Create Atomic Planes in FCC, NaCl and Simple Cubic Crystals with *Crystal Viewer*

1. Log in to nanoHUB or create a free nanoHUB account at https://nanohub.org/register.

2. Go to Crystal Viewer on nanoHUB.org (https://nanohub.org/tools/crystal_viewer/) and click the **Launch Tool** button 

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3. Click the **Settings** button in the lower right corner 

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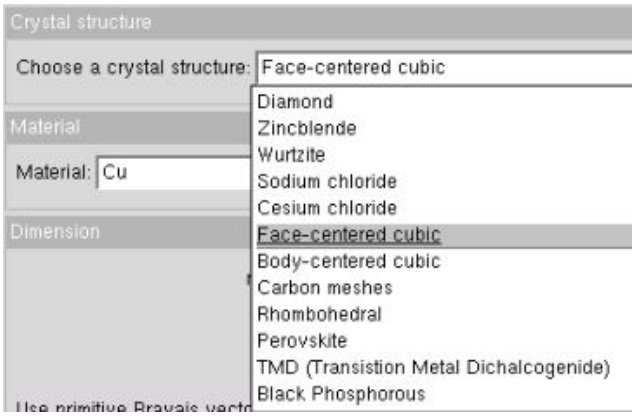
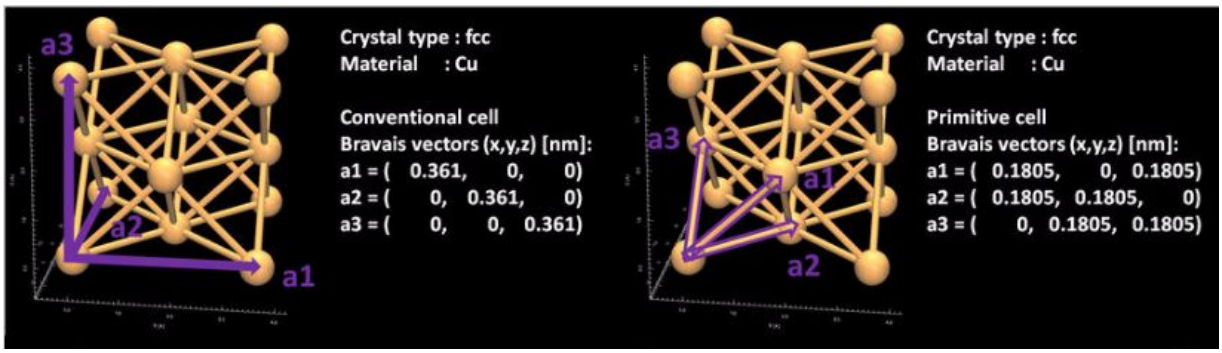
Instructions for viewing the (110) Plane in FCC copper

4. In the **Crystal structure** window, **Choose a crystal structure**, select **Face-centered cubic**.


5. Use the default **Material**, **Cu** (Copper). Copy down the unit cell parameters that are provided. Be sure Draw miller plane is set to **no** to be able to see all of the information. Copper is a cubic crystal, so a1=a2=a3= 0.361 nm in the conventional unit cell.


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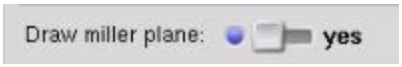
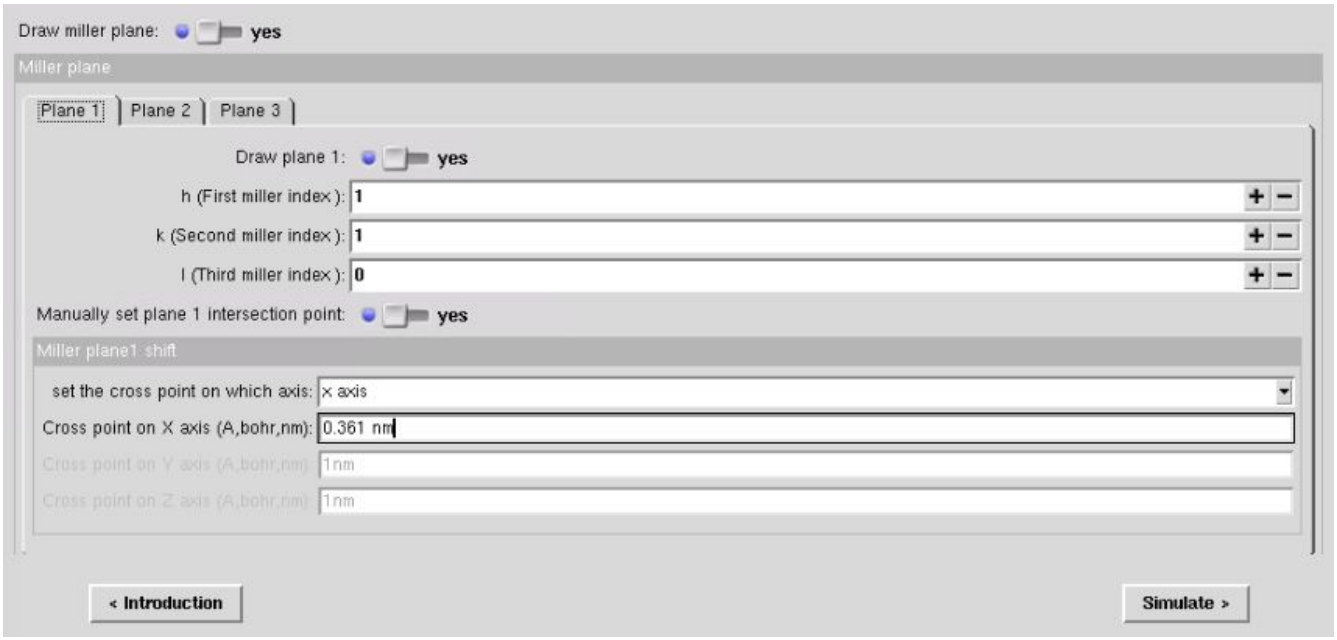
6. At the bottom of the page, change the **Draw miller plane** option to **yes**.


7. Set Plane 1 to be (110) and manually set its intersection point. In order to place this plane diagonally across the center of the unit cell, set its intersection point to be on the x-axis or on the

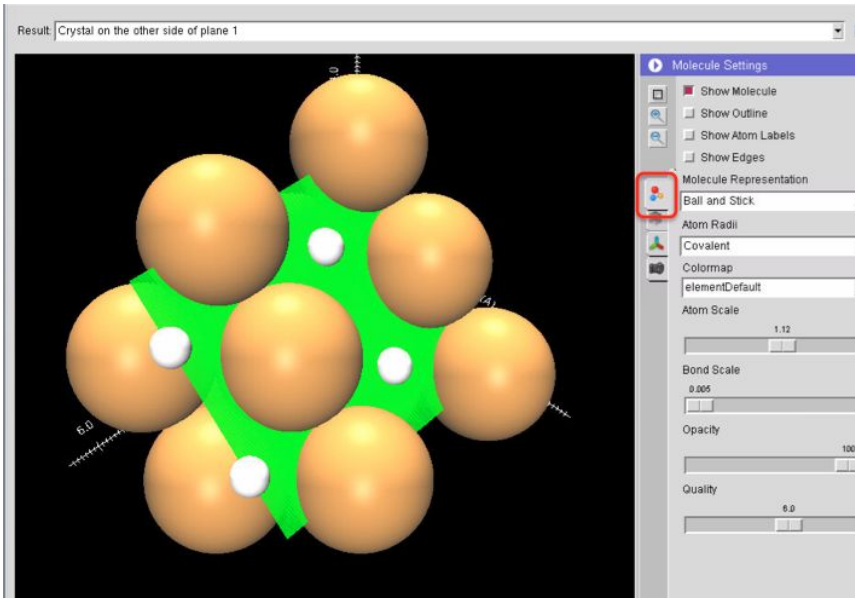
y-axis, crossing at a distance of one unit cell parameter (0.361 nm). Note that this plane is parallel to the z-axis, so has no intersection there.



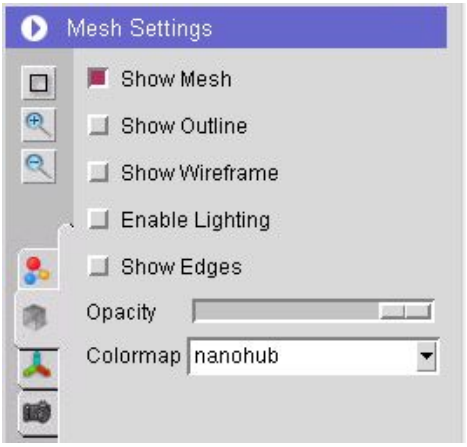
8. Click the **Simulate** button 

. Optionally, you can access a saved run of this simulation and continue from here.
https://nanohub.org/tools/crystal_viewer/invoke?params=file(simset):/data/tools/shared/faltens/crystal_viewer/cu110/cu110.sav

