Reference Material

VMD Software Download:
https://www.ks.uiuc.edu/Research/vmd/

3D-SNFG plugin for VMD:
http://glycam.org/docs/othertoolsservice/2016/06/03/3d-symbol-nomenclature-for-glycans-3d-snfg/

GPUs that VMD can use:
https://developer.nvidia.com/cuda-gpus

My GPU: GeForce GTX 1060 6GB GDDR5X

LiteMol: litemol.org

GlycoproteinBuilder: glycam.org/gp
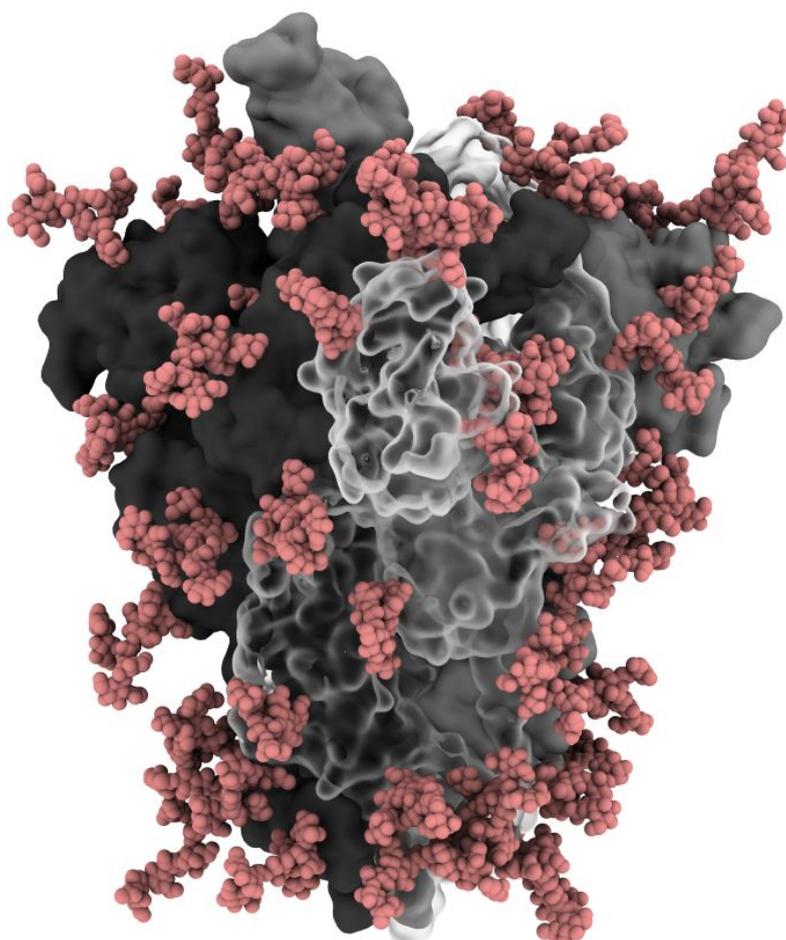
Aim: Learn how to make this render of the SARS-CoV2 Spike Glycoprotein.

Tutorial

Go to https://www.modelarchive.org/doi/10.5452/ma-zykoq and download the 3D structure. Launch VMD using the icon or from a terminal by typing "vmd" and hitting enter.

In the display window, hold left click to rotate the molecule and mouse wheel to zoom. Press T on your keyboard and then left click to translate the molecule. Press R to go back to rotate mode.

Load in your 3D structure:
Menu**:** File -> New Molecule
Click on "Browse…" and navigate to the 3D structure file you wish to load (ma-zykoq.cif).
Click Load and then close the Molecule File Browser window.
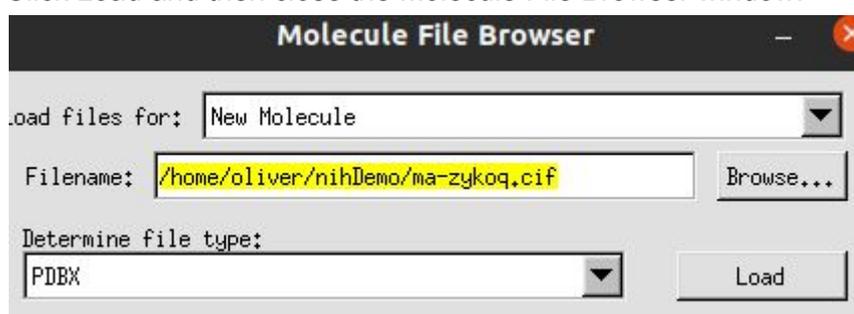
Enable Ambient Occlusion and Ray Tracing:
Menu**:** Display -> Display Settings
Set "Shadows" and "Amb. Occl." to On.

