winmostar tutorial

LAMMPS/Gromacs Automatic Force Field Editing

V11.3.0

1st Oct. 2022

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 requires Winmostar V11 Professional Elite edition. Once set up, simulations can be run with both LAMMPS and Gromacs, with rigid structures supported exclusively in LAMMPS.

1. **Assignment of the OPLS-AA Force Field**
   Assign the OPLS-AA force field to ethanol using mktop. Unlike the conventional method using acpype with OPLS-AA/L+GAFF, OPLS-AA is applied also to intramolecular potentials.
2. **Automatic Parameter Assignment for Rigid Structures**
   - Automatically assign UFF or Dreiding LJ parameters to graphene. Unlike conventional methods, there is no need for manual input of LJ parameters.
3. **Auto-Completion for Failed Assignments**
   - Assign a combination of GAFF and Dreiding parameters to silanol. Unlike conventional methods, there is no need to interrupt the process even if some degrees of freedom lack parameter definitions.
4. **Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations**
   - Adjust the force field parameters of the PF_6^- ion based on equilibrium bond lengths and angles obtained from GAMESS calculations. This approach helps prevent structural distortions that can occur when using the default values from general-purpose force fields.

Note

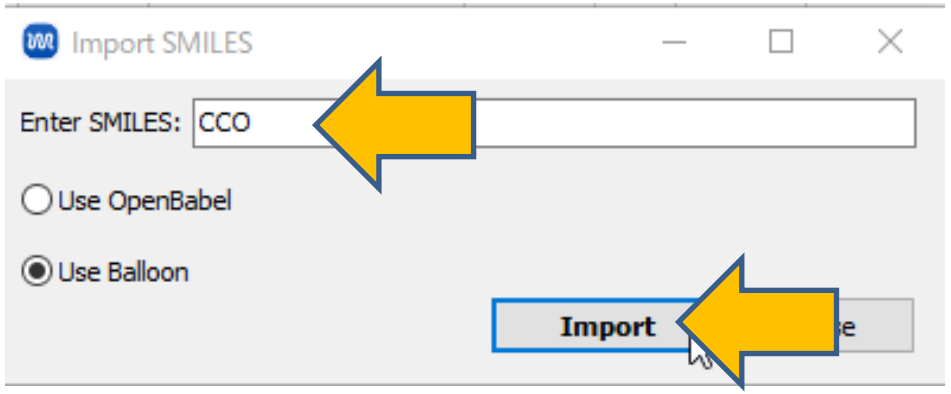
- When editing charges or force fields, it is recommended to run actual simulations and evaluate the structure and various properties to assess the impact of the changes.

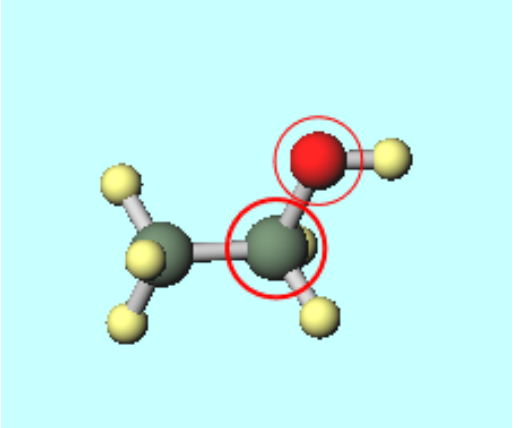
A. Auto-assignment of the OPLS-AA Force Field

Refer to LAMMPS Basics Tutorial for basic operation methods.

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

B. Click **Import SMILES** on the toolbar, enter 'CCO' (in all uppercase), and then click **Import**. After the process completes, when the message 'Successfully finished.' appears, click **OK**.



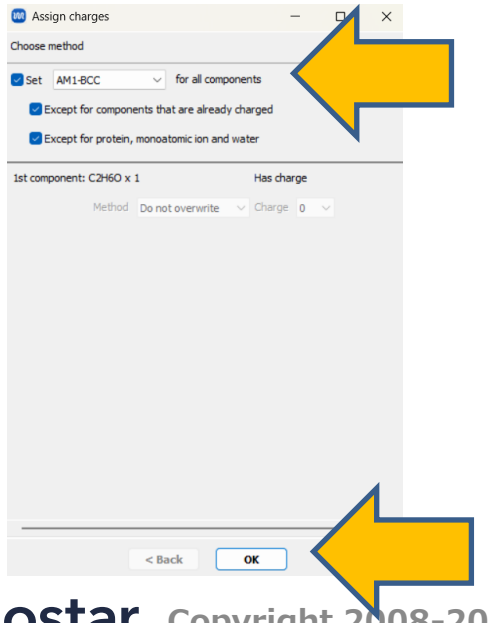


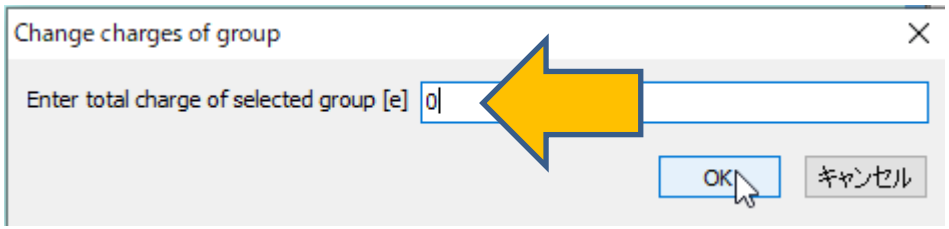
A. Auto-assignment of the OPLS-AA Force Field

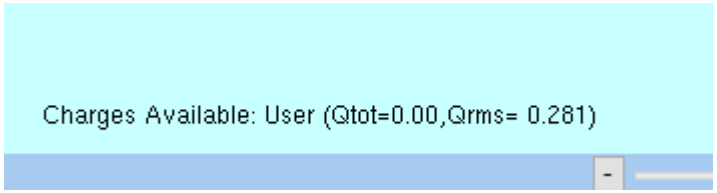
A. Click  **Assign Charges Automatically** and then click **OK**.

B. Select the desired type of charge using '**Set ... for all components**' and click **OK**. If you want to use OPLS-AA charges, select 'OPLS-AA'.

C. When using OPLS-AA charges for ethanol, a message will appear stating: 'Total charge OPLS-AA obtained by mktop is not an integer value.' If you want to force the total charge to be an integer, click **Select | Select All** then click **Edit | Modify Selected Group | Change Charges of Group**, enter an appropriate value (e.g., "0" for neutral molecules like ethanol), and click **OK**. You can check the total system charge under "Qtot=" at the bottom of the molecule display area.

