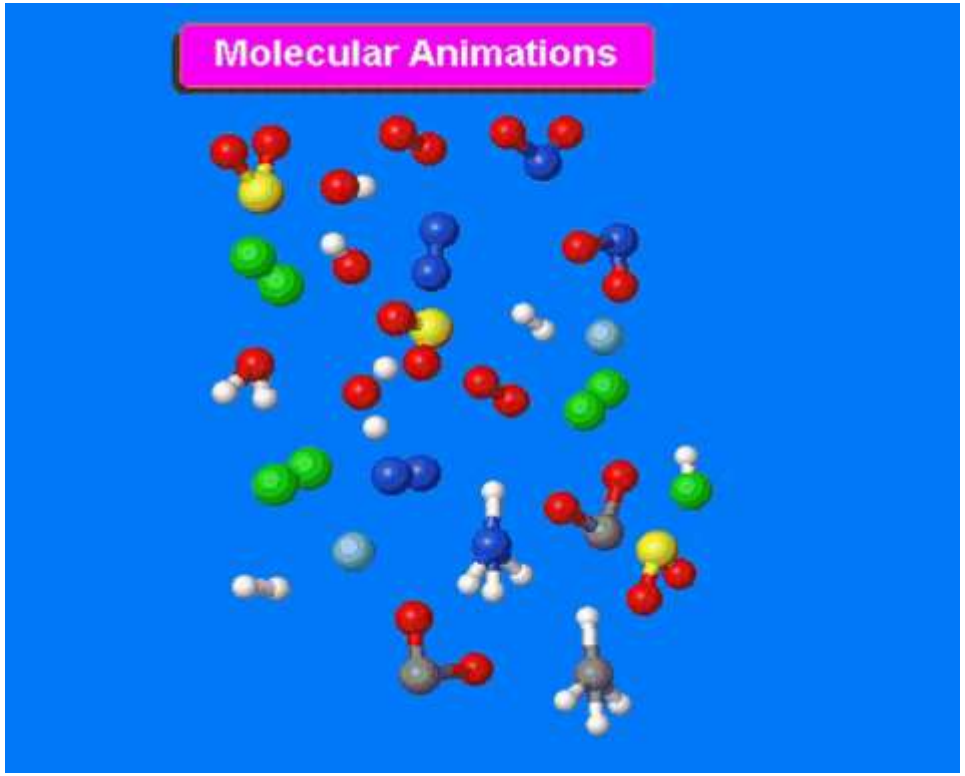
Molecular Workbench

Interactive simulations for teaching and learning science



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TGT Science

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Why interactive simulations in science?

- Experience the science of atoms and molecules in most versatile way .
- Visualize the scientific phenomena that appear in textbooks.
- Learn science in more engaging way and nurture natural curiosity.

The Software - Molecular Workbench

- **A free and open source software.**
- A modeling tool for designing and conducting computational experiment across science.
- An interactive learning environment.
- License under Creative Commons Attribution-Non-Commercial 3.0.

System requirements

- MW runs on Windows, Mac OS X and Linux, provided that the computer has at least 128 MB of RAM and a Java Runtime Environment (JRE)

- **Jmol -** It is used as a 3D renderer. It is also used as a molecular viewer to show molecular structures.

Java 2D Graph Package Version 2.4(GPL License)- It is used as an X-Y graph that displays simulation results.

The website- http://mw.concord.org/modeler/

Windows users

File name - mw.jar

1. Install the latest Java software, if you have not.
2. Click this link to save mw.jar on your disk. Do not rename the file--the file name must be exactly "mw.jar".
3. Double-click once and only once on mw.jar to launch MW. On some old machines, the launching process will take a while. Please wait.
4. To run MW again, just double-click mw.jar. You need not repeat the first two steps when you want to run it again.

Mac OS X users

You must have OS 10.4 or higher version and Java 1.5 or higher version. If you do not have the required Java version, please update through the Software Update utility. Once you make sure that you have the required Java software, right-click or CTRL+click this link: mw.jar and save the file to your disk. Do not rename the file--the file name must be exactly "mw.jar". After downloading it, simply double-click once and only once on it to launch MW.

Linux users

You need to install the latest Java Runtime Environment first, then download the file given by the following link: mw.jar. Double-click on mw.jar to launch MW. If it does not launch, open a x-terminal, change to the directory where it is located, and type in the following command: java -jar mw.jar. If the java command is not recognized, please also include the path (e.g. /usr/local/jdk1.6/bin, if Java is installed in the /usr/local/jdk1.6 directory).

