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Winmostar Tutorial

Molecular Modeling
（Modeling Supramolecules）

V7.016

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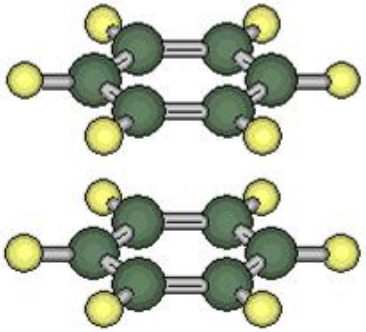
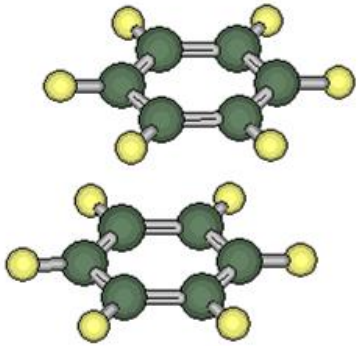
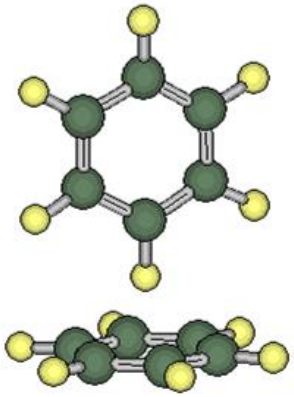
I. Configurations



Sandwich

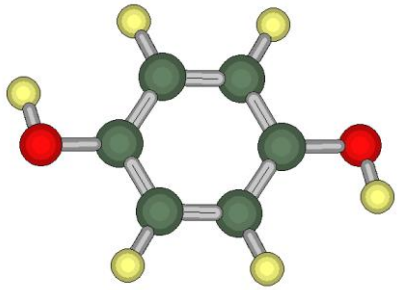


Parallel-displacement



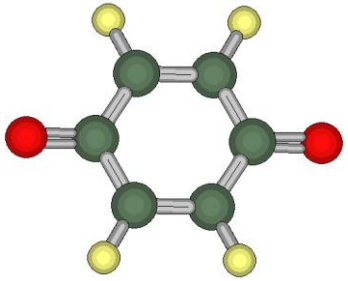
T-shaped

Benzene Dimer



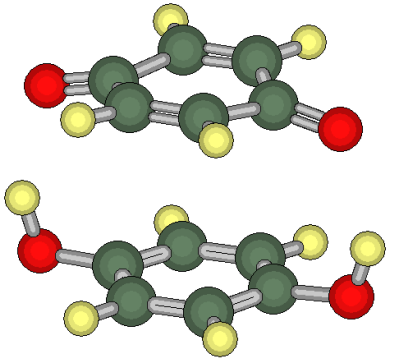
Donor

+



Accepter

→



Complex

Charge Transfer Complex

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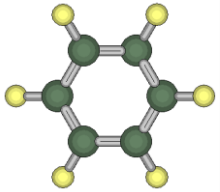
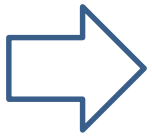
II. Modeling Benzene Dimer – Sandwich

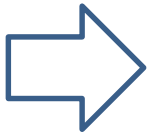
1. Model a benzene, click **x-axis POV** in toolbar

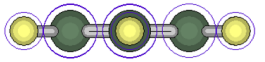
2. Hold down **Shift** and click on the molecule (select molecule)