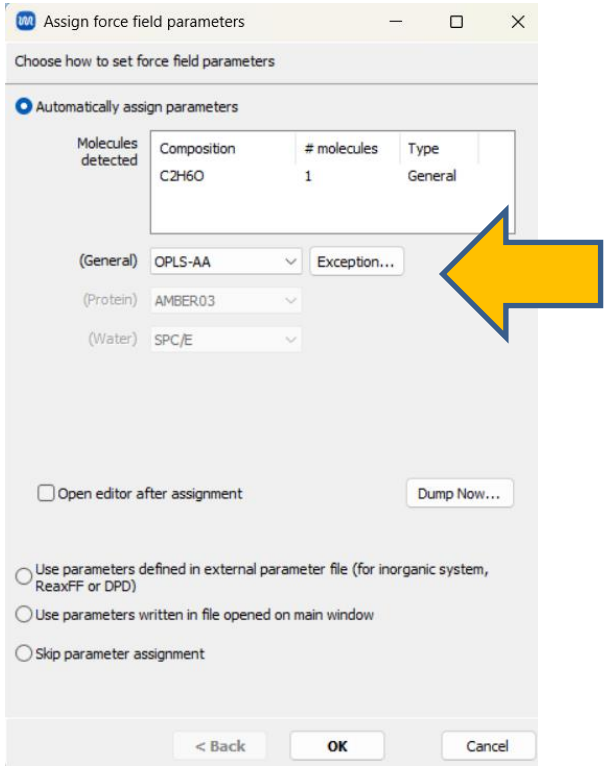






A. Auto-assignment of the OPLS-AA Force Field

A. Select **LAMMPS** or **Gromacs** as Solver, and click **(Workflow Setup)**
B. When the 'Create Cell' / 'Enter Margin' dialog appears, simply click **OK**.
C. Select the force field you want to use (e.g., OPLS-AA) at (General) in **Automatically assign parameters**.
D. The subsequent steps follow the procedures outlined in LAMMPS Basics Tutorial and related guides.



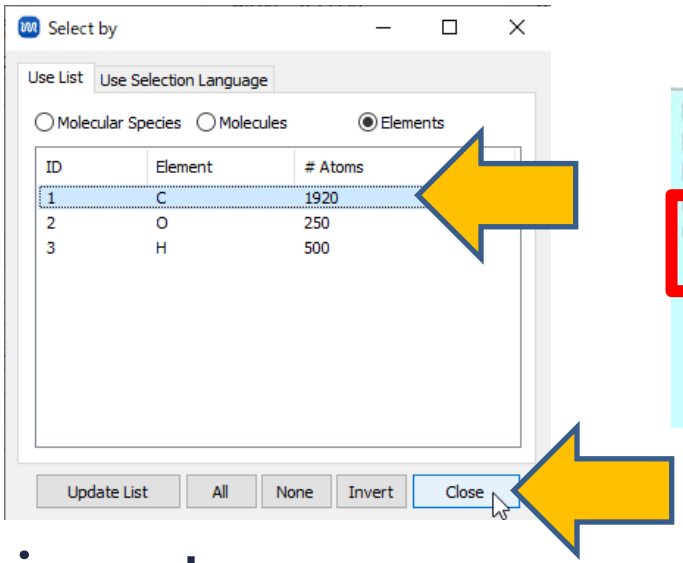
B. Automatic Parameter Assignment for Rigid Structures

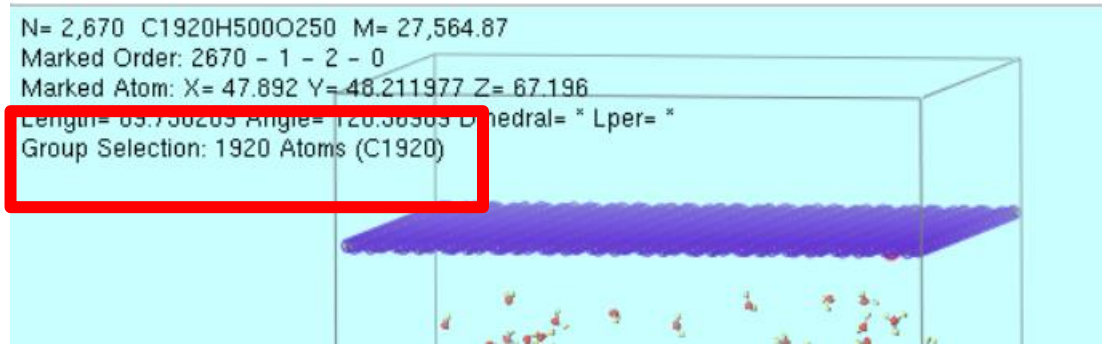
Refer to LAMMPS Basics Tutorial for basic operation methods.

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

B. Click **File | Import | Samples File | graphene_water_graphene.mol2**.
- If you wish to load a different file at this stage, use File | Import File instead.

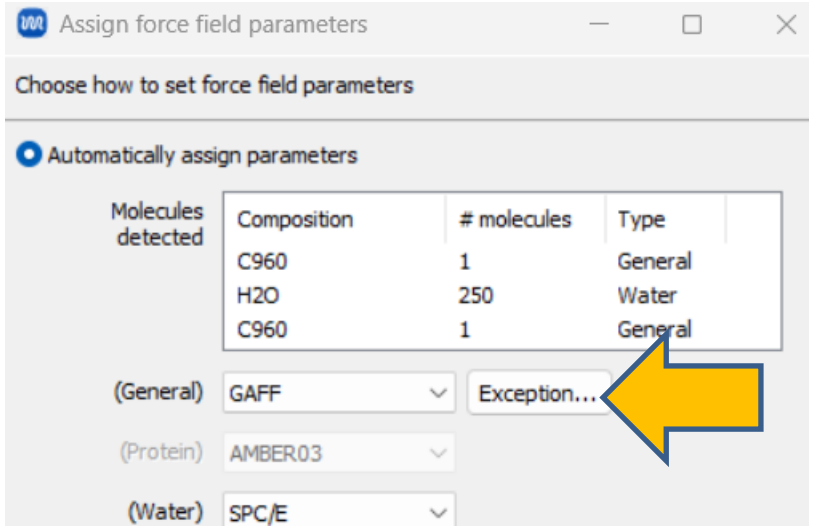
C. Click on the row labeled '1 C 1920' and click **Close**. Click **Select | Register Selected Group**, enter '**graphene**' as **Group name**, and click **OK**.
(Although this guide does not cover running MD simulations, the procedure described here is necessary to set up rigid structure for the simulation.)

