Mapping Electrostatic Potential on a Density Isosurface in Gaussview

MGCF - College of Chemistry, University of California, Berkeley

Read a checkpoint file into Gaussview.
Select the Menu: **Results > Surfaces/Contours...**
On the **Surfaces and Contours** window, in the **Cubes Available:** section, select the pulldown: **Cube Actions > New Cube > Type > ESP** and click **Ok** (change the **Grid** if you want a better picture).
Repeat these **Cube Actions**, but now select **Total Density** instead of ESP.
In a few minutes (longer for large molecules and basis sets), two entries will appear in the **Cubes Available** section.
Select (highlight) **Electron density from Total SCF Density**.
Then, in the **Surfaces Available:** section, select the pulldown: **Surface Actions - New Mapped Surface**.
This opens the **Surface Mapping** window.
On that window, choose **Electrostatic potential from Total SCF Density** in the **Cubes Available** field, and check the box to **Use an existing cube**. Then click **Ok**. It may take a few minutes before the display appears.
Adjust the isosurface size by adjusting the **Isovalue**.
In the upper left and right corners of the window displaying the surface, there are fields for the upper and lower bounds for charges. You can set these so they are the same for different molecules, so that the color regions can be compared between molecules.