3. **Ctrl+C** to copy, **Ctrl+V** to paste





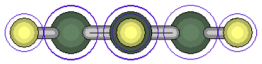


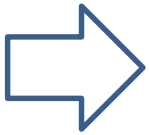


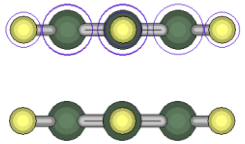
4. Drag cursor upward

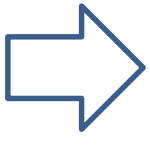
5. Adjust view angle

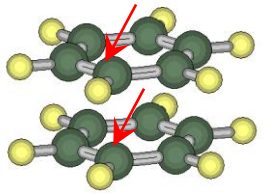
6. Click two atoms indicated below







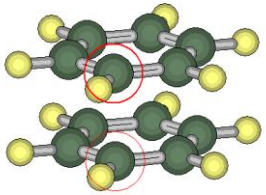


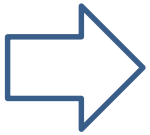


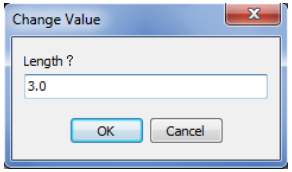
7. Select **Edit | Set | Bond Length**

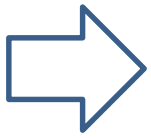
8. Set the **Length** at **3.0** and click **OK**

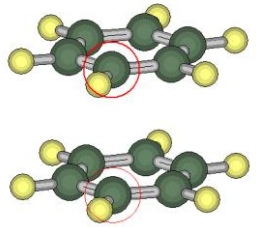
9. Save as needed











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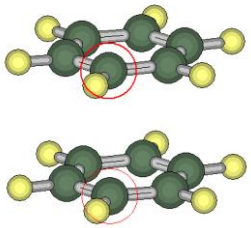
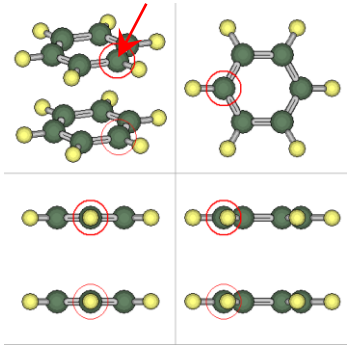
III. Modeling Benzene Dimer – Parallel Displaced

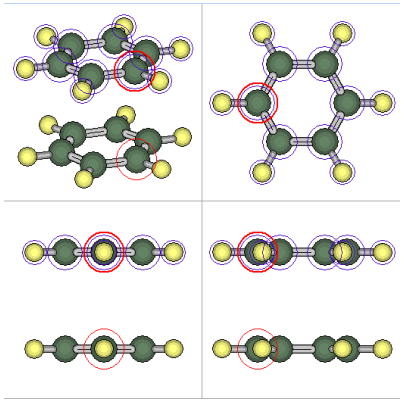
1. Start with Benzene Dimer – Sandwich configuration, click **Three View** icon



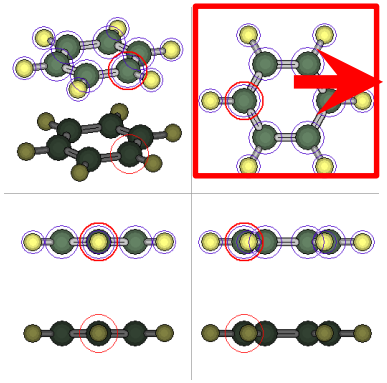
2. Hold down **Shift** and click on the atom indicated by the red arrow



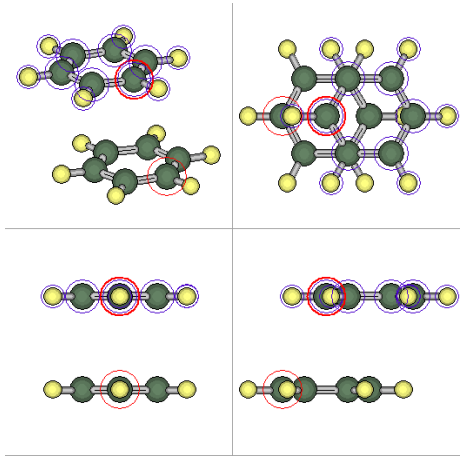
3. Hold down **Ctrl + M** (Partial move)