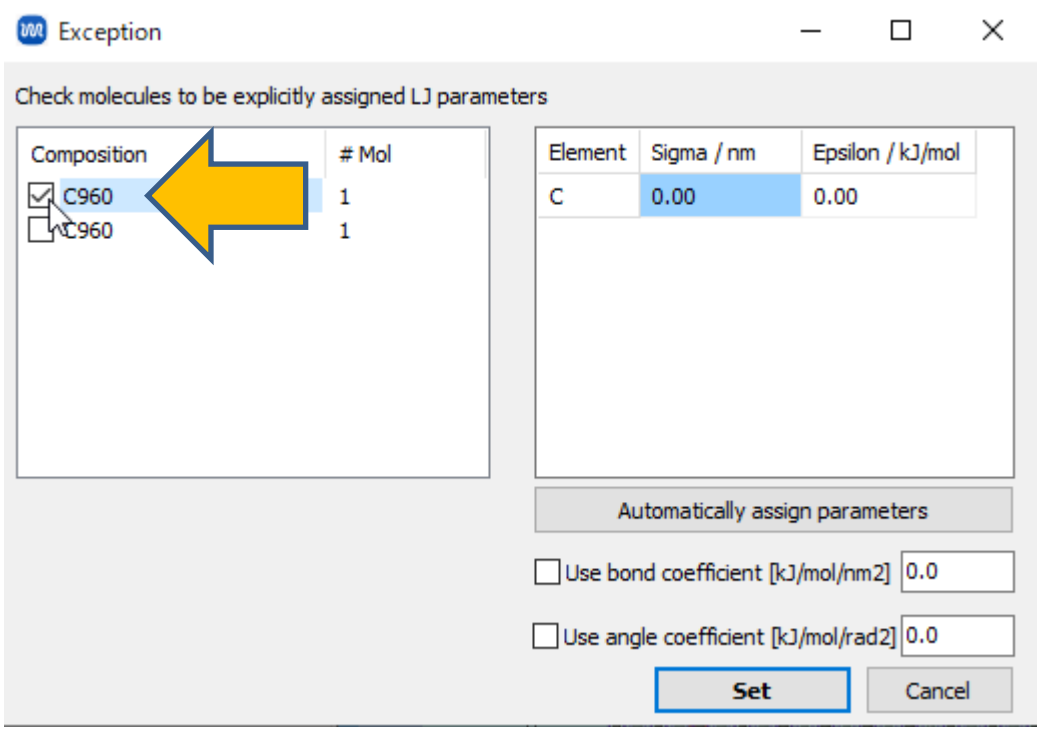




B. Automatic Parameter Assignment for Rigid Structures

A. Select **LAMMPS** from **Solver** and click **(Keyword Setup)**.
B. If prompted with '**Some molecules do not have charges. Do you want to assign charges now?**', click **No**.
C. Click **Exception**.
D. Check the first **C960** in the list on the left



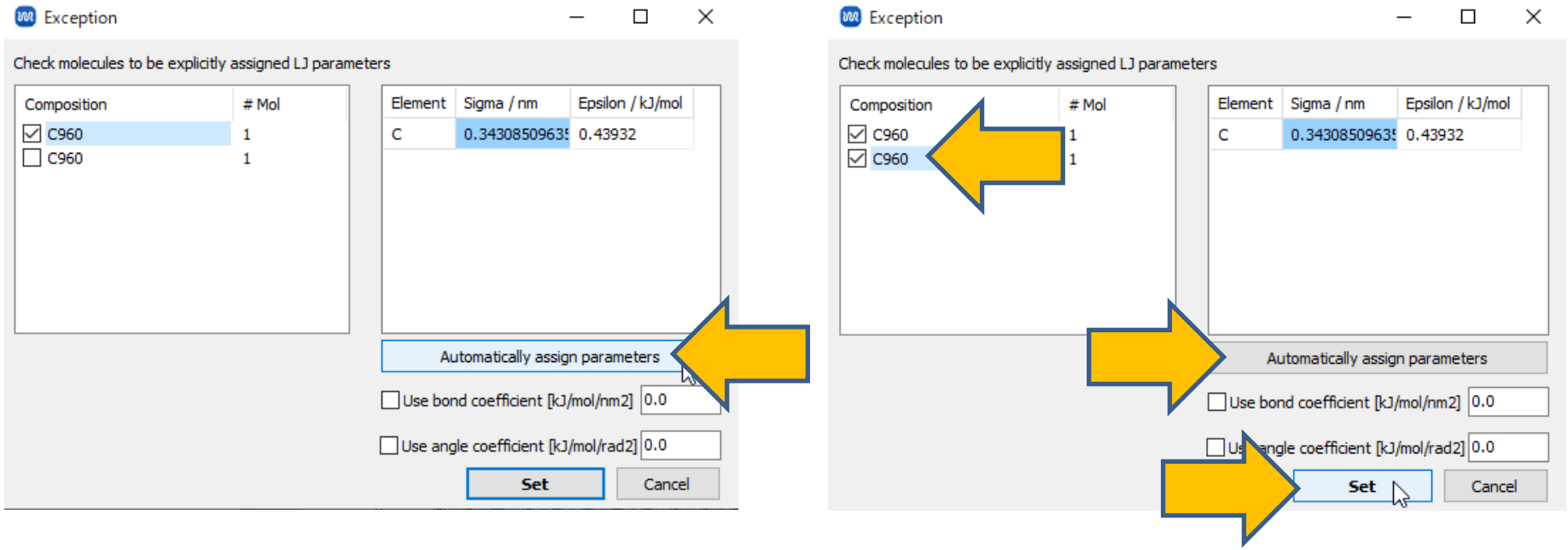


B. Automatic Parameter Assignment for Rigid Structures

A. Click **Automatically assign parameters**, select ‘UFF’ or ‘Dreiding’ under ‘Select force field,’ and the parameters will be automatically populated in the list above.

B. Check ‘C960’ in the second row of the **Composition** section, then similarly click **Automatically assign parameters** and select either ‘UFF’ or ‘Dreiding’.

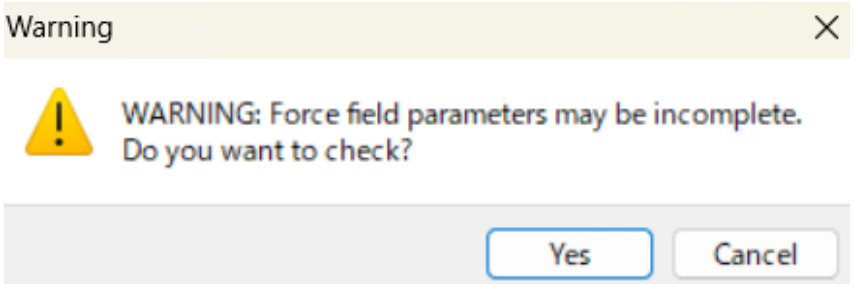
C. Click **Set**. The subsequent steps follow the procedure outlined in the LAMMPS tutorial for systems with solid walls.



C. Auto-Completion for Failed Assignments

Refer to LAMMPS Basics Tutorial for basic operation methods.

A. Click **File | New Project**, enter 'silanol_gaff_dreiding' in **Project name**, and click **Save**.
B. Click **File | Import | Samples File | silanol_resp.mol2**.
C. Select **LAMMPS** or **Gromacs** as Solver, and click **(Workflow Setup)**
D. When the 'Create Cell' / 'Enter Margin' dialog appears, simply click **OK**.
E. In "Assign force field parameters' window, click **OK** with the default settings (GAFF). When the message 'Force field parameters may be incomplete. Do you want to check?" appears, click **Yes**.

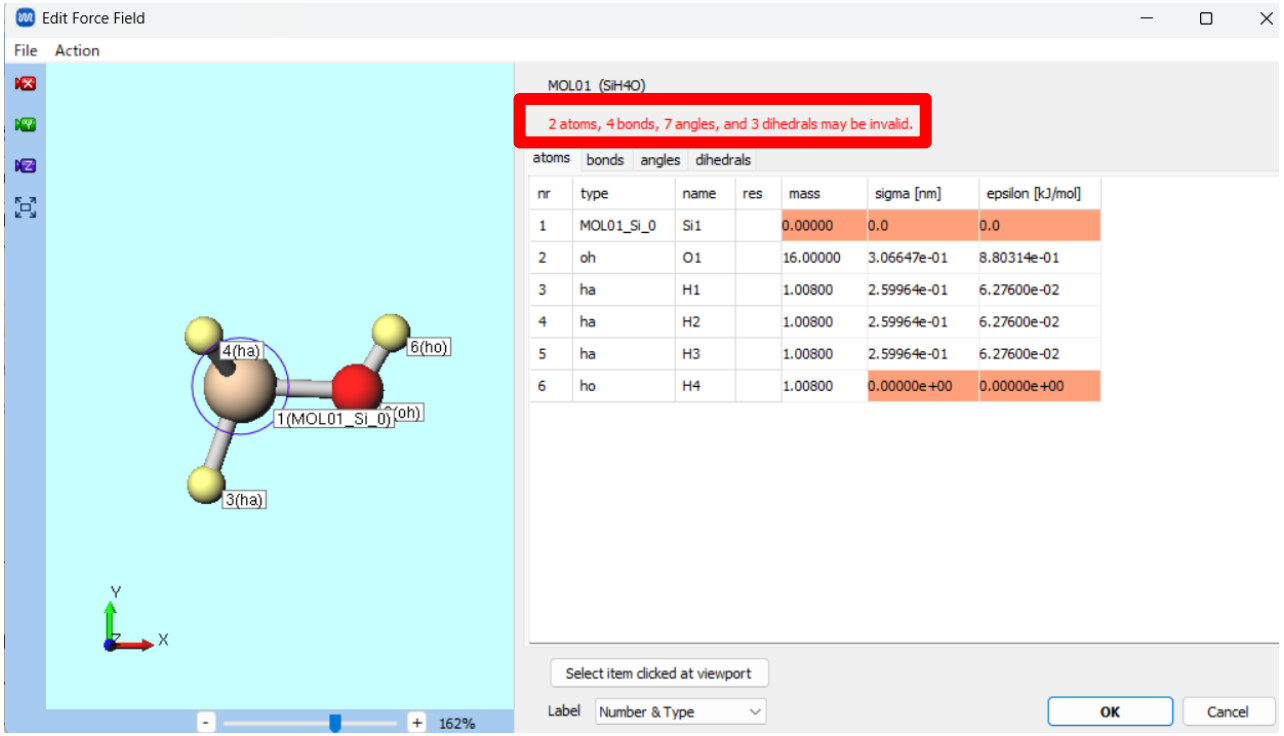


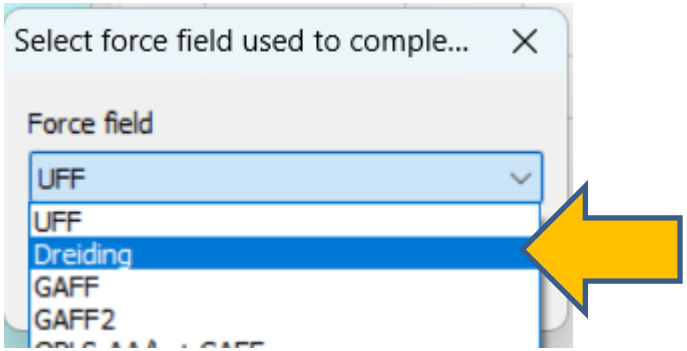
C. Auto-Completion for Failed Assignments

A. At the top of **Edit Force Field** window, a warning in red text will appear stating '2 atoms, 4 bonds··· may be invalid', indicating that some degrees of freedom failed to be assigned using GAFF.

B. Click **Action** | **Complement,** change the Force Field from 'UFF' to 'Dreiding', and then click **OK**.

C. When the message 'Complemented 1 atoms···' appears, click **OK**.

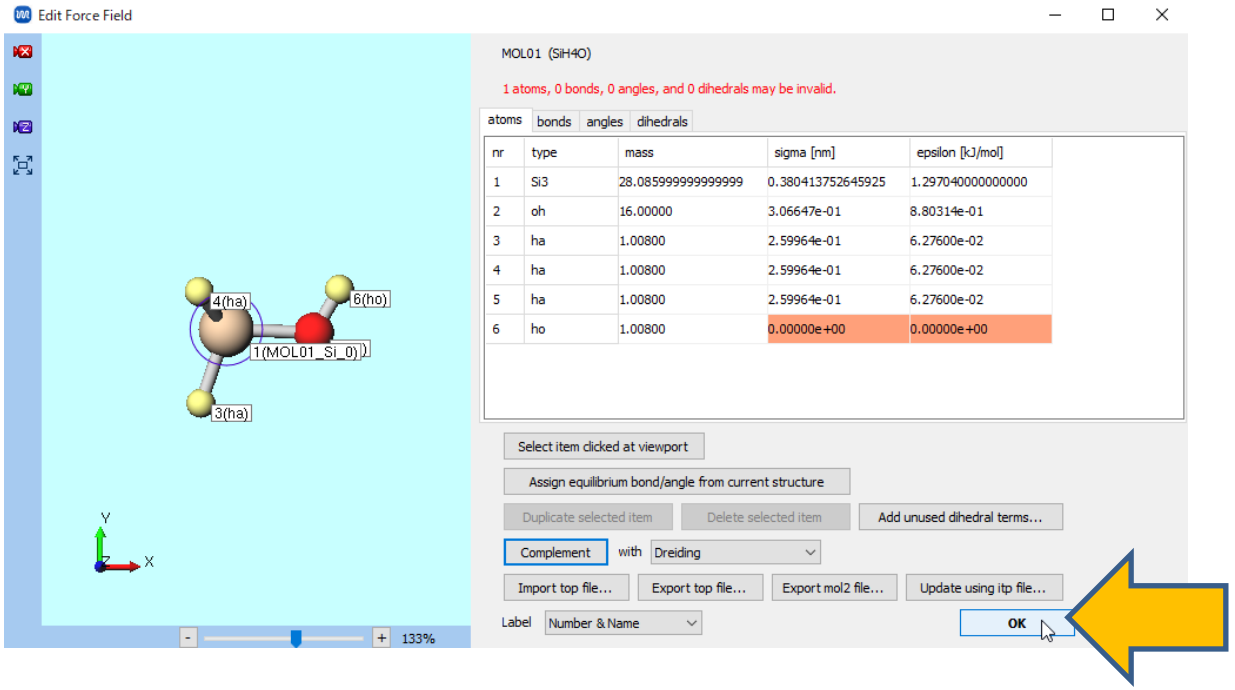




C. Auto-Completion for Failed Assignments

A. Basically, continue using **Complement** with different force fields or manually input values into the list in the center of the window until the warning at the top disappears. In this case, since the atom causing the warning (the hydrogen atom of the OH group) originally has sigma = 0 and epsilon = 0 in the force field definition, the warning can be safely ignored, and we will proceed without modification.

B. Click **OK** at the bottom of the window. The subsequent steps follow the procedures outlined in [LAMMPS Basics Tutorial] and related guides.



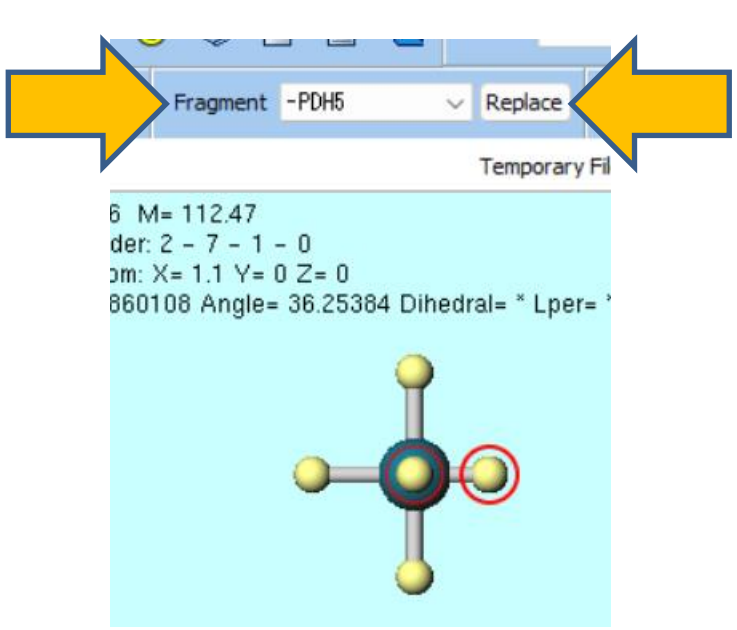
D. Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations

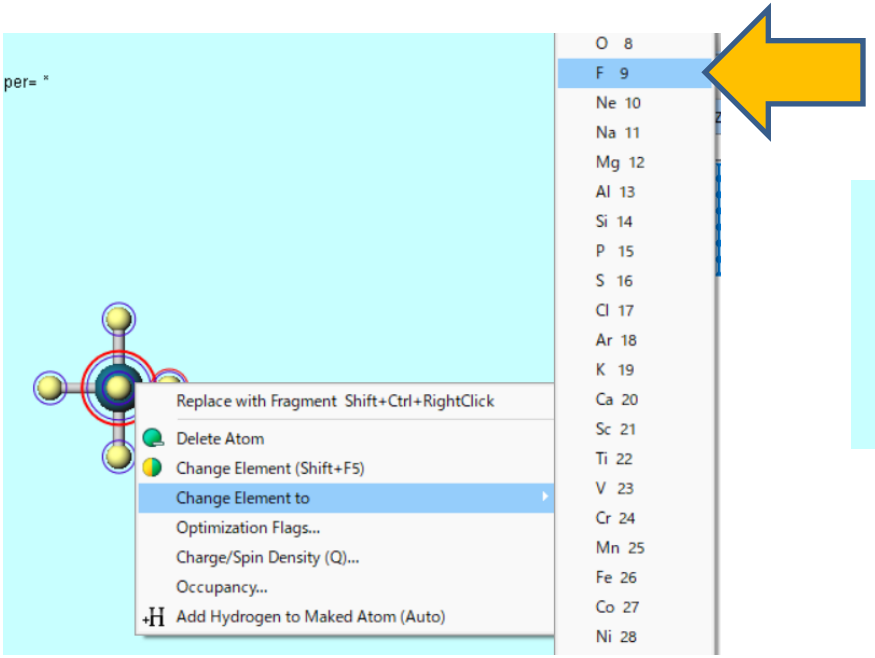
Refer to LAMMPS Basics Tutorial for basic operation methods.

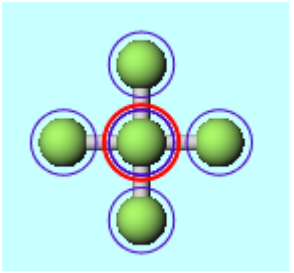
A. Click **File | New Project**, enter 'lipf6' in **Project name**, and click **Save**.

B. On the toolbar, select '-PDH5' under **Fragment** and click **Replace**.

C. Click **Select | Select All,** then right-click any atom, select **Change Element to** and click **F 9** to change all atoms to fluorine (F).







D. Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations

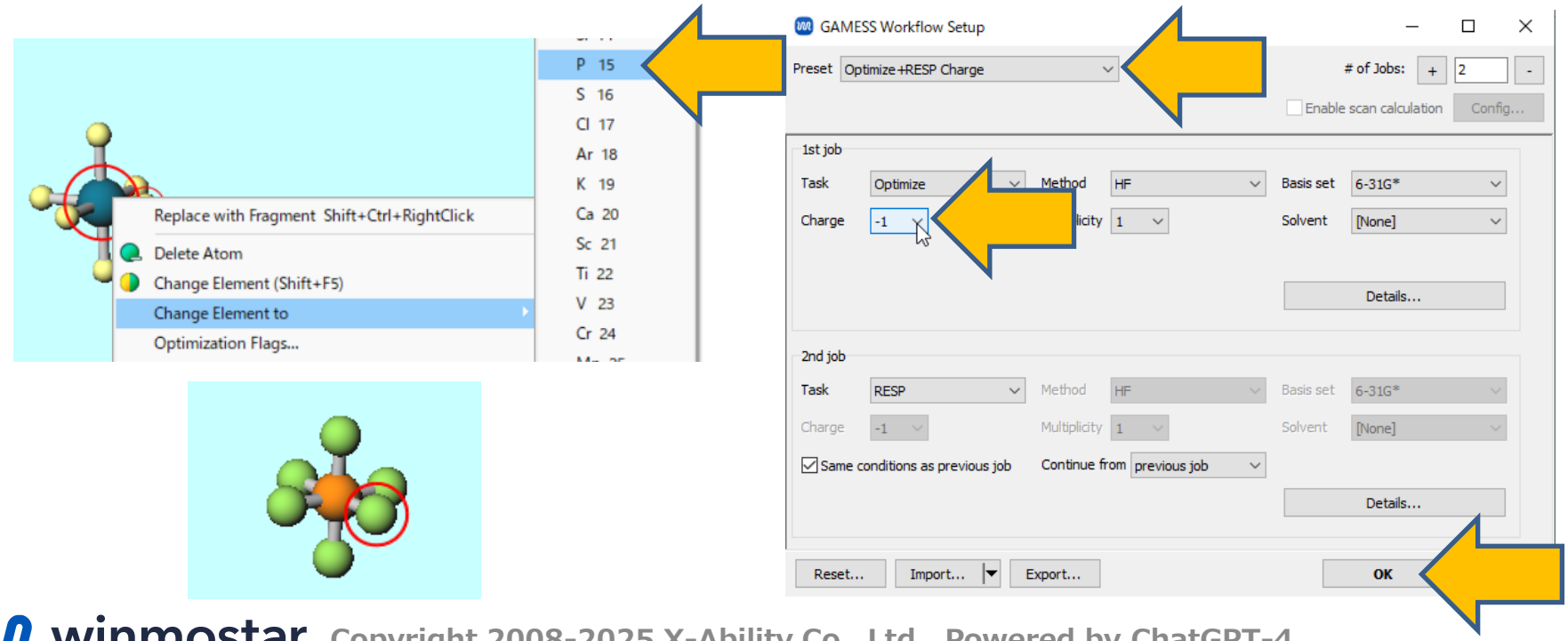
A. Click **Select | Select None**

B. Drag the Viewport to adjust the camera angle so that the central atom is clearly visible.

C. Right-click the central atom, select **Change Element to** and click **P 15** to set it as PF_6.

D. QM | GAMESS | Workflow Setup

E. Change the **Preset** to 'Optimize + RESP Charge', set the **Charge** of the **1st job** to '-1', and click **OK**.



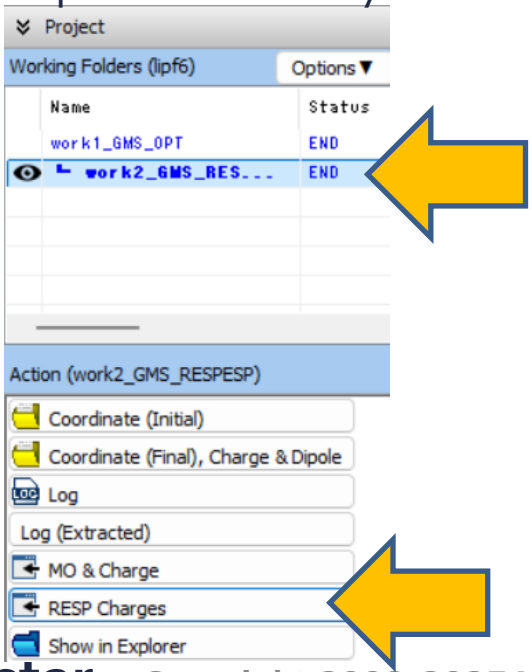
D. Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations

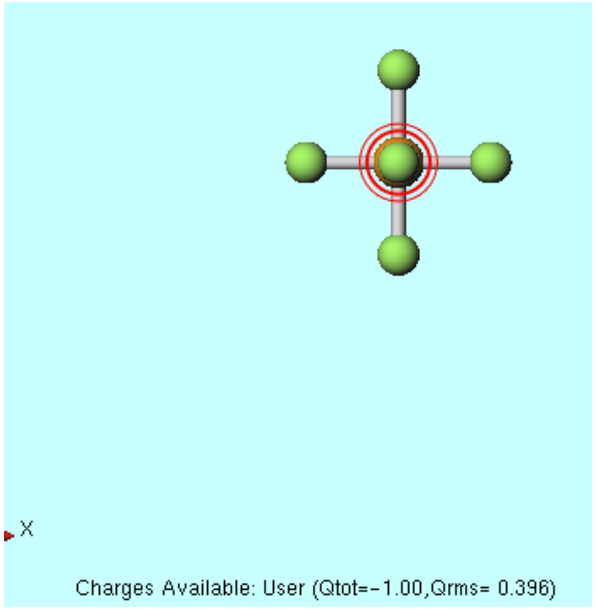
A. Click OK in GAMESS **Workflow Setup** window, set as appropriate in Job Setting window, and then click **Run**.

B. After the work2 calculation finishes, click ‘work2_GMS_RESPESP’ in **Working Folder**, then click **RESP Charges** under the **Action**.

C. When prompted with ‘Do you want to assign the same charge to equivalent atoms in terms of topology?’, click **No**.

D. When the message "Charge has been assigned to User Charge." appears, click **OK**. When prompted with "Do you want to display charges?", click **No**.

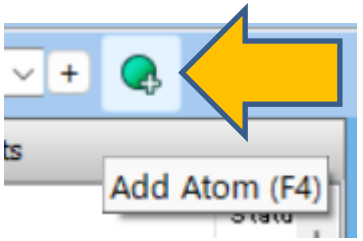


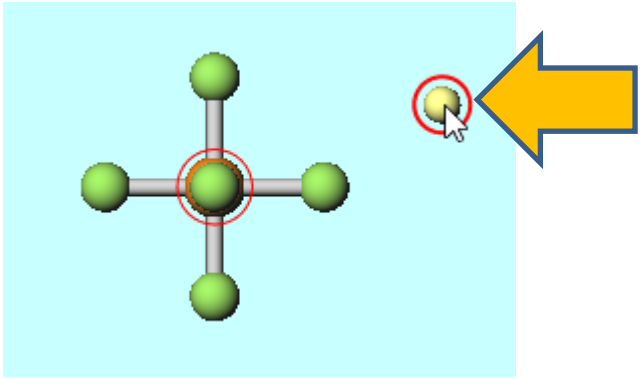


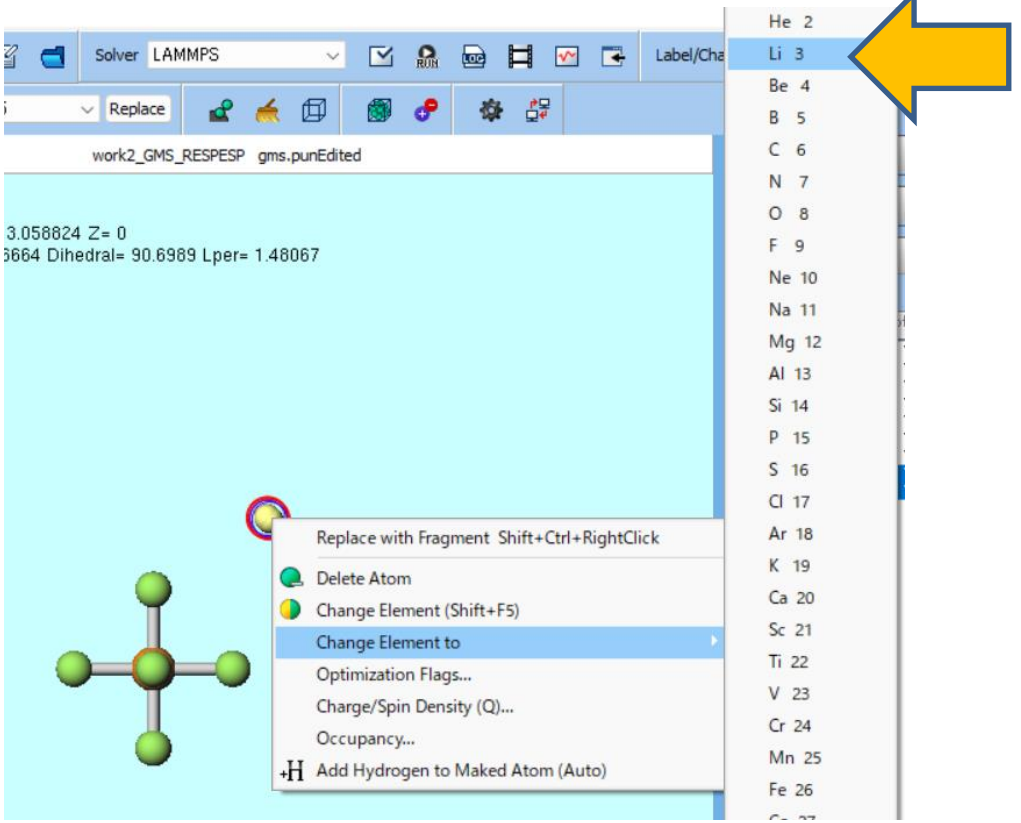
D. Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations

A. Click **Add Atom** on the toolbar, then click an appropriate location slightly away from the PF_6 molecule.

B. Right-click the added atom, select **Change Element to** and click **Li 3**.

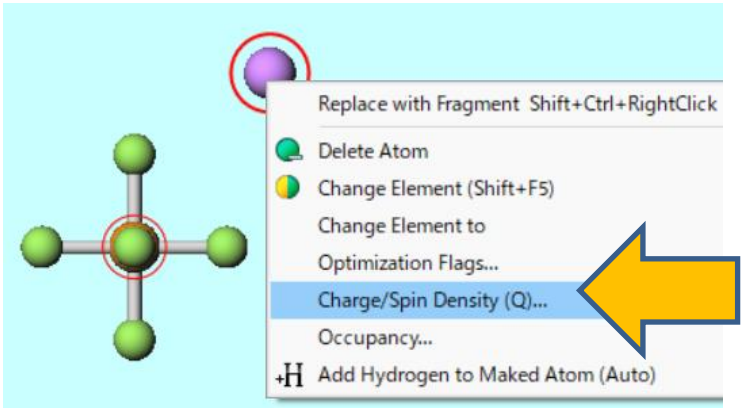


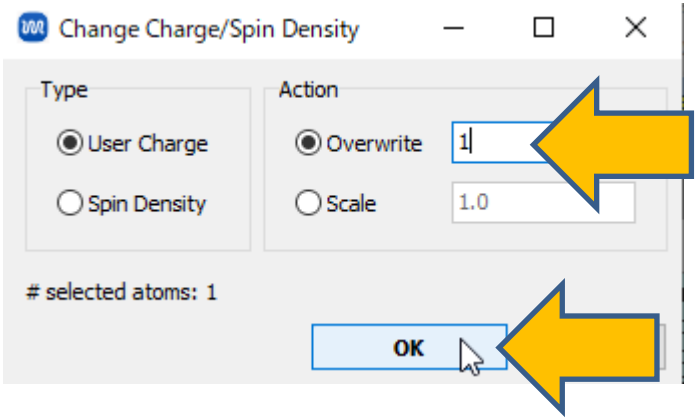


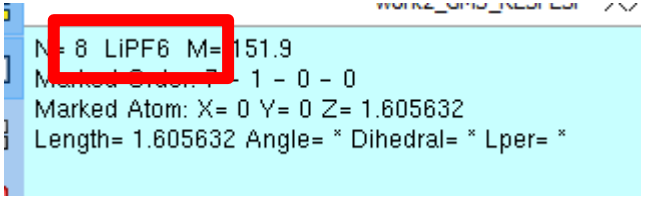


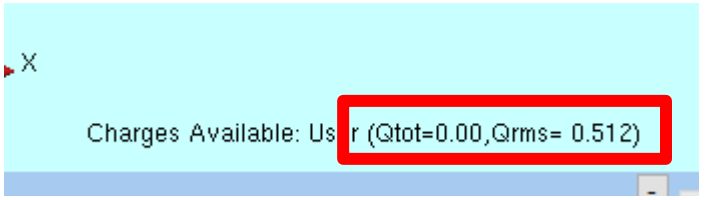
D. Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations

A. Right-click the added atom and click **Change Charge/Spin Density (Q)**.
B. Enter '1' next to **Overwrite** under **Action**, then click **OK**.
C. At the top of Viewport area, confirm that the composition is shown as 'LiPF6', and at the bottom, that Qtot is 0 and Qrms is nonzero.





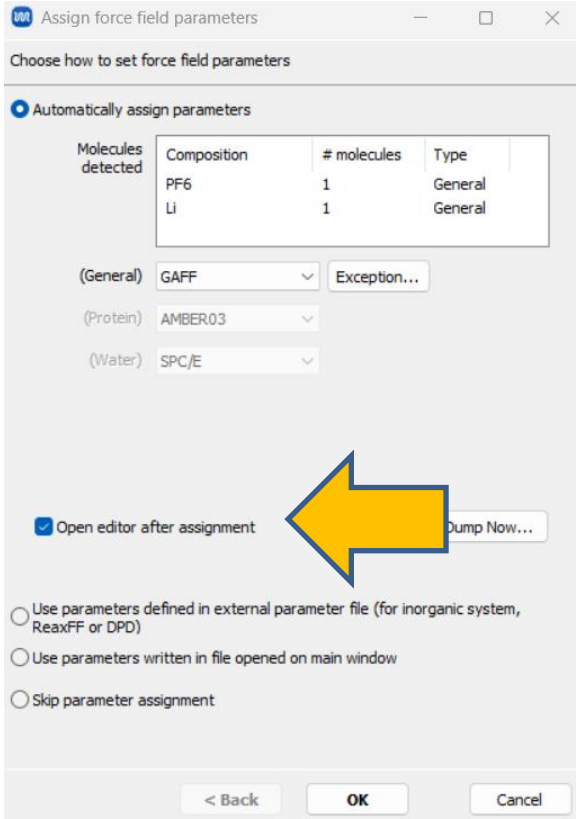




D. Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations

A. Select **LAMMPS** as Solver, and click **(Workflow Setup).** When **Create Cell** / 'Enter Margin' dialog appears, simply click **OK**. When 'Residue names of monoatomic ions will be automatically corrected.' dialog appears, click **OK**.

B. In **Assign Force Field Parameters** window, select the desired force field type (this tutorial uses the default GAFF and AMBER03), check **Open editor after assignment**, and click **OK**.



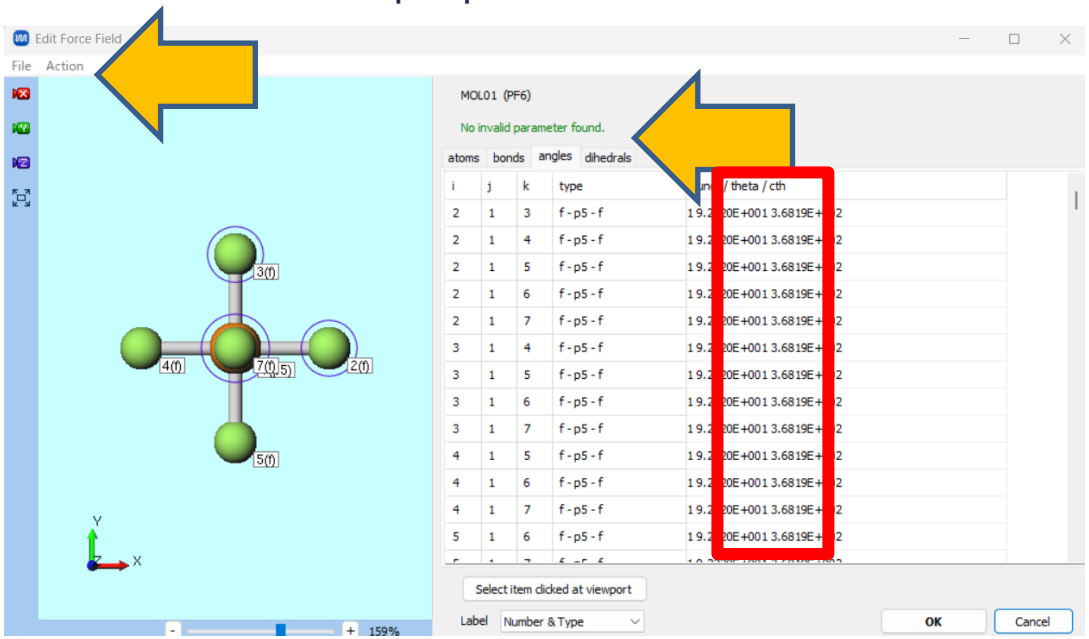
D. Automatic Extraction of Equilibrium Bond Lengths and Angles from Quantum Chemical Calculations

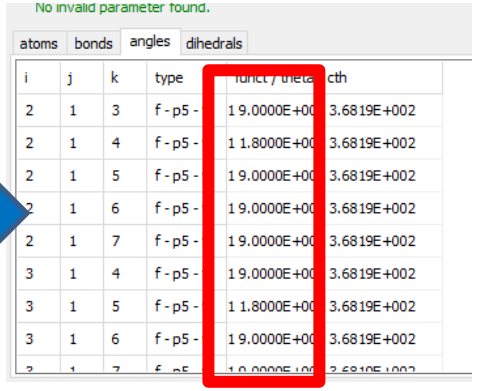
A. In **Edit Force Field** window, click the **angles** tab on the right. You will see that all F-P-F equilibrium angles are set to 92.22°. If MD calculations are run as is, the octahedral structure will collapse.

B. Click **Action** | **Assign equilibrium bonds/angles from current structure** to update the equilibrium bond lengths and angles based on the loaded structure.

C. Click **OK**. The subsequent steps follow the procedures outlined in [LAMMPS Basics Tutorial] and related guides.

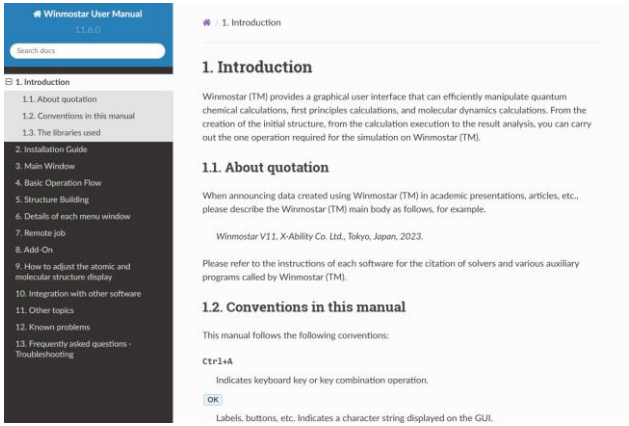
   – Since the original force field has been modified, please verify the resulting structure and properties after each calculation.





Finally

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



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact page, detailing the steps to reproduce the issue and attaching any generated files at that time.