

# Nanocarbon

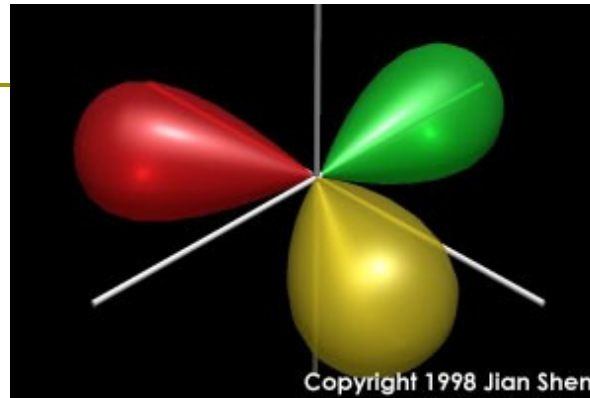


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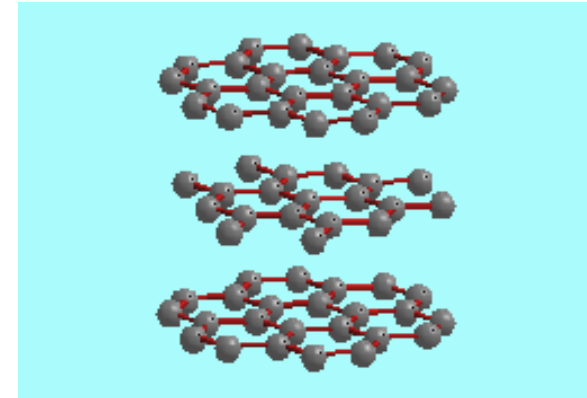
## graphite



## $sp^2$ hybridised



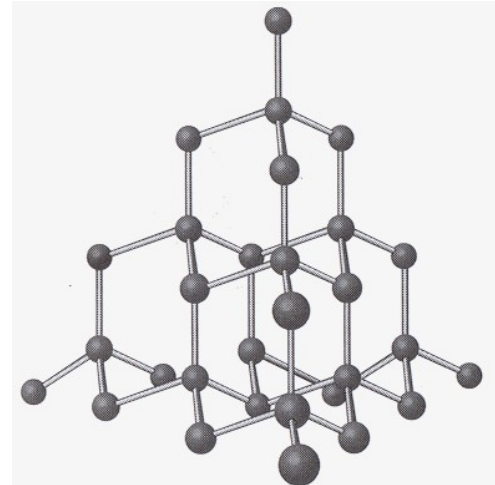
The lowest-energy state of elemental carbon at ambient pressure and temperature is graphite



## diamond



## $sp^3$ hybridised

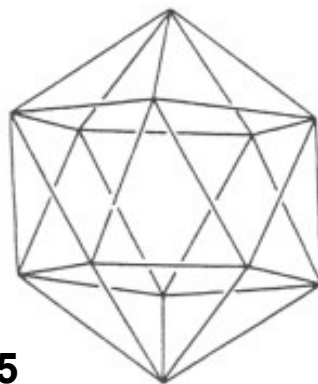
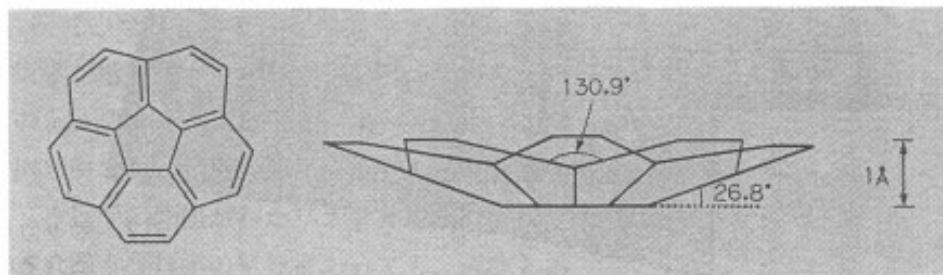


**E. Osawa, a quantum chemist, had predicted the possibility of a stable  $C_{60}$  molecule in 1970 using a simple Hückel model. The only article he ever published in Japanese!**

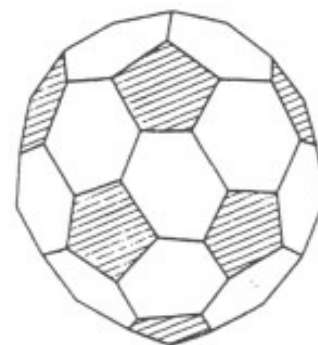
Russian quantum chemists D. Bochvar and E. Galpern predicted the stability of  $C_{60}$  "footballene" in 1973 [Doklady Akademii Nauk 1972]

В 1973 году московские химики Дмитрий Бочвар и Елена Гальперн подсчитали, что квантовая химия теоретически допускает существование и некой новой разновидности углерода, молекула которого должна быть копией футбольного мяча: сфера, составленная из шестигранников или пятигранников.

サッカーボール分子  $C_{60}$  の発想のきっかけとなったコランニュレン分子の構造



(12)



**"Buckminsterfullerene" discovered 1985**

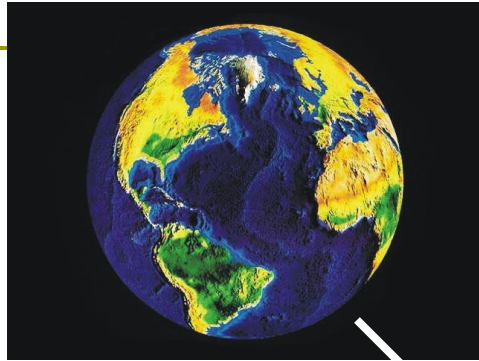
**Nobel prize in chemistry, 1996**

**Produced as pure material in 1990  
(Krätschmer und Huffman)**

## Size Comparison

New "nanomaterial" with a wide range of interesting properties

- light weight and record-high elastic modulus
- strongest fibres that can be made
- high thermal conductivity
- metallic or semi-conducting (depending on geometry)



Earth  $10^7$  m

$10^{-8}$

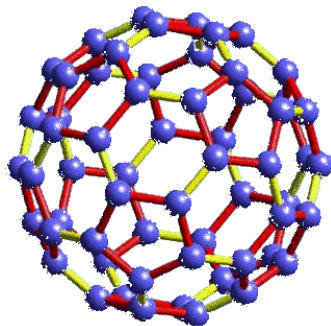
Football 0.1 m



Fullerene

$10^{-9}$  m

$10^{-8}$

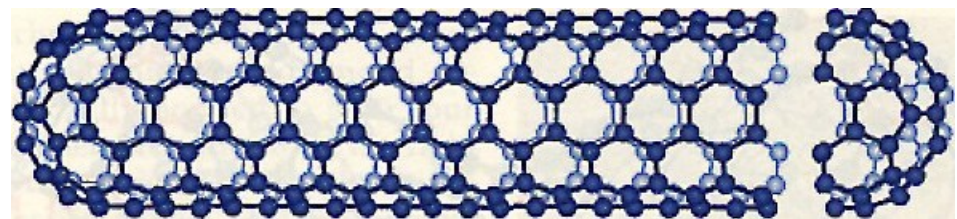


Bulk material is interesting for composite materials e.g. smart clothing, conducting paper, modifying polymer properties.....

Quasi-one dimensional structures -  
Theoreticians love them!

100 000 nm

1 nm



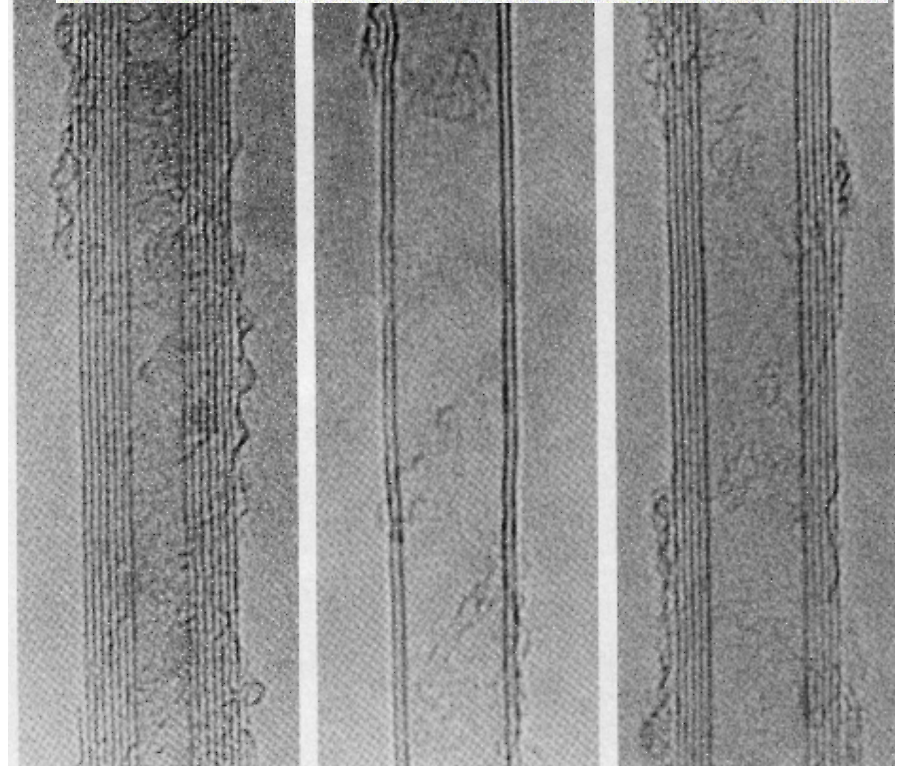
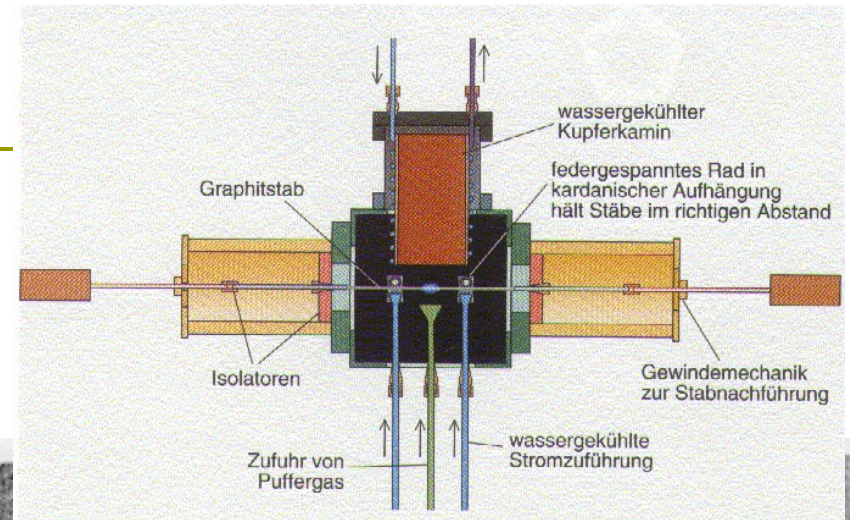
# "Helical microtubules of graphitic carbon", S. Iijima, Nature 354, 56 (1991)



**MWNT discovered in 1991 by Sumio Iijima**

- Diameter of  $\sim 5\text{-}10\text{ nm}$
- Concentric cylinders of carbon with a length of several mm

**SWNT in 1993**



Rolled up graphite sheets,  
 no unsatisfied surface bonds  
 Single walled or multi-walled  
 Metallic or semiconducting  
 Band gap of SWNTs =  
 $f(\text{chirality, diameter})$   
 or 'wrapping vector'  $(n,m)$   
 Multi-walled are metallic

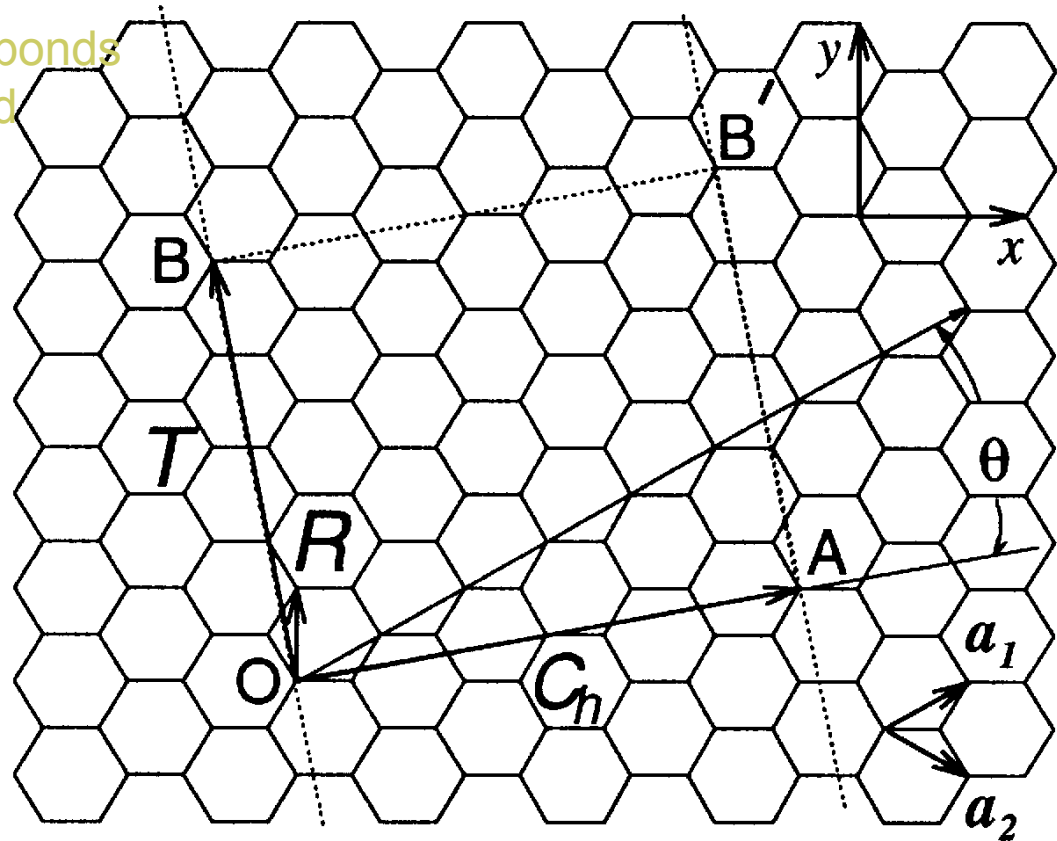
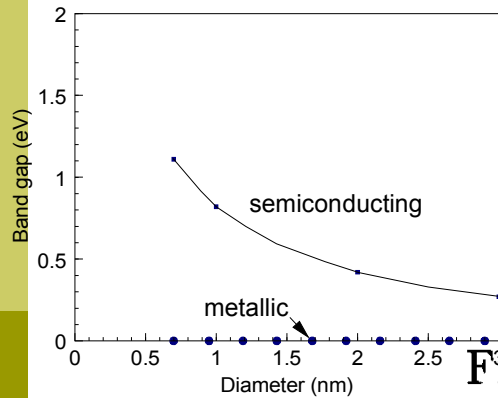
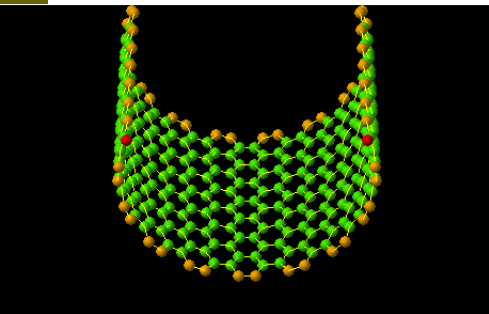


Fig. 3.2: The unrolled honeycomb lattice of a nanotube. When we connect sites  $O$  and  $A$ , and  $B$  and  $B'$ , a nanotube can be constructed.  $\vec{OA}$  and  $\vec{OB}$  define the chiral vector  $\mathbf{C}_h$  and the translational vector  $\mathbf{T}$  of the nanotube, respectively. The rectangle  $OAB'B$  defines the unit cell for the nanotube. The vector  $\mathbf{R}$  denotes a symmetry vector (see Sect. 3.4). The figure corresponds to  $\mathbf{C}_h = (4, 2)$ ,  $d = d_R = 2$ ,  $\mathbf{T} = (4, -5)$ ,  $N = 28$ ,  $\mathbf{R} = (1, -1)$ .

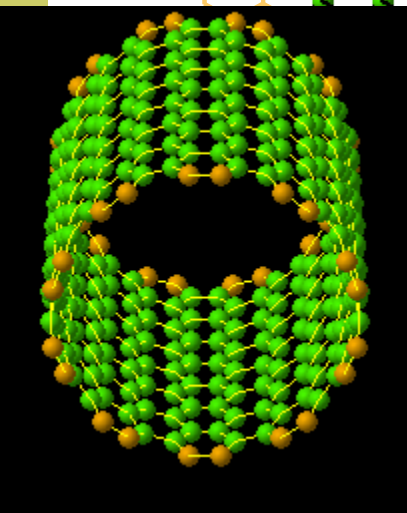
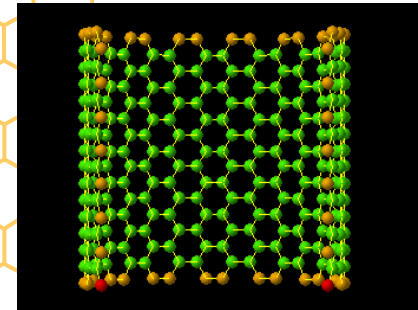
# Wrapping (10,10) SWNT



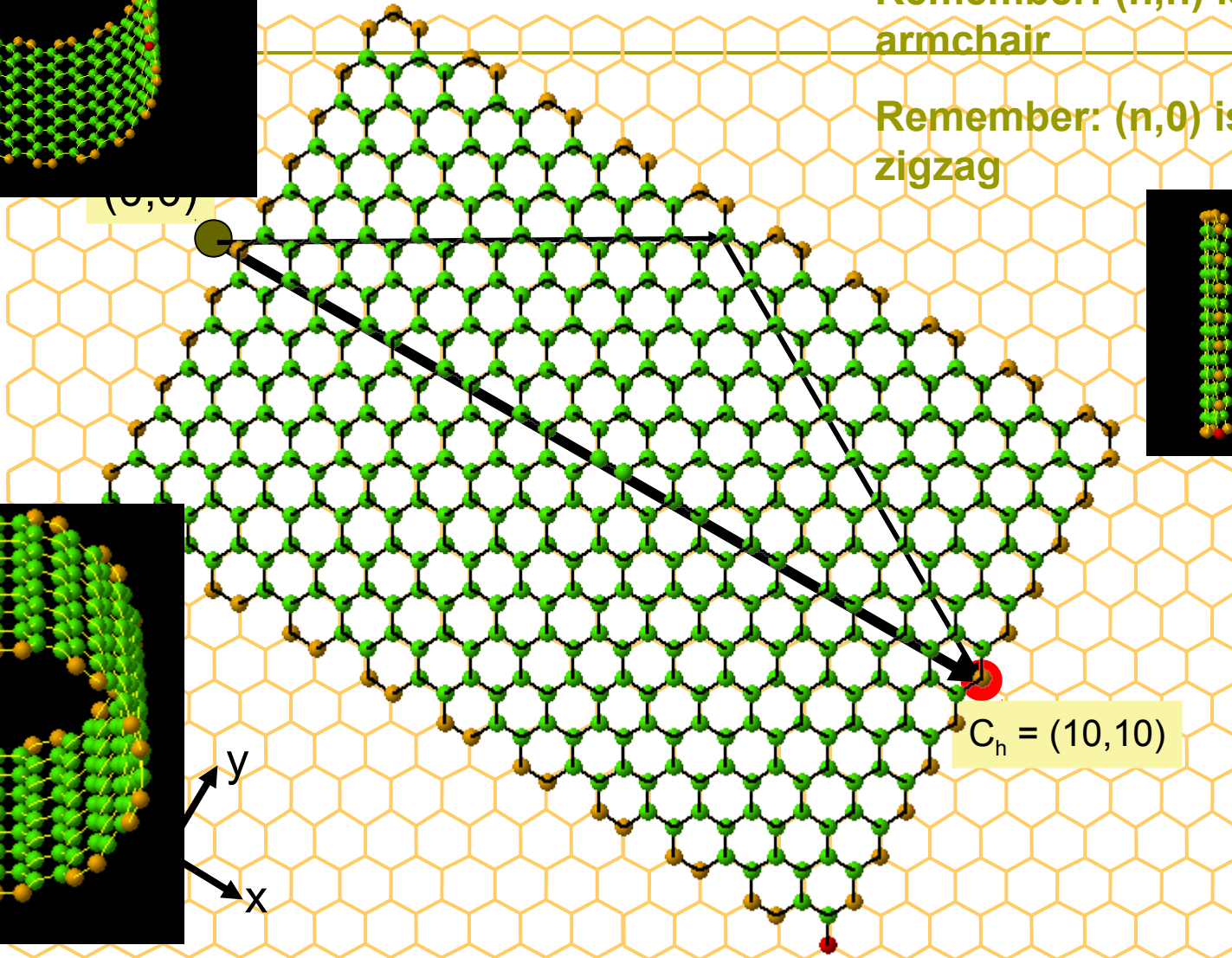
$(0,0)$

Remember:  $(n,n)$  is always armchair

Remember:  $(n,0)$  is always zigzag

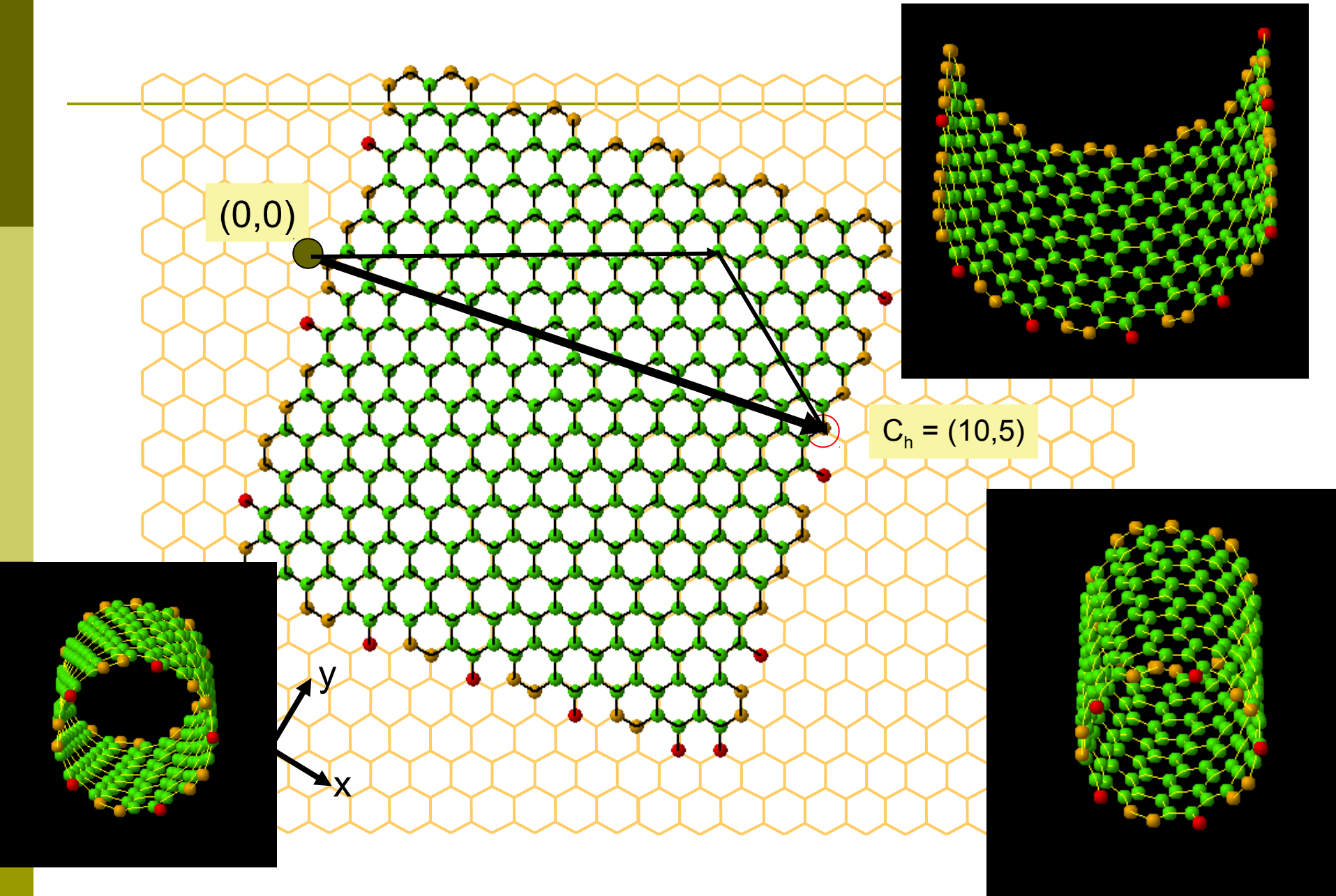


y  
x



$C_h = (10,10)$

# Wrapping (10,5) SWNT (chiral)

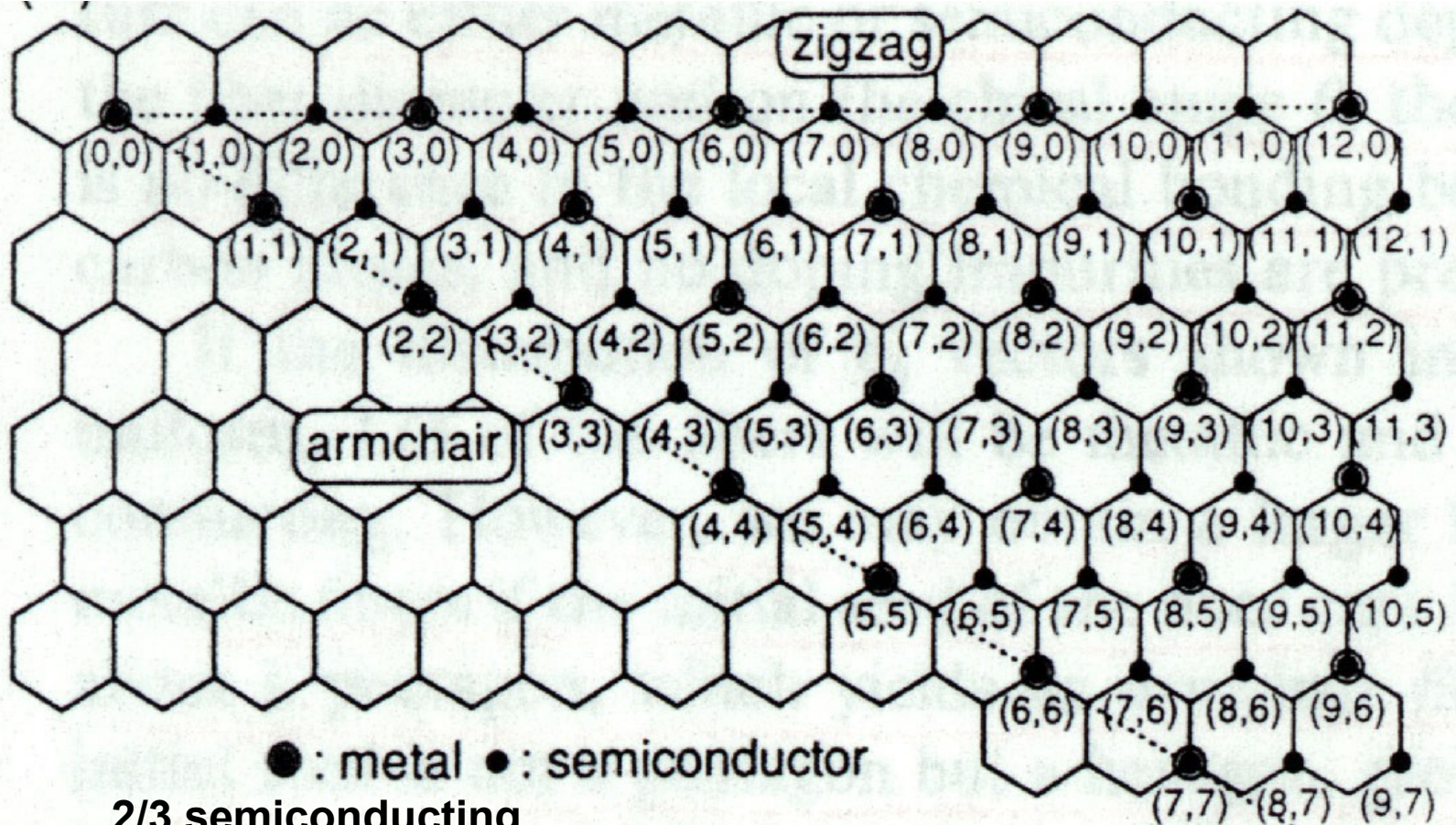


**All Armchair (n,n) tubes are metallic**

**Zigzag tubes (n,0) are metallic if n is a multiple of 3**

**Chiral tubes are semiconducting, bandgap scales with 1/d**

**or metallic if  $n-m = 3q$**



**2/3 semiconducting**

**1/3 metallic**

# Nanotubes coordinates

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- <http://k.1asphost.com/tubeasp/tubeASP.asp>
  - XMOL (xyz)
  - SIESTA
- <http://turin.nss.udel.edu/research/tubegenonline.html>
  - Gaussian (PBC)
  - WIEN2k
  - XYZ
  - CIF