Setup 3D structure for the image:
Menu**:** Graphics -> Representations.
"Material" select a representation starting with "AO…" e.g. AOChalky.
"Selected Atoms" box write "chain A" and hit enter.
"Drawing Method" QuickSurf.
"Coloring Method" ColorID, then change from 0 (blue) to 8 (white).

Click on the representation in the box and then click "Create Rep". It will create a copy of this representation that we can edit.
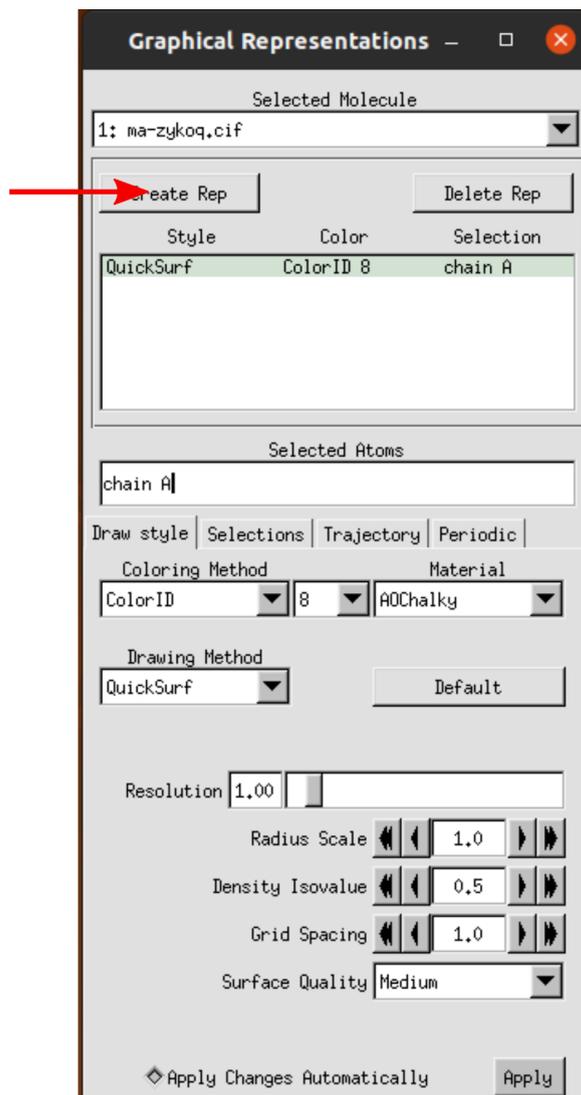
"Selected Atoms" change the text to "chain B" and hit enter.
Change the color to "6 Silver"

Click "Create Rep" to create another copy. Edit the text to "chain C" and change the color to "2 Gray".

Click "Create Rep" again. Edit the text to say "Hetero noh". This means hetero atoms but not hydrogen.
"Drawing Method" VDW. This will show the atoms as van der Waal surfaces.
Set the color to "9 pink".
The final result should look like this:

Make a render with these representations:

Menu**:** File -> Render…

In File Render Controls, change the Renderer from Snapshot to **Tachyon**. Snapshot will reproduce what is in the display window, Tachyon will actually render with Ray Tracing and Ambient Occlusion. If you have a **TachyonL-OptiX** (interactive, GPU-accelerated) option, use that instead as it's much faster.
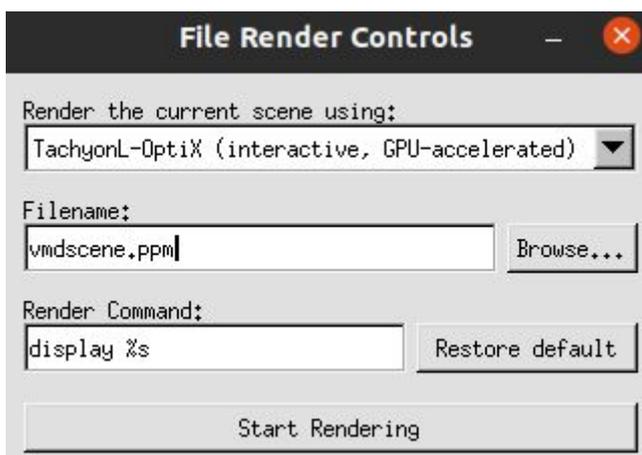
Change the filename and location as desired.

Click "Start Rendering"

Congratulations! You've made a nice image. Let's go a little bit further and learn how to edit colors/materials and use transparent surfaces.

Color editing:

You'll see in your image that the grey/silver isn't very distinct. Let's make the grey darker.

Menu: Graphics -> Colors.

In the bottom left under Color Definitions click on "2 gray". Select "Grayscale" and move one of the dials down to ~25. Now when you render the protomer colors are more distinct.
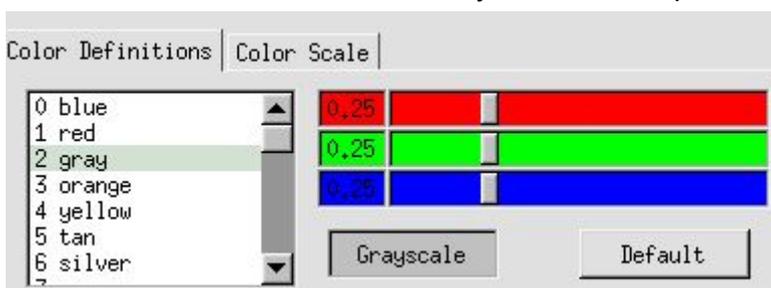
Transparent surfaces:

In Graphical Representations, select the "chain A" representation and change the material to "glass bubble". Then render. Note renders with transparent surfaces can take much longer. This representation is too transparent, let's edit it.

Material editing:
Menu**:** Graphics -> Materials
Click on ClassBubble and set the following:
Opacity to 0.3
Ambient to 0.3
Diffuse to 0.7
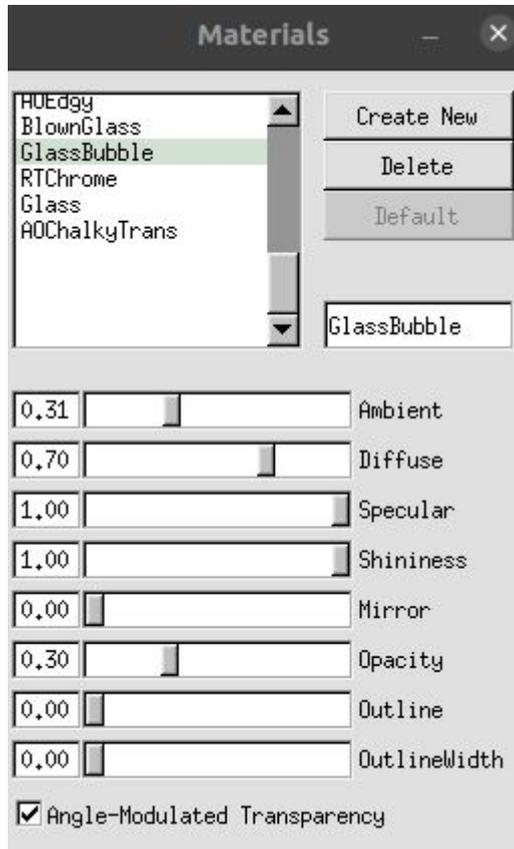
Then render. You will have an image close to that shown at the beginning. If you mouse over each of the settings in Materials it will explain what it does. If you have a GPU and can render quickly, I suggest learning what each does by adjusting it and rendering an image.

Video:
Menu: Extensions -> Visualization -> Movie Maker.
In Format select gif or as desired.
Set Working directory as desired.
In Movie Settings -> Rotation about Y axis
Set Rotation angle to 360.
Set Movie duration to 20 seconds.
In Renderer select Tachyon (or TachyonL-OptiX if available).
Optional: In Movie Settings, deselect "Delete Image files" if you wish to use other software to compile the movie from the individual frames.

Press Make Movie to start the process. This can take a very long time depending on your settings (transparent surfaces, large images, long movies, no GPU).

You can save your session:
Menu: File -> "Save Visualization State"
Then when you reopen VMD and haven't moved or renamed the 3D structure file:
Menu: File -> "Load Visualization State". May take some time to load.

Suggested Next Steps:
Learn more about VMD selections. Search for "VMD selections" online in a search engine.
Learn how to install and use 3D-SNFG shapes in VMD. Search for "VMD 3D SNFG".
Join the VMD mailing list to ask for help or email/tweet me at olivercgrant@gmail.com or @olivercgrant.