

# Computing Molecular orbitals and electron densities using Gaussian + Avogadro/GaussView

Avogadro is open-source !!

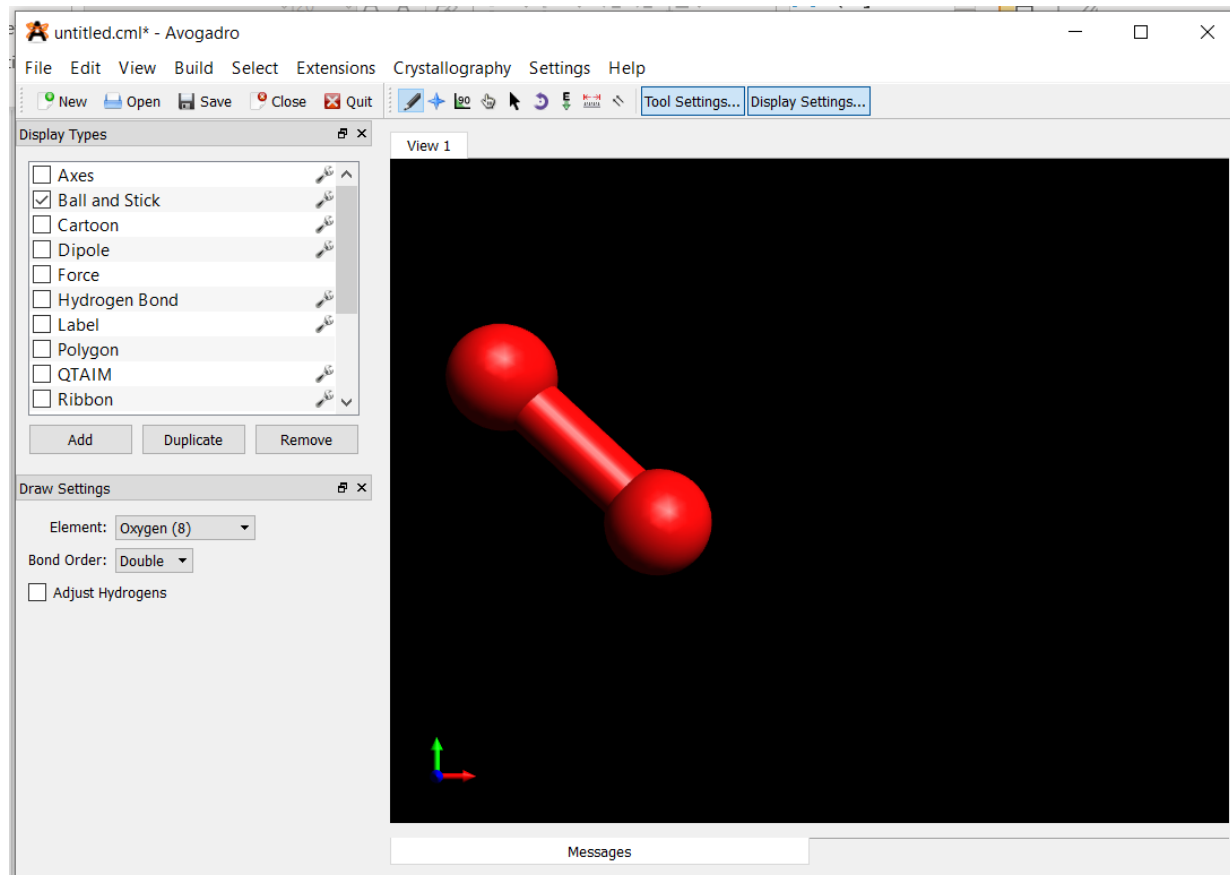
Compiled by Harin

Professor Fabrikant's Group

# Assuming you have installed Gaussian and GaussView or Avogadro.....

## Step 1. Create an input file for Gaussian

GaussView or Avogadro makes it easy to create input files for Gaussian



