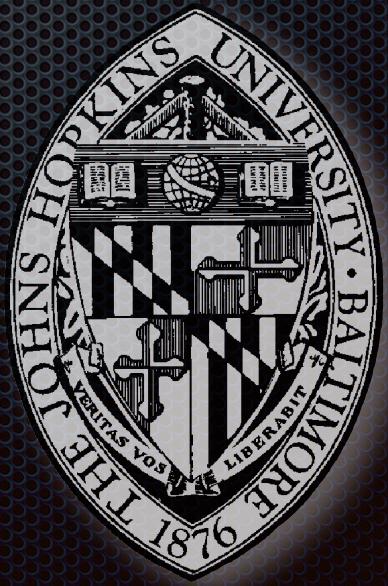
Project D
Build Your Own Carbon Nanotube

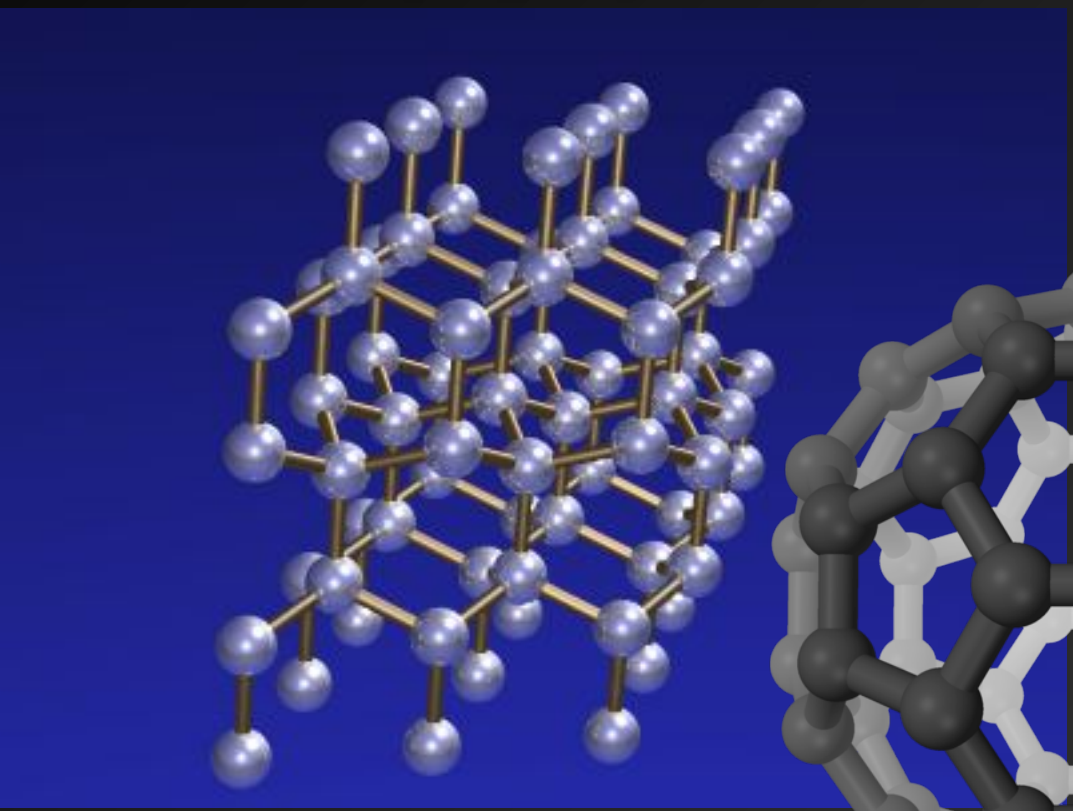
EN500.113 Gateway Computing: Python

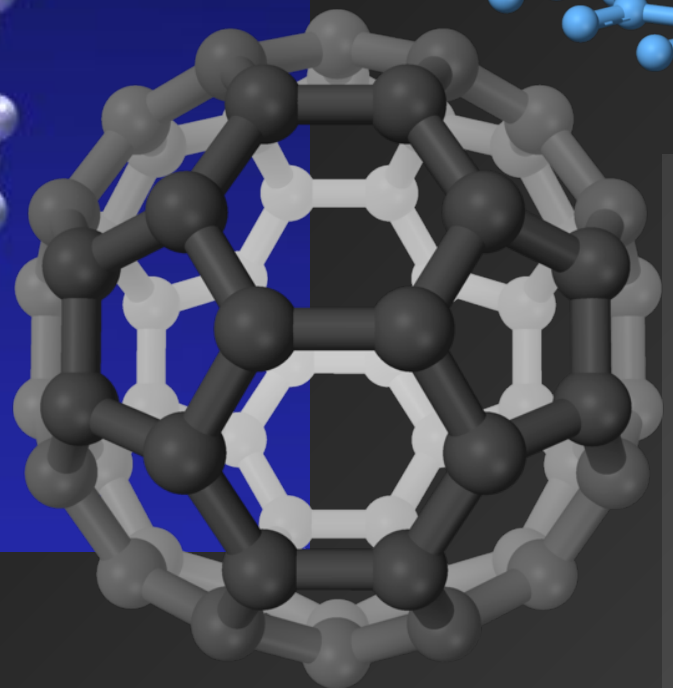
Whiting School of Engineering,
Johns Hopkins University

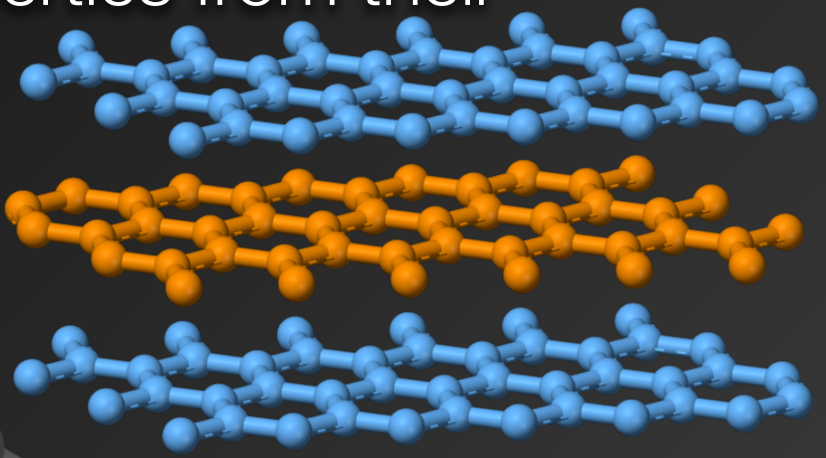


Crystal Structures in Materials

- Many materials derive their properties from their underlying crystal structure.







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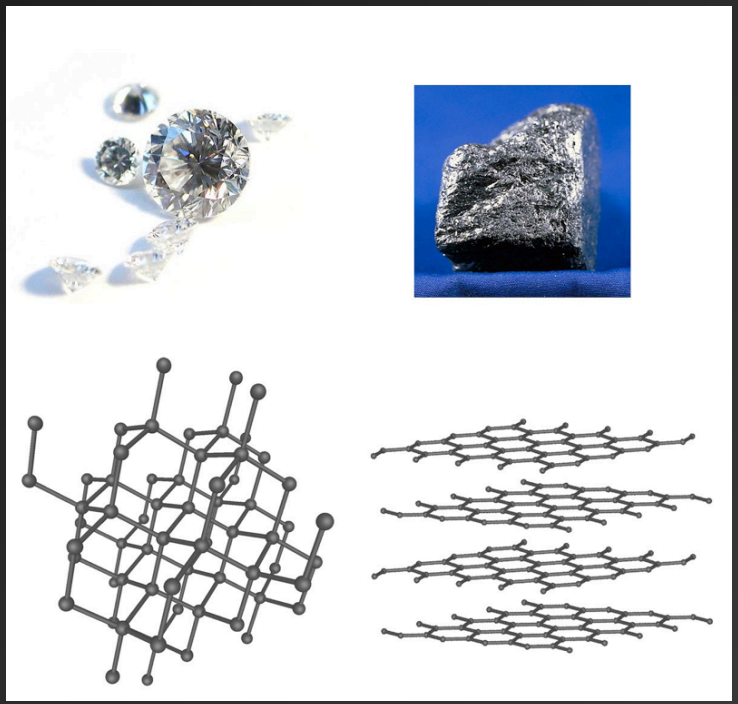
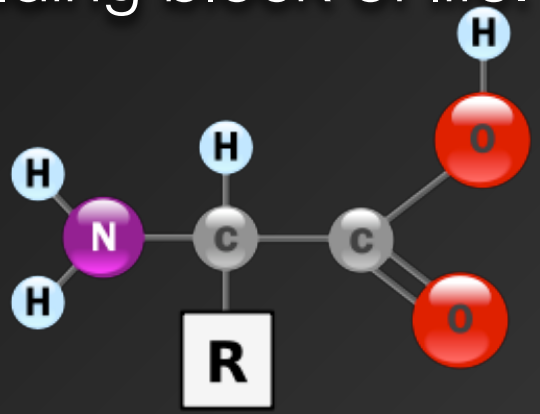
- Carbon is perhaps the most versatile of atoms.
- Typically pure carbon is found as carbon or graphite.
- Hydrocarbon compounds are the foundation of our fossil fuel based energy economy.
- C is a critical building block of life.





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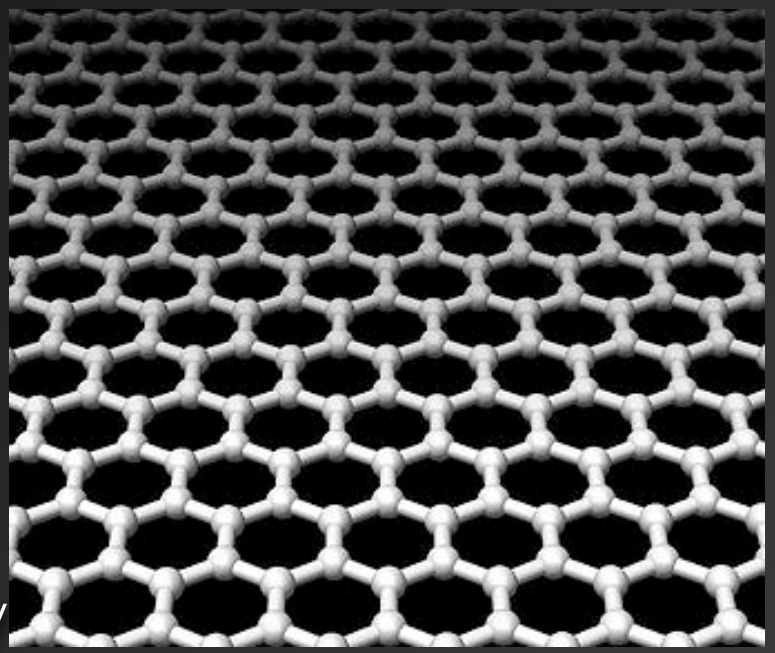
- Graphene is a single sheet of graphite
- First isolated in 2004 graphene is interesting for its unique electron transport characteristics and possible applications in spintronics.
- Graphene costs have dropped from nearly $300 per gram (Gold costs $50/gram) to as low as $0.10 per gram, making it feasible to compete with Silicon in electronic applications.



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- 2010 Nobel Prize was awarded for Graphene research:

  Geim and Novoselov extracted the graphene from a piece of graphite such as is found in ordinary pencils. Using regular adhesive tape they managed to obtain a flake of carbon with a thickness of just one atom. This at a time when many believed it was impossible for such thin crystalline materials to be stable.

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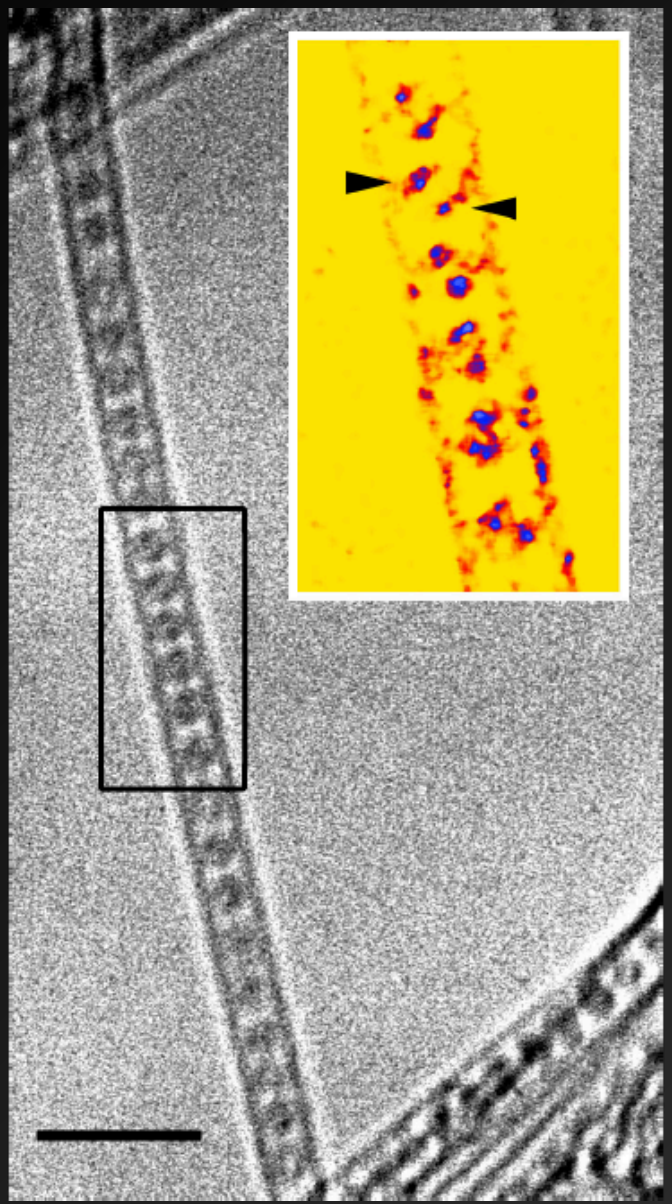
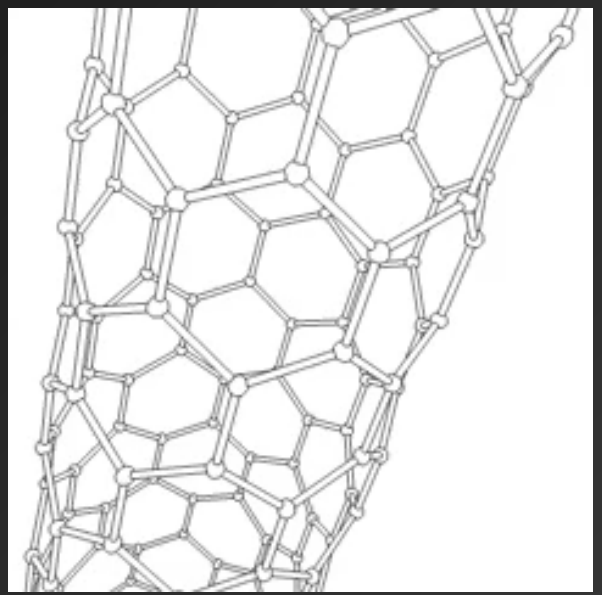


- First observed in 1991, carbon nanotubes are one of the linchpins of nanotechnology research.
- They consist of a graphene sheet rolled up into a tube.



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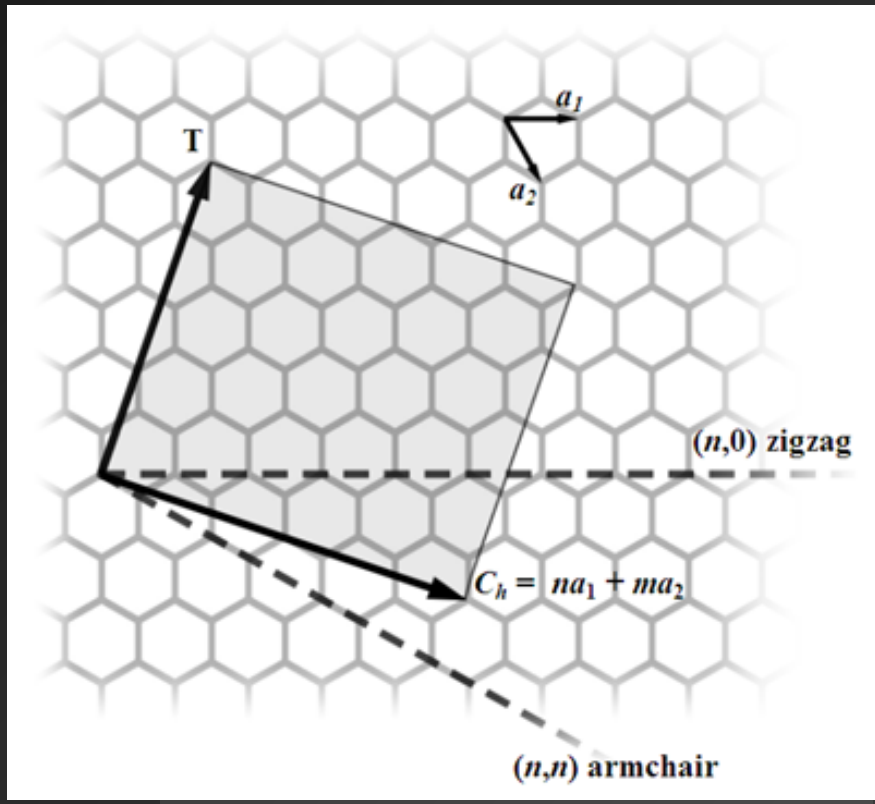
- There are a countable, but infinite number of ways to construct nanotubes.
- Each nanotube type is denoted by two positive integers n and m such that n>=m.
- The value of n and m determine if the tube acts like a metal or a semiconductor.
- When m=0 the tube is zig-zag, and when m=n it is armchair. Otherwise it is chiral.
- In this diagram C_h is the direction that will be rolled up and T is the direction of the tube axis.



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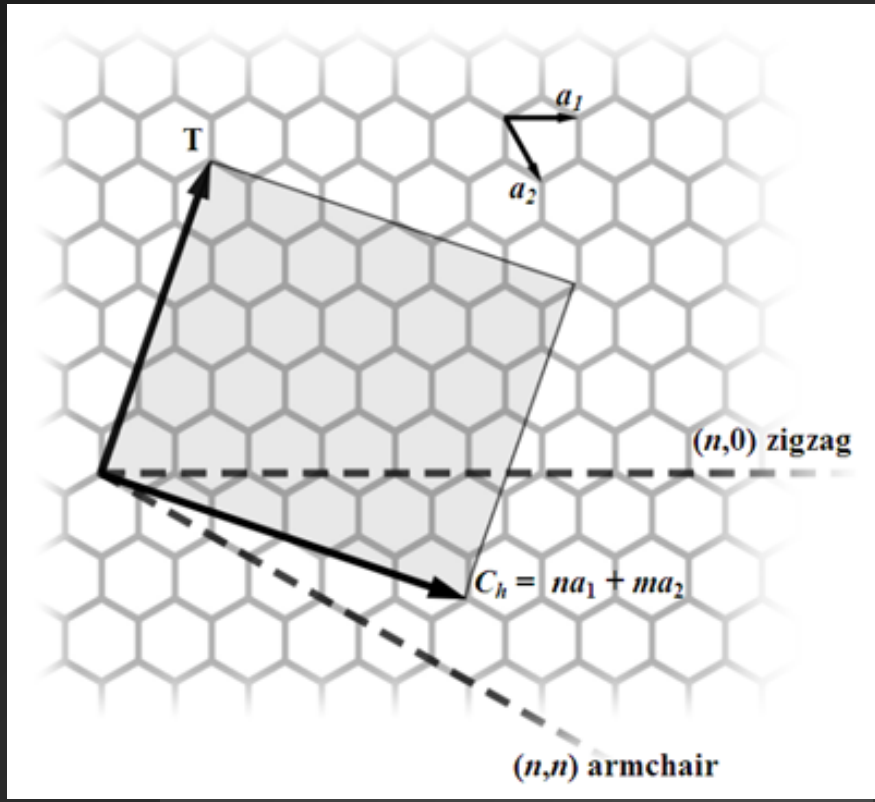
- To construct the vector C_h, we hop n times in the a_1 direction and m times in the a_2 direction.
- $C_h = n\,a_1 + m\,a_2$
- Your job will be do make a program that
  - Makes a rectangle of carbon sheet described by the numbers n and m and a third number l that gives the length of T.
  - Makes a carbon nanotube from this same sheet by rolling it up.



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- First run your code to create a list of atom positions for the graphene and the nanotube, i.e.
  pos_gr, pos_nt =Graphene(5,2,5)
- Then you should be able to type
  atomplot(pos_gr, pos_nt)
  to plot the tube using the **atomplot** function provided.
- Make sure to test zig-zag, chiral and armchair tubes.
- Quantitatively check against the examples provided.
- Answer the application question about encapsulation of a drug within a nanotube.