

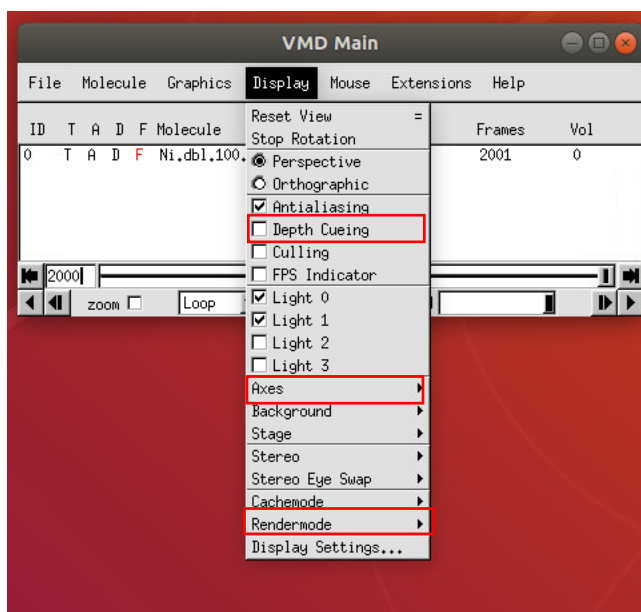
Tutorial for trajectory visualization using VMD

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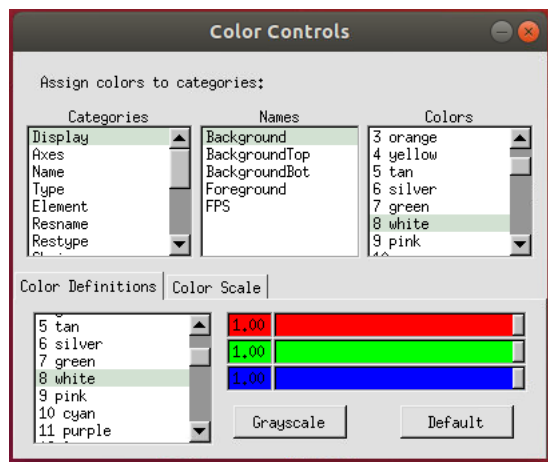
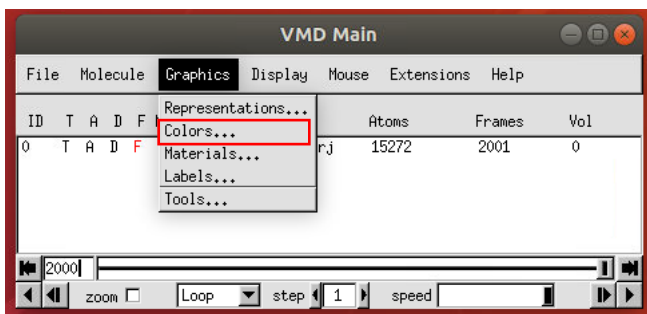
Example: Nano Lett. 2019, 19, 8638–8643, Figure 1a

A. Set up VMD settings and background color

1. After loading the LAMMPS trajectories into VMD, we need to change three options under **Display** tab: **Depth Cueing** has to be turned off; **Axes** to be turned off; **Rendermode** to be turned to GLSL for better quality (As shown below).

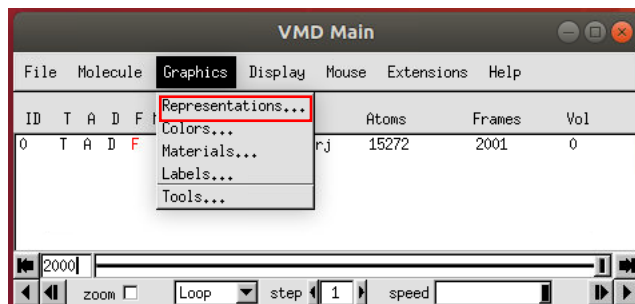


2. Next, we have to set the background color to white. Under the **Graphics** tab, select **Colors...** (Shown as left figure below). Then in Color Controls, select **Category:** Display -> **Names:** Background -> **Colors:** White.



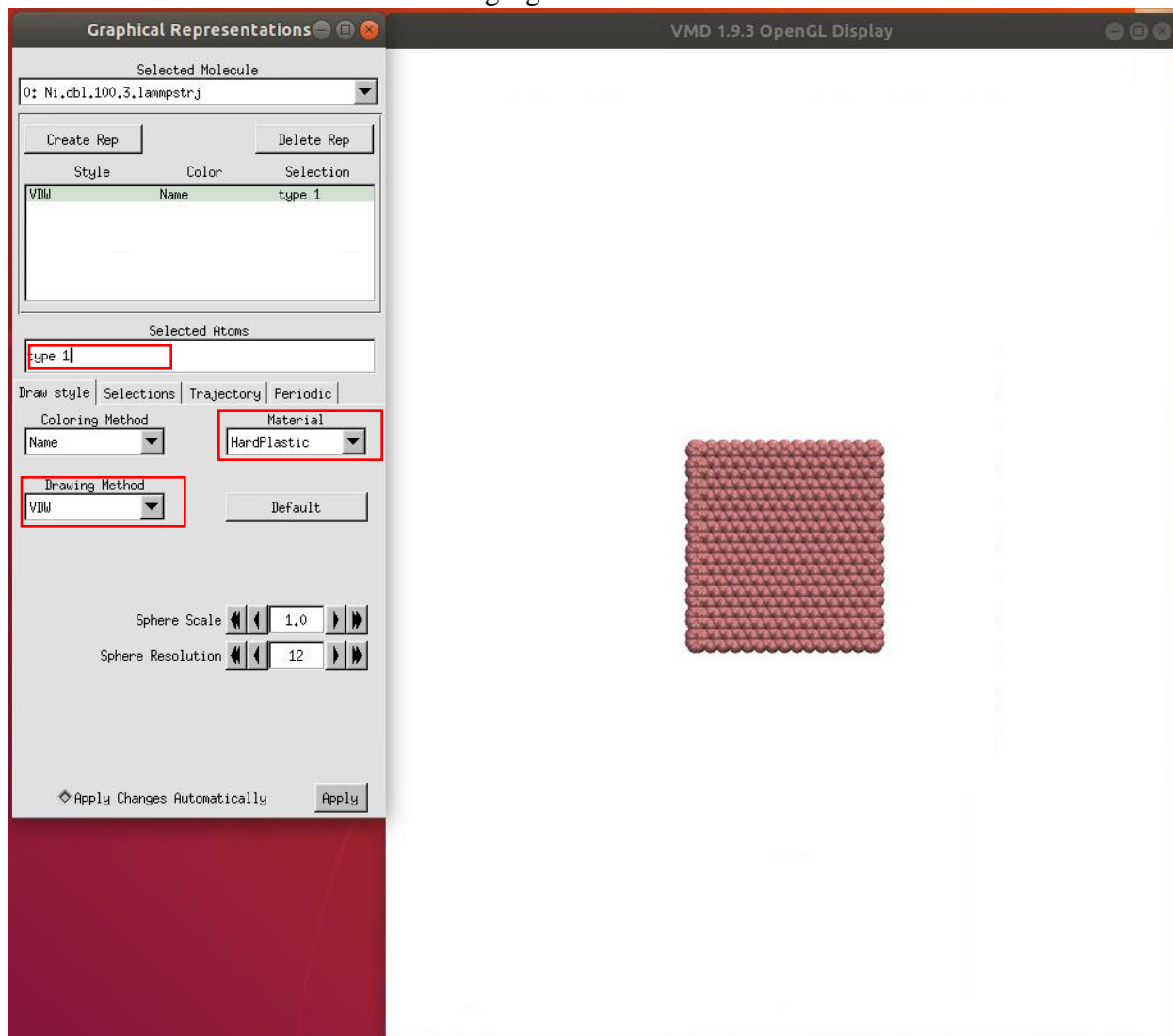
B. Set up representations for each atom type

In our Figure 1a, we have shown four groups of atoms including: 1. Graphene piston 2. MOF 3. Water and 4. Ions. Each of them will have different representations. We will modify representations of each atom in **Graphics** tab -> **Representations...** (Shown below)



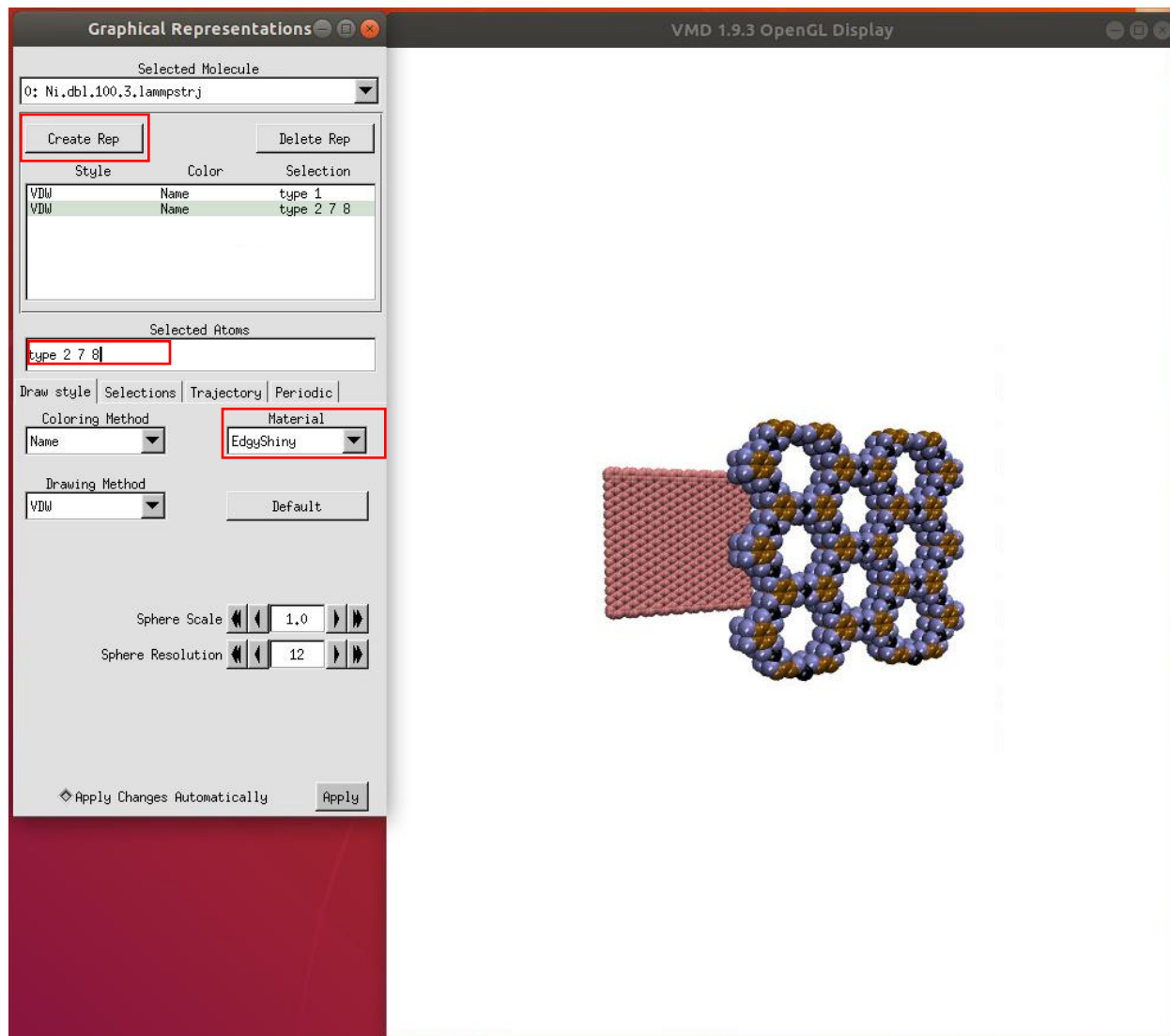
1. Graphene piston:

In our simulation, carbon atoms in graphene piston is type 1. So we change the **Selected Atoms** of this representation to be type 1. Then we change the **Drawing Method** to VDW, **Material** to be HardPlastic, and you can choose whatever **Coloring Method** you like. The result will be as following figure:



2. MOF membrane:

Next step is to visualize MOF membrane. We create a new representation by **Create Rep** button. Notice the new representation will have exactly same setup as the previous one. Click the new representation to make sure it is highlighted. Atoms in our MOF membrane is type 2, 7 and 8, therefore we select type 2 7 8. Then we change the **Material** to EdgyShiny for aesthetic purpose. Result is shown below:



3. Water:

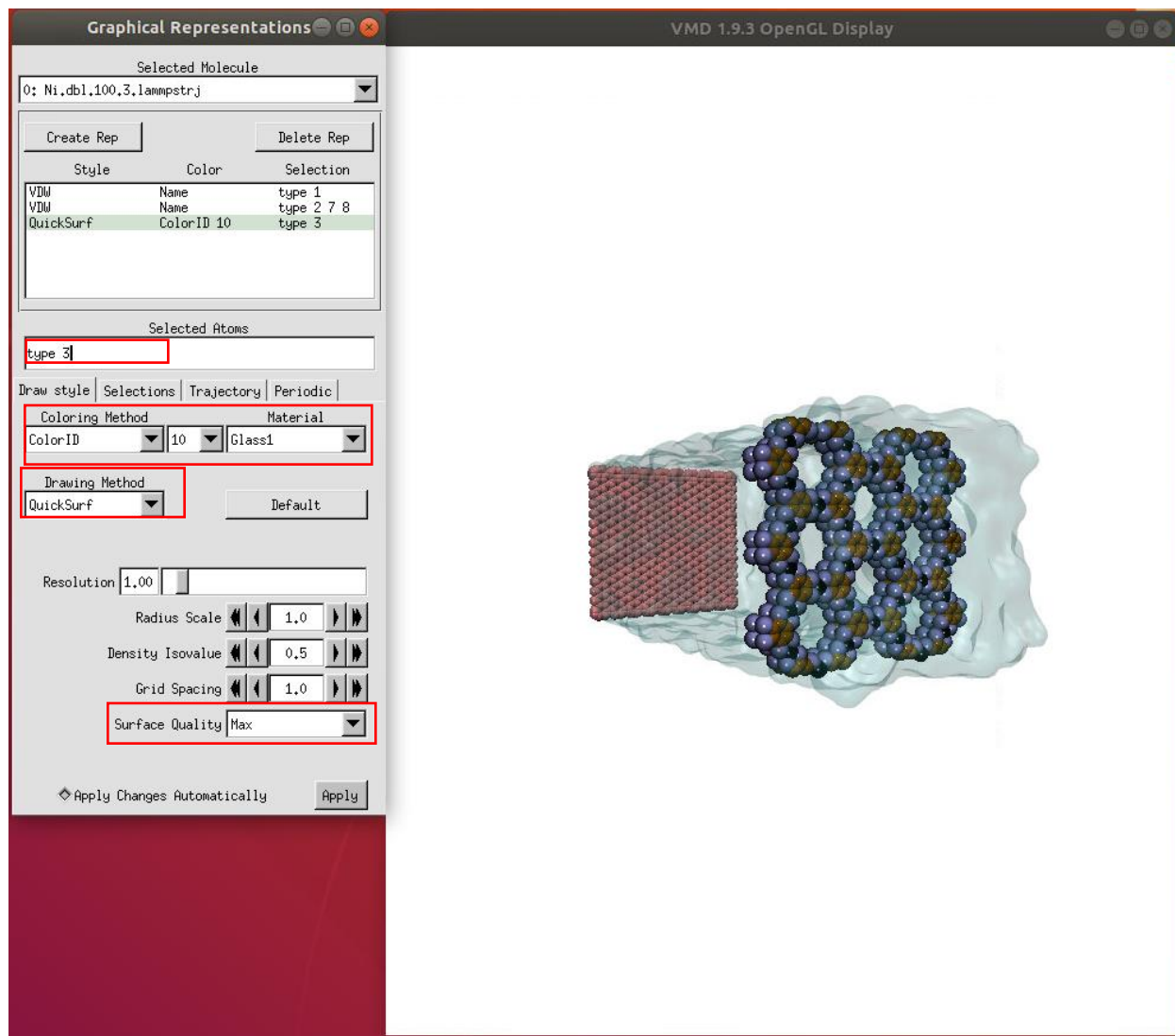
The third group is water. Water molecule contains oxygen and hydrogen atoms.

However, when visualizing water as fluid, we can simply use oxygen to represent water.

Since oxygen is type 3 in our simulation, we create a new representation of atom type 3.

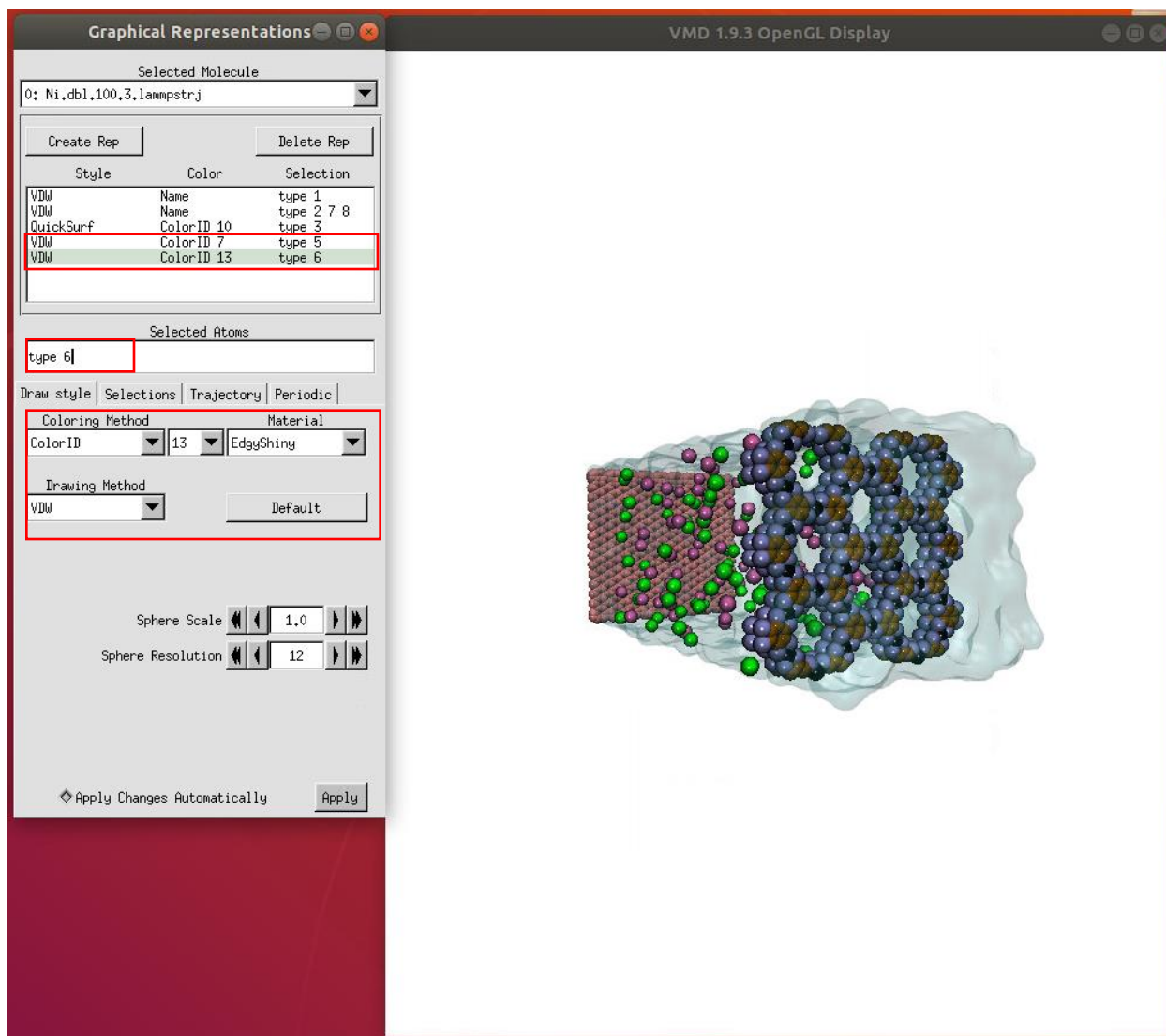
Then we change the **Coloring Method** to Color ID 10 (cyan), **Drawing Method** to

QuickSurf and **Material** to Glass1. Then we modify the **Surface Quality** to Max. Result is shown below:



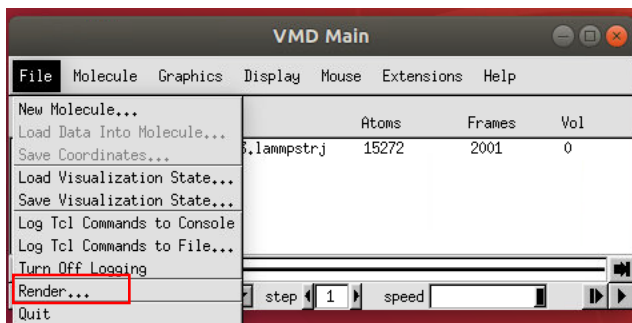
4. Ions:

Ions include Cations and Anions, and in our case they are atom type 5 and 6. To show them in different colors, we create two different representations for atom type 5 and 6. We use EdgyShiny for **Material** and VDW for **Drawing Method**. You can choose whatever color you like to accommodate your aesthetic taste. The result is shown below:

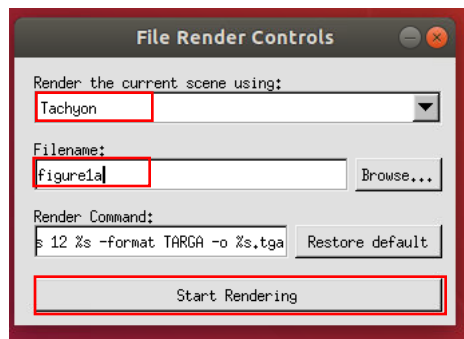


C. Render visualization to a picture

After we set up the representations, we can render a high resolution picture using VMD. In VMD Main window, select **render...** under **File** tab (as below).



Then in the render control window, change the rendering method to **Tachyon**, and change **Filename** to whatever you want (figure1a in our case). Then click on **Start Rendering Button** (as below).



A rendered picture will be in your working directory. Notice that the picture will be in .tga form. You may need to convert that to .jpg or .png format before using it through online tools.