Plotting Density differences

1. **On your (optimized) geometry run a TD job using the density=current keyword in the input file for the calculation of the excitation energies. Use a chk file for TD-DFT calculation**.

Example (input file)

```
%rwf=............/3sn_td_dd.rwf
%Nosave
%chk=............/3sn_td_dd.chk
%nprocshared=20
%mem=20GB
#p td=(nstates=20) density=current b3lyp/6-311+g(d,p)
scrf=(solvent=dmso) int=(grid=ultrafine,acc2e=12) scf=verytight

SNAFR3 dendiff DMSO

0 1
 C                  1.99589800   -1.79836900    0.01395500
 C                  3.10188600   -2.59268300    0.01071800
……..
```

2. **Once the job is finished, format the chk file using the formchk utility:**

Example (run formchk utility)

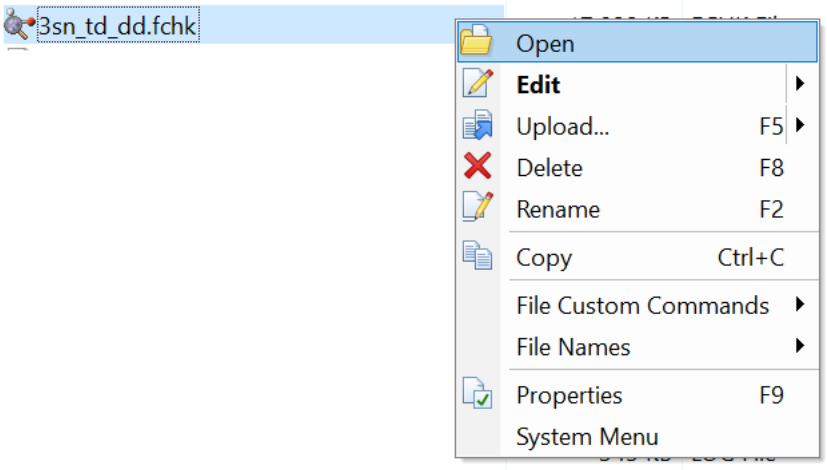
```
[                              ]$ formchk 3sn_td_dd.chk
```

and you will obtain the .fchk file (i.e., 3sn_td_dd.fchk)

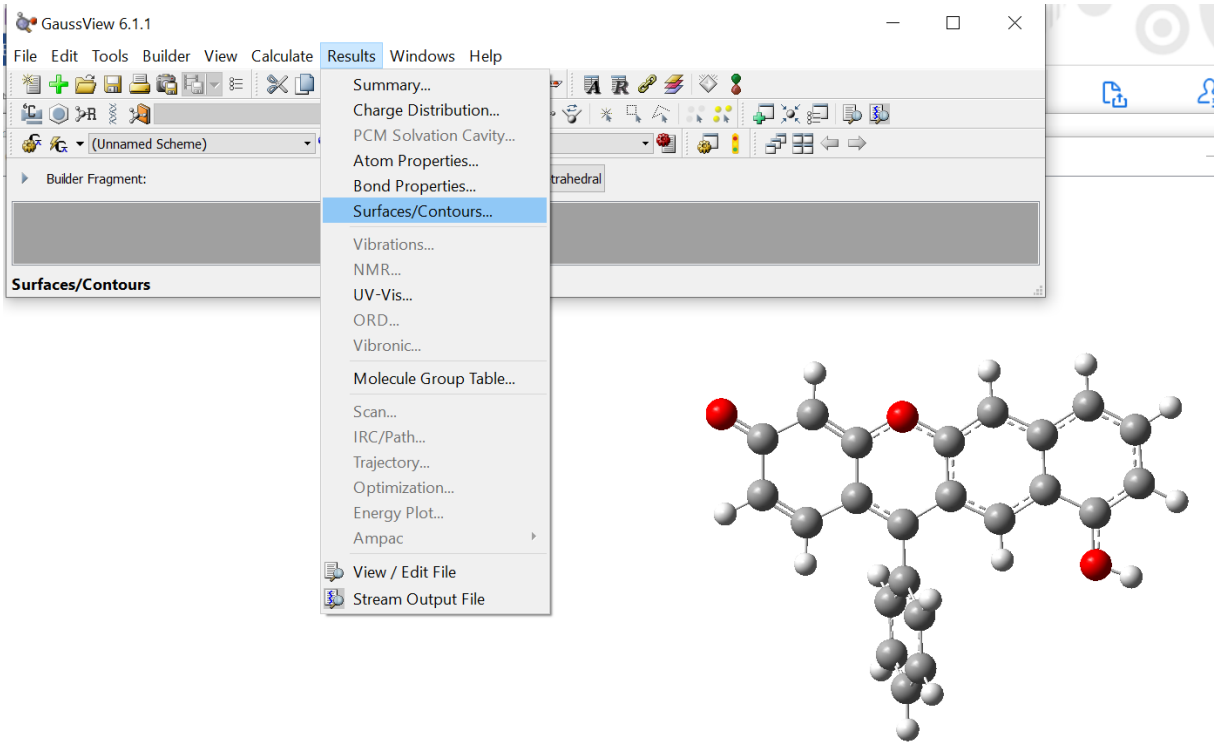
(The chk file can also be used but it is usually much larger than the formatted fchk.)

I am using GaussView for Windows OS so that I have to transfer the fchk file from the Linux computer to the Windows workstation.

