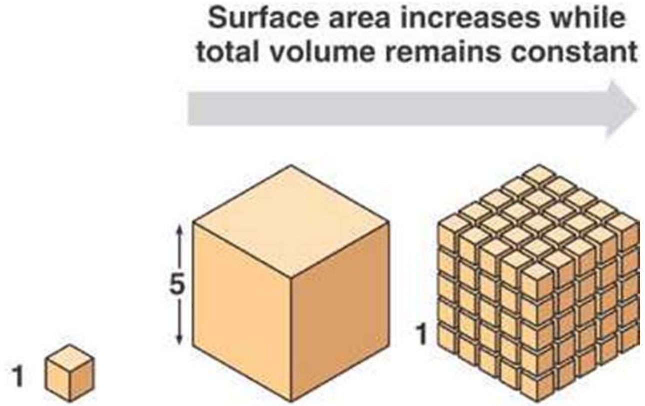
Second letter

First letter	U	C	A	G	Third letter
U	UUU Phe UUC Phe UUA Leu UUG Leu	UCU Ser UCC Ser UCA Ser UCG Ser	UAU Tyr UAC Tyr UAA Stop UAG Stop	UGU Cys UGC Cys UGA Stop UGG Trp	U C A G
C	CUU Leu CUC Leu CUA Leu CUG Leu	CCU Pro CCC Pro CCA Pro CCG Pro	CAU His CAC His CAA Gln CAG Gln	CGU Arg CGC Arg CGA Arg CGG Arg	U C A G
A	AUU Ile AUC Ile AUA Ile AUG Met	ACU Thr ACC Thr ACA Thr ACG Thr	AAU Asn AAC Asn AAA Lys AAG Lys	AGU Ser AGC Ser AGA Arg AGG Arg	U C A G
G	GUU Val GUC Val GUA Val GUG Val	GCU Ala GCC Ala GCA Ala GCG Ala	GAU Asp GAC Asp GAA Glu GAG Glu	GGU Gly GGC Gly GGA Gly GGG Gly	U C A G

Nanomaterials

- Metals and Alloys
  - Fe, Al, Au
- Semiconductors
  - Band gap, CdS, TiO_2, ZnO
- Ceramic
  - Al_2O_3, Si_3N_4, MgO, , SiO_2, ZrO_2
- Carbon based
  - Diamond, graphite, nanotube, C60, graphene
- Polymers
  - Soft mater, block co-polymer
- Biological
  - Photonic, hydrophobic, adhesive,
- Composites

Surface to Volume Ratio



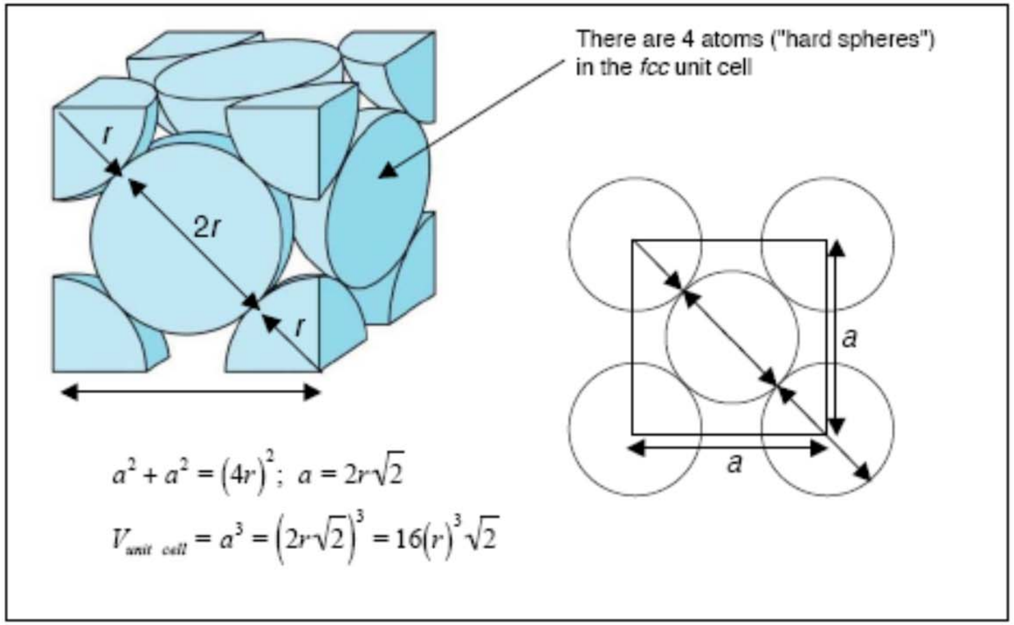
Total surface area (height × width × number of sides × number of boxes)	6	150	750
Total volume (height × width × length × number of boxes)	1	125	125
Surface-to-volume ratio (surface area / volume)	6	1.2	6

