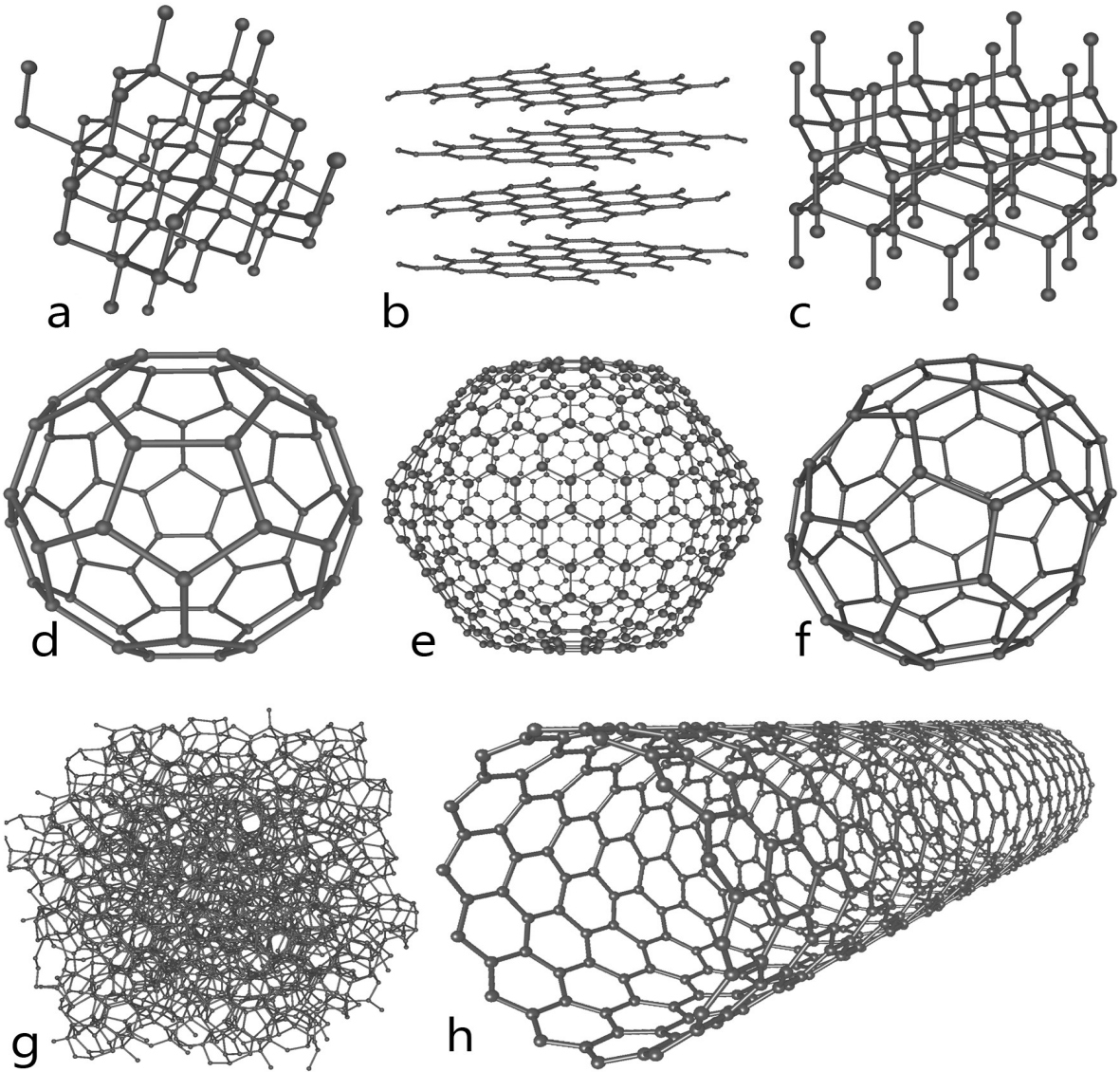

Carbon-Carbon bonds: Hybridization

Gina Peschel
05.05.2011

Content

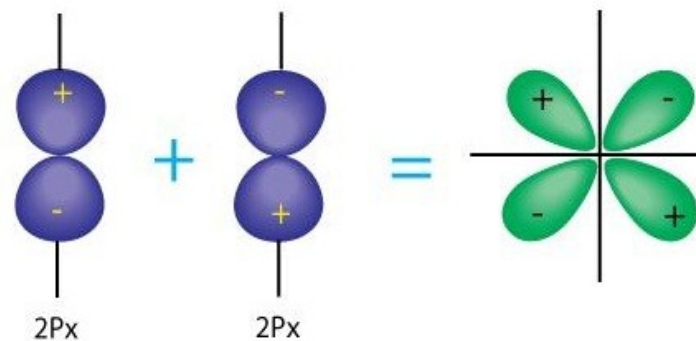
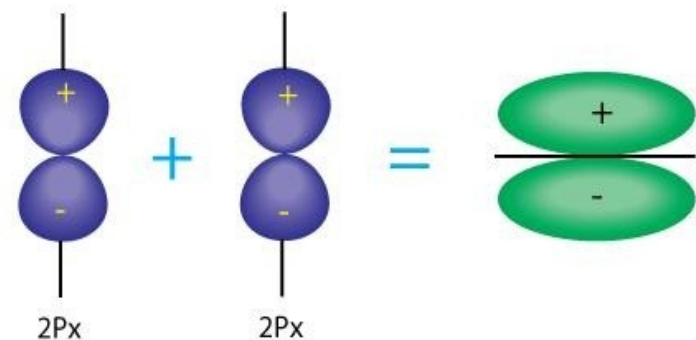
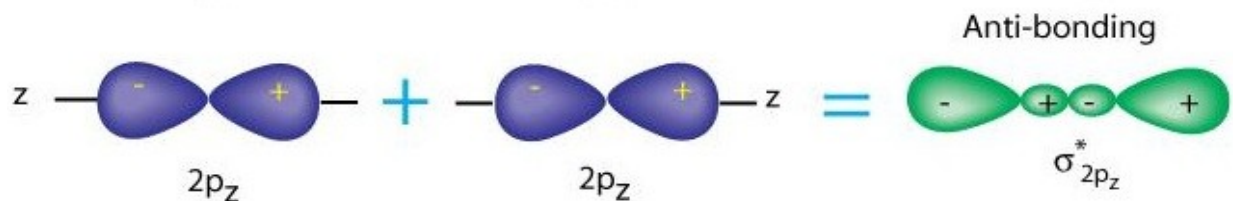
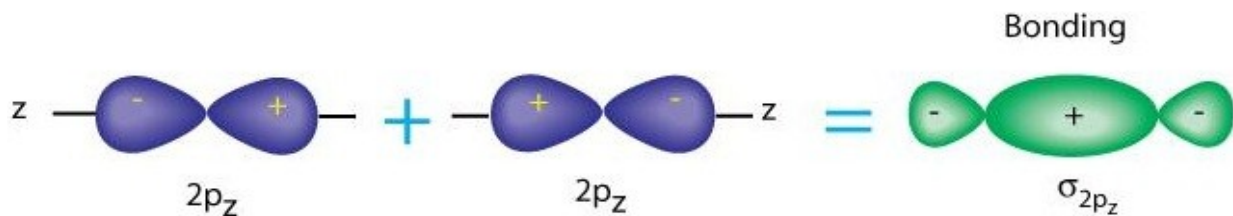
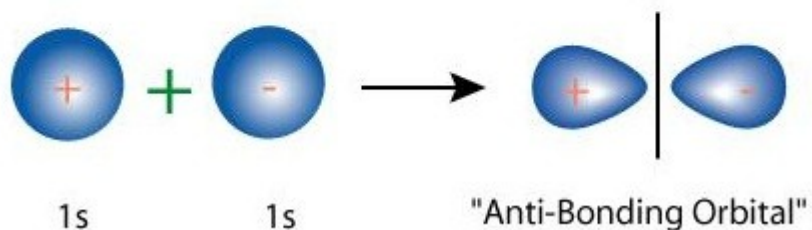
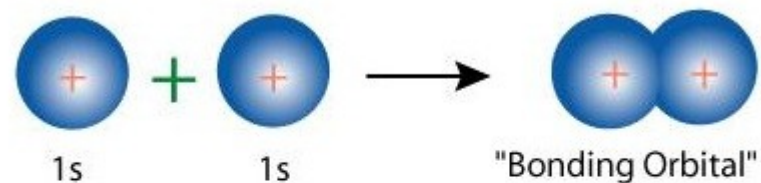
- Manifestation of Carbon
- sp^3 -, sp^2 - and sp - Hybridization
Graphite and diamond
- Rolled carbon materials
 - Rehybridization
 - Reactivity

