A novel way for drawing electrostatic potential distribution plots

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Electrostatic potential(ESP) is one of the commonly used methods for analyzing the electronic structure of molecules, and it is also the best tool for illustrations. How to draw high-quality, clear and persuasive ESP distribution plots is the pursuit of scientific research workers. Via GaussView program, it can be made quickly (sobereva.com/253). However, due to the limitations of GaussView program itself, it will be leaded that the subsequent processing of the image is not better. On the other hand, the method via Multiwfn not only can analyze the surface of molecules quantitatively to get the maximum and minimum of ESP, but also can plot the high-quality maps of ESP with VMD (sobereva.com/196). Unfortunately, the resulting plots are often like these based on the most computer graphics cards:

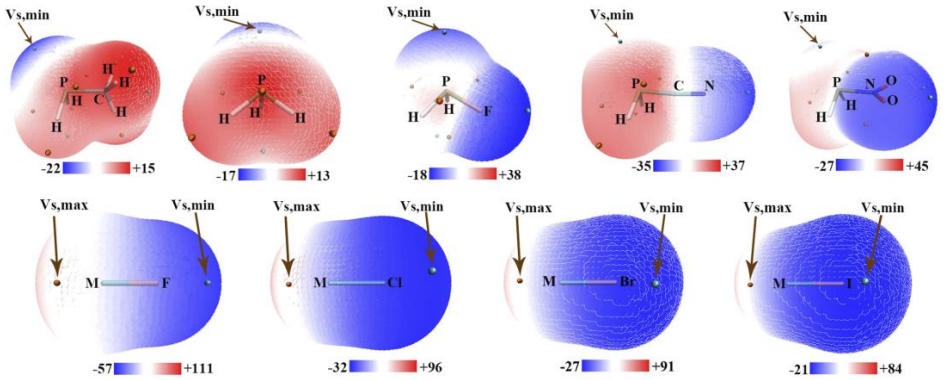


FIG. 1. Electrostatic potentials on the monomers' van der Waals surfaces of XH_2P (X = H, CH_3, F, CN, NO_2) and MY (M = Cu, Ag, Au; Y = F, Cl, Br, I). The units are kcal/mol. Red and blue regions represent positive and negative molecular electrostatic potential (MEP) values, respectively. The orange and cyan spheres represent the position of maximum and minimum points of MEP on the surface, respectively.

Fig 1 in JCP 148, 194106 (2018)

It can be found that there are some cracks on the surface of ESP. It does not affect the analysis of the problem but the appearance of plot, which may cause the reviewer's picky and whisper. In fact, there is another method to plot the surface of ESP of molecule via Multiwfn and VMD.

The ESP plots are drawn though the ESP is projected onto the Van der Waals surface of molecule, the isovalue surface of electron density which the isovalue equals 0.001 a.u.. So, via the projection method, the smooth ESP plots can be obtained though computed ESP is projected onto the Van der Waals surface of molecule. HF molecule can be taken in this article as an example.

Initially, the geometry and wavefunction file of HF molecule have been received after geometry optimization. In this article, the geometry of HF molecule is computed in the level of M06-2X/6-311G* by Gaussian 09 D.01 program package. The wavefunction file, .fch file is transferred by the formchk module of Gaussian 09.

Starting the Multiwfn program (in this article, the development version 3.6 has been used) and loading the HF.fch file.

HF.fch

5 // grid point file computation

1 // electron density computation

2 // medium quality grid

2 // export the Gaussian type .cub file (density.cub)

0 // return main menu

5 // grid point file computation

12 // Total ESP computation

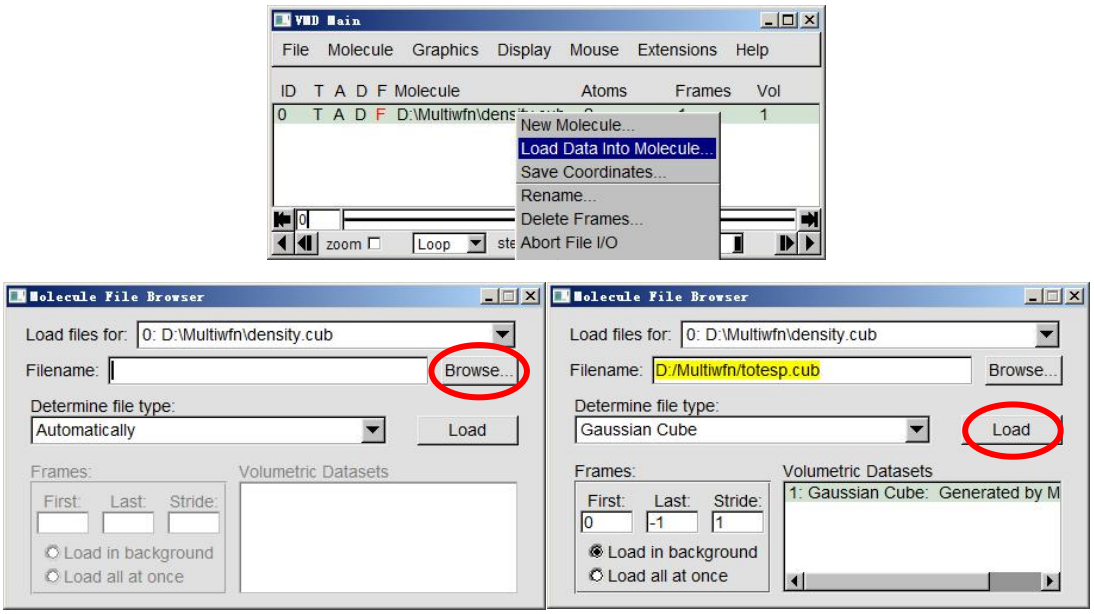
2 // medium quality grid

2 // export the Gaussian type .cub file (totesp.cub)

PS: Multiwfn has been updated after Augest 7th 2018. After this version, the cubegen module of Gaussian can be called by Multiwfn. You can modify the path of cubegen in setting.ini to borrow the cubegen module and accelerate the ESP computations.

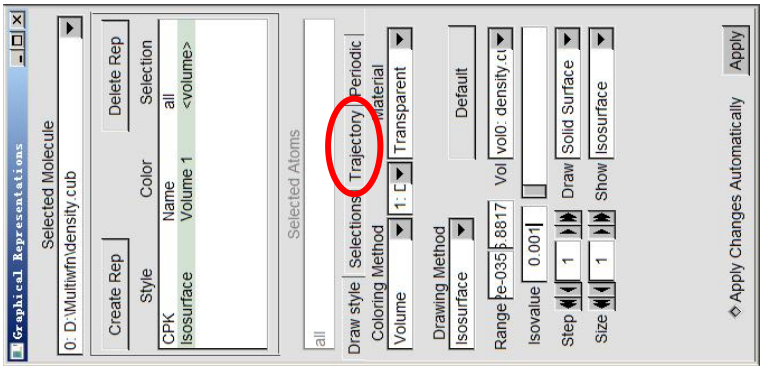
Now, there are two files, density.cub and totesp.cub, in the folder of Multiwfn. It is recommended to put two .cub files with the surfanalysis.pdb file that may be used next in the VMD folder. After this, it is the time to call the strongest plotting features of VMD software.

Starting VMD software and dragging the density.cub file into the VMD main interface. After this, click the right mouse on the item that appears and choose “Load Data into Molecule”. When the new dialog box has been appeared, click the button of “Browse”, choose totesp.cub and close the dialog box. There is another fatal suggestion that transfer the display style of “perspective” into “orthographic” in the item of “Display”.

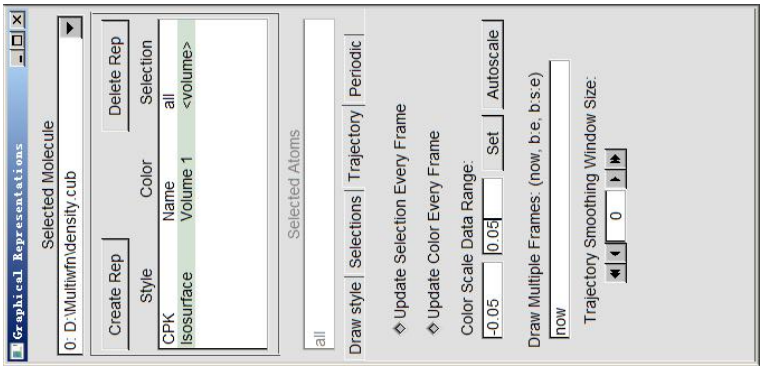


Click the “Representation” in the “Graphics” of VMD main interface and make the “Drawing Method” transfer to CPK. Then click “Create Rep” for creating a new level to display the isovalue surface. In the dialog box of “Representation”, set the “Drawing Method” to “Isosurface” that the

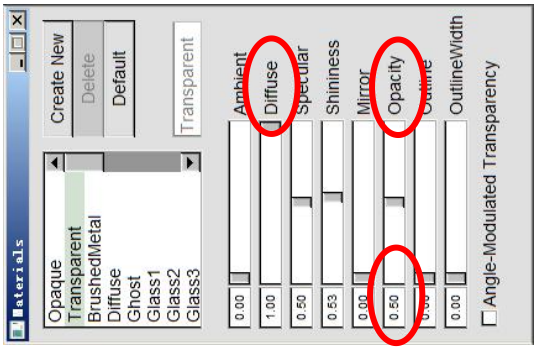
Isovalue is 0.001. The item “Vol” transfers to “Vol0: density.cub”. The item “Draw” transfers to “Solid Surface”. And The item “Show” transfers to “Isosurface”. The item of “Coloring Method” transfers to Volume, and the right side of it transfers to “1:”. The item of Material transfers to “Transparent”. All of setting is shown below:



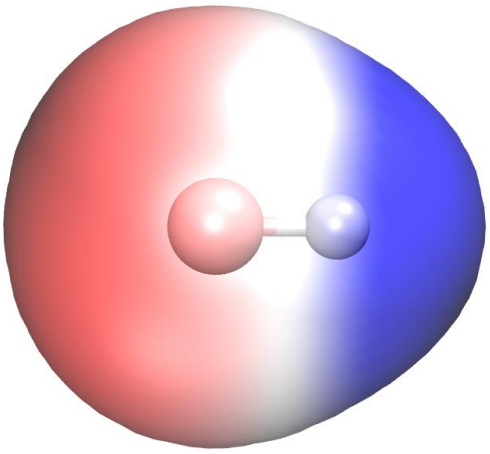
In the bookmark page of “Trajectory”, input the “-0.05” and “0.05” into the two boxes under the “Color Scale Data Range”, respectively, and pass enter. Please be careful that DO NOT input one and press enter. You should enter two of them one time and pass enter. Of course, you can modify the value of number if the consequent has been found that is not suitable.



For adjusting the effect of plots, click the “Materials” in the item “Graphics” of VMD main interface. In the item of “Transparent”, set the scale of “Opacity” to 50. This is because, when more the value of “Opacity” is , less the transparency of color-filling isosurface will be, which may be obvious for color of surface. At that time, set the value “diffuse” to the maximum. Others can be adjusted freely.

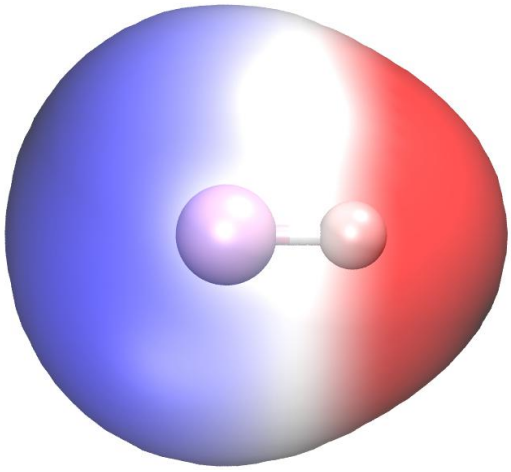


Now, the ESP plot can be gotten below:



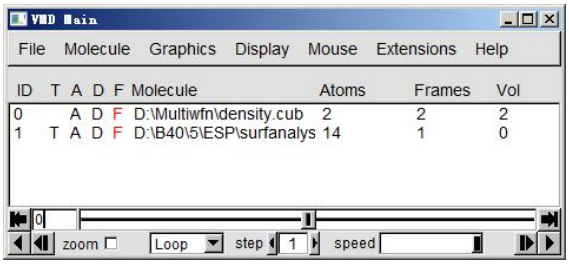
Habitually, the negative ESP should be shown in blue, and the positive should be in red. So it has to be modified. It is OK that choose the item “Color scale” in the item “Colors” under the “Graphics” of VMD main interface and transfer the RWB, a default option, to BWR.

The new one:



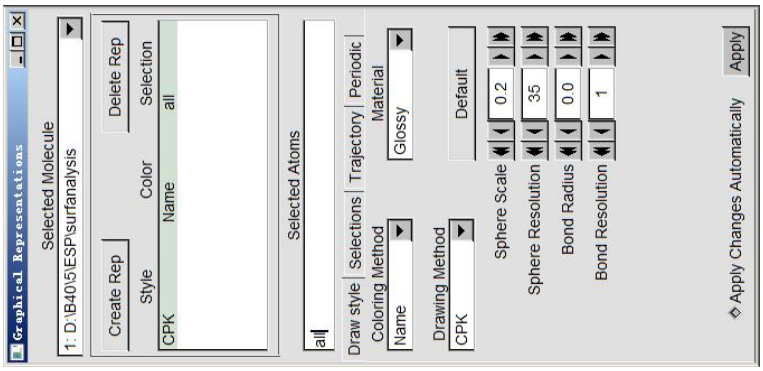
Most of works have been finished now, and you can put it into your paper.

You can read further if you have additional requirements about ESP plots.
The first requirement: I want the maximum and minimum points of ESP can be shown in the plot.
Answer: Quantitative analysis of molecular surface should be done(sobereva.com/196). After done, the file of surfanalysis.pdb obtained the maximum and minimum point of ESP can be gotten. Drag the file of surfanalysis.pdb into the VMD main interface.

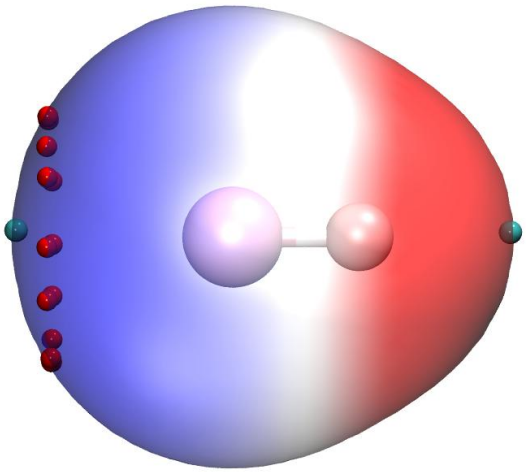


In the “Representation” under “Graphics” of VMD main interface, set the “Drawing Method” to CPK, where the values of “Bond Radius” and “Bond resolution” are zero, of “Sphere Scale” is 0.2

as shown in the picture.



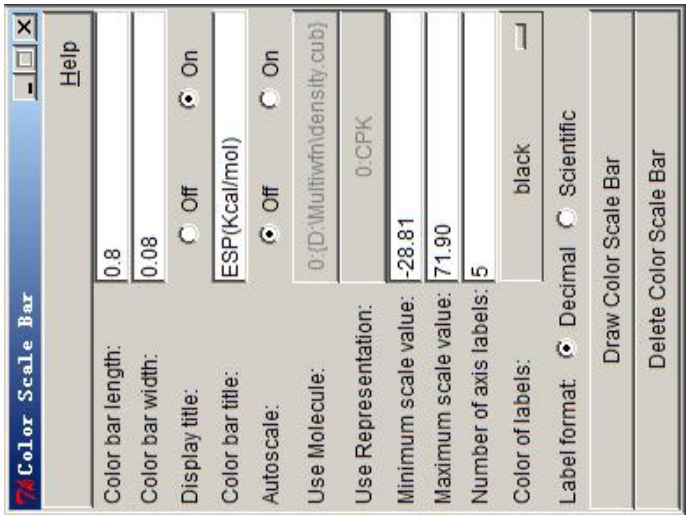
Here is the result:



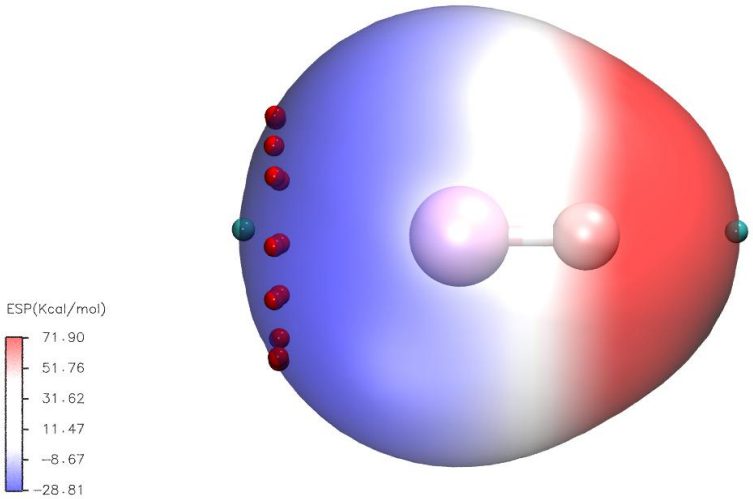
The second requirement: I want color scale bar can be shown in the plot.

Answer: Choose the “Color Scale bar” in the item “Visualization” of “Extensions”. The value of “Color bar width” is 0.08. Turn “on” the “Display title”. Input “ESP (Kcal/mol) into “Color bar title” and minimum and maximum of ESP (the values are in surfanalysis.pdb) into scale, respectively. “Number of axis labels” is 10. “Color labels” is black. “Label format” is Decimal. After clicking the button of “Draw Color Scale bar”, the color scale bar has been shown, and the item named “Color Scale bar” has listed in VMD main interface. Double click the item named “Color Scale bar” to make the label “F” be red (as well make the label “F” NOT be frozen in the plot), then the size and position of color scale bar can be modified. When it can be suitable, double click the item named “Color Scale bar” to make the label “F” be black again (as well make the label “F” be frozen in the plot).

The setting about “Color Scale bar” is there:



The plot has been finished:



You may say that it is too complex to repeat the process of ESP plotting. Actually, when you finish the plot of ESP successfully, the VMD script can be saved. You can call the script directly to plot ESP quickly. It is what you should do that click the “Save Visualization state” in the item “File” of VMD main interface after the plot has been finished successfully, and input the “ESP.vmd” into the new dialog box. So as you want to do the plot of ESP again, put the density.cub, totesp.cub and surfanalysis.pdb in the VMD folder, click the “Load Visualization state” in the File of VMD main interface and choose the ESP.vmd after starting VMD.

Conclusion:

Via projection, the smooth, no-cracks ESP plots can be made without Super anti-aliasing functions of Nvidia graphic cards and without enduring the choking up of computer when the high-quality grid point has been used. I believe that you can love the method for ESP and plot your own ESP more pretty and pleasing to the eye.