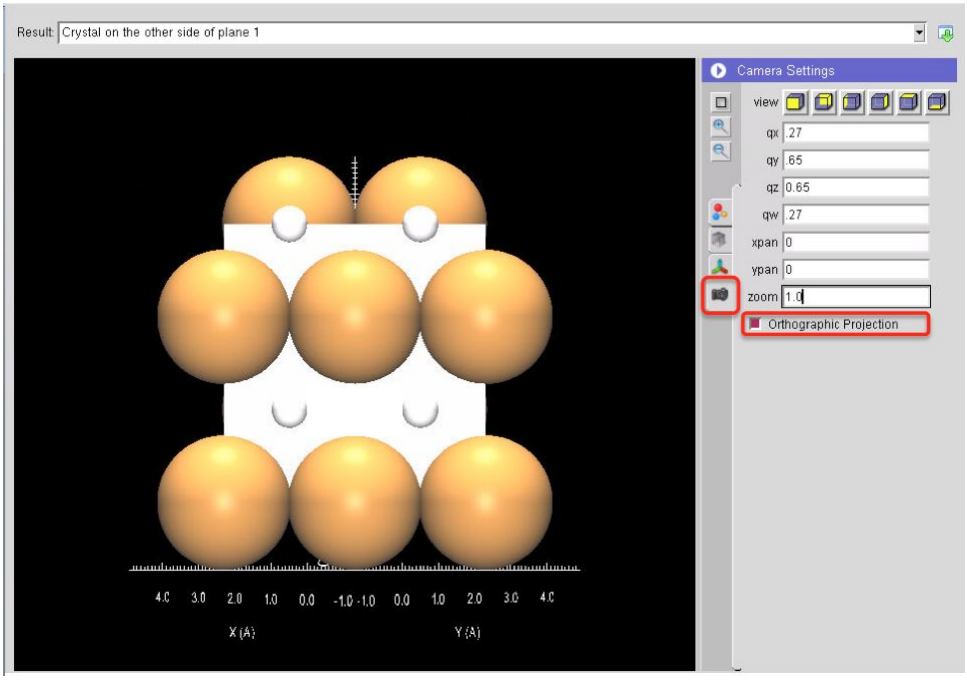
9. Once the simulation is complete, select **Crystal on the other side of plane 1** from the **Result** drop down menu.
10. In the **Molecule Settings** menu (click the icon of 3 colored balls to open), select:
    a. Atom scale: change this until the closest atoms appear to be just touching, about **1.12**
    b. Bond scale: about **0.005**
    c. Opacity: **100**
    d. Quality: about **6**



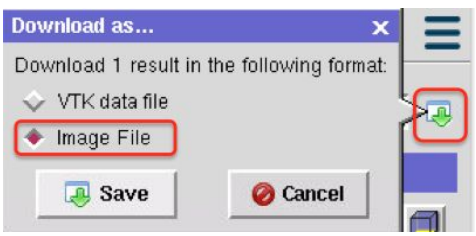
11. In the **Mesh Settings** tab,
    a. Adjust the **opacity** as you like
    b. Select the nanoHUB **colormap**



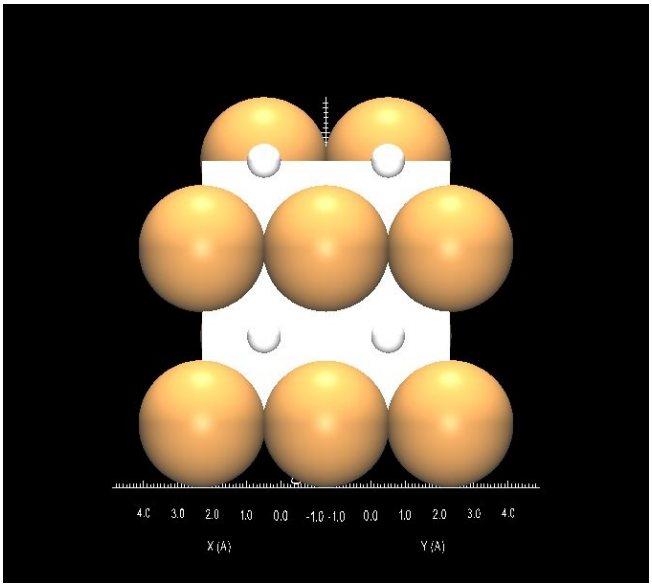
12. In the **Camera Settings** tab:
    a. Select Orthographic Projection
    b. Set **qx = qw = 0.27** and **qy = qz = 0.65** to get the <110> view.
    c. To get other views, click on one of the cube icons for the desired face.
13. You can also use your mouse to rotate the structure to the desired view.



