

## How can the structural aspects of carbon nanotubes explain their extraordinary properties?

Carbon nanotubes have the following structural features:

1. Six membered carbon ring: This is the basic building block of carbon nanotubes. Six carbon atoms are covalently bonded in a hexagonal formation through SP<sup>2</sup> hybridized orbitals. This leads to the formation of a planar structure with six delocalized  $\pi$  electrons residing on both the sides of the plane.
2. Graphene sheet: Unsatisfied carbon valencies at the corners of the hexagonal rings lead to replication of the six membered ring structure to form a two dimensional sheet called as a 'graphene sheet'. Thus a graphene sheet is a planar network of adjoining aromatic rings which facilitates the delocalization of  $\pi$  electrons across the sheet. This graphene sheet is one atom thick. Hence all the carbon atoms lie on the surface and are exposed to the surroundings.
3. Tubular structure: Graphene sheet when rolled up and bonded edge to edge forms a tubular structure called a single wall nanotube (SWNT). The tube is 1~10 micron long and 1 nm in diameter. Due to this tubular structure at the atomic level, the movement of the electrons is confined along the cross section in two dimensions. The delocalized  $\pi$  electrons possess great mobility along the length of the tube. Hence nanotubes are considered one dimensional nanostructure.
4. Anisotropy: There are two sources of anisotropy. First is due to the high aspect ratio (~1000) causing 2D quantum confinement. The second is due to chirality which arises from the orientation of rolling of the graphene sheet with reference to the hexagonal structure. The direction of rolling is called the chiral vector. If the direction of rolling is parallel to the two opposite sides of hexagon, the resultant tube is called 'armchair' nanotube based on the shape of the edge at the end of the tube. If the direction of rolling is perpendicular to the two opposite sides of the hexagon, then the tube is called as 'zig-zag' nanotube describing the edge of the end. There are many other intermediate configurations possible which are known as 'chiral' nanotubes.

5. Number of walls: Carbon nanotubes may be single walled (SWNT) or multi-walled (MWNT), formed by co-axial cylindrical tubes of progressively higher diameter. The number of walls can vary from 3 to 15.
6. End caps: Edges of the nanotubes may be open or closed. These ends are highly reactive due to the imbalance in bond structure.
7. Inter-tube attraction: The  $\pi$  electrons on the tube surface induce dipole character in the tubes which leads to strong van der Waals forces operating among the tubes at the point of contact.

With the above back ground, the characteristics of the nanotubes can be explained as shown in Figure 1 below:

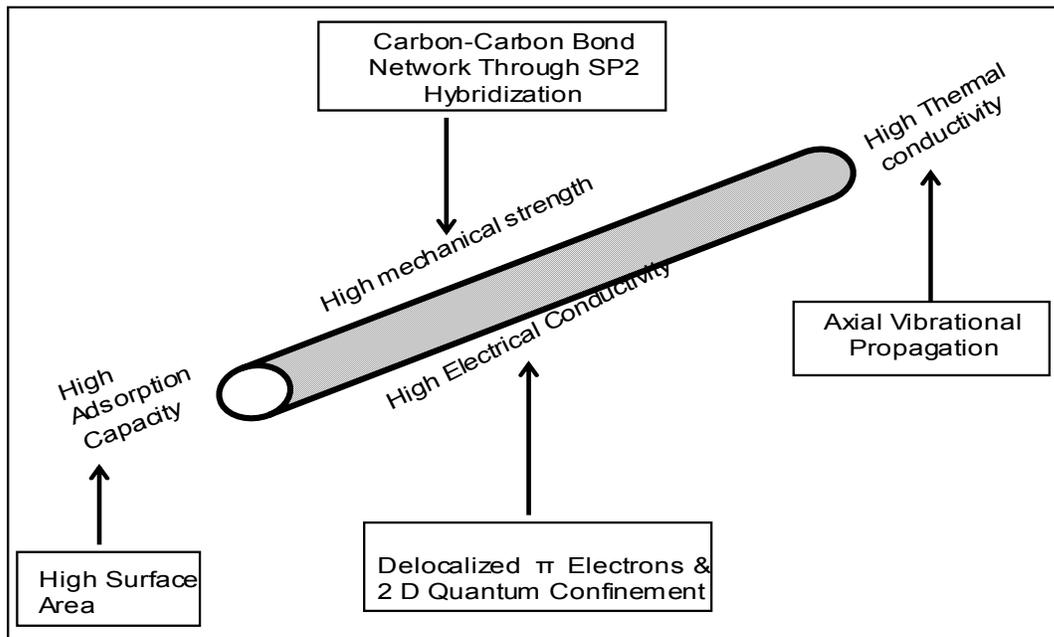


Figure: Properties of Carbon Nanotubes

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