Quick and Easy Guide to Carbon Structure Simulations using Crystal Viewer Tool

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The **Crystal Viewer** tool in nanoHUB.org can be used to build three carbon nanostructures: graphene sheets, Buckminsterfullerene, "Bucky balls" (C_{60}), and carbon nanotubes. This document provides step-by-step instructions for building these structures and provides some interesting information about each of them.

In order to use the simulation tools on nanoHUB.org, you must register an account. Registration is **free** and is a simple 3-step process:

1. Visit www.nanoHUB.org/register
2. Create your account
3. Click on the link in the confirmation email you will receive to complete your registration.

Launch the Crystal Viewer Tool

There are several ways to find the Crystal Viewer Tool. The easiest way is to type Crystal Viewer in the search box. You can also click on Resources and select Tools from the drop-down menu. Crystal Viewer Tool can be found in the Resources window that opens up. Here is a direct link: http://nanohub.org/resources/crystal_viewer

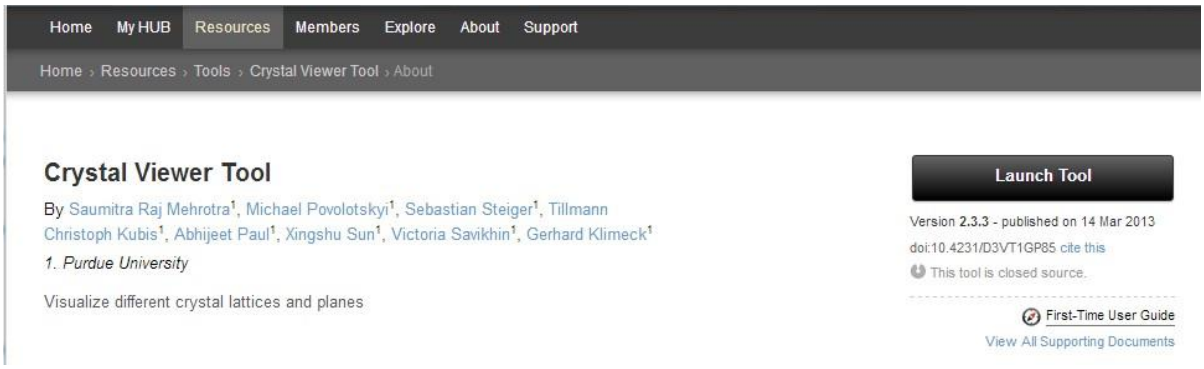


Figure 1: Crystal Viewer Tool

- Click on the black "Launch Tool" button to enter the simulation. You may need to install Java in your browser the first time you run the simulation.

To make the carbon nanostructures, you will change a few of the parameters.

Create a Graphene Sheet

To make a sheet of graphene, select the following parameters:

- Material or Crystal System?: **Material**
- Lattice Structure: **Carbon Meshes**
- Material: **Graphene/Graphite**
- Lx: **4** (you can change this number)
- Ly: **4** (you can change this number)
- C-C bond length: 0.142 nm
- Num. Sheets: **1**
- Layer separation: 0.335nm (this number will not matter for a single graphene sheet.)

Your window should look something like this:

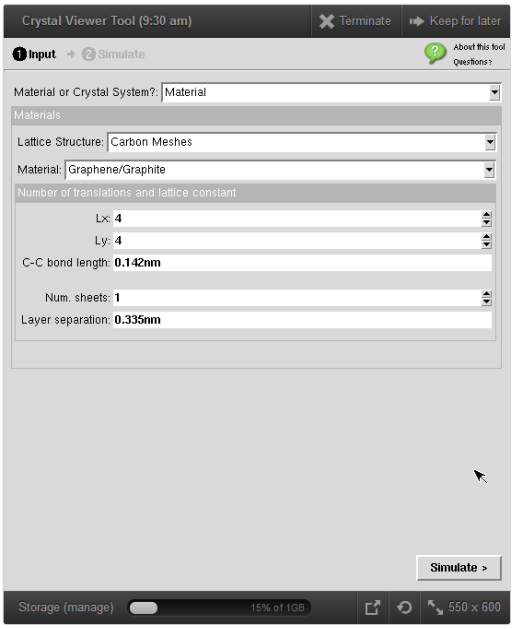


Figure 2: Graphene Parameters

Once you have selected these parameters, click on the **Simulate** button, and wait a moment for the simulation to complete and send you the structure, which will look like figure 3. Click and hold the left mouse button as you drag the mouse around to rotate the image in 3 dimensions.

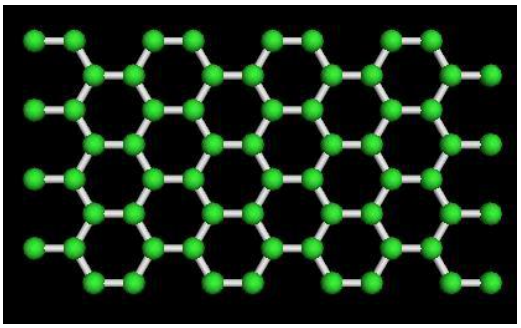


Figure 3: Graphene Sheet with Lx=4, Ly=4

The toolbar on the right side of the simulation window gives you more control options:

- Download the file:
  - As a .pdb file if you have an application that uses this file format
  - As an image file in JPEG, TIFF or PNG formats.
- Open or close the side bar
- Reset the view to the default zoom level
- Zoom in (magnify)
- Zoom out
- Show or hide the atom labels
- Rock the structure back and forth
- Use perspective or orthoscopic projection
- Open / Close the sidebar for Settings

Using the download option, you can download the image as a high quality image file, and also change the background color. I downloaded this graphene sheet as a JPEG file, and selected a white background. This is the result:

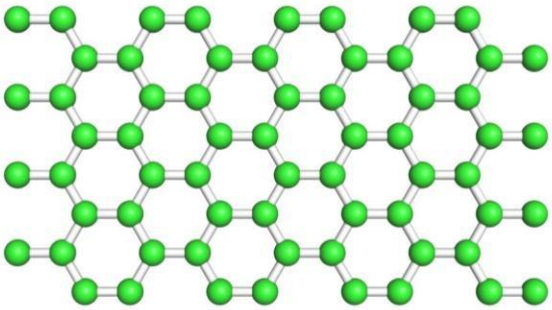


Figure 4. Graphene Sheet JPEG image on white background

<u>Create a Carbon Nanotube (CNT)</u>

To make a Carbon Nanotube, select the following parameters:

- Material or Crystal System?: **Material**
- Lattice Structure: **Carbon Meshes**
- Material: **Carbon Nanotube (CNT)**
- n: **6** (you can change this number)
- m(>=n): **6** (you can change this number)
- C-C bond length: 0.142 nm
- Num. Unit Cells: **3** (you can change this

number) Your window should look something like this:

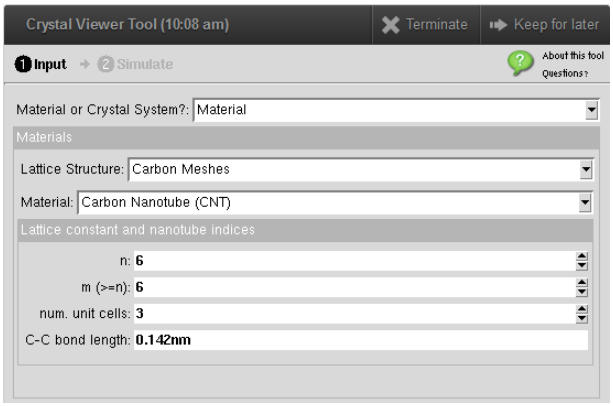


Figure 5. Carbon Nanotube Parameters Window

After clicking **Simulate**, the simulation window will look like this:

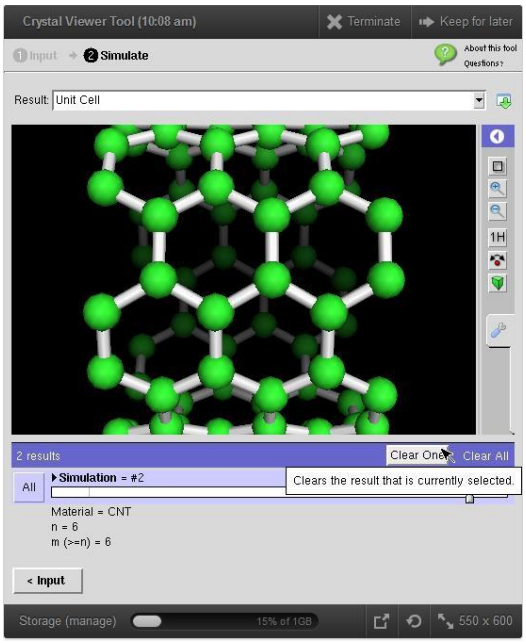
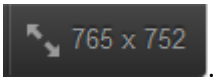


Figure7. Carbon Nanotube Simulation Window without rescaling

To rescale the CNT to fit the windowbetter, use the **Zoom Out** control. 

. You can also use the window controls at the bottom of the frame to pop out the window  or resize it 

. If you pop out a new window, you can resize that window by dragging the bottom right corner. You can download the file after rearranging it the way you like:

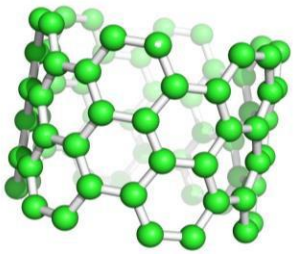


Figure 8. Carbon Nanotube (n = 6, m = 6, 3 unit cells) JPEG image on white background

<u>Create a Bucky Ball</u>

To make a Bucky Ball, select the following parameters:

- Material or Crystal System?: **Material**
- Lattice Structure: **Carbon Meshes**
- Material: **Bucky Ball (C60)**

Press **Simulate**.

Your output should look like this:

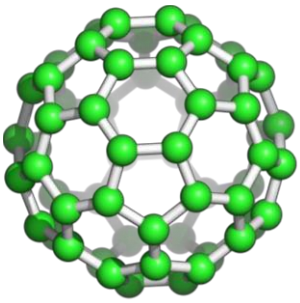


Figure 9. Bucky Ball (C60)

<u>Interesting information about the carbon structures</u>

Graphene Sheets

- 2-Dimensional
- Very thin → Transparent, yet electronically conductive
- Essentially one layer of the layered graphite mineral structure
- Andre Geim and Konstantin Novoselov won **the2010 Nobel Prize in Physics** for groundbreaking experiments regarding graphene.
- Graphene sheets may be used as a transparent conductor in future display technologies.

Carbon Nanotubes (CNTs)

- 1-Dimensional
- Three different structures for single-walled CNTs
    - Armchair (metallic) n=m
    - Zigzag (m=0)
    - Chiral
- Can be a metallic conductor or a semiconductor.
- Could be used as the smallest wires in future electronics
- Semiconducting nanotubes can be used in future transistors.

"Bucky Balls", Buckminsterfullerene, (C60)

- "zero -dimensional"
- Discovered in 1985
- The first "new" form of carbon known. Previously only graphite and diamond.
- Kroto, Curl and Smalley won the **1996 Nobel Prize in Chemistry** for this work.
- Voted molecule of the year
- Very stable
- Roundest molecule
- Bucky balls might be used as carriers in future drug delivery