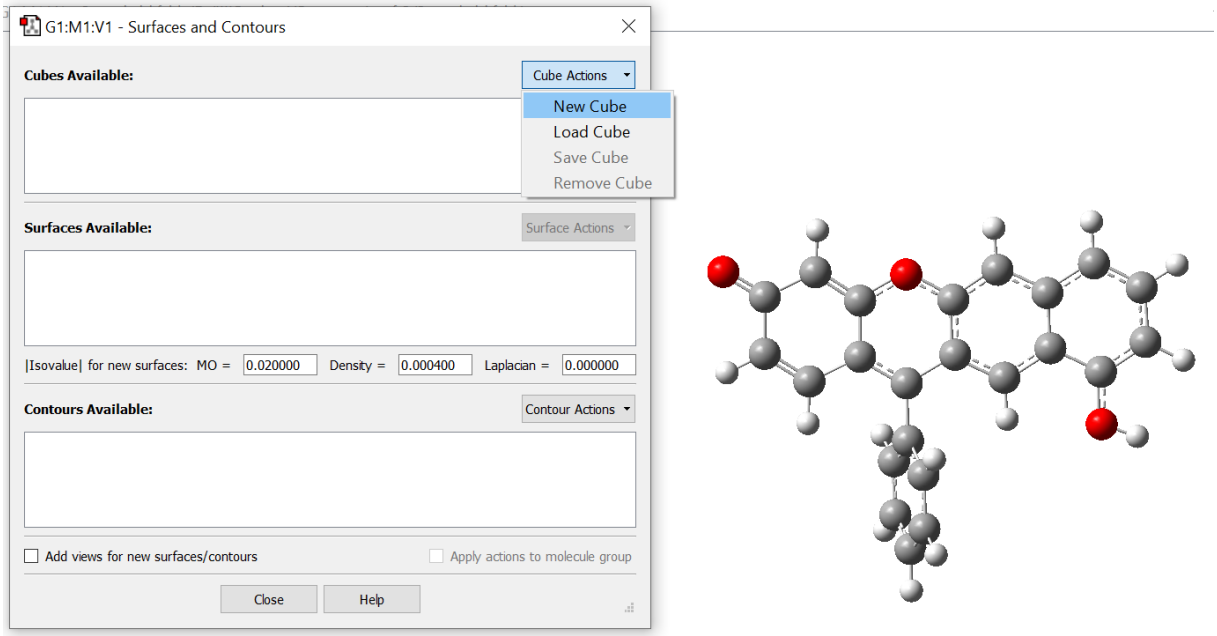
3. **Open the .fchk file in GaussView.**



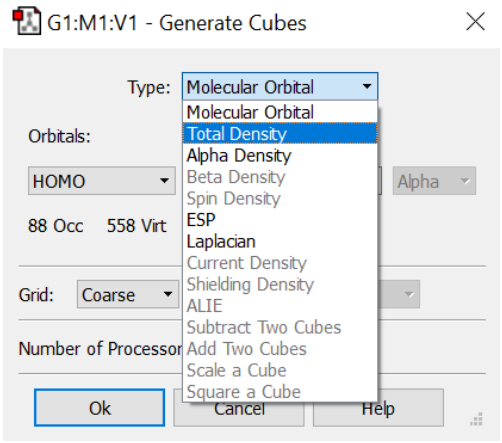
4. **From "Results" menu choose "Surfaces/Contours…"**



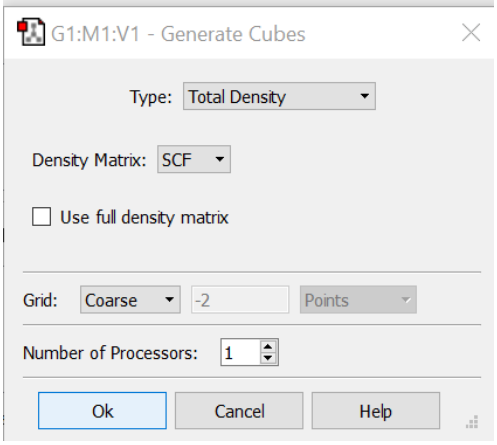
5. **Choose "Cube Actions" and "New Cube":**



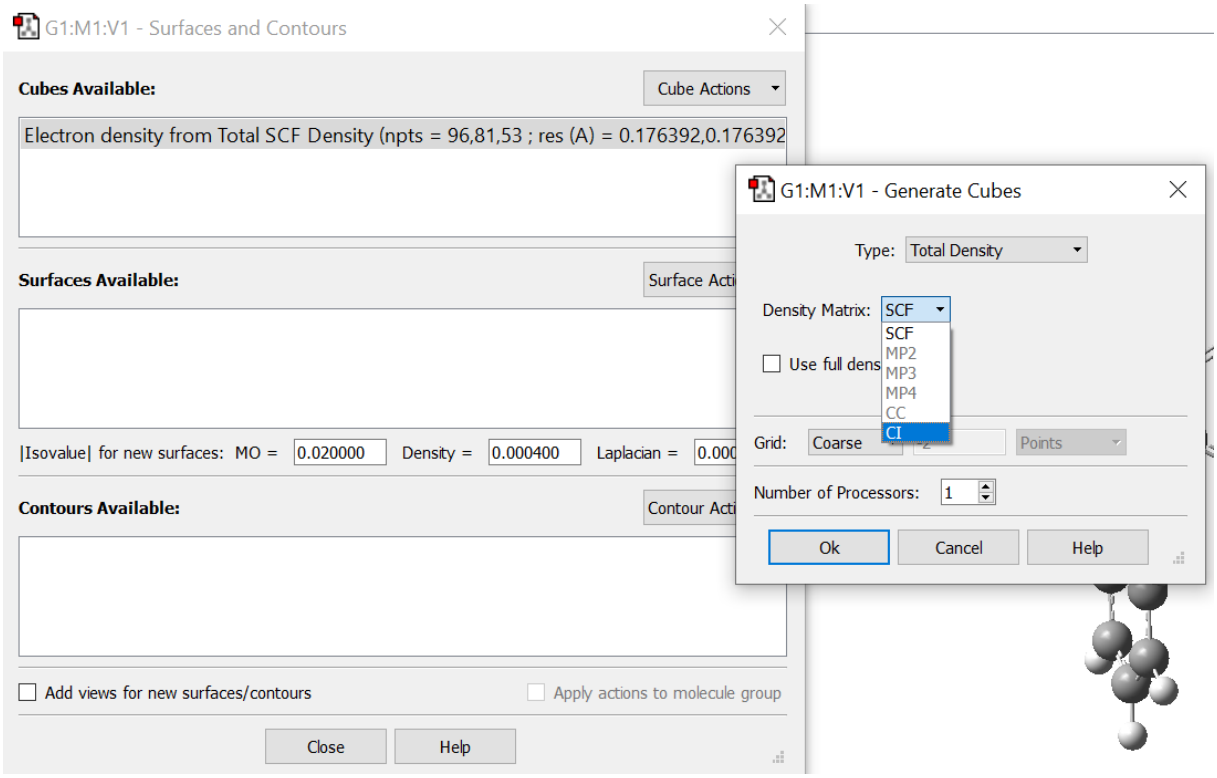
6. **Choose "Total Density" for the type of cube:**



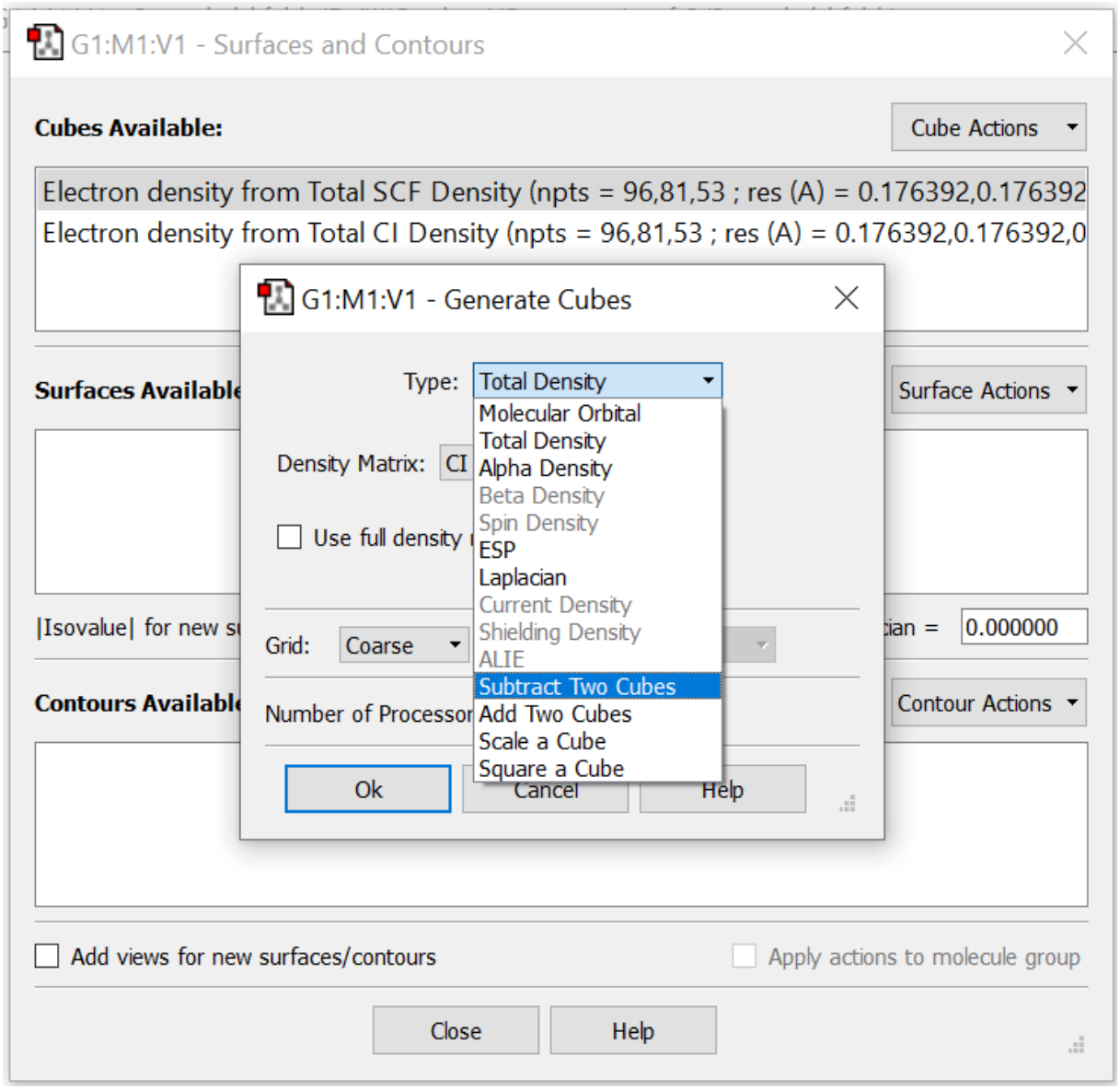
Leave SCF for Density matrix. Select the appropriate number of processors, then click OK.