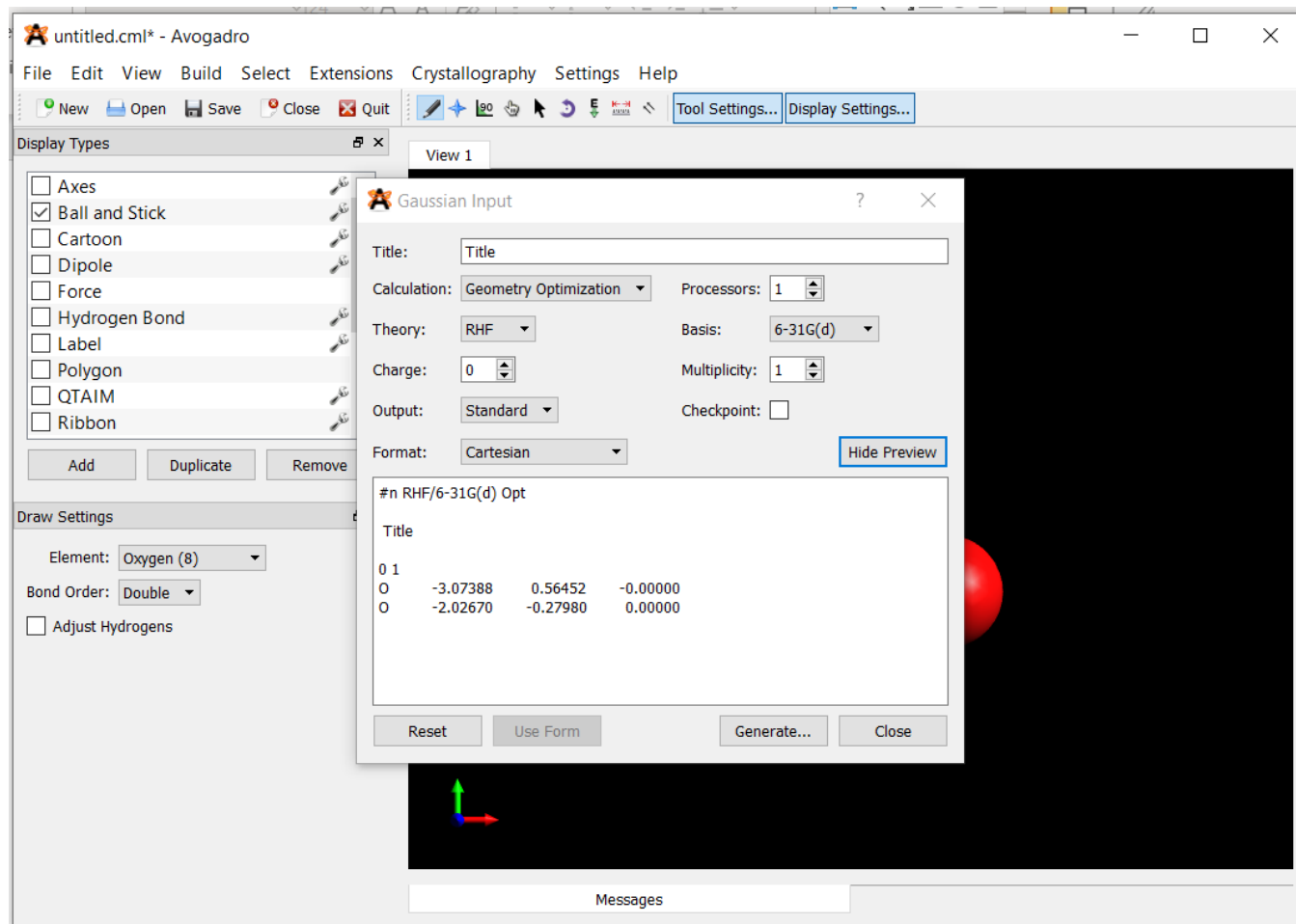
Select an Element from the drop-down menu

Left click anywhere on the black panel to place the element

Drag the element (left click on) to make bonds

Right click to delete an element

## Step 1. Create an input file for Gaussian



From the “Extensions” menu, select “Gaussian”