Manifestation of Carbon

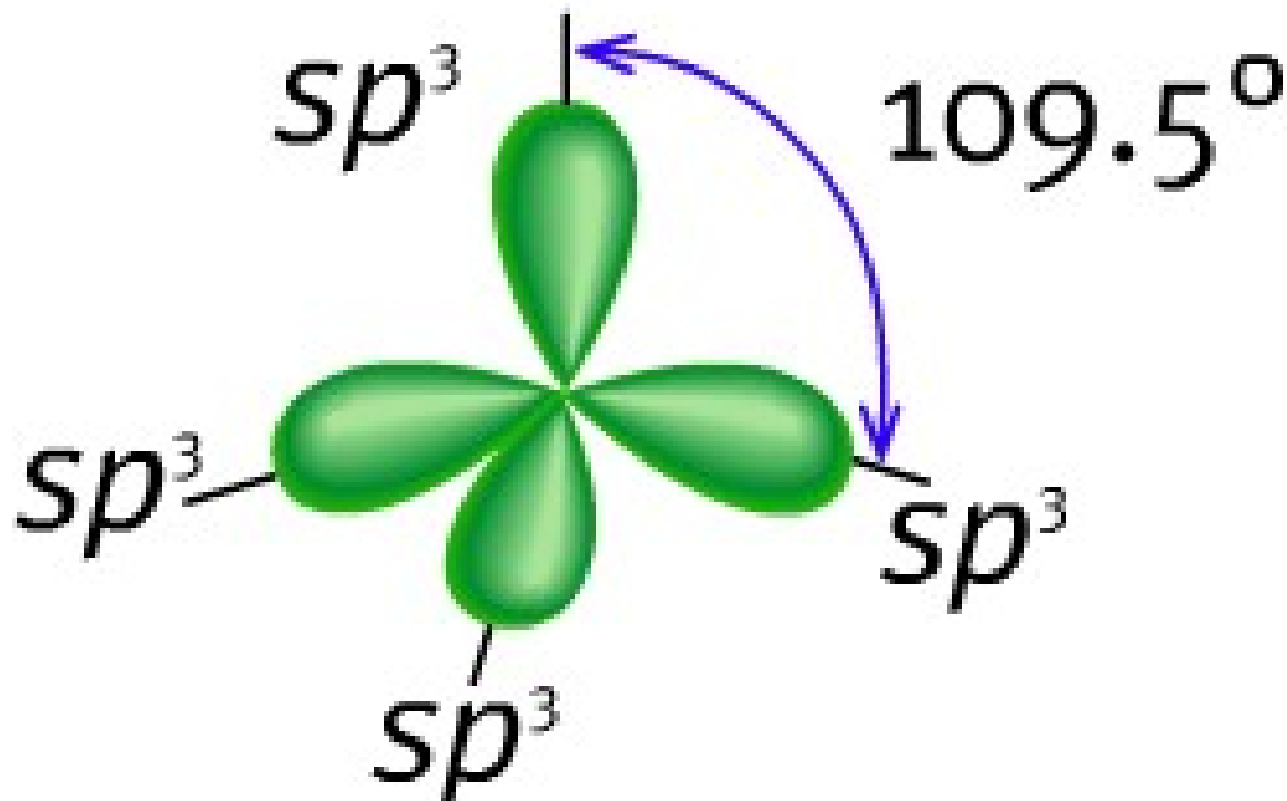


- a) Diamond
- b) Graphite
- c) Lonsdaleite
- d-f) Fullerenes (C₆₀, C₅₄₀, C₇₀)
- g) Amorphous carbon
- h) Carbon nanotube.

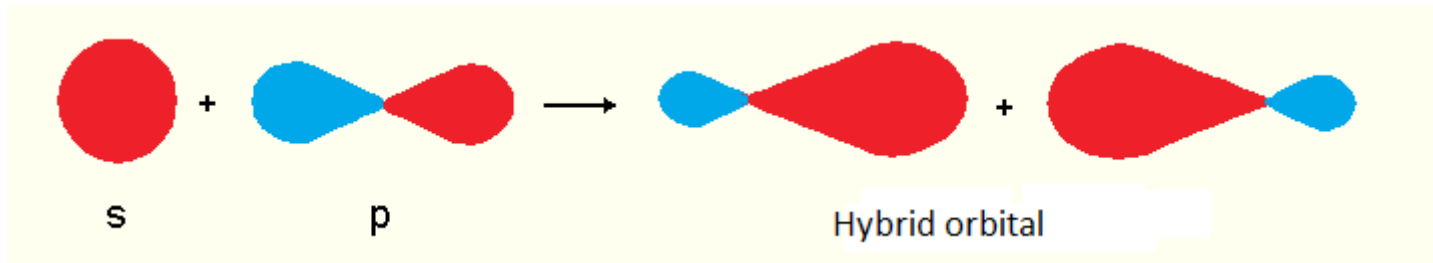
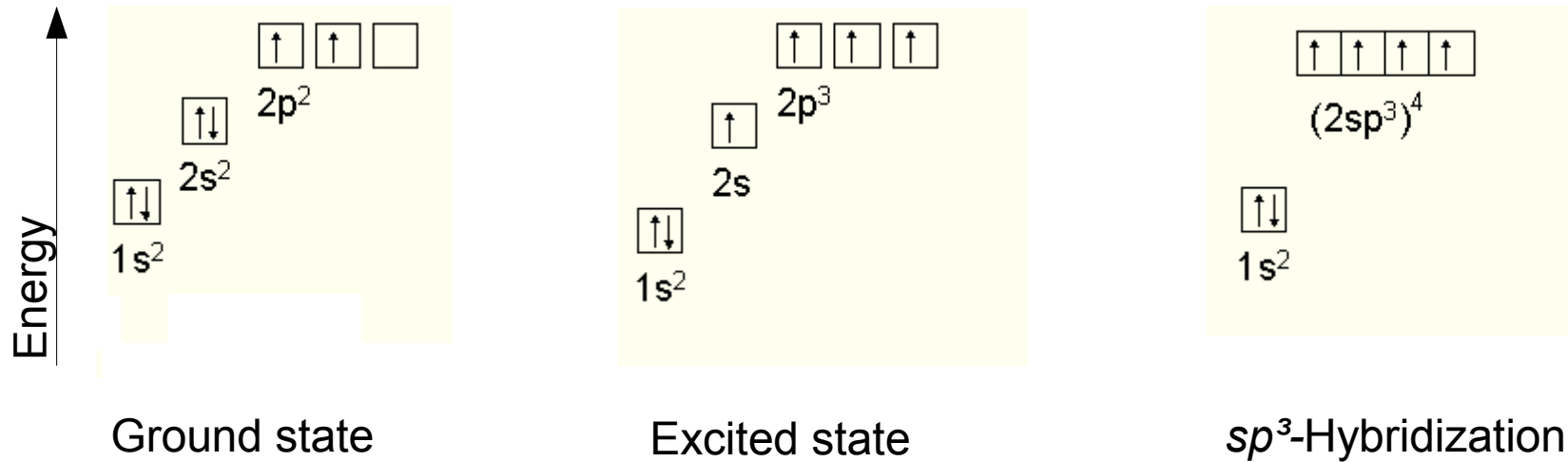
Bonding of molecular orbitals



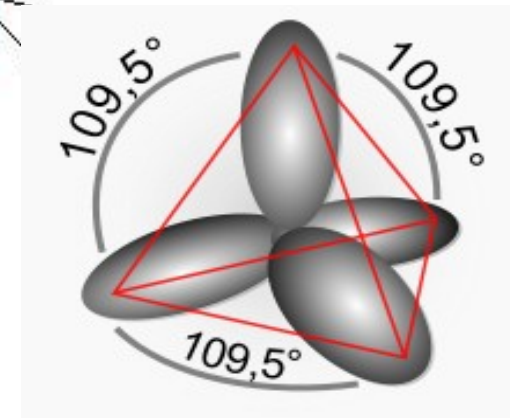
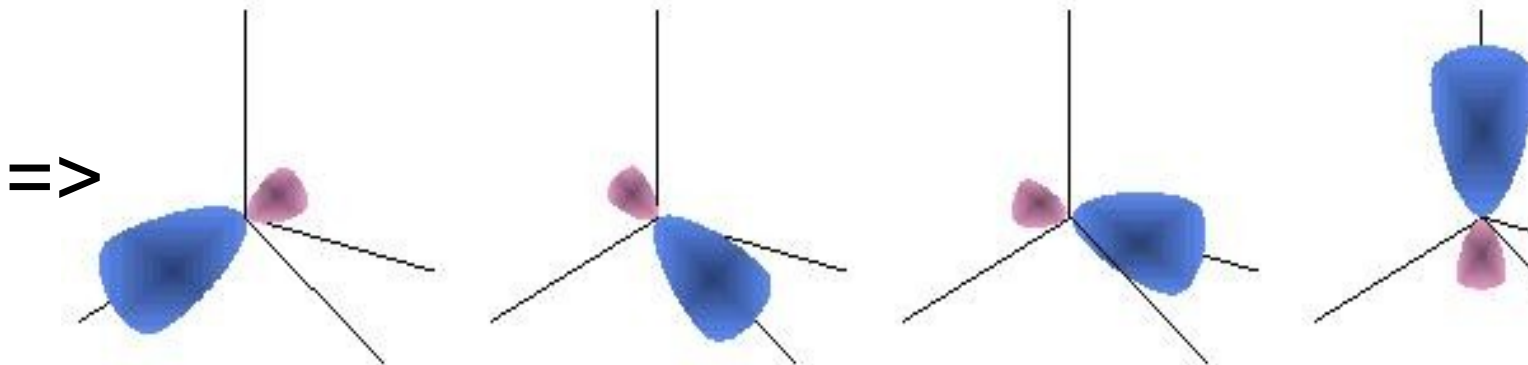
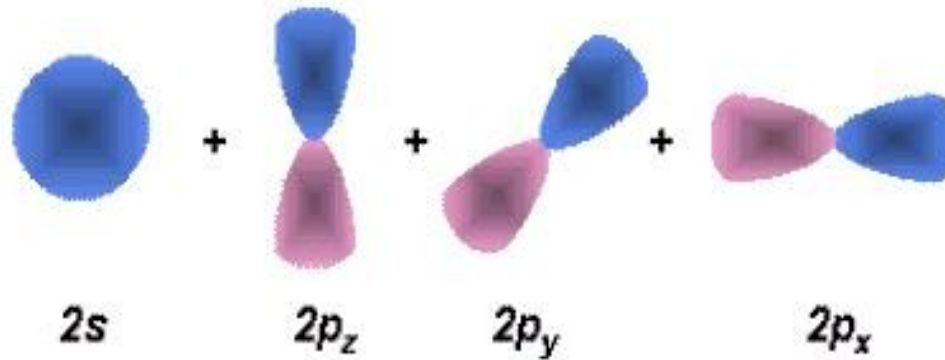
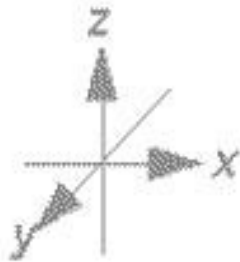
Hybridization