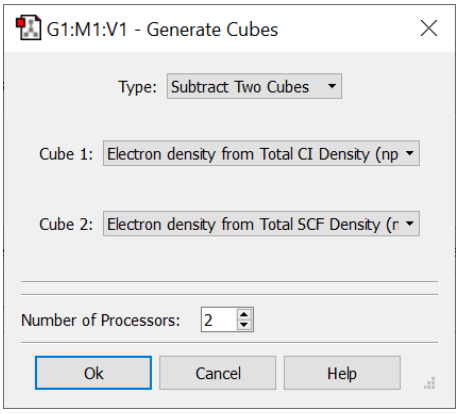
7. **Wait for the cube to be generated. Then select "Cube Actions" again, New Cube, then choose CI for the Density matrix and click OK:**



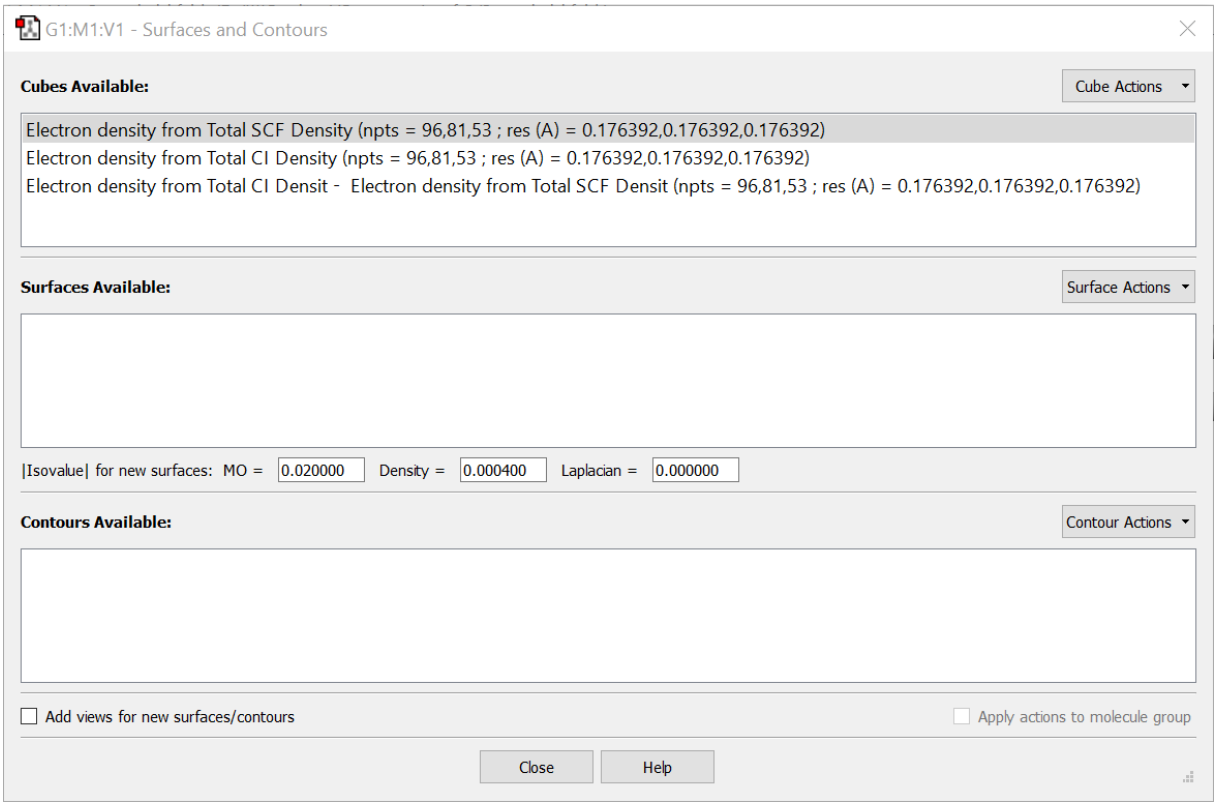
8. **Substract the SCF cube from CI cube.**
   Select "Cube Actions", then "New"Cube" and Select "Substract Two Cubes" for the type of cube:



9. **In the next window select "Electron density from total CI density" for the first cube and "Electron density from total SCF density":**



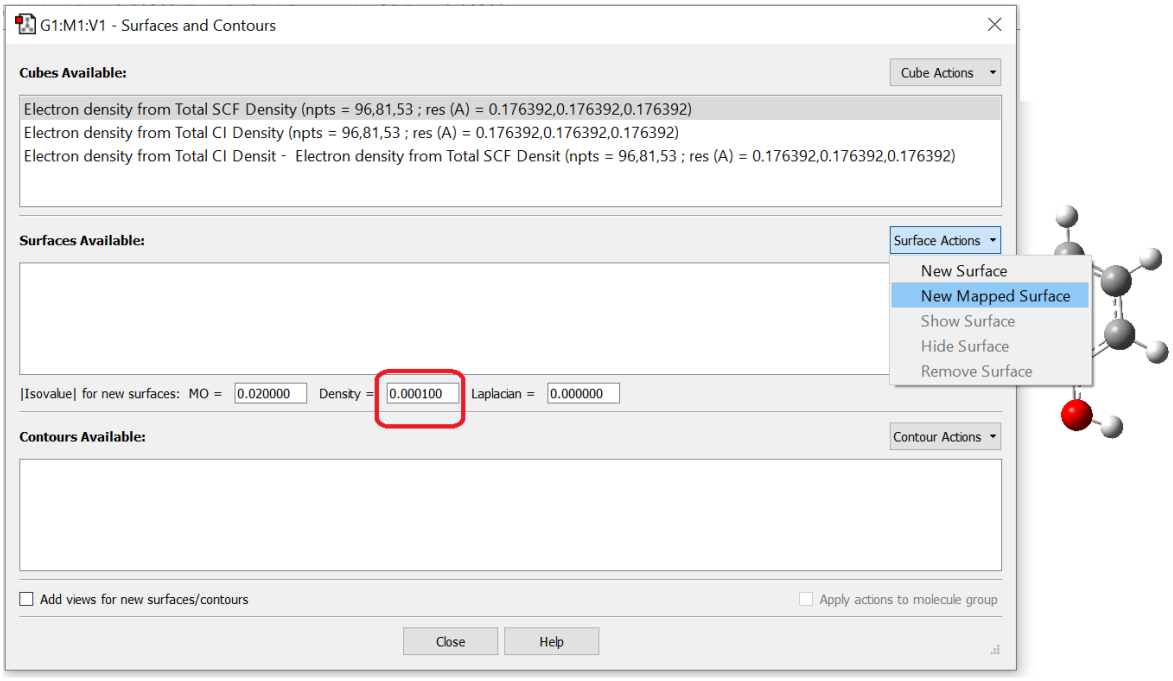
10. Click OK and you will have the three generated cubes:



11. Now you can construct a mapped surface.

This will be the "Electron density from Total CI Density – Electron density from total SCF Density" mapped on the isosurface "Electron density from total SCF Density".

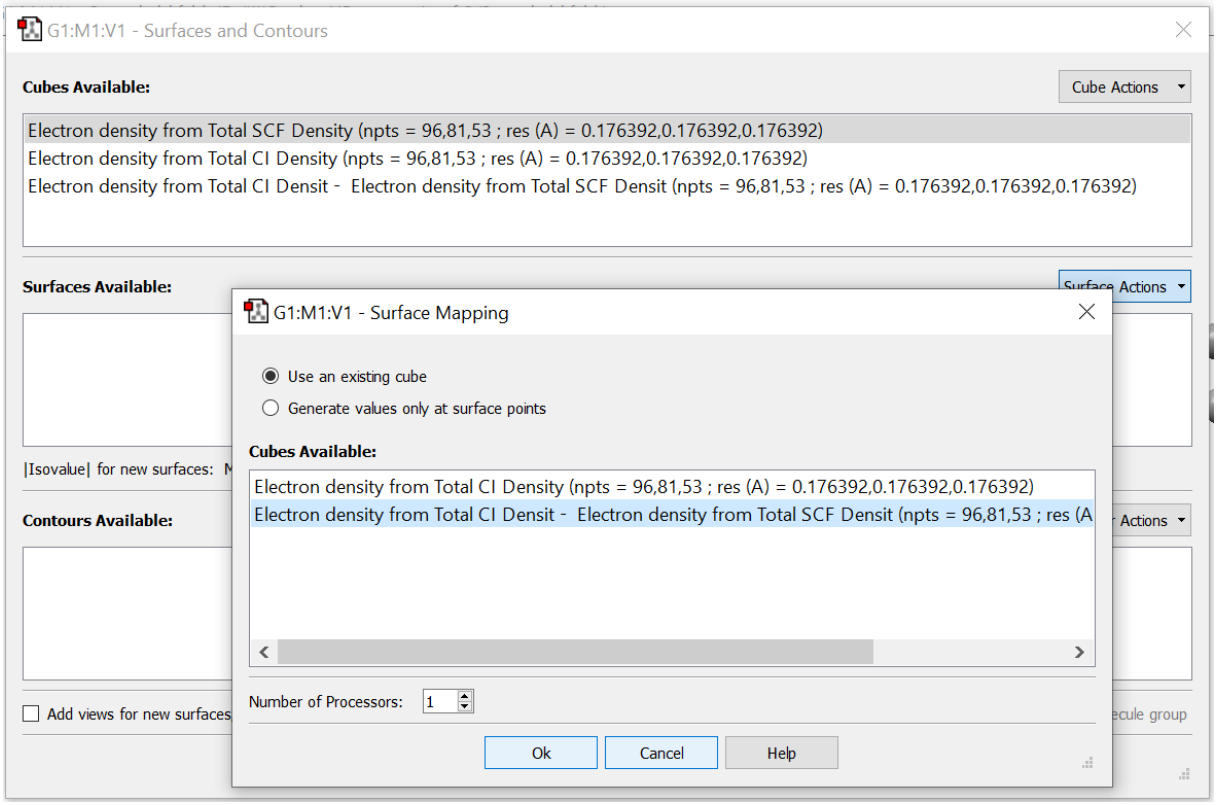
In "Cubes available" section click on "Electron density from Total SCF Density", then click "Surface actions" and then choose "New Mapped Surface":



Here you might want to play with the Density isovalue.