Surface to Volume Ratio

Au: AAA
Atomic mass: 196.967
Density 19.31
Radii =0.144 nm

Number of Au atoms in 1 m	$3.4\ 10^{9}$
Volume of Au atom	$4.19\ 10^{28}$
Surface area Au atom	$7.22\ 10^{19}$
Surface/volume ratio	$1.72\ 10^{-9}$

fcc



$$V_{unit\ cell} = a^3 = \left(2r\sqrt{2}\right)^3 = 16(0.5\text{nm})^3\sqrt{2} = \mathbf{2.828\ nm^3}$$

$$\frac{10^{27}\ \text{nm}^3}{2.828\ \text{nm}^3} = \mathbf{3.536x10^{26}\ nano\ \ unit\ cells}$$

$$\text{Collective Area} = 3.536x10^{26}\ \text{nano unit cells}\left(\frac{4\ \text{spheres}}{\text{unit cell}}\right)\left(\frac{4\pi r^2}{\text{sphere}}\right) = \mathbf{4.44x10^{27}\ nm^2}$$

$$\frac{S_{spheres}}{S_{unit\ cell}} = \frac{4.44x10^9\ \text{m}^2}{6.0x10^9\ \text{m}^2} = \mathbf{0.74}$$

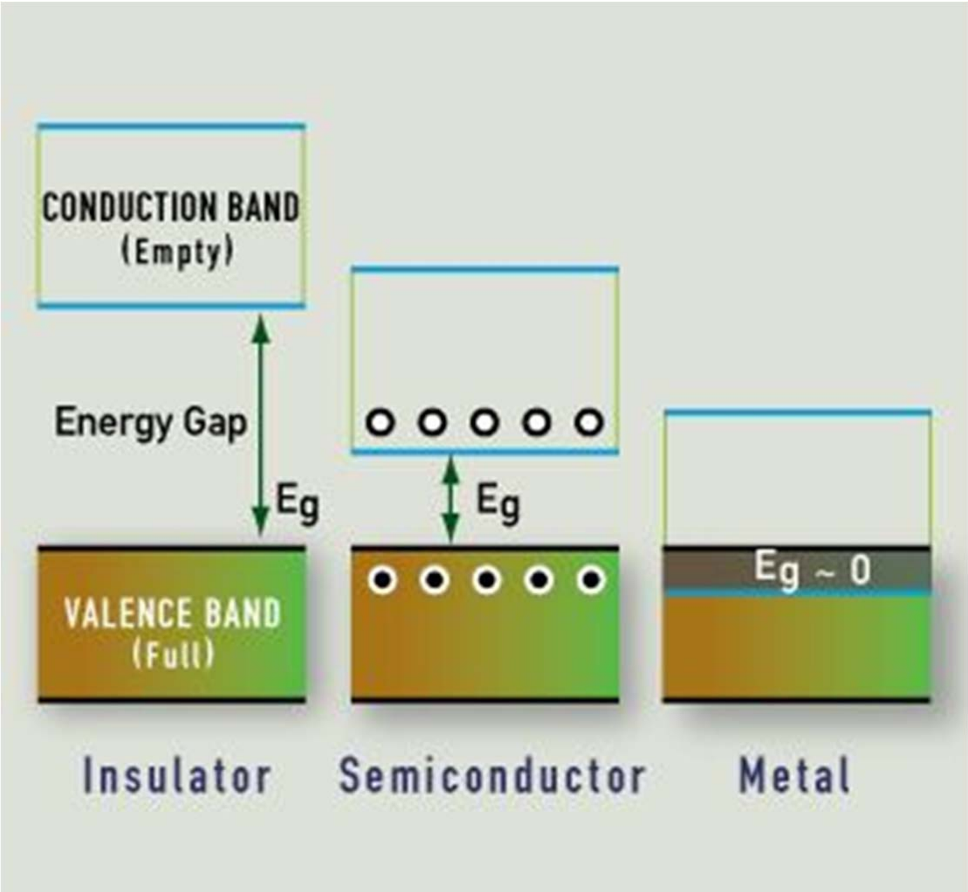
Packing Fraction

$$\mathrm{APF} = \frac{N_{\mathrm{atoms}} V_{\mathrm{atom}}}{V_{\mathrm{crystal}}}$$

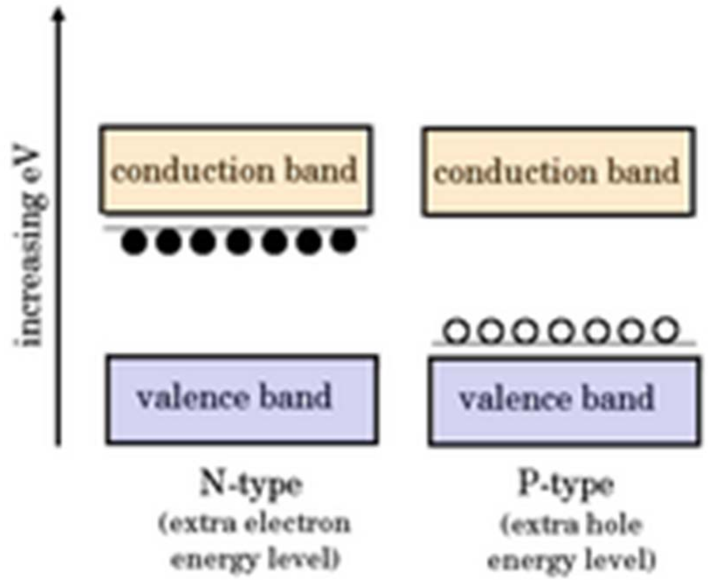
Surfaces

- Collective surface area of nanocube 1 nm
- Porous materials
  - Micropore (<2 nm)
  - Mesopore (2 nm ~ 50 nm)
  - Marcopore (> 50nm)
- Void volume
  - $V_{pore}/V_{material}$

Bandgap

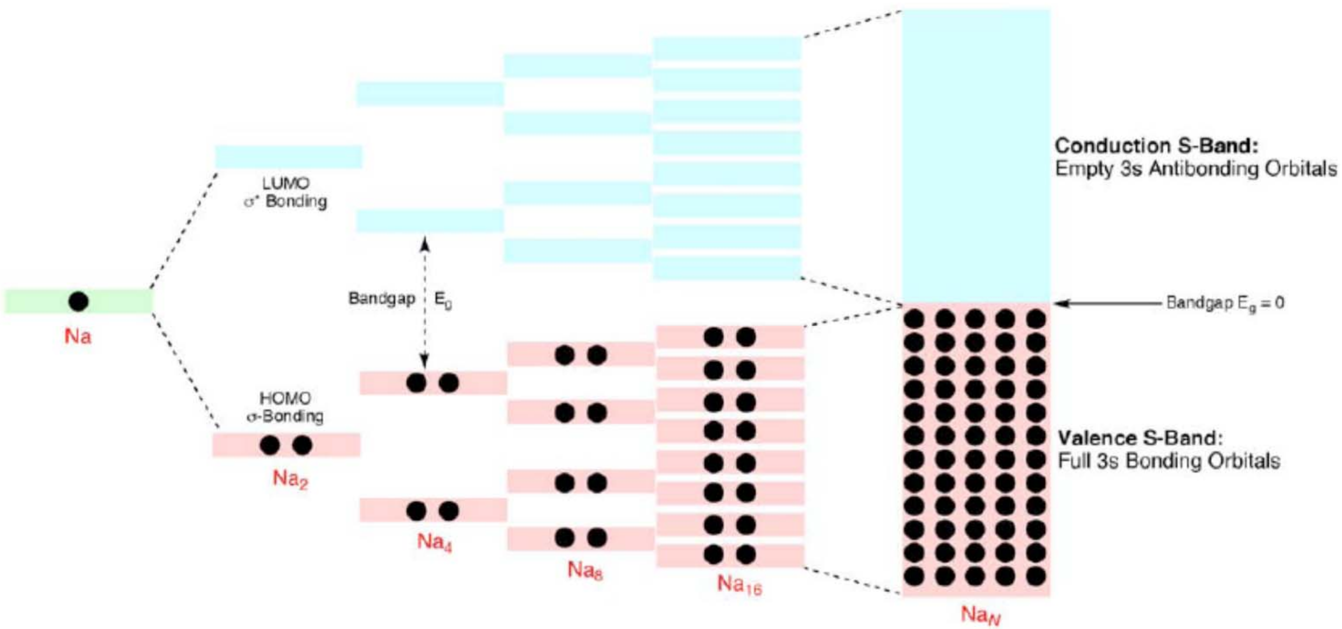


CONDUCTION BAND
(Empty)
Energy Gap
Eg
Eg
Eg ~ 0
VALENCE BAND
(Full)
Insulator
Semiconductor
Metal



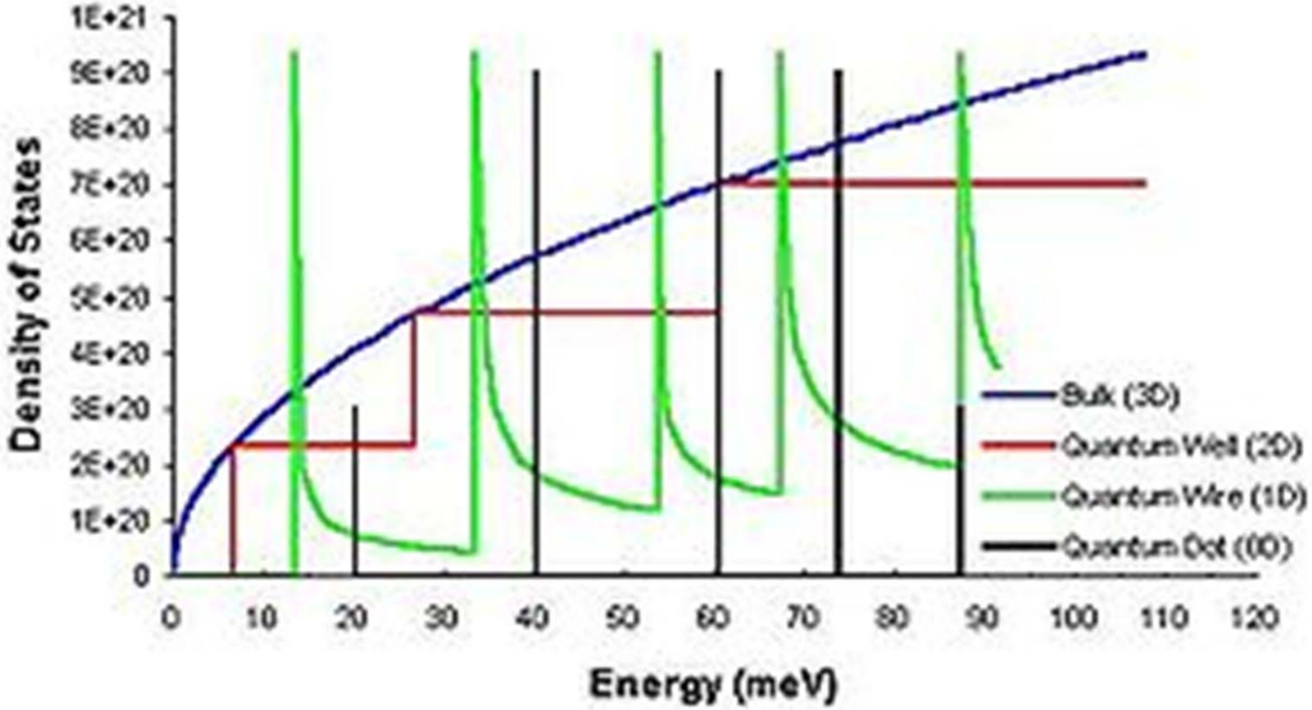
increasing eV
conduction band
conduction band
valence band
valence band
N-type
(extra electron energy level)
P-type
(extra hole energy level)

Bandgap



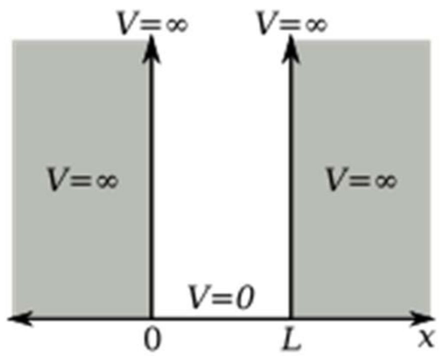
LUMO
σ* Bonding
Bandgap
E_0
HOMO
σ-Bonding
Na
Na_2
Na_4
Na_8
Na_{16}
Na_N
Conduction S-Band:
Empty 3s Antibonding Orbitals
Bandgap $E_g = 0$
Valence S-Band:
Full 3s Bonding Orbitals

Density of State



Particle in a Box

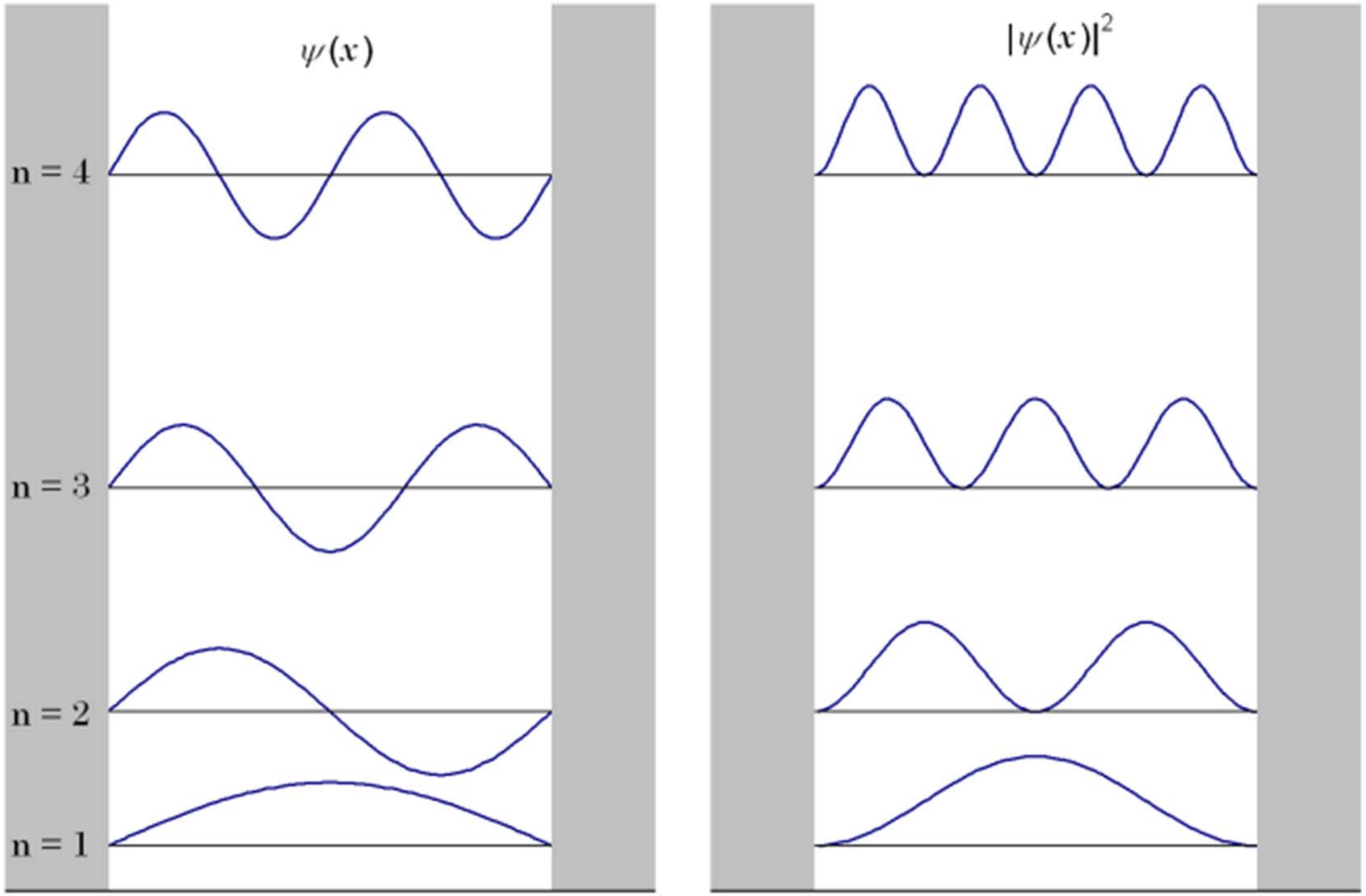
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (1)$$



$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2$$

Particle in a Box



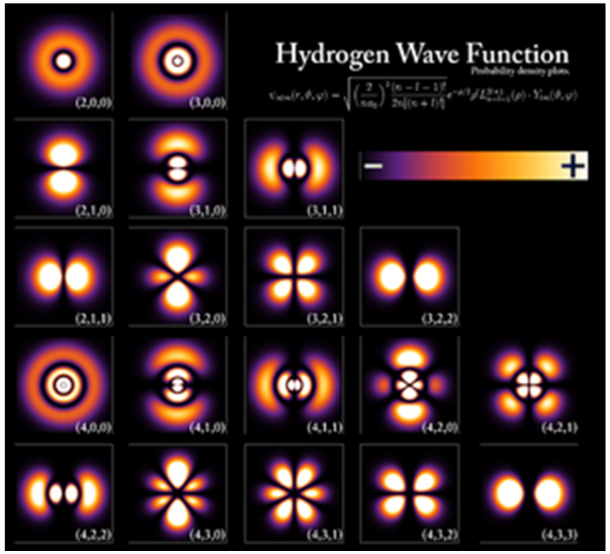
$$\psi_{n_x,n_y} = \sqrt{\frac{4}{L_x L_y}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right)$$

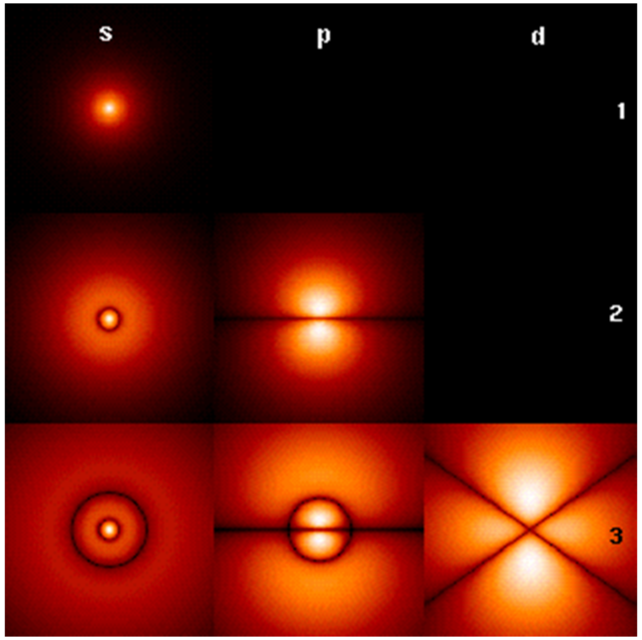
$$E_{n_x,n_y} = \frac{\hbar^2 \pi^2}{2m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right]$$

$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{L_x L_y L_z}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right) \quad (22)$$

$$E_{n_x,n_y,n_z} = \frac{\hbar^2 \pi^2}{2m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2 + \left(\frac{n_z}{L_z}\right)^2\right] \quad (23)$$

Wave Functions





$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},\, t) = \hat{H}\Psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\Psi(\mathbf{r},\, t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},\, t)+V(\mathbf{r})\Psi(\mathbf{r},\, t)$$

$$V(r) = -\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}$$

$$\psi_{n\ell m}(r,\vartheta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-\ell-1)!}{2n(n+\ell)!}}e^{-\rho/2}\rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho)\cdot Y_\ell^m(\vartheta,\varphi)$$

Linear combination of atomic orbitals molecular orbital method

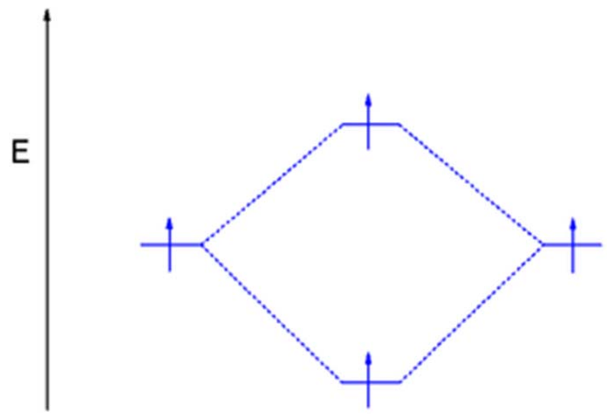
$$\phi_i = c_{1i}\chi_1 + c_{2i}\chi_2 + c_{3i}\chi_3 + \cdots + c_{ni}\chi_n$$

$$\psi_i = \sum_{\mu} c_{\mu i}\phi_{\mu}$$

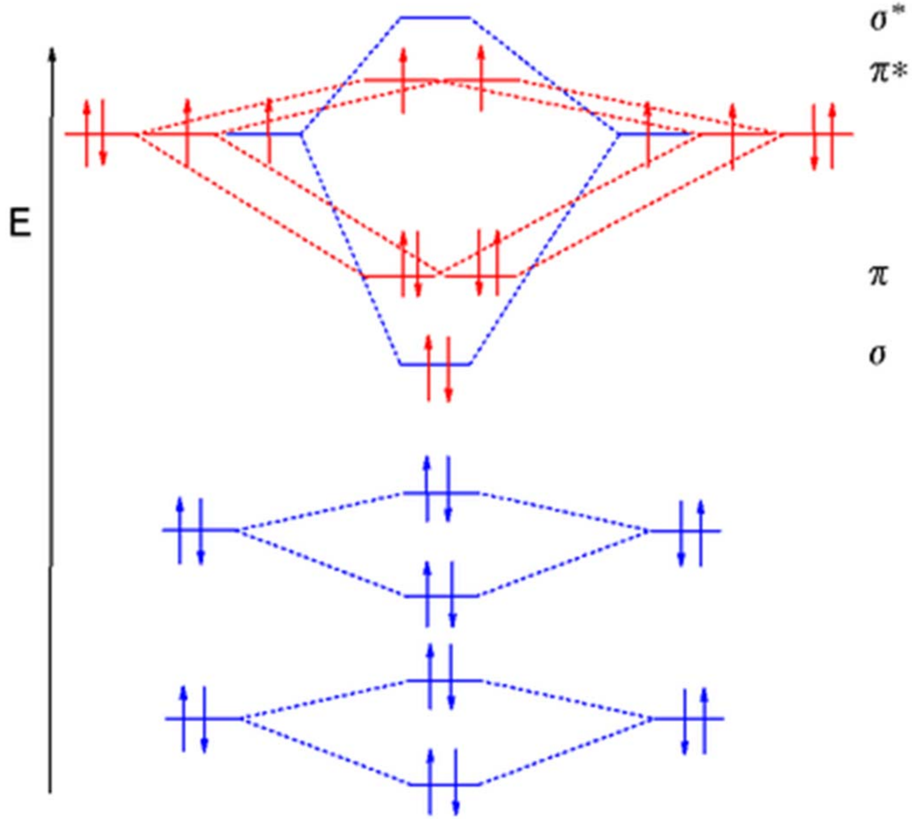
MO

