Removing the excess dangling atoms around metal coated Carbon Nanotube

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Executable program files to create hollow cylindrical Carbon Nanotube (CNT) structures are available. But, as the lattice parameter of Nickel (Ni) and its crystal structure (BCC) are different from CNT, those files are futile in order to create a Ni layer over CNT. Hence, a suitable hollow cylindrical tube is trimmed from cubical structure of Ni and it is then added to the CNT using LAMMPS, a Molecular Dynamics (MD) Simulation code, as shown in Figure *1*.

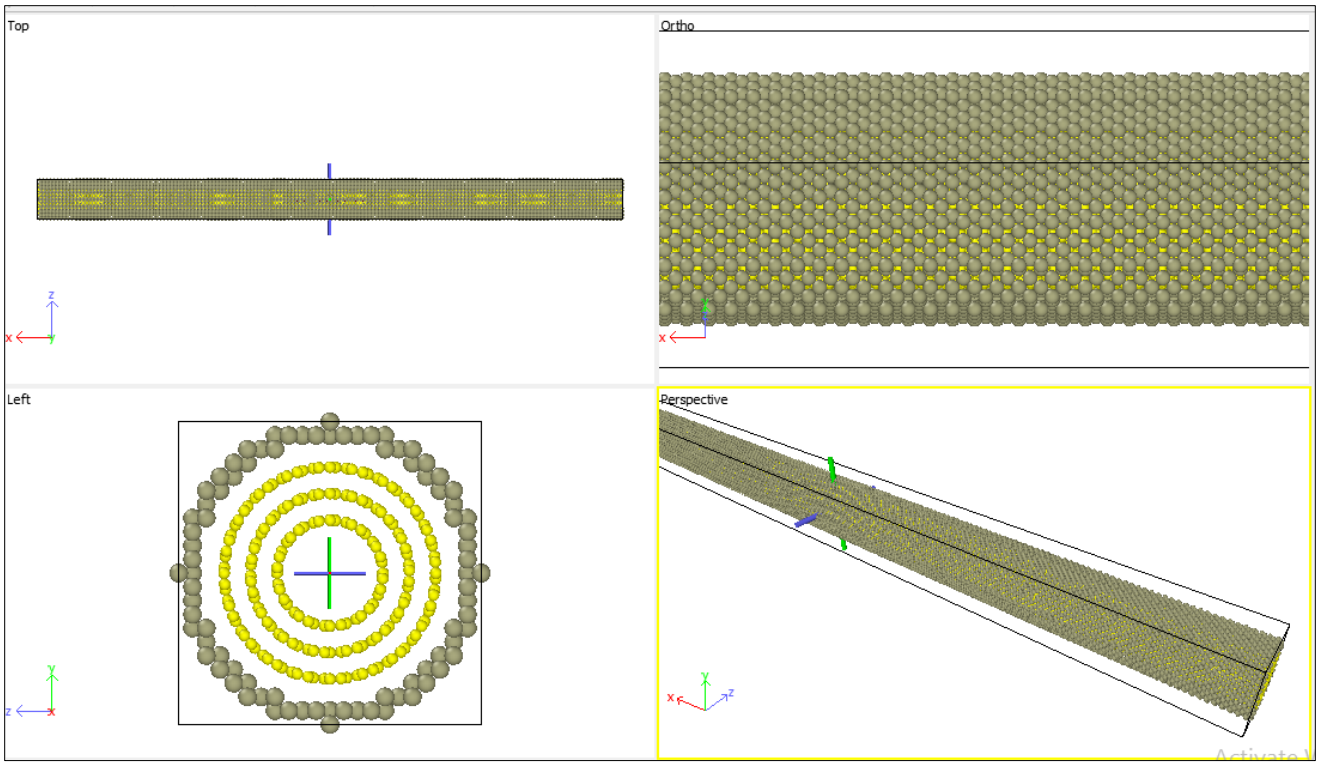


Figure 1

In MD simulations, the Potential Energy (PE) of each atom can be calculated at the end of every timestep during the run and can be dumped in a file. That dump file can be opened in **Ovito**, a visualization software, to view the atomic movements and variations in PEs of each atom at every timestep throughout the simulation.

