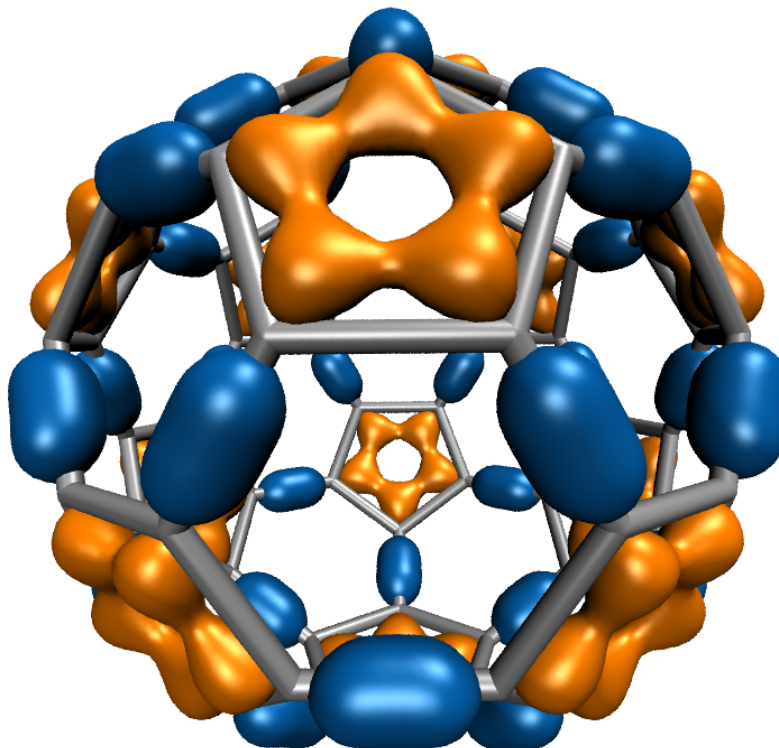


# VMD Quantum Chemistry Visualization Tutorial

## A tutorial for the visualization of quantum chemistry calculations using VMD

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## 1. Introduction

VMD [1] can be used to load files that contain quantum mechanics (QM) data such as GAMESS log files and Molden files. With QM data loaded, VMD can display molecular orbitals, as well as access the calculated energy levels and various other data present in the loaded files [4, 3].

In this tutorial output from the GAMESS [2] program will be used to provide input for visualization of QM Data using VMD. GAMESS is available free of charge from:

<http://www.msg.ameslab.gov/GAMESS/>

It can be used for *ab initio* calculations of molecular structure, vibrational spectra, etc. It can calculate multiple wavefunctions, corresponding to different levels of theory (e.g. Hartree-Fock, Coupled Cluster methods, DFT, etc.). Depending on the calculation type, GAMESS output can, in addition to atomic coordinates, contain various different data like wavefunctions, input parameters, energies, normal mode vibrations, etc. The output from a GAMESS calculation can be loaded into VMD. VMD can then be used to plot molecular orbitals, wavefunctions, electron densities and access the QM data present in the loaded file via the Tk Console.

## 2. Visualizing Molecular Orbitals

Let's explore the orbital representation starting with a simple molecule: water. To start VMD, in the terminal type

```
> vmd
```

Once VMD is started the VMD Main and VMD Display windows will be shown. The VMD console will be shown in the terminal window from which VMD was started. GAMESS output can be directly loaded into VMD in the same way that any other molecule is loaded. Once loaded, the final structure of the molecule from the GAMESS log file will be shown shown in the Display window, where it can be rotated and inspected.



**Naming convention:** Note that in VMD, a file ending `.log` is assumed to be a GAMESS file. This is due to the convention of saving GAMESS output in `.log` files, however it is a common ending for many different file formats.

### Orbital Representations

- Some files may contain multiple wavefunctions. You can choose which wavefunction you would like to see from the Wavefunction Type drop-down list.

- A maximum of 20 orbitals can be listed in the Orbital drop-down list. To quickly get to a specific orbital, use the OrbList arrows to skip to the correct decade before selecting the orbital of interest in the Orbital list.
- Higher Grid Spacings draw the orbital surface with less detail but can improve performance greatly.
- Wavefunction properties in drop-down menus that don't exist for the selected wavefunction type are disabled (greyed out).

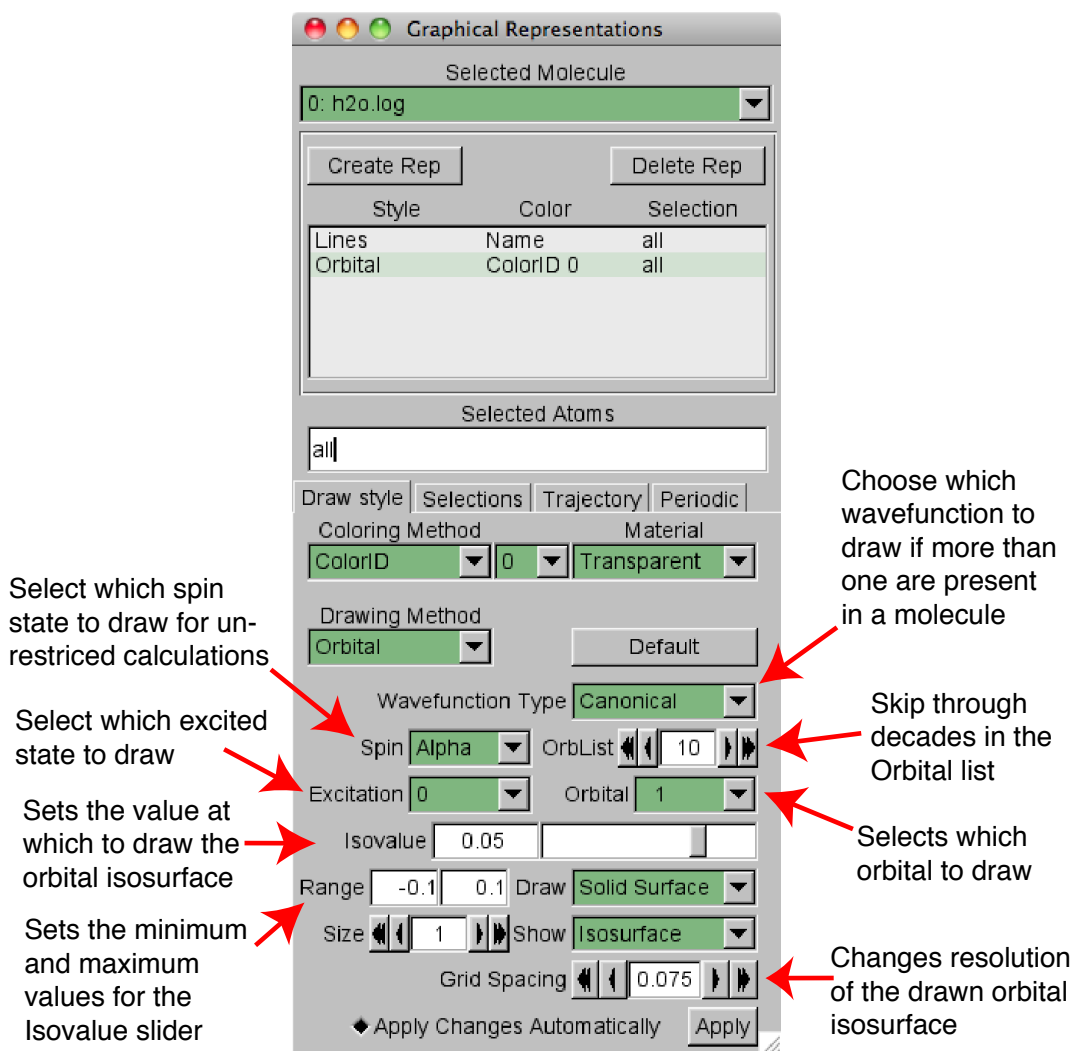


Figure 1: The Orbital drawing method in the Graphical Representations dialogue.

## Loading QM Data

1. Load the `h2o.log` file:

Select File→New Molecule. In the Molecule File Browser window click on the "Browse..." button. In the new window, browse to the directory that the GAMESS output file `h2o.log` is located. Select the output file and click "OK". Notice that the file type has been identified as "GAMESS". Click "Load" to load the file into VMD. Once this step is done, you can close the Molecule File Browser.

Alternatively you can type

```
mol new h2o.log
```

in the Tk Console (substituting in the correct path to `h2o.log` where necessary).

2. Create a new representation and select "Orbital" for Drawing Method:

In the "Graphics" menu, select "Representations...". Make sure the selected molecule is `h2o.log`. Click on "Create Rep" to create a new representation of the molecule. In the "Graphical Representations" window select "Orbital" from the "Drawing Method" drop down list.

3. Next to Isovalue type in 0.05.

4. Click Apply

This step will plot, as a solid surface, the lowest energy molecular orbital of water, which consists primarily of the 1S orbital from the oxygen. The displayed orbital can be made to look like orbital #1. in Fig. 2. by changing the material to "Transparent" and the coloring method to "ColorID".

For older computers and those without CUDA enabled graphics cards, it may be preferable to increase the grid spacing for the drawn orbitals. This will make the orbital appear coarser, but will greatly speed up calculation and drawing of the orbital isosurfaces.

The drawn isosurface denotes the surface where the value of the wavefunction, for the

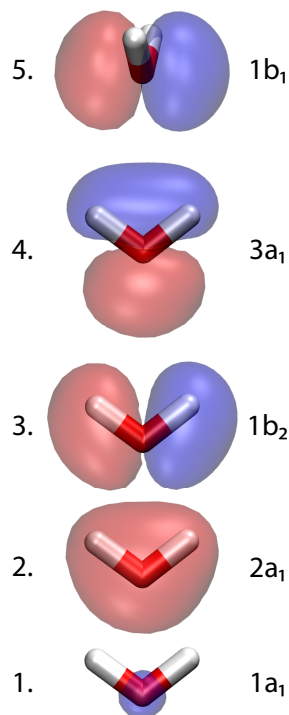


Figure 2: The occupied orbitals of water.

selected molecular orbital, is equal to to the specified isovalue (see the “Selecting the isovalue” box for more details).

To see the second lowest energy orbital, select 2 from the Orbital drop down list and set the isovalue to -0.05. The isosurface at -0.05 will then be drawn. By sliding the Isovalue slider to 0.1, you can scan through the node of the orbital function (where no orbital volume is drawn) towards 0.1 where you see volume encompassing the whole water molecule. The range of isovalues in the slider can be changed by modifying the “Range” values in the “Graphical Representations”.



**Selecting the isovalue.** For smaller absolute values of the wavefunction, we get surfaces that include a large volume. Conversely for a large absolute values of the wavefunction, we get surfaces that include a smaller volume and are closer to the most likely volume for the electrons in the selected wavefunction.

By changing the range to allow a maximum isovalue of 0.5 and adjusting the isovalue slider to 0.36, you can see that the most likely position for an electron in this orbital is between the oxygen and the hydrogens. This shows how the electrons in this orbital contribute to the O-H bonds in water.

Orbital  $1b_1$  is primarily responsible for the “lone pair” effect on the oxygen atom, and contributes to the hydrogen bonding ability of water. To see the orbital:

1. Select orbital 5 from the Orbital drop down menu.
2. Set the Isovalue to -0.05.
3. Change the Coloring Method to ColorID.
4. Set the Material to Glass 3.
5. To draw the second lobe of the orbital, click on Create Rep. Repeat the above steps for the new representation but set the Isovalue to +0.05 and choose ColorID 1.

### 3. Using the TkConsole and QM Data Interface

The information stored in the log file can be accessed via the TkConsole in VMD. Load the file containing the water molecule `h20.log`

1. From VMD Main window open the console by selecting Extensions→Tk Console
2. In the Tk Console type in `mol new h2o.log`

The basic data interface is:

```
molinfo top get <keyword>
```

where <keyword> is replaced by one of:

```
numorbitals, multiplicity, scfenergy, gradients, nimag, nintcoords,  
numbasis, numshells, num_basis_funcs, numelectrons, totalcharge,  
nproc, memory, runtime, scftype, basis_string, runtime, geometry,  
qmversion, qmstatus, num_shells_per_atom, num_prim_per_shell,  
basis, numavailorbs, wavef_type, wavef_spin, wavef_excitation,  
wavef_energy, orbenergies, orboccupancies, wavefunction,  
wavef_tree, qmcharges, carthessian, inthessian, normalmodes,  
wavenumbers, intensities, imagmodes
```

To get the energy levels of the computed molecular orbitals type in

```
% molinfo top get orbenergies
```

The returned values are the energy levels (in Hartree) for each orbital in the order that they are in the "Orbital" list of the representations window. From these values we can see that the lowest energy orbital is -20.54 Hartree (-558.9 eV). To get the occupancies of the orbitals, type in

```
% molinfo top get orboccupancies
```

The returned list gives the number of electrons in each orbital. We see here that the lowest 5 orbitals are completely occupied. Summing up the occupancies will give the total number of electrons, which can be confirmed by

```
% molinfo top get numelectrons
```

Further detail on the other keywords can be found in the VMD Users Manual.

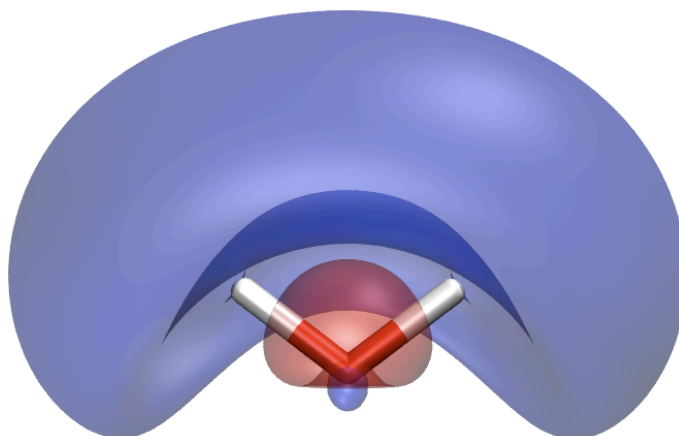


Figure 3: Lowest unoccupied molecular orbital of water

**Exercise:** Find the energy level of the lowest unoccupied molecular orbital (LUMO) and generate a figure showing both positive and negative isovalue volumes of this orbital. Your results should resemble Fig. 3.

#### 4. Viewing Geometry Minimization Steps

To view a minimization trajectory generated by GAMESS, the log file containing the optimization calculation can be loaded into VMD.

1. Load the `met.log` file

Optimization steps can be visualized as if it were a molecular dynamics trajectory. Some minimization calculations, depending upon input parameters from the user, do not write out the molecular orbitals for all steps but do so for only the last, or only the first and last frame.



**Orbitals for each step.** The default output from geometry optimizations contain molecular orbitals for only the final structure. Adding `$CONTRL NPRINT=8 $END` to the GAMESS input will print the molecular orbitals for each step.

Often the orbitals of greatest interest are the highest occupied and lowest unoccupied. An example function to find the highest occupied molecular orbital is shown below:



```
proc find_homo { m_ind } {  
  set i 0  
  while { [lindex [lindex [lindex [molinfo $m_ind get  
    orboccupancies] 0] 0] $i] > 0 } {  
    incr i  
  }  
  puts "Highest Occupied Molecular Orbital: [expr $i-1]"  
}
```

The highest occupied molecular orbital can be found by then copying and pasting the above function into the Tk Console and typing the command: `find_homo 0`. For methionine the HOMO is orbital 39. To view this orbital create a new representation and change the Drawing Method to Orbital. Click the right triangle next to “Orblist” until it reads 30. Then select orbital 39 in the Orbital drop-down list. Enter 0.05 for the Isovalue. Create a new representation identical to the last but set the isovalue to -0.05. The resulting displayed volumes correspond to the molecular orbital 39 with an absolute value greater than 0.05, shown in figure 4.

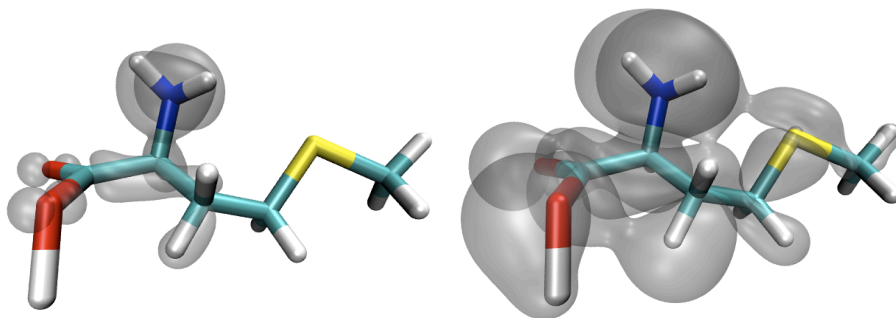


Figure 4: The highest occupied molecular orbital of methionine plotted at isovalues  $\pm 0.05$  (left) and  $\pm 0.01$  (right).

## 5. Following Molecular Orbitals Through a Trajectory

QM Trajectories can also be loaded into VMD. The primary difference, in terms of visualization, between a trajectory and a simple minimization is that the trajectory contains the molecular orbitals for each step and not only the first and last (note minimization runs can also be set to write

the molecular orbitals at each step, see the “Orbitals for each step” info box).

Load `ammonia.log`. This trajectory corresponds to the inversion of ammonia. To do this a dummy atom (labeled `X` in the structure) was introduced. Change your selection to: `all` and `not name X` so that the dummy atom is not drawn. Then create representations for isovalues at  $\pm 0.05$  for the second and third lowest energy molecular orbitals. Set the material to `Glass 3` and color the different orbitals different colors.

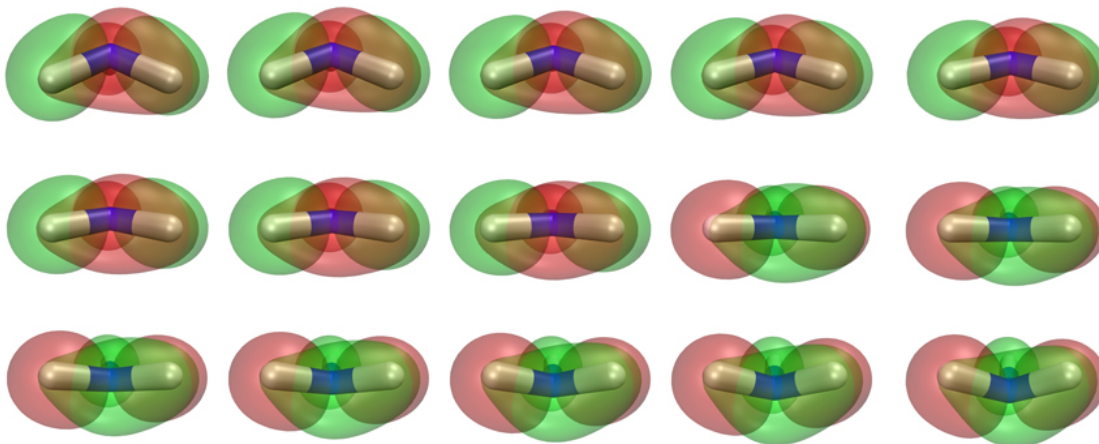


Figure 5: The inversion of ammonia showing the swapping of the 2nd and 3rd lowest orbitals' energy levels.

By stepping through the trajectory (or playing it slowly) you notice that at frame 9, the orbitals swap color. Swapping of the colors occurs because the two orbitals switch their relative energy levels, thus the previously second-lowest energy orbital becomes the lowest energy orbital, and vice versa. It is important to note that the orbital numbers are always ordered by increasing energy level for each individual frame, thus by selecting an initially drawn orbital does not necessarily correspond to the same orbital in other frames.

## Acknowledgments

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