Later we will discuss the options in the new Pop-up menu,

Click on “Generate” and save the file , for example: O2molecule.com ( file extension is .com)

Open O2molecule.com in your favorite text editor,  
We are going to add more commands to it

## Step 1. Create an input file for Gaussian

A typical Gaussian input file(.com):

```
#n RHF/6-31G(d) Pop=Full FormCheck Opt
```

Root section

```
O2 molecule
```

Title section

```
0 1
```

Charge and spin multiplicity

```
O    -9.89176    0.75266    0.00000
```

```
O    -9.05751    -0.25659    0.00000
```

Z-matrix / coordinates of the atoms before  
Geometrical optimization (in Angstroms)

### Root section

**#n**- for standard print out of the results

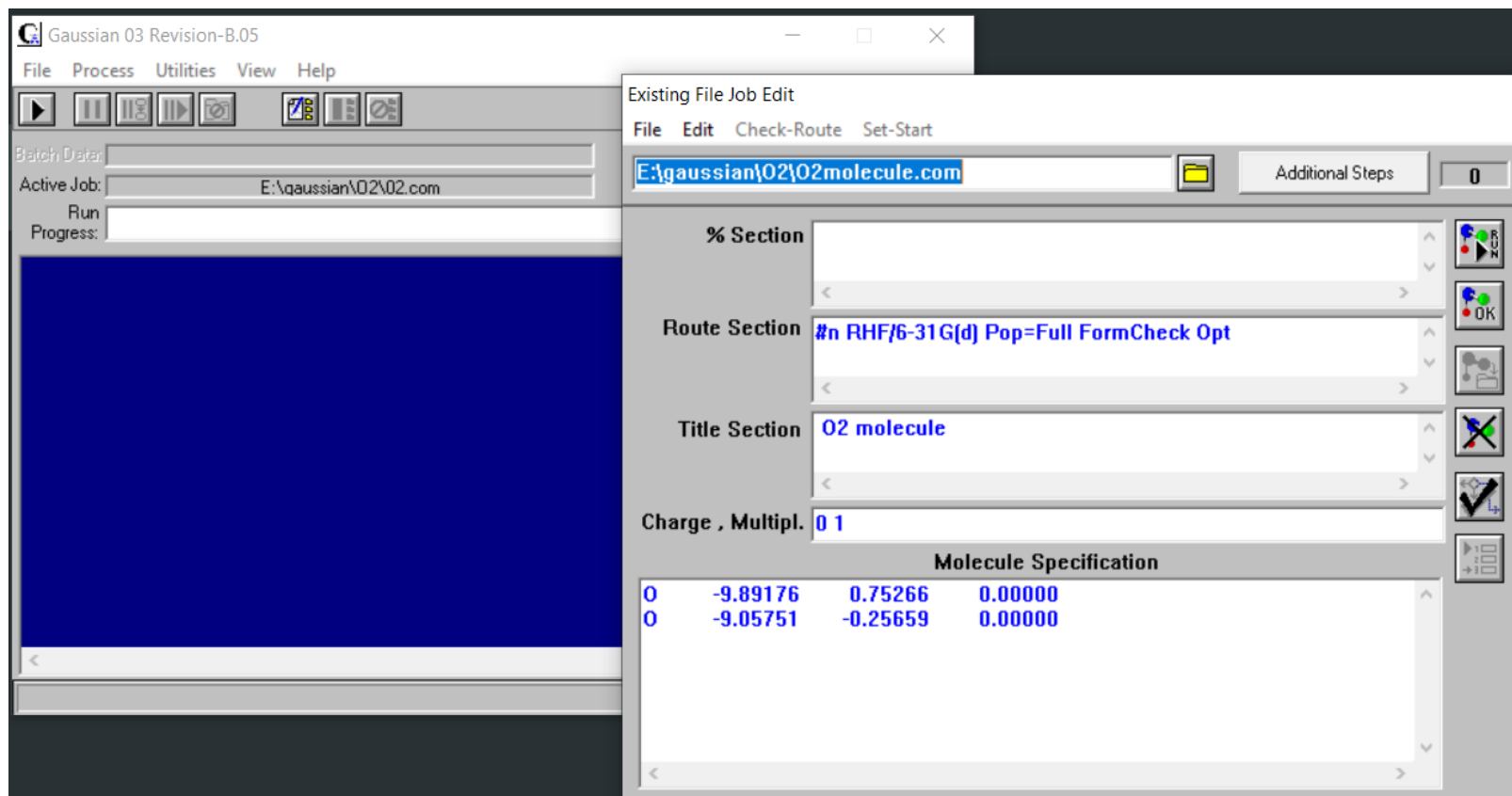
**RHF/6-31G(d)** –Restricted Hartree-Fock calculations, 6-31G(d) is the basis

**Pop=Full** - population analysis, “Full” gives all the details of occupied/valence orbitals and electron density

**FormCheck** – will create a file named “**Test.fchk**” in the scratch directory. We will need this .fchk file later

**Opt**-command for geometrical optimization

## Step 2. Run the “O2molecule.com” file in Gaussian



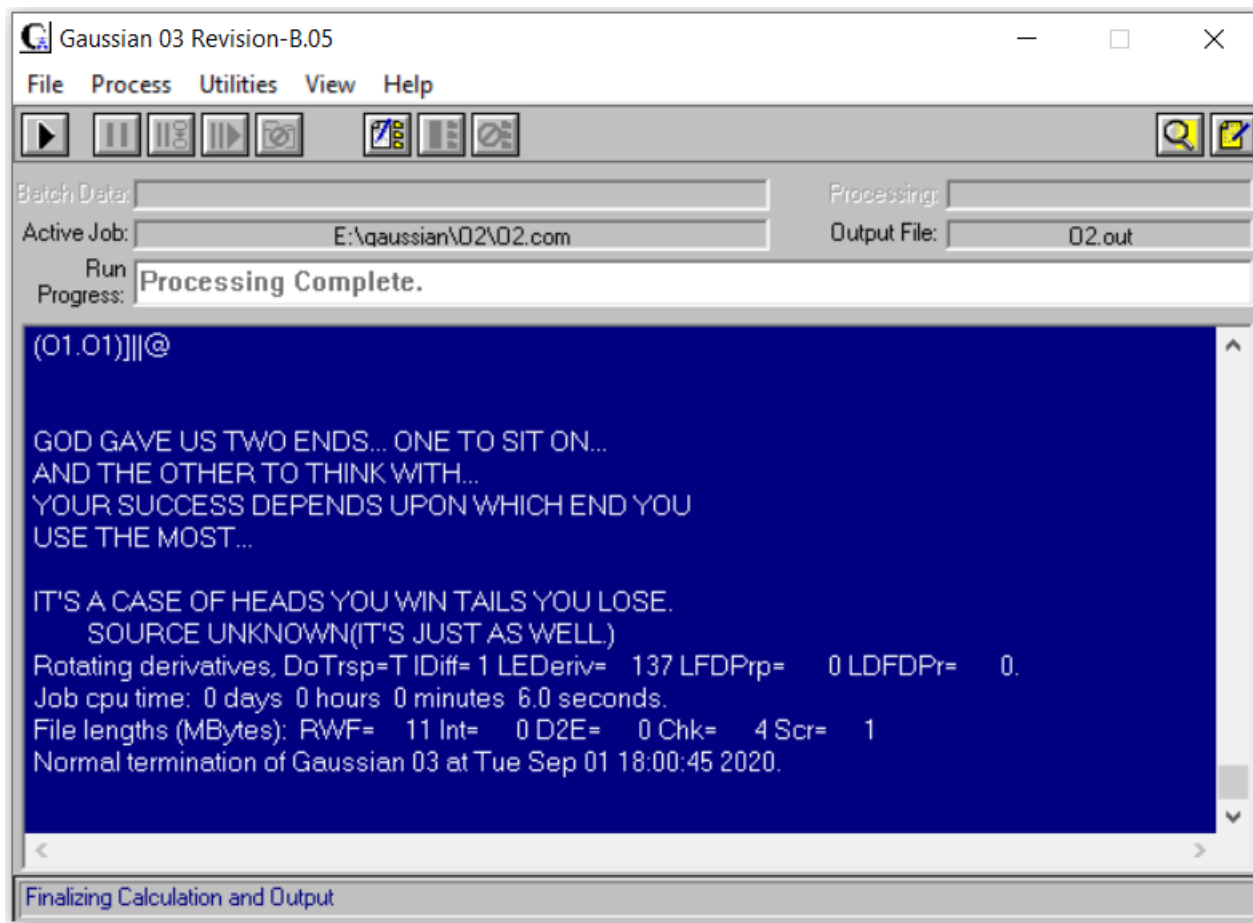
Start Gaussian , File->Open->  
“O2molecule.com”

Double check the input commands  
“%Section” for multiprocessor/intermediate  
File check options.

Click “Run”

Save the gaussian output, example:  
“O2molecule.out”

## Step 2. Run the “O2molecule.com” file in Gaussian



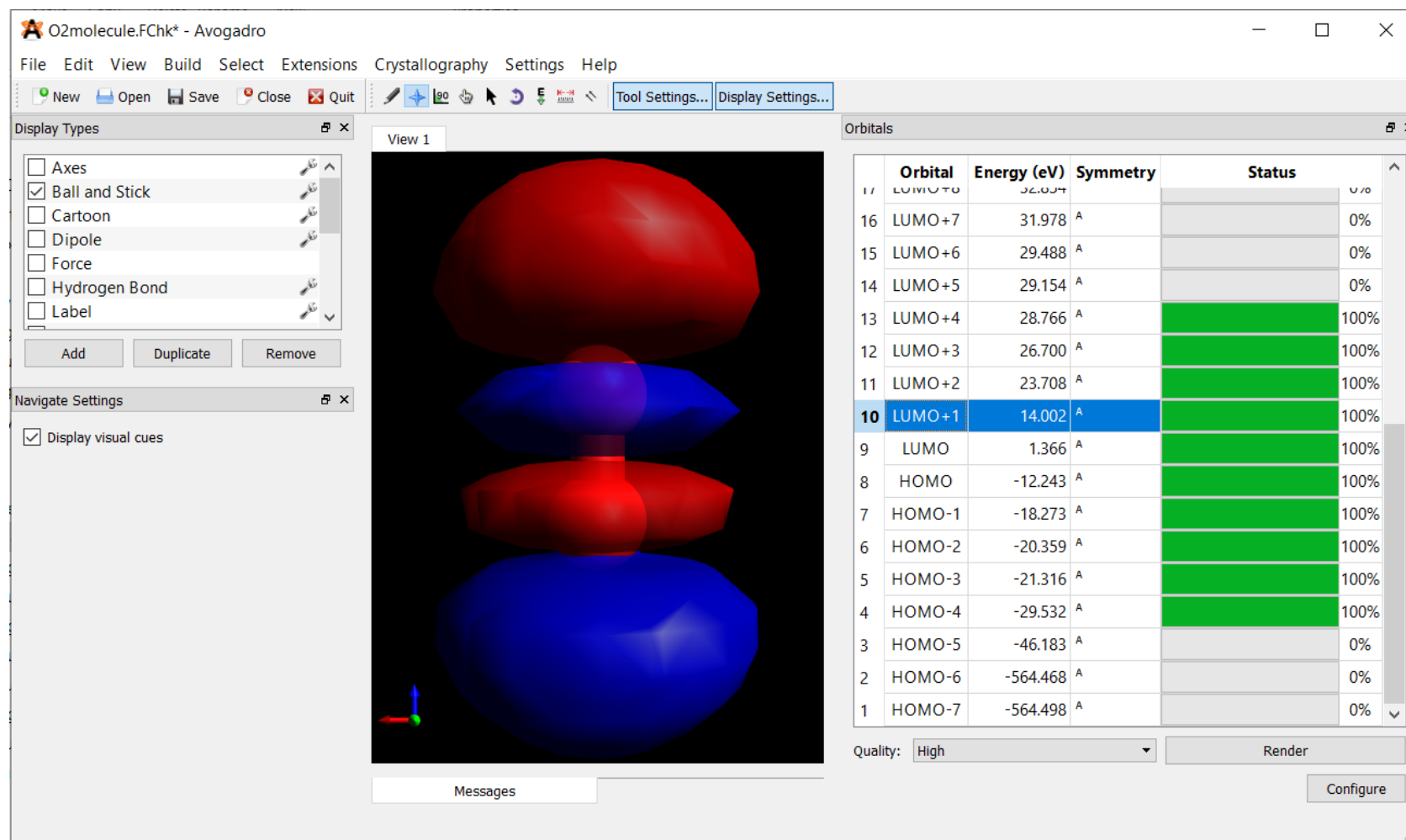
A successful run always ends with a Quote. We must Read it!

Open the “O2molecule.out” or “Test.fchk” files and explore, check for convergence, orbital energies, Symmetries, etc.

You may want to rename “Test.fchk” file and copy it to the working directory. Ex: O2molecule.fchK

Both .out and .fchk files contain the expansion coefficients of MO's and electron density.

### Step 3. Visualize the MO's or Electron density (Fun begins !)



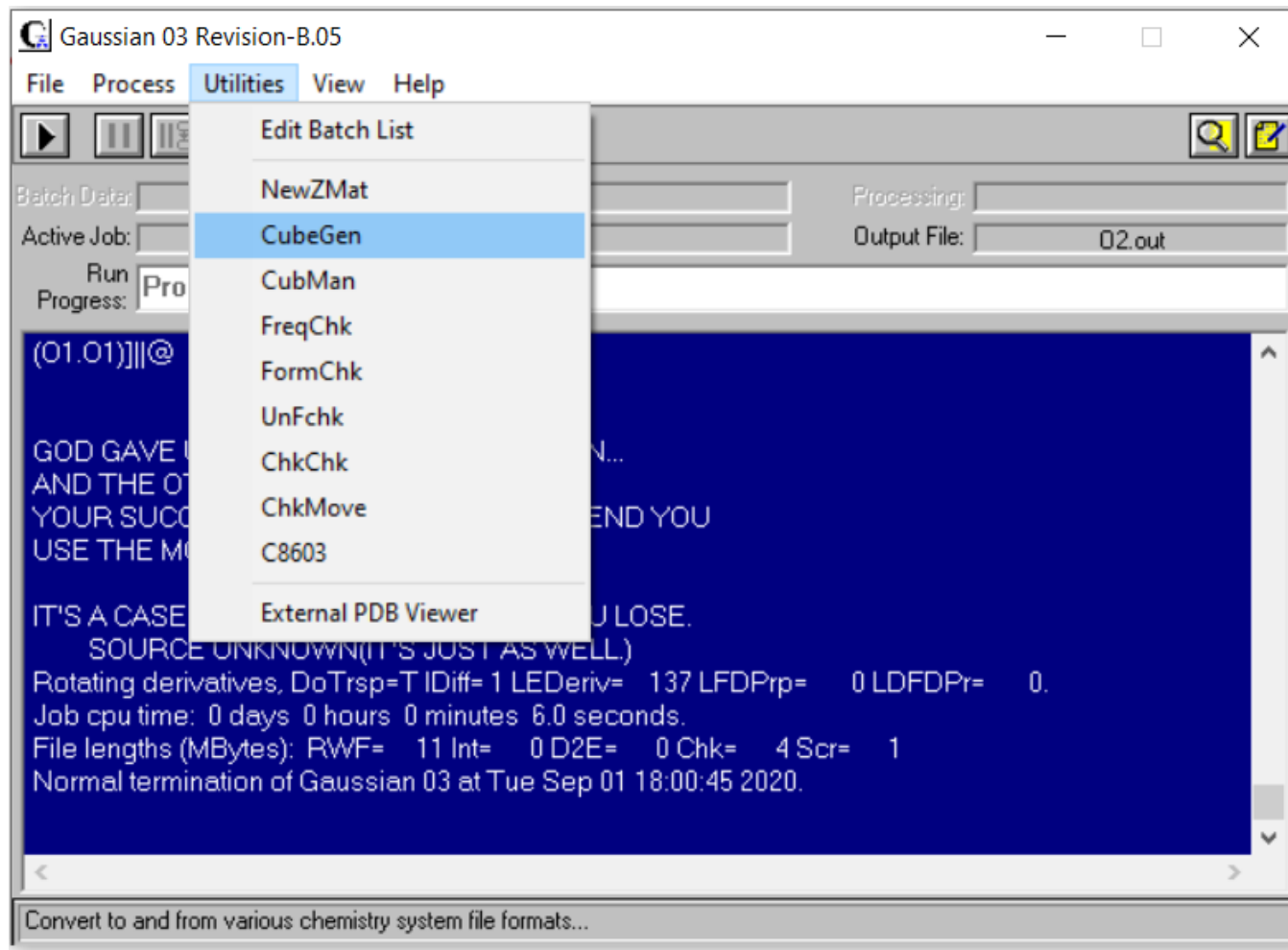
Open the “O2molecule.fchk”  
file in Avogadro

Click on any orbital to visualize

For electron density:

Extensions->Create Surfaces-> Surface Type

## Step 4. Post-calculations with .cub files



From Gaussian Utilities , click “CubeGen”

Proceed as follows:

```
Property [Density]? MO=1
Formatted Checkpoint file? O2molecule.fchk
Cube file [ ]? O2molecule.cub
Approximate points per side [0]? 40
Header in cube file [H]? Y
```

**MO=1**, prints the data for 1<sup>st</sup> occupied orbital

Save the output in “O2molecule.cub” file



## Step 4. Post-calculations with .cub files

Part of O2molecule.cub file (all in atomic units)

O2 molecule MO=1

Alpha MO coefficients

-2 -4.970736 -4.970736 -6.072059

○ A number denoting how “fine” is the grid

Starting points of the coordinates X0,Y0,Z0

37 0.272495 0.000000 0.000000

37 0.000000 0.272495 0.000000

46 0.000000 0.000000 0.272495

} # points and increments along each direction

8 8.000000 0.000000 0.000000 1.101323

8 8.000000 0.000000 0.000000 -1.101323

} # atomic number,charge,  
XYZ points of each atom

1 1 ignore, molecular orbital number

2.80708E-12 5.54800E-12 1.05243E-11 1.91601E-11 3.34751E-11 5.61224E-11

9.02842E-11 1.39354E-10 2.06364E-10 2.93185E-10 3.99620E-10 5.22626E-10

6.55947E-10 7.90452E-10 9.15293E-10 1.01982E-09 1.09582E-09 1.13957E-09

1.15299E-09 1.14341E-09 1.12191E-09 1.10054E-09 1.08907E-09 1.09237E-09

1.10907E-09 1.13191E-09 1.14973E-09 1.15054E-09 1.12457E-09 1.06673E-09

9.77605E-10 8.63070E-10 7.32669E-10 5.97409E-10 4.67591E-10 3.51190E-10

2.53066E-10 1.74952E-10 1.16038E-10 7.38416E-11 4.50863E-11 2.64156E-11

1.48519E-11 8.01372E-12 4.14999E-12 2.06274E-12

5.71755E-12 1.13003E-11 2.14362E-11 3.90258E-11 6.81831E-11 1.14312E-10

1.83894E-10 2.83840E-10 4.20328E-10 5.97168E-10 8.13959E-10 1.06450E-09

Orbital wavefunction at each grid point,  
Read and store in an array, example:

```
do 1 n1=1,n1pts
  do 1 n2=1,n2pts
    read(11,'(6e13.5)')(orbital(n1,n2,n3),n3=1,n3pts)
  1 continue
```

Example calculations of the H2 orbitals from the .cub files

