# Computational Nanoscience
## Spring 2008
## Physics C203 & NSE C242

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## Homework Assignment #3 - Due February 26

**Molecular Dynamics Simulation of Carbon Nanotubes**

In this exercise, you will perform molecular dynamics simulations to calculate various properties of carbon nanotubes using LAMMPS and Tersoff potentials.

Please use our **class nanoHUB tool** with the LAMMPS code for this work.

## Setup

Use a timestep of 0.2 fs for most of your work. You can generate coordinates for a carbon nanotube from many different sources. One example is the website: **TubeGen Online**. Be sure you get the correct cell size in the z-dimension. If you use the tubegen website, it will correspond to the "Tubular Height" multiplied by the number of replication counts.

## Some things to do:

- Start with **this tube**, and relax it to its energy minimum. What are 3 different ways in which you could compute the frequency of its radial breathing mode? Now compute that frequency using 2 of these 3 methods and compare the results. You may find **this coordinate file** useful - it's the same tube but the coordinates are stretched in the direction of the breathing mode. For both coordinate files the cell dimensions are listed in the subject lines.

- Use the coordinates for a C60 fullerene molecule provided by our tool. Optimize the

structure, and compare its binding energy per atom with that of the nanotube. Which one is more stable? Is the difference what you would expect? Now find the relative binding energies at 800K and explain any differences.

- As a follow-up to our in-class simulations, pick any nanotube you like and do one of the following two simulation experiments:
    - Either compute the Young's modulus as a function of nanotube radius,
    - or, compute the Young's modulus for a pristine carbon nanotube and then for the same carbon nanotube with a Stone--Wales defect. How does the defect affect the modulus?
    - BONUS: Explain how the Young's modulus for the nanotube changes at finite temperature.