

Computational Materials Science and Mechanics Laboratory (CMSML)

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Tutorial:

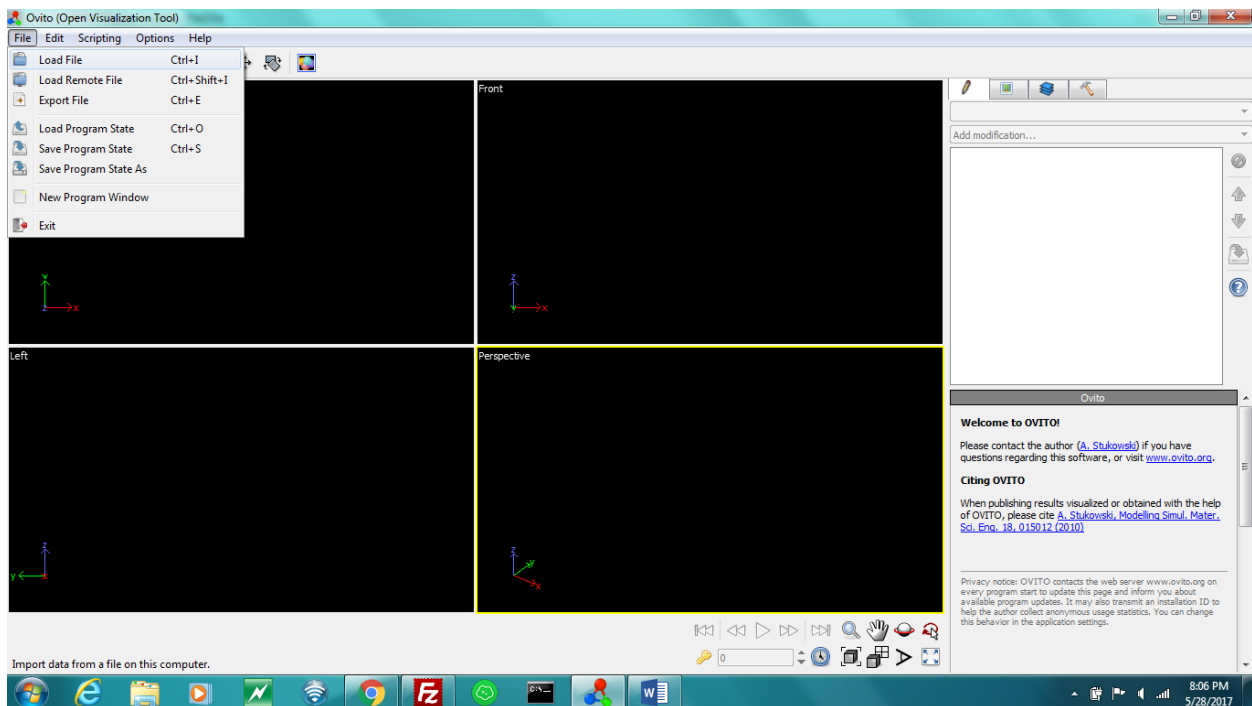
Using OVITO for Atomic Group Selection and Deletion

Prepared by: Alexander Snyder

When visualizing and post processing simulation results using OVITO, it may be desirable to track the motion of only certain chemical groups or a certain region of a sample. Consider the following example of hydroxyapatite tension test simulation post processing.

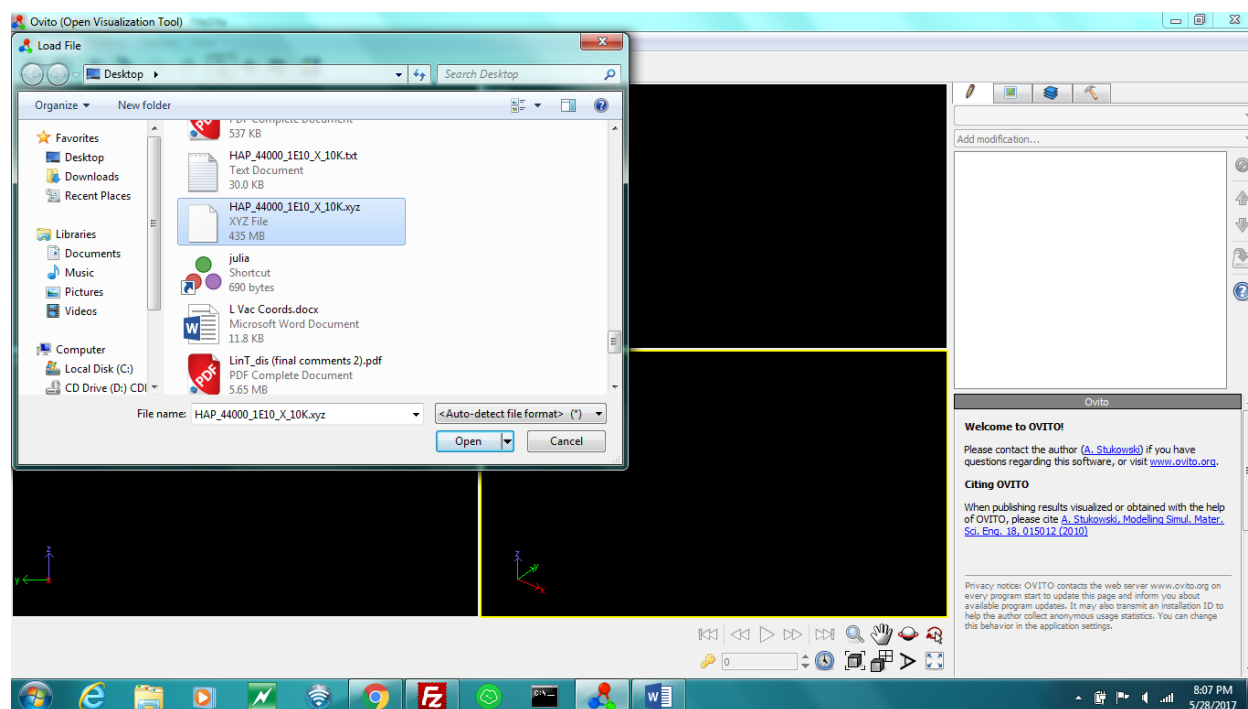
Import the appropriate file into OVITO.

File-Load File

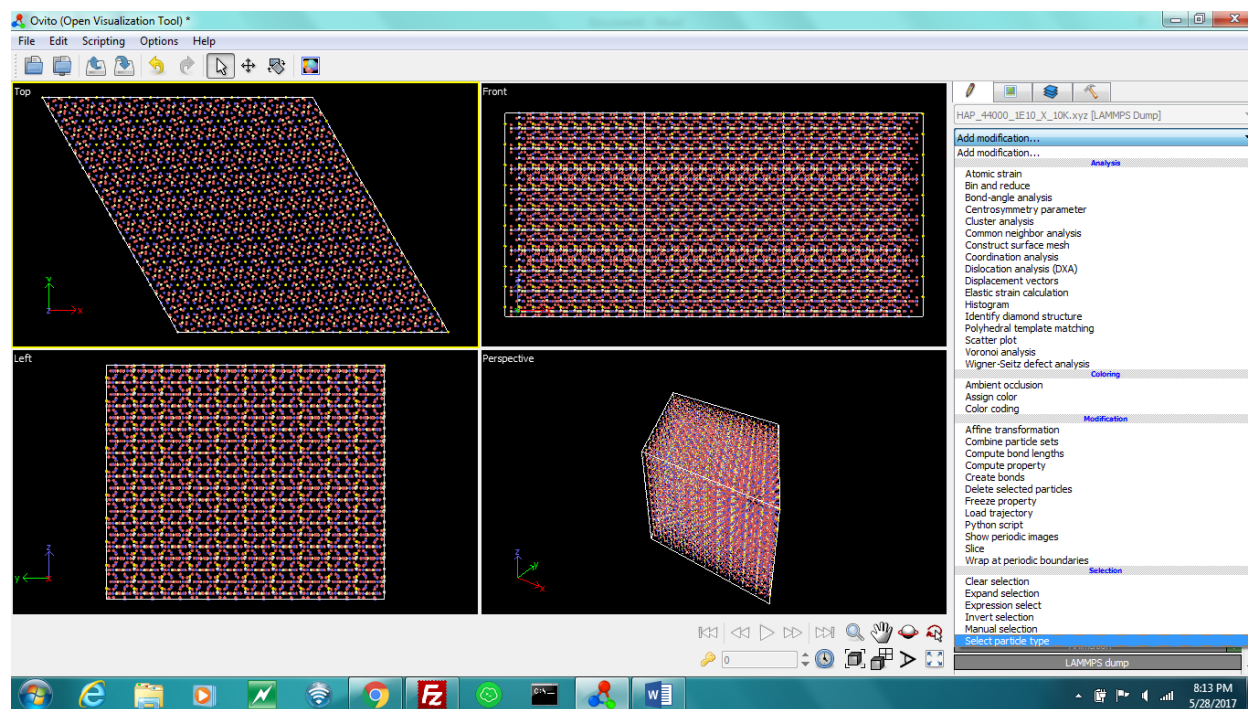


Select the file that is to be imported.

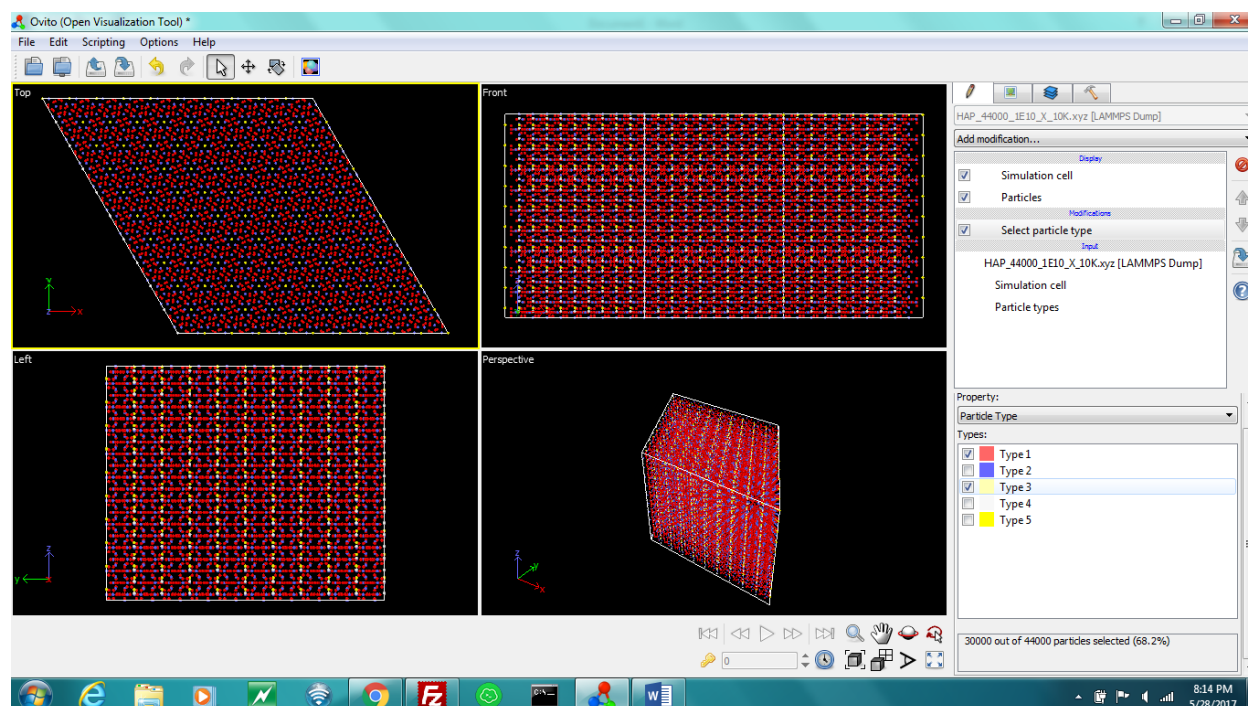
Click on File-Open



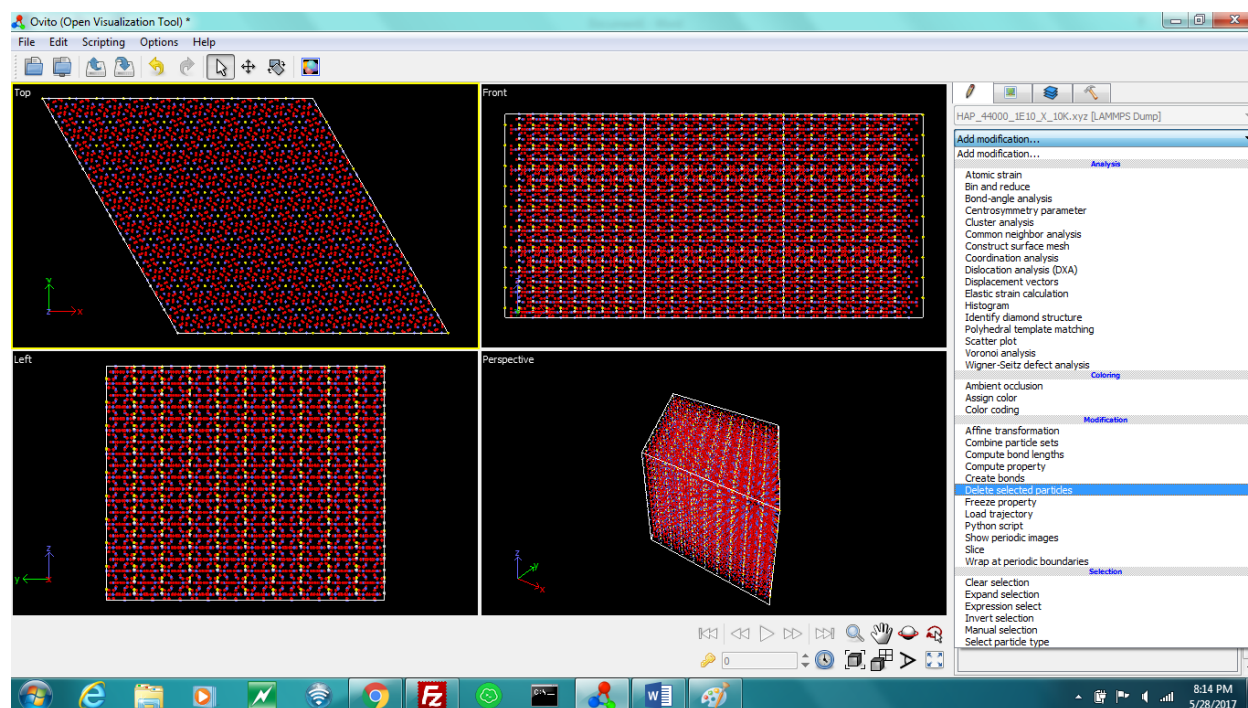
Particle types, i.e. atomic species, may be selected in different ways using OVITO. The easiest way is to select them explicitly, using the Select Particle Type Option.



It is possible to select one or more particle types by checking the boxes next to the available types. A refreshed count will show below the selection area with a count of how many particles in total are currently selected.

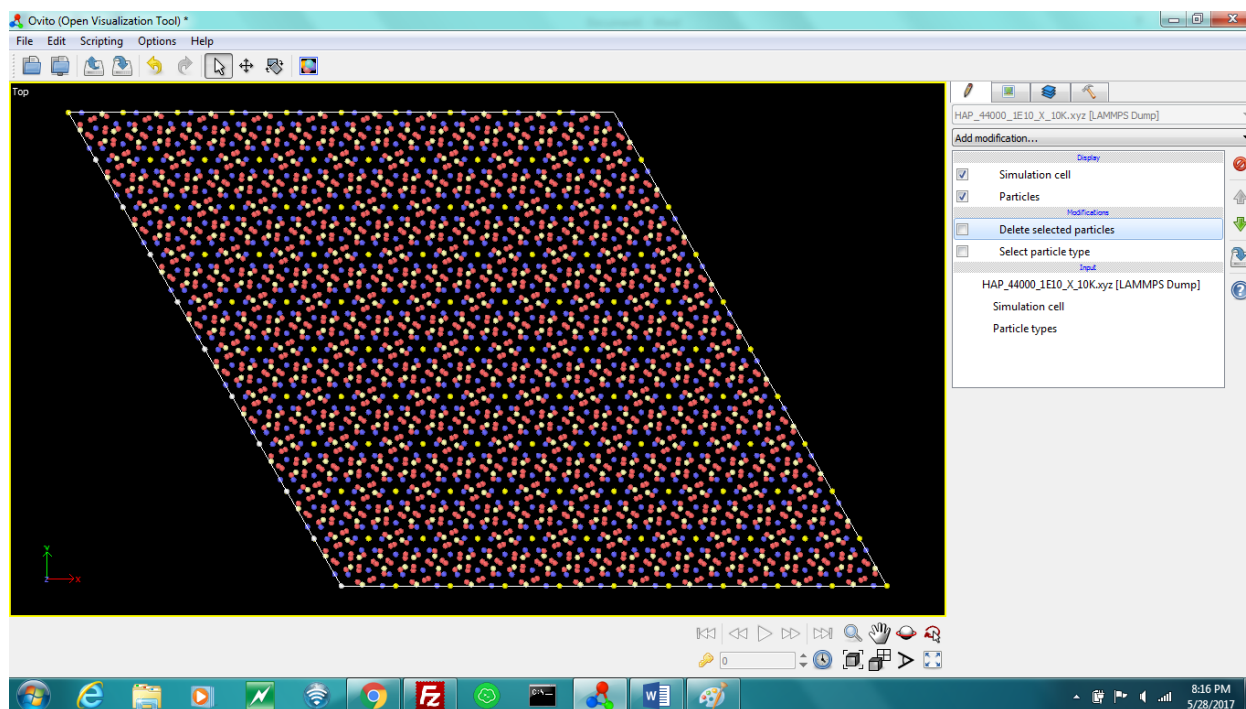


To delete these particles, use the Delete Selected Particles Option.

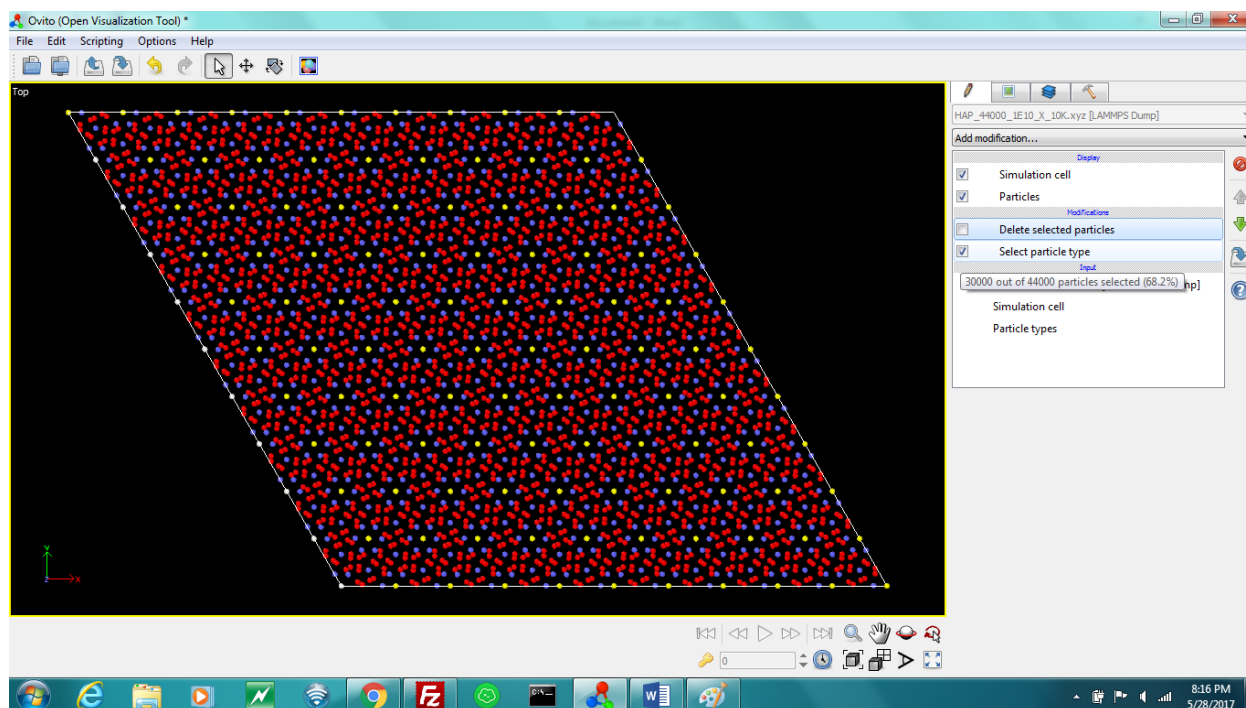


When using the preceding options on this system, the simulation box will show the following progression of images:

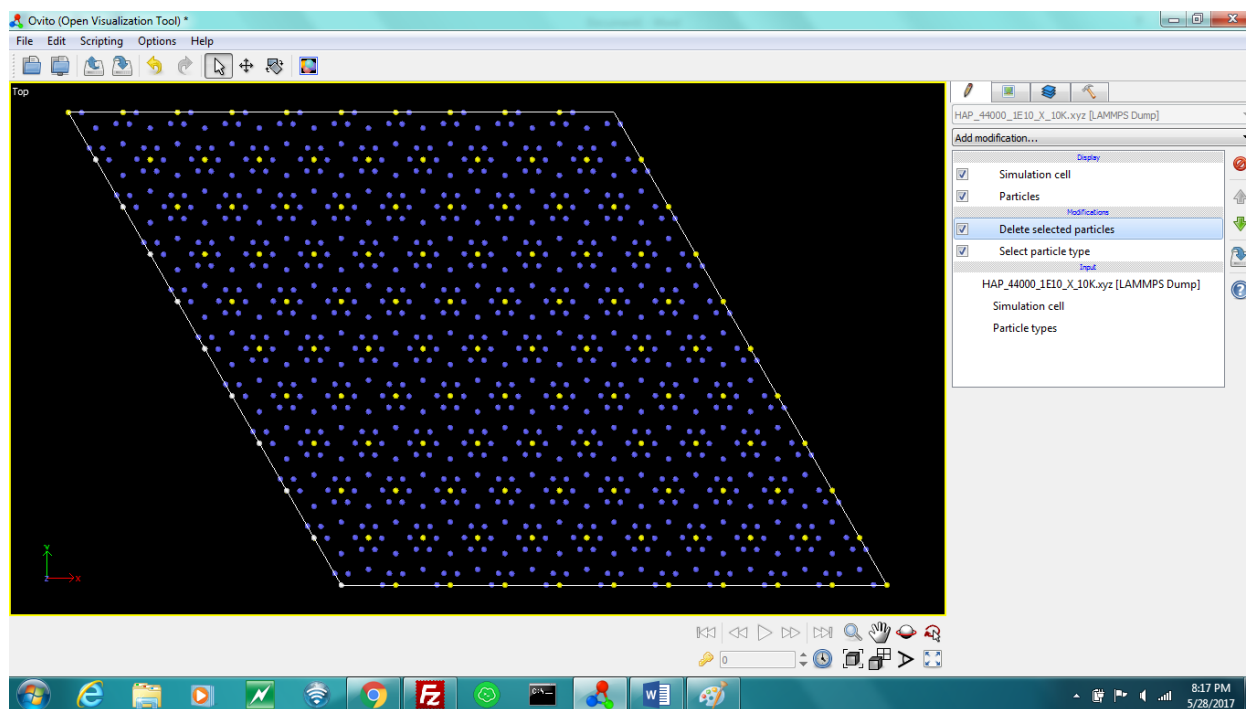
1. The original simulation box. No particles are selected.



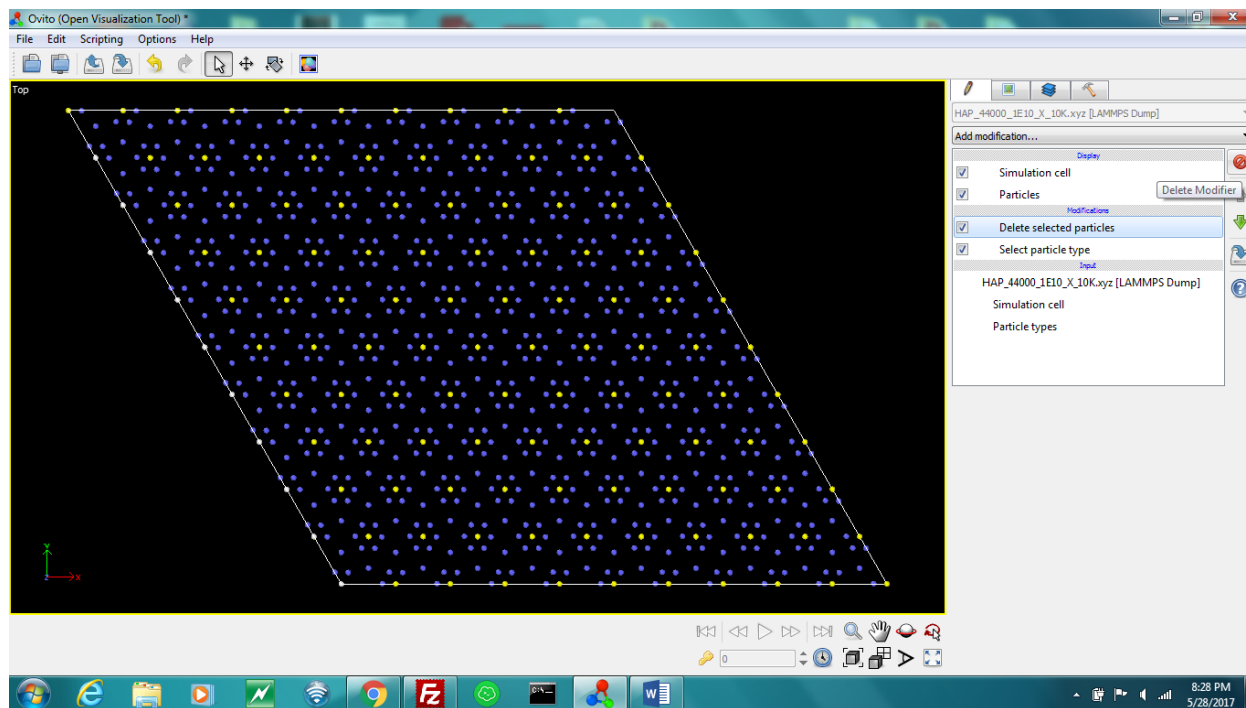
2. The simulation box with Particle Types 1 and 3 selected.

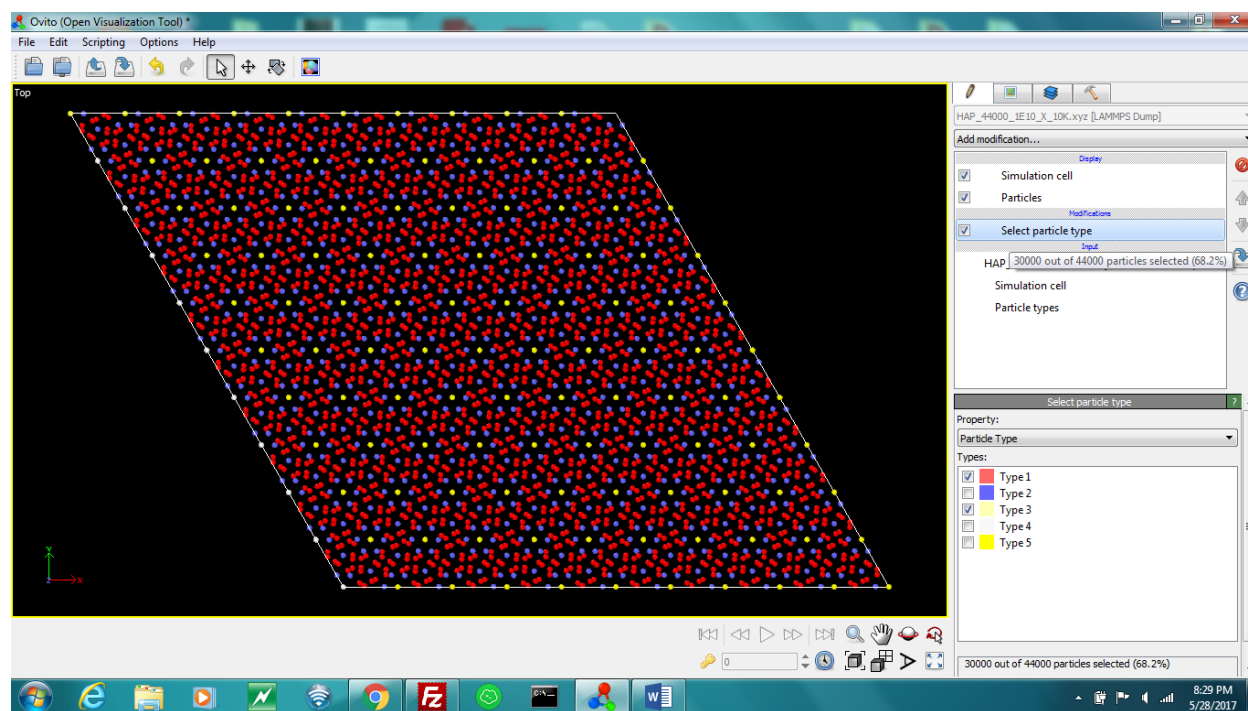


3. The simulation box after deletion of Particle Types 1 and 3.

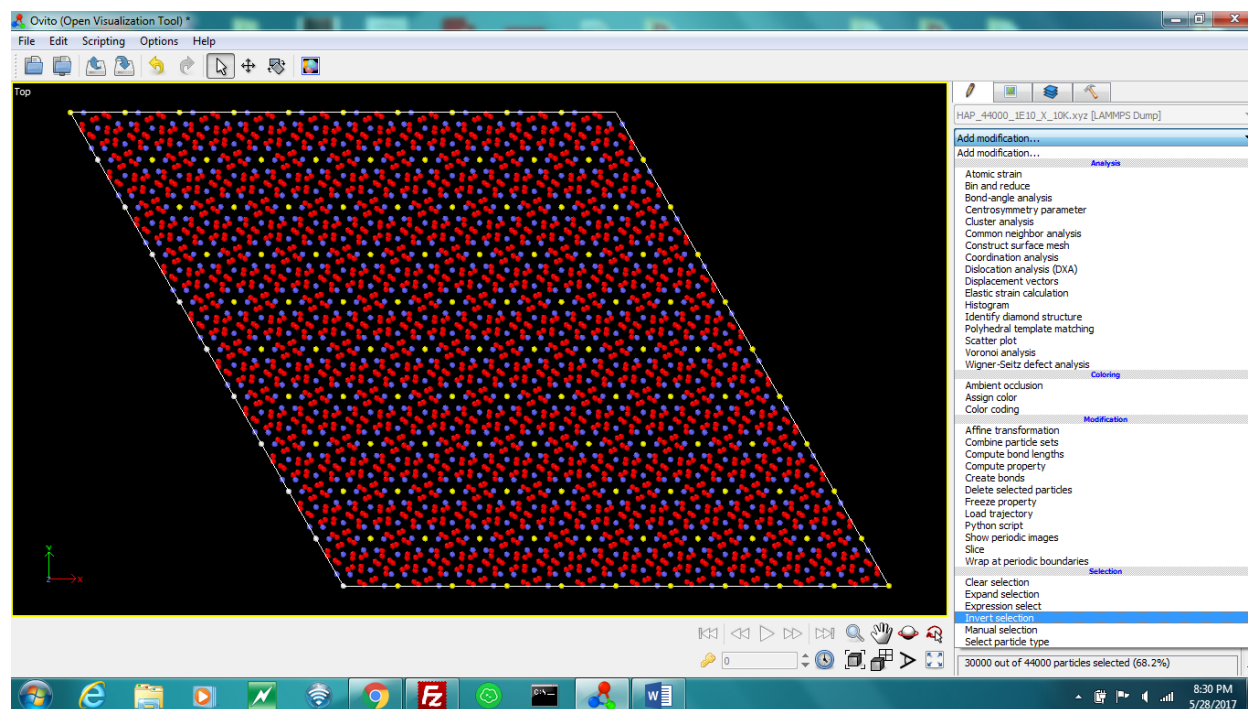


To delete every other Particle Type that is not 1 or 3, delete the previous particle deletion option and reselect the Select Particle Type option that was already set.

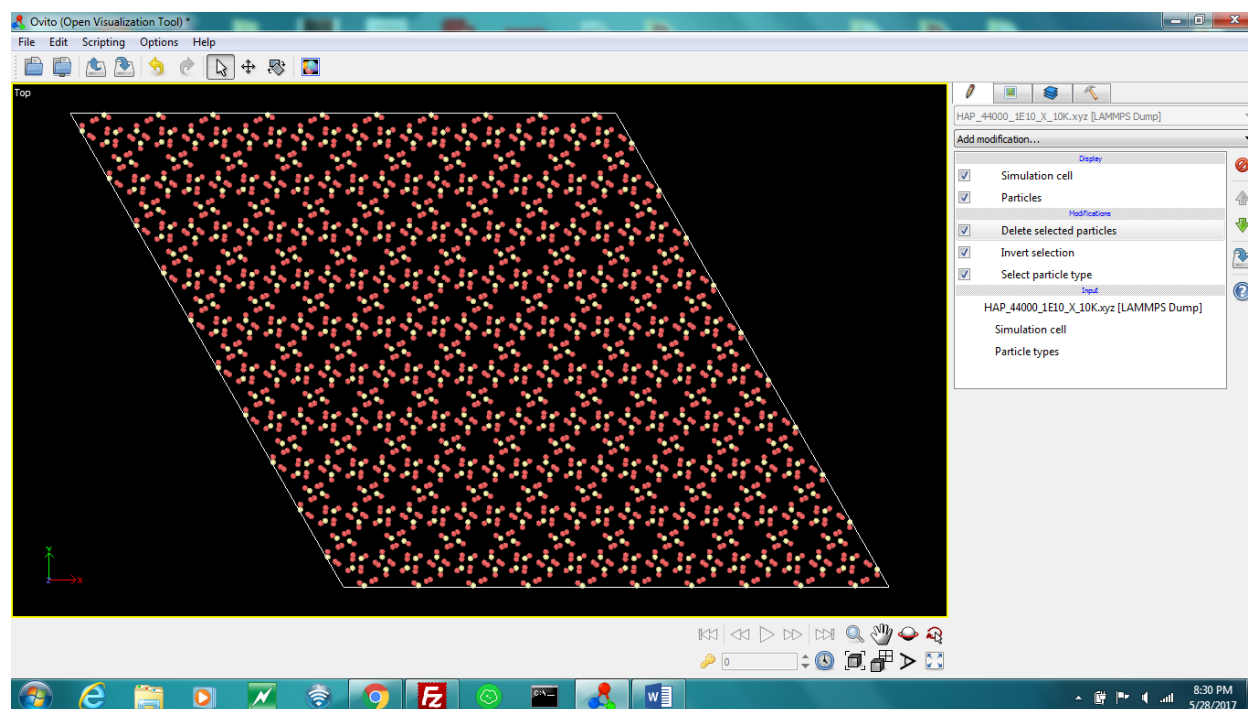




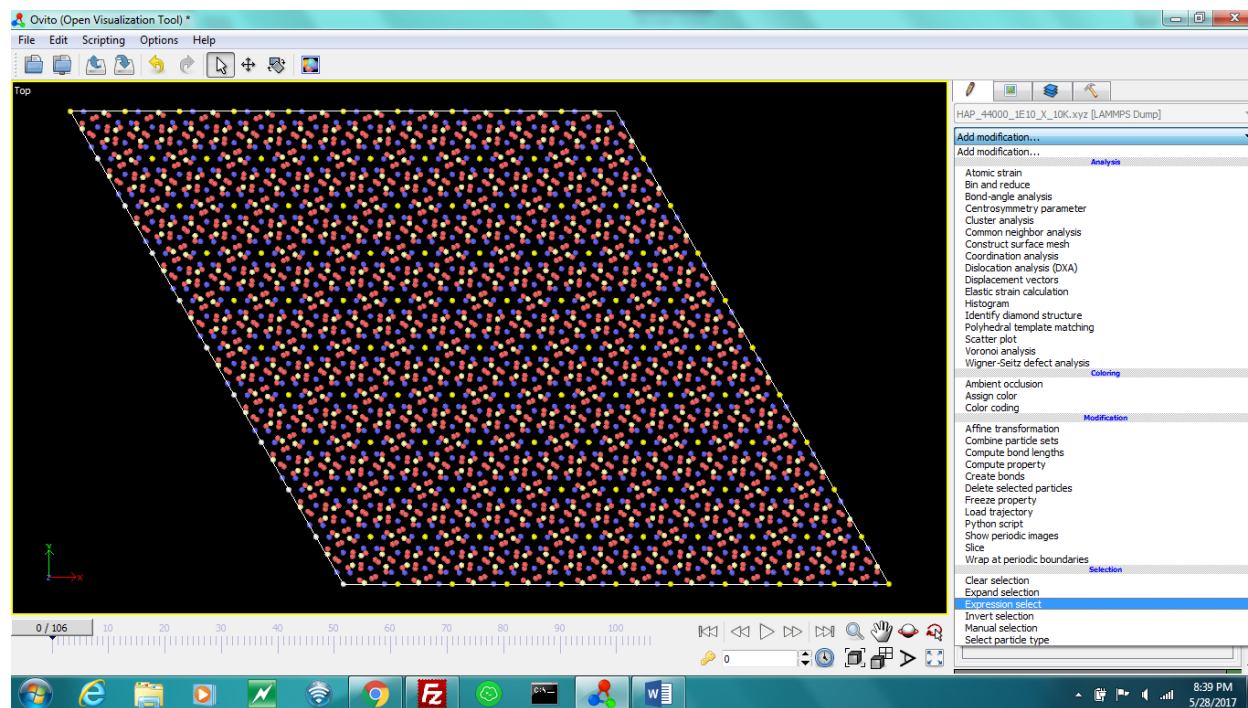
Click on Invert Selection.



Repeat the Delete Selected Particles selection option. The current file has 5 Particle Types, so deletion of types 2, 4, and 5 yields the following image:

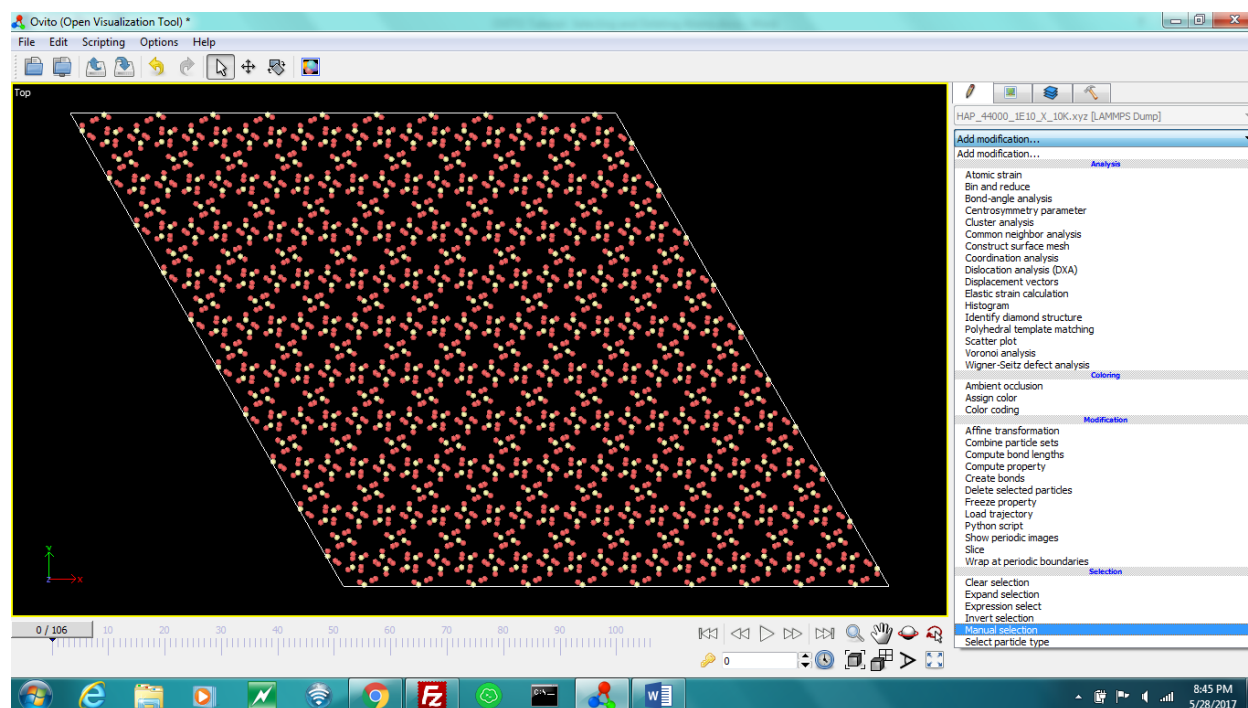


An equivalent way to perform this procedure is by replacing the Select Particle Type Option with an equivalent selection of particles by using a Boolean expression. To do this, start by choosing Expression Select from the drop-down toolbar.

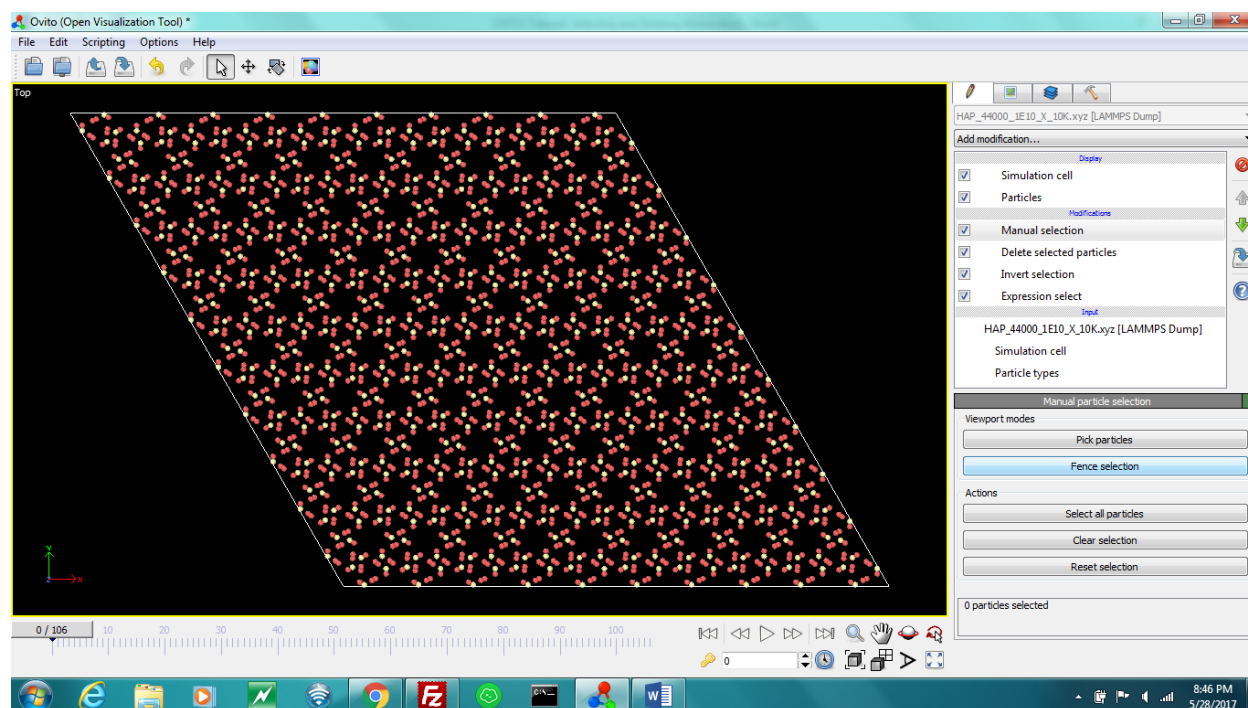


Enter `ParticleType==1||ParticleType==3` in the box provided and press Enter on the keyboard. Particle Types 1 and 3 should show as selected.

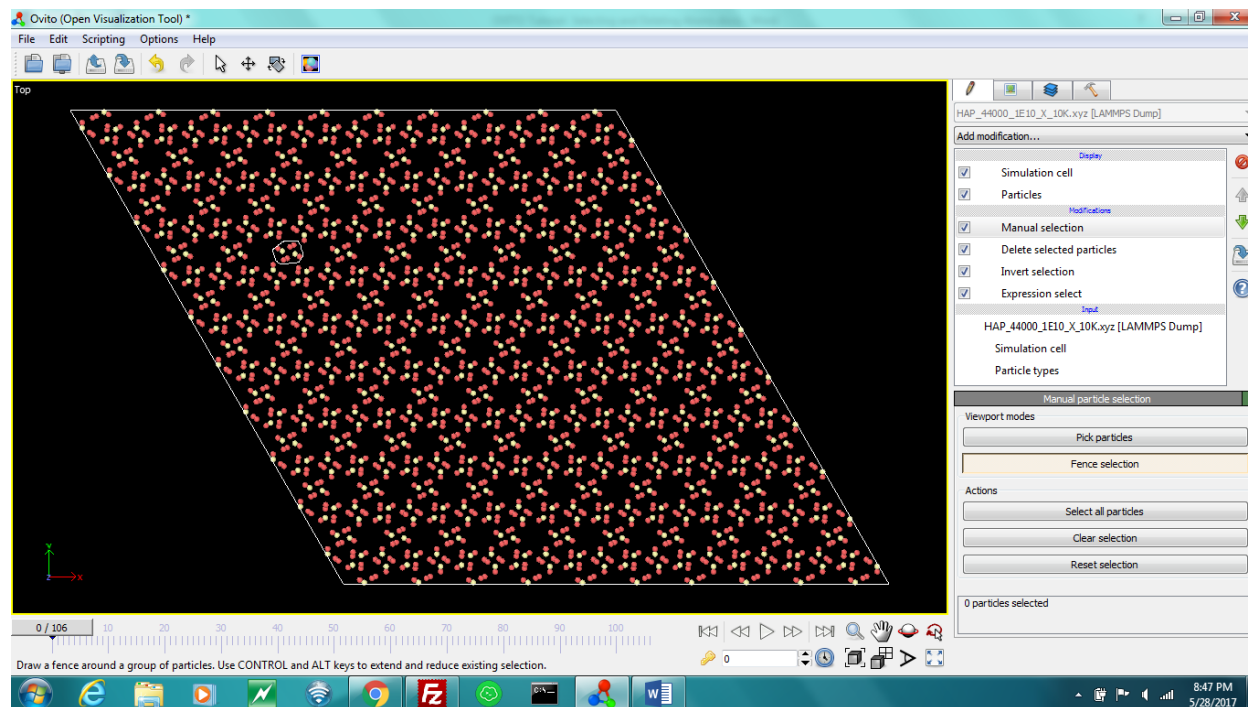
Sometimes, tracking the motion of only one particle or group of particles is desirable. Use the manual selection tool in this situation. Starting from the image obtained after deletion of the inverted selection, choose Manual Select from the drop-down toolbar.



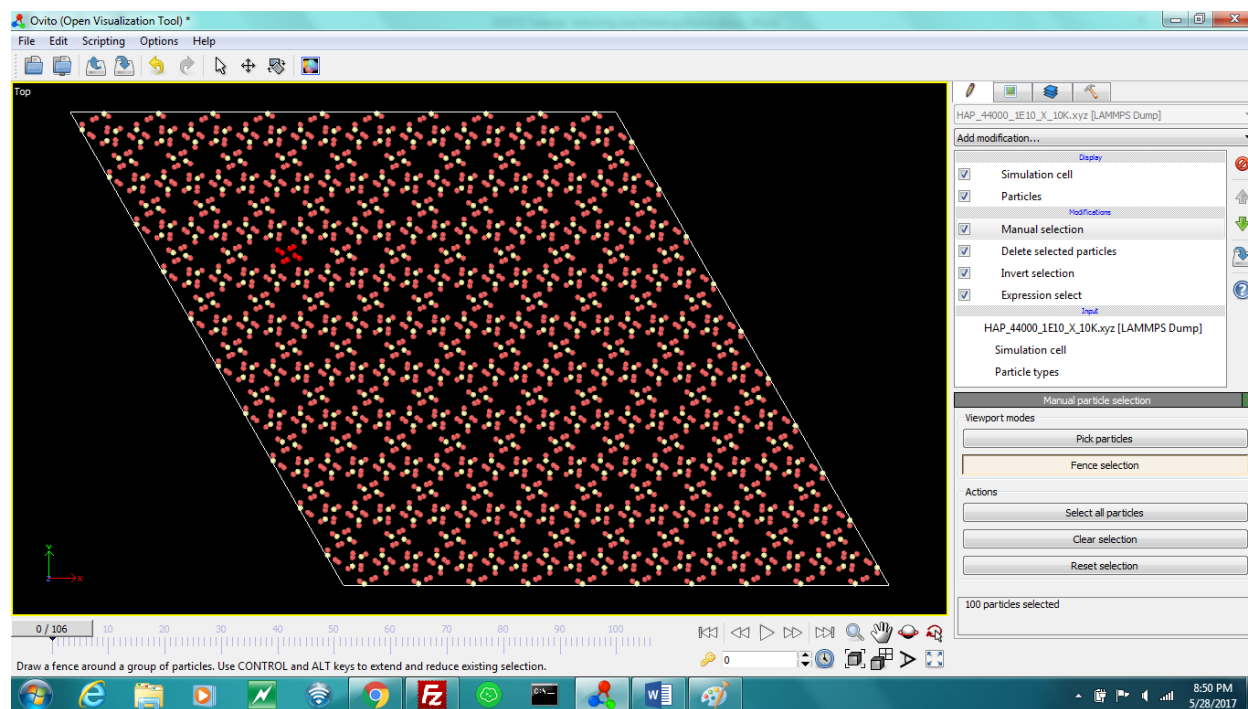
To select a group of atoms, click on Fence Selection.



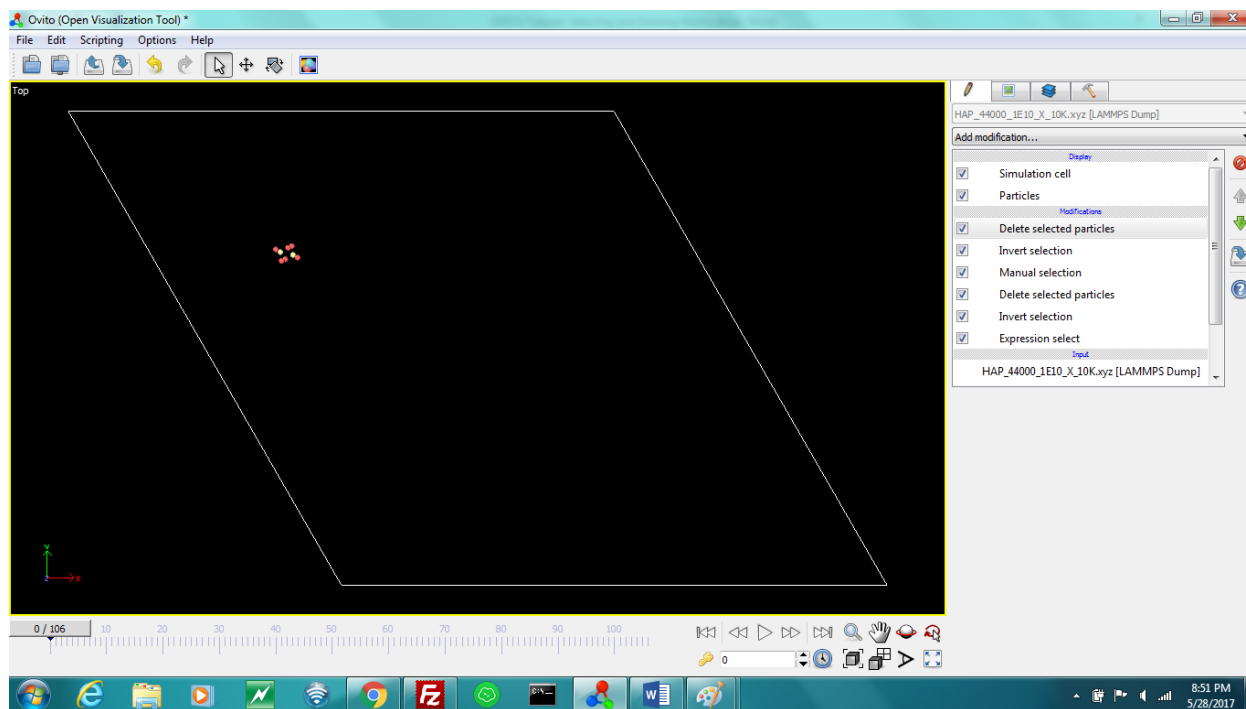
Start at a point bordering the group of interest, and hold down the left mouse button. Draw a shape around the group of interest and release the left mouse button to complete the selection.



The group should show as selected.



If the selection was not properly made, click Clear Selection and try again. To show just the selected group, use the inversion and deletion tools as before.



Feel free to explore the other manual selection options, such as Pick Particles. These are not covered in this tutorial, but are easy to use and understand.