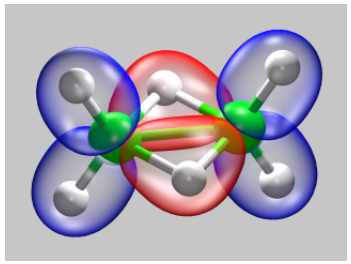
Introduction to the VMD program

Visual Molecular Dynamics (VMD)

- toolkit for visualization and analysis of MD data
- `http://www.ks.uiuc.edu/Research/vmd/`, download, manual, examples



Customizing your VMD Setup

adapt file `.vmdrc` in your home directory

Customization

orthographic projection, grey background, green C, light green F.

```
# make sure, that the main menu is active
menu main on

# modify display settings
display projection orthographic
axes location off
color Display Background silver

# redefine some colors
color Name C green
color Name F lime
color Type C green
color Type F lime
```

Extending script and plugin search path

Make additional Tcl scripts or plugins available to VMD *via* `.vmdrc`. Assume the directory `vmd` in home and therein `scripts`, `scripts/tcl`, `scripts/extensions`, and `plugins`.

```
# search for new/updated molfile plugins in $HOME/vmd/plugins/$VMDARCH/molfile
# type 'vmdinfo arch' to find your name for $VMDARCH
vmd_plugin_scandirectory [file join $env(HOME) vmd/plugins [vmdinfo arch] molfile] *.so

# add local (autoloaded) scripts to the search path
set auto_path [concat $env(HOME)/vmd/scripts/tcl $auto_path]

# command extensions (e.g. vmd_draw_vector) have to be sourced
foreach ext [glob  nocomplain $env(HOME)/vmd/scripts/extensions/*.tcl ] {
        source $ext
}
unset ext
```

Loading and visualising structures

`#vmd GEOMETRY.xyz`

Or via `File/Load`.

Standard drawing method for visualisation representation is Lines (via `Graphics/Representatio`
`Method`) - find CPK, find Isosurface, volume slice.

Change color of atoms via `Graphics/Colors/Name`.

Save presentation, render presentation.