14. To Download this image, click the **download icon** (Green down arrow) and select **Image File,** then **Save.**



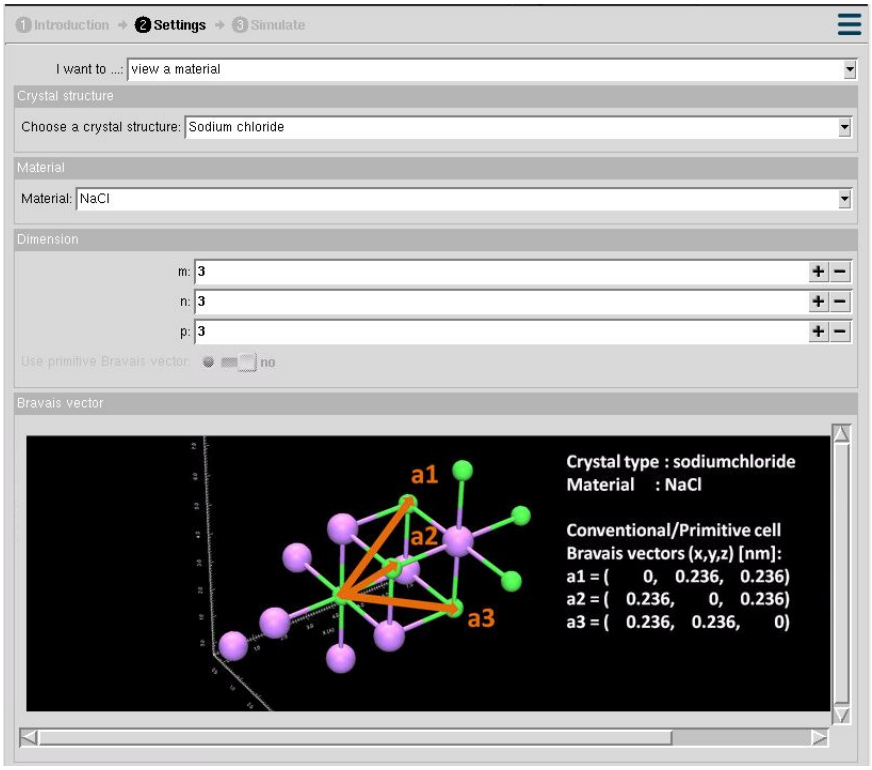
15. In the Pop Up window, click **Save As…**, then select a location on your local drive where you want to save the jpeg image. Here is the saved image from this lesson:



In this image, you see the (110) plane in white, with the 6 Cu atoms that are sitting on this plane. Ignore the small white spheres, they are artifacts of the program and needed to draw the plane and cut the structure, but are not atoms or part of the structure.

Instructions for Viewing the (100) plane in NaCl

1. In crystal viewer, select **Crystal structure**: ***Sodium Chloride.***
2. Select **Material**: ***NaCl***
3. Set the **Dimensions** to ***3x3x3.***



4. Record the lattice parameter information. For sodium chloride, the primitive unit cell vectors are provided. If the distance from a vertex to a face center is (0, 0.236 nm, 0.236 nm), then the distance from vertex to vertex is twice that, or 0.472 nm. (Check the geometrical calculations for yourself to be sure you understand how this works.) The conventional lattice cell parameter is 0.472 nm.

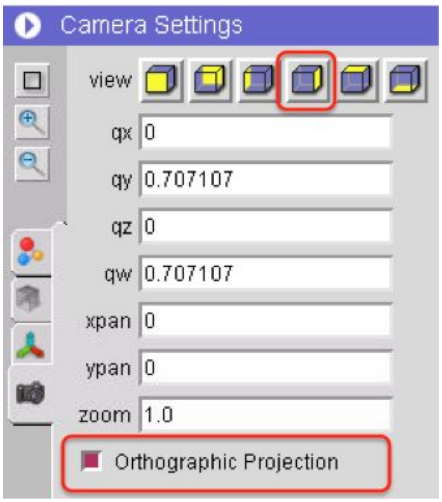
5. Toggle the switch to draw the Miller Plane (this will hide much of the structural information). View the (100) plane.