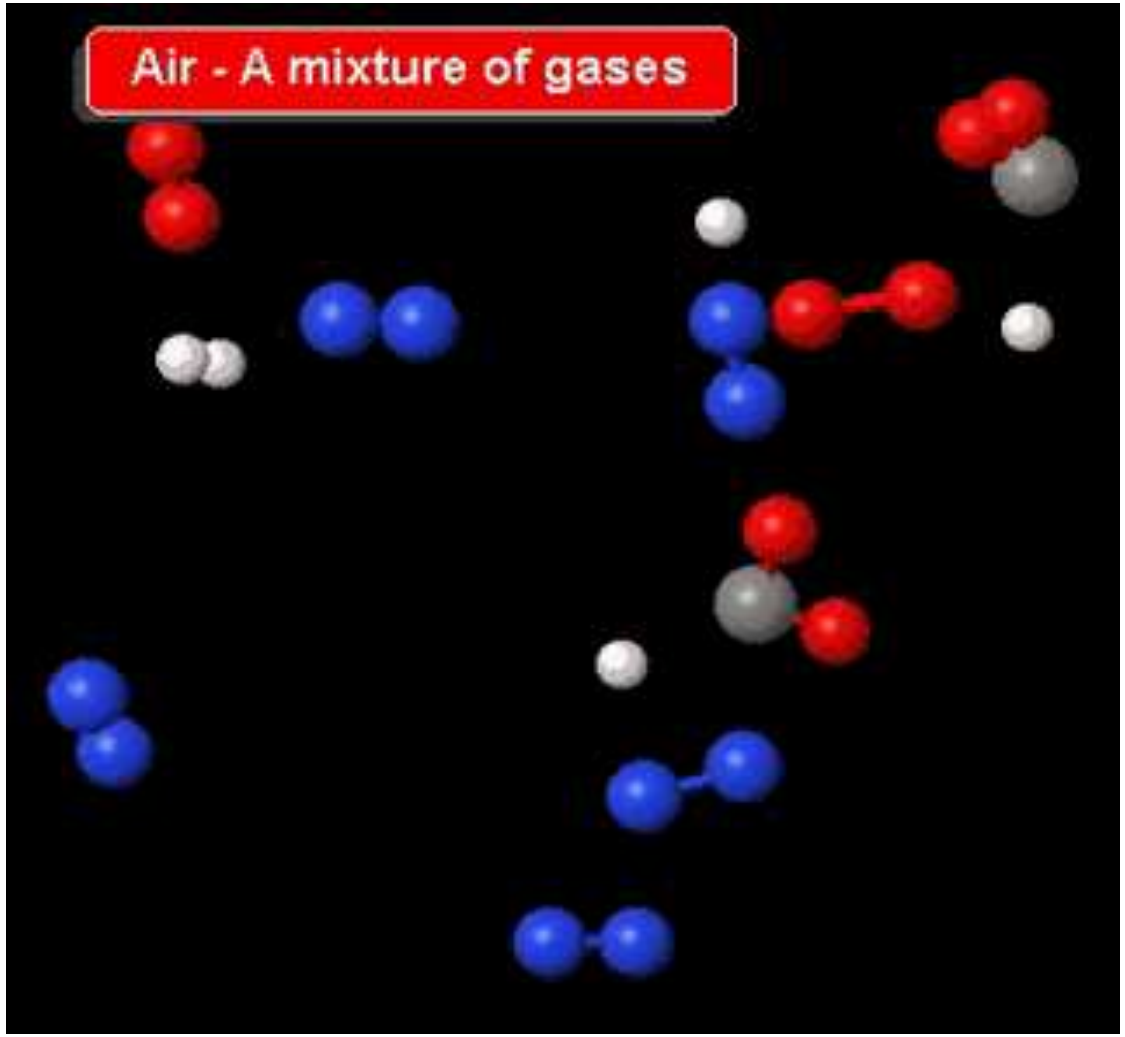
MW covers a range of topics

- Chemical Bonding
- Chemical Reactions
- The Genetic Code
- Protein Synthesis
- Gas Laws

- Fluid Mechanics
- Properties of Materials
- States of Matter
- Phase Change
- Heat Transfer

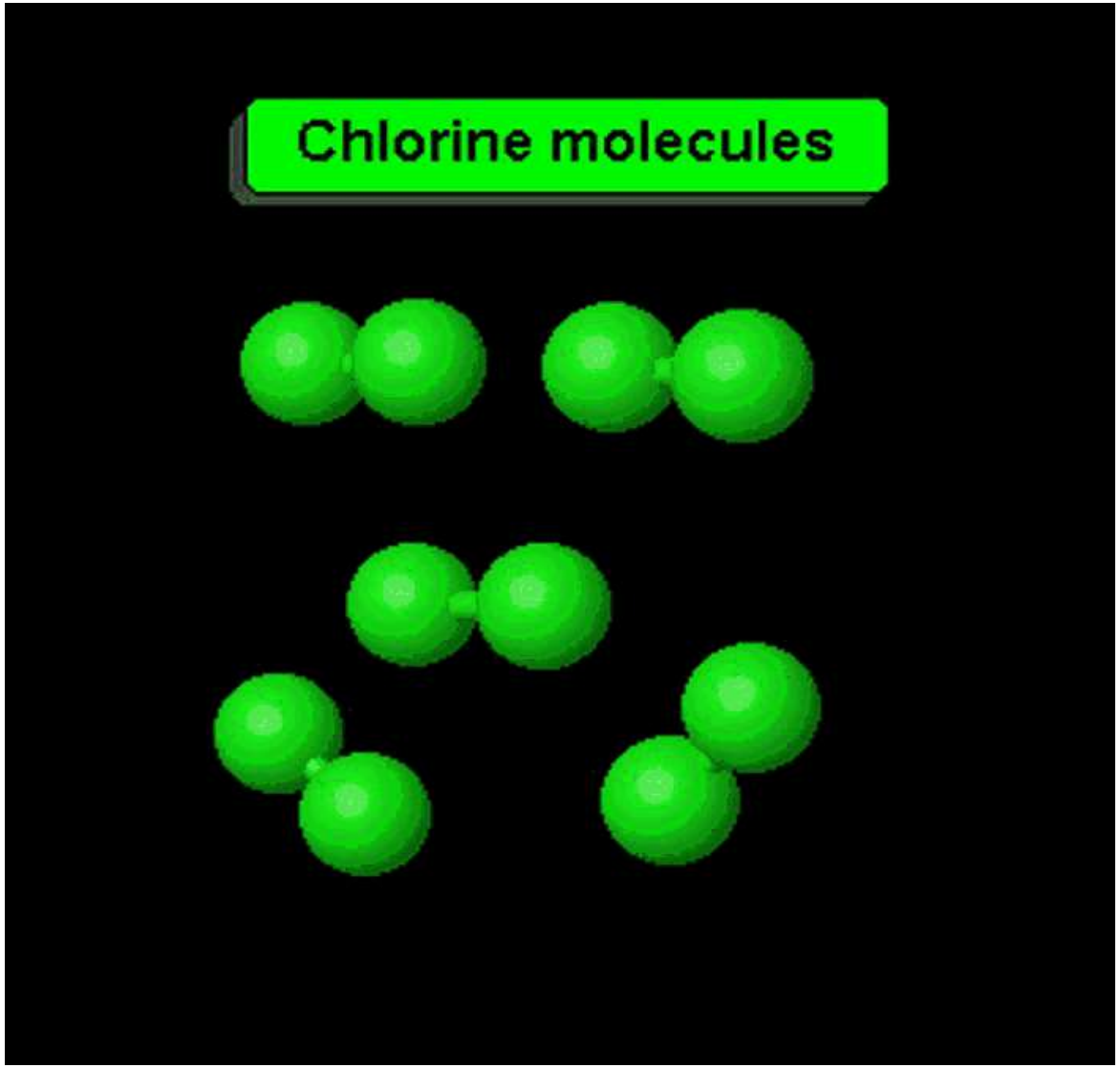
Air : A mixture of gases

This simulation shows the components of air as a particle model in a small container. A mixture of elements and compounds are shown in this model.



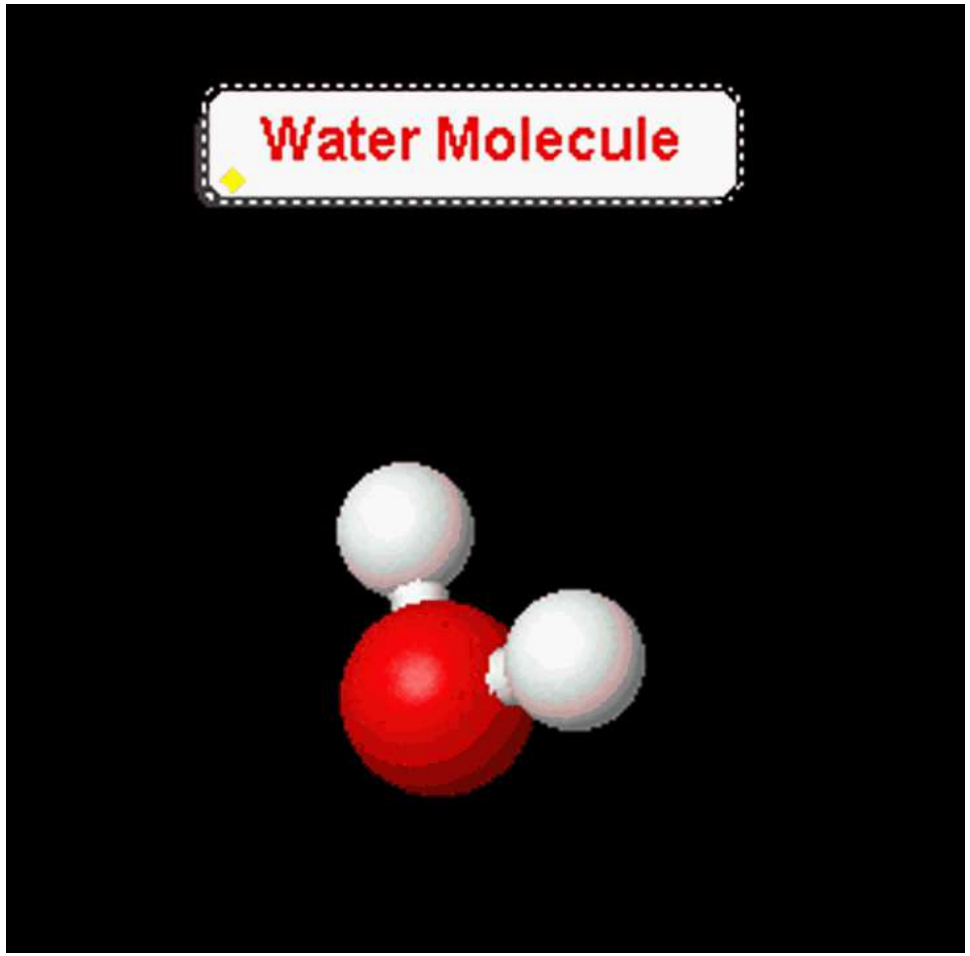
Chlorine Molecules

Chlorine is diatomic gas with symbol **Cl** . Two atoms of chlorine combine to make one molecule.



Water Molecule

Its chemical formula is **H_2O**.
Its molecule contains
one oxygen and
two hydrogen atoms

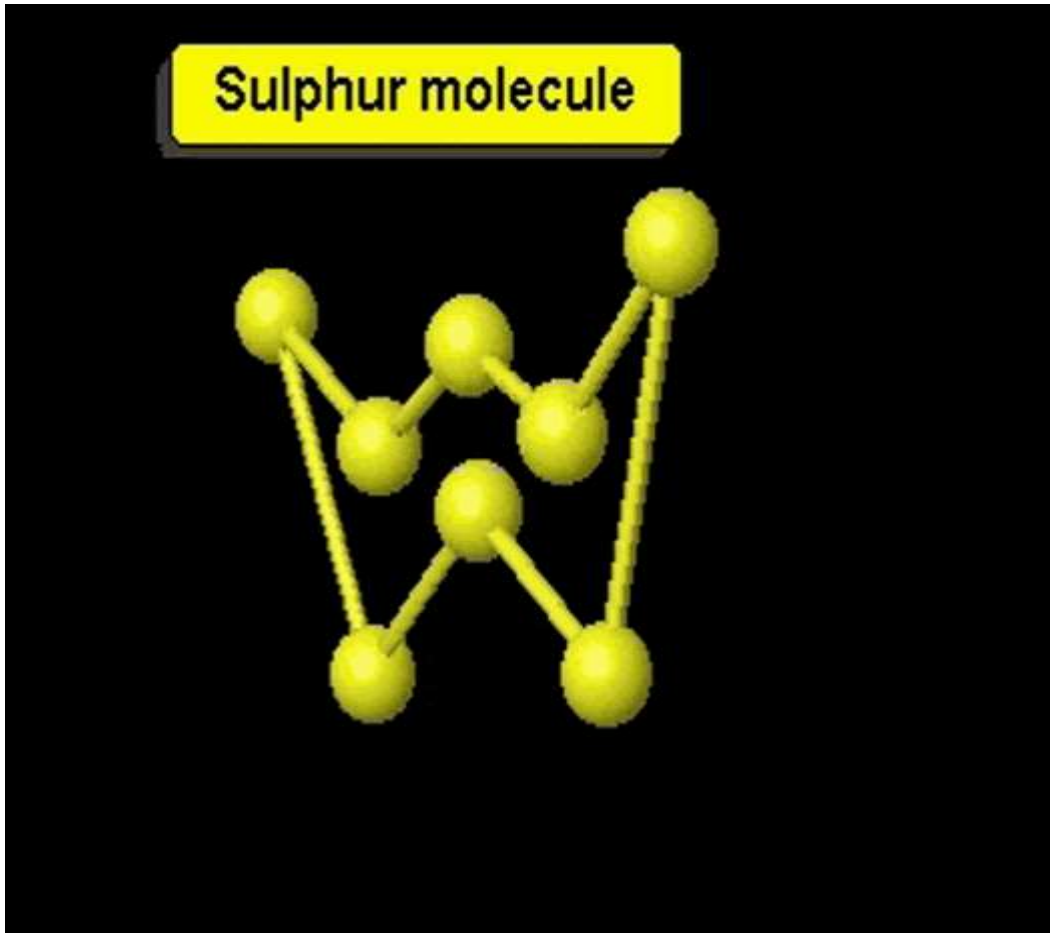


Oxygen atom

Hydrogen atom

Sulphur Molecule

Sulfur or **sulphur** is a chemical element with symbol **S** and atomic number 16. It forms a puckered ring structure of 8 atoms.

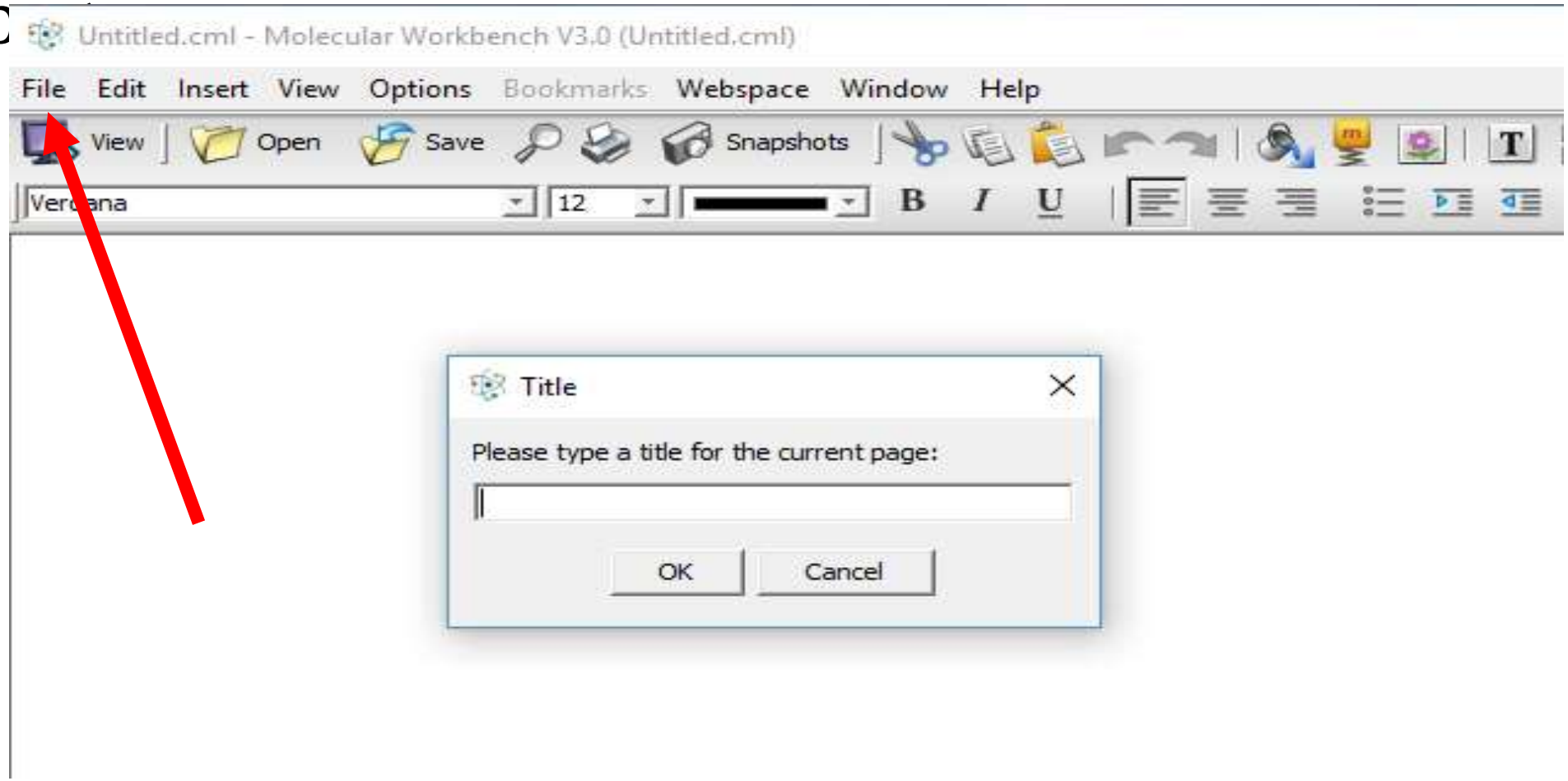


Sulphur atom

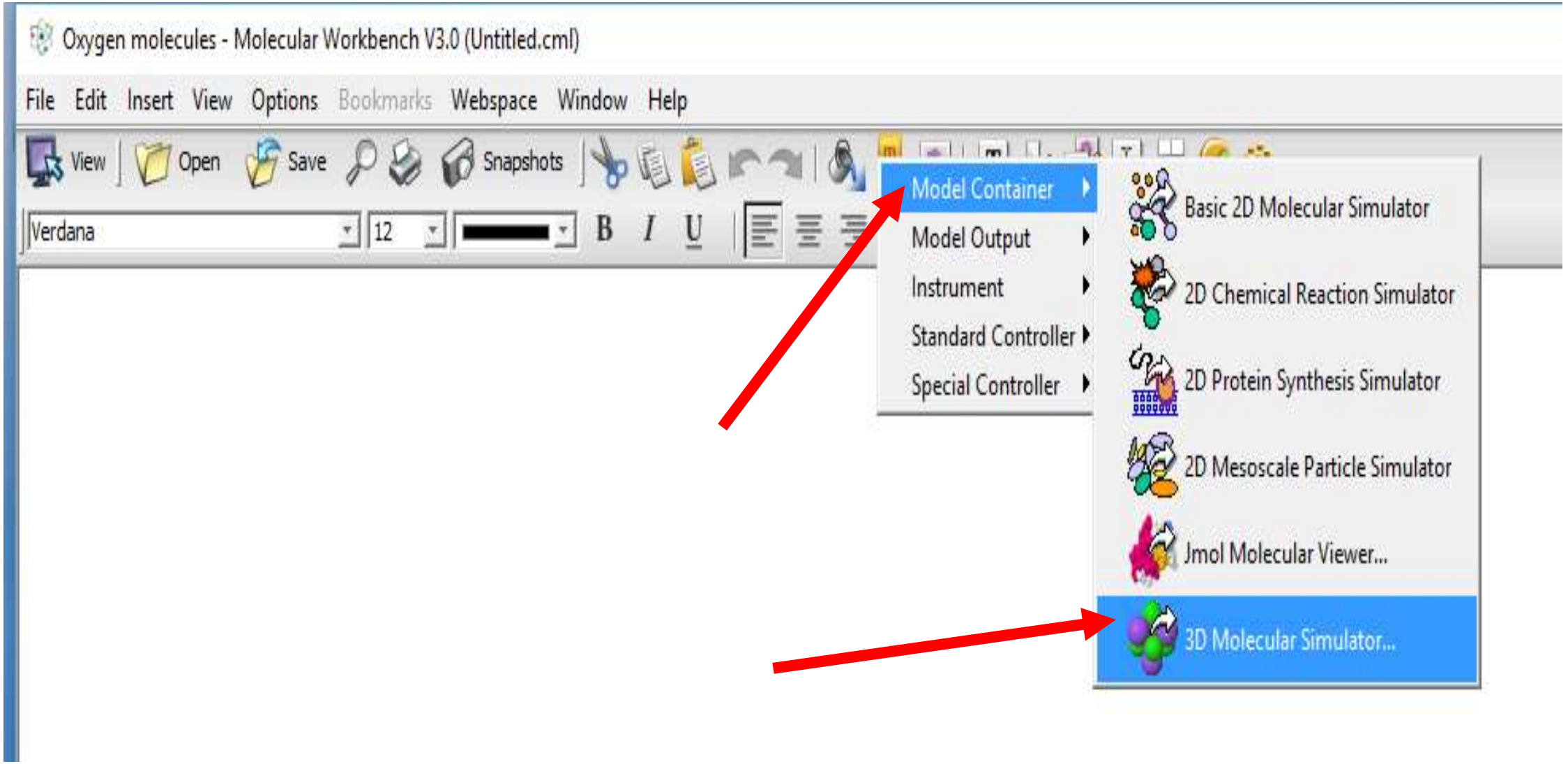
Exploring Molecular Workbench
&
Designing molecular models

Steps to design a model of molecule

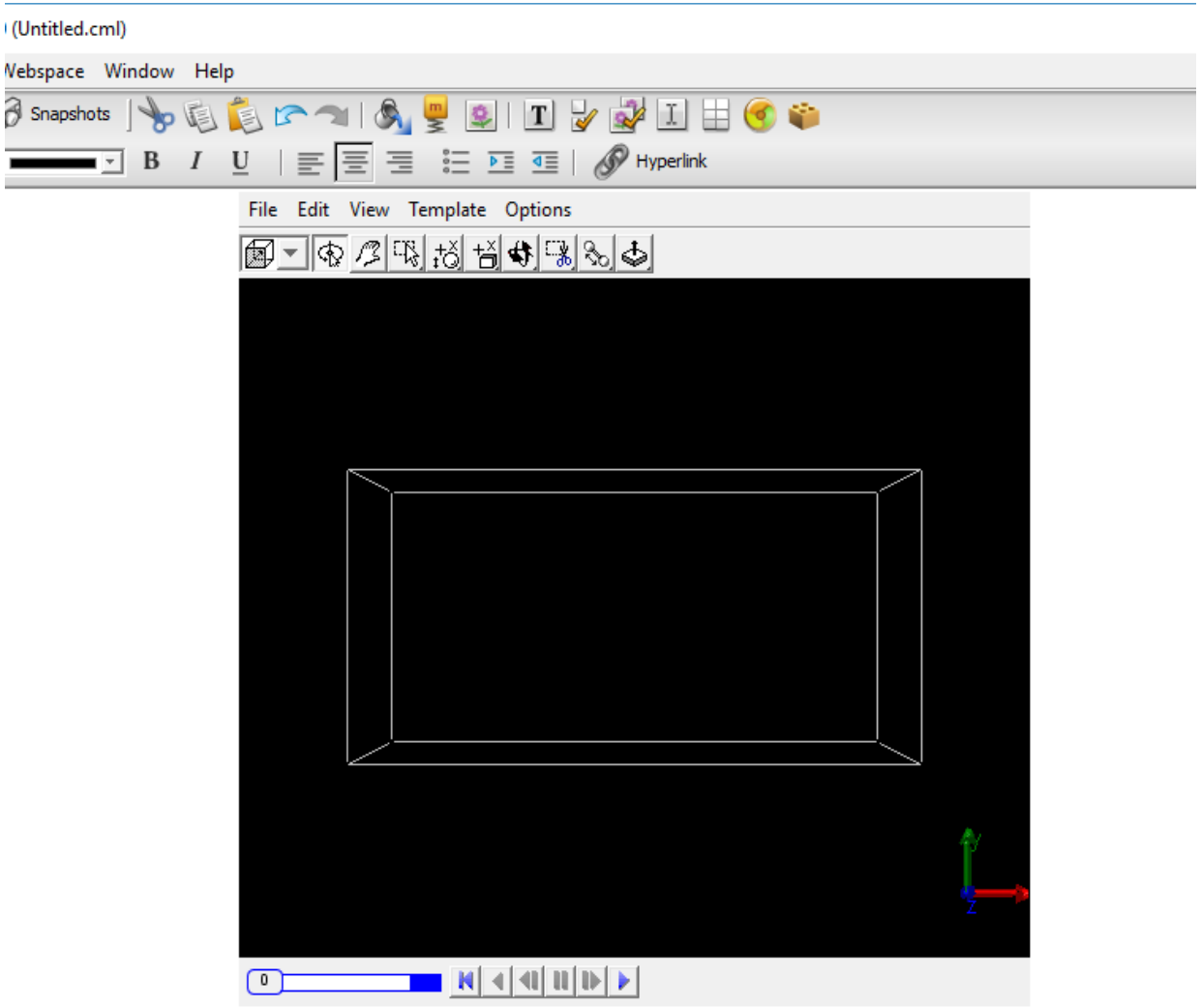
Step I. Click file menu to open a blank page and type the title of p



Step II-Insert a model component and select 3D molecular simulator from drop down menu.



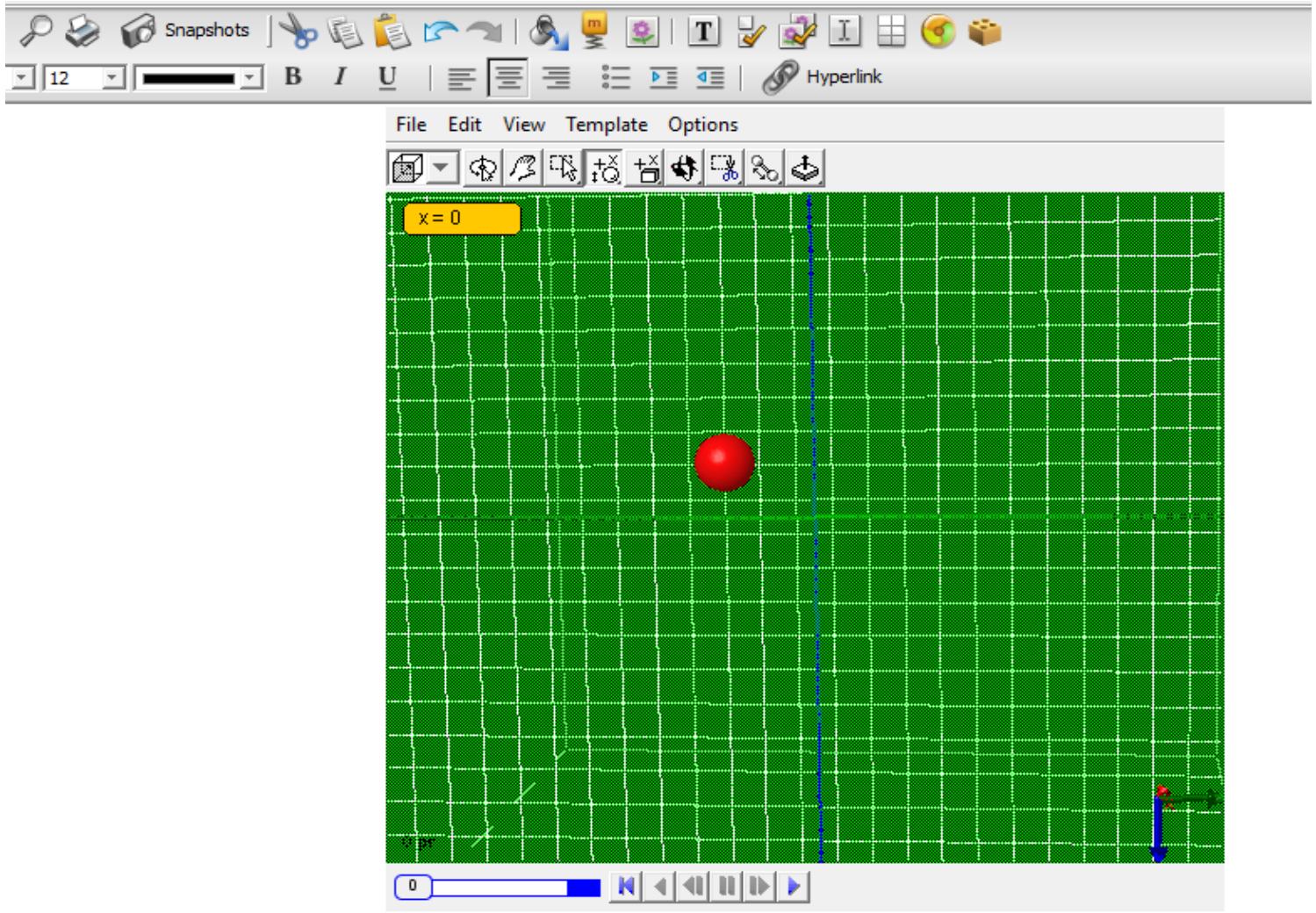
Step III - Customize the size of the container width 600 and Height 600. You can choose borders also. Align model paragraph centre.



- **Step IV-** Drop an atom on a plane perpendicular to X axis

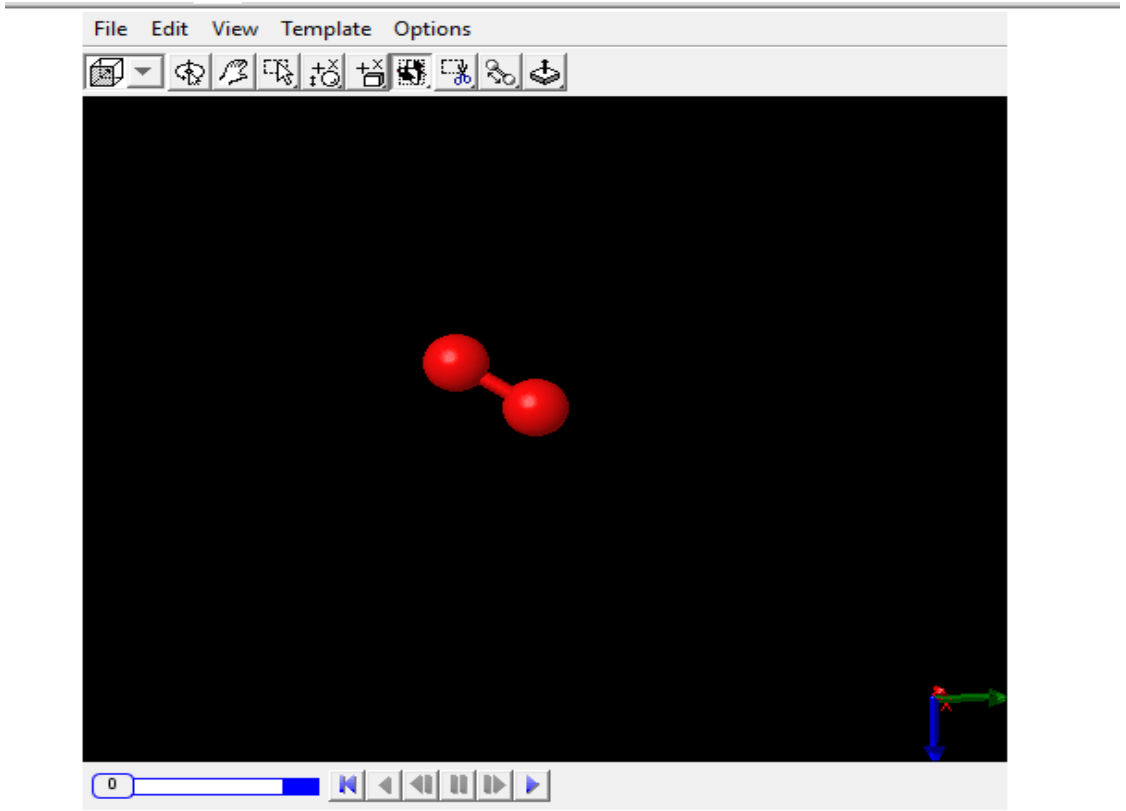
- **Step V-** Select element say for example Oxygen . Graph can be seen by tilting the model by dragging the cursor.

Step VI- Double click on screen of green bar . Atom can be seen

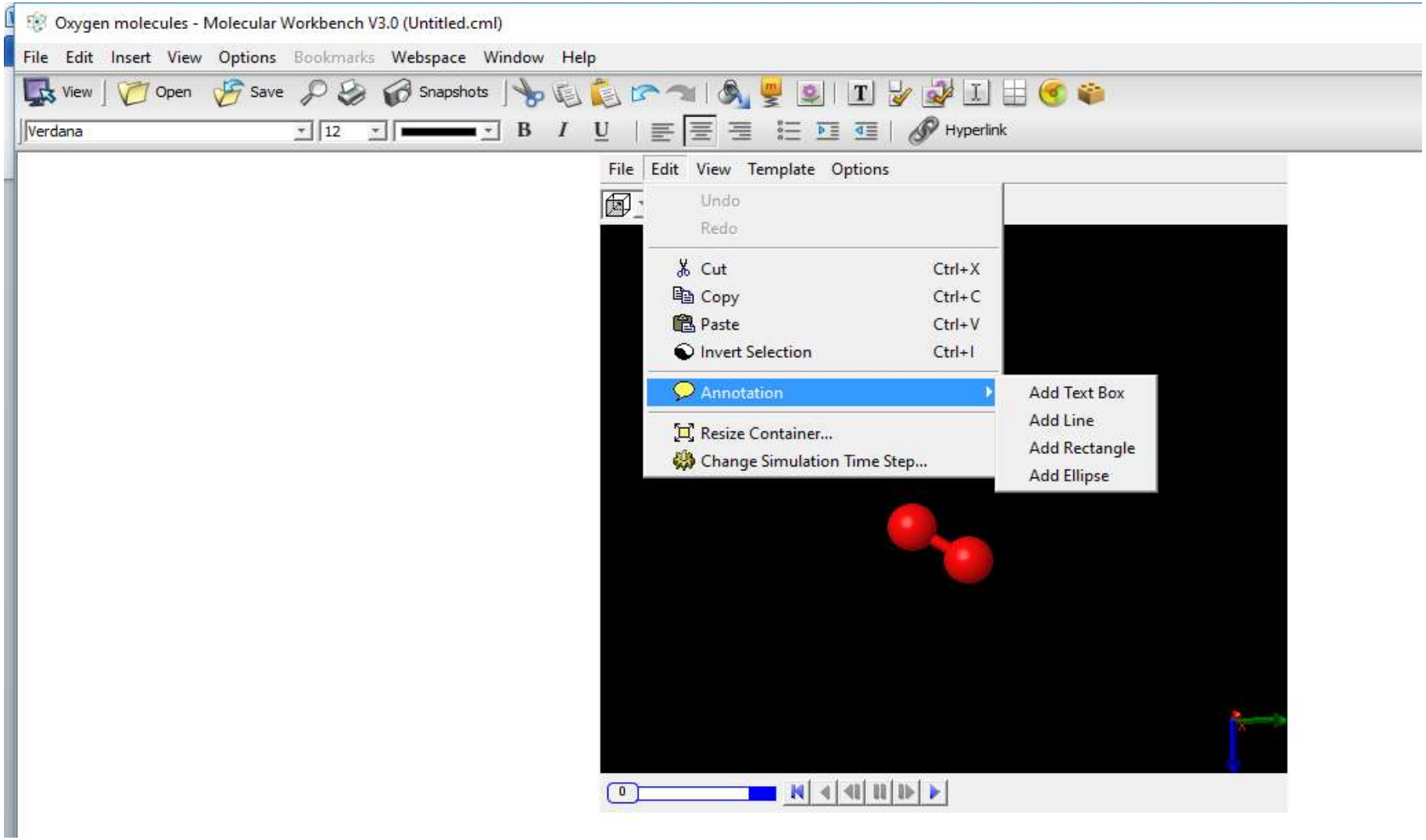


Step VII – Drop another atom of Oxygen and build a radial bond between two atoms by first clicking on radial bond icon and then atoms with pressing ALT key

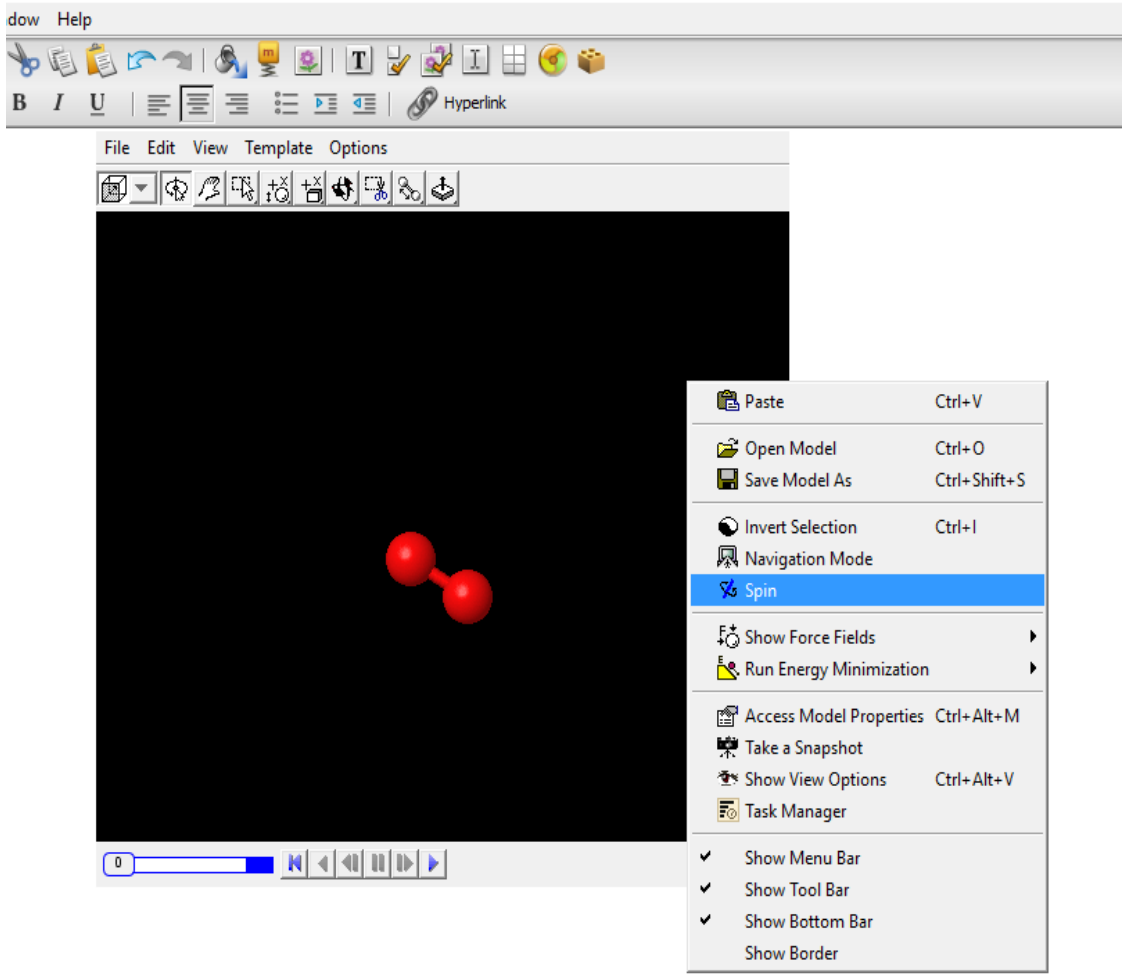
Step VIII- Click on rotate TAB



Step IX- Put annotation by clicking Edit TAB



Step X - Spin the model by right clicking on model



Credits

- **Soft wares used for creating Molecular Models**
- **Molecular Workbench** a free, open source software - **http://mw.concord.org/modeler/index.html**
- **Jmol (LGPL License) -**an open-source Java viewer for chemical structures in 3D
- **Java 2D Graph Package Version 2.4(GPL License)**

Thanks

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