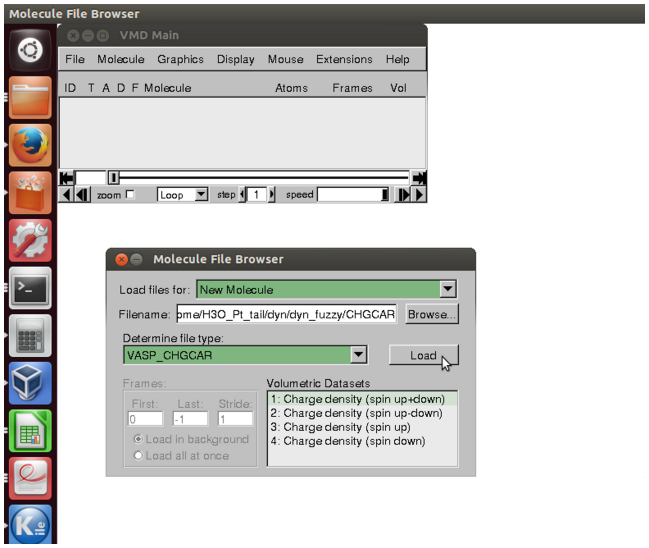
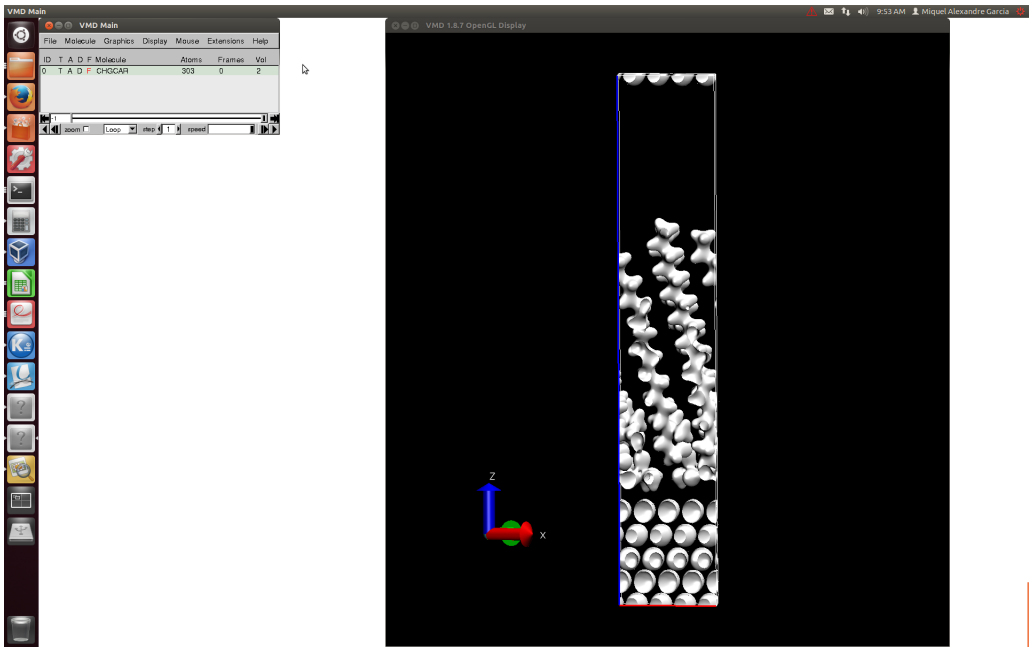
How to plot the molecular electrostatic potential (MEP) from VASP files using VMD