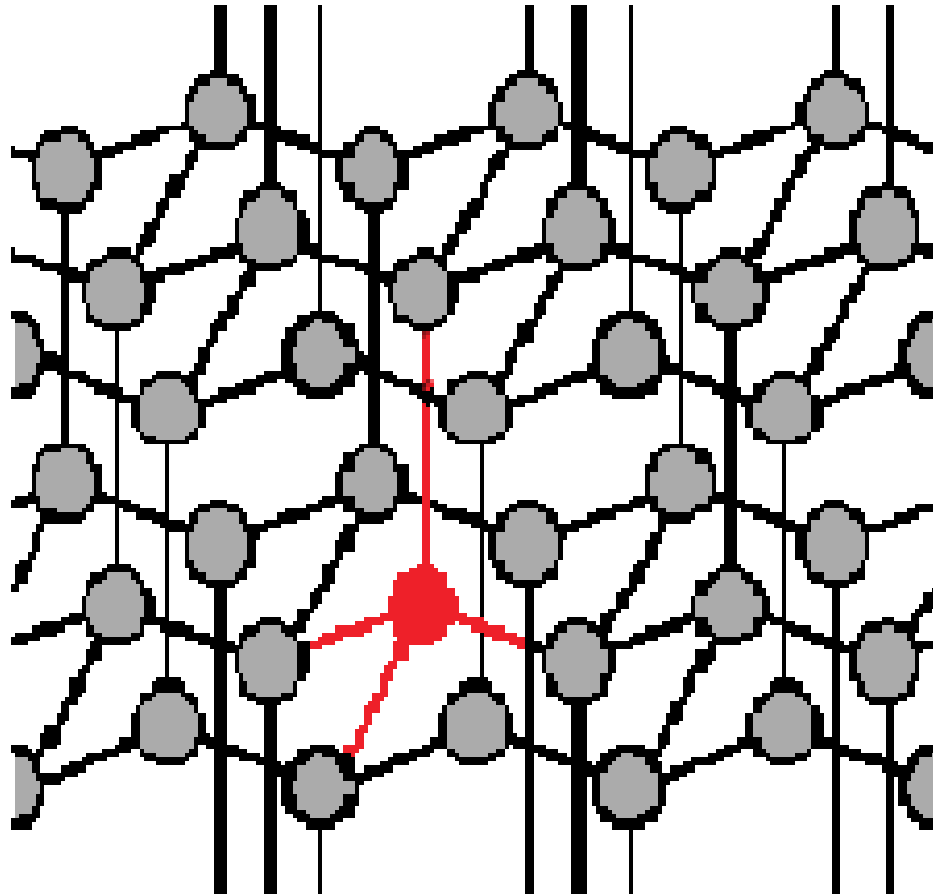
sp^3 - Hybridization



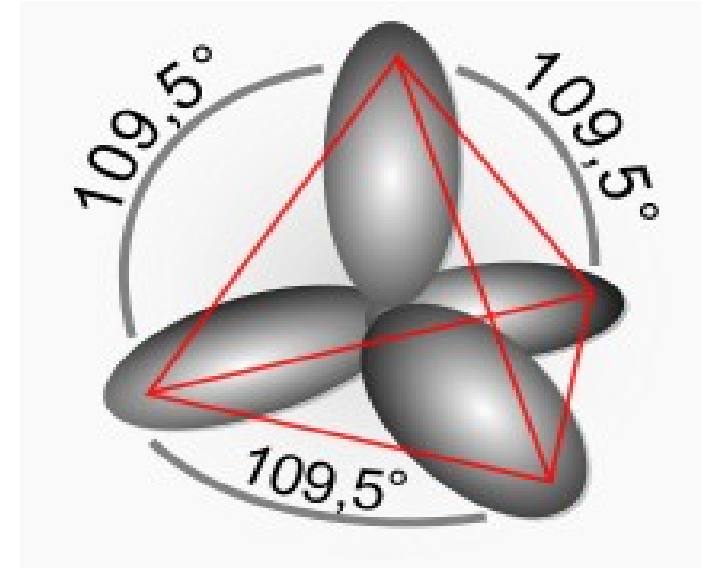
sp^3 - Hybridization



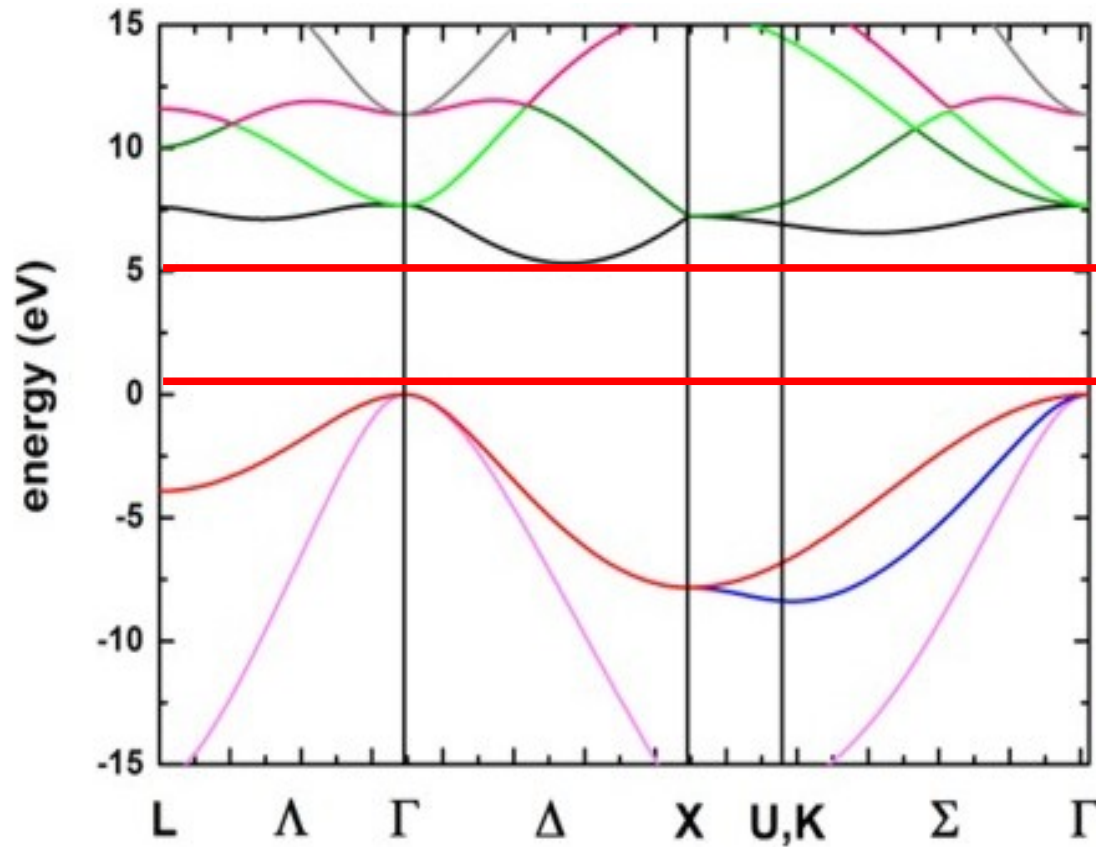
sp³ - Hybridization



Diamond



Bandstructure of diamond



$E_g = 5 \text{ eV}$



Diamond

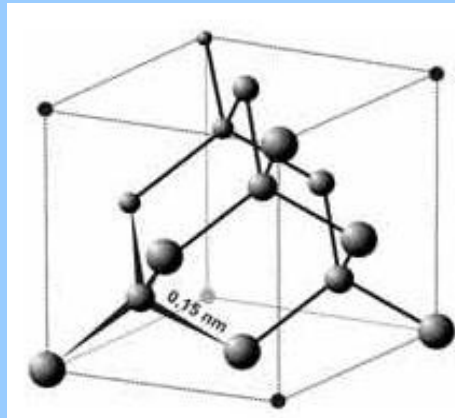
Hardness



Color



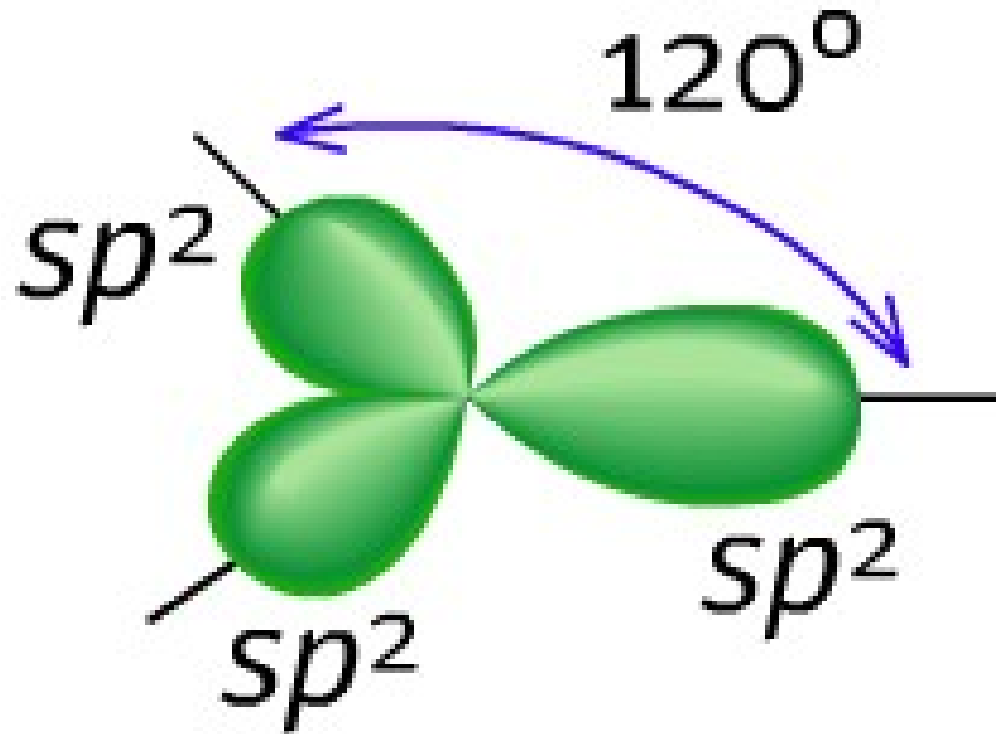
Crystal structure



Electr. conductivity

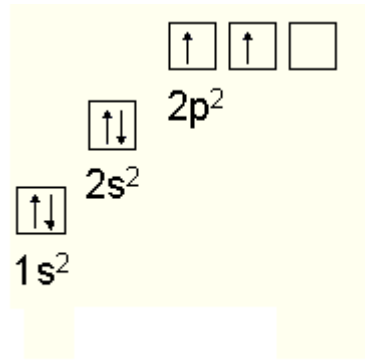


Hybridization

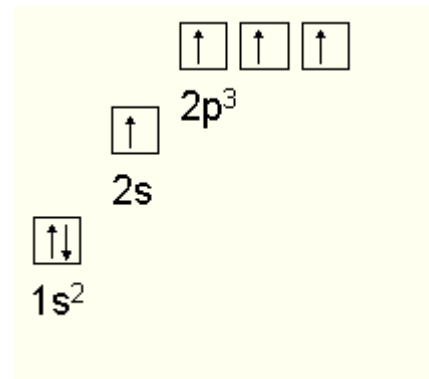


