winmostar tutorial

GAMESS Bimolecular Calculations (Dispersion Force Corrections)

V11.6.5

14 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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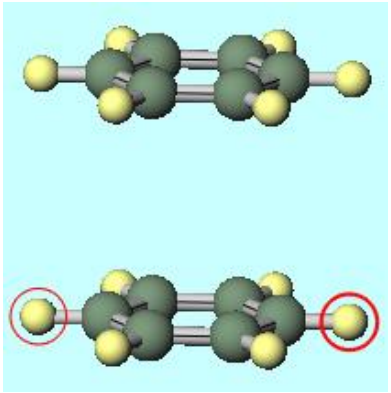
Overview

- Traditional methods like HF or conventional DFT (B3LYP, PBE, etc.) cannot handle dispersion forces (also known as weak interactions) such as van der Waals forces or π-π interactions. To accurately calculate dispersion forces, methods that correct for dispersion based on interatomic distances (like B3LYP-D3), improved DFT functionals (such as cam-B3LYP, M06 series), or high-precision second-order perturbation (MP2) methods are needed. This tutorial describes the calculation of a benzene dimer using the B3LYP-D3 method.



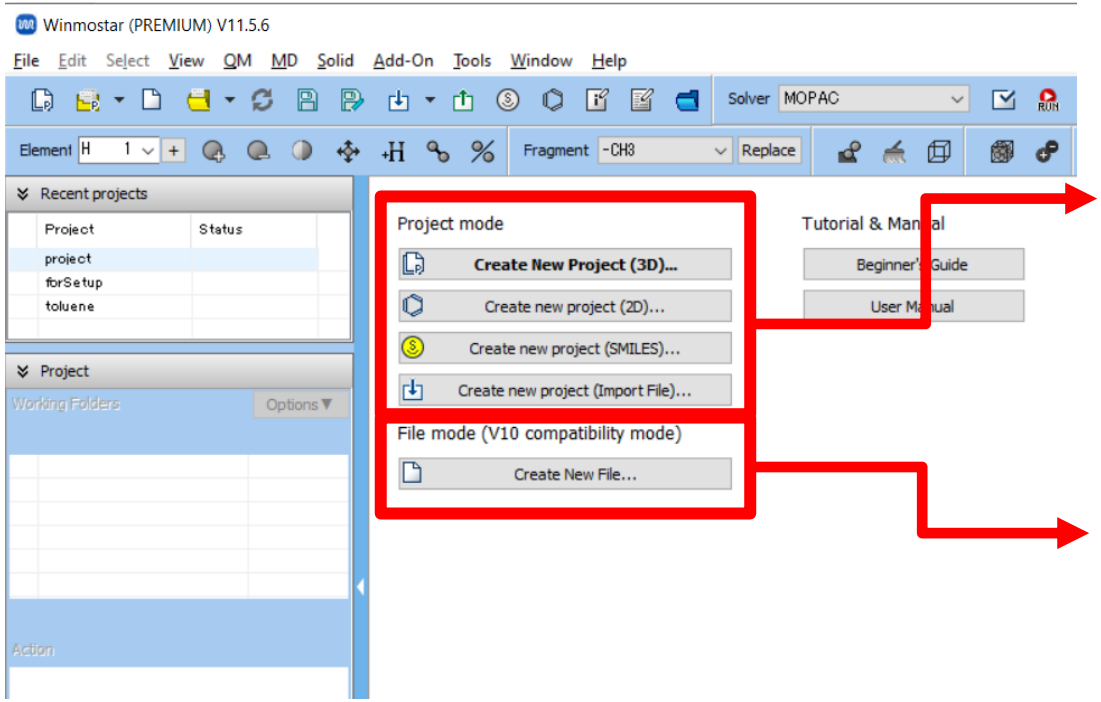
Preference of Operating Environment

- For GAMESS

Follow the GAMESS Installation Manual at https://winmostar.com/en/manual_en/installation/GAMESS_install_manual_en_win.pdf to install GAMESS.

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.