6. Toggle the switch to manually set the plane intersection point to x=0.472 nm.

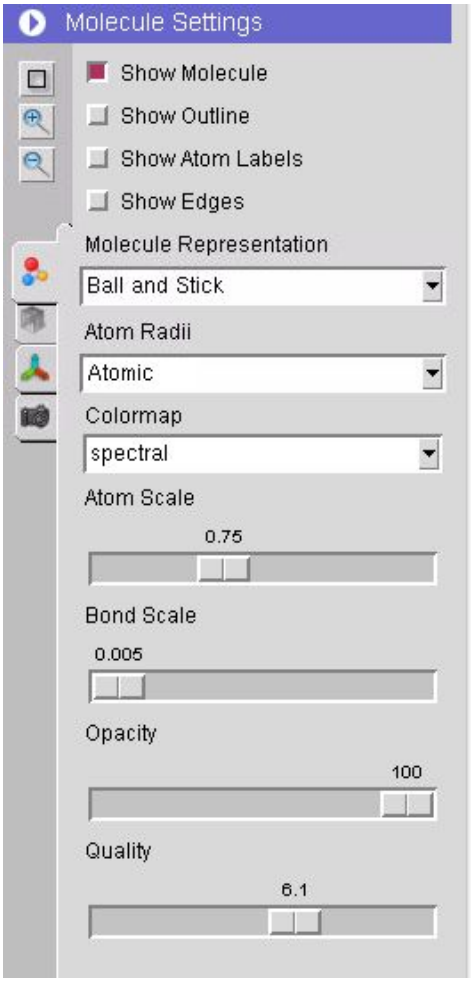
7. **Simulate** the structure. Optionally, you can access a saved run and continue from here.
https://nanohub.org/tools/crystal_viewer/invoke?params=file(simset):/data/tools/shared/faltens/crystal_viewer/NaCl100/NaCl100.sav

8. Select "**Crystal on other side of plane 1**"

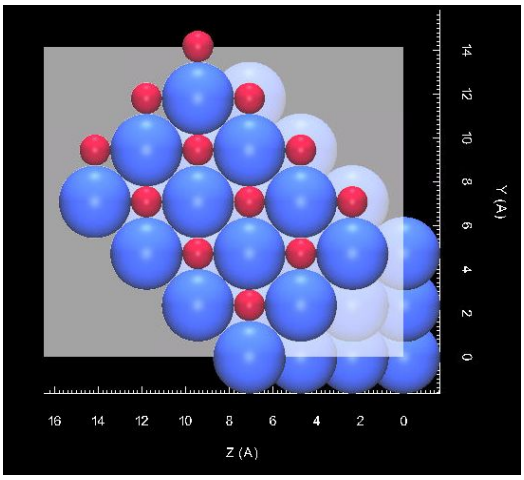
9. In **Camera Settings**, view from the **right** (4th option) as an **Orthographic Projection**.



10. In **Molecule Settings**, select:
    a. Molecule Representation: **Ball and Stick**
    b. Atom Radii: **Atomic**
    c. Colormap: **Choose one you like**
    d. Atom Scale: change this until the closest atoms appear to be just touching, about **0.75**
    e. Bond Scale: minimum (**0.005**)
    f. Opacity: **100**, or as you like
    g. Quality: About **6**



You will see a view of the (100) plane of NaCl.



There are many more options to play with. Feel free to explore!

Instructions for Viewing the Simple Cubic Crystal Structure

There are no commonly found materials containing only one element that have the simple cubic crystal structure, thus this is not an option in the drop-down menu. You can still create this structure yourself.

Select: I want to …. **view Bravais lattice**
Crystal System: **Cubic**
Bravais Lattice: **Simple cubic**
Bravais lattice parameters:**0.334 nm**
Dimension: **2x3x3**
Simulate!
Adjust the molecule, mesh and camera settings as you like, and view the structure from the right.
There is no option for cutting the structure on a plane, so be sure to place the plane where it is easiest to view.
Here is a saved run with a (100) plane in a simple cubic structure.
https://nanohub.org/tools/crystal_viewer/invoke?params=file(simset):/data/tools/shared/faltens/crystal_viewer/SC100/SC100.sav

Here is a download of the jpeg file showing a view of the (100) plane in the simple cubic crystal structure: