

Praktikum Physikalische Chemie

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Molecular Dynamic Simulations

VMD Installation

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1 VMD installation for UNIX systems

Create an account and download file

Use the link below to create an account:

<https://www.ks.uiuc.edu/Development/Download/download.cgi?UserID=&AccessCode=&ArchiveID=1585>

Install VMD

1. Extract the file and change (`cd`) to the extracted directory:

`"vmd-1.9.4a38.bin.LINUXAMD64-CUDA10-OptiX600-RTX-OSPRay170.opengl.tar.gz"`

2. Edit the following two paths in the `configure` script:

`install_bin_dir`

This is the location of the startup script 'vmd'. It should be located in the path of users interested in running VMD.

`install_library_dir`

This is the location of all other VMD files. This includes the binary and helper scripts. It should not be in the path.

3. Generate the Makefile based on these configuration variables by running the command

`sudo ./configure`

4. After configuration is complete `cd` to the `src` directory and type

`sudo make install`

5. After this, you can use `vmd` with the path you defined previously for the `install_bin_dir` variable. For instance, if you did not change the path you can run `vmd` with the following command:

`/usr/local/bin/vmd`