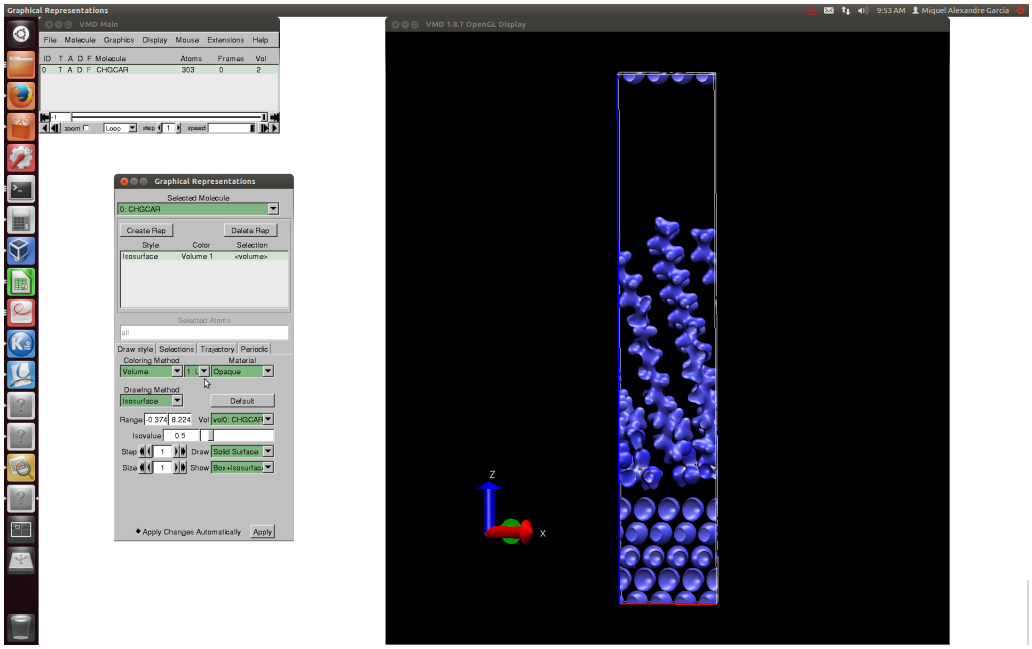
- First of all you should run a VASP calculation. One needs to generate the CHGCAR file (`LCHARG=.TRUE.`) that contains the data for the electronic charge density in space and the LOCPOT file which contains the electrostatic potential data. The LOCPOT file should contain only the electrostatic contribution to the local potential. To do so we need to set `LVHAR=.TRUE.` in the INCAR file.
- When the calculation stops, run vmd from terminal.
- Select **/File/New Molecule** on the menu bar and search for the corresponding CHGCAR file. Choose VASP_CHGCAR on the **Determine file type** tab.



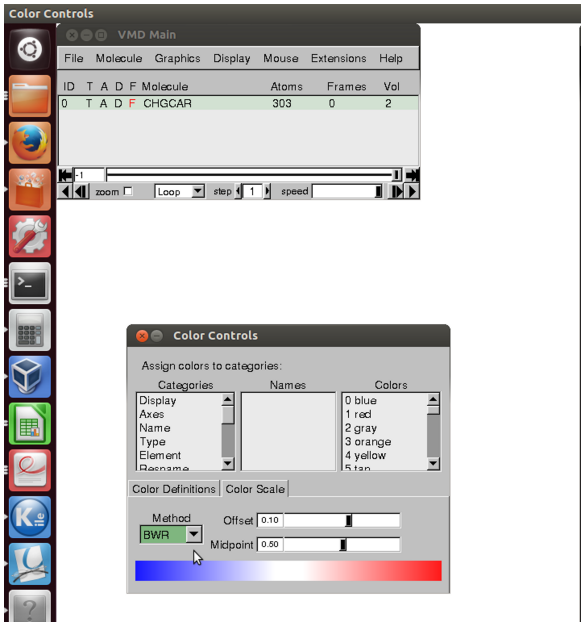
- Once the CHGCAR file is loaded, right-click on the line where the CHGCAR name appears and select **Load Data into Molecule**. Once there, search for the LOCPOT file (choose VASP_CHGCAR on the **Determine file type** tab).
- After loading both the CHGCAR and the LOCPOT files, the VMD Main screen looks like:



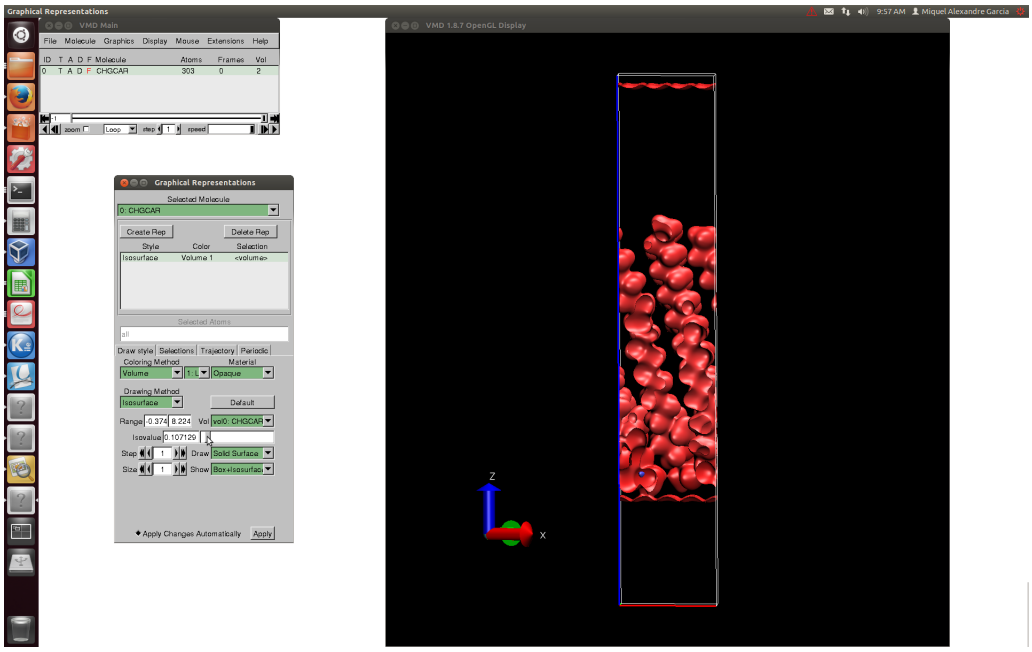
- On the Menu **/Graphics/Representations** click on the **Draw Style** tab. Once there, select Volume in the **Coloring Method** and choose the LOCPOT file on the same row. The **Drawing Method** should be Isosurface. On the tab **Vol** choose vol0: CHGCAR. When doing so, your isosurface will be colored in the same way everywhere (see snapshot below).



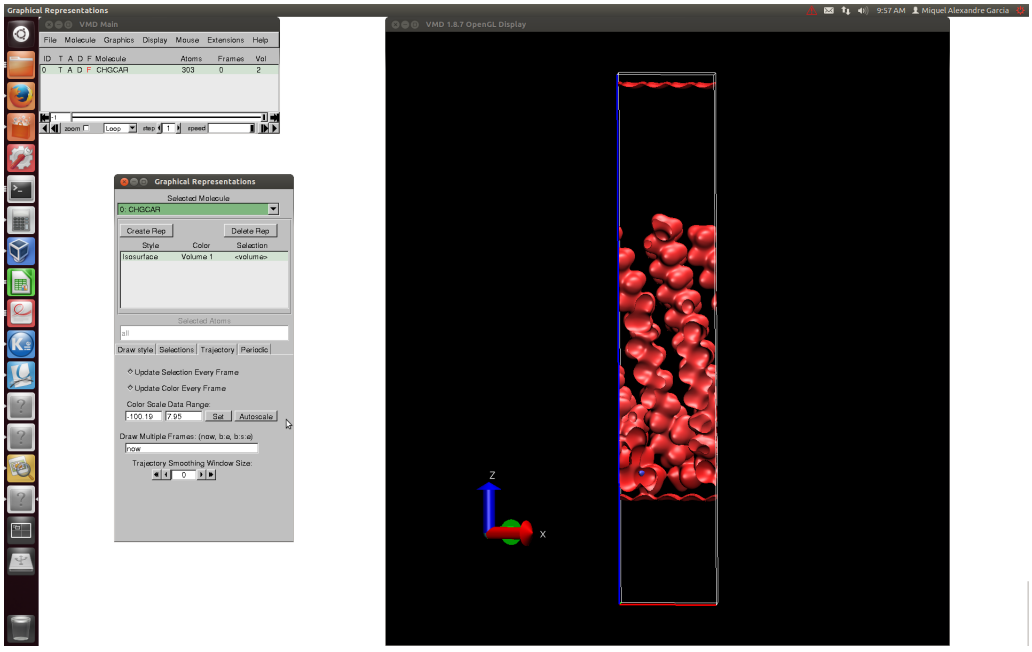
- Before doing more adjustments we need to change the color scale. Attractive regions (for a unit positive charge) should be colored in red while repulsive regions in blue. On the menu bar, click on **/Graphics/Colors**, and then click on the **Color Scale** tab. Choose BWR on the **Method** tab.



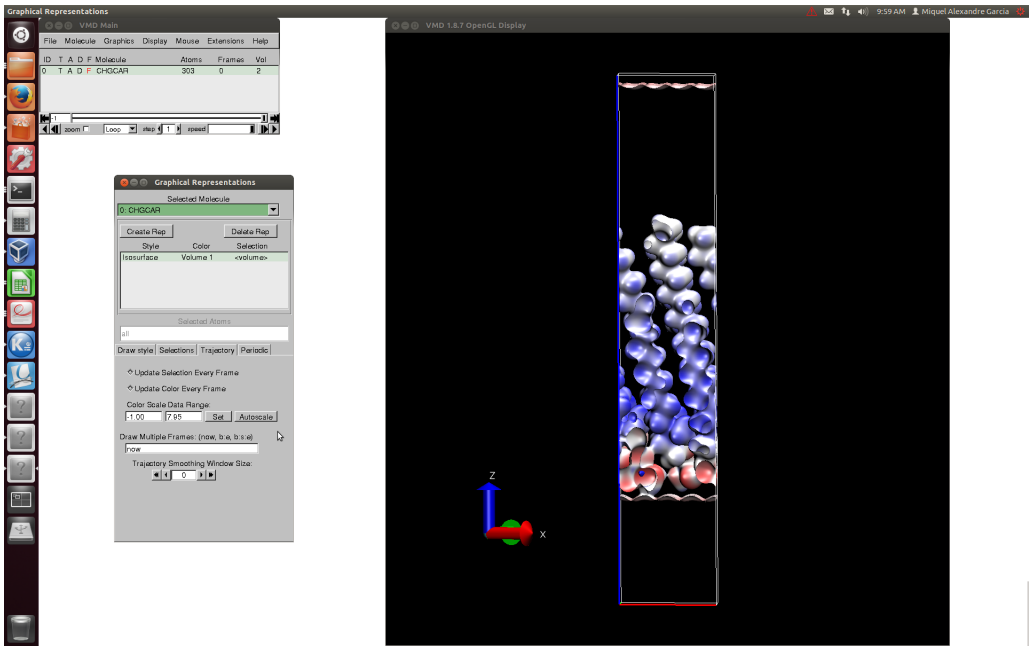
- After doing so, we need to adjust the **Isovalue** for the charge density isosurface to the desired value. Vmd plots the charge density in units of $e/\text{Å}^3$. Look at the Display and change the isovalue until you get the desired isosurface shape (see snapshot below).



- Now we need to adjust the range for the electrostatic potential values that will be projected on the charge density isosurface. Select the **Trajectory** tab on the **Graphical Representations** menu to know the range of values. The upper and lower limits for the electrostatic potential data are given in the **Color Scale Data Range**. Take into account that if the values that have some physical meaning are for instance between -1 and 7.95 (in the units of the electrostatic potential) then if you choose the range [-100.19 : 7.95] all the isosurface will be colored in red (as we can see below).



- Then, we change the **Color Scale Data Range** to [-1.00 : 7.95] and now the MEP plot looks like:



Of course, the user could play a bit more with the adjustments until the MEP plot looks as desired.