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Introduction to Molecular Dynamics Showcase

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1 Introduction

The Molecular Dynamics (MD) showcase project aims to create web-based platforms to showcase and share molecular structures and MD simulation trajectories. It has resulted in two tools: the visualization tool (Molecular Dynamics Showcase) and the builder tool (Molecular Dynamics Showcase Builder). Both tools are hosted at <https://nanohub.org/> and are free to everyone:

- Molecular Dynamics Showcase <https://nanohub.org/tools/mdshowcase>
- Molecular Dynamics Showcase Builder <https://nanohub.org/tools/mdshowbuilder>

The visualization tool allows users to visualize and interact with MD simulation trajectories online, without installing any visualization or simulation software or having any simulation experience. The builder tool allows users familiar with molecular visualization software (e.g. VMD), to showcase either a molecular structure or a simulation trajectory to everyone. The author of the showcase can use it to collaborate with other scientists or to create a lesson about a microscopic world.

In this tutorial, we will focus on using the builder tool to create a showcase. We will start with the simplest example – creating a showcase from a PDB file – before exploring, step-by-step, more complicated examples. We will cover how to add a description, change perspective, and add frame-related comments. **It is assumed that the reader of this tutorial has finished the VMD tutorial** (<http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/>). If you encountered any problems or bugs while using this tutorial, please don't hesitate to contact Aksimentiev group (<http://bionano.physics.illinois.edu/people/aleksei-aksimentiev>).

Prerequisites:

- VMD program
- A command-line interface terminal
- A Java-enabled web browser

1.1 Content of the tutorial files

The hierarchy of subdirectories extracted from “mdshowcaseTutorial.tar.gz”:

- mdshowcaseTutorial

- * 1h_WI_dna.pdb
- * 1h_npt_dna.tcl
- * example_output
- ch3
 - * 1h_WI_dna.pdb
 - * 1h_npt_dna.tcl
 - * example_output
 - * replicate.tcl
 - * rockandroll.tcl
 - * rotate.tcl
 - * view_example_0.tcl
 - * view_example_1.tcl
- ch4
 - * 1h_WI.psf
 - * 1h_WI_npt.dcd
 - * 1h_npt.tcl
 - * example_output
 - * funnel_E100mV.tcl
 - * funnel_WI_cS_f_rm_c_aC_dna.psf
 - * funnel_WI_cS_f_rm_c_aC_lip.psf
 - * funnel_WI_cS_f_rm_c_aC_pot.psf
 - * loadFunnel.tcl
 - * movie_dna_E100mV.xtc
 - * movie_lip_E100mV.xtc
 - * movie_pot_E100mV.xtc
- ch5
 - * 1h.bib
 - * 1h_npt_comment.html
 - * 1h_npt_description.html
 - * 1h_npt_snapshot.tga
 - * 1h_npt_view.tcl
 - * example_output
 - * funnel.bib
 - * funnel_E100mV_description.html
 - * funnel_E100mV_snapshot.tga

Each subdirectory (ch2, ch3, ch4 and ch5) contains the associated files for each section. If your archive does not contain all the files in the list, please download the latest version from Aksimentiev group website (<http://bionano.physics.illinois.edu/>).

1.2 Introduction to a showcase

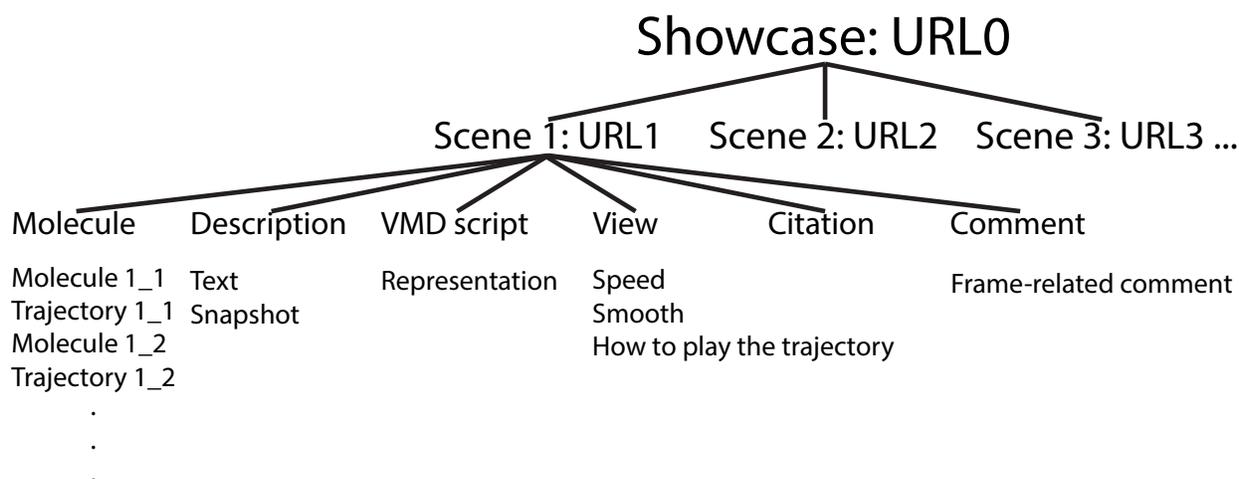


Figure 1: The structure of a showcase.

The basic structure of a showcase can be illustrated in Figure 1. Once a showcase is shared, a URL will be assigned to it. A showcase can contain many scenes, and each scene has its own URL. A scene contains the following:

- Molecule: A collection of molecules (PSF and PDB files), and their trajectories (DCD, XTC or other trajectory file format).
- Description: Description text and a thumbnail image.
- VMD script: VMD script for defining representation and perspective.
- View: Speed, smoothness, and how to play the trajectory. You can also add custom script to rotate or zoom while playing the trajectory.
- Citation: The citation for the current scene.
- Comment: The comment or description which only appear at certain frames.

1.3 Found a bug in the tool

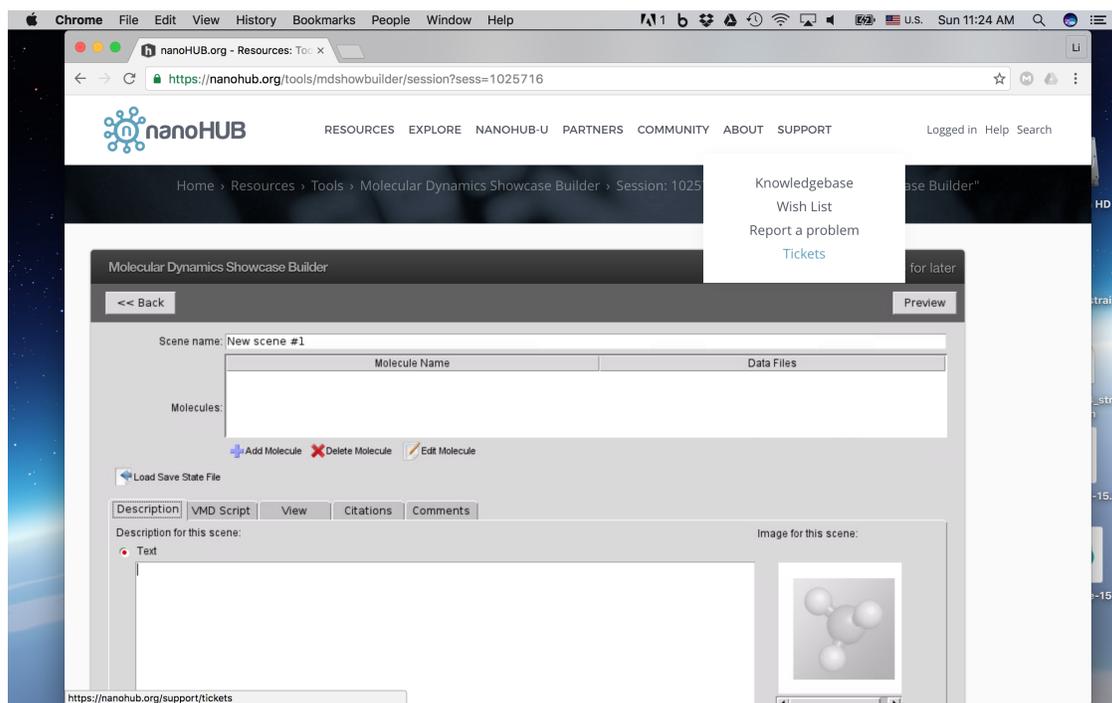


Figure 2: Go to “SUPPORT” > “Tickets” to submit a ticket.

If the MD showcase or MD showcase builder tool crashes for unknown reasons, please submit a ticket directly through nanoHUB. You can submit a ticket by going to “SUPPORT” > “Tickets” on the nanoHUB web page (Figure 2).

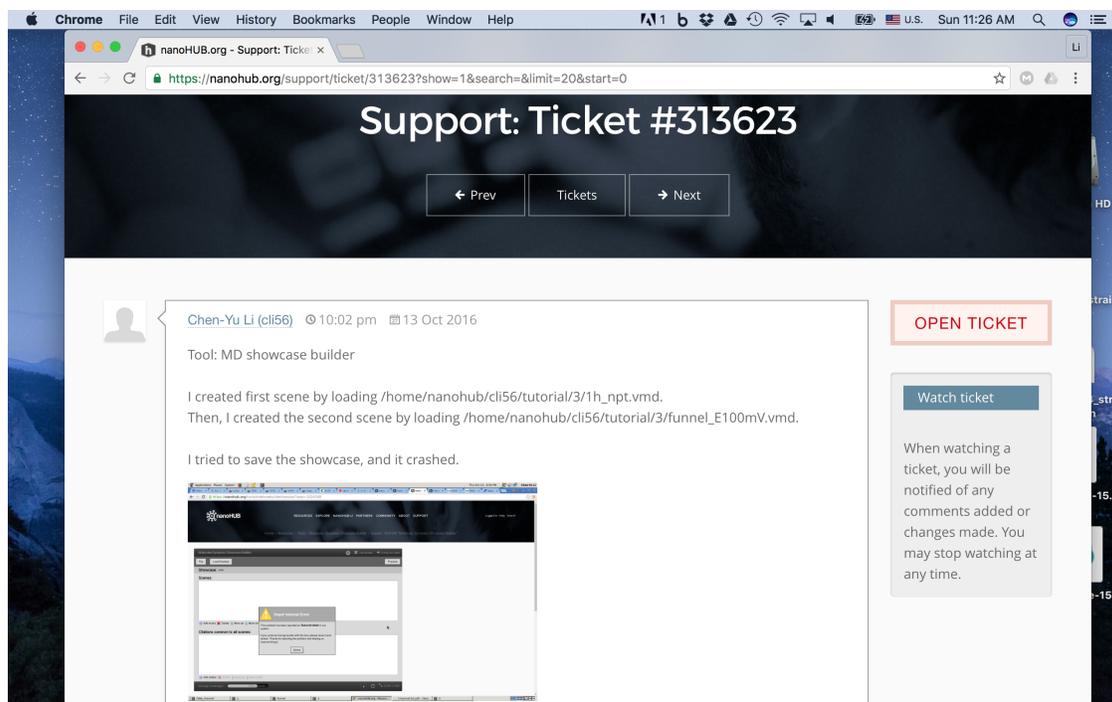


Figure 3: An example ticket. It is best to provide the name of the tool, steps needed to reproduce the bug (if applicable) and a snapshot of the error or error message.

Figure 3 is an example of a ticket. To make the communication (ticket) more effective, please specify the name of the tool, the detailed steps needed to reproduce the bug (if applicable) and a snapshot image of the bug.

We apologize for any inconvenience caused by bugs in the beta versions of the tools, and we appreciate your report to help us improve them!

2 Create the first showcase

Please navigate to the ch2 folder.

For this section, the guide use a PDB file (“1h.WI.dna.pdb”) containing a DNA duplex. [1] Feel free to use your own PDB file in its place. The DNA duplex is functionalized with 6 porphyrin groups. First, let’s load the PDB file in VMD. Next, let’s create some nice representation for this molecule. You can use your favorite text editor to open the PDB file and examine what residues are in this PDB file. Alternatively, you can use the following command in the TkConsole to display each chain and rename:

```
set all [atomselect top all]
# get all unique resname
lsort -unique [$all get resname]
# get all unique chains
lsort -unique [$all get chain]
```

You can choose any representation you like. For details about VMD representation, please refer to VMD tutorial (<http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/>) or VMD User's Guide (<http://www.ks.uiuc.edu/Research/vmd/current/ug/>). Here, we also provided an example representation in the "1h_npt_dna.tcl" (However, if you use your own PDB file, the example representations may not work well.) You can simply type the following command in the TkConsole to use the example representation:

```
source 1h_npt_dna.tcl
```

Once you are satisfied with the representation and viewpoint, you can save the VMD state by going to "File" > "Save Visualization State" (Figure 4). Let's save it as "1h_1.vmd".

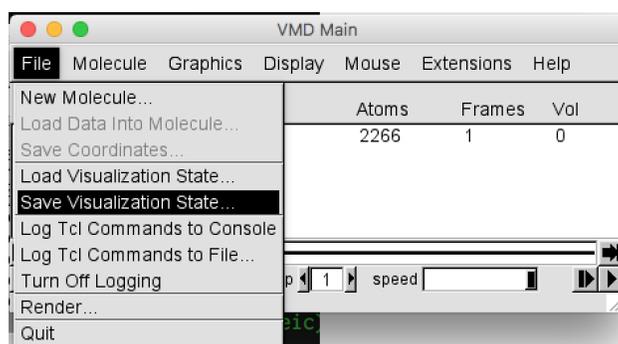


Figure 4: Save VMD state.

Next, open a web browser and go to <https://nanohub.org/tools/mdshowbuilder>, the page of MD showcase builder (Figure 5) and launch the MD showcase builder.

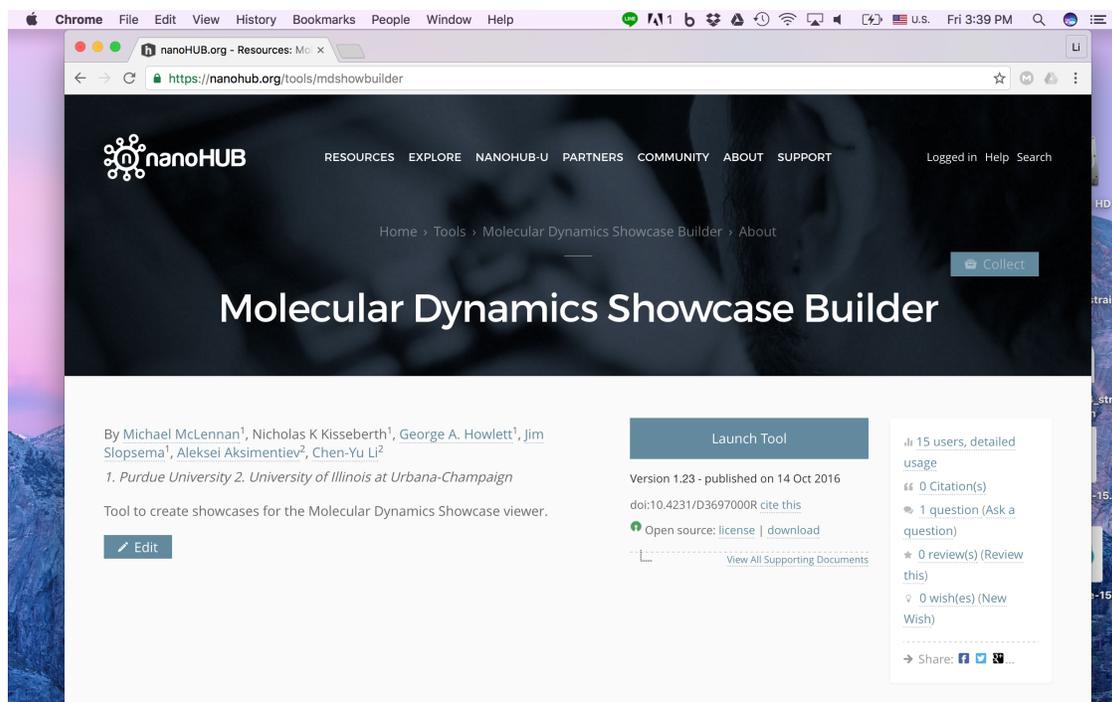


Figure 5: The MD showcase builder tool page. Click “Launch Tool” to start MD showcase builder.

2.1 Create a scene in the showcase

Now, we will create our first showcase. If you are unable to finish the [previous section](#), you can use the “example_output/1h_1.vmd” to continue.

We provide complete step-by-step snapshots for this section, from Figure 6 to Figure 20. You can finish this section by simply following the snapshots. However, if you would like to know more detail or encounter any issue, we suggest going through the description.

Figure 6 is the main window of the MD showcase builder. From the left of the first row, the “File” button allows you to open a previously saved showcase file, save a showcase file, share a showcase file, upload a file to your nanoHUB workspace or download a file from your workspace to your desktop. The “Load Example” button allows you to load example showcase files to get started. The “Preview” button allows you to preview the showcase you loaded or made. The middle part is the scene section, where you can add, delete, reorder or copy scenes. The bottom part is the citation section, where you can add, delete or reorder citations. Since now we are at the showcase level (the top level in Figure 1), the citation is for the entire showcase.

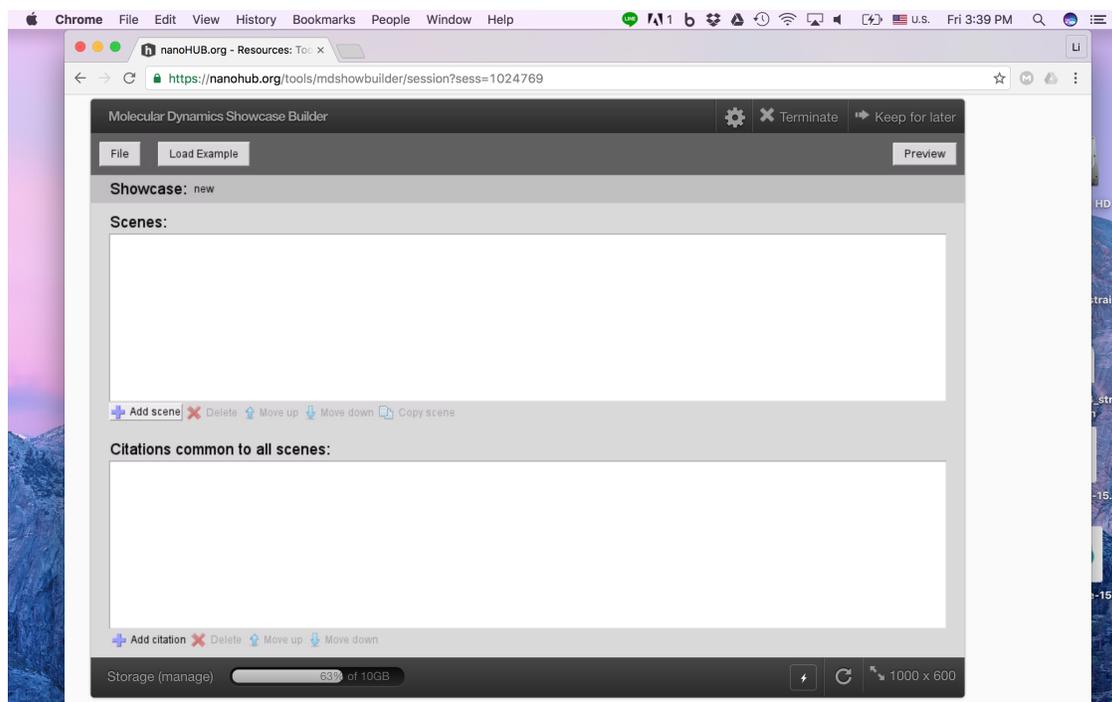


Figure 6: The MD showcase builder main window. Click “Add Scene” to add a new scene.

By default, we are at a new showcase. Let’s click “Add Scene” to add a new scene (Figure 6). Then, move the mouse to “New scene #1” and the “Edit” button will appear. Click “Edit” to edit the scene (Figure 7).

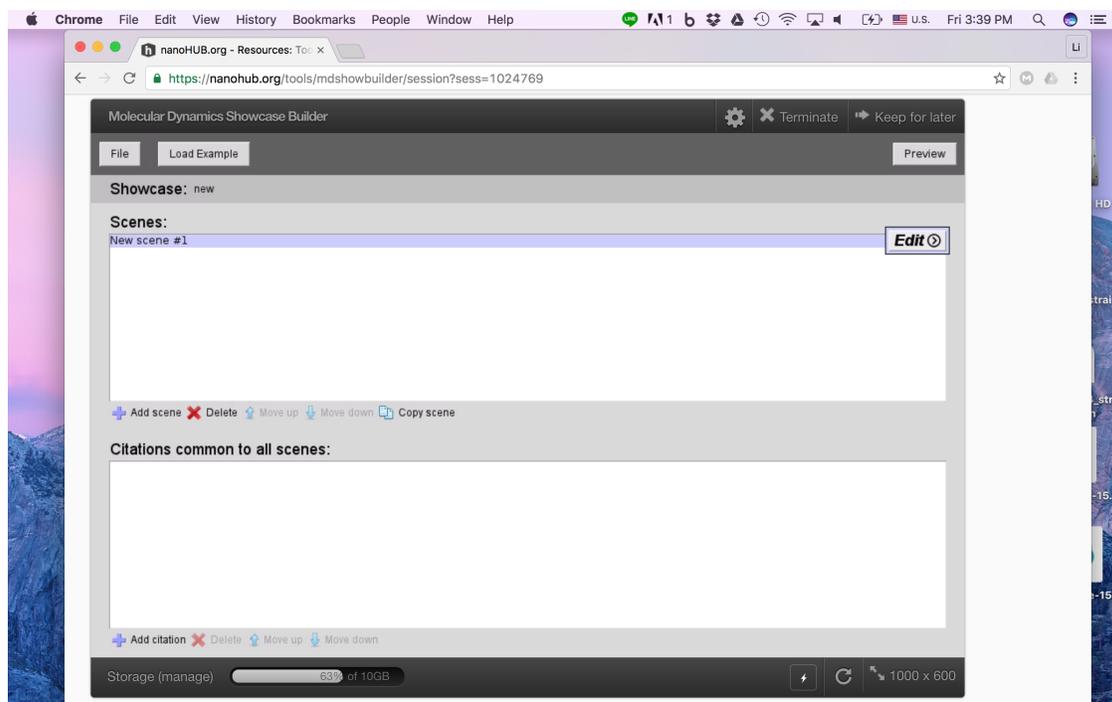


Figure 7: Move the mouse to “New scene #1” and the “Edit” button will appear. Click “Edit” to edit the scene.

Figure 8 is the scene window of the MD showcase builder. The top column is the scene name. The second part is the molecule section, where you can add, delete and edit molecules. The molecule section corresponds to the molecule component in Figure 1. On the bottom left of the molecule section, there is a “Load Save State File” button, which you can use the VMD state file to create a scene. At the last section of the window, there are five tabs “Description”, “VMD script”, “View”, “Citation” and “Comment”, corresponding to the other five components of a scene in Figure 1.

Although you can also create a scene from scratch (adding molecule and adding VMD script), in this tutorial you will create a scene using VMD state file (Figure 7).

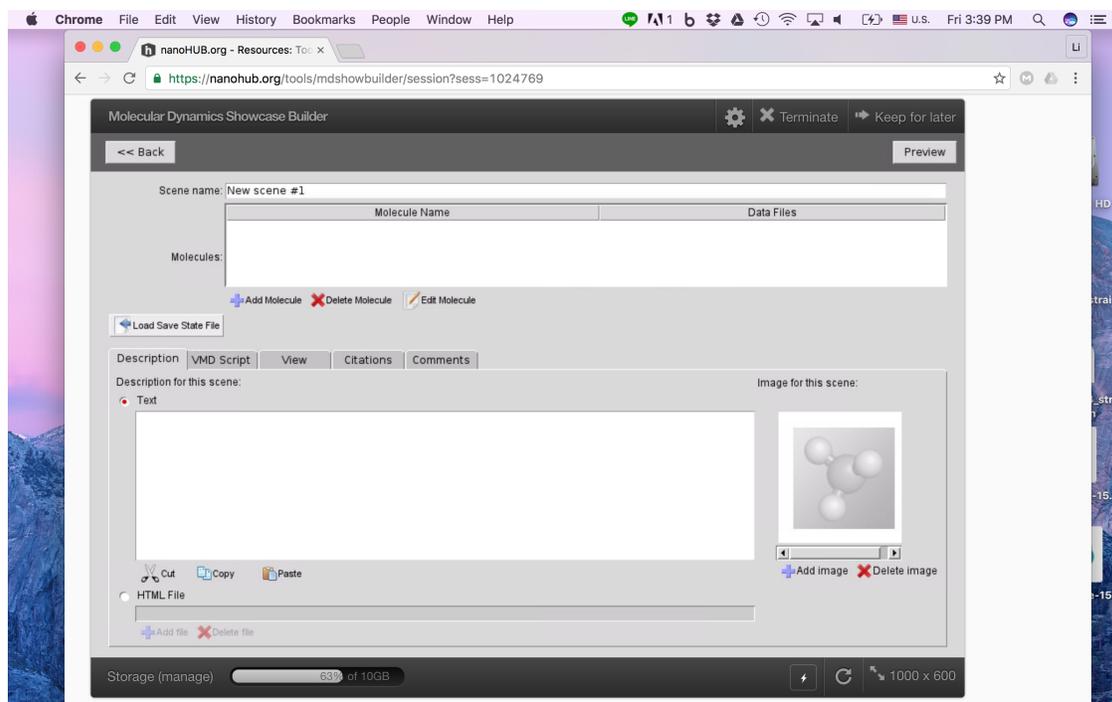


Figure 8: Click “Load Save State File” to create the scene with the VMD state file.

When we create a scene with the VMD state file, all of the related files (PSF, PDB, DCD and so on) have to be in the same folder. So, let’s create a “mdshowcaseTutorial” folder and a “ch2” folder inside it (Figure 9 to Figure 11).

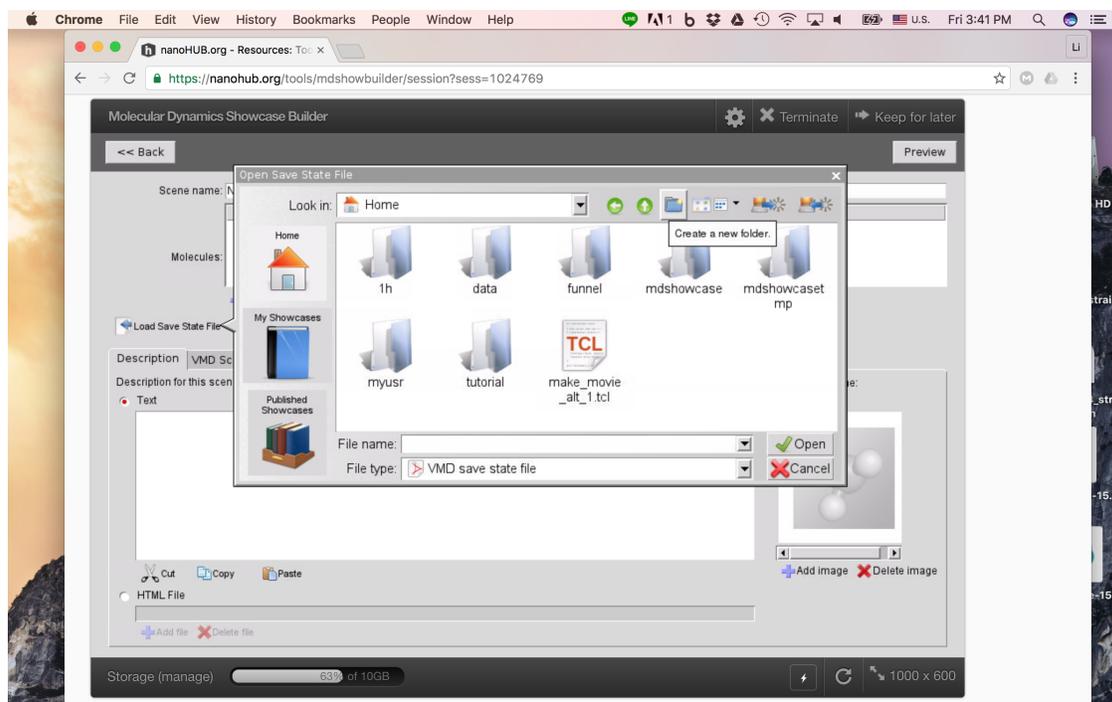


Figure 9: Click “Create a new folder”.

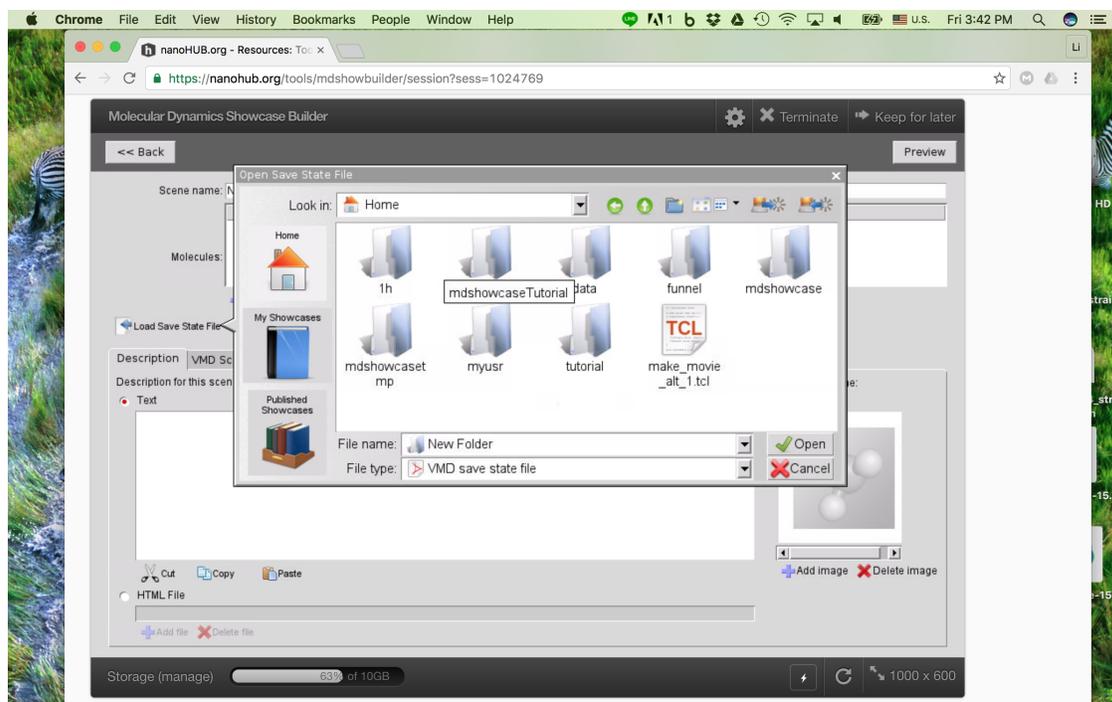


Figure 10: Right-click on the new folder to rename it. Let’s call it “mdshowcaseTutorial”.

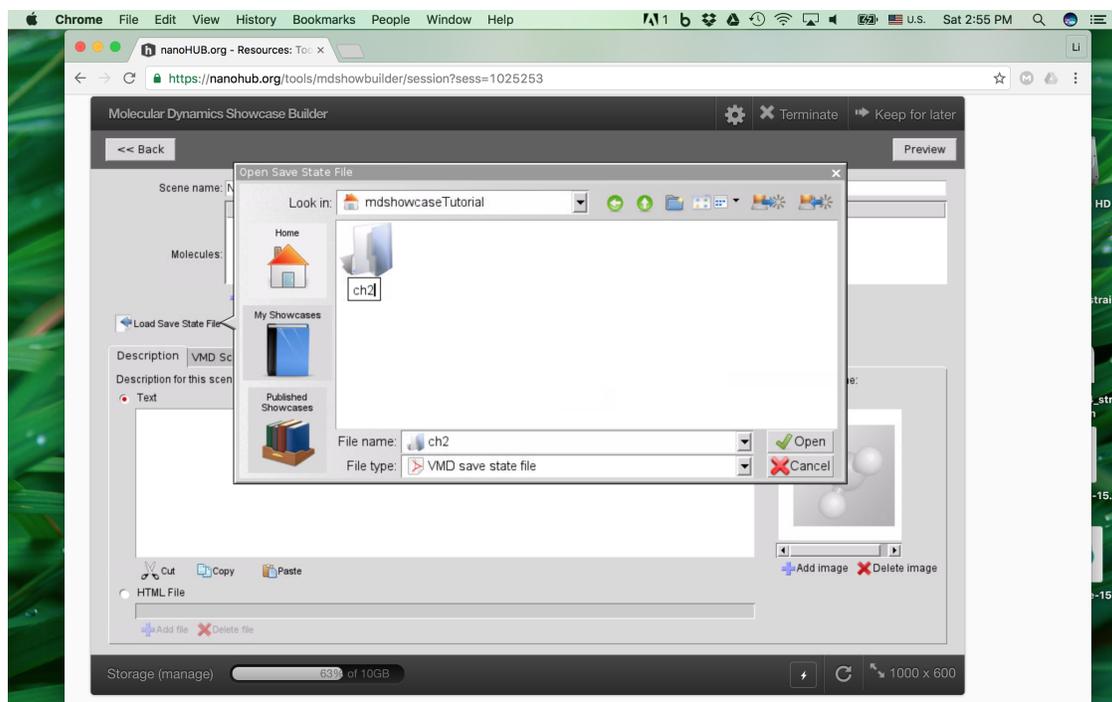


Figure 11: And create another folder “ch2” inside “mdshowcaseTutorial”.

Then, we have to upload the PDB file (“1h_WI_dna.pdb”) and the VMD state file (“1h.1.vmd”), Figure 12 to Figure 14

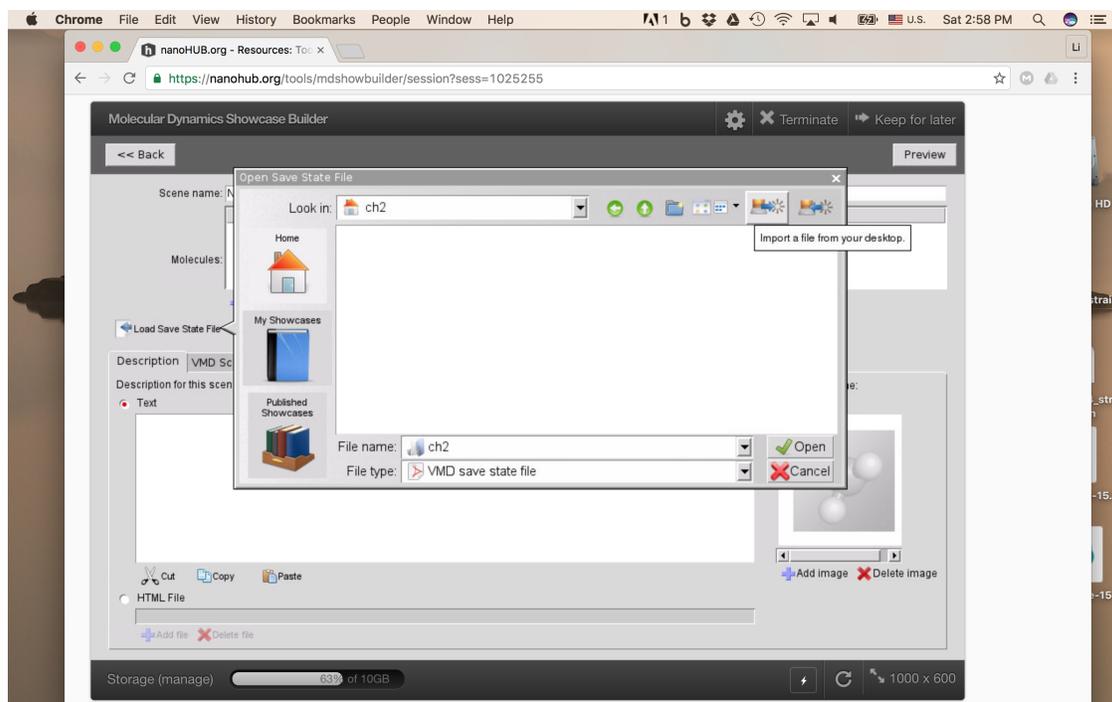


Figure 12: Click “Import a file from your desktop”.

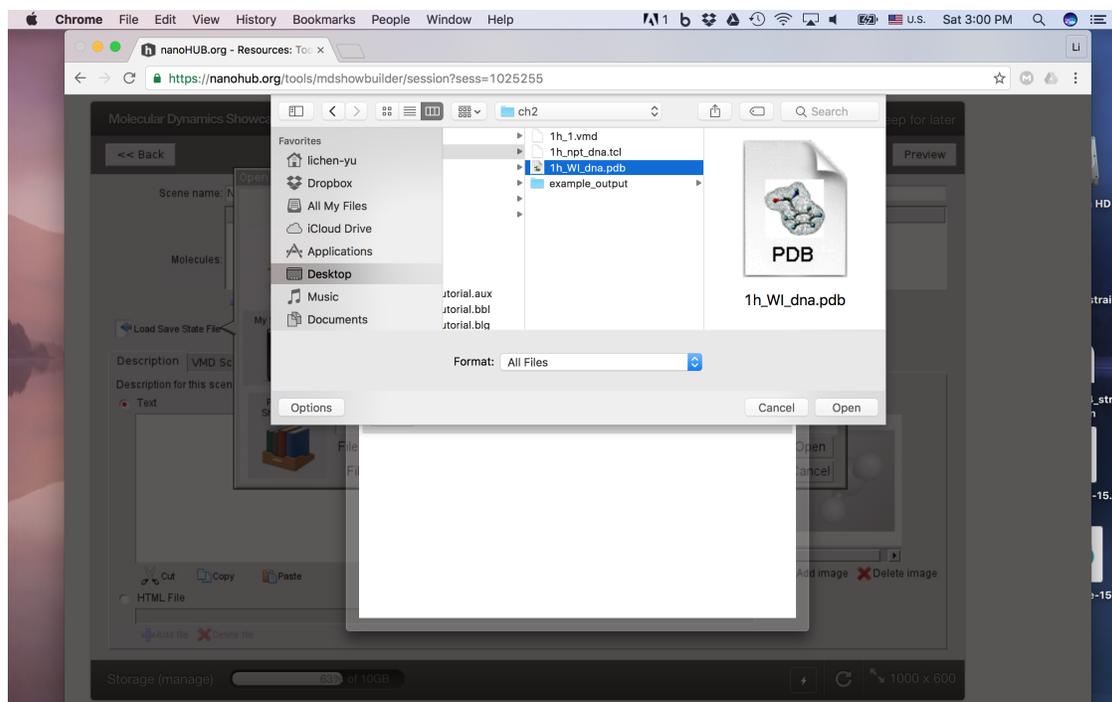


Figure 13: First, select the PDB file.

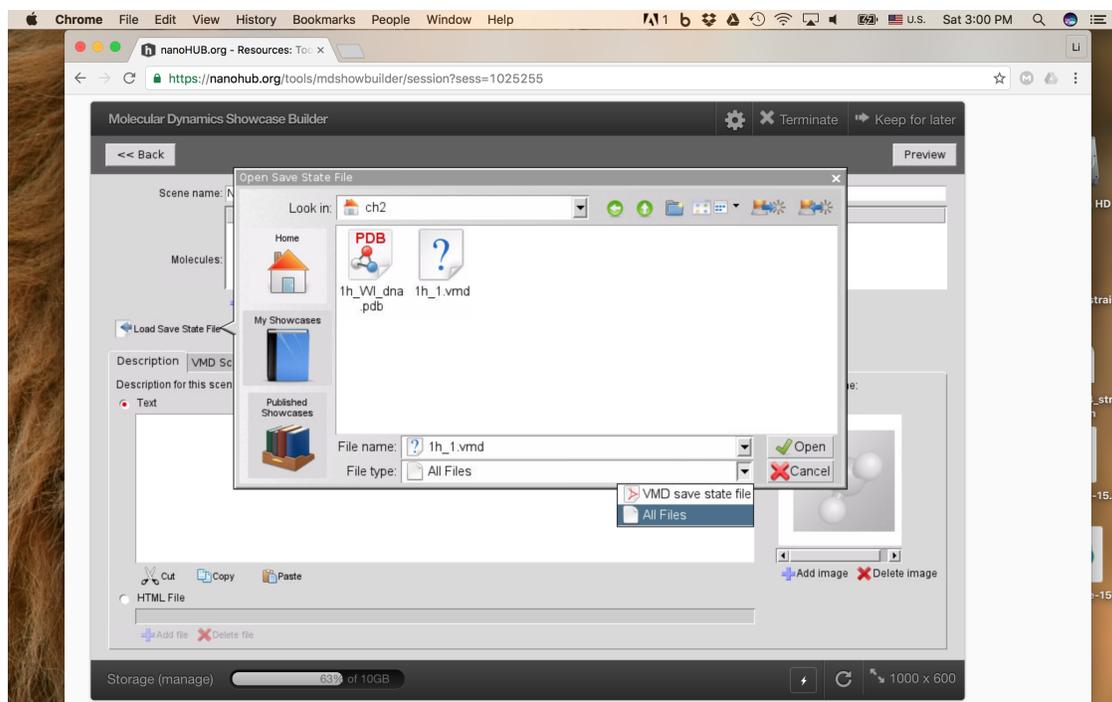


Figure 14: Then, import the VMD state file. Change the file type to “All Files” to make sure both files are present.

After we open the VMD state file, the information from the VMD state file will be extracted (Figure 15).

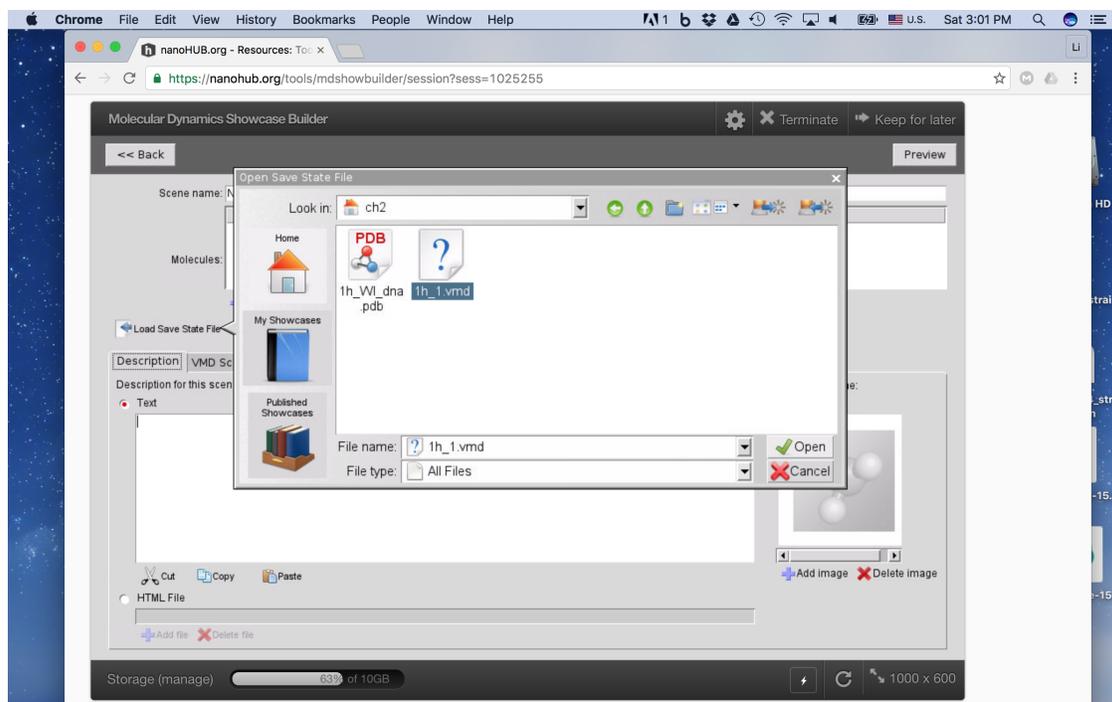


Figure 15: Click the .vmd file and “Open” to open the VMD state file.

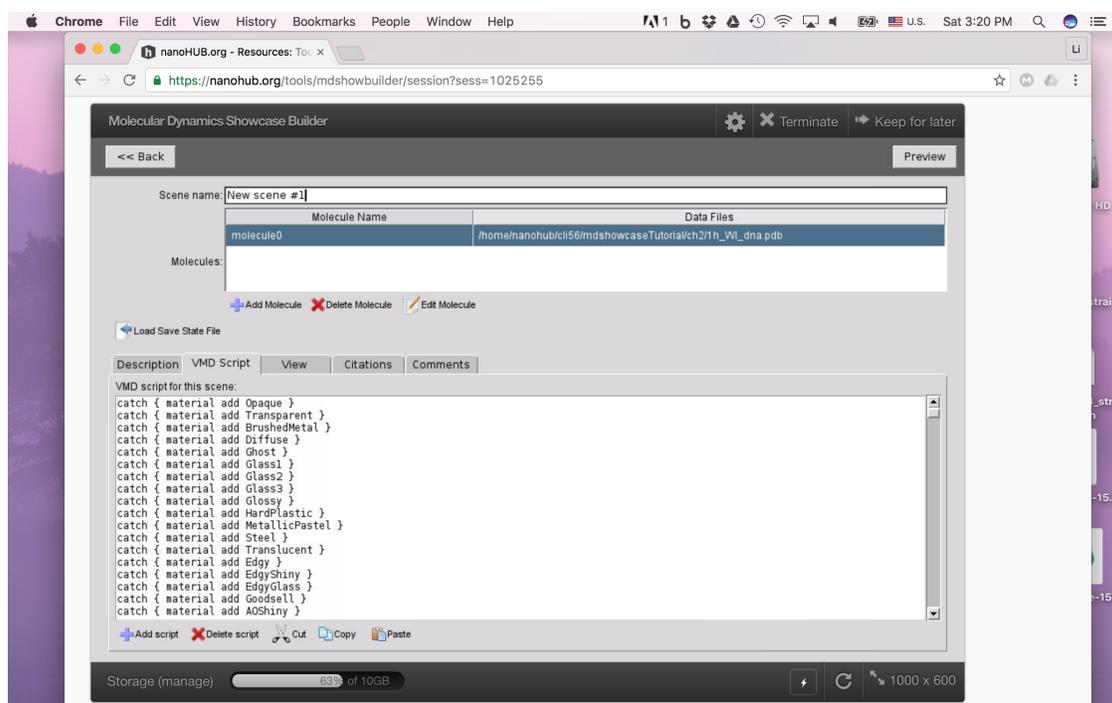


Figure 16: The molecule and the “VMD script” tab will be populated with information from the VMD state file.

The molecule section and the VMD script section will be populated with the information from the VMD state file (Figure 16).

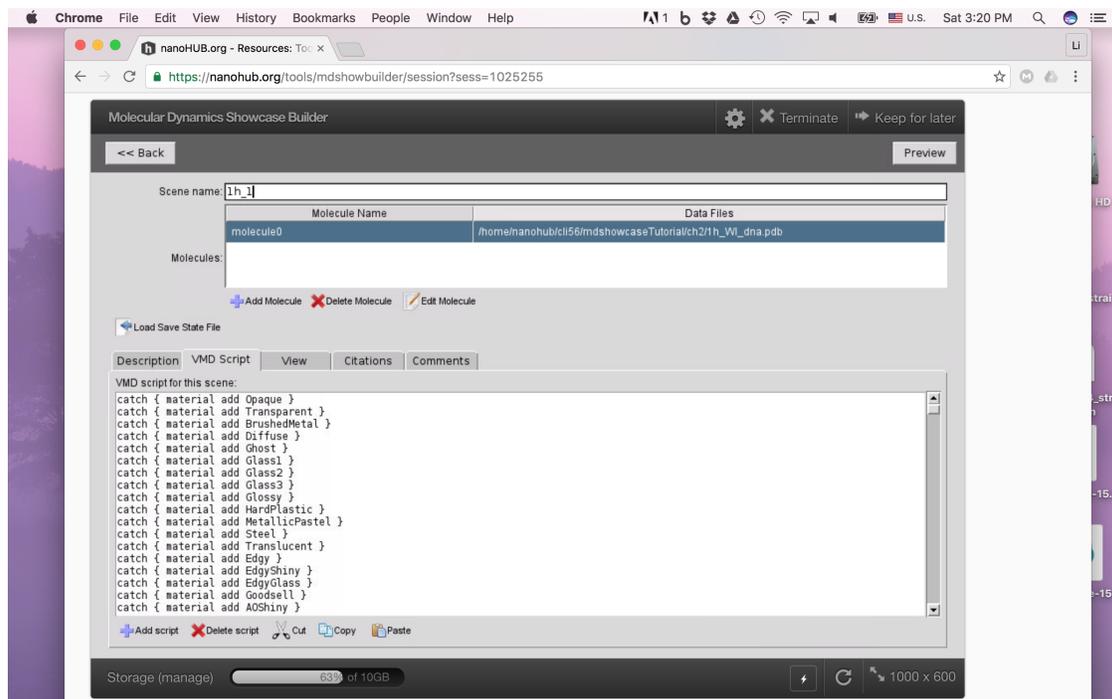


Figure 17: Change the name of the scene.

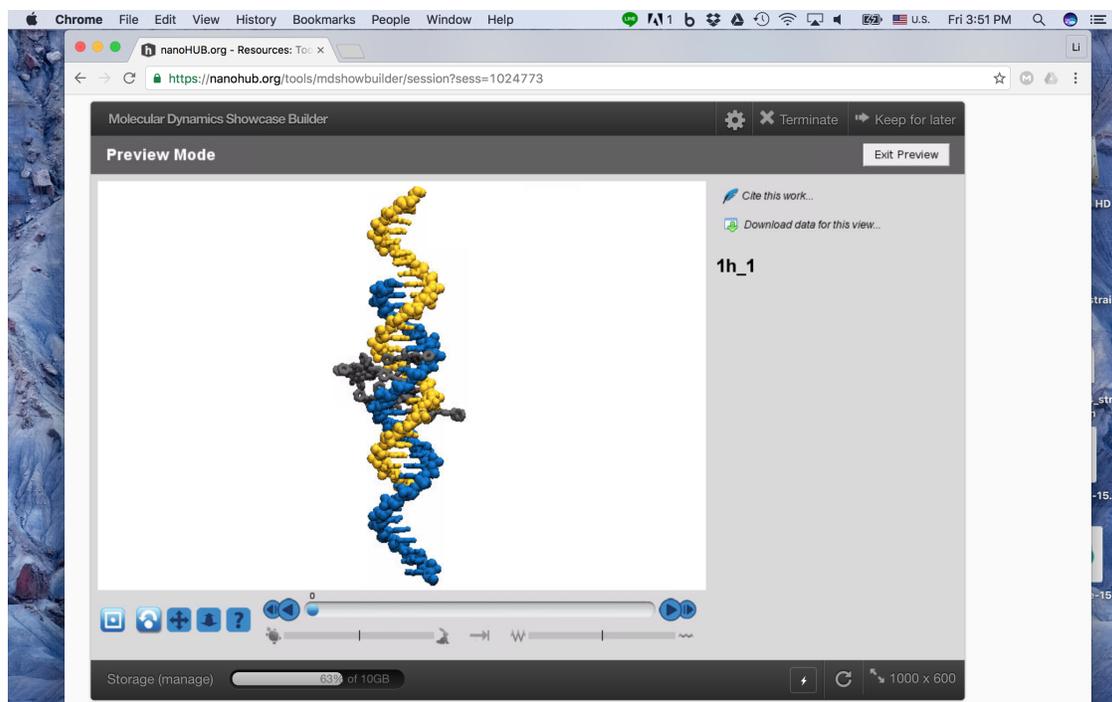


Figure 18: Click “Preview” to preview the scene. It should look exactly as we saw it in VMD.

Now, we can change the name of the scene (Figure 17) and preview our first scene (Figure 18).

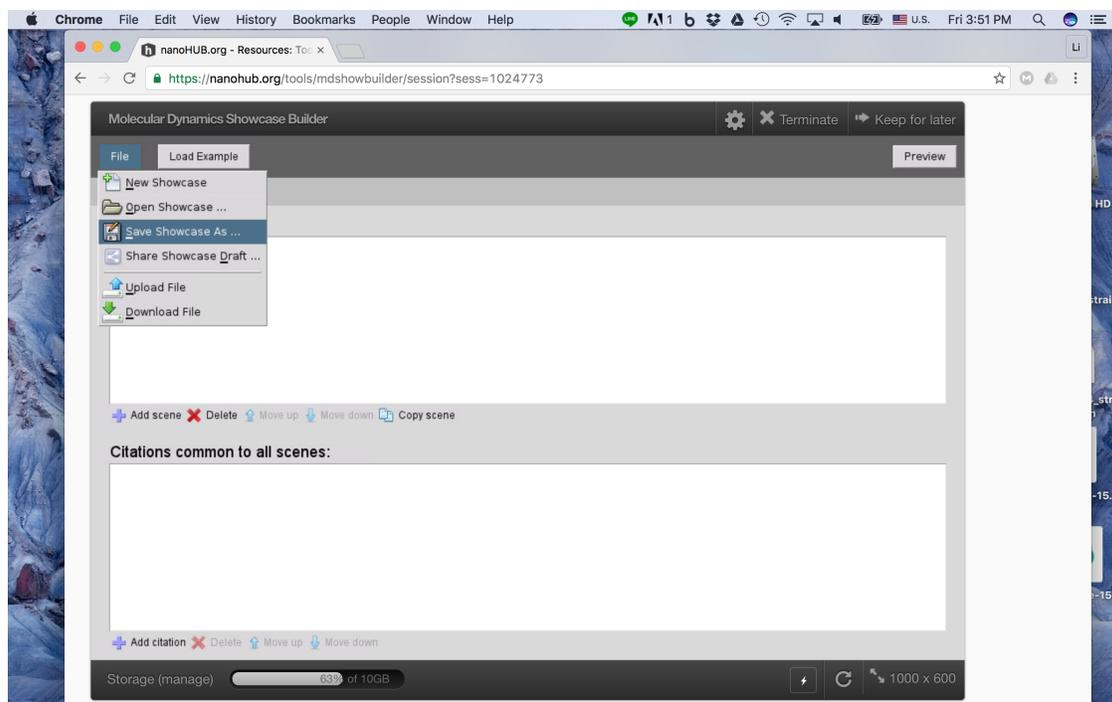


Figure 19: Click “Exit Preview” and then “Back” to go back to the main window. Click “File” > “Save Showcase As”.

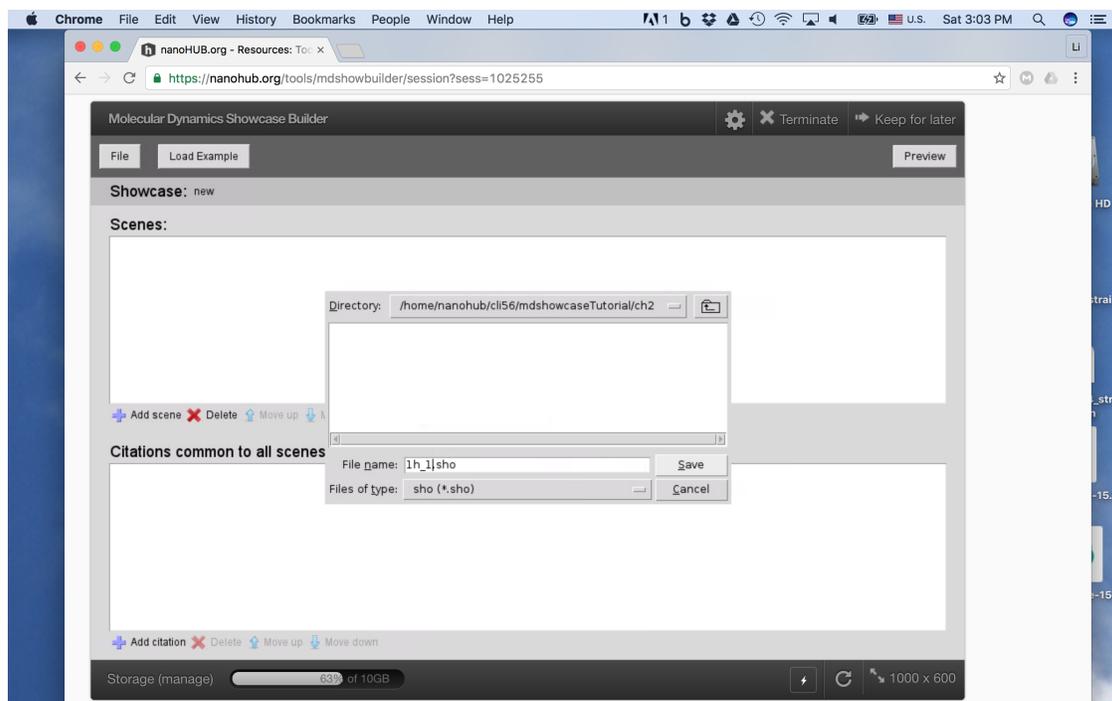


Figure 20: Save it as 1h_1.sho.

Finally, to save our work, we need to go back to the main window. Then, we need to click “File” > “Save Showcase As” to save the showcase file (Figure 19). Let’s save it as “1h_1.sho” (Figure 20).

2.2 Share the showcase

We have saved the showcase file in the workspace. Now, how can we share it?

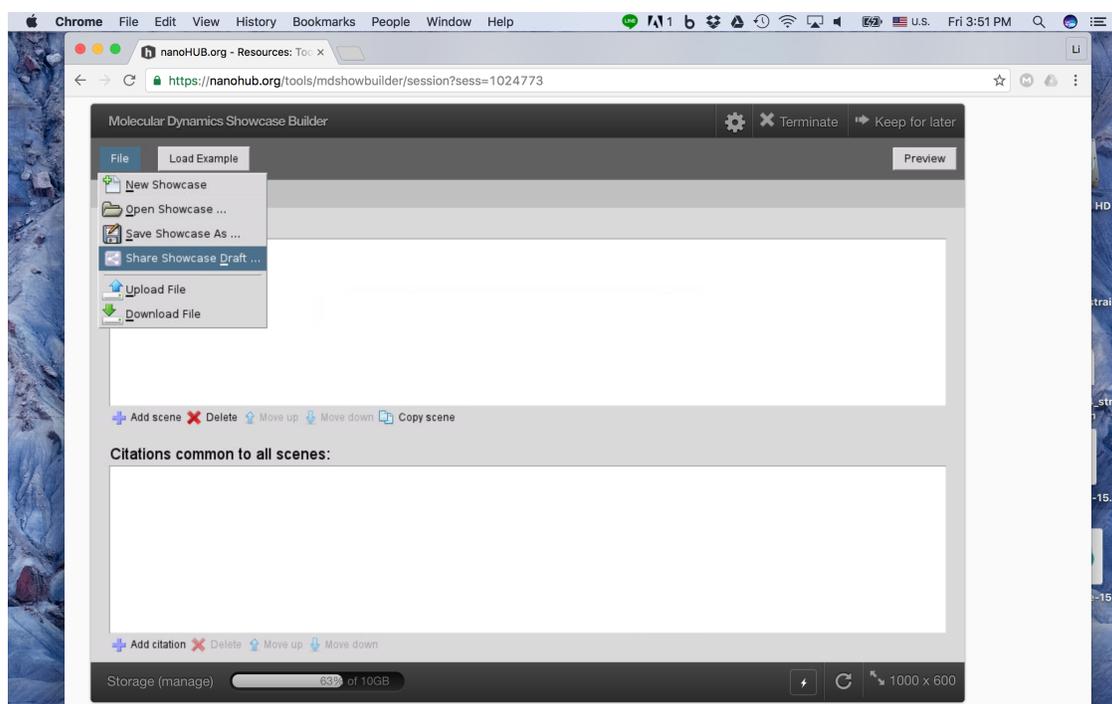


Figure 21: Click “File” > “Share Showcase Draft”.

First, Click “File” > “Share Showcase Draft” in the MD showcase main window (Figure 21).

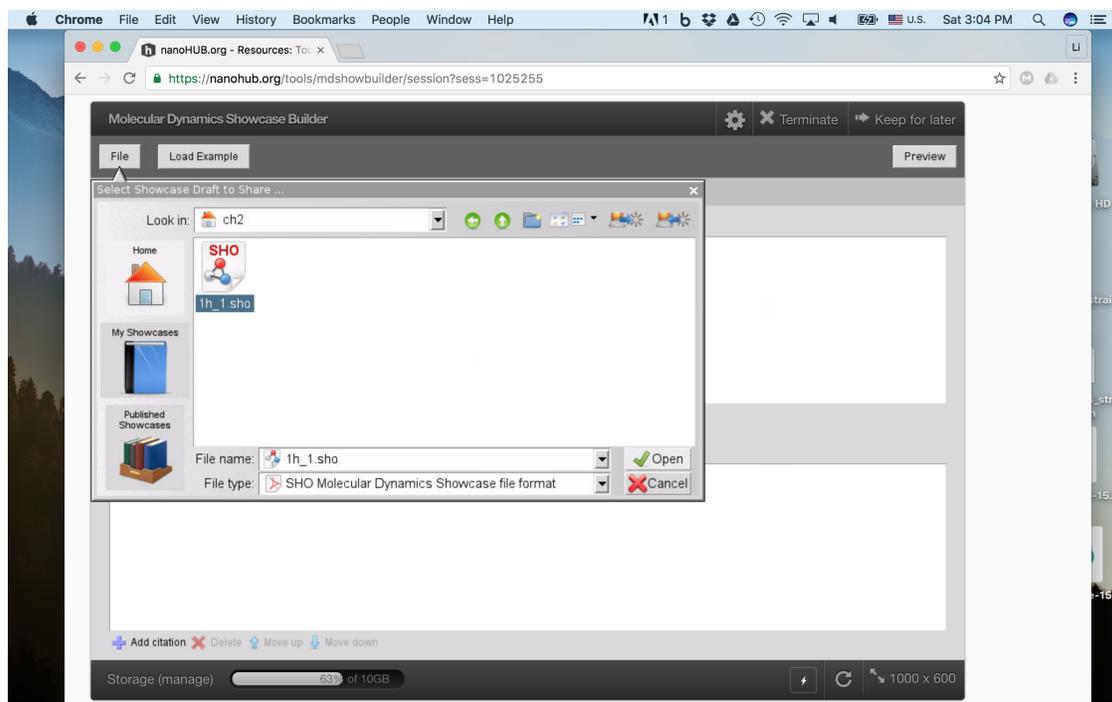


Figure 22: Select the “1h.1.sho” and click “Open”.

Then, select the “1h_1.sho” and click “Open” (Figure 22).

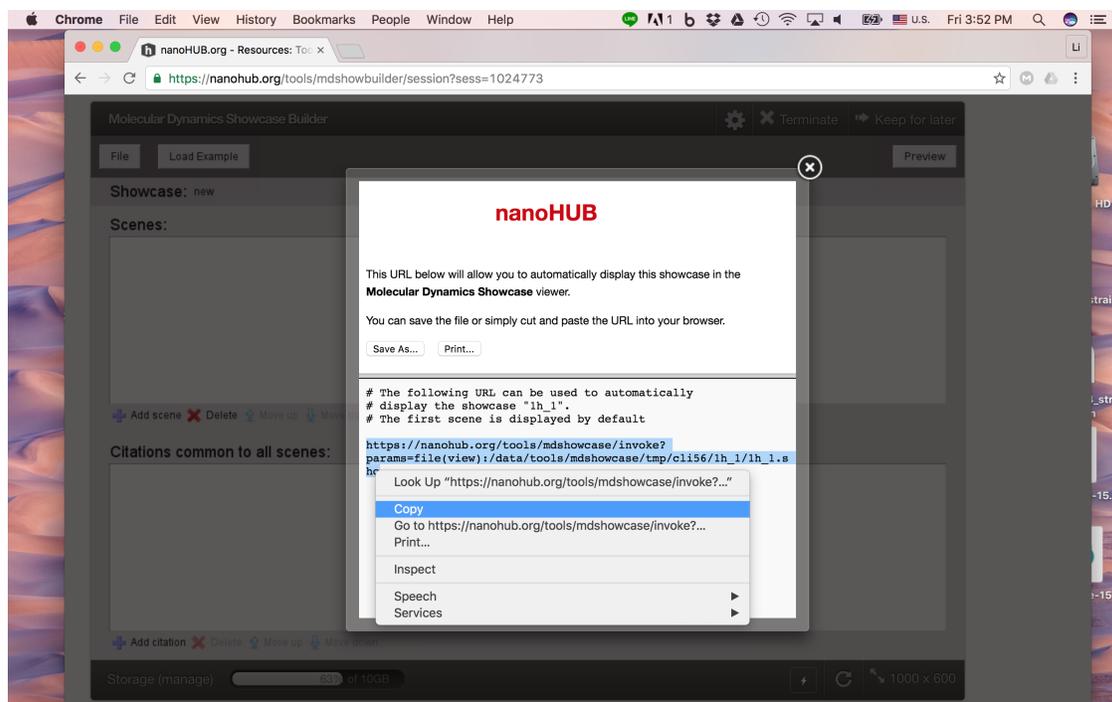


Figure 23: Copy the URL.

A pop-up window will appear, displaying the URL of the shared showcase. If there are multiple scenes in the showcase, it will also show all the URLs to each scene. Let's copy the URL (Figure 23).

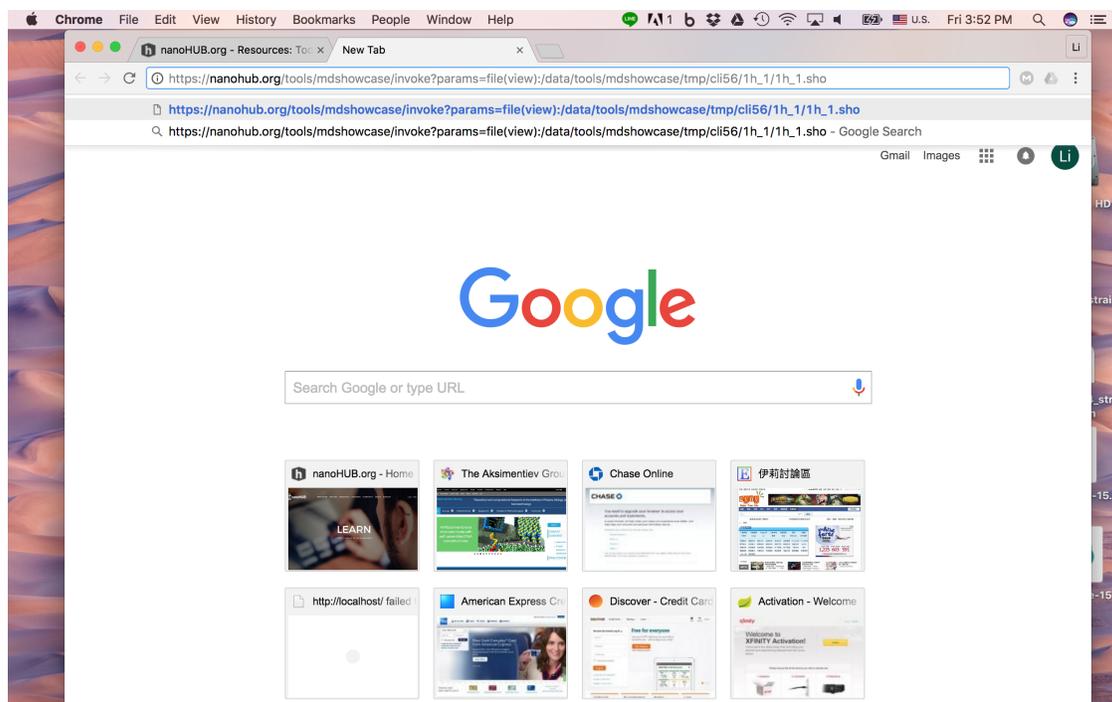


Figure 24: Paste it in the browser.

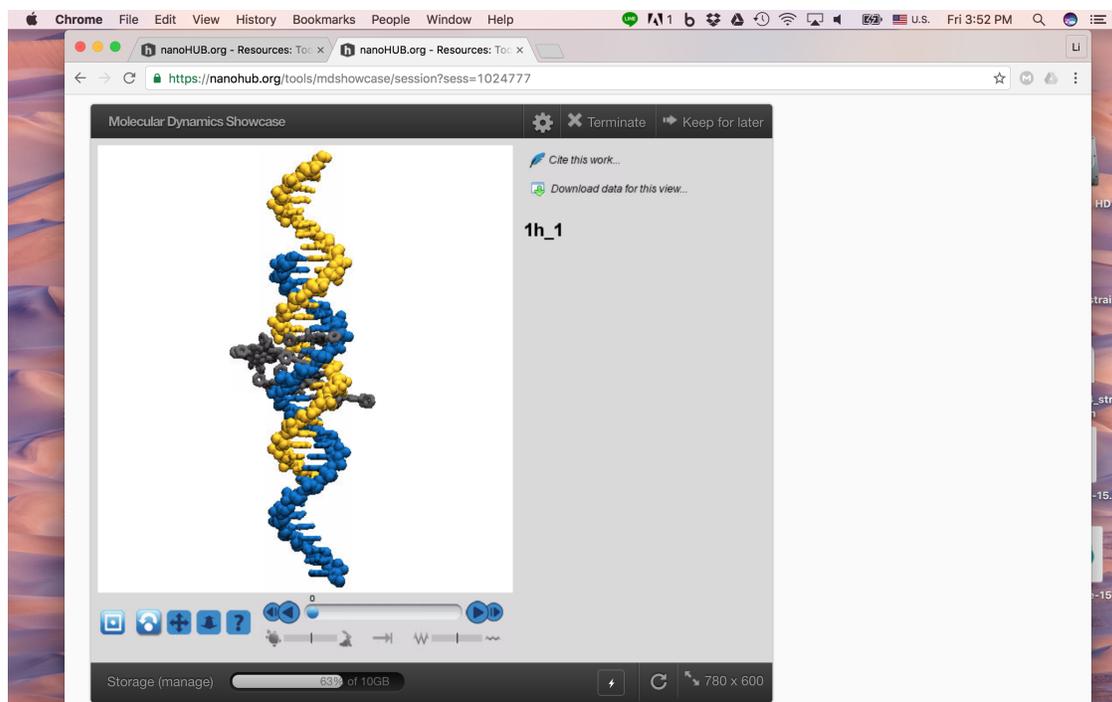


Figure 25: It will launch MD showcase, displaying the showcase we just created.

Finally, just paste the URL in the browser (Figure 24). It will launch MD showcase, displaying the showcase we just created (Figure 25). You can share the URL with others, and they can interactively explore your molecular system.

Congratulations on creating your first showcase!

3 Create an animated showcase

Please navigate to the ch3 folder.

In the [previous section](#), we created a showcase with a PDB file. Most PDB files downloaded from RCSB Protein Data Bank (<http://www.rcsb.org/>) contain the coordinates of each atom in only one configuration. In other words, it contains only a single frame of a movie or trajectory. As a result, if you click the play button in VMD or in the showcase we made in the [previous section](#), it will not play because there is no “next frame”. In this section, we will introduce some tricks to create an animated showcase using a PDB file with only one frame.

3.1 Rotation

One of the simplest and most commonly used molecular animations in scientific presentations is the rotation of a molecule (ex. protein). Here, we will use a script to create a rotating trajectory from the PDB file we used in the [previous section](#).

Please type the following command in a terminal:

```
vmd -dispdev text -args 1h_WI_dna.pdb rotate.dcd 180 360 z < rotate.tcl
```

This script takes 5 arguments, the name of PDB (1h_WI_dna.pdb), the name of output DCD (rotate.dcd), the number of frames (180), the degrees of rotation (360) and the axis of rotation (z).

If you had difficulty creating the file “rotate.dcd”, you can use the example file in “example_output/rotate.dcd” to continue the tutorial.

Next, you can load the PDB file “1h_WI_dna.pdb” and the DCD file “rotate.dcd” in VMD and define the representation you like. You can again use the same example representation in “1h_npt_dna.tcl” Next, you can save the VMD state “rotate.vmd” as we did in the [previous section](#).

If you were unable to create the file “rotate.vmd”, you can use the example file in “example_output/rotate.vmd” to continue the tutorial.

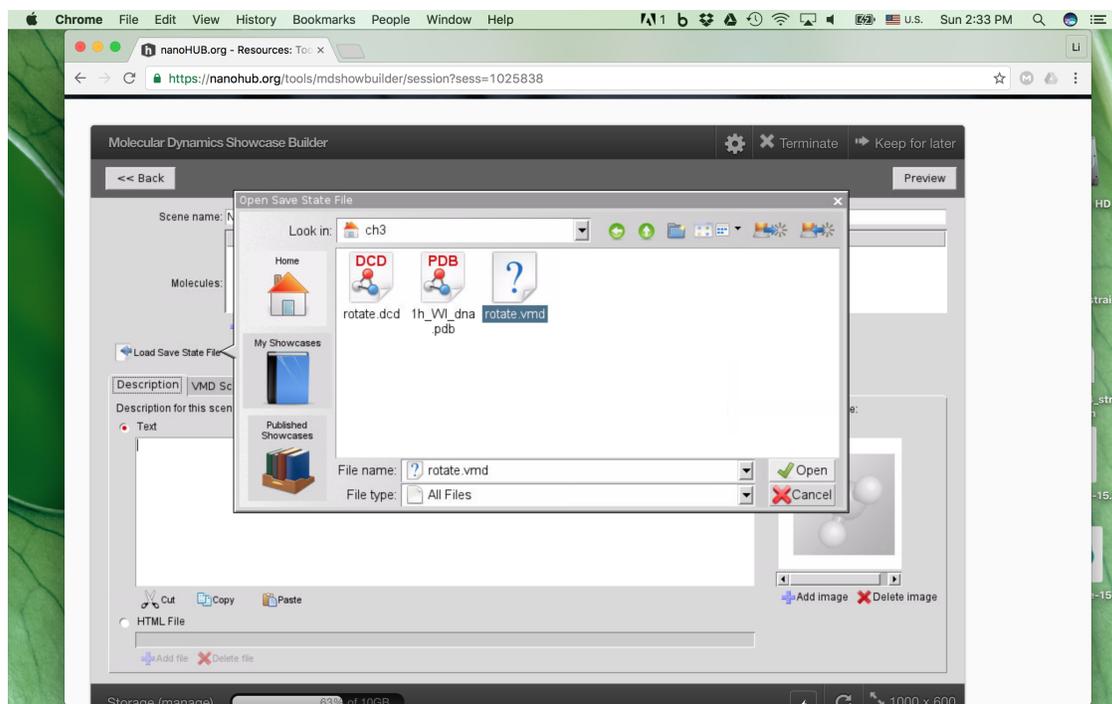


Figure 26: Upload “1h_WI_dna.pdb”, “rotate.dcd” and “rotate.vmd” and use “rotate.vmd” to create the scene.

Finally, launch the MD showcase builder, create the “mdshowcaseTutorial/ch3” folder in your workspace, upload the PDB file “1h_WI_dna.pdb”, the DCD file “rotate.dcd” and the VMD state file “rotate.vmd”, Figure 26. Then, you can create the scene using the VMD state file, save the showcase and share the showcase as we did in the [previous section](#).

3.2 Rock and roll

In this section, we will create an animated trajectory with a fancier “Rock and Roll” motion.

Please type the following command in a terminal:

```
vmd -dispdev text -args 1h_WI_dna.pdb rockandroll.dcd 180 < rockandroll.tcl
```

Except for the file name of PDB and DCD, the only argument is the number of frames you want. Then, you can follow the same process as in the [previous section](#) to make and share the showcase.

In case any problem occurs, we provided “rockandroll.dcd” and “rockandroll.vmd” in the “example_output” folder. You can use them to continue the tutorial.

3.3 Controlling the camera with a “view script”

The “View” tab in the MD showcase builder (Figure 1 and Figure 8) provides extensive functionality for designing how to play the trajectory. To test how it works, let’s create a “static” trajectory in which each frame is the same.

Please type the following command in a terminal:

```
vmd -dispdev text -args 1h_WI_dna.pdb replicate.dcd 180 < replicate.tcl
```

Except for the file name of the PDB and output DCD, the only argument is the number of frames you want. Then, follow the same process as in the [previous section](#) to make the showcase. After loading the VMD state file, let’s go to the “View” tab, Figure 27.

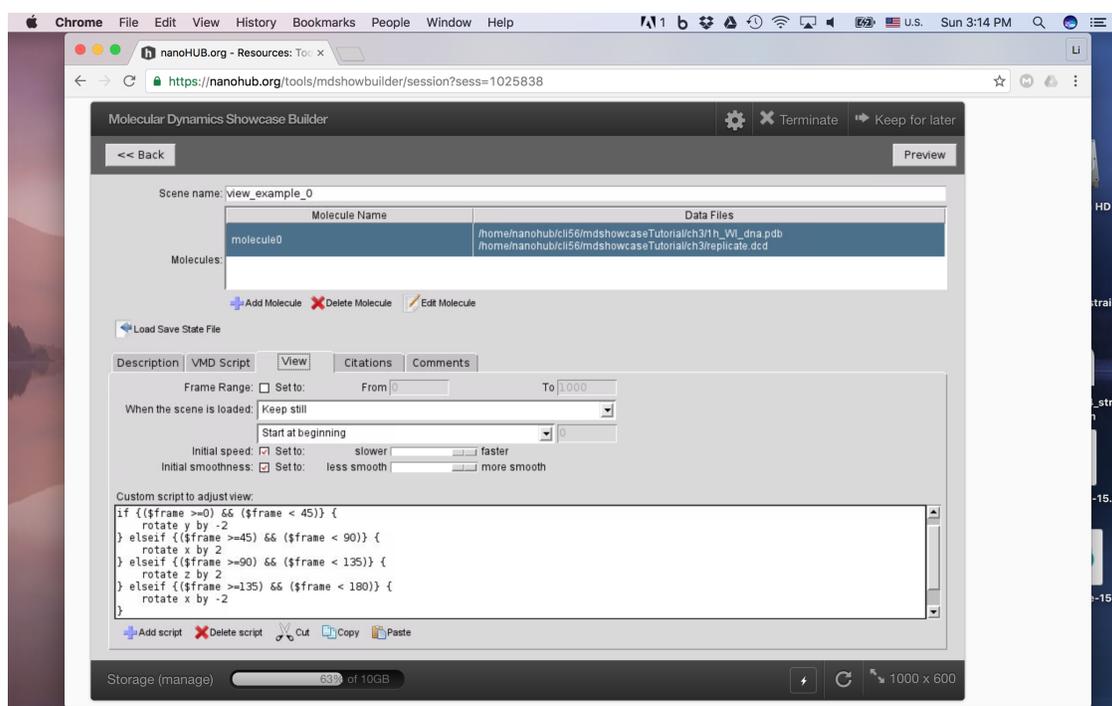


Figure 27: The “View” tab.

In the “View” tab, the “Frame Range” defines where those view functions below take effect. “When the scene is loaded” defines how you want it to play, including once, in a loop, forward, backward and back forth. You can also tune the default playing speed and smoothness. In the last part, you can adjust the view using a script. Let’s click “Add script” and upload the “view_example_0.tcl”.

The content of the script is the following:

```
if {($frame >=0) && ($frame < 45)} {  
    rotate y by -2  
} elseif {($frame >=45) && ($frame < 90)} {  
    rotate x by 2  
} elseif {($frame >=90) && ($frame < 135)} {  
    rotate z by 2  
} elseif {($frame >=135) && ($frame < 180)} {  
    rotate x by -2  
}
```

The script divides the trajectory into 4 parts. In each part, the view rotates along different axes. In the end, the script will rotate the view back to the original perspective.

Now you can follow the same process as in the [previous section](#) to save and share the showcase.

In case any problem occurs, we provided “replicate.dcd” and “replicate.vmd” in the “example_output” folder. You can use them to continue the tutorial.

3.4 Combine previous examples with a view script

In this section, we demonstrate how to combine the animated trajectory ([Rotation](#) and [Rock and roll](#) section) with a view script ([Design animation with a view script](#) section).

Please open the showcase you made in the [Rock and roll](#) section. Go to the “View” tab and add “view_example_1.tcl”. Click “Preview” and you should see the power of combining the two methods.

Then, you can follow the same process as in the [previous section](#) to save and share the showcase.

4 Create multiple scenes with MD simulation trajectories

Please navigate to the ch4 folder.

So far, we have only animated trajectories created by a script and a static PDB file. What if we have a simulation trajectory? The process is the same.

4.1 Create a showcase with a MD trajectory

First, let’s load “1h_WI.psf” and “1h_WI_npt.dcd” into VMD and visualize with the representation defined in “1h_npt.tcl”. Next, save the VMD state as “1h_npt.vmd”. Launch the MD showcase builder and create “mdshowcaseTutorial/ch3” folder in your workspace.

Then, upload “1h_WI.psf”, “1h_WI_npt.dcd” and “1h_npt.vmd” into the “ch4” folder and use “1h_npt.vmd” to create the scene, Figure 28.

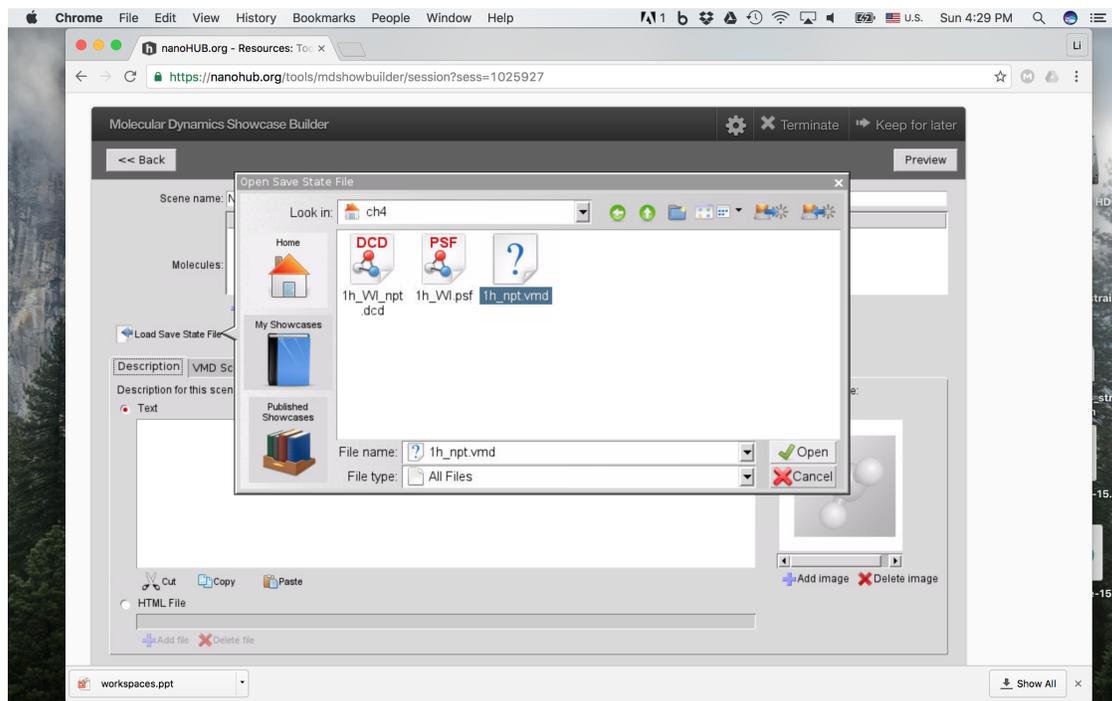


Figure 28: Use “1h_npt.vmd” to create the scene.

If the trajectory file size is too large (ex. > 1GB), it is recommended to use sftp (ex. “sftp username@nanoHUB.org”, read the [sftp tutorial](#) for details).

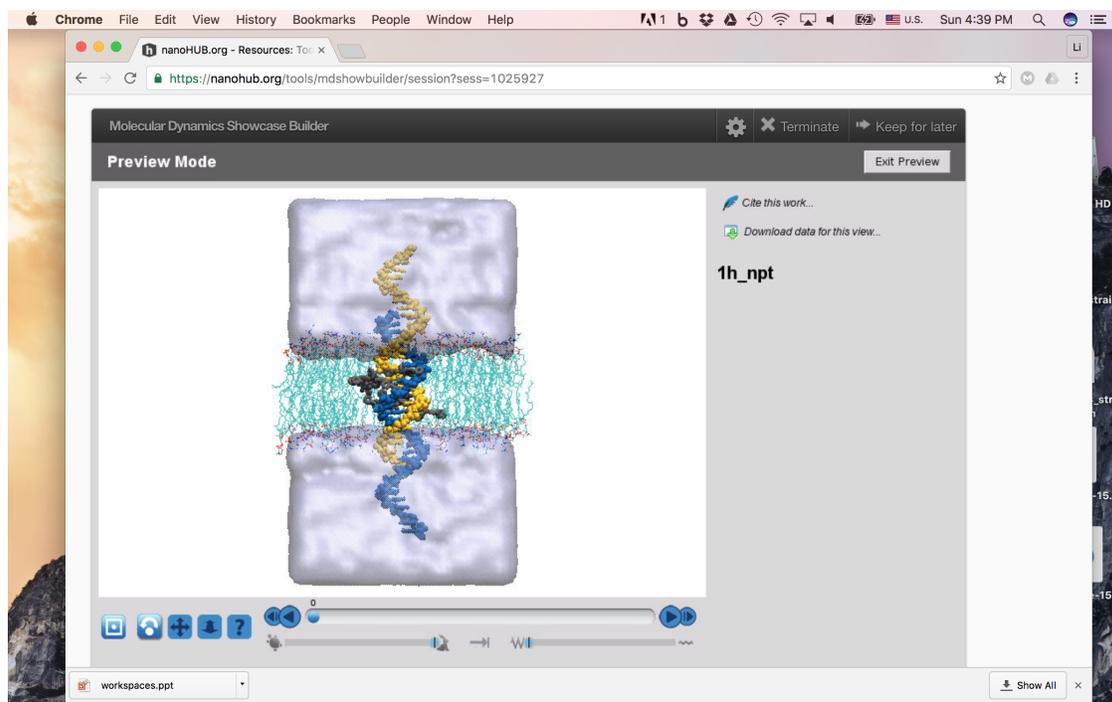


Figure 29: Preview of the showcase made with a simulation trajectory.

Then, if you set the playing speed to the maximum and smoothness to the minimum in the “View” tab and change the scene name to “1h_npt”, your showcase should look like Figure 29 when you click “Preview”.

Please save the showcase. We will continue to use it in the next section.

4.2 Add another scene with multiple molecules

As we illustrated in Figure 1, a showcase can contain more than one scene and a scene can contain more than one molecule and trajectory. In this section, we will demonstrate how to add another scene with multiple molecules. We will use a system containing a funnel-shaped DNA origami channel [2]. The channel is functionalized with 19 cholesterol groups and inserted into the lipid bilayer membrane. The entire system contains 8 million atoms. For systems of such size, it is common to split the simulation trajectory into different parts based on atom groups to reduce memory usage, for example, the trajectory of DNA channel “movie_dna_E100mV.xtc”, lipid membrane “movie_lip_E100mV.xtc” and potassium ions “movie_pot_E100mV.xtc”. The original PSF is also split into “funnel_WLcS_fm_c.aC.dna.psf”, “funnel_WLcS_fm_c.aC.lip.psf” and “funnel_WLcS_fm_c.aC.pot.psf”. Then, we can load what we need and skip what we do not need (ex. water) to minimize memory usage. The splitting of PSF and DCD is beyond the scope of this tutorial. Please refer to [psfgen User’s Guide](#) and [CatDCD manual](#) for more information.

You might also notice that we are not using the common DCD files created by NAMD, but XTC files. The XTC file is a more compressed trajectory format, commonly used in GROMACS. Since MD showcase is powered by VMD, all file formats recognized by VMD, such as GROMACS trajectory file format, can also be used in MD showcase. For the conversion of DCD file to XTC file format, please refer to [CatDCD manual](#) and [GROMACS trjconv utility](#).

Now, please launch VMD within the “ch4” folder. Then, load the PSF files and the trajectories and define the representations by typing the following command in the TkConsole:

```
source loadFunnel.tcl
source funnel_E100mV.tcl
```

Next, save the visualization state as “funnel_E100mV.vmd”.

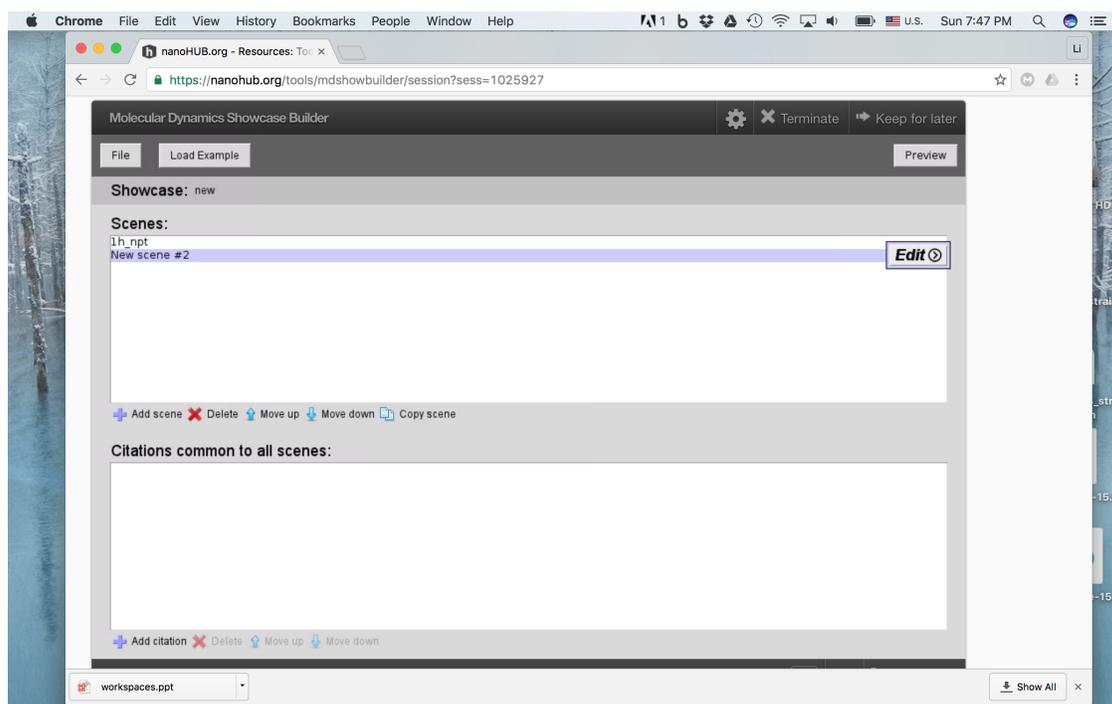


Figure 30: Add the second scene and click “Edit”.

Go back to MD showcase builder and open the showcase we made in the [previous section](#). Add the second scene and click “Edit”, Figure 30. Upload the VMD state file, all the PSF and XTC files. Then, create the scene by “funnel_E100mV.vmd”.

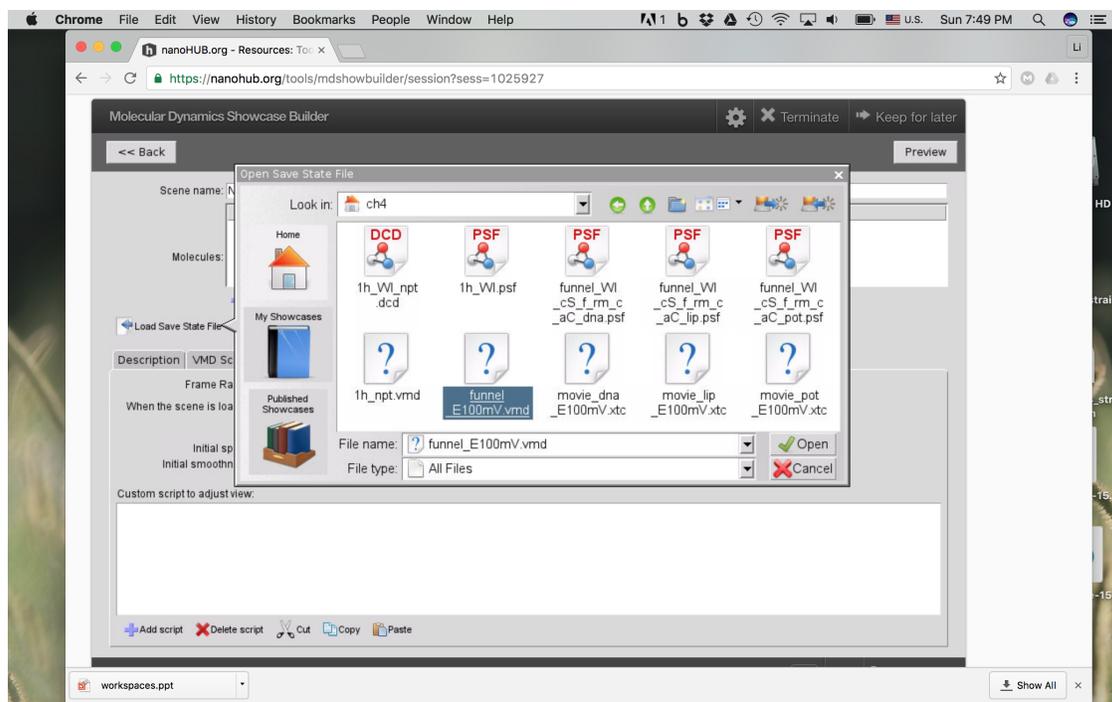


Figure 31: Create the scene by “funnel.E100mV.vmd”.

Change the name of the scene to “funnel_E100mV” and click “Preview”. The result should look like Figure 32.

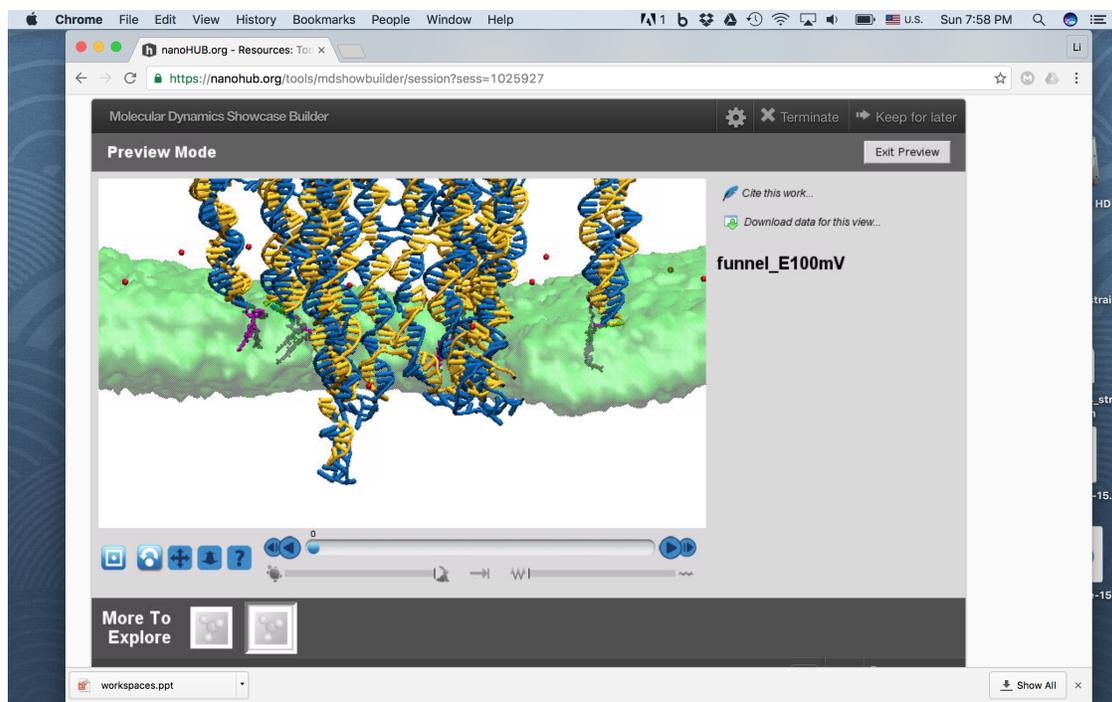


Figure 32: Preview the second scene.

Now, you would see that there are two thumbnails at the bottom. If you click the first one, it will show the first scene we made in the [previous section](#).

Please keep the session or save the showcase We will continue to build on this showcase in the next section.

5 Enrich the showcase

Please navigate to the ch5 folder.

Now, we have a nice showcase with two scenes. In this section, we will demonstrate how to enrich the content of the showcase.

5.1 Add snapshots for each scene

Although we have two scenes in a showcase and thumbnails switching between them (Figure 32), it is hard to know which one is which without a proper image. So, let's add images for each scene as snapshots. Although we will use the example images in the “ch5” folder to proceed, you can take snapshots of your system in VMD as well.

First, let's create “mdshowcaseTutorial/ch5” folder in your workspace. Next, click “Edit” the first scene and go to the “Description” tab.

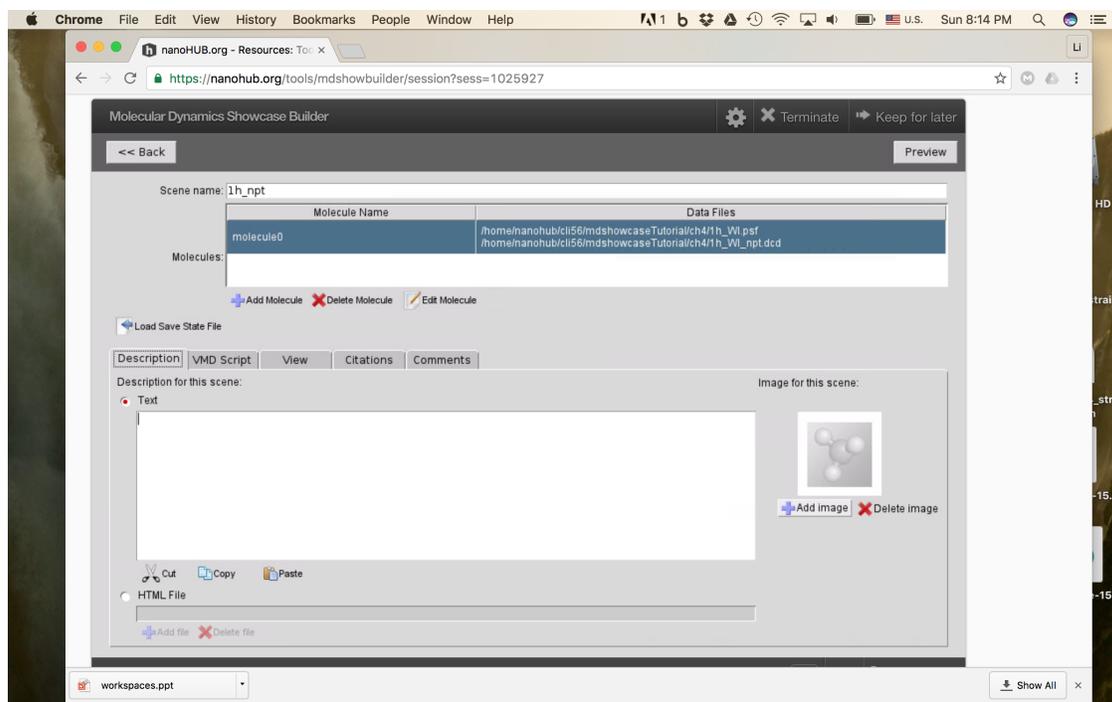


Figure 33: Click “Add image” to add snapshot.

Click “Add image” to add snapshot (Figure 33). Upload the two images “1h_npt_snapshot.tga” and “funnel_E100mV_snapshot.tga” and use the “1h_npt_snapshot.tga” for the first scene (Figure 34).

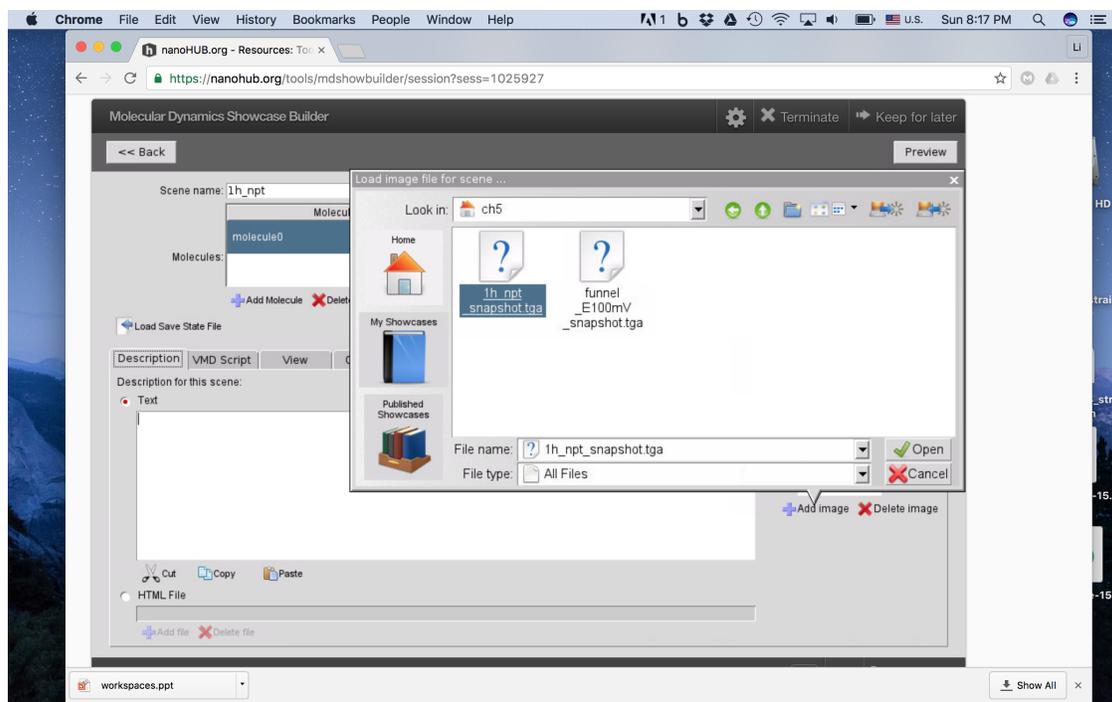


Figure 34: Use “1h_npt_snapshot.tga” for the first scene.

And, use “funnel_E100mV_snapshot.tga” for the second scene (Figure 35).

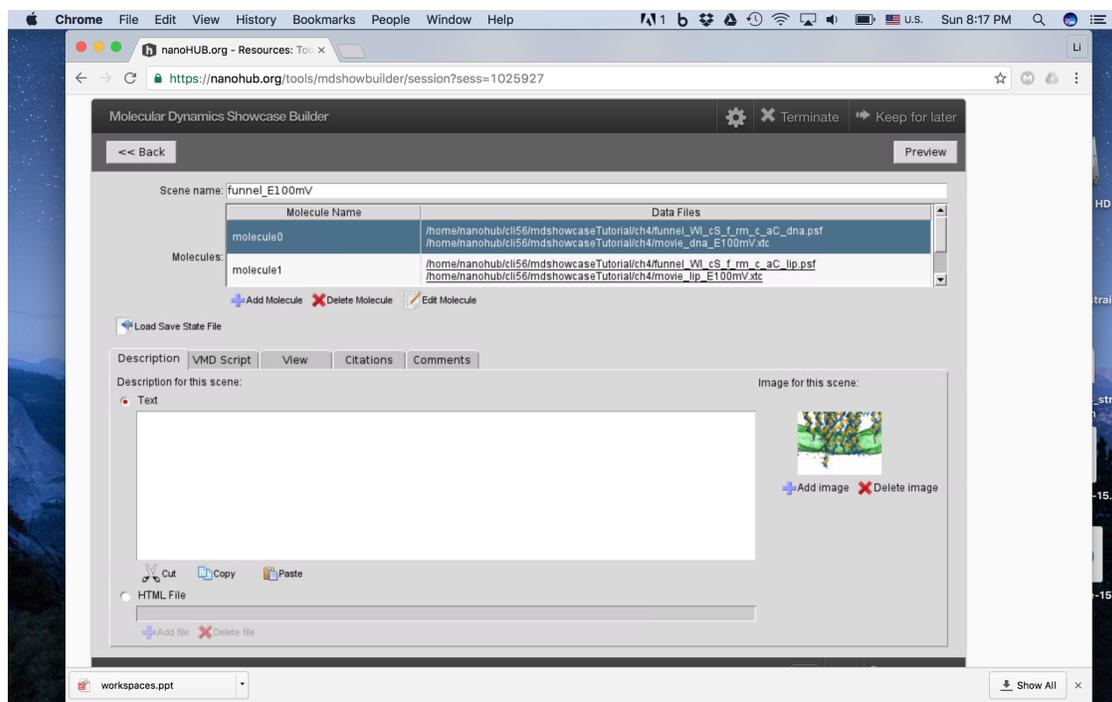


Figure 35: Use “funnel_E100mV_snapshot.tga” for the second scene.

Now, if you click “Preview”, you should see that the snapshot images have been used for thumbnails (Figure 36).

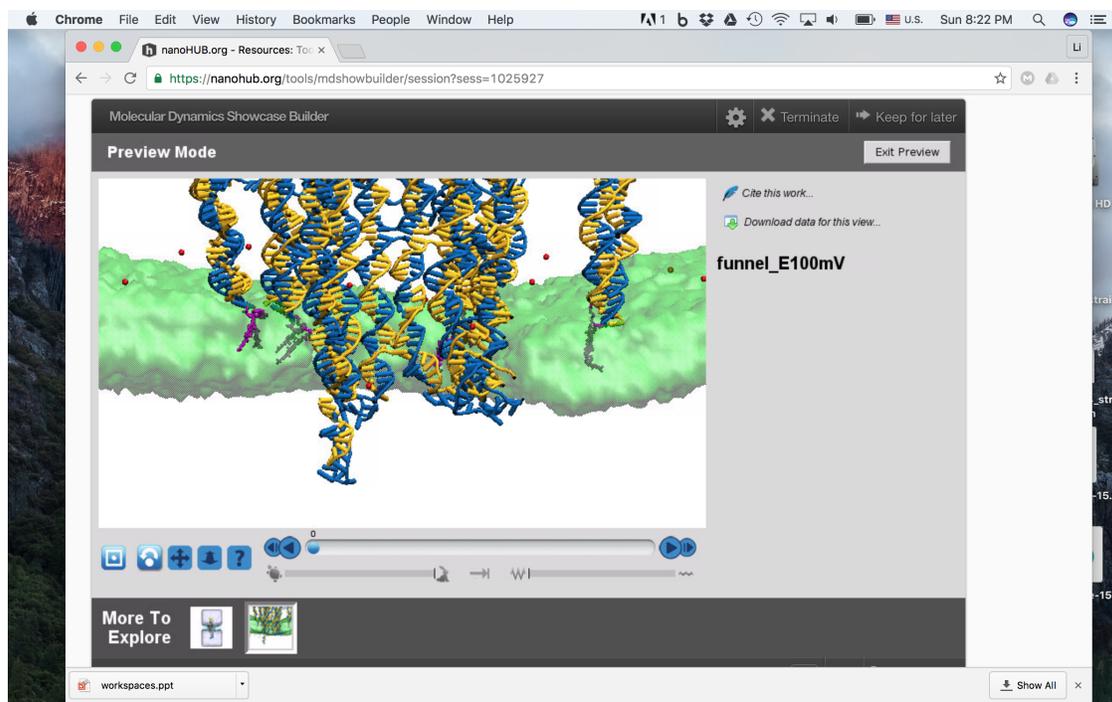


Figure 36: Snapshot images are used for thumbnails.

5.2 Add description

Now, we have the snapshots as thumbnails and names for each scene. But, it would be better if there are some descriptions about what each scene shows. Let's exit preview, click "Edit" on the first scene and go to the "Description" tab. MD showcase builder supports two ways of adding description: plain text or HTML. Adding plain text is easy: just type the text in the block.

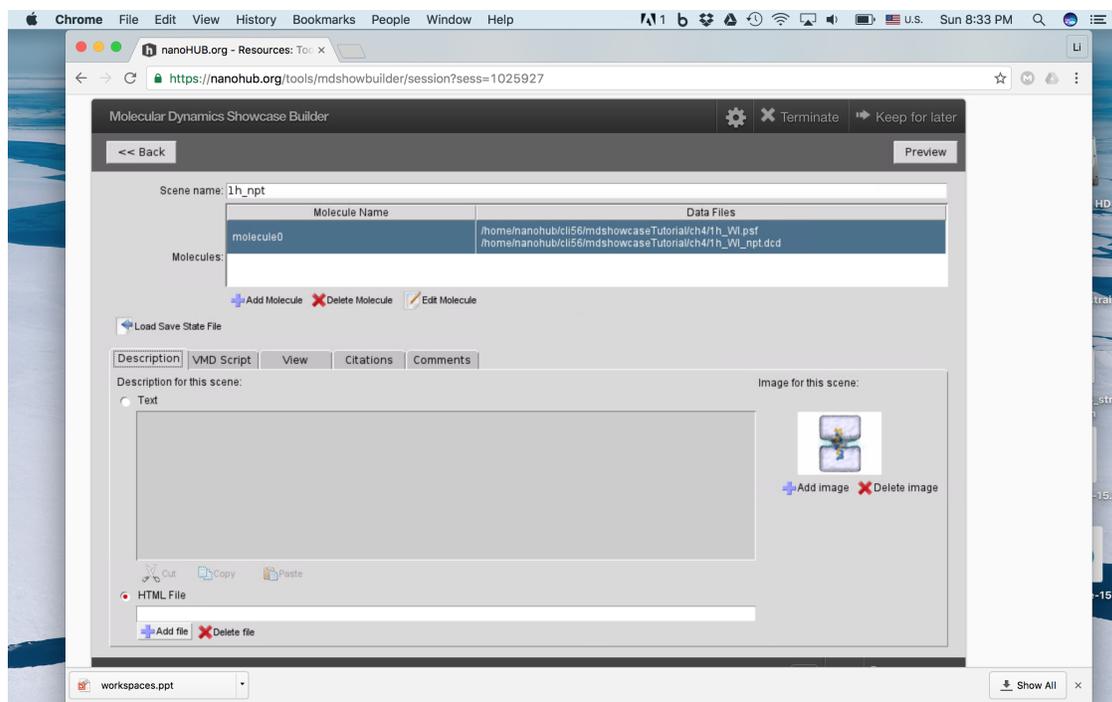


Figure 37: Click “HTML File” and “Add file”.

Here, we will show how to add HTML description. Using HTML description, you can easily change text font, color or adding a hyperlink. We provided two example HTML file “1h_npt_description.html” and “funnel_E100mV_description.html”. Please refer to [HTML tutorial](#) for basic usage of the HTML language.

Click “HTML File” and “Add file” in the “Description” tab (Figure 37). Go to “mdshowcaseTutorial/ch5” and upload “1h_npt_description.html” and “funnel_E100mV_description.html”.

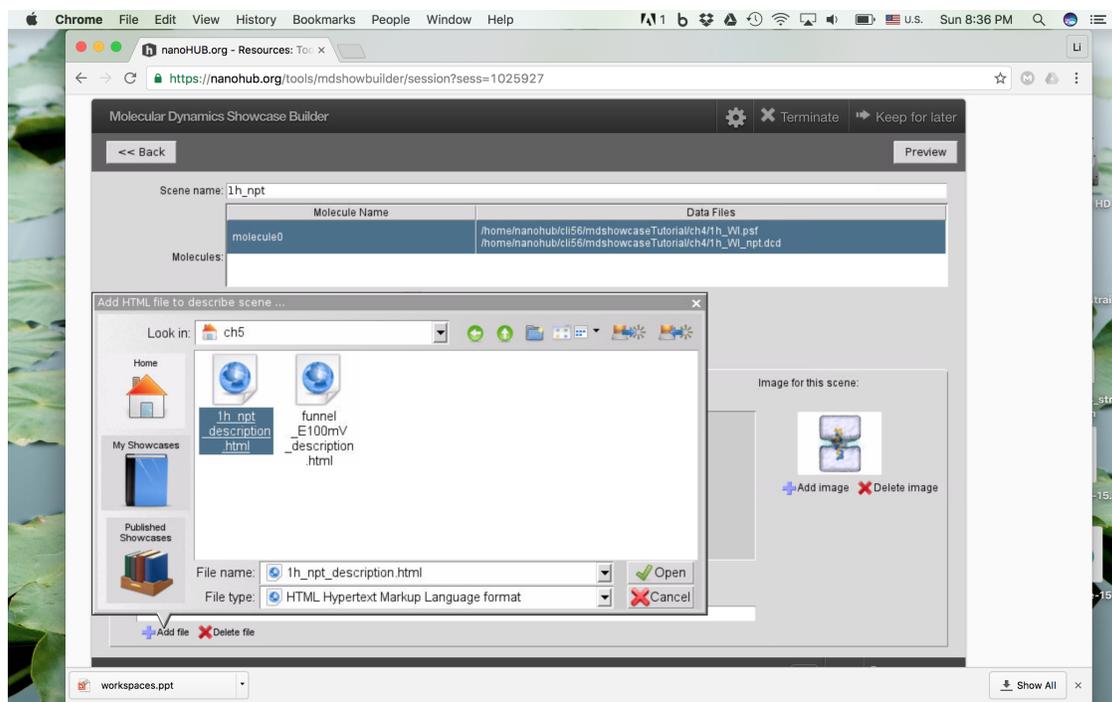


Figure 38: Use “1h_npt_description.html” for the first scene.

Use “1h_npt_description.html” for the first scene and “funnel_E100mV_description.html” for the second scene (Figure 38).

The result should look like Figure 39 and Figure 40.

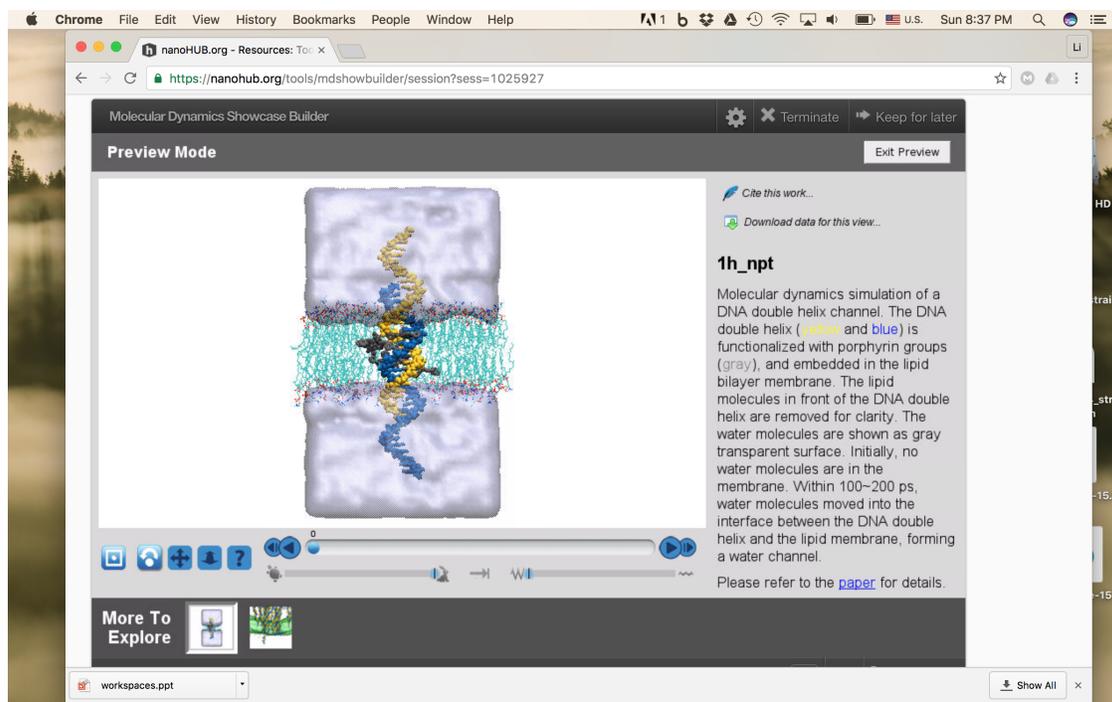


Figure 39: The first scene with description.

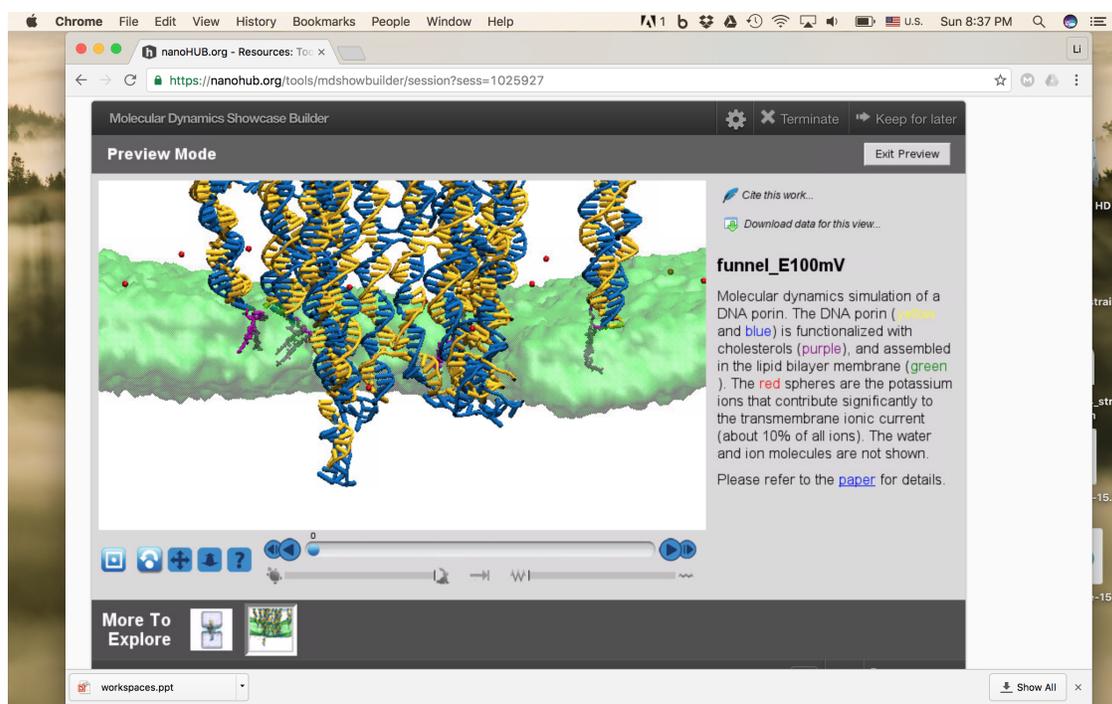


Figure 40: The second scene with description.

5.3 Add frame-related comment

Sometimes, we want to highlight certain part of a trajectory, for example, the conformation change of a protein. And, we may also want to add some specific comment to further explain what happened during that period. Here, we will demonstrate the usage of adding frame-related comments using the first scene as an example.

In the first scene, the presence of a DNA duplex in the lipid bilayer membrane caused water molecules to move into the lipid membrane, covering the DNA duplex and forming a water channel. However, the transparent water channel is not very visible in the presence of the DNA duplex. So, let's hide the DNA from frame 50 ~ 100. We can achieve that by using a view script. Let's exit preview, click "Edit" on the first scene and go to the "View" tab.

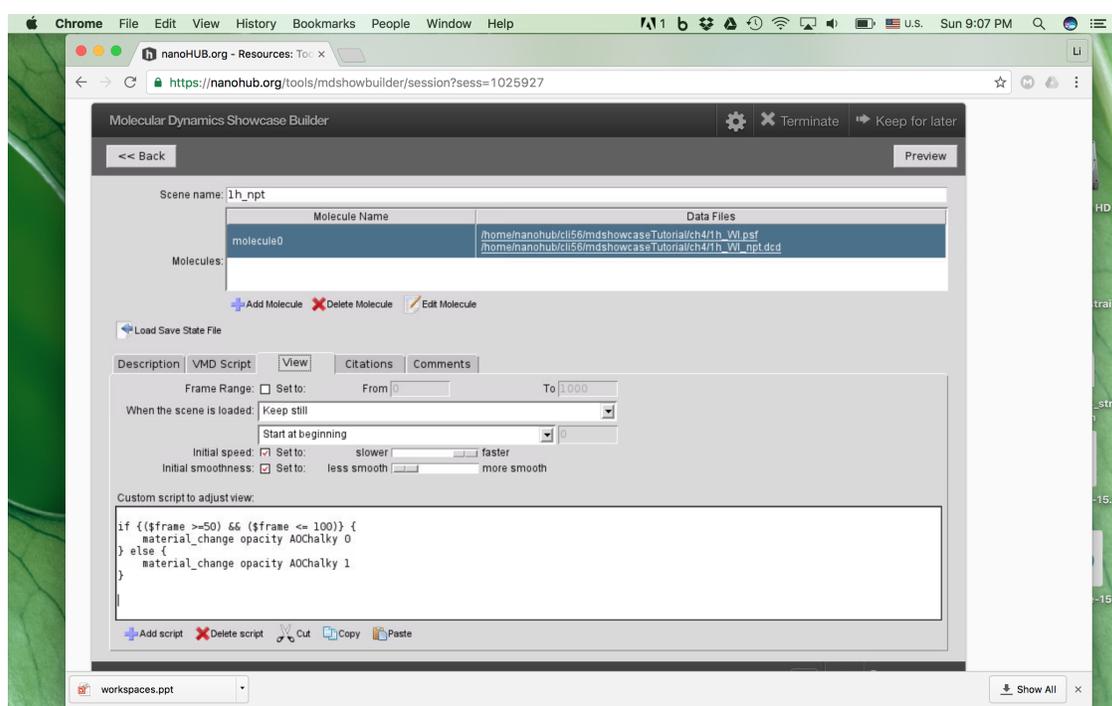


Figure 41: Add "1h_npt_view.tcl" as the view script.

Add "1h_npt_view.tcl" as the view script (Figure 41). In the script, we hide the DNA by changing the material opacity used for DNA to 0 in frame 50 ~ 100.

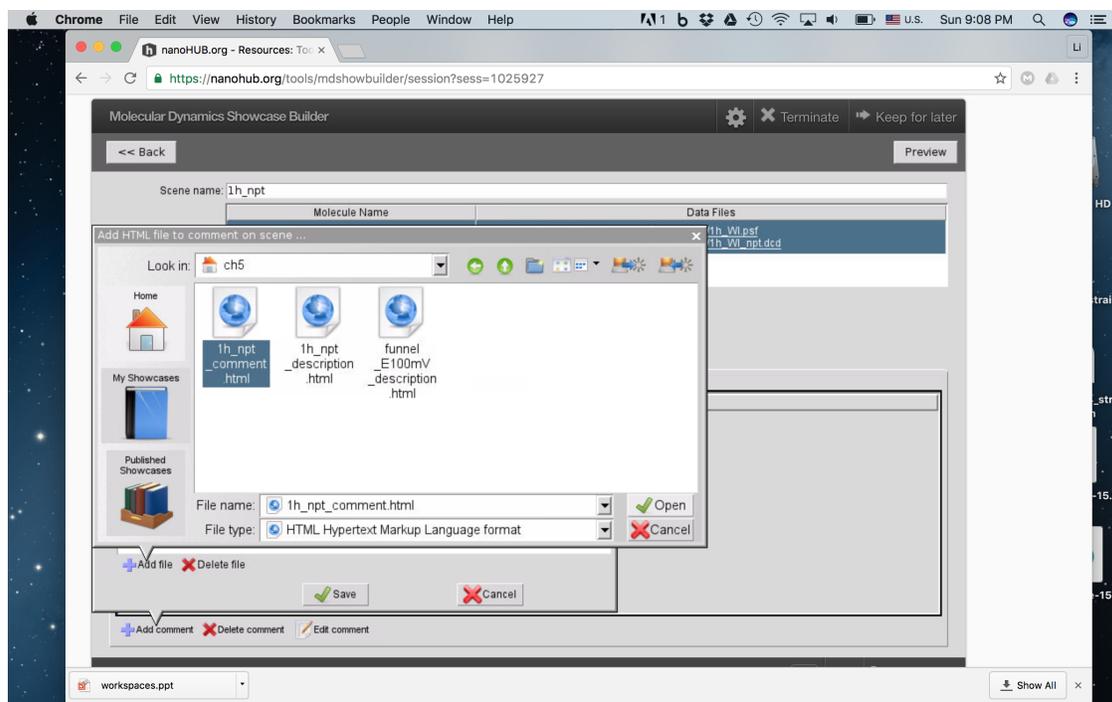


Figure 42: Add “1h_npt_comment.html” as the frame-related comment.

Then, go to the “Comment” tab. Add a comment in frame 50 ~ 100 and add “1h_npt_comment.html” as the content of the comment (Figure 42).

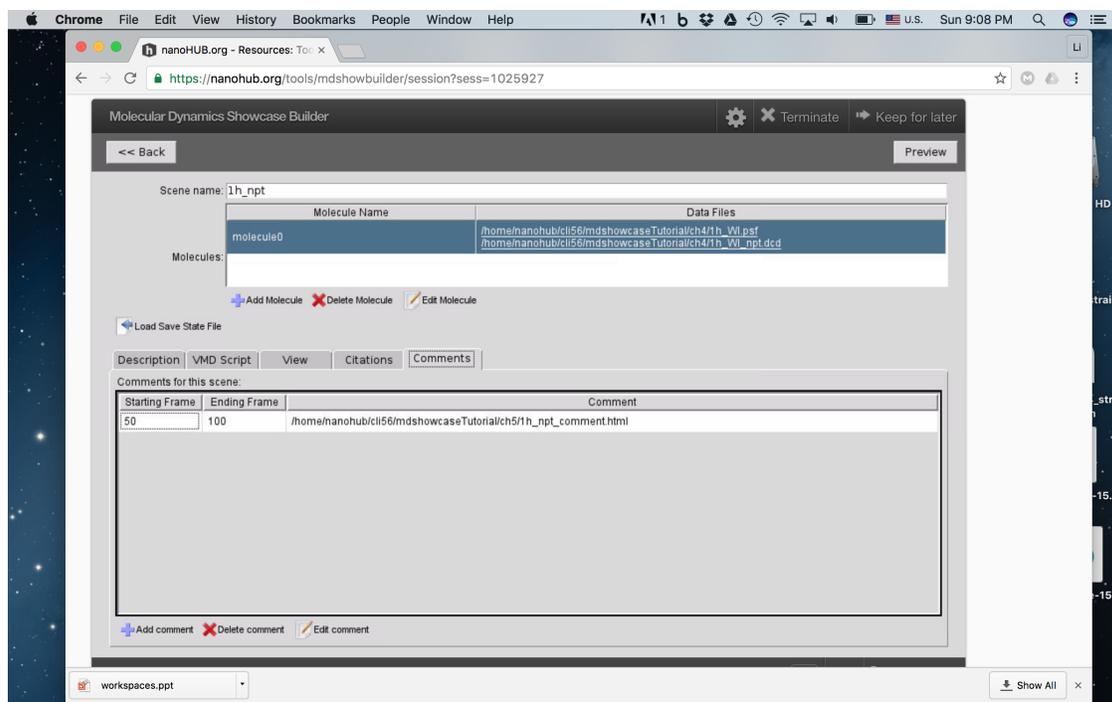


Figure 43: The comment will show up in frame 50 ~ 100.

The “Comment” tab should look like Figure 43. You can add multiple comments with different frame ranges. If the ranges of the comments overlap, the latter one will replace the former one.

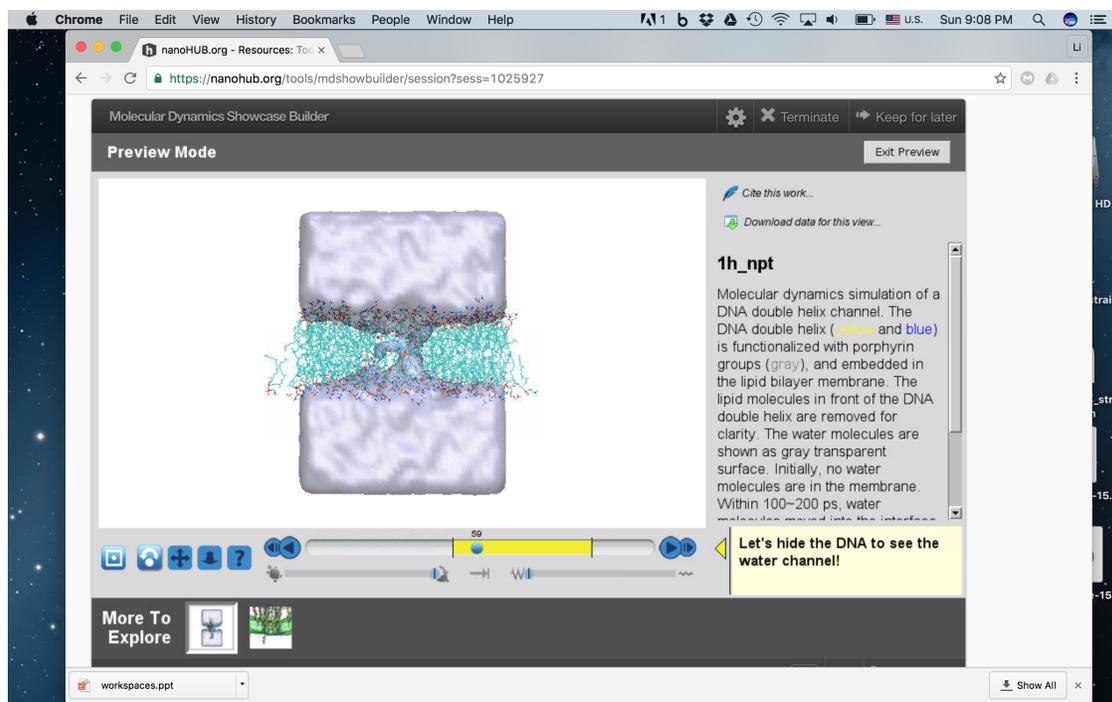


Figure 44: The DNA disappeared and the comment appeared.

If we click “Preview”, it should look like Figure 44. There is a yellow region in the slide bar, showing that comment will appear during this period. As we play into this period (the slide bar move into the yellow region), the DNA disappears and the comment appears.

5.4 Add citation

In the last section, we will show how to add citations. You can add citations in the main window (Figure 6) for the entire showcase, or add citations for each scene. Here, we will show how to add citation for the first scene. The process is the same for adding citations of the entire showcase.

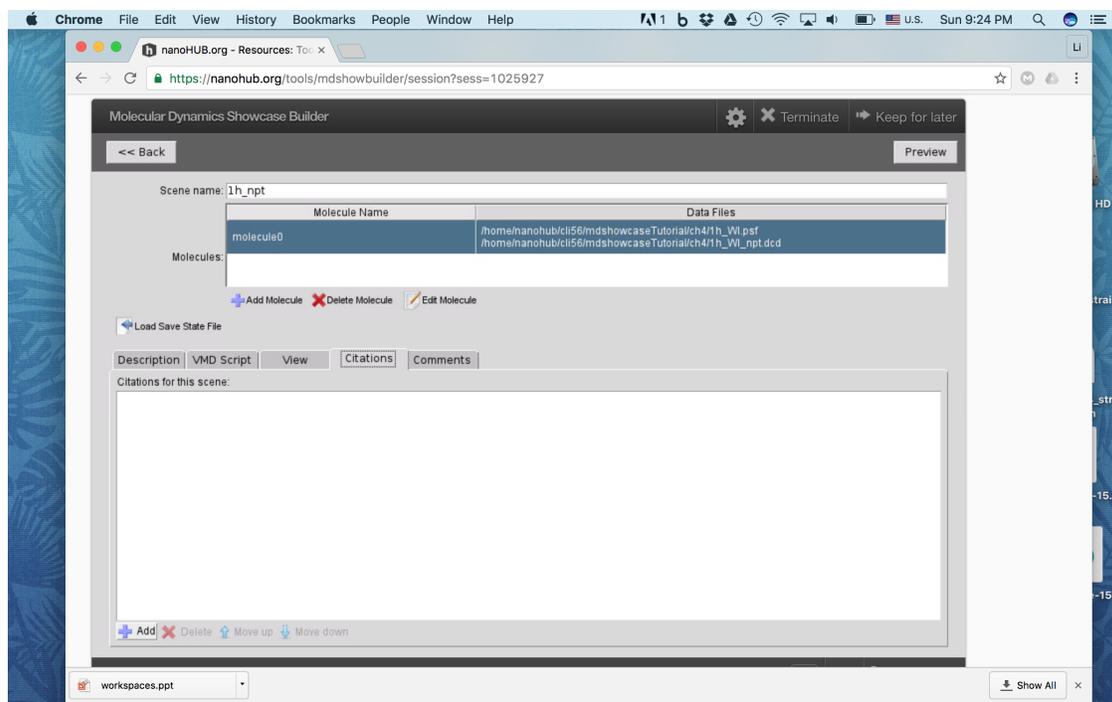


Figure 45: Go to “Citation” tab and click “Add”.

First, let’s go to the “Citation” tab and click “Add” (Figure 45).

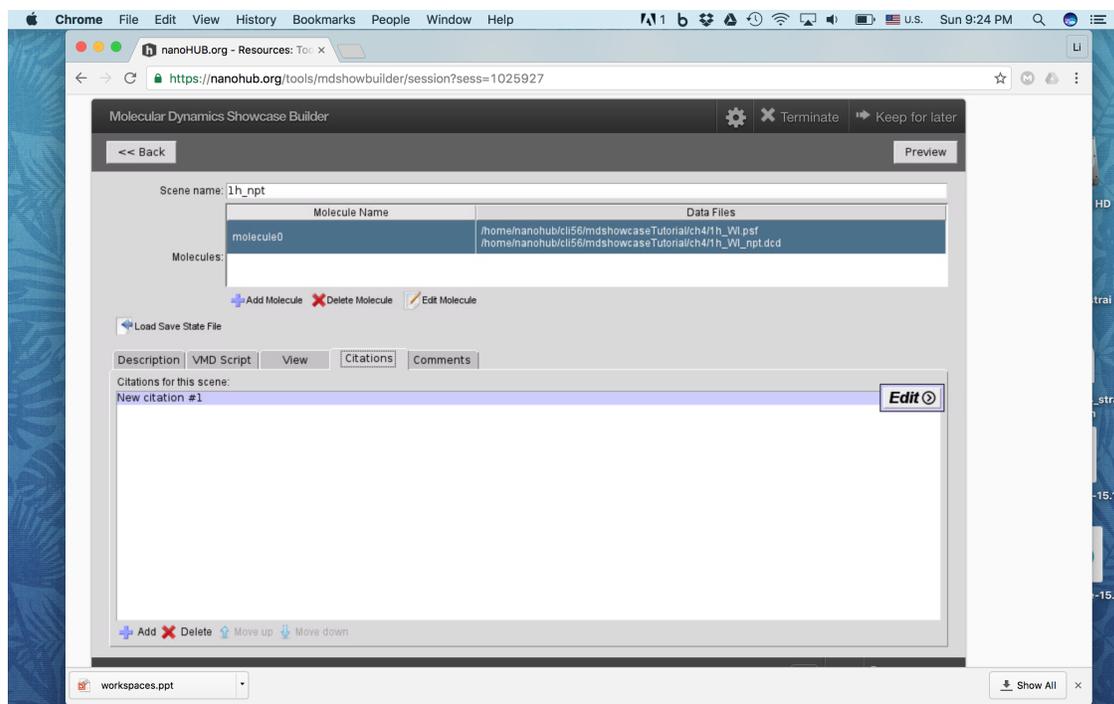


Figure 46: Click “Edit”.

Next, click “Edit” (Figure 46).

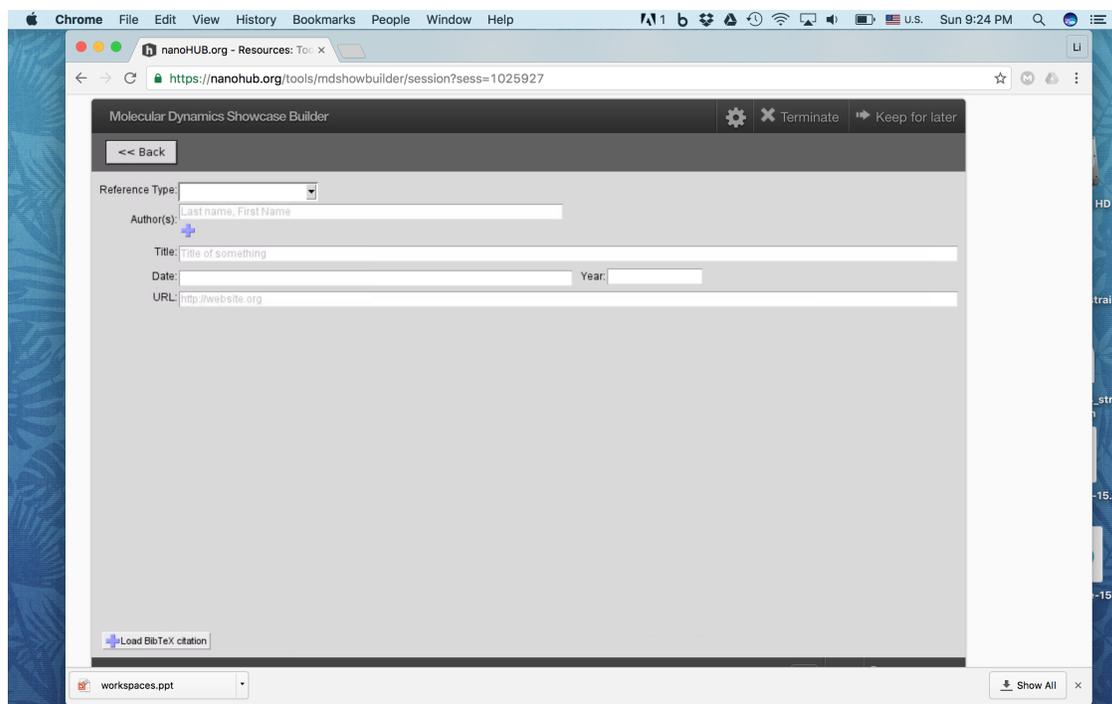


Figure 47: Click “Load BibTeX citation”.

Click “Load BibTeX citation” on the bottom left (Figure 47).

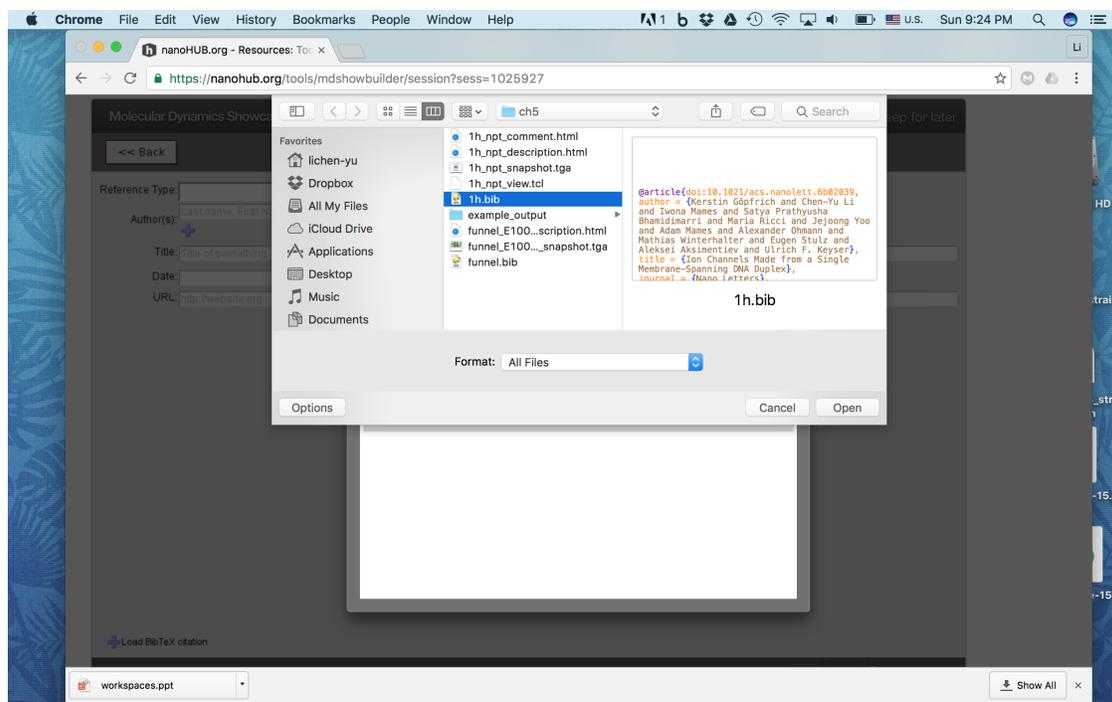


Figure 48: Select “1h.bib” on the desktop.

Select “1h.bib” on the desktop (Figure 48).

The screenshot shows a web browser window with the URL <https://nanohub.org/tools/mdshowbuilder/session?sess=1025927>. The page title is "Molecular Dynamics Showcase Builder". The interface includes a "Back" button, a "Reference Type" dropdown menu set to "Journal Article", and a list of authors: Kerstin Göpflich, Chen-Yu Li, Iwona Mames, Satya Prathyusha Bhamidimarri, Maria Ricci, Jejoong Yoo, Adam Mames, Alexander Ohmann, Mathias Winterhalter, Eugen Stulz, Aleksei Aksimentiev, and Ulrich F. Keyser. Each author name has a red "x" icon to its right. Below the authors is a "Title" field containing "Ion Channels Made from a Single Membrane-Spanning DNA Duplex". The "Journal Name" is "Nano Letters". The "Pages" field contains "4665-4669", "Volume" is "16", "Number" is "7", and "Year" is "2016". The "Keywords" field contains "keyword, keyword, ...". The "DOI" field contains "10.1021/acs.nanolett.6b02039". At the bottom left, there is a "Load BibTeX citation" button. The browser's address bar and menu bar are visible at the top.

Figure 49: Each column will be filled with data in the “1h.bib”.

The MD showcase builder will extract information in the “1h.bib” and fill each column (Figure 49).

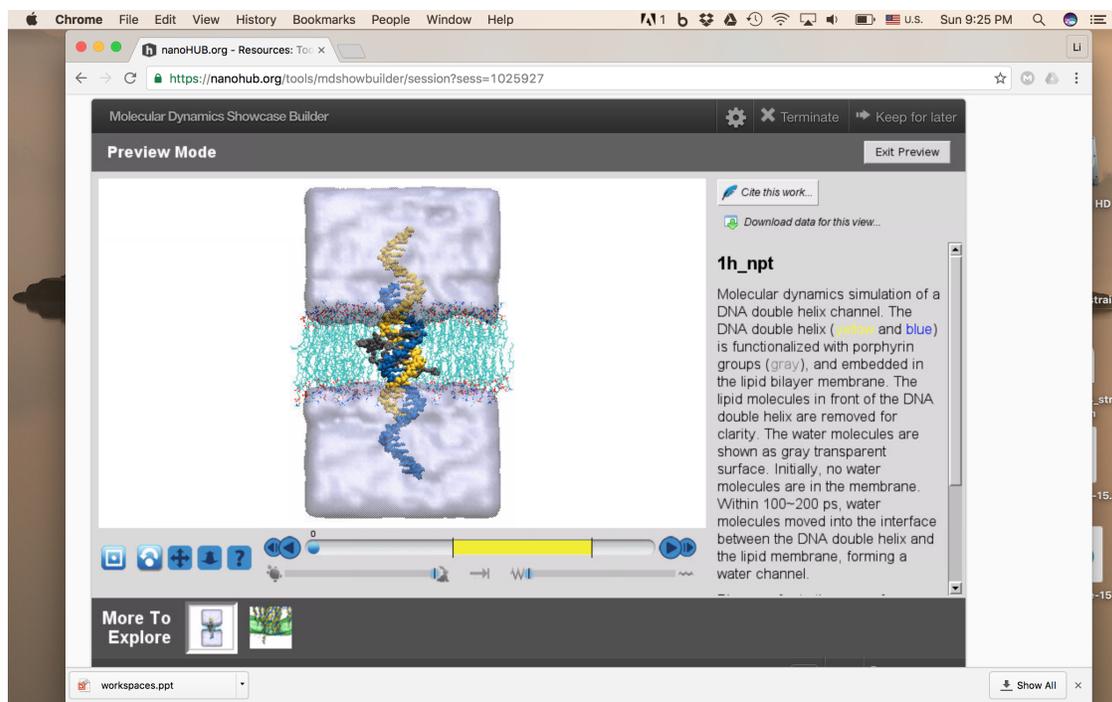


Figure 50: Click “Preview” and “Cite this work”.

Finally, let’s click “Preview” and “Cite this work” to see if it works (Figure 50).

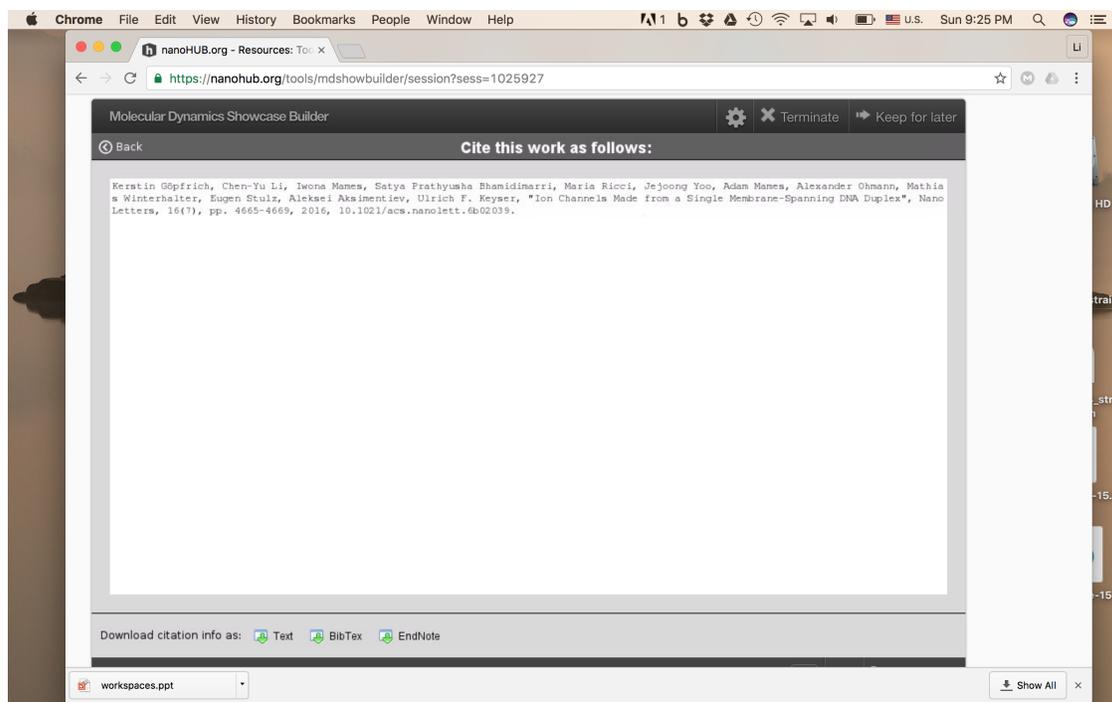


Figure 51: The citation will appear and can be downloaded in different formats.

The citation will appear and can be downloaded in different formats (Figure 51).

Then, you can also add citation for the second scene using “funnel.bib”. Since the process is the same, we will not repeat it again.

Congratulation!! You have completed the entire MD showcase tutorial. It’s time for you to try it using your own molecule or trajectories.

References

- [1] Kerstin Göpfrich, Chen-Yu Li, Iwona Mames, Satya Prathyusha Bhamidimarri, Maria Ricci, Jejoong Yoo, Adam Mames, Alexander Ohmann, Mathias Winterhalter, Eugen Stulz, Aleksei Aksimentiev, and Ulrich F Keyser. Ion channels made from a single membrane-spanning DNA duplex. *Nano Lett.*, 16(7):4665–4669, 2016.
- [2] Kerstin Göpfrich*, Chen-Yu Li*, Maria Ricci, Satya Prathyusha Bhamidimarri, Jejoong Yoo, Bertalan Gyenes, Alexander Ohmann, Mathias Winterhalter, Aleksei Aksimentiev, and Ulrich F Keyser. Large-conductance transmembrane porin made from DNA origami. *ACS Nano*, 10(9):8207–8214, 2016.