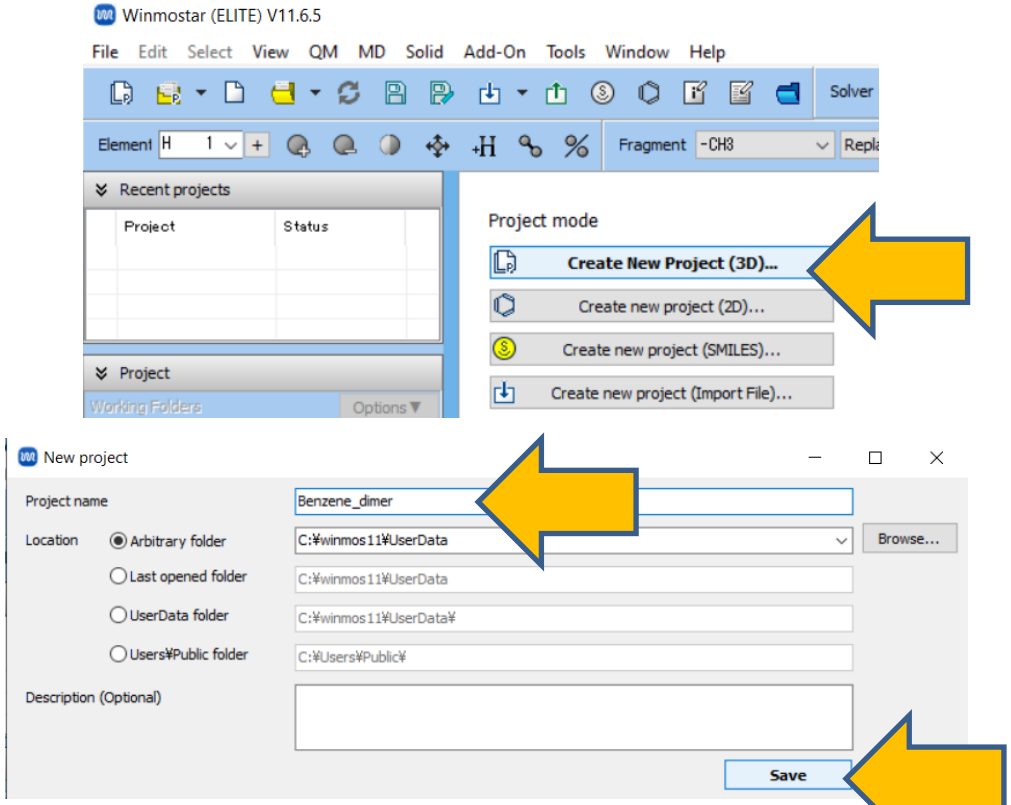
When creating a continuation job, in file mode or versions prior to V10, it is necessary to display the final structure of the original job each time. However, in project mode, the final structure is automatically carried over.

A. Modeling of the System

For basic operation instructions, please refer to GAMESS Fundamentals tutorial.

A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already open, click on **File | Close** first.

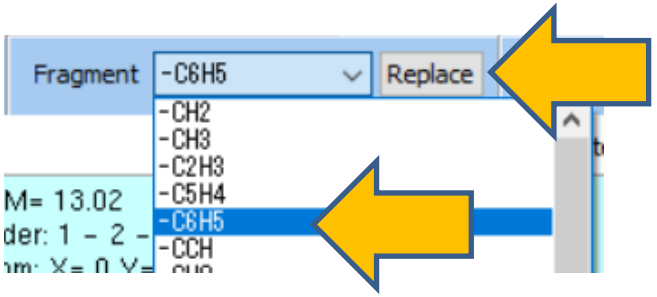
B. Enter 'Benzene_dimer' as **Project name** and click **Save**.

