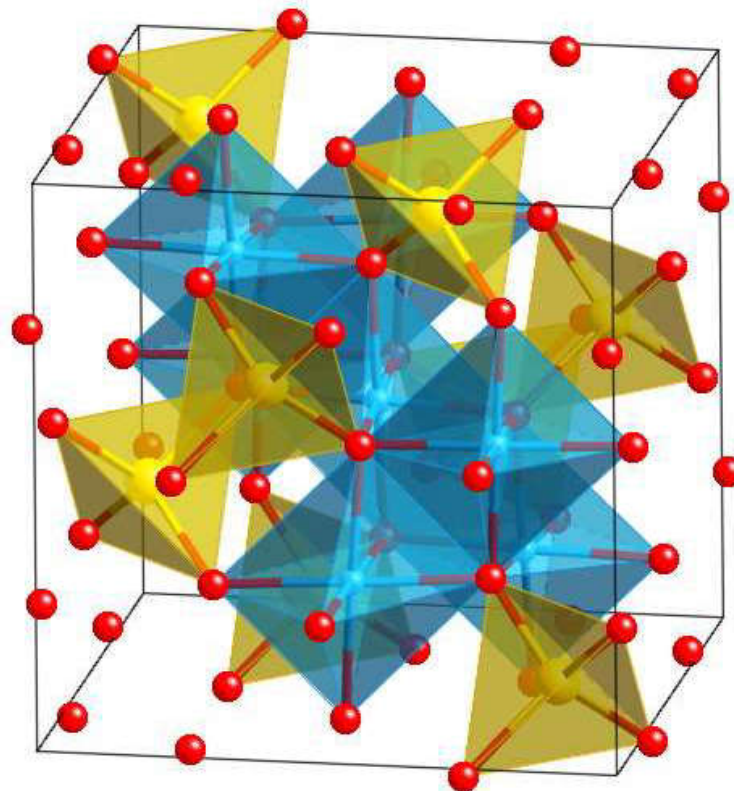
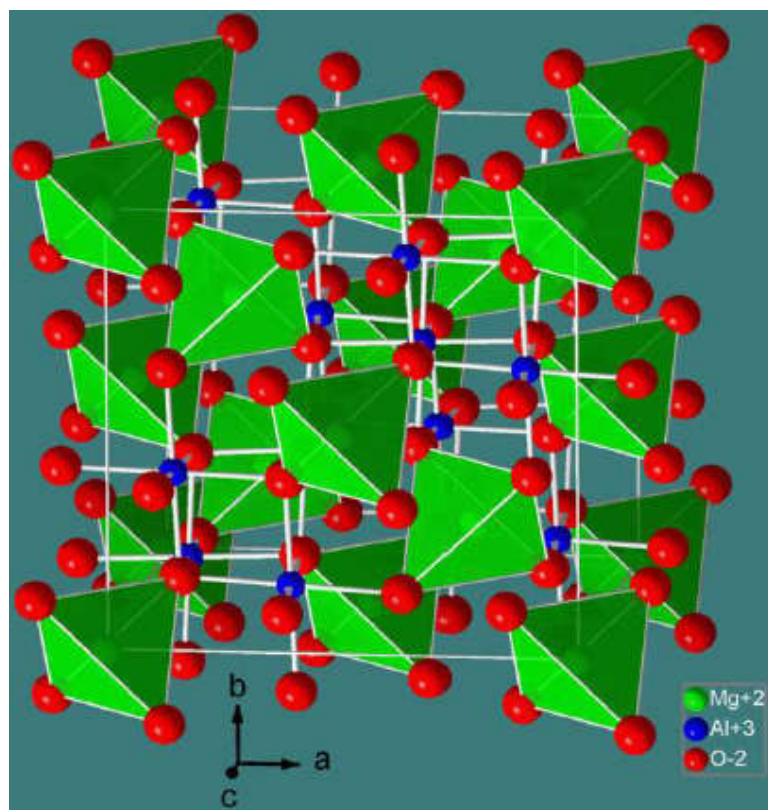
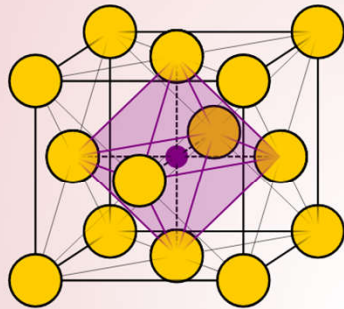


Normal spinel structures are usually cubic close-packed oxides with one octahedral and two tetrahedral sites per formula unit.

B^{3+} ions occupy half the octahedral holes, while A^{2+} ions occupy one-eighth of the tetrahedral holes.

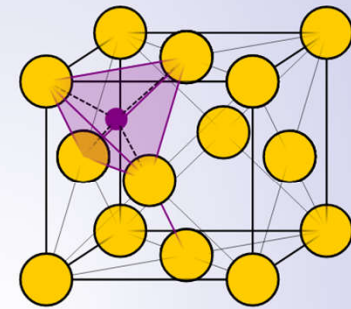


Octahedral Sites in FCC



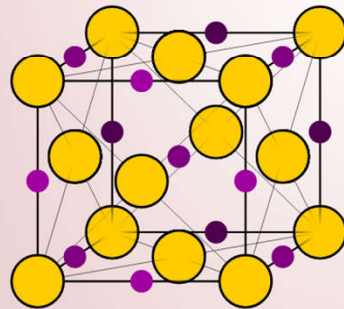
An **interstitial site** ●
among neighboring
host atoms ○

Tetrahedral Sites in FCC

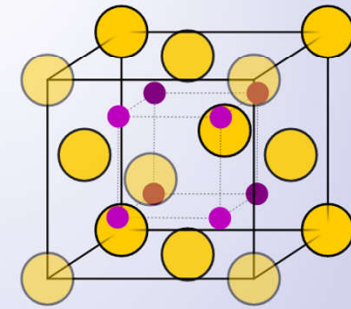


An **interstitial site** ●
among neighboring
host atoms ○

Octahedral and Tetrahedral Interstitials in FCC



All **interstitial site**
positions within
FCC unit cell



All **interstitial site**
positions within
FCC unit cell

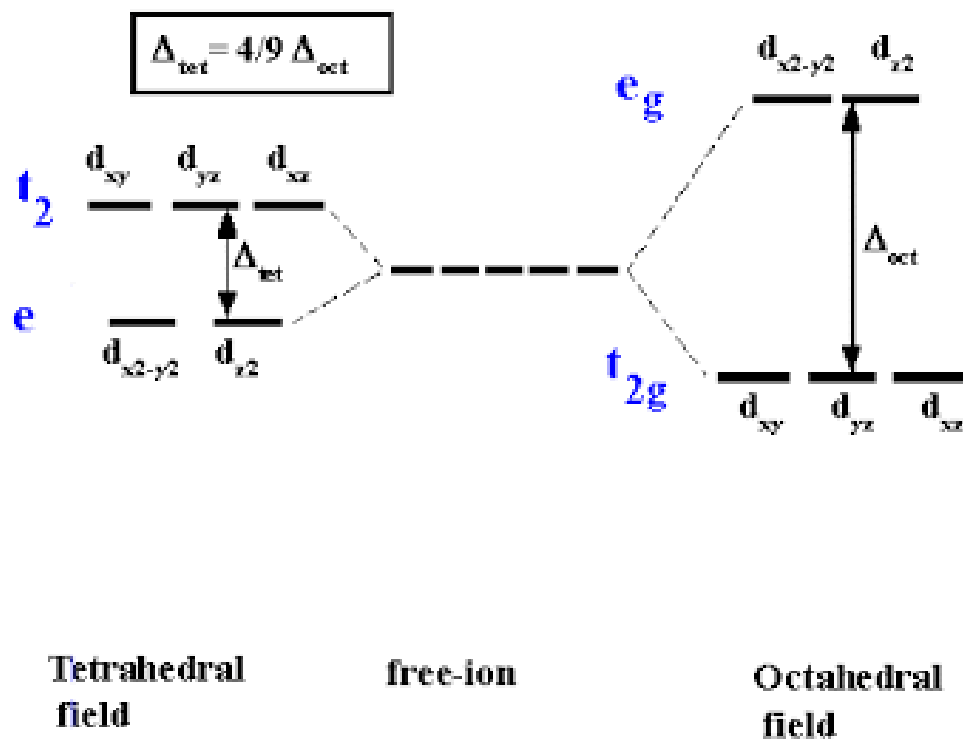
Crystal Structure	Face-centered Cubic (FCC)
Unit Cell Type	Cubic
Relationship Between Cube Edge Length a and the Atomic Radius R	$a = 2R\sqrt{2}$
Close-Packed Structure	Yes
Atomic Packing Factor (APF)	74%
Coordination Number	12
Number of Atoms per Unit Cell	4
Number of Octahedral Interstitial Sites	4
Number of Tetrahedral Interstitial Sites	8
Size of Octahedral Voids	$r = 0.414 R$
Size of Tetrahedral Voids	$r = 0.225 R$

Inverse Spinels usually have alternate arrangement.

The **A^{II}** ions occupy the **octahedral** voids, whereas half of **B^{III}** ions occupy the **tetrahedral** voids

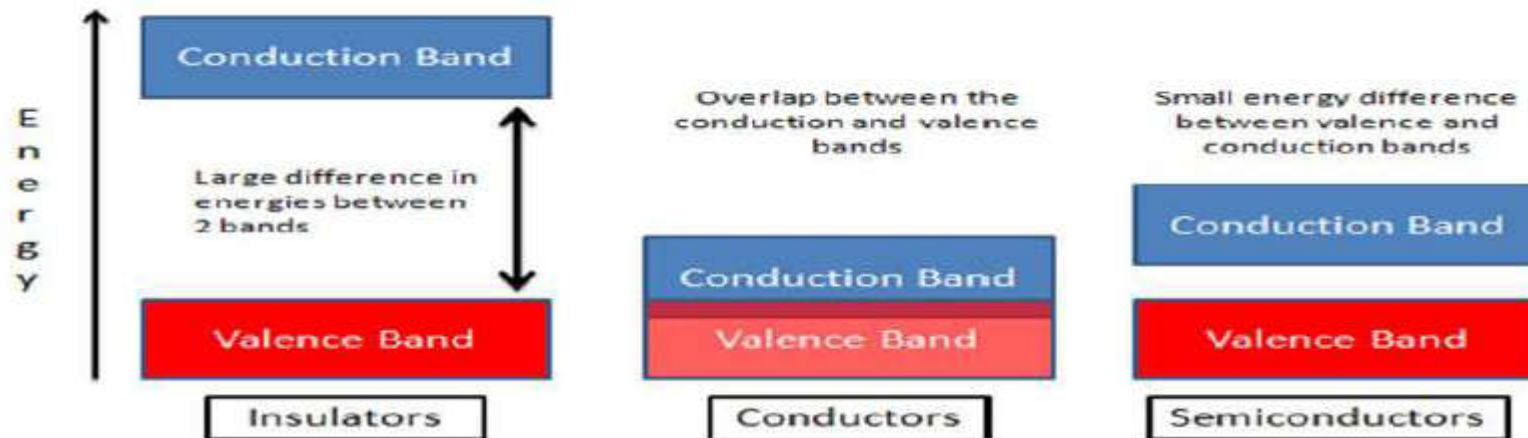
It can be represented as: **(B^{III})^{tet}(A^{II}B^{III})^{oct}O₄**

Energy levels of the d-orbitals in common stereochemistries



Semiconductors:

A Semiconductor is a material which has Electrical Conductivity between that of conductor and that of an insulator.

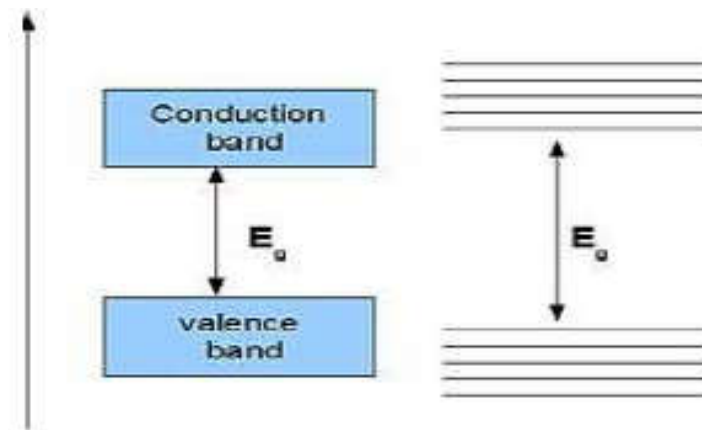


Quantum confinement is the spatial confinement of electron hole pairs in one or more dimensions within a material.

-1D confinement-quantum wells

-2D confinement- quantum wires

-3D confinement-quantum dot



- Electron hole pairs become spatially confined when the diameter of a particle approaches the de Broglie wavelength of electrons in the conduction band.
- As a result the energy difference between energy bands is increased with particle size decreasing.

Relativity

$$E = mc^2$$

Photoelectric effect

$$E = hf = \frac{hc}{\lambda}$$

The de Broglie Hypothesis

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

$9.1093837 \times 10^{-31}$ kilograms

Planck's constant =
 $6.62607015 \times 10^{-34} \text{ m}^2 \text{ kg / s}$

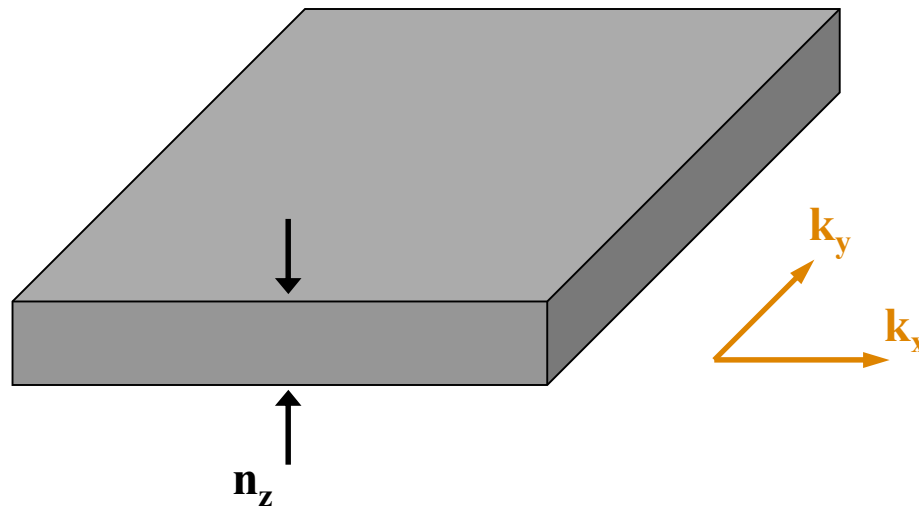
1. Thin Films & Quantum Wells

Electrons are **Confined in 1 Direction:**

⇒ They can easily have

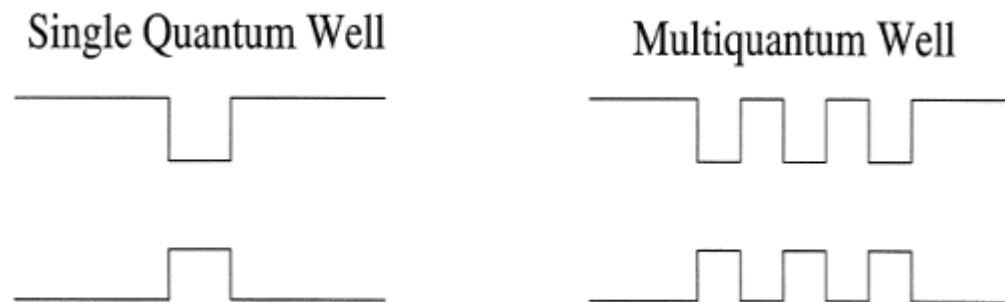
Motion in 2 Dimensions!

⇒ **There is 1 Dimensional Quantization!**



The quantum well in nanotechnology is formed by **sandwiching a material (fore example GaAs) between the two layers of another material having broader gap** (For example aluminium arsenide). The layers are prepared by the chemical vapor deposition or epitaxy.

Quantum well lasers with one active are called single-quantum-well (SQW) lasers and lasers with multiple quantum well active region



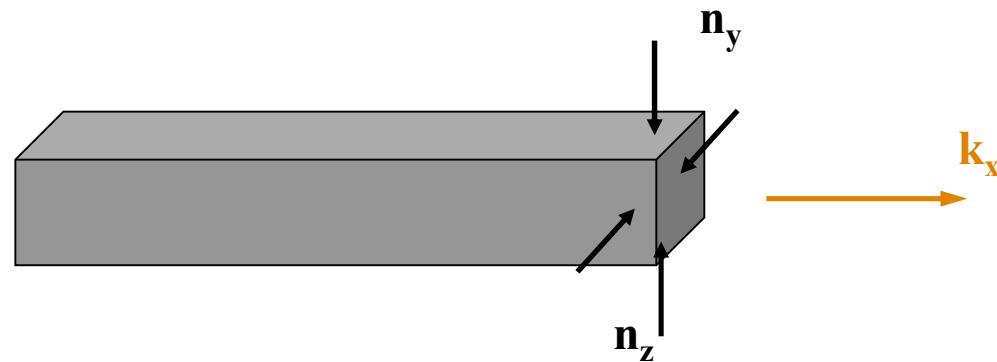
2. Quantum Wires

Electrons are *Confined in 2 Directions*:

⇒ They can easily have

Motion in 1 Dimension!

⇒ *There is 2 Dimensional Quantization!*



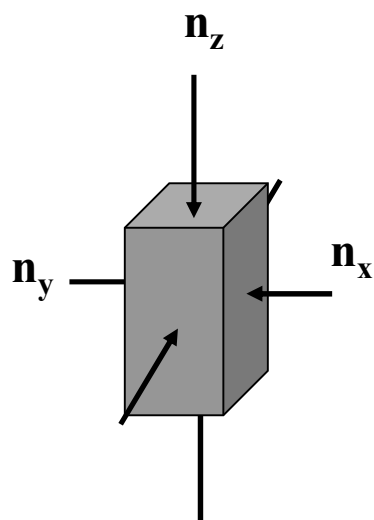
3. Quantum Dots

Electrons are *Confined in 3 Directions*:

⇒ They can easily have

Motion in 0 Dimensions!

⇒ *There is 3 Dimensional Quantization!*

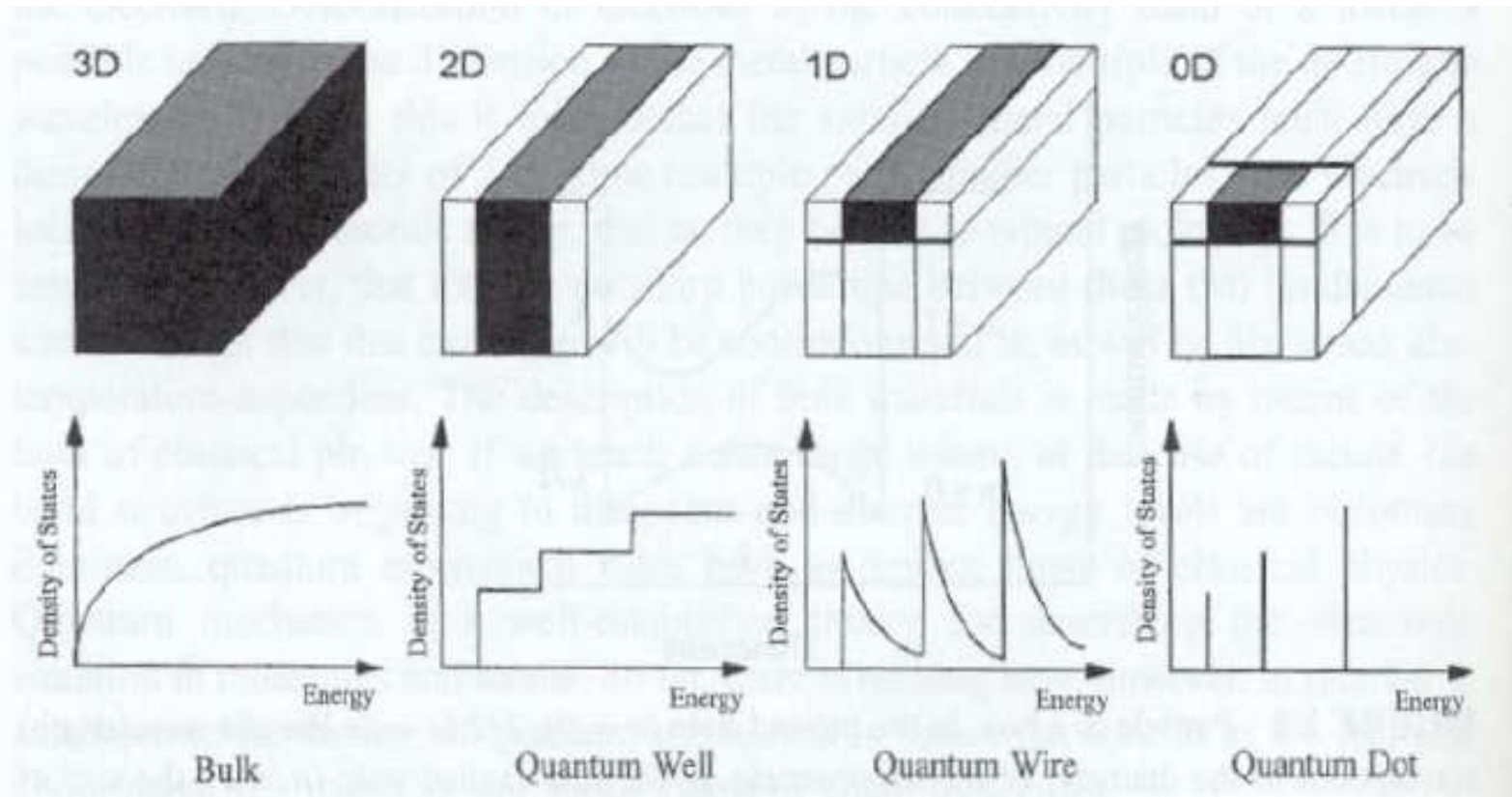


Each further confinement direction

*changes a continuous component
to a discrete component*

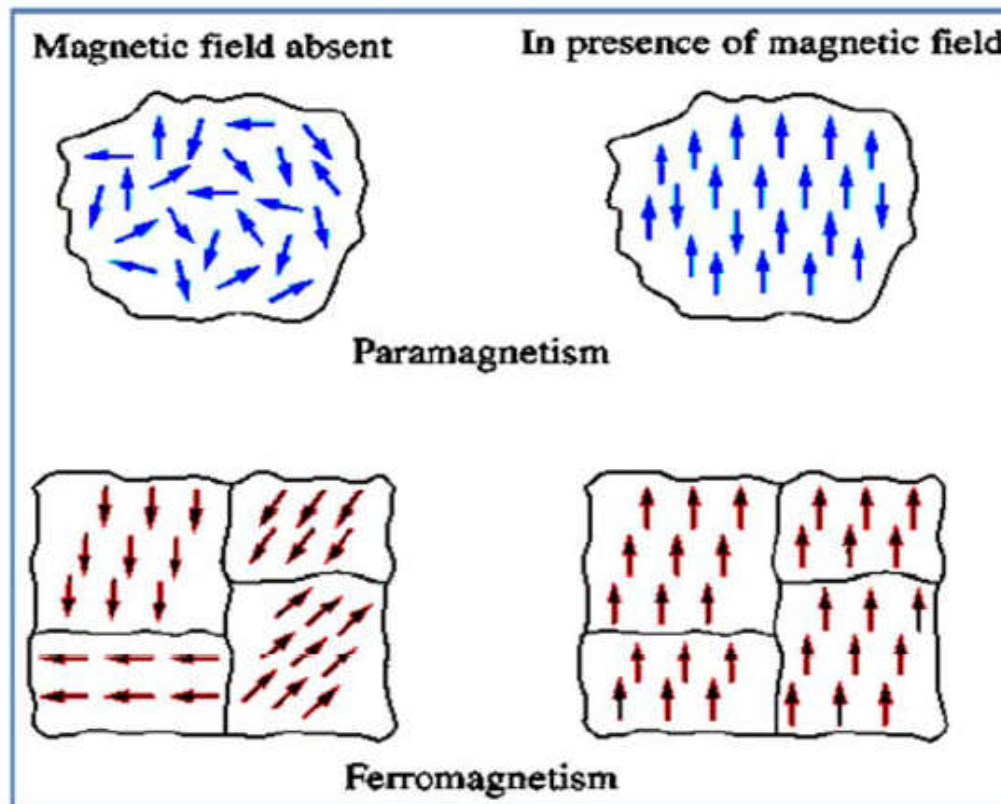
characterized by

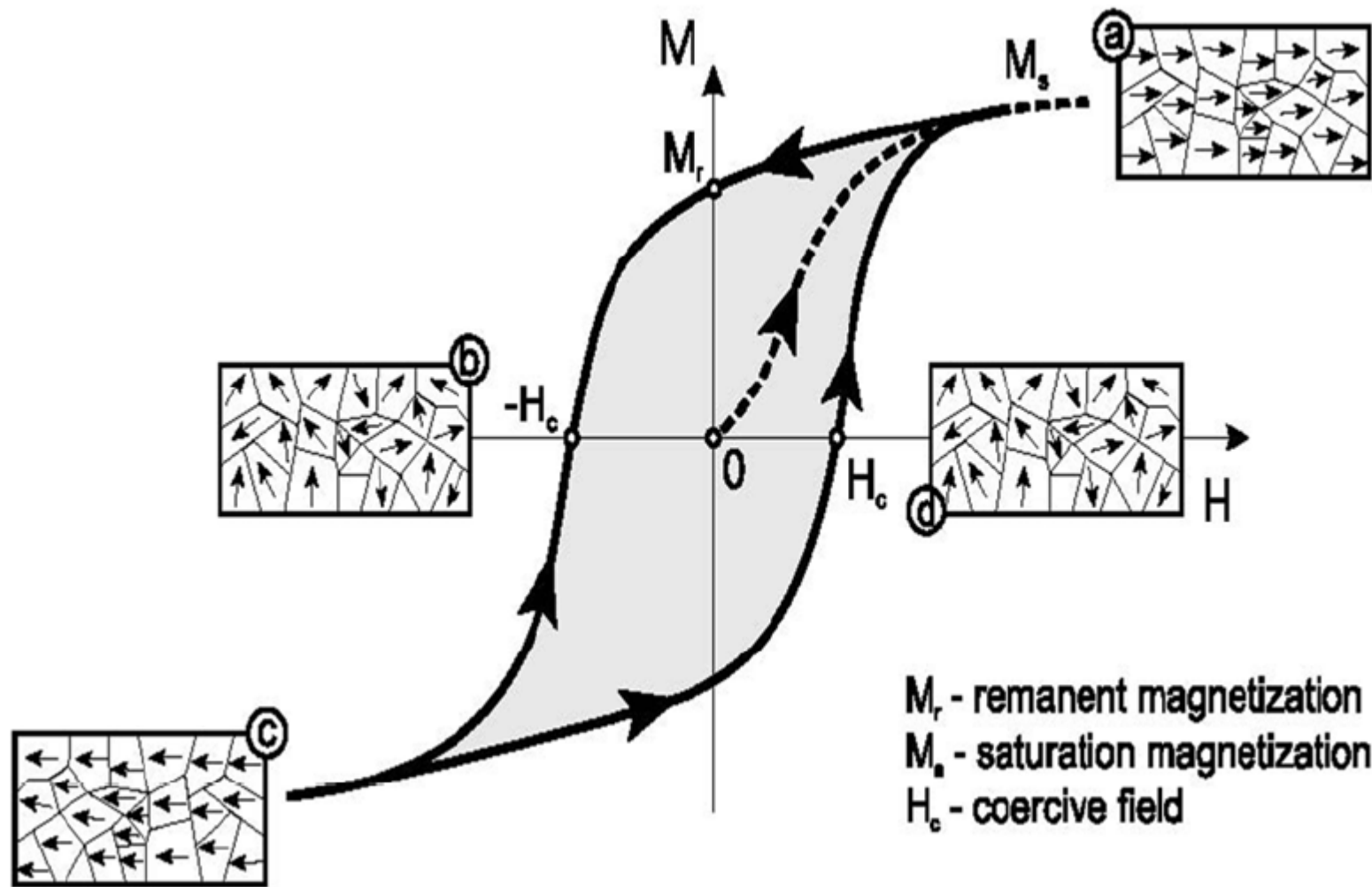
a quantum number n .



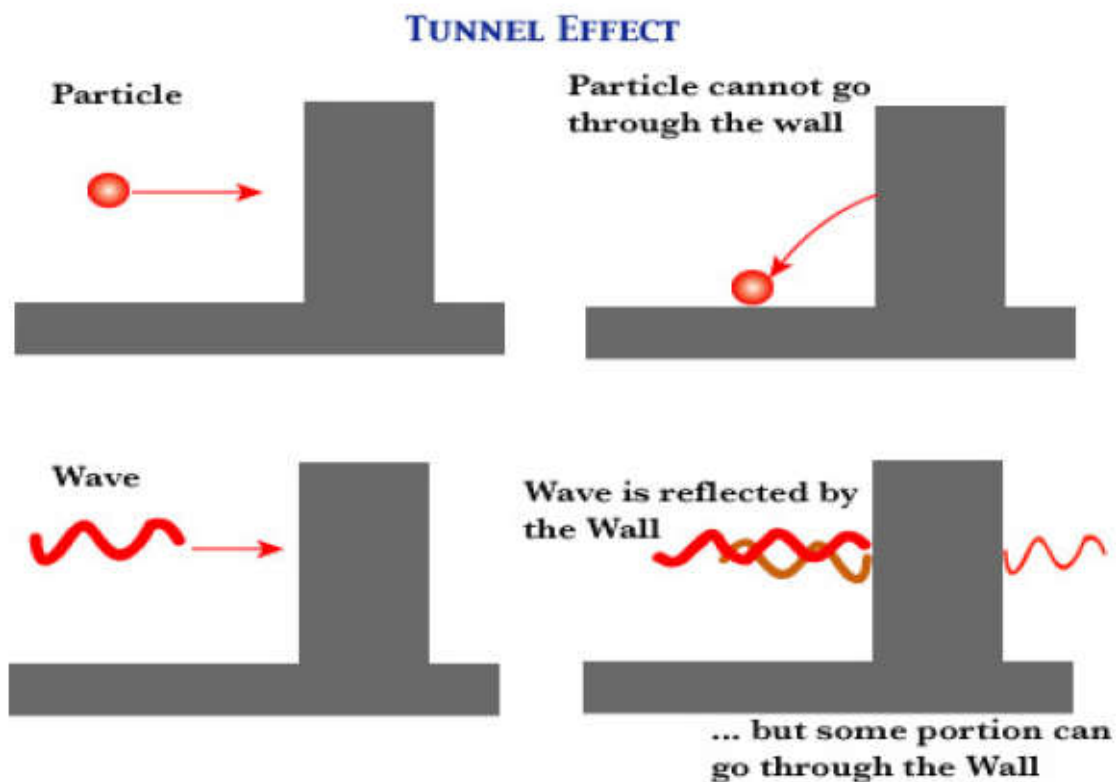
Magnetic Properties:

- The Magnetic Moment of Nano particles is found to be very less when compared them with its bulk size.

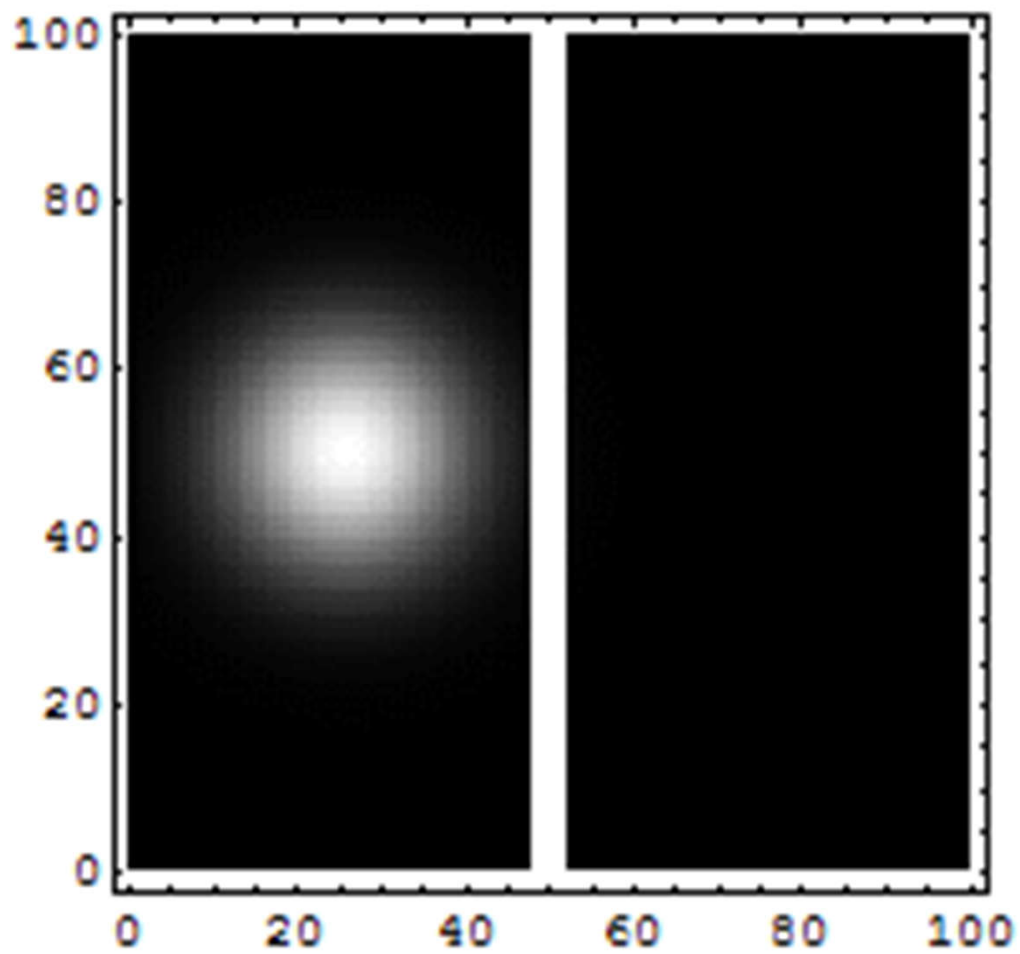




Consider a ball trying to roll over a hill. The following table gives a picture how the perception differs from classical mechanics to that of quantum mechanics:

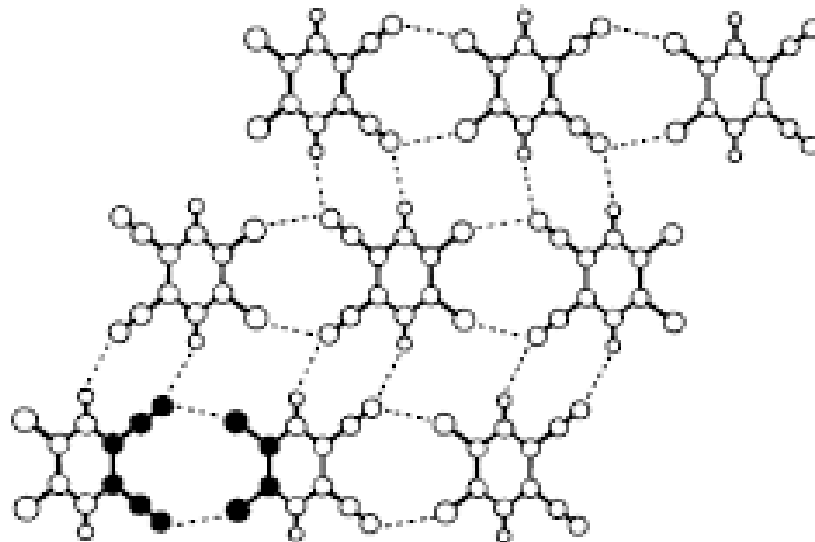
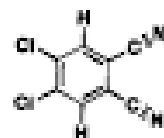


Classical Mechanics	Quantum Mechanics
<ul style="list-style-type: none">• The ball does not have enough energy to classically surmount a barrier and thus will not be able to reach the other side. Thus, a ball without sufficient energy to surmount the hill would roll back down• Lacking the energy to penetrate a wall, it would bounce back (reflection)• In the extreme case, the ball may bury itself inside the wall (absorption).	<ul style="list-style-type: none">• The ball can, with a very small probability, tunnel to the other side, thus crossing the barrier.• Here, the ball could, in a sense, borrow energy from its surroundings to tunnel through the wall or roll over the hill, paying it back by making the reflected electrons more energetic than they otherwise would have been



Supramolecular Structures:

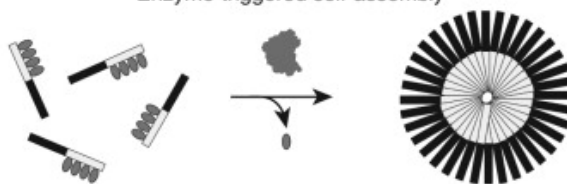
More complex than a molecule, also: composed of many molecules



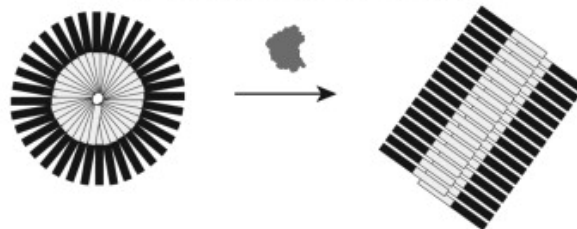
Enzyme-induced disassembly



Enzyme-triggered self-assembly

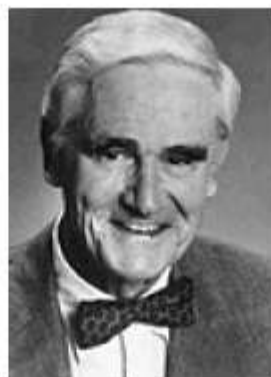


Enzyme-induced morphological changes



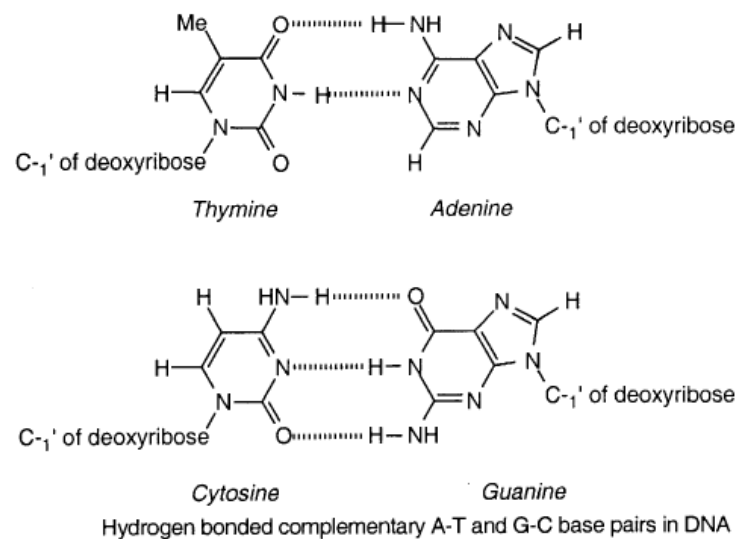
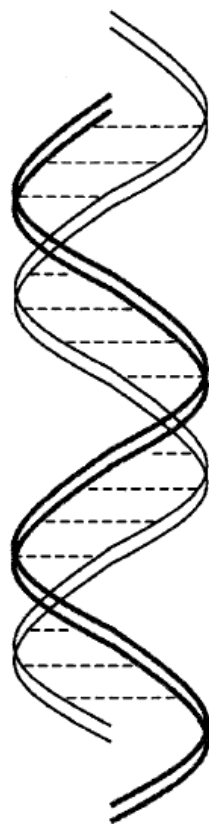
Supramolecular Chemistry:

A term introduced by Jean-Marie Lehn, is “chemistry beyond the molecule”, i.e. the chemistry of molecular assemblies using noncovalent bonds.



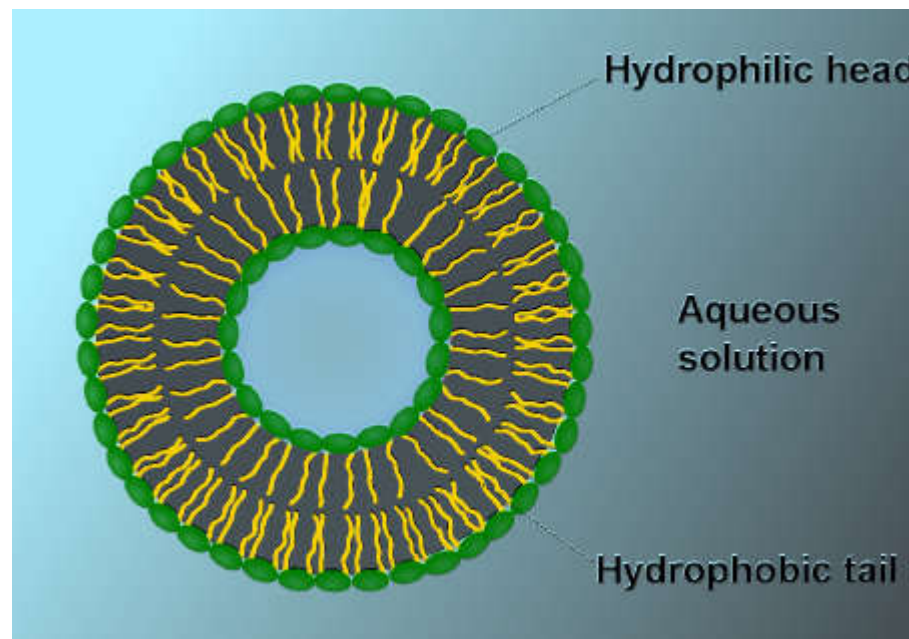
Nobel Prize in 1987: Pederson C , Cram D J, Lehn J M

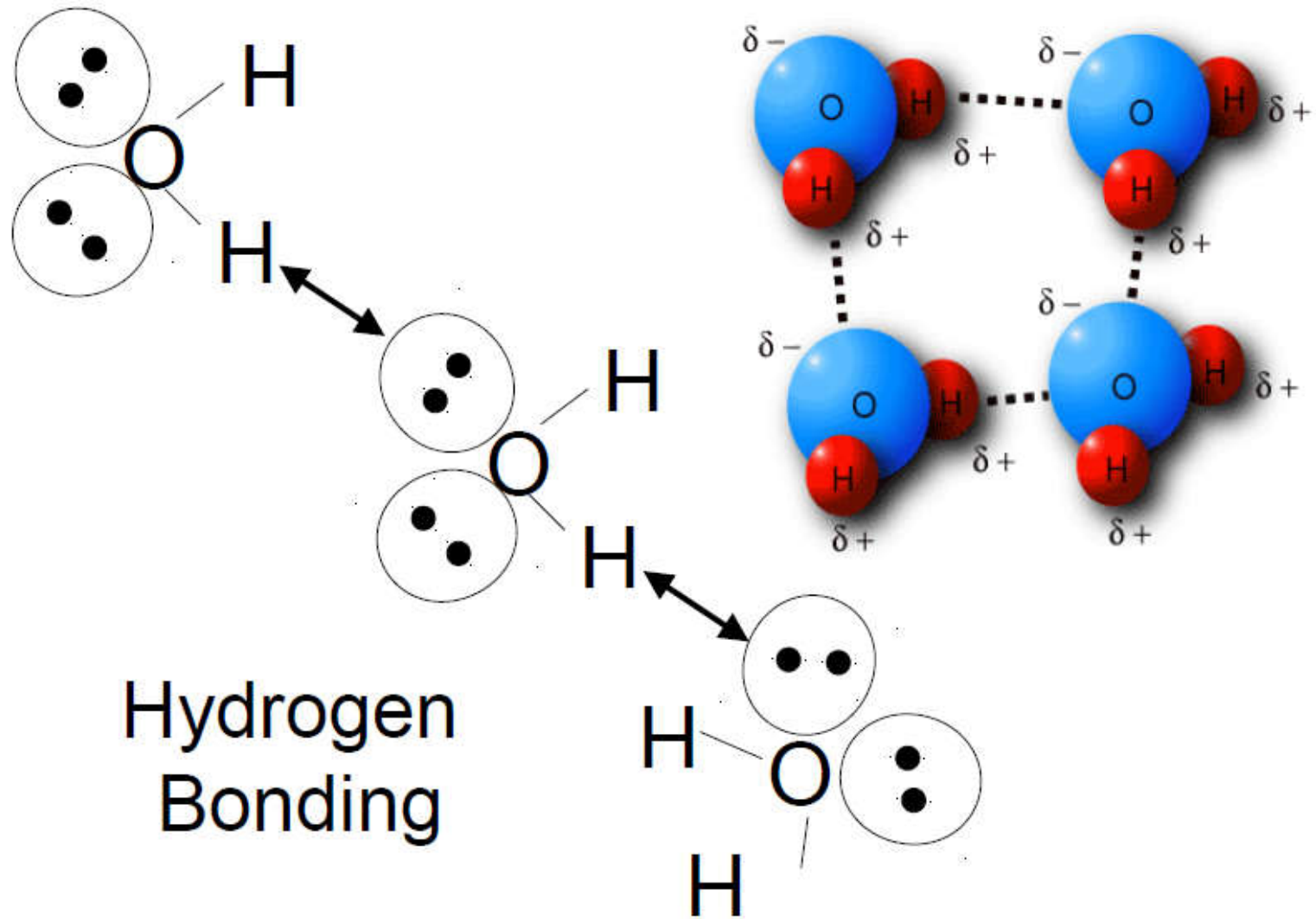
Two DNA strands form a helical supramolecular assembly **through hydrogen bonding interactions that form between the bases**. Thymine can hydrogen bond preferentially with adenine. Cytosine hydrogen bonds preferentially with guanine.



Self Assembly:

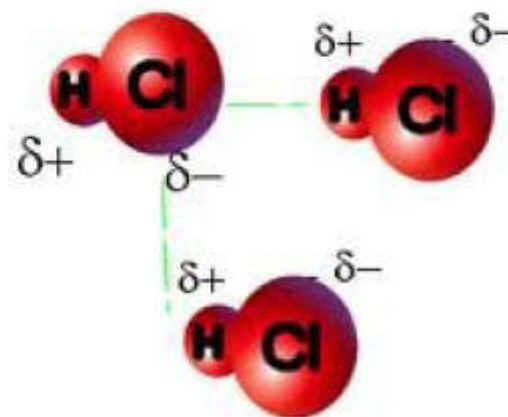
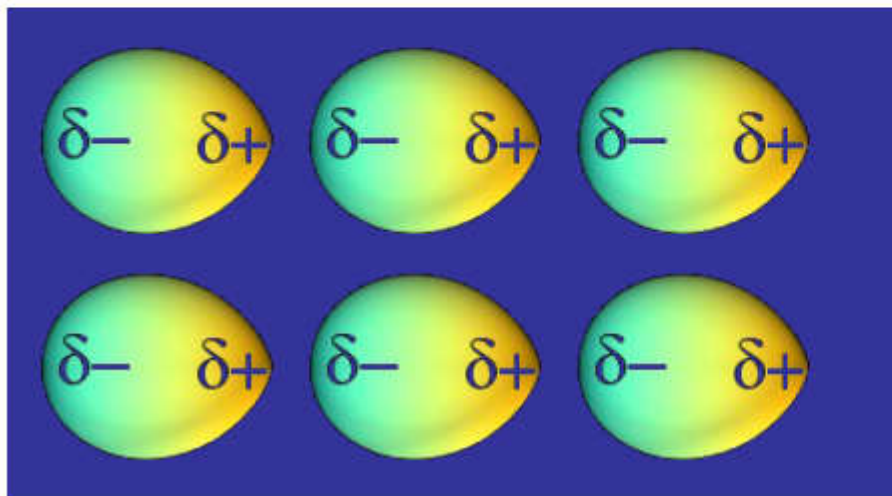
Self Assembly is defined as the spontaneous association of numerous individual units of material into well organized, well defined structures without external instruction.





Dipole Interaction

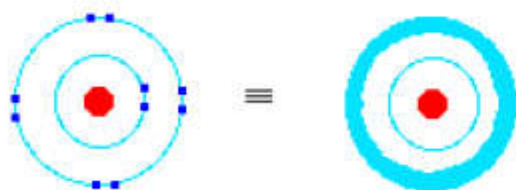
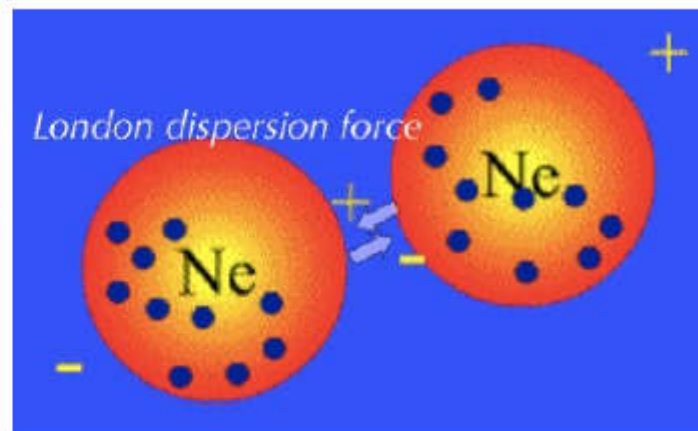
- The partial positive and negative ends of the molecules hold the molecules together.



London Dispersion Forces (LDF)

instantaneous dipole–induced dipole forces,

London forces are induced dipoles caused by temporary rearrangement of the electron cloud.

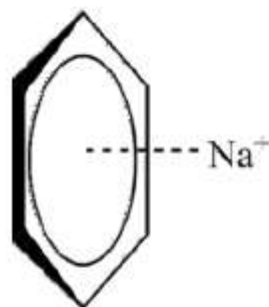


Neon

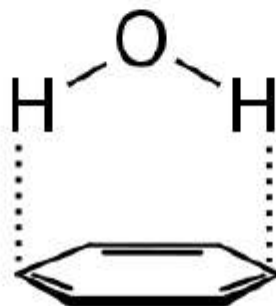
no permanent dipole

Assembled by π - π interaction

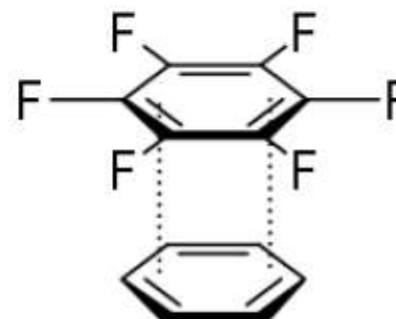
Some simple models:



Cation- π interaction bn
benzene and a
Na cation.

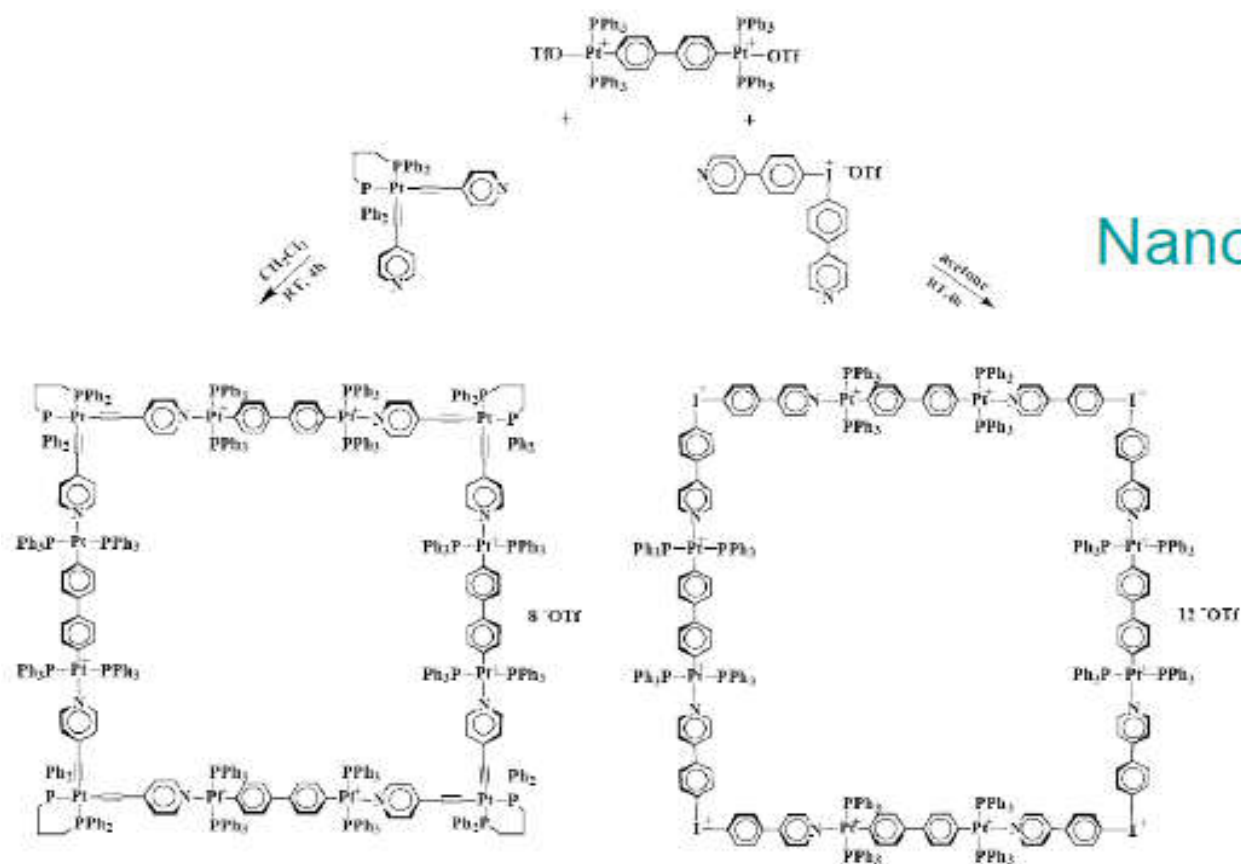


Polar π interaction bn
water molecule
and benzene



π - π interaction bn
e rich benzene
& e poor
hexafluorobenzene

Assembled by metal-ligand



Nanosized cavities

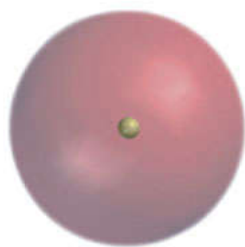
Valence Bond Theory and Molecular Orbital Theory:

s and p orbitals most important in organic and biological chemistry

s orbitals: spherical, nucleus at center

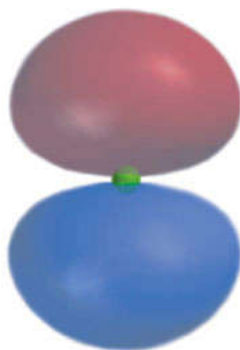
p orbitals: dumbbell-shaped, nucleus at middle

d orbitals: elongated dumbbell-shaped, nucleus at center

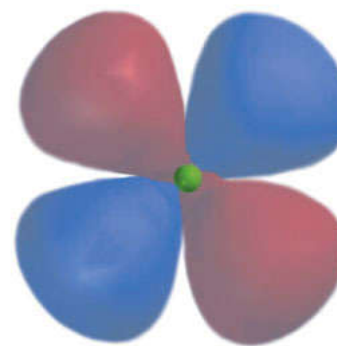


An s orbital

© 2007 Thomson Higher Education

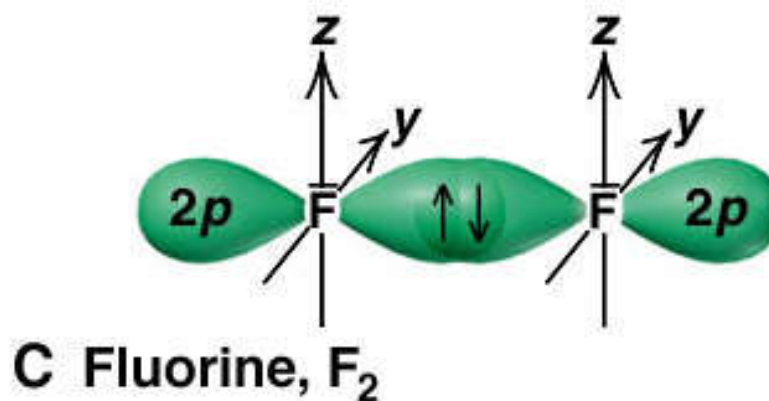
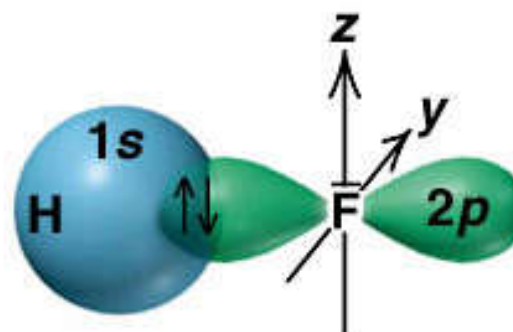
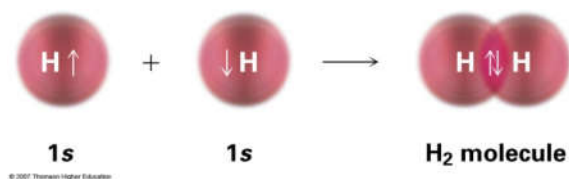
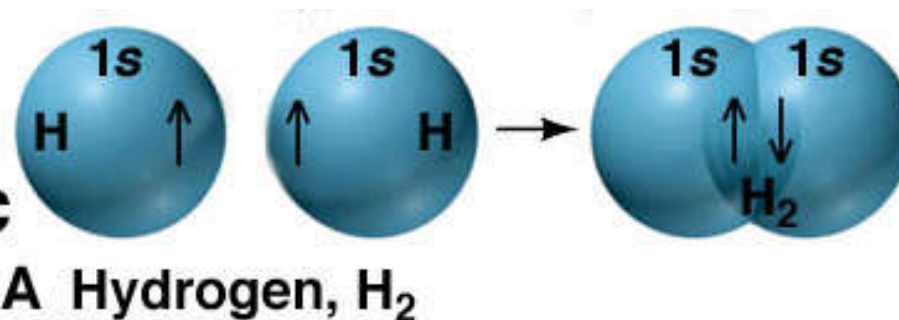


A p orbital



A d orbital

Orbital Overlap and Spin Pairing in Three Diatomic Molecules



1. sp^3 Orbitals and the Structure of Methane

Carbon has 4 valence electrons ($2s^2 2p^2$)

In CH_4 , all C–H bonds are identical (tetrahedral)

sp^3 hybrid orbitals: s orbital and three p orbitals combine to form four equivalent, unsymmetrical, tetrahedral orbitals (sp^3)