sp^2 - Hybridization

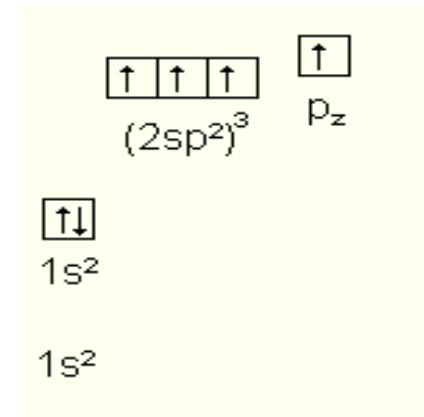
Energy ↑



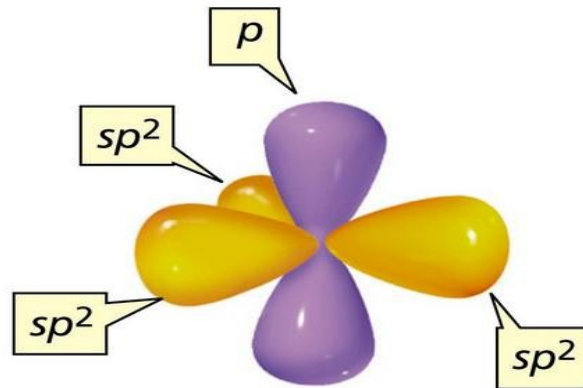
Ground state



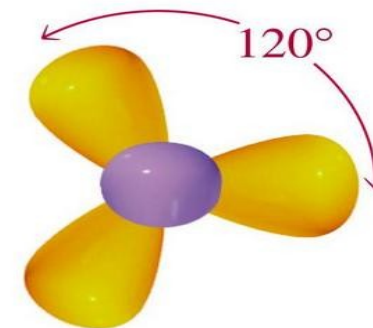
Excited state



sp^2 - Hybridization

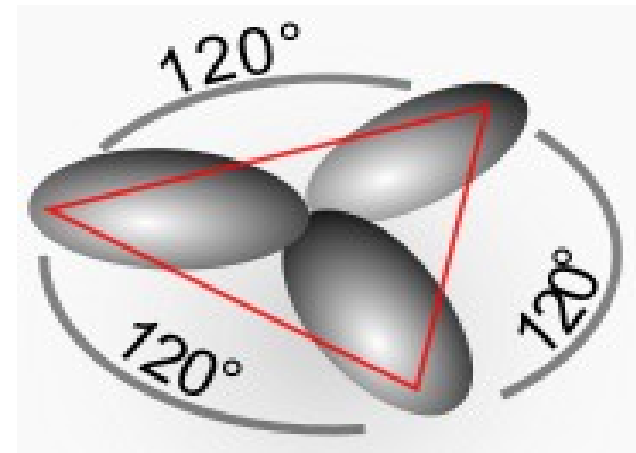
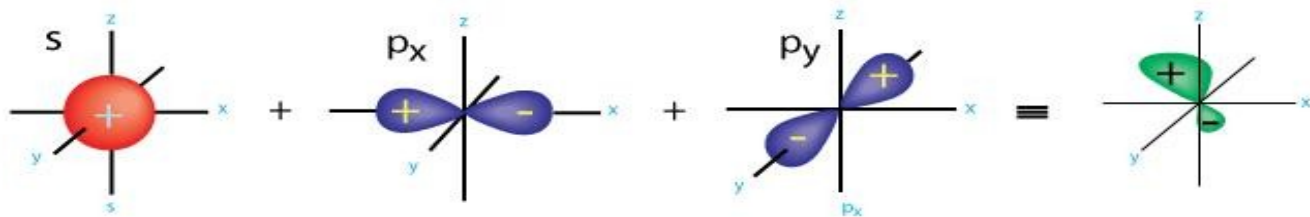
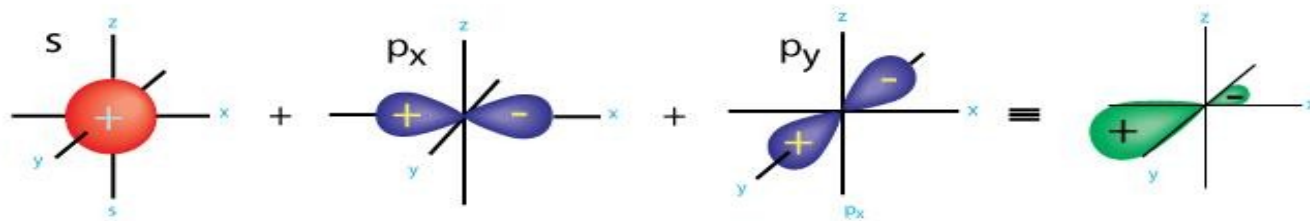


side view

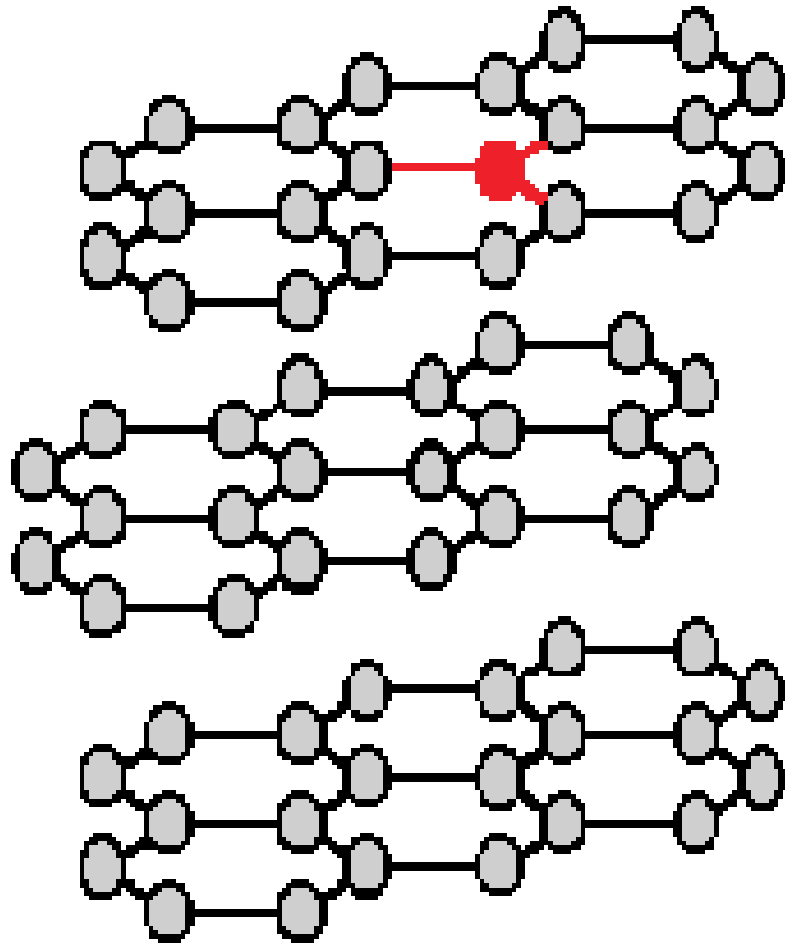


top view

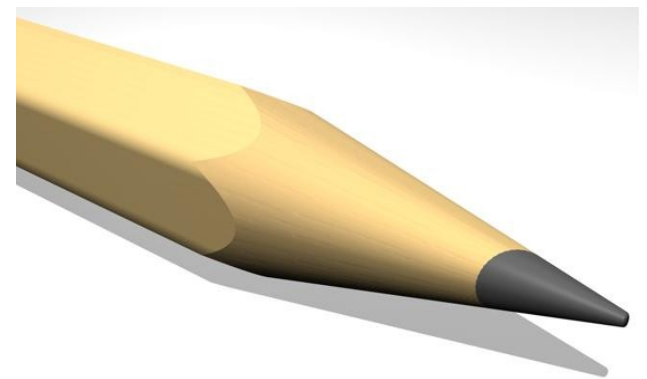
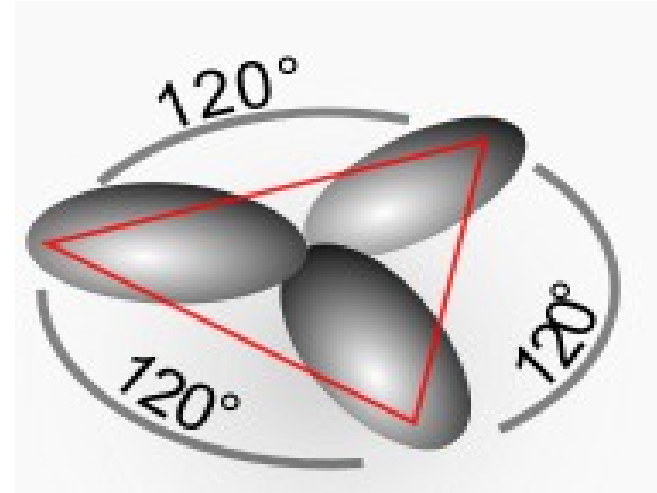
sp² - Hybridization



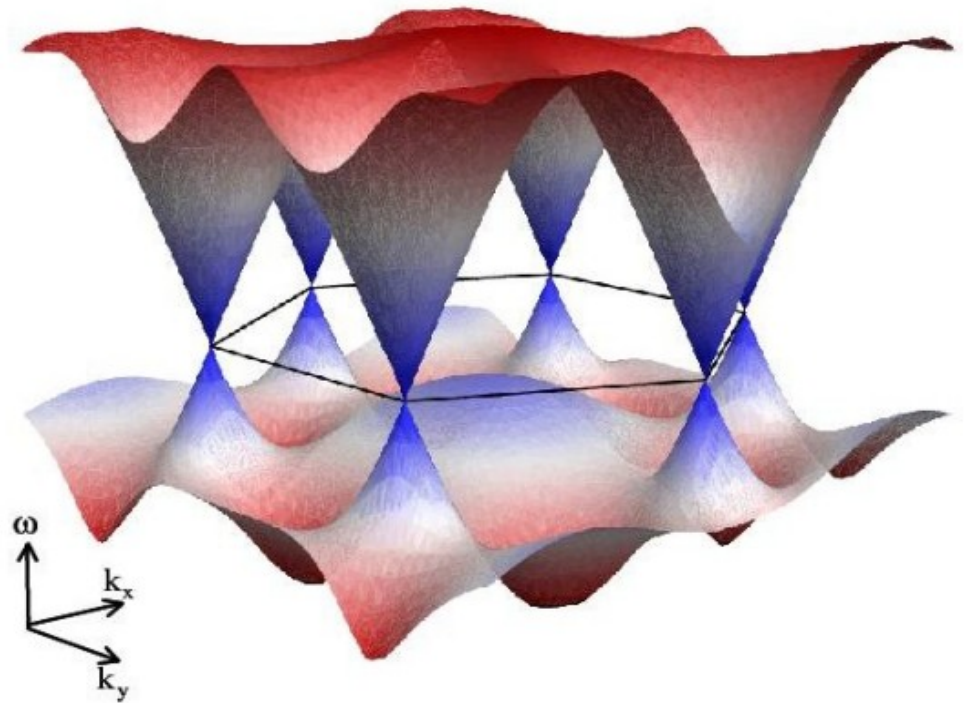
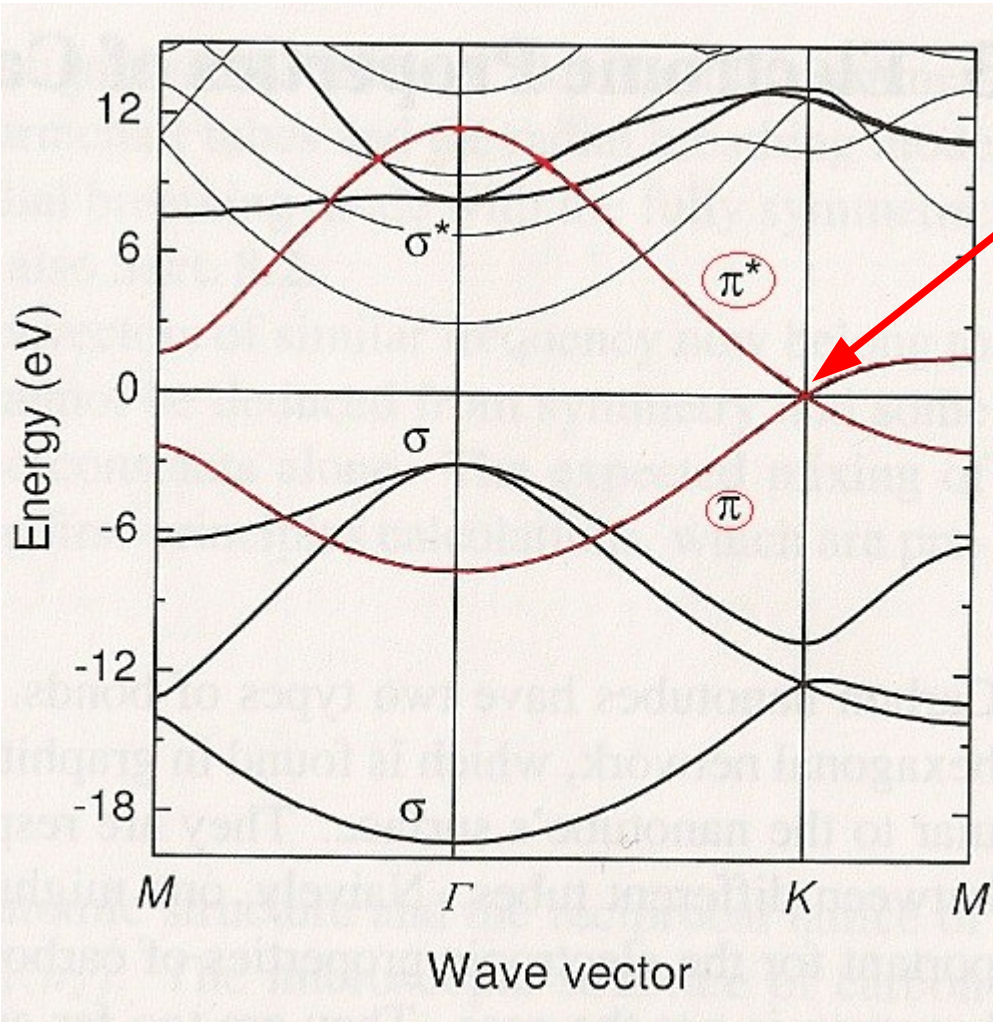
sp² - Hybridization



Graphite

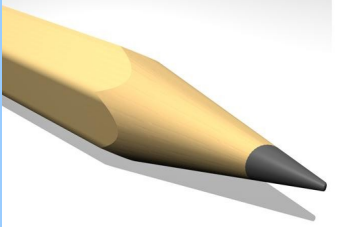


Bandstructure of graphene



Graphite

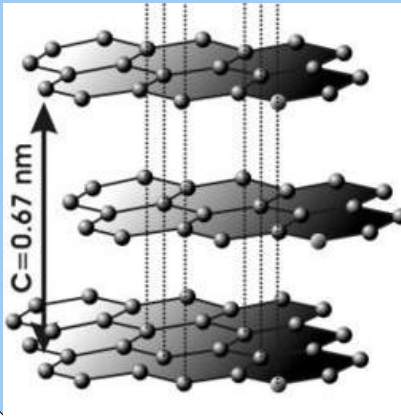
Hardness



Color



Crystal structure

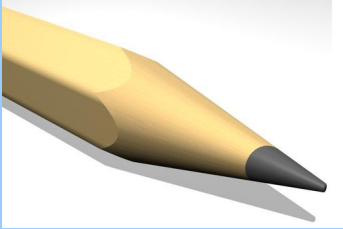


Electr. conductivity



Diamond and graphite

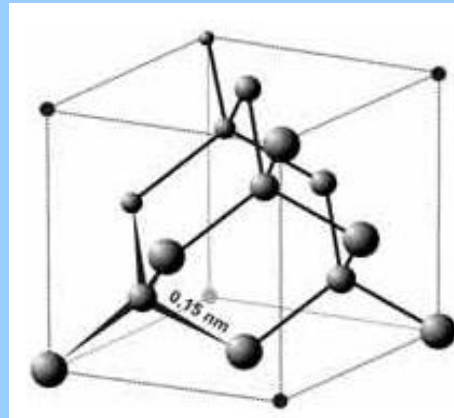
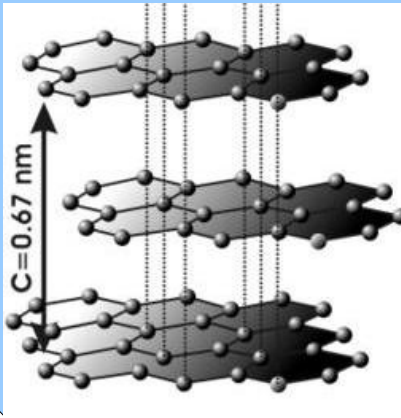
Hardness



Color



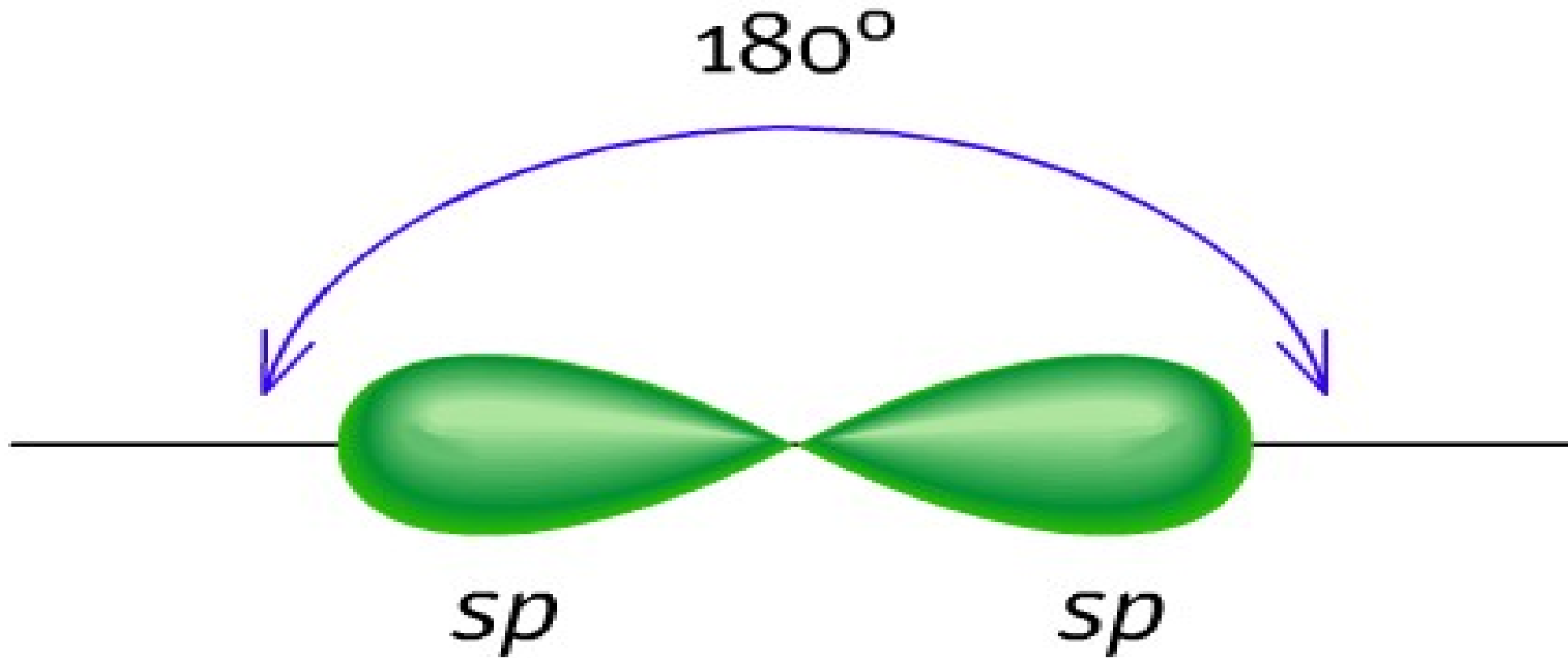
Crystal structure



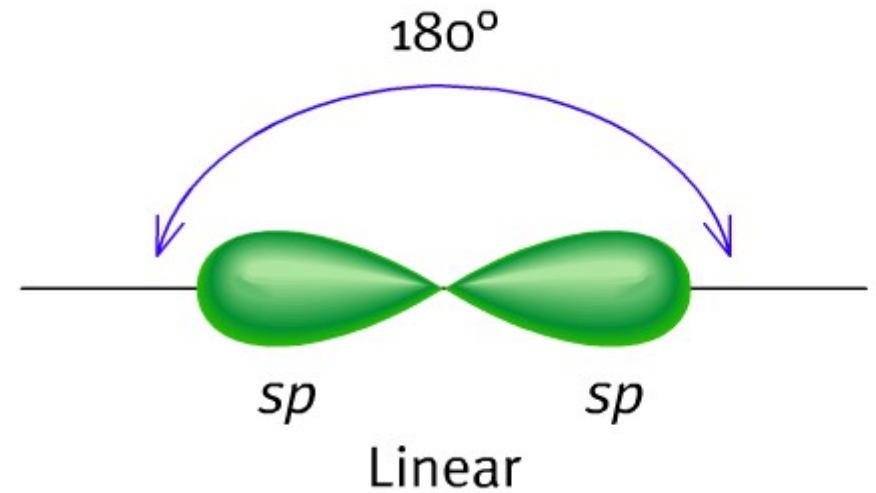
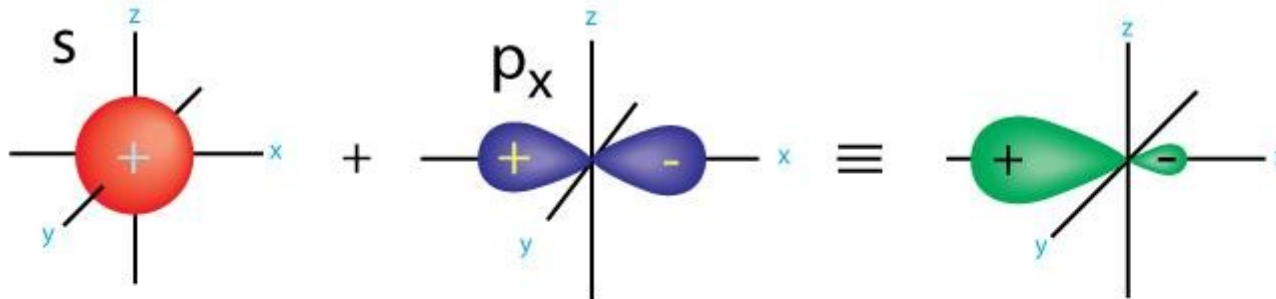
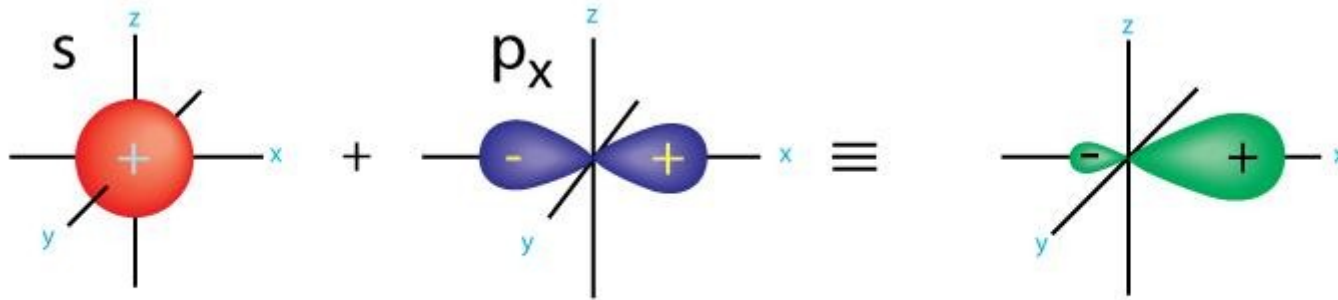
Electr. conductivity



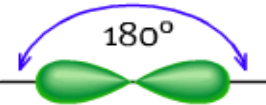
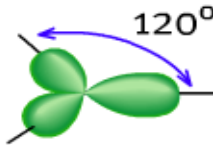
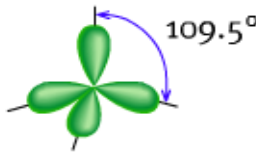
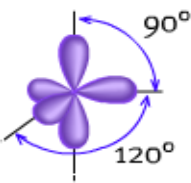

Hybridization



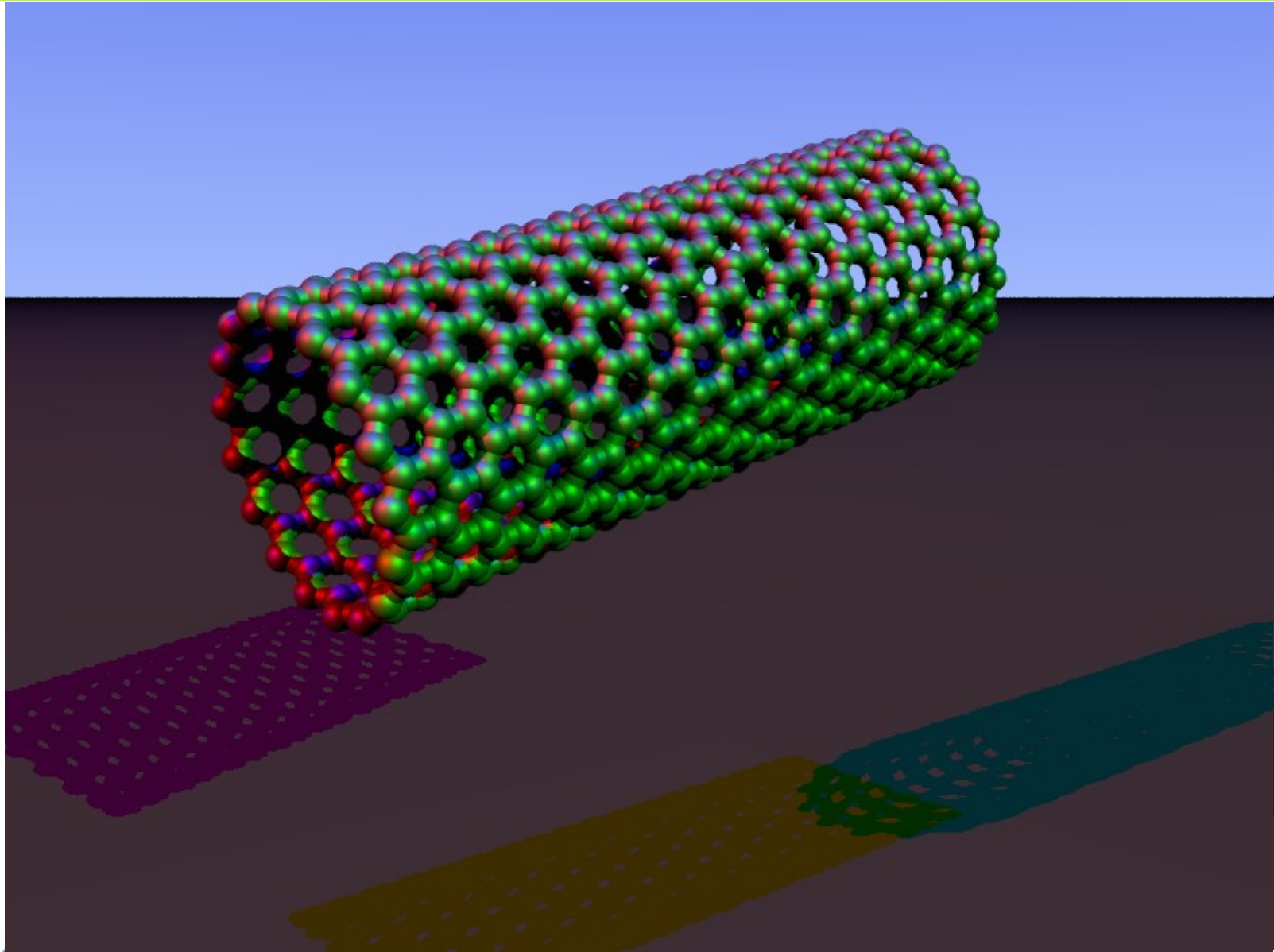
sp - Hybridization



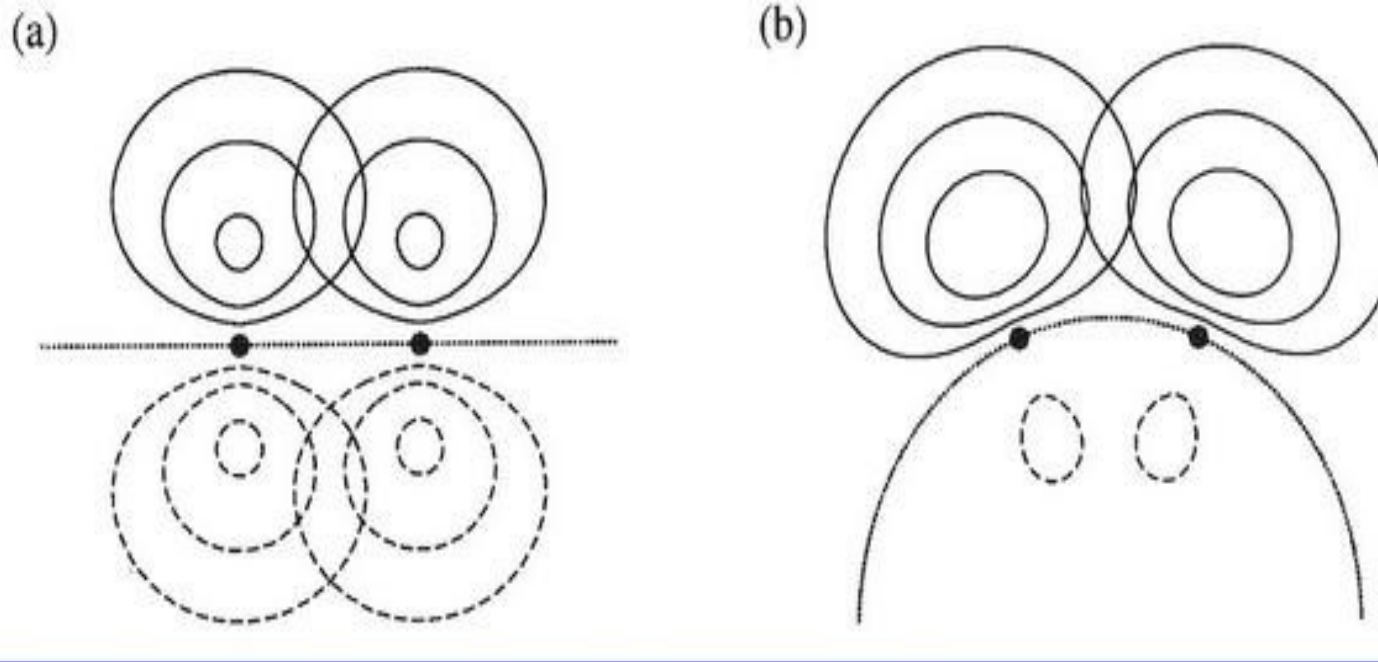
Hybridization - summary

Pure atomic orbitals of central atom	Hybridization of the central atom	Number of hybrid orbitals	Shape of hybrid orbitals
s,p	sp	2	Linear 
s,p,p	sp ²	3	Trigonal Planar 
s,p,p,p	sp ³	4	Tetrahedral 
s,p,p,p,d	sp ³ d	5	Trigonal Bipyramidal 
s,p,p,p,d,d	sp ³ d ²	6	Octahedral 

Curved carbon materials - Carbon nanotubes



Curved carbon materials - Rehybridization

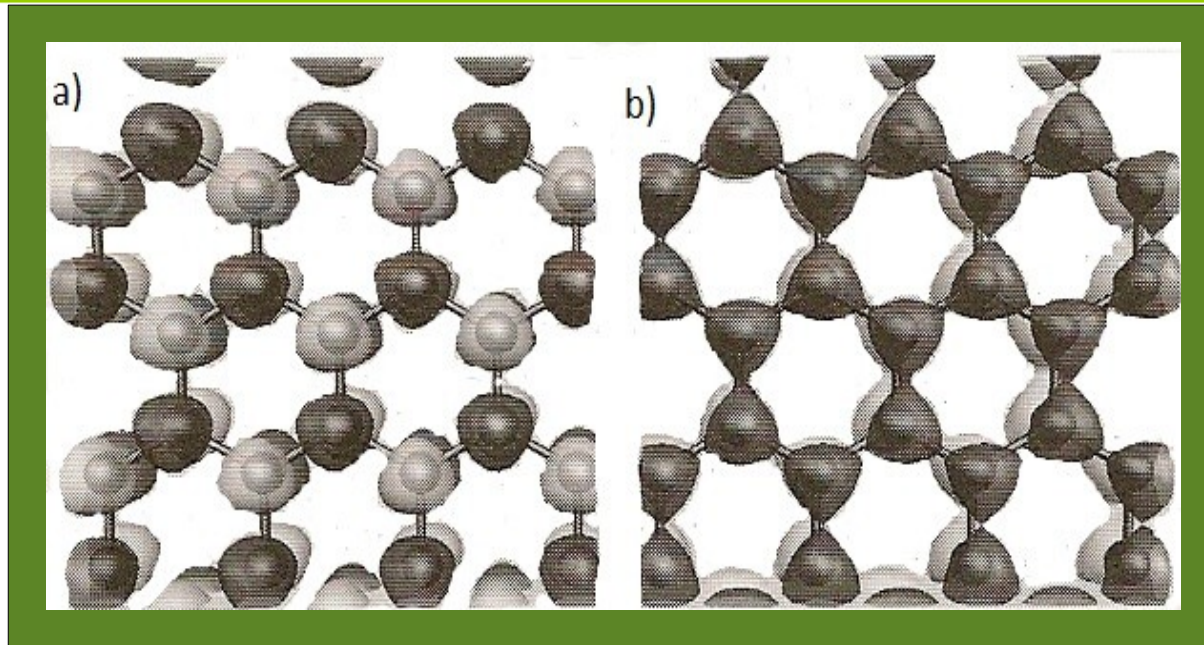


a) Graphene

b) C20

- Tilting angles of π -orbitals $\delta = a/(2 \sqrt{3} d)$
- Wavefunction of π - and σ - orbitals
- Degree of hybridization $sp^{2+\eta}$

Curved carbon materials - Rehybridization



Graphene

a) Antibinding π^* orbital
(conduction band)

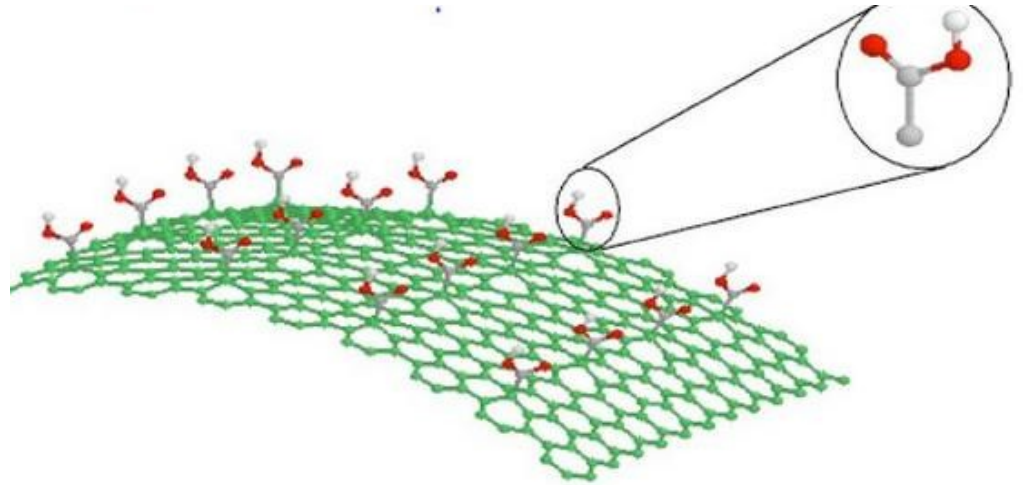
b) Binding π orbital
(valence band)



Carbon nanotube

Rehybridization orbital

Curved carbon materials - Reactivity

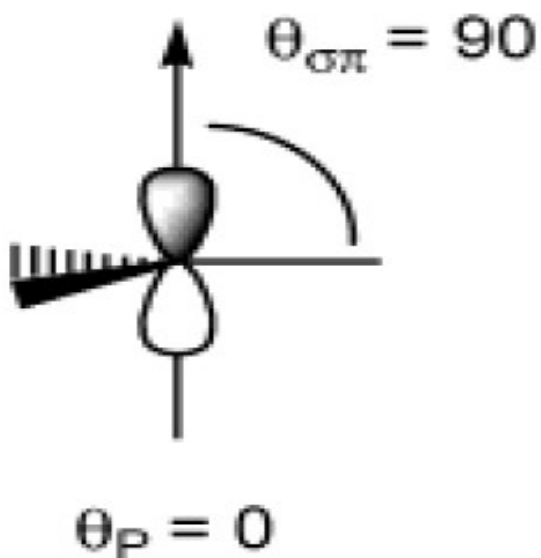


Reactivity

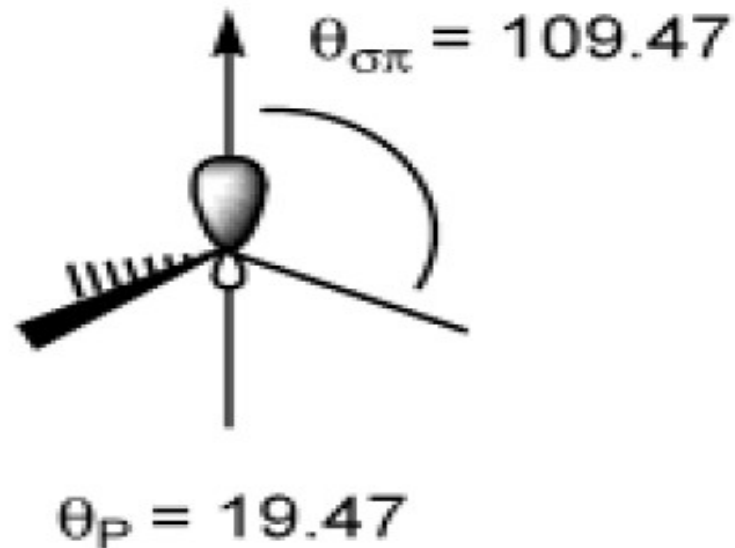
Curved carbon materials - Reactivity

$$\text{Pyramidalization Angle: } \theta_P = (\theta_{\sigma\pi} - 90)^\circ$$

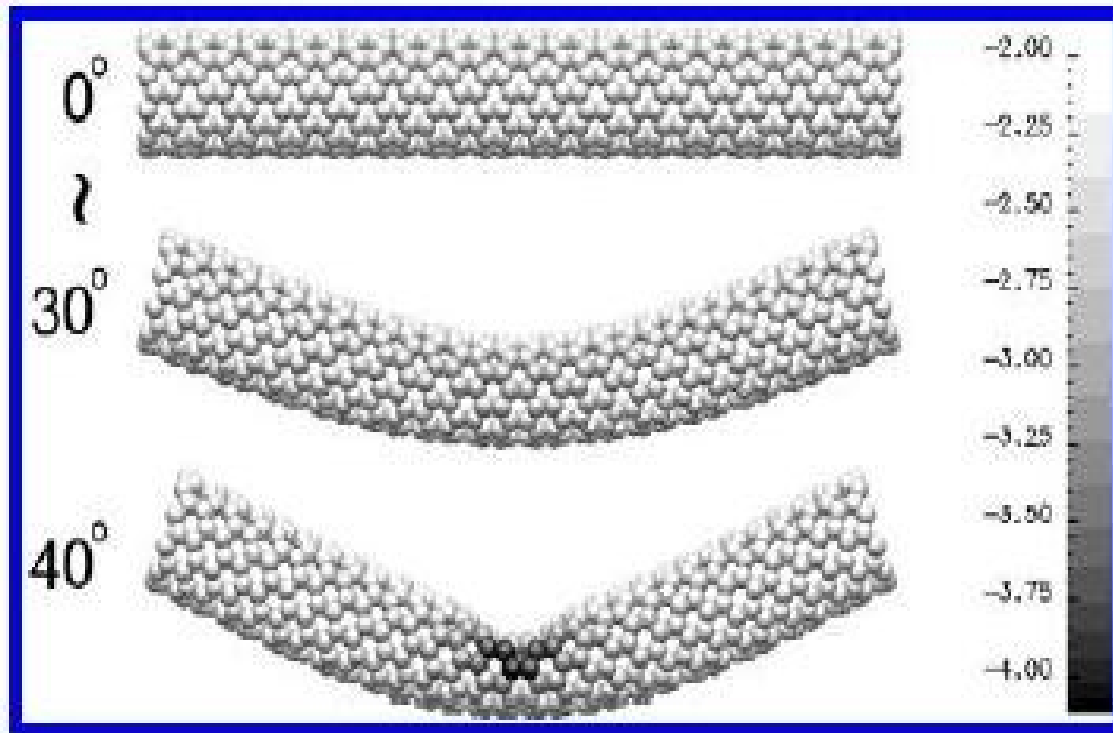
TRIGONAL



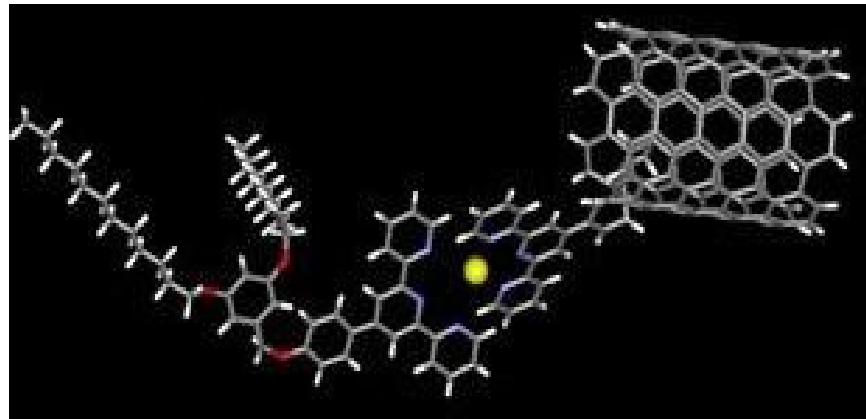
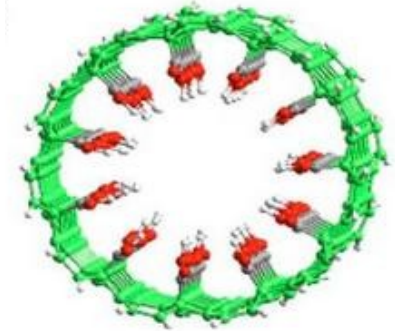
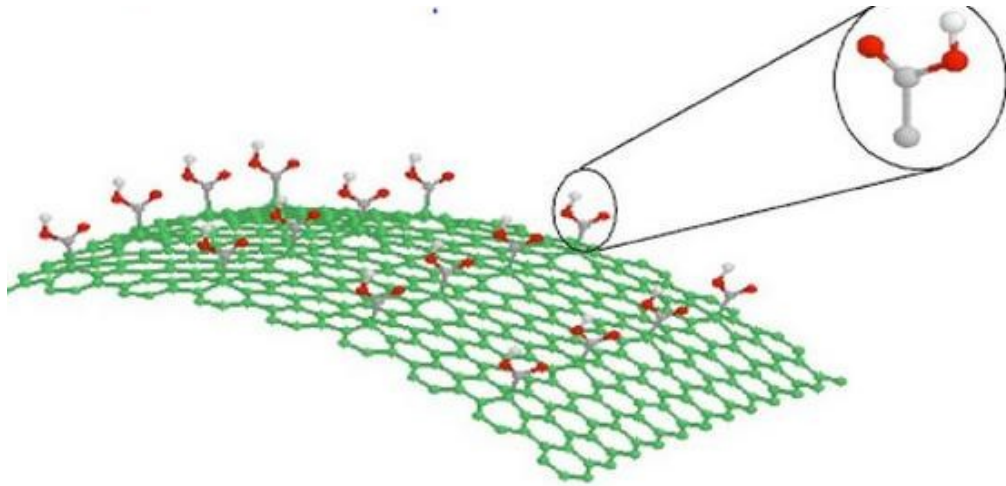
TETRAHEDRAL



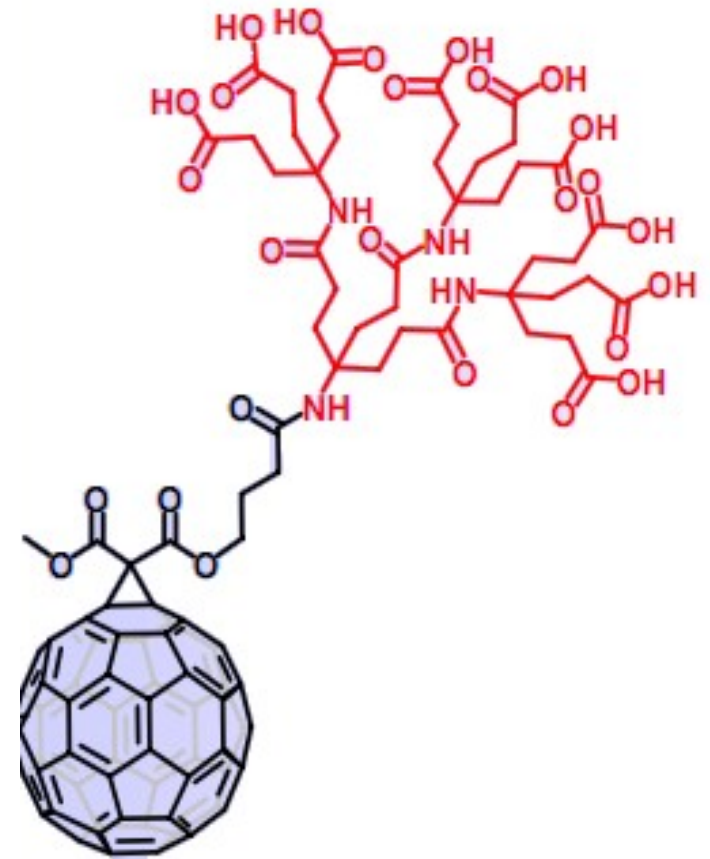
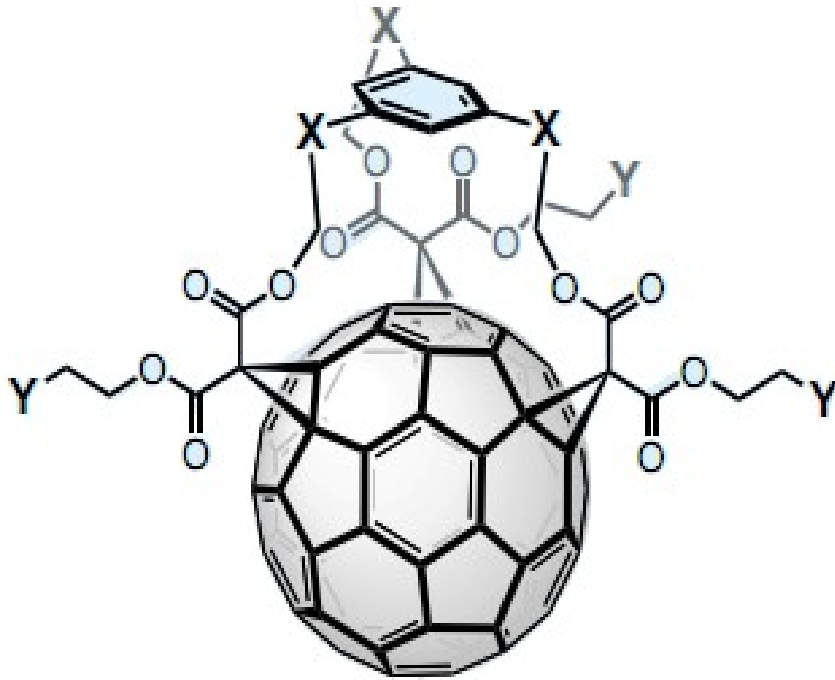
Curved carbon materials - Reactivity



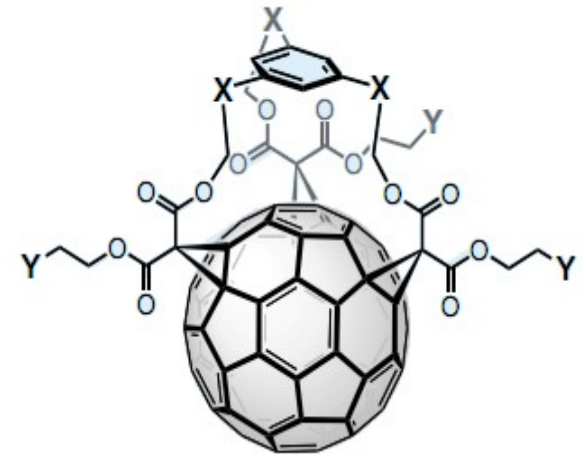
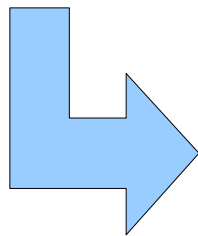
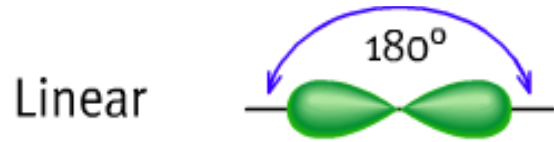
Curved carbon materials - Reactivity



Curved carbon materials - Fullerene



Summary



Thank you for your attention!