

Loading the file

- 1- Go to the files location at the black vmd terminal:

>cd dir (dir=your working directory)

e.g.

>cd (to go to your home)

>cd Desktop (to go to your Desktop)

>dir (to see what is inside the repository)

- 2- File > New Molecule>Browse

- a. You choose the *name-dens.cube* file

- b. ON THE SAME WINDOW (do not repeat the File>New Molecule process) you load the *name-grad.cube* file

Drawing the NCI surface

- 1- Graphics > Representations > Create Rep

- a. Drawing Method : Isosurface

- b. Isovalue:

+ Enter

- c. Coloring Method: Volume

- d. In Trajectory (3rd tab): Color Range Data Range :

Other settings

- Changing the background color to white
Graphics>Colors>Display (in Categories)> 8 white (in Colors)
- Getting rid of the axes
Display>Axes>Off
- Not showing perspective
Display>Orthographic

Saving your picture

File > Render > Filename:

Saving your state for ulterior use

File > Nom du fichier: yourname.vmd