When this whole structure is relaxed to room temperature using proper force fields, Ni gets uniformly adhered to the CNT. However, due to some variabilities in crystal structure, some Ni atoms be suspended over the uniform layer of Ni as shown in Figure *2*. This phenomenon cannot be controlled in MD simulations and hence, to maintain the uniformity of layer thickness, we get rid of those dangling atoms in Ovito tool.

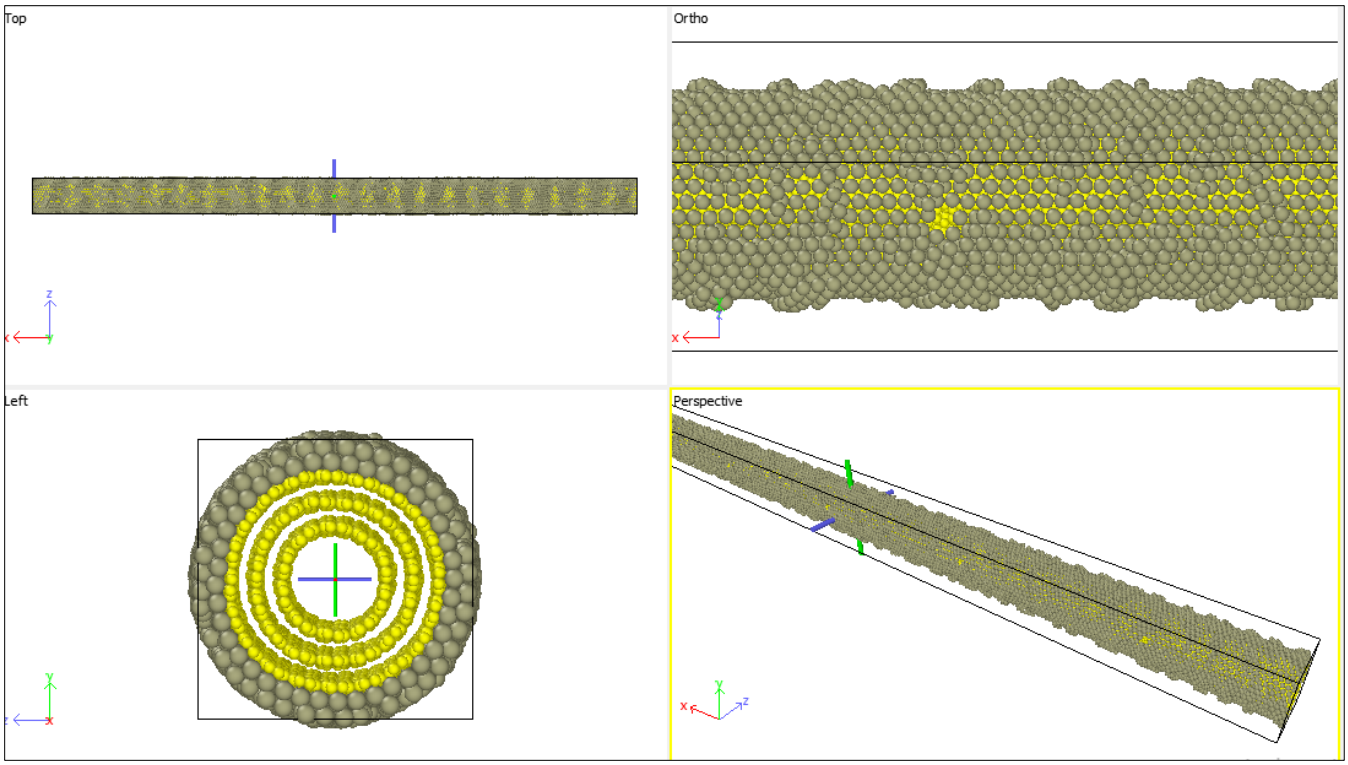


Figure 2

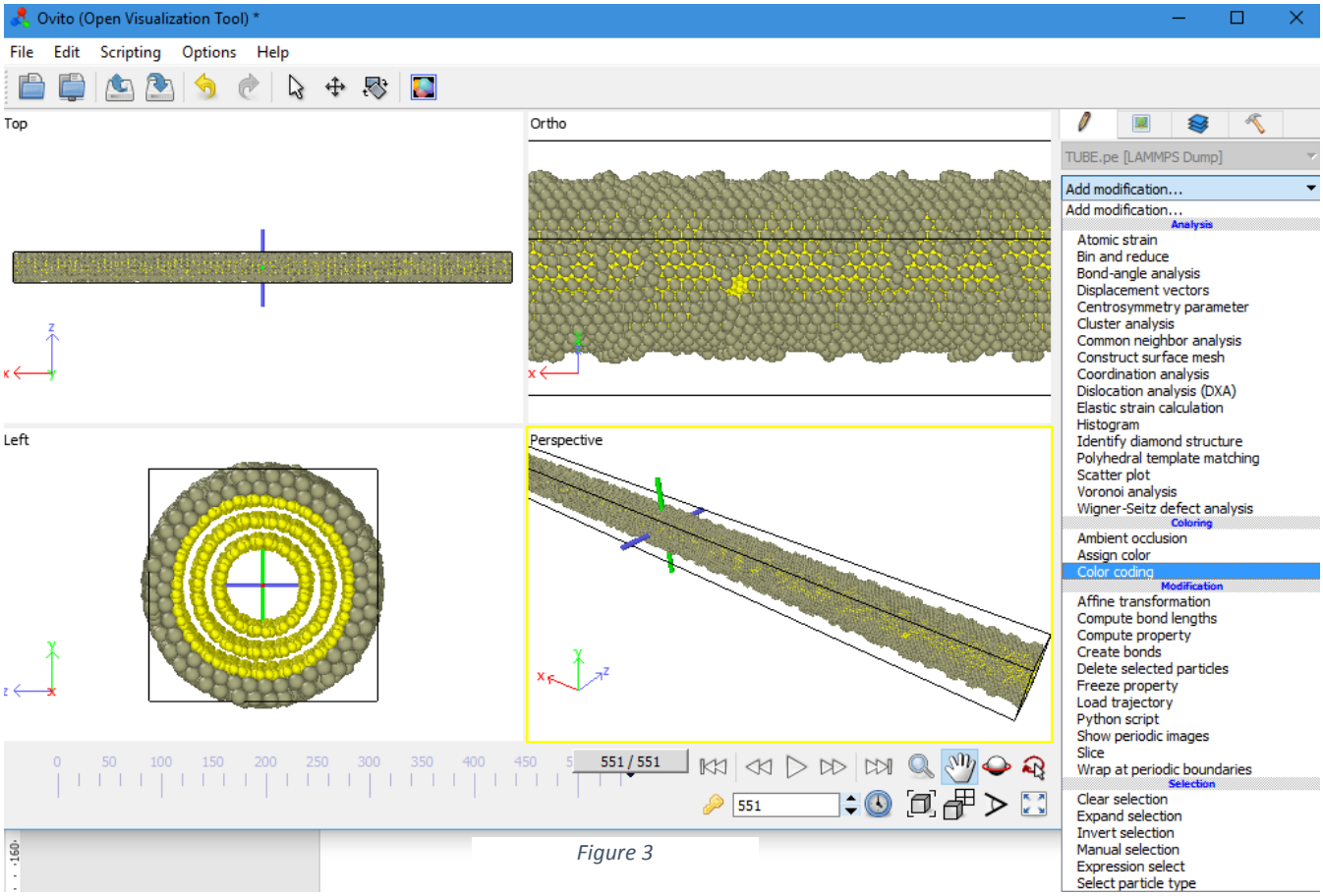


Figure 3

The dangling atoms possess higher Potential Energy due to more unpaired bonds at the surface and this can be viewed by adding Color Coding Modifier. To add this modifier, go to the drop down menu, ***Add modification*** → ***Color Coding*** on the top right of the window as shown in Figure *3*.

Then in the bottom right section of the window, select the Potential Energy (c_pe) in the drop down menu of Particle Property. ***Particle property*** → ***c_pe*** as shown in Figure *4*.

