

# Drawing ELF isosurfaces with different colors for different domains

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In this tutorial I will show how to use Chimera 1.8.1 (<http://www.cgl.ucsf.edu/chimera/>) in combination with Multiwfn 3.3.7 (<http://sobereva.com/multiwfn>) to draw ELF isosurfaces with different colors for different ELF domains. Both of them are freely available. Ethanol will be taken as example.

First, boot up Multiwfn and input

*ethanol.wfn*

5 // Generate grid data

9 // ELF

2 // Medium quality grid

2 // Export cube file as ELF.cub in current folder

Then we obtain .pdb file for ethanol by following below steps.

0 // Return to main menu

100

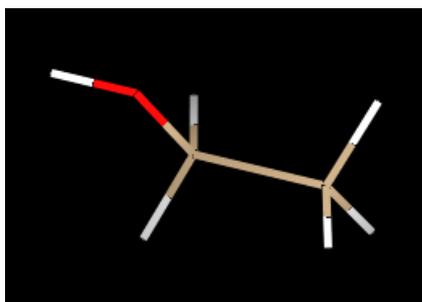
2

1

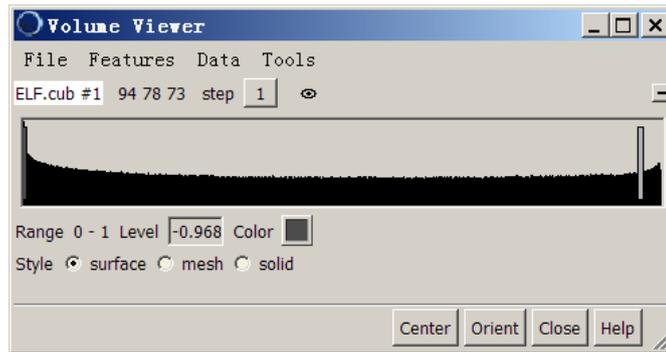
*ethanol.pdb*

Now we have .pdb file of ethanol in current folder.

Close Multiwfn and boot up Chimera, open the ethanol.pdb, then select "Actions-Atoms/Bonds-wire", and then "Actions-Atoms/Bonds-wire width-5", you will see



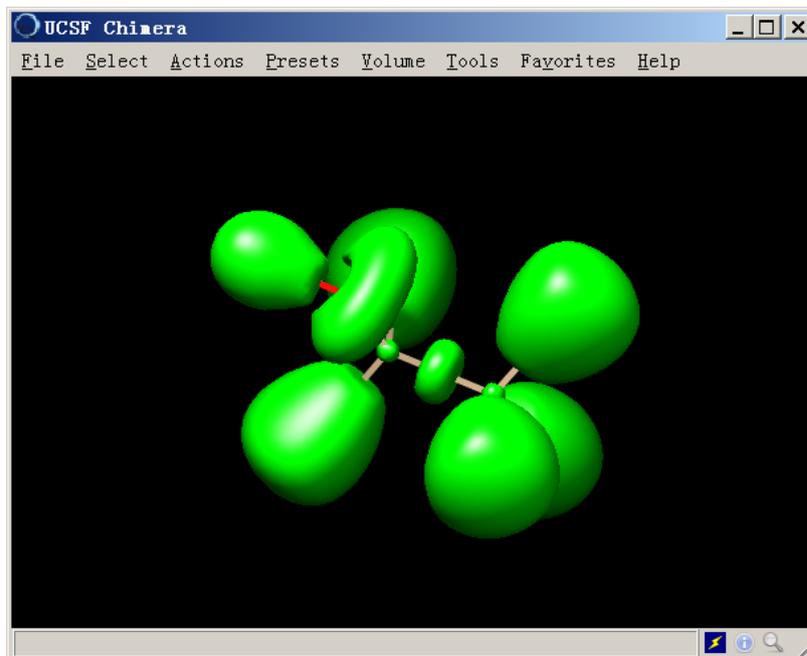
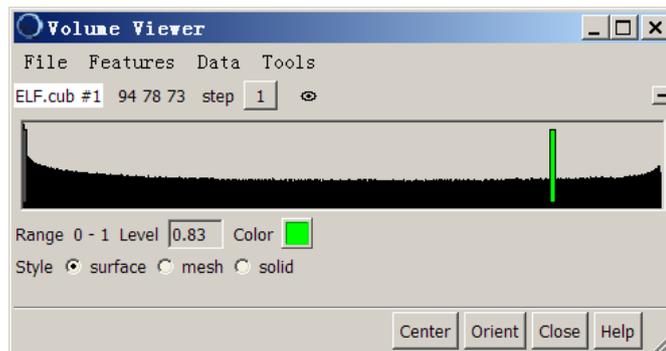
Use Chimera open the ELF.cub, the ELF isosurfaces will be immediately shown, and "Volume Viewer" window pops up:



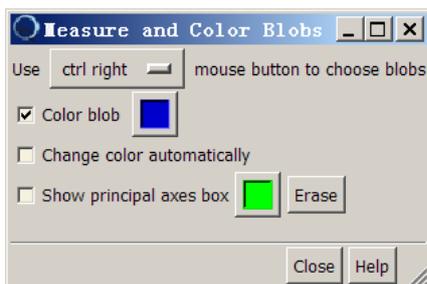
The vertical bar corresponds to the value of isosurface, the black shaded curve exhibits the amount of grid points in each interval of the function value.

Click the vertical bar to active it, assume that we would like to draw ELF=0.83 isosurfaces, input 0.83 in the text box and press ENTER.

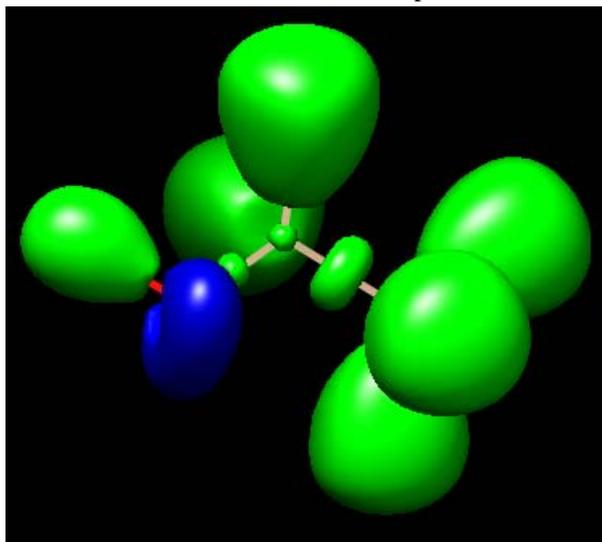
Assume that we want green as default isosurface color, click the box at the right-hand side of "Color" text, then drag the "G" bar to the maximum, and drag "R" and "B" bars to their minima, now the window and graph should be



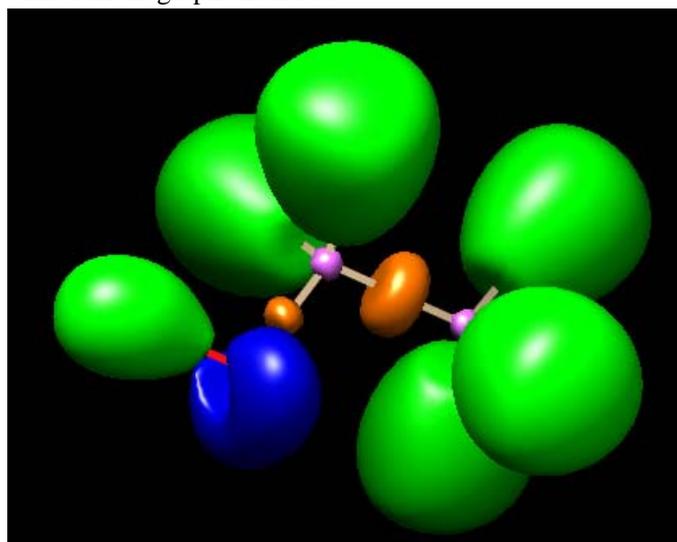
In the Volume Viewer window choose "Tools-Measure and color blobs", you will see



That means, if you hold "Ctrl" button and click an isosurface by right mouse button, then the isosurface will be shaded as blue. Now we do this for lone pair domain of oxygen, you will see



Then click the color box and change the color from blue to orange, then click the isosurfaces corresponding to C-O and C-C bonding domains to shade them as orange. Similarly, color the core domains are purple. The current graph should be



To make the isosurfaces transparent, choose "Actions-Surface-transparency-40%". To change the background color as white, choose "Actions-Color-all options-background", then click white.