**Useful commands VMD (TkConsole)**

1) Make a selection of atoms: it can be done with any selection criteria of VMD such as atom type, name, residue, distances,... For example:

set seleccio [atomselect top "protein"]

set seleccio [atomselect top "all and not x\*x+y\*y<36"]

2) Obtain **information** from atom selection

*Number of atoms in a selection:*

$seleccio num

*Maximum and minimum values of coordinates from a selection*

measure minmax $seleccio

*Calculate charge from a selection*

eval vecadd [$seleccio get charge]

*Center of coordinates from a selection*

measure center $sel weight mass

*Save coordinates of a selection in a pdb*

$seleccio writepdb myselection.pdb

*Save structure/topology of a selection in psf format*

$seleccio writepsf lamevaseleccio.psf   
   
3) **Modify** a selection of atoms

*Change atom properties (such as charge, mass,...)*

$seleccio set charge 0.060 #changes the charge of seleccio

*Move selected atoms (for example move -6.0 in z coordinate)*

$seleccio moveby {0 0 -6.0}

*Move selected atoms in a way that the geometric center will be in 0,0,0*

set com [measure center $seleccio]

$seleccio moveby [vecscale -1.0 $com]

*rotate respect to axis not passing from the CM of the molecule (for example a protein)*

set com [measure center $seleccio weight mass]

set matrix [transaxis z 45]

$seleccio moveby [vecscale -1.0 $com]

$seleccio move $matrix

$seleccio moveby $com

*Define periodic boundary conditions: one component of ( a b c) or the full vector:*

molinfo top set a 17.194

pbc set {17.194 17.018 40} -all -molid top

**-NOTE:**  To save memory, when finishing with a selection use: $seleccio delete