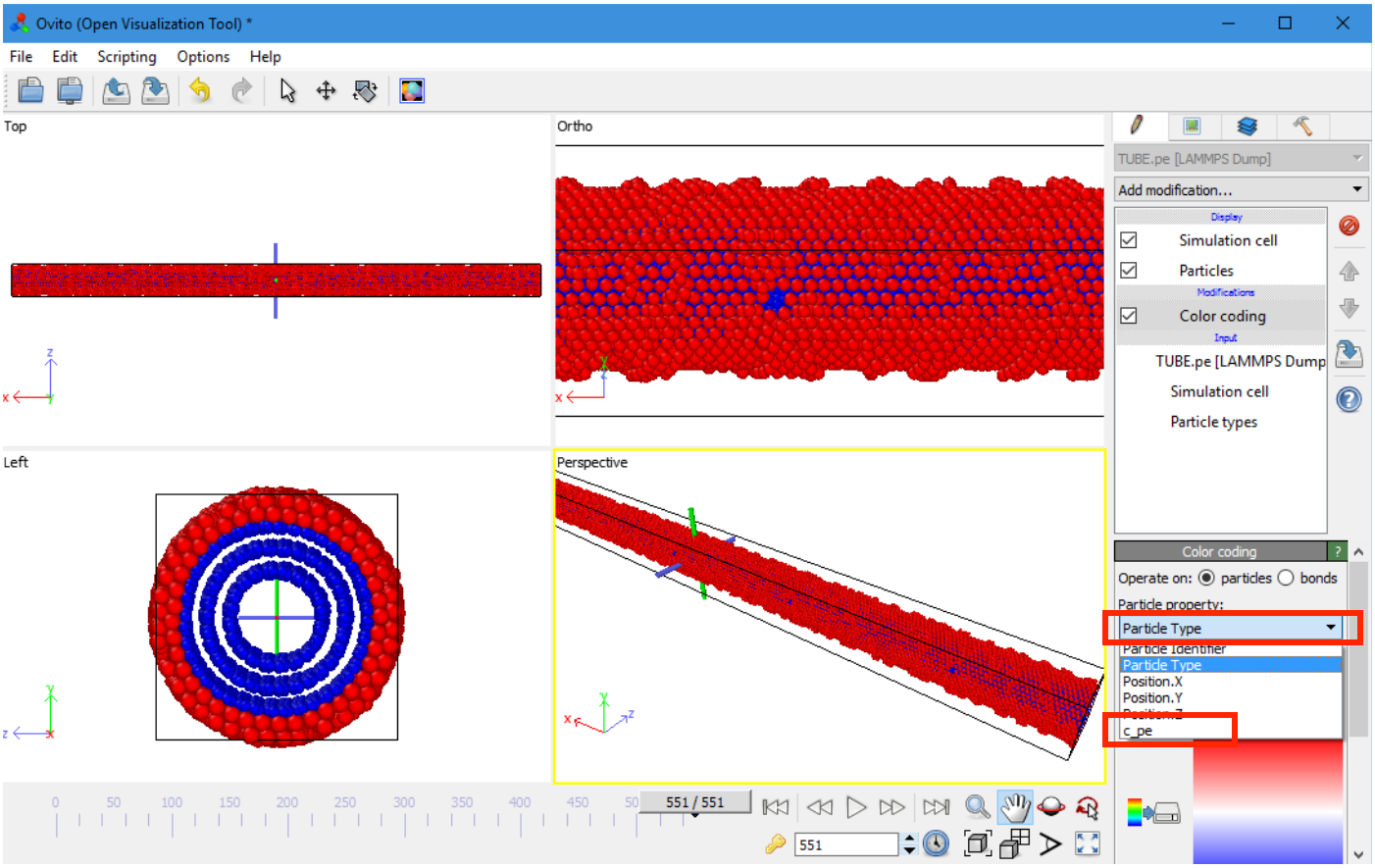


Figure 4

After selecting any of the Particle properties, it is recommended to click on ***Adjust Range*** - to automatically modulate the vacillating start and end values. It is even possible to set the range manually if desired. Then the ***Color gradient*** can also be selected from the different available options.

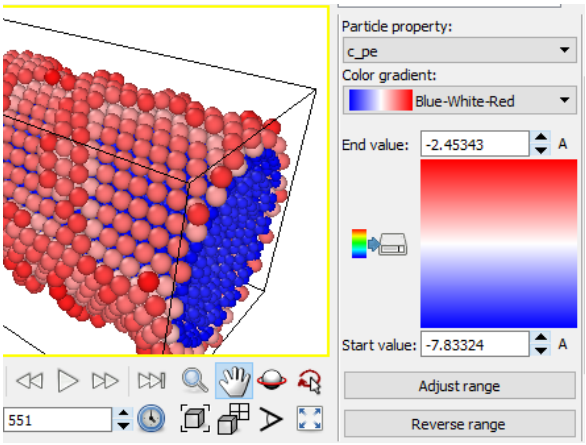
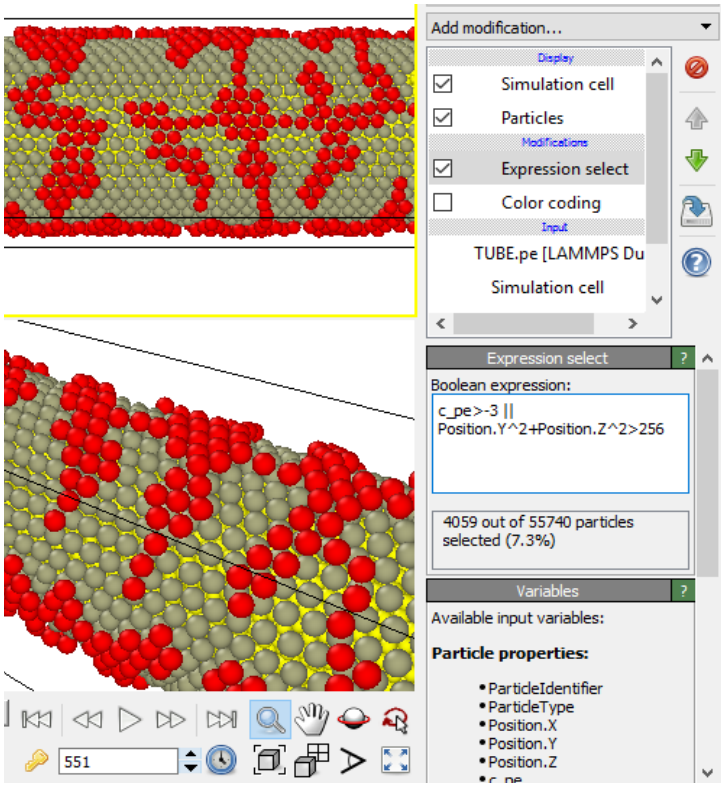


Figure 5

When we have thousands of atoms in the structure, it is difficult to hand-pick the atoms just by visualizing them. Therefore, ***Expression Select*** modifier can be used to select multiple atoms having a common quality (***Add modification → Expression Select***). One or more conditions to be applied on the atoms can be given in the form of ***Boolean Expression.*** The proper syntax and information about various operators are given in the ovito manual.

https://www.ovito.org/manual/particles.modifiers.expression_select.html

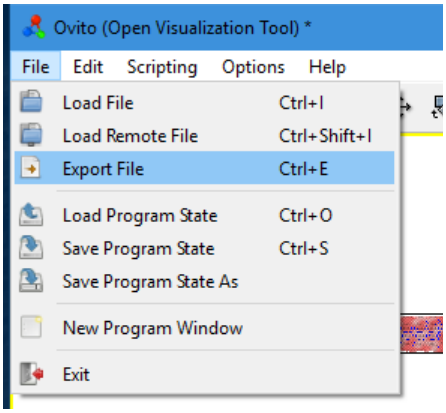
E.g: In this case, as already discussed, the dangling atoms would have high PE when compared to the atoms below them. Also as all those atoms are hanging to the first layer of Ni, they would be at much far distance from the center of the CNT. Hence, the PE range being -2.45 to -7.83, all the atoms with PE greater than -3 (c_pe>-3) **OR** all the atoms that lie exterior to circular region with radius 16 ($Position.y^2+Position.z^2>16^2$) are selected.



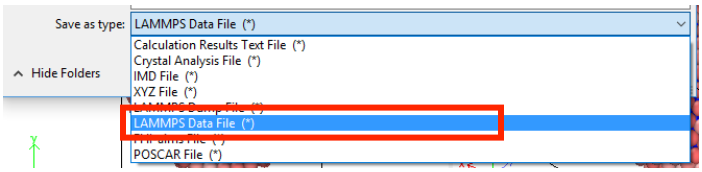
The above set criteria for PE and Radius may vary depending on the structure or the problem. So, the user should be able to estimate them accordingly with good judgement.

Note: Here, the atoms with high range of PE would be in red color and by default the atoms that are selected through Boolean expression would be in red color too. Hence, Color coding modifier is unchecked to have a better illustration of the selected atoms.

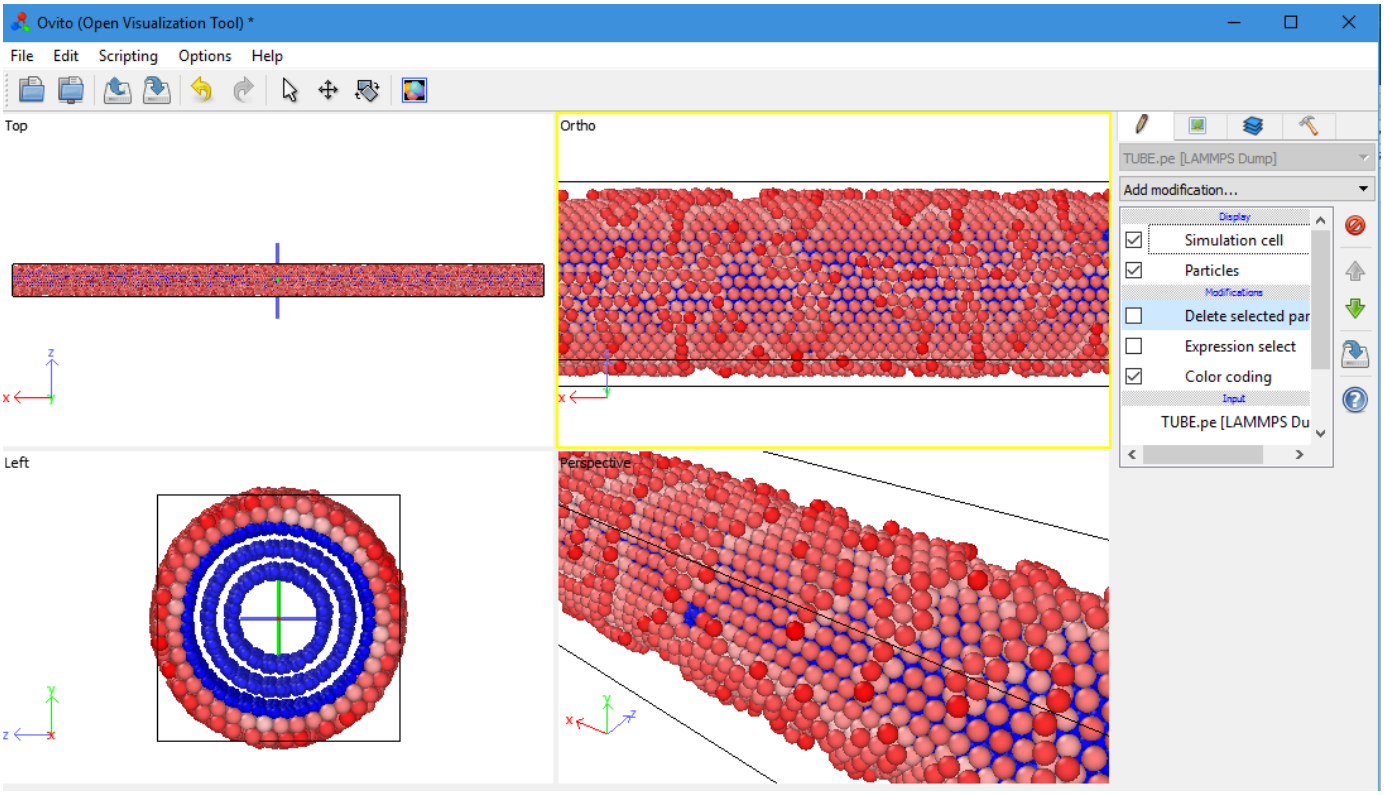
Lastly, all the above selected atoms can be deleted by using the Delete Selected Particles modifier (***Add Modification → Delete Selected Particles***).



To use the current state of the structure as an input file for the MD simulation, it must be exported to a format that can be read by LAMMPS. (On the Menu Bar, ***File → Export File.*** Then, in the *Save as type* drop down menu, *XYZ file* or *LAMMPS Data file* is selected.)



Before removal of hanging atoms:



After the removal of hanging atoms: