Electrophilic frontier density using Gaussian, Multiwfn, and Jmol

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in Gaussian, optimize and do MO calculation for H_2O. (“formcheck” option saves the formatted checkpoint file necessary for Multiwfn operations.)
#N B3LYP/6-31G(d,p) SP GFINPUT POP=FULL formcheck

From WebMO, export job archive, expand the .zip file, rename Test.Fchk to water.fchk. Move or copy to the folder with Multiwfn program (/home/sally/Downloads/Multiwfn_3.8)

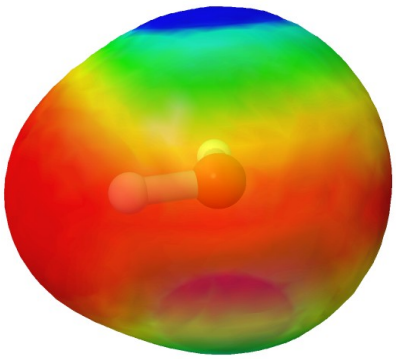
Gaussian must be installed. Follow WebMO instructions for G16 (webmo.net), and run test job per instructions as user Sally. Prior to starting Multiwfn, set the g16 environment:
$ source g16setup

Run Multiwfn:
$ Multiwfn water.fchk

5 / Output and plot specific property within a spatial region
1 / Electron density
2 / Medium quality
2 / Export data to a Gaussian-type cube file (saves density.cub in current directory)
0 / Return to main menu

22 / Conceptual DFT analysis
1 / Generate .wfn files for N, N+1, N-1 electrons states
(enter theory, e.g. B3LYP/6-31G(d,p))
enter (Input the net charge and spin multiplicity for N electrons state, e.g. 0 1
Note: If pressing ENTER button directly, (0 1), (-1 2) and (1 2) will be employed for N, N+1 and N-1)
y (to invoke Gaussian to calculate these .gjf files now to yield .wfn files)
4 / Set delta in orbital-weighted (OW) calculation
enter 0.08
7 / Calculate grid data of OW Fukui function
2 / Medium quality
6 / Export grid data of orbital-weighted f- as OW_f-.cub in current folder
0 / Return
0 / Return

26 / Structure and geometry related analyses
2 / Various geometry operations
-2 / Output system to .pdb file
-10 / Return
0 / Return
q / exit



In Jmol:
cd home/sally/Downloads/Multiwfn_3.8;
load water.pdb; background white; color bonds gainsboro;
isosurface efd cutoff 0.001 density.cub color absolute 0.000 0.0005 map OW_f-.cub;
isosurface fullylit translucent 90;
