VMD Cheat Sheet

https://lixinsun.mit.edu/blog/vmd-cheat-sheet

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	GUI-interface	TK Console	note
Load a molecule	Control panel → Files → New molecules	mol new <filename> type <POSCAR/lammpstrj/pdb/…>	In terminal: $vmd a.lammpstrj For VASP output POSCAR / CONTCAR, the automate detection won't work. You need to select file type manually
Add a layer of selected atom (i.e. "sqrt((x-2)**2+(y-2)**2)<3 and z>4 and type 2")	Control panel → Graphics → Representation → create Rep → type "sqrt((x-2)**2+(y-2)**2)<3 and z>4 and type 2" in "Selected Atoms"	mol selection {sqrt((x-2)**2+(y-2)**2)<3 and z>4 and type 2 } mol addrep top	
Delete a layer	Control panel → Graphics → Representation → select the layer → Delete Rep. (or double click to just hide the layer)	mol delrep 0 top	
Change background color	Control panel → Graphics → color → Display → Background	color Display {Background} white	
Change view	Control panel → Display → perspective / orthographic	display projection Orthographic or display projection Perspective	
Change coloring method	Control panel → Graphics → Representation → select "Coloring method" as "ColorID"	mol color ColorID 0 then redefine the current presentation	

	GUI-interface	TK Console	note
Change drawing method	Control panel → Graphics → Representation → select “Drawing method” as “cpk” or “point” or line	mol representation CPK <sphere radius> <bond radius> <sphere resolution> <bond resolution>	
Change transparency of atoms	Control panel → Graphics → Representation → select “Material” as “Transparent”	mol material <Transparent/Opque/…>	
Read coordination	Visualization window → keyboard “1” → mouse click		
Read bond length	Visualization window → keyboard “2” → mouse click		
Rotate configuration	Keyboard “R” → use mouse Keyboard g/h/j/k/l	rotate y by 90	
Output / render image	Control panel → Files → Render → choose the software, usually povray or tachyon	render Tachyon outputfilename “<executable of tachyon” -aasamples 12 %s -format PNG -o %s.png"	
Change default setting	Control panel → Extension → VMD preference	Edit .vmdrc	
Save the current setting in a file	Control panel → File → save visualization state		
Load a previous setting	Control Panel → File → load visualization state		