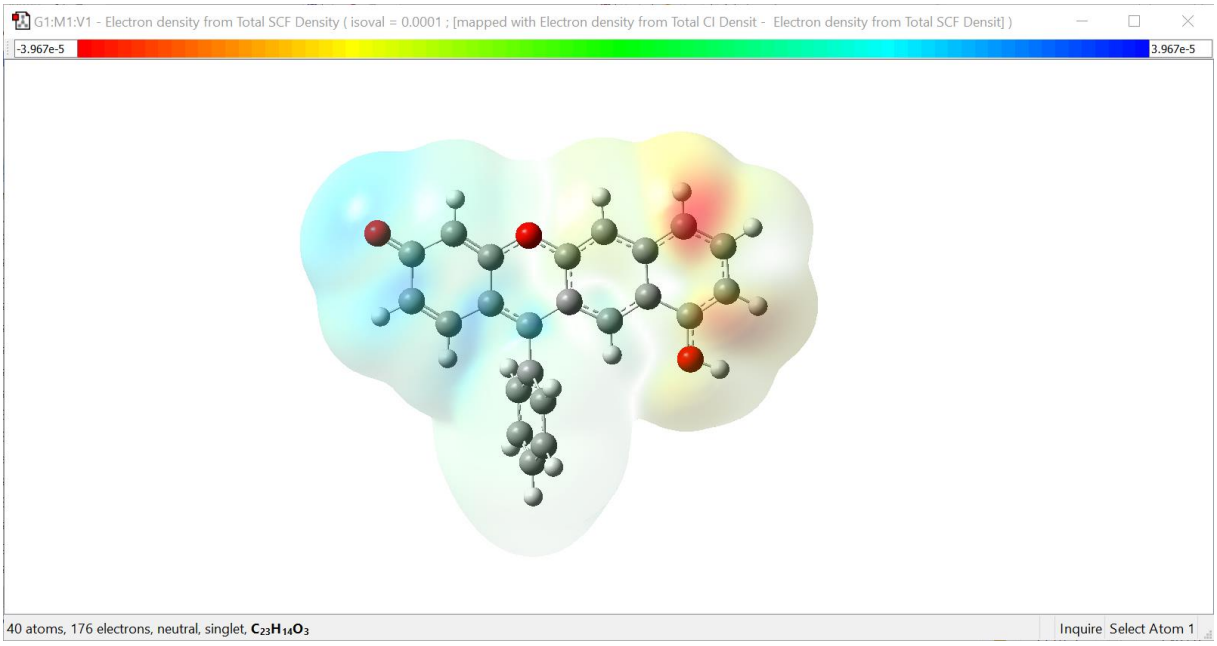
12. Plot the mapped surface

Keeping selected the "Electron density from total SCF Density" in the "cubes Available" from the "Surface and Contours window, choose "Electron density from Total CI Density – Electron density from total SCF Density" in the "Surface Mapping" window and then click OK:

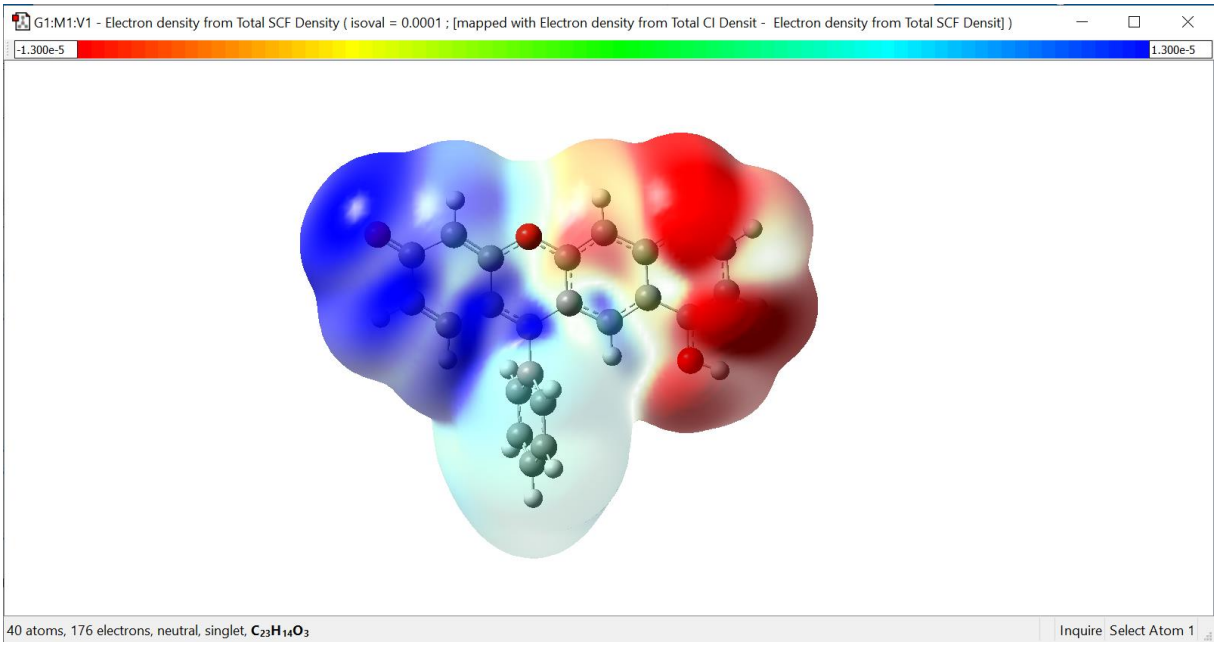


13. Refine your generated mapped surface

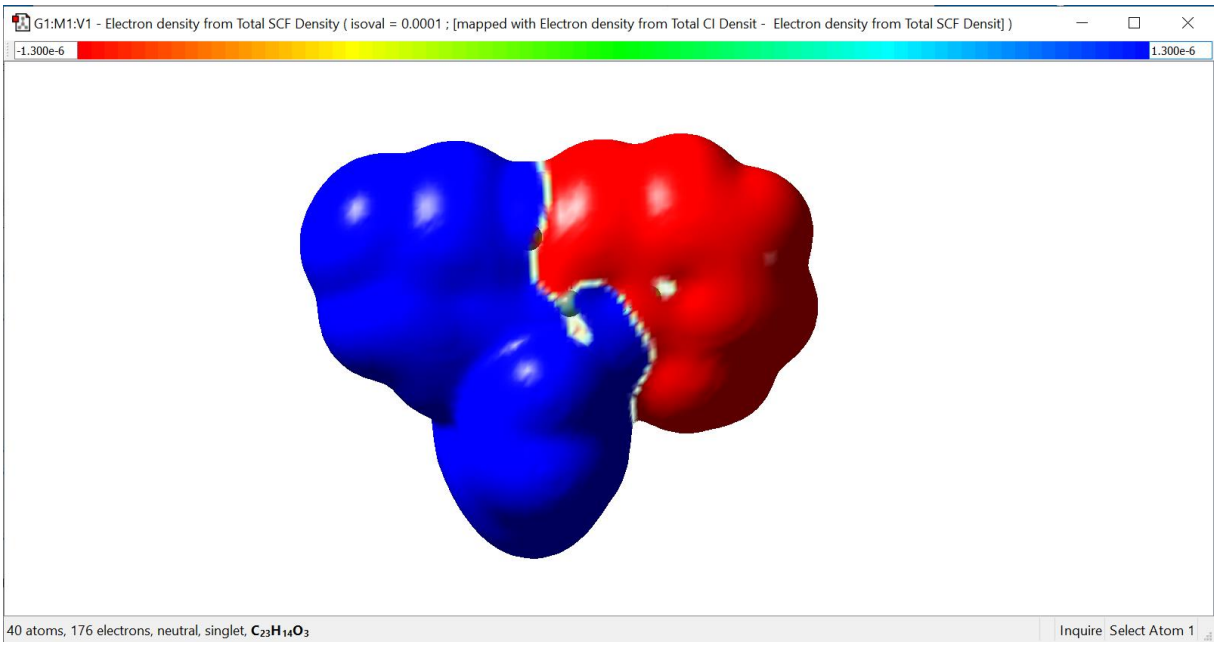
Now you should see the mapped CI-SCF density on the isosurface of the SCF density:



You can play with the max and min values of the density difference:

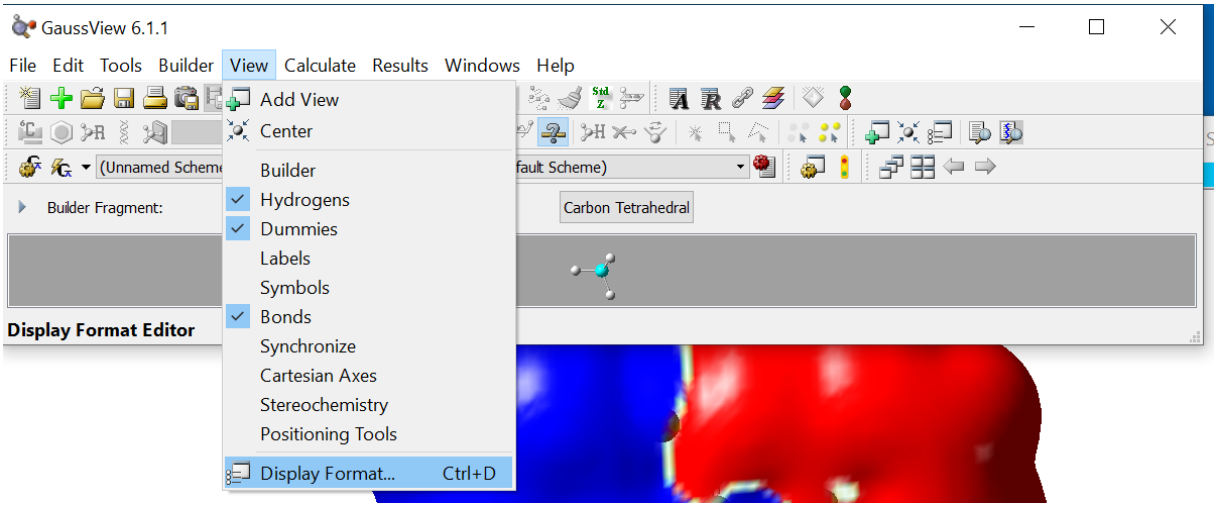


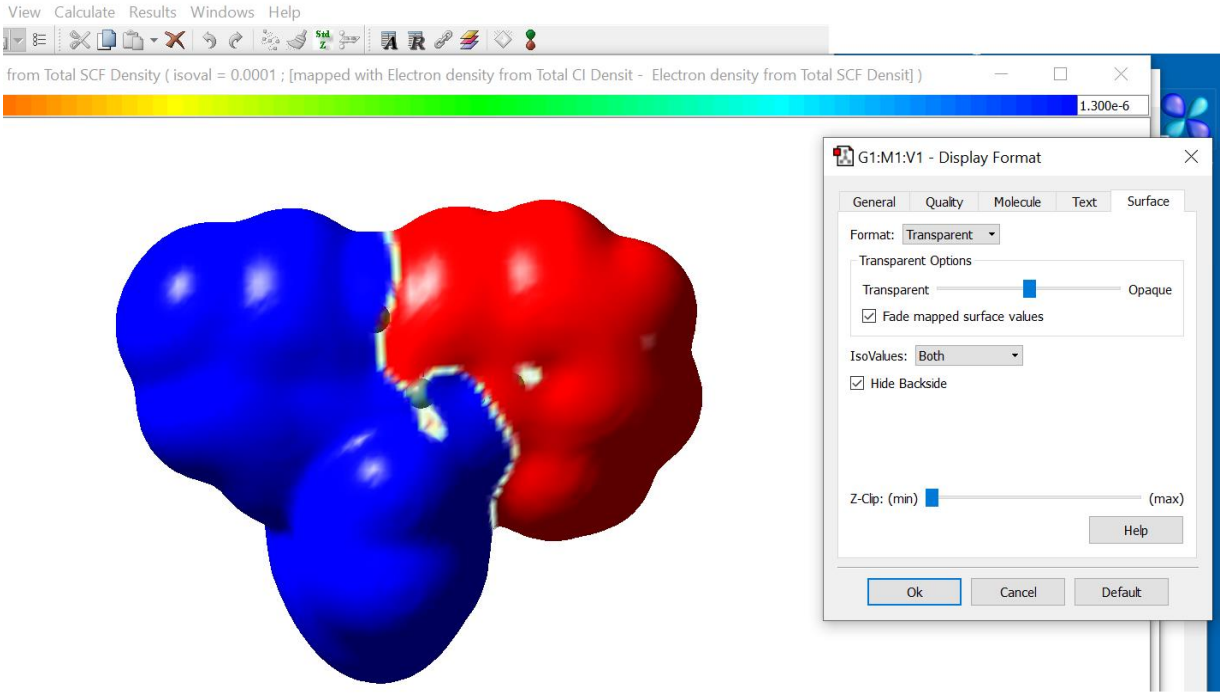
or:



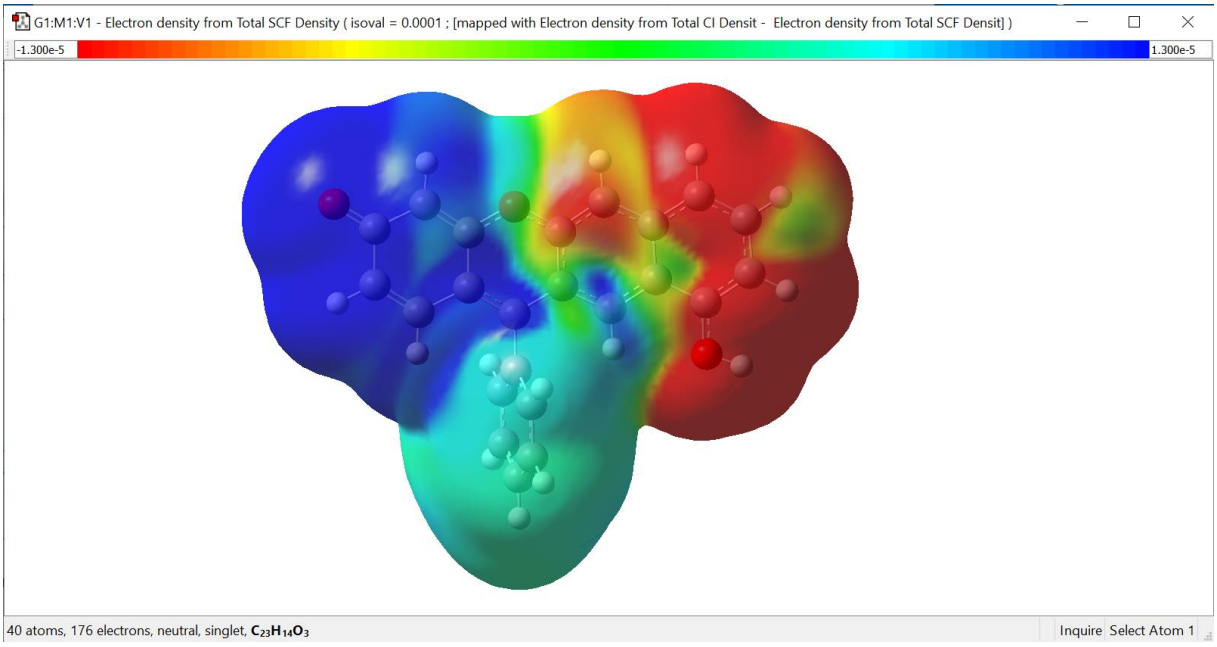
14. Change the appearance of the mapped surface

You can play with the parameters found in View -> Display Format -> then Surface tab:





Here you can change the transparency, activate or inactivate the "Fade mapped surface values" or "Hide Backside":


G1:M1:V1 - Electron density from Total SCF Density (isoval = 0.0001 ; [mapped with Electron density from Total CI Densit - Electron density from Total SCF Densit])
-1.300e-5
1.300e-5
40 atoms, 176 electrons, neutral, singlet, C23H14O3
Inquire Select Atom 1