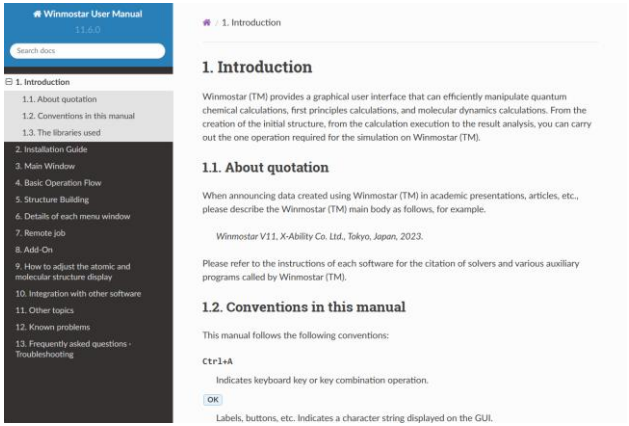
B. Select **Target Group** for which you wish to calculate the self-diffusion coefficient (for LAMMPS, choose MOL01_C4H6O3 for PC, MOL02_BF4 for BF4, MOL03_Li for Li; for Gromacs, select MOL01 for PC, MOL02 for BF4, LI for Li) and click **Draw**.
   - Using the Nernst-Einstein equation allows for the estimation of ionic conductivity from **Diffusion Constant**.



# 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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