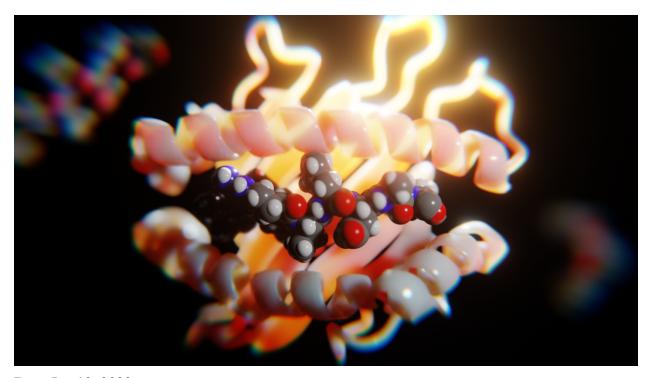
Lesson 1: The 3D Viewport and Lighting



Day: Jan 18, 2023

Time: 10:30 – 11:30AM

Room: 56-154

Lesson Summary

For many of you, this will be your first introduction to the world of 3D modeling. At first it will feel foreign, and you will likely find yourself wondering, *how can I possibly remember all this?* Don't worry! Everyone feels this way when they start. In fact, this first lesson is designed to make you feel that way. By the end of this lesson, you will have seen EVERYTHING you need to make a high-quality journal cover. The next three lessons will reinforce what we learn today and introduced more advanced topics.

Class Schedule

1.	20.S947: Intro to 3D Scientific Rendering	5 min
2.	Converting molecular structures to 3D meshes	10 min
3.	Basics of manipulating molecular structures in Blender	15 min
4.	Experimenting with Blender materials for molecules	10 min
5.	Experimenting with lighting for molecular scenes	5 min
6.	The compositor and final render settings	10 min

Total Time 55 min

1. Converting molecular structures to 3D meshes (10 min)

Before we jump into Blender, we will need a structure. In this lesson, we will be rendering the MHC from assignment 2 of 20.420. Some of you may remember it! As this is the first class, many won't have the software downloaded yet, so I have provided the starting file: **Start.blend**. Now sit back and relax. It isn't necessary to follow along for section 1. However, I do want to show you every step so you can replicate it on your own later.

- Download ChimeraX: https://www.rbvi.ucsf.edu/chimerax/
- Download the PDB file: https://files.rcsb.org/download/2BVP.pdb
- Open the PDB in ChimeraX
 - Delete waters → delete :HOH
 - O Delete everything but the MHC \rightarrow delete /B /A:181-274
 - o Hide interacting amino acids → hide /A atoms
 - \circ Increase cartoon width \rightarrow cartoon style width 3.5
 - \circ Increase cartoon thickness \rightarrow cartoon style thickness 1
 - Update colors → color byelement
 - o Add in hydrogens → addh /C
 - Depict peptide as spheres → style /C sphere
 - o Save as a model → save structure.glb format gltf instancing true

2. Basics of manipulating molecular structures in Blender (15 min)

Now that you have a model of your structure, we can open it in Blender and begin practicing with the interface. This is where you can follow along if you'd like, although some may prefer to just watch depending on their learning style.

- Download Blender: https://www.blender.org/download/
- Open Blender

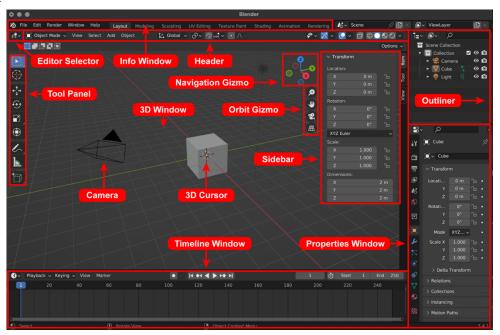


Figure 1. Getting to know the 3D viewport. I will use these terms in the tutorial.

- Delete default cube Click on the cube $\rightarrow x \rightarrow d$
- Import the molecular structure → File → Import → glTF (.glb/.gltf)
- Clean up the structure
 - o Create new collection called Complex → C
 - Create new collection called MHC \rightarrow C
 - Create new collection called Peptide → C
 - **Hint:** If you press **C** while after selecting a folder in the **Outliner**, it will automatically create a collection inside the selected collection
 - o Right-click and delete 2bvp.pdb
 - o Drag and drop **ribbons** inside the new **MHC** collection
 - o Right-click and delete Atoms
 - O Drag and drop all **atoms** inside the new **Peptide** collection
- Right click MHC and Select Objects
 - Set the origin to your object → Object → Set Origin → Origin to Geometry
- Center the object at World Origin
 - o Click on an orthographic viewpoint in the Navigation Gizmo
 - o Move the object with **Move** in the **Tool Panel** on the left-hand side
 - o Repeat with the other orthographic viewpoints in the Navigation Gizmo
- Scale Complex by selecting Scale in the Tool Panel
- Fit the molecule to the camera view
 - \circ View (Sidebar) \rightarrow Camera to View
 - o Use Scale, Rotate, and Move in the Tool Panel to position the molecule
- Lastly, let's learn how to copy objects as the scene would look better if there were more substrates floating in the background
- In the Outliner, Right-click Peptide and Duplicate Collection
- Select the new peptide Right-click → Select Objects
 - o Maneuver it to the back of the scene using the Move button in the Tools Panel
- Repeat this as many times as you'd like.
 - o I think two looks best. One on the left and one on the right.

3. Experimenting with Blender materials for molecules (10 min)

- Switch to render view by selecting **Viewport Shading** in the **Header** bar
 - o You will notice that the colors are dull and uninteresting
- Adjust the colors of the MHC by selecting it and going to the Material Properties tab in the Properties Window
 - Press New
 - \circ Subsurface = 2.0
 - \circ Roughness = 0.2
 - Check Screen Space Refraction
 - Check Subsurface Translucency
- Adjust the colors of each atom (you only need to change one of each type)
 - \circ Metallic = 0.0

- \circ Roughness = 0.2
- o **Base Color** to full saturation

4. Experimenting with lighting for molecular scenes (5 min)

- Change the background to black in World Properties of the Properties Window
 - \circ Color \rightarrow Hex \rightarrow 000000
- Select Light
- Change the light type in the **Object Data Properties** tab in the **Properties Window**
 - o Area
 - o Move Light around until you get some interesting shadows
- Add back light
 - Duplicate Light with Shift+D
 - o Move it behind the protein
 - o Change the **Power** to 750

5. The compositor and render settings (10 min)

- Adjust the camera settings
 - Select Camera in the Outliner panel
 - o Select the Object Data Properties tab in the Properties Window
 - Check Depth of Field
 - o Expand the **Depth of Field** option
 - Expand **Aperture** by selecting the arrow on the left-hand side
 - $\mathbf{F-Stop} = 0.05$
 - o The image now looks blurry
 - Expand Viewport Display
 - Select Limits
 - A green crosshair just appeared in the **3D Window**
 - Maneuver it to wherever you would like to be in focus
- Go to Render Properties tab in the Properties Window and check:
 - Ambient Occlusion
 - o Bloom
 - Screen Space Reflections
 - \circ Color Management \rightarrow Look \rightarrow High Contrast
- Post processing adjustments in the compositor
 - o Go to the Compositing tab in Info Window
 - Check Use Nodes
 - \circ Shift+A \rightarrow Search \rightarrow Lens Distortion
 - Drag and drop it between Render Layers and Composite
 - Dispersion = 0.175
 - Shift+A \rightarrow Search \rightarrow Glare
 - Drag and drop it between Render Layers and Lens Distortion
 - Streaks → Fog Glow

- Medium → High
- Now let's render the image
 - o Select Render from the Info Window
 - o Render Image
 - We are using **Eevee**, which is lower quality but very fast. It should finish in less than a minute.