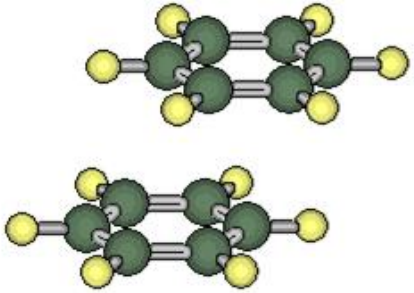
4. Drag molecule on upper-right window



5. Adjust view angle



6. Save as needed



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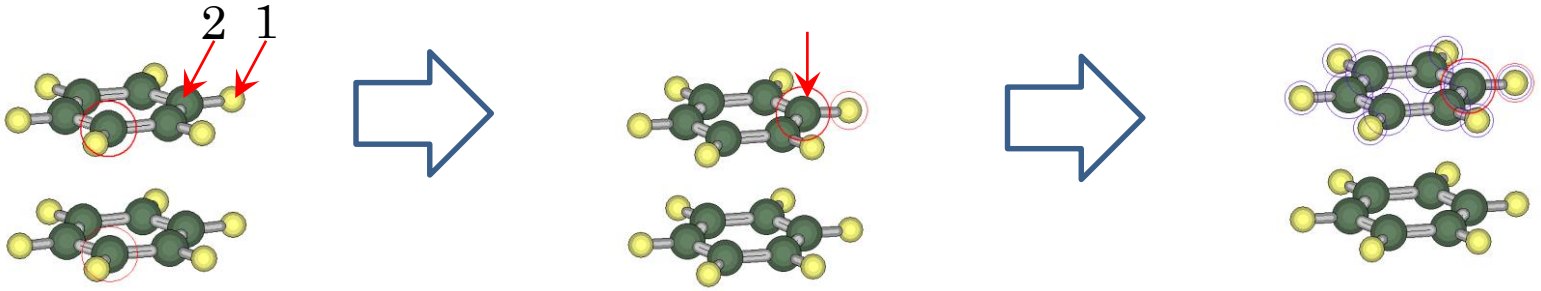
IV. Modeling Benzene Dimer – T-Shaped

1. Start with Benzene Dimer – Sandwich configuration, click atoms in order shown below (define axis)

2. Hold down **Shift** and click on molecule indicated by red arrow (select molecule for reorientation)

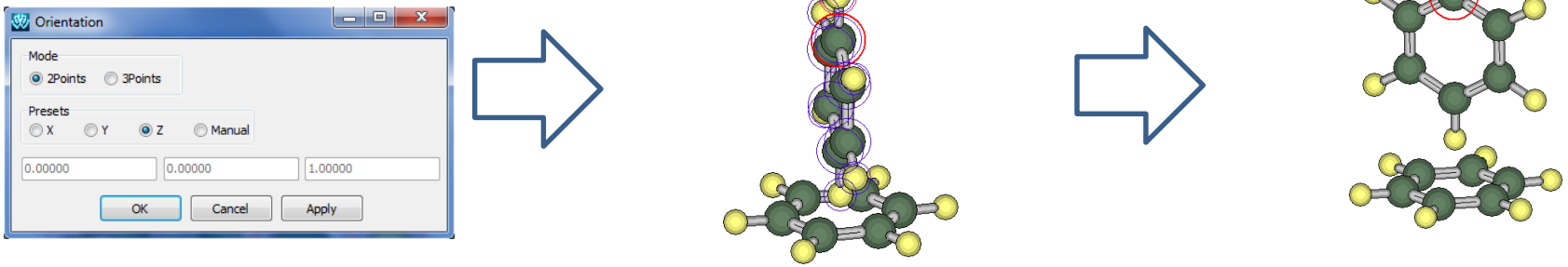
3. Select **Edit | Partially Edit | Partially Orientate**



4. Select **2 points** for **Mode**, Z for **Presets,** click OK

5. Adjust molecule spacing using **Multi-view** and **Partial movements**

6. Save as needed



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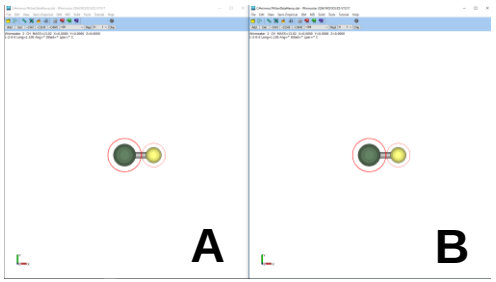
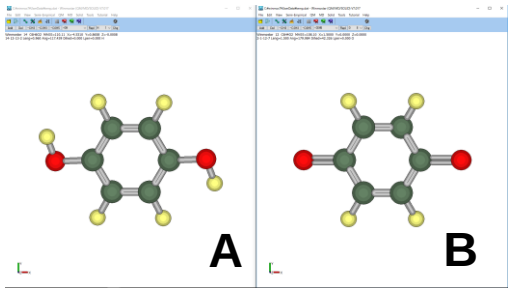
V. Modeling Charge Transfer Complex

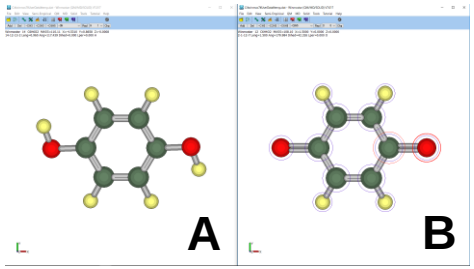
1. Open 2 Winmostar windows. Here, they will be called windows A and B

2. Model molecules on both windows A and B.

3. Select molecule in window B by **Shift+Click**, then **Ctrl+C (partial copy)**.



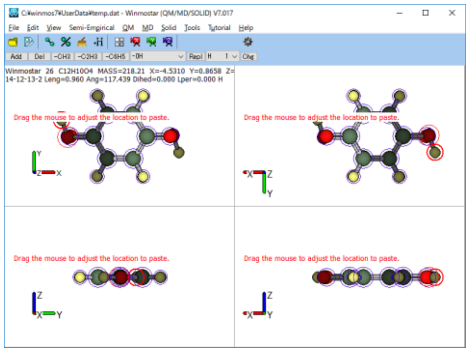


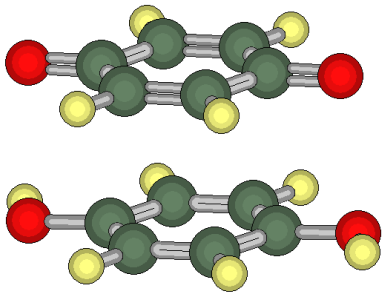


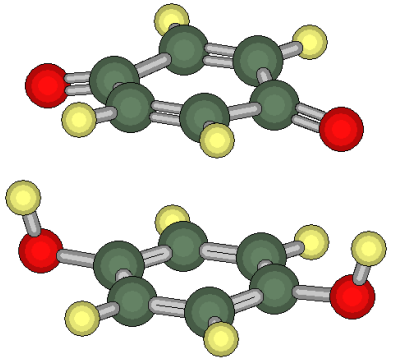
4. Click windowA and press **Ctrl+V (partial paste)** adjust molecule position as needed.

5. Optimize the configuration using GAMESS.
(for example: b3lyp/6-31G*)

6. Molecular configuration after optimization.







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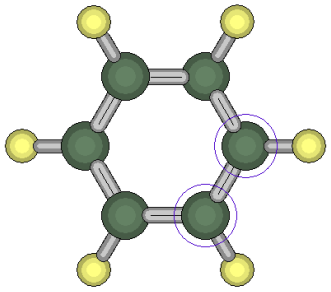
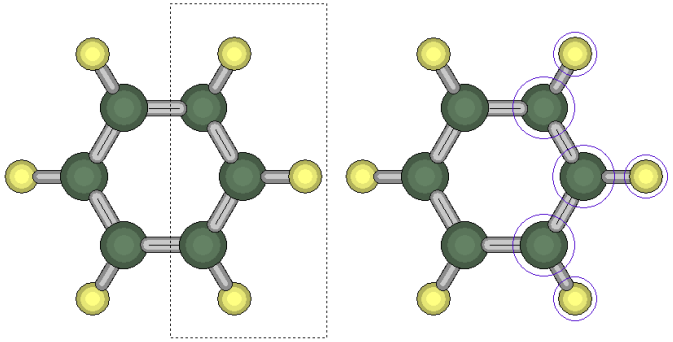
Appendix (Partial Selection)

