winmostar tutorial

NWChem
Dimer Calculation (Dispersion Force Correction)

V11.6.5

18 April 2024 X-Ability Co., Ltd.

Note: This manual was created for version V11.6.5.
If you are using version V11.4.X or earlier, please use the file mode.

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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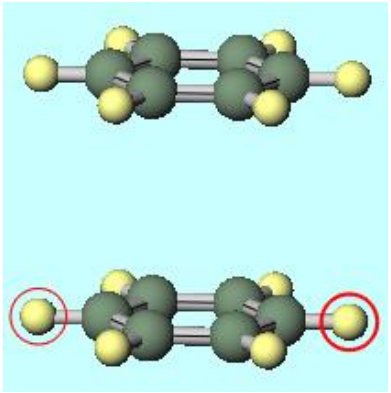
Overview

- Hartree-Fock methods and traditional DFT methods (such as B3LYP and PBE) cannot handle weak interactions such as van der Waals forces or π-π interactions. To calculate these interactions, methods that correct for dispersion forces based on interatomic distances (such as B3LYP-D3), improved DFT functionals (like cam-B3LYP, M06 series), or high-precision second-order perturbation (MP2) methods are required. This tutorial will explain the calculation of a benzene dimer using the B3LYP-D3 method.

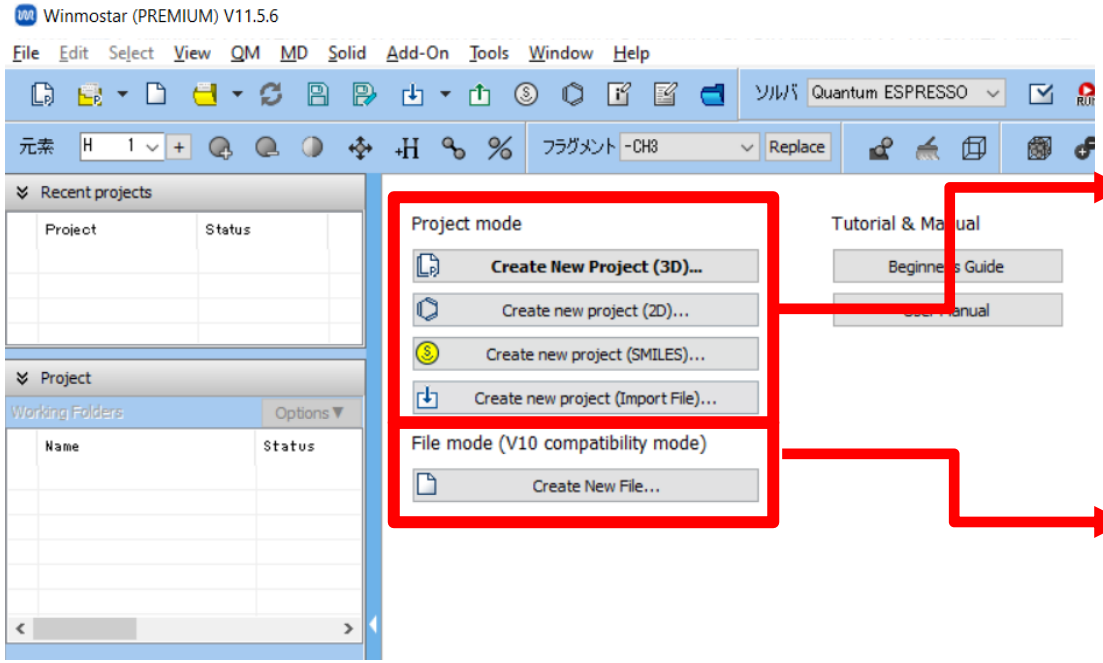


Operating Modes of Winmostar V11

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 NWChem Tutrial for V10.



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 before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

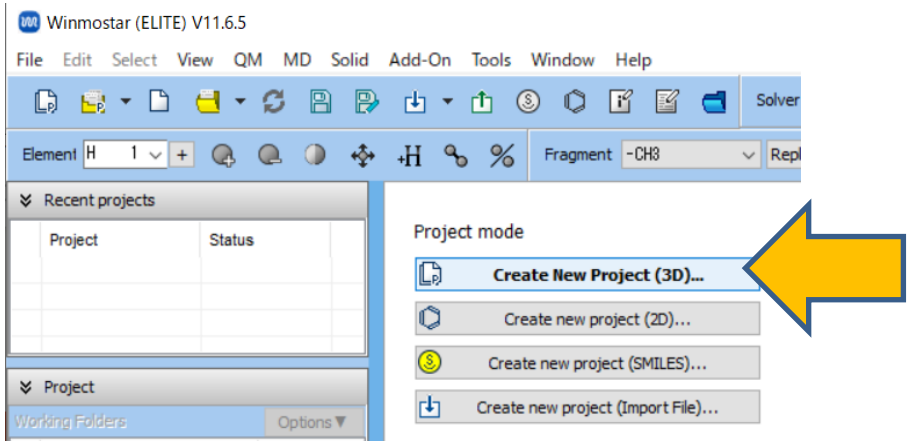
Preferences

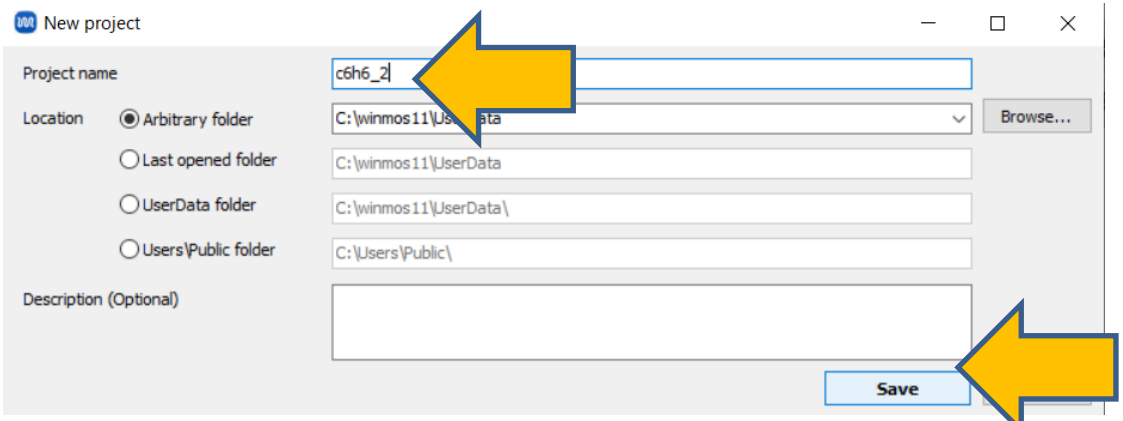
Please set up NWChem according to Windows version NWChem Installation Manual.

A. Modeling of the System

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

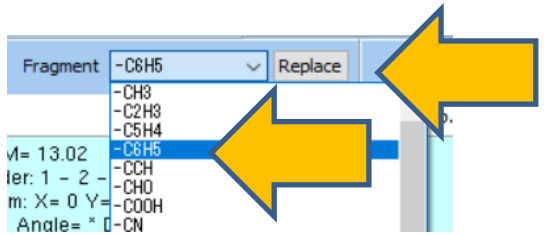
B. Enter 'c6h6_2' for **Project name** and click **Save**.

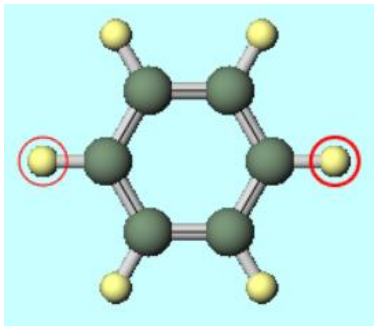


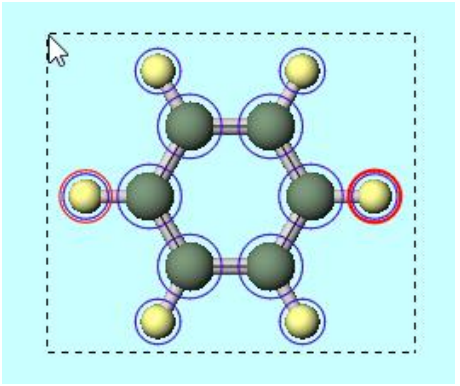


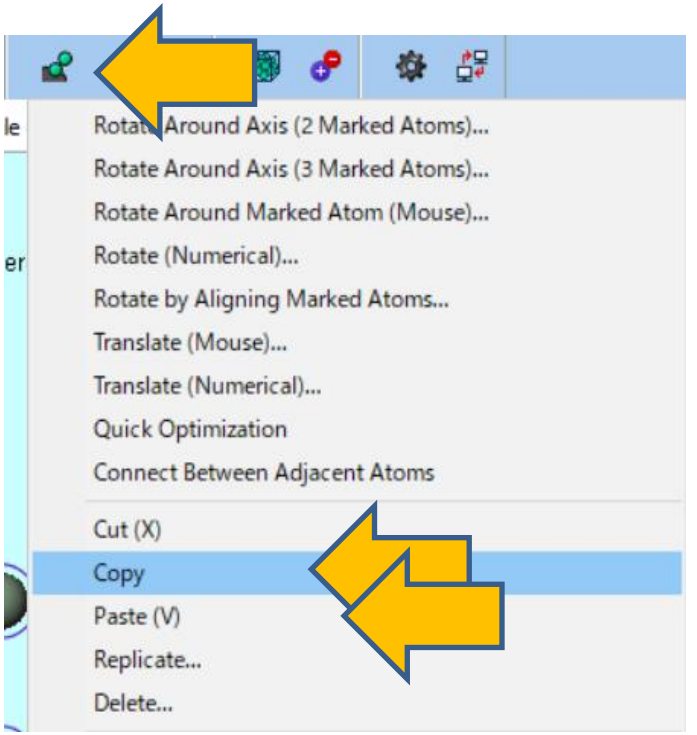
A. Modeling of the System

A. Select **Fragment -C6H5** and click **Replace** on the right once to create benzene.
B. While holding **Ctrl**, drag across the entire benzene to group select all atoms (selected atoms will be marked with a blue circle).
C. Click **Modify Selected Group | Copy**, then click **Modify Selected Group | Paste**.



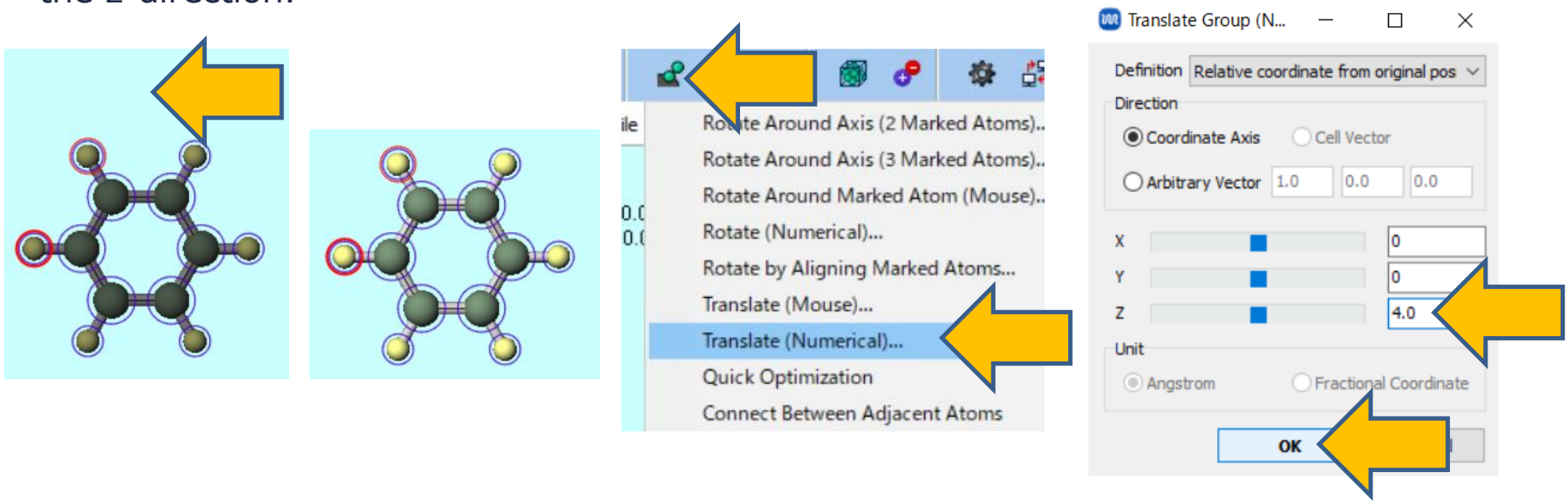






A. Modeling of the System

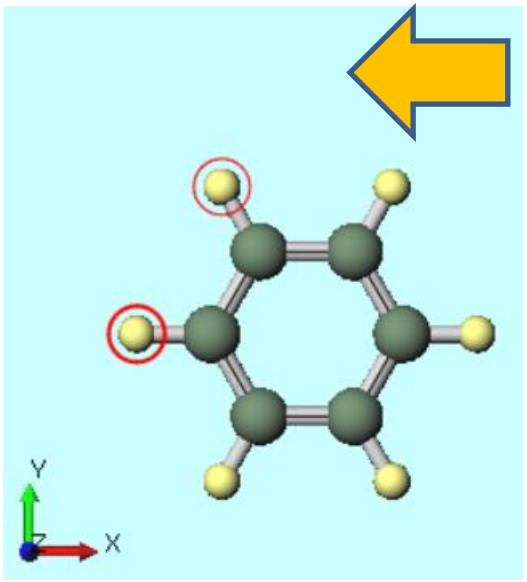
A. Clicking on Viewport (the light blue area) where benzene is shown will paste the copied molecule in the same location as the original, with only the copied molecule group selected.
B. Click **Modify Selected Group | Translate (Numerical)**.
C. Enter '**4.0**' in z box and click **OK**. All the group-selected atoms will be moved 4.0 Å in the z-direction.

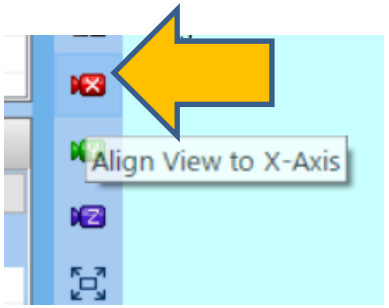


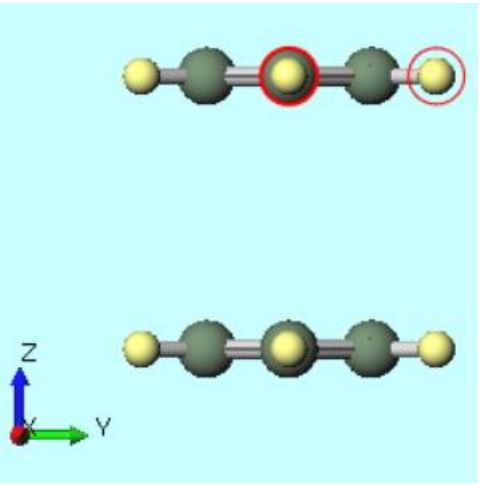
A. Modeling of the System

A. Click in the light blue area around the molecule to deselect the group (blue circles will be removed).

B. Click Align View to X-Axis to view from the x-axis direction, and check if the translation in the z-direction has been successful.

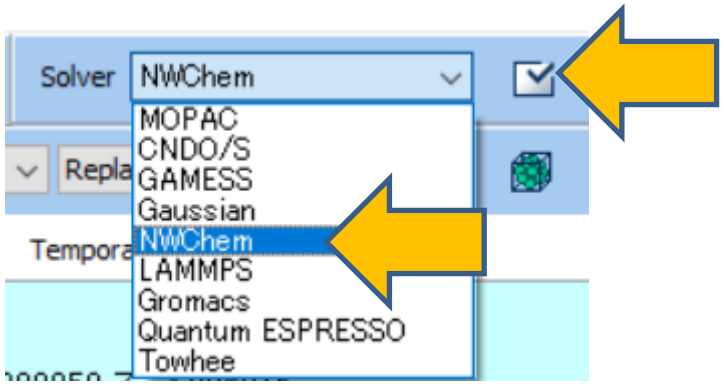


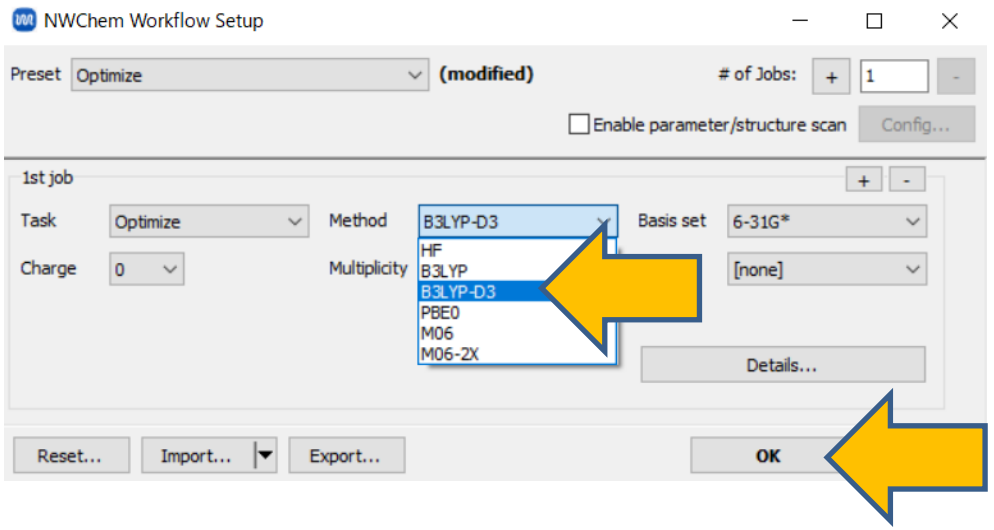




B. Execution of Calculate

A. Select **NWChem** from **Solver** and click **Workflow Setup**.
B. Change **Method** to '**B3LYP-D3**' and click **OK**.
C. In **Job Setting** window, click **Run**.

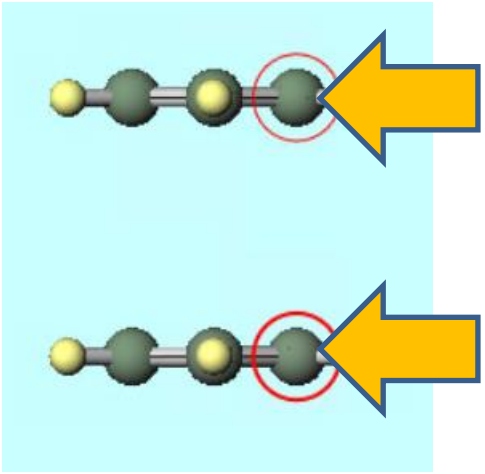


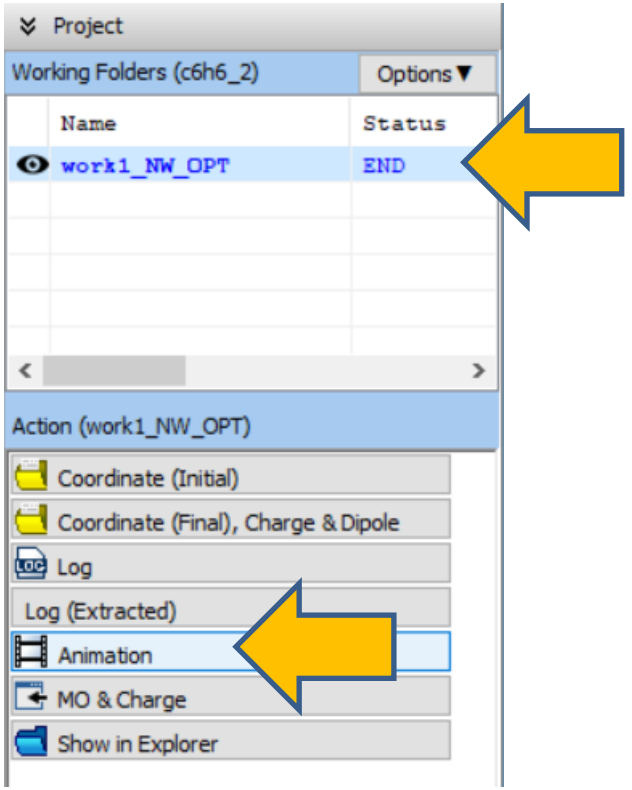


C. Result Analysis

A. After the calculation is completed and the status of **work1_NW_OPT** changes to **END**, click on the corresponding carbon atoms of the upper and lower benzene molecules to examine the changes in the distance between them.

B. Click **work1_NW_OPT** in **Working Folders**, then click **Animation** under **Action**.

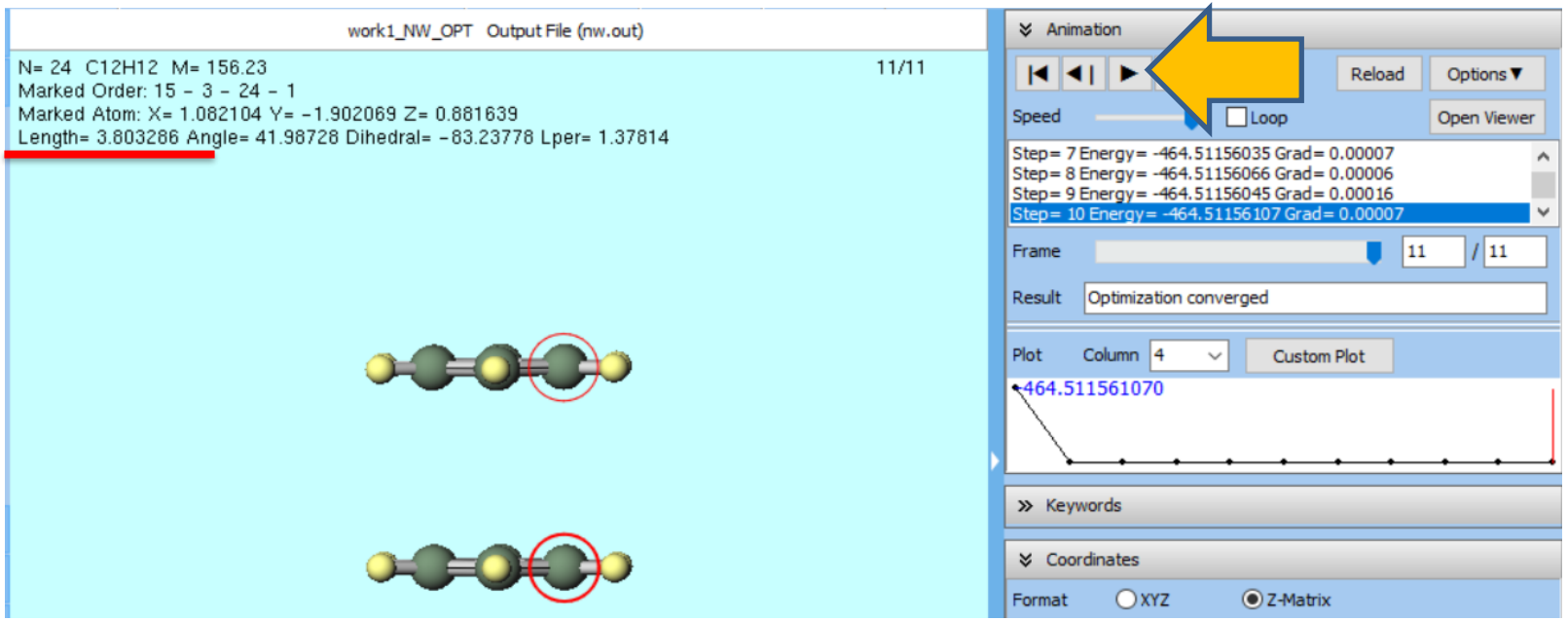




C. Result Analysis

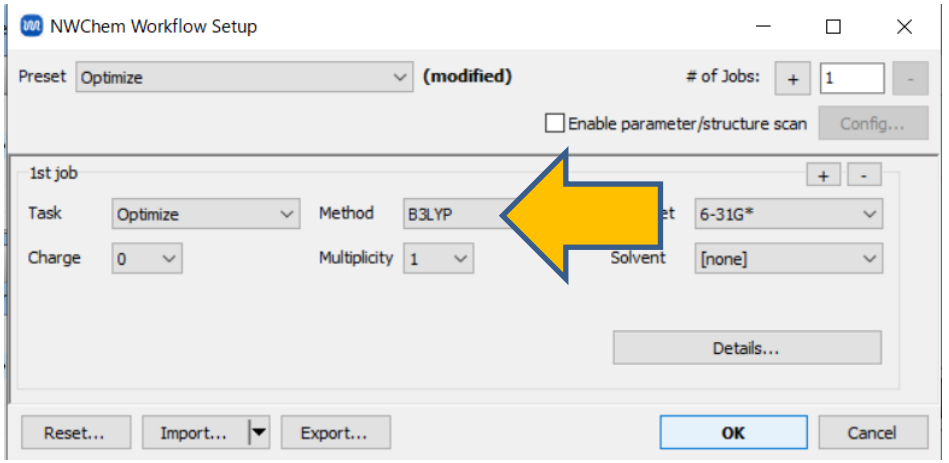
A. Click ▶ (**Play** button) in **Animation** Panel to play the animation and display the final optimized structure.

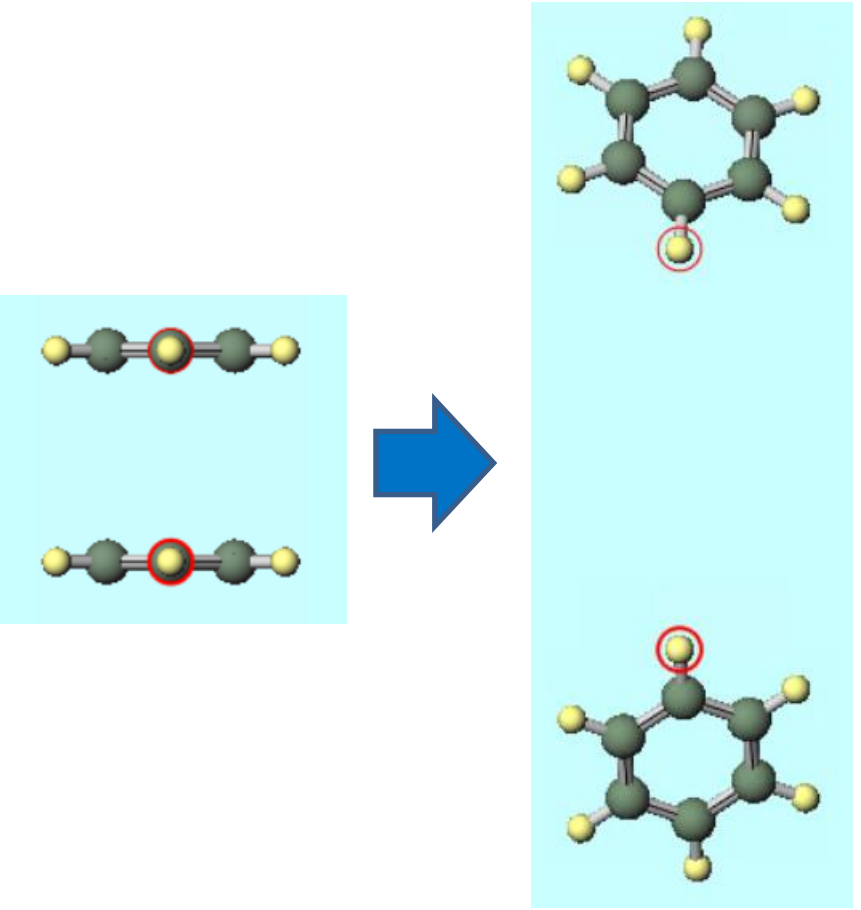
B. Confirm that a stable structure is formed at a distance of approximately 3.8 Å, as indicated by the Length value for the plane of the benzene dimer.



D. Comparison of B3LYP and B3LYP-D3

✓ Change **Method** to **B3LYP** for comparison and perform a similar calculation. Play in **Animation** to observe how the two benzene molecules separate.

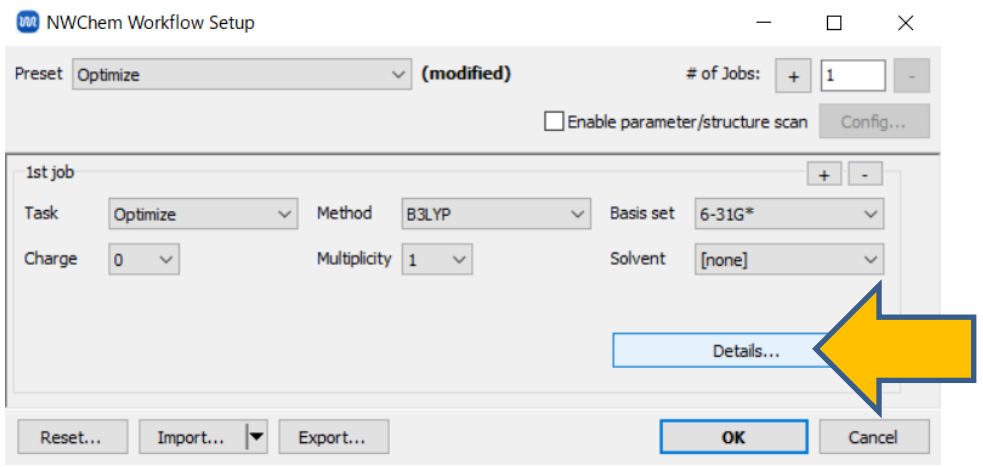


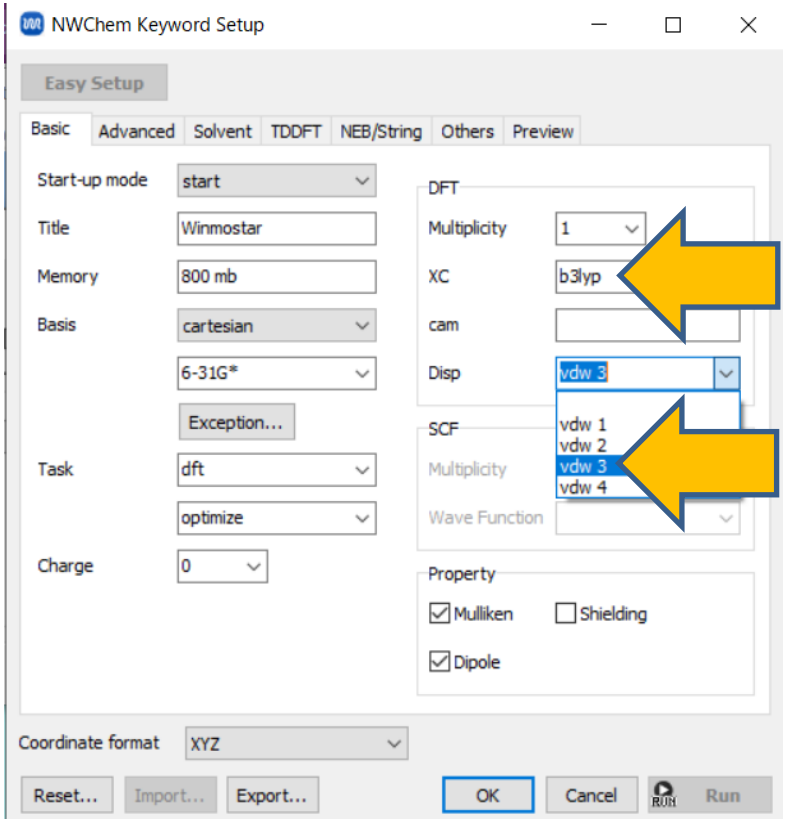


Supplement:
Specifying -D3 with Functionals Other than B3LYP

A. In **NWChem Workflow Setup** window, click **Details**.

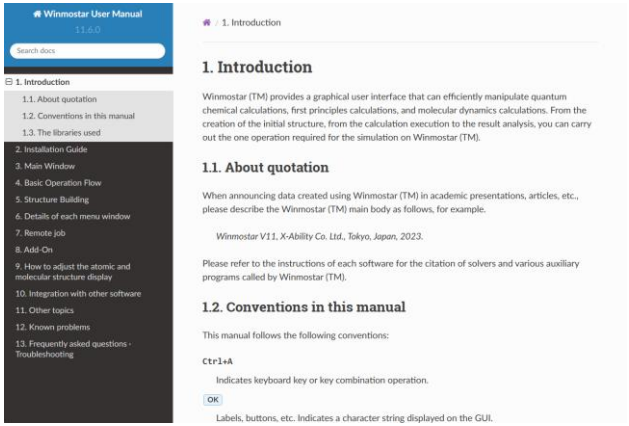
B. In **NWChem Keyword Setup** window, change **XC** to the desired functional, select '**vdw 3**' for **Disp**, and click **OK**.





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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