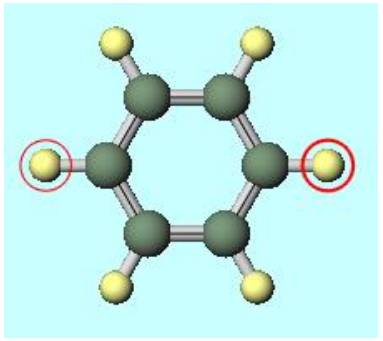


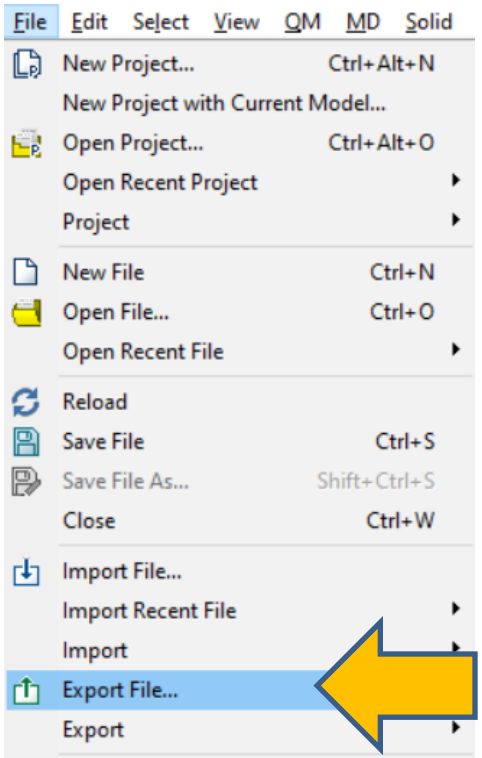
A. Modeling of the System

A. Select **-C6H5** from **Fragment** at the top of Main Window, and click **Replace** once to create benzene.

B. Click **File | Export File**, enter ‘benzene‘ as the file name, and click **Save**. When ‘Successfully exported benzene.wmm‘ is displayed, click **OK**. This completes the saving of this benzene structure file.

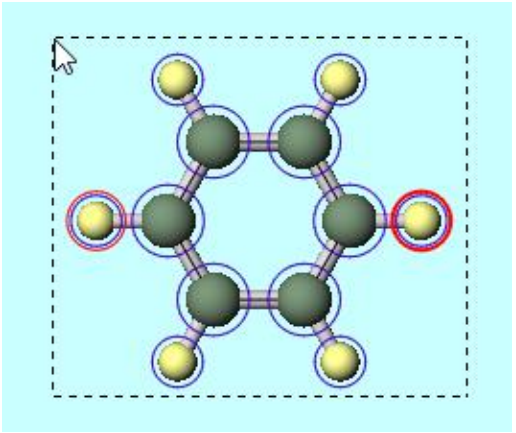


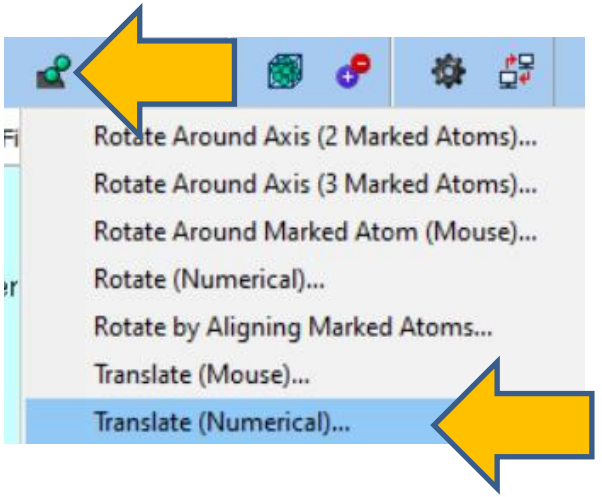


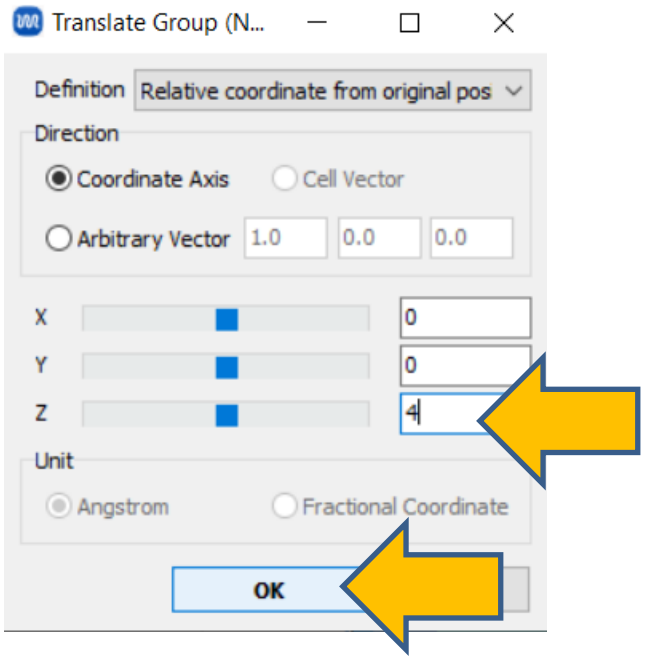


A. Modeling of the System

A. Hold **Ctrl** and drag over the entire benzene to select all atoms as a group.
B. Click  **(Modify Selected Group)** and select **Translate(Numerical)**.
C. In **Translate Group** window, enter **4.0** in **Z** field and click **OK**.

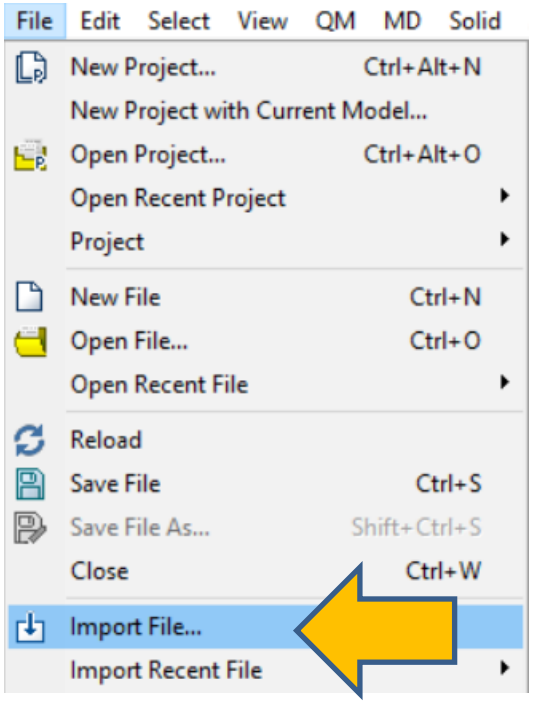


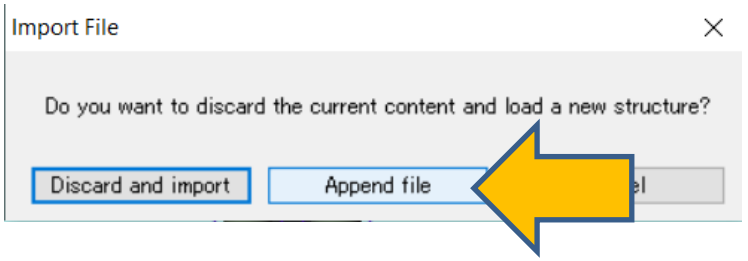


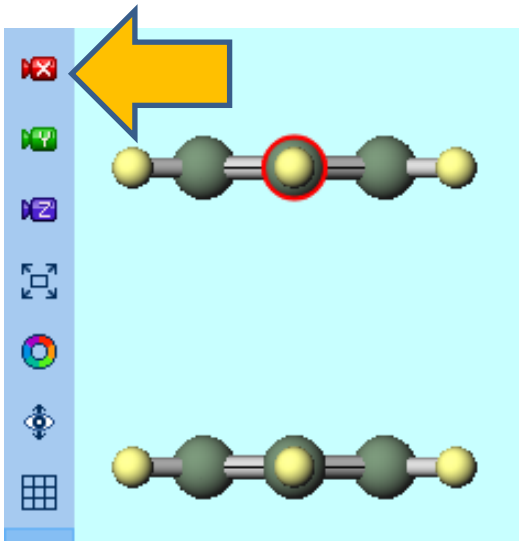


A. Modeling of the System

A. Click **File | Import File**, select ‘benzene.wmm‘ file saved in p.7, and click **Open**.
B. When prompted with ‘Do you want to discard the current content and load a new structure?‘, click **Append file**.
C. Click **(Align View to X-Axis)** to confirm that the benzene dimer has been successfully created.



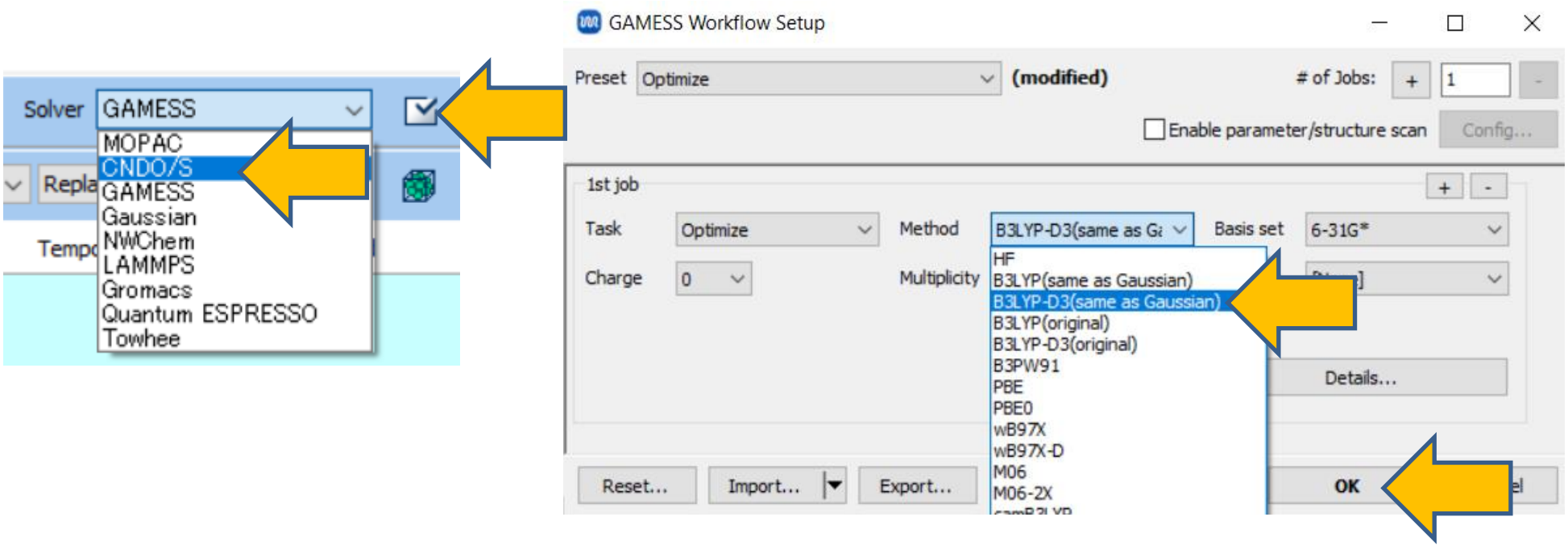




B. Execution of Calculate

A. Select **GAMESS** from **Solver** and click **Workflow Setup**.
B. In **GAMESS Workflow Setup** window, change **Method** to **B3LYP-D3 (same as Gaussian)**.
C. Click **OK**.

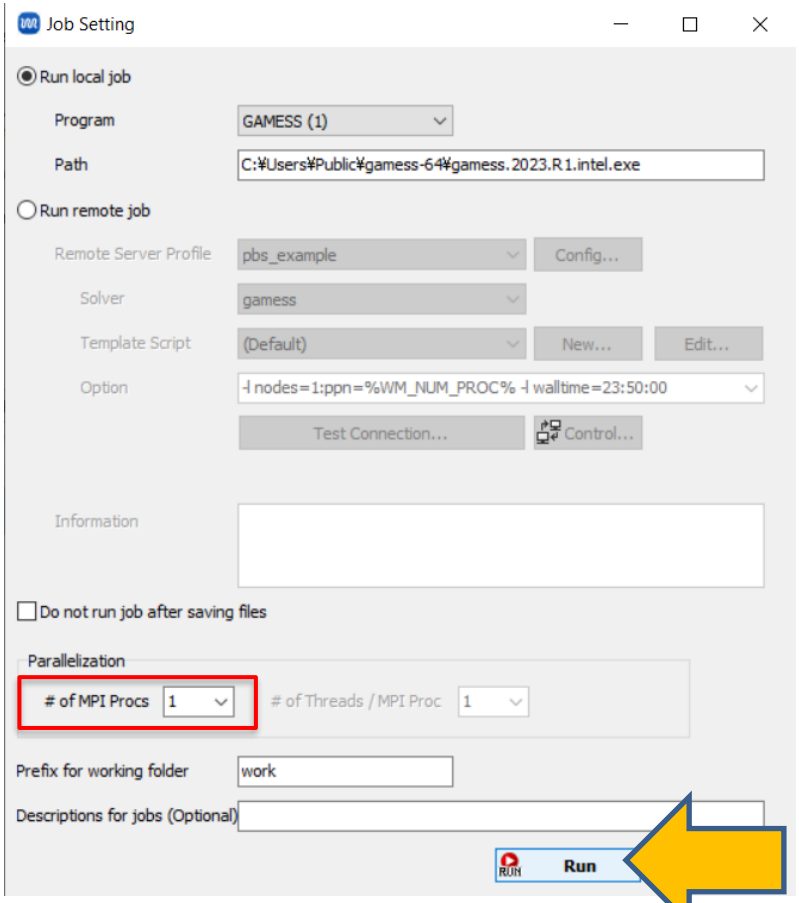
・ To speed up the calculation by reducing accuracy, change **Basis set** to **STO-3G**.



B. Execution of Calculate

A. Set the # of MPI Procs according to the number of cores in your computer. When running on a remote machine, also set up profiles and other settings.

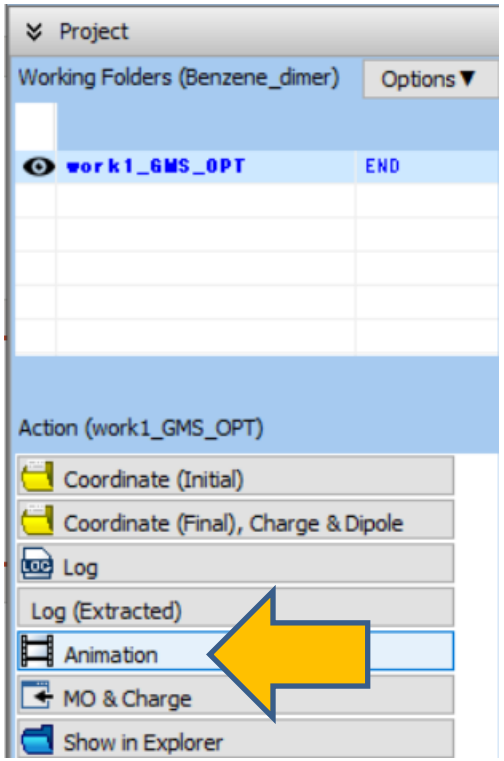
B. Click **Run**.

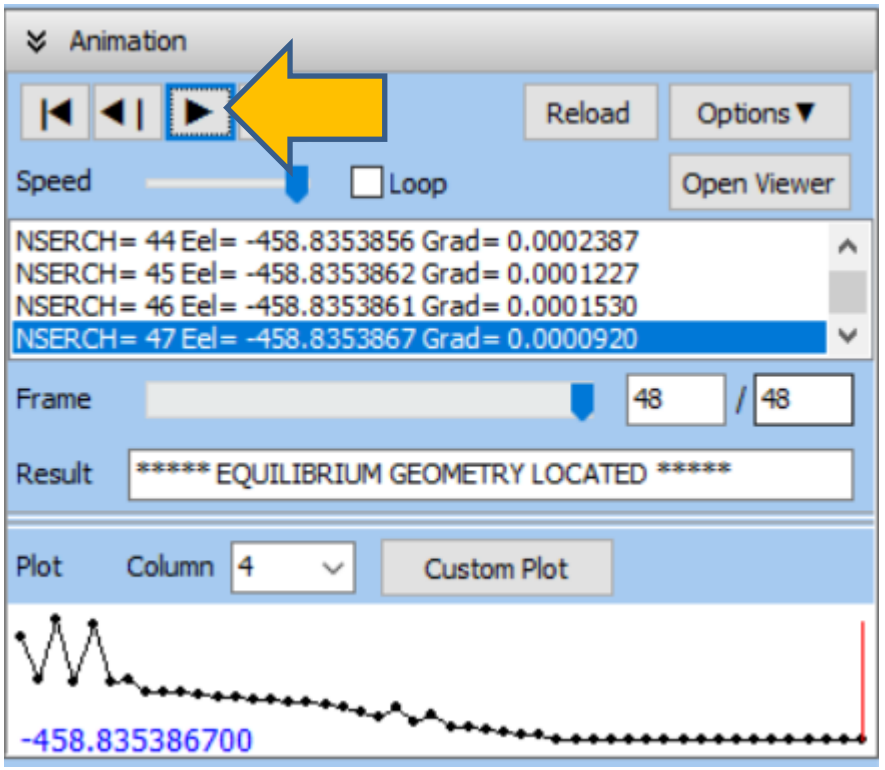


C. Computational Analysis

A. After the calculation has finished and the status of the work folder changes to **END** or **END(-)**, click **Animation** in **Action** at the bottom right of Main Window to display the results of the structure optimization calculation in Animation area.

B. Click ▶ **lay)** button to play the animation and display the final optimized structure.

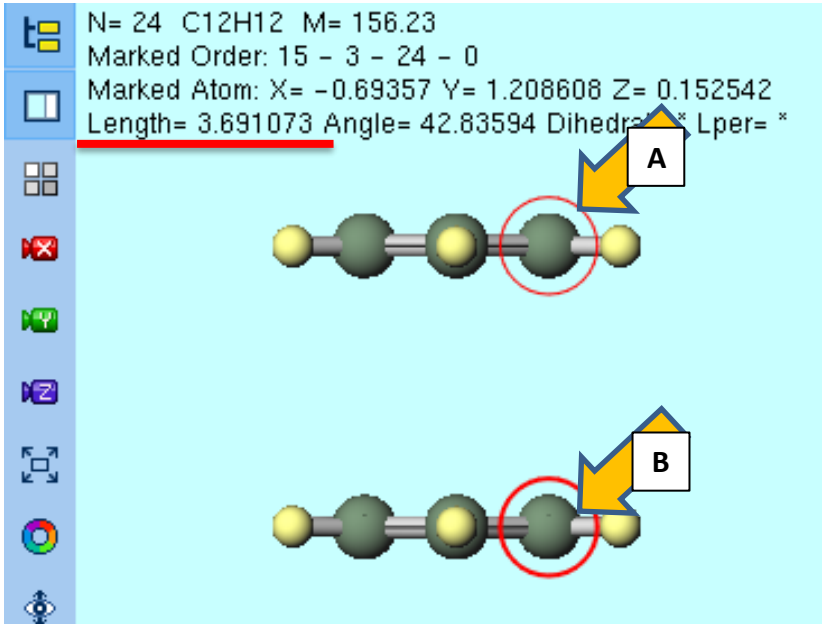




C. Computational Analysis

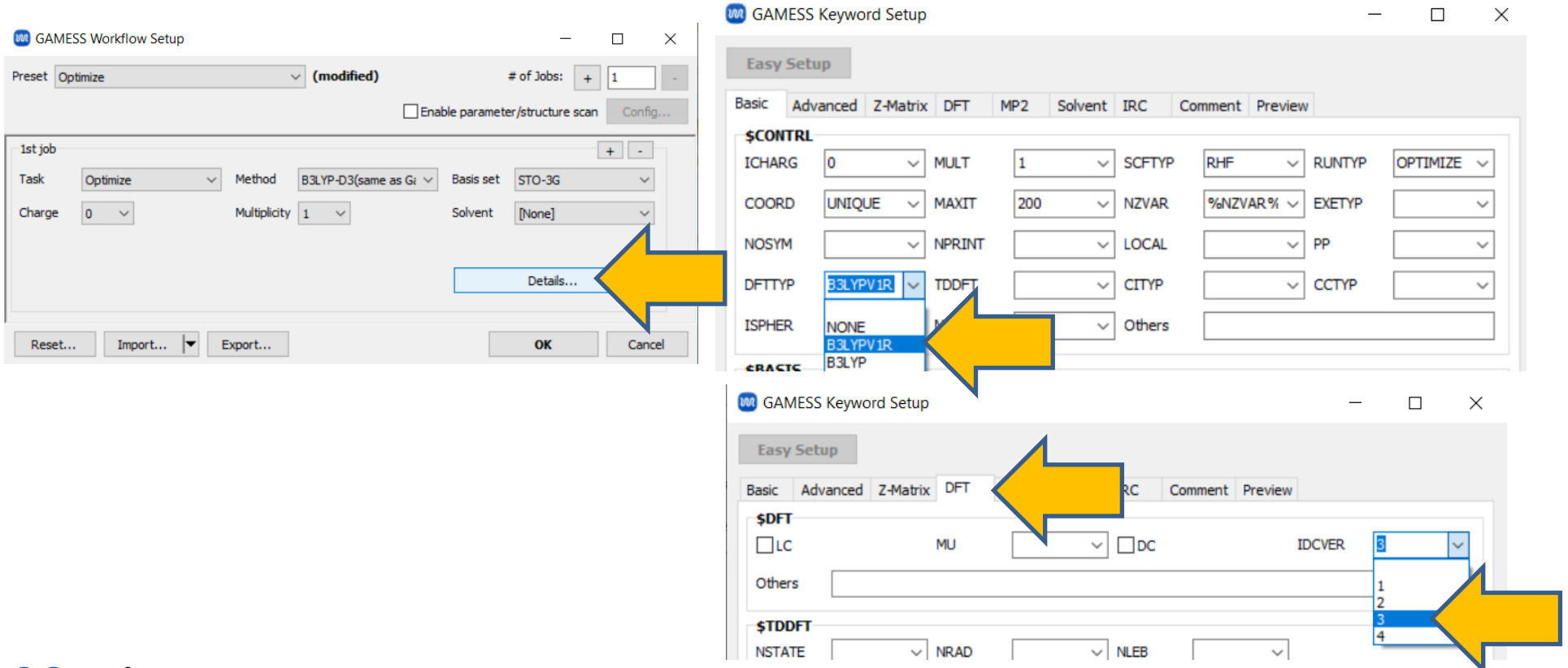
A. Click  **(Align View to X-Axis)**, then click on two carbon atoms in overlapping positions when viewed from above the benzene rings. Verify that the distance between the planes of the benzene dimer, indicated by the Length value, is approximately 3.7Å.

・(Comparison) When the structure optimization calculation is performed using **B3LYP** instead of **B3LYP-D3**, as **Method** on p.10, the two benzene molecules become more stable as they move apart, and the energy change becomes negligible at around 6Å, at which point the calculation ends.



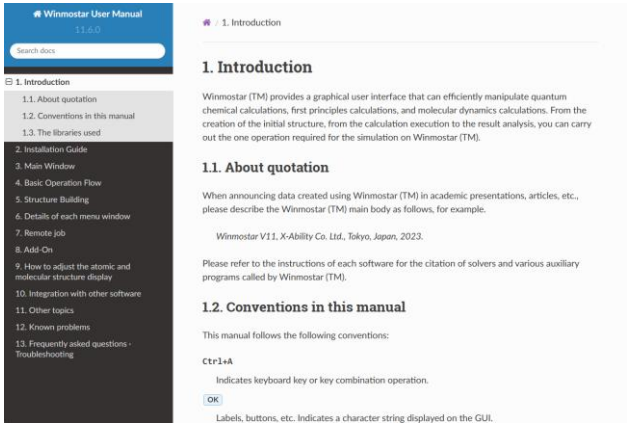
Supplement: Specifying -D3 with Other Functionals

A. Click **Details** in **GAMESS Workflow Setup** window.
B. In **GAMESS Keyword Setup** window, change **DFTTYP** in **$CONTRL** section to the desired functional.
C. Click **DFT** tab and change **IDCVER** in **$DFT** section to **3**.



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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