There are three ways for partial selection (blue circle)

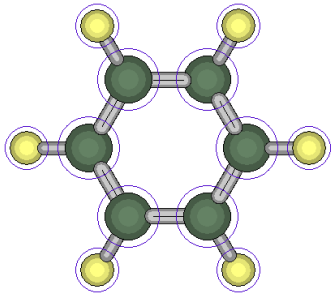
Hold down **Ctrl** and select atom (partial selection)



Hold down **Ctrl** and drag cursor on window (areal selection)



Hold down **Shift** and click molecule (selection of molecule)



A blue circle indicates partial selection.
Edit | Partially Edit feature allows users to model molecules with flexibility.

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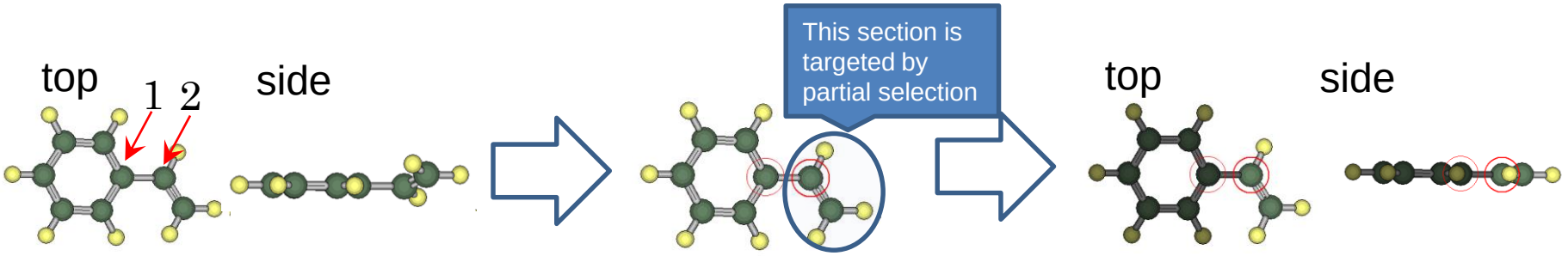
Appendix (Partial editing)

Two ways of utilizing **Edit | Partially Edit**

Editing with no partial selection (useful for monomolecular modeling)

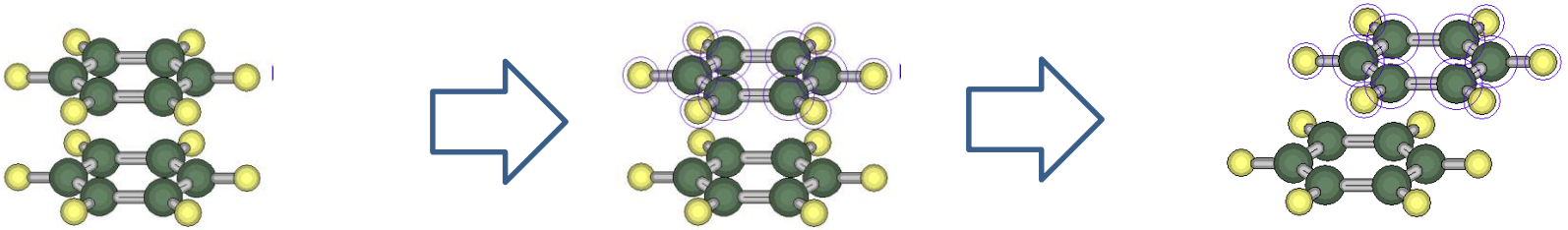


Click on atoms in orders indicated

Ctrl + R
(Partially rotate)

Drag and rotate molecules as needed

Editing with partial selections (useful for multiple molecules)



Hold down **Shift** and click on molecule

Ctrl + M
(Partially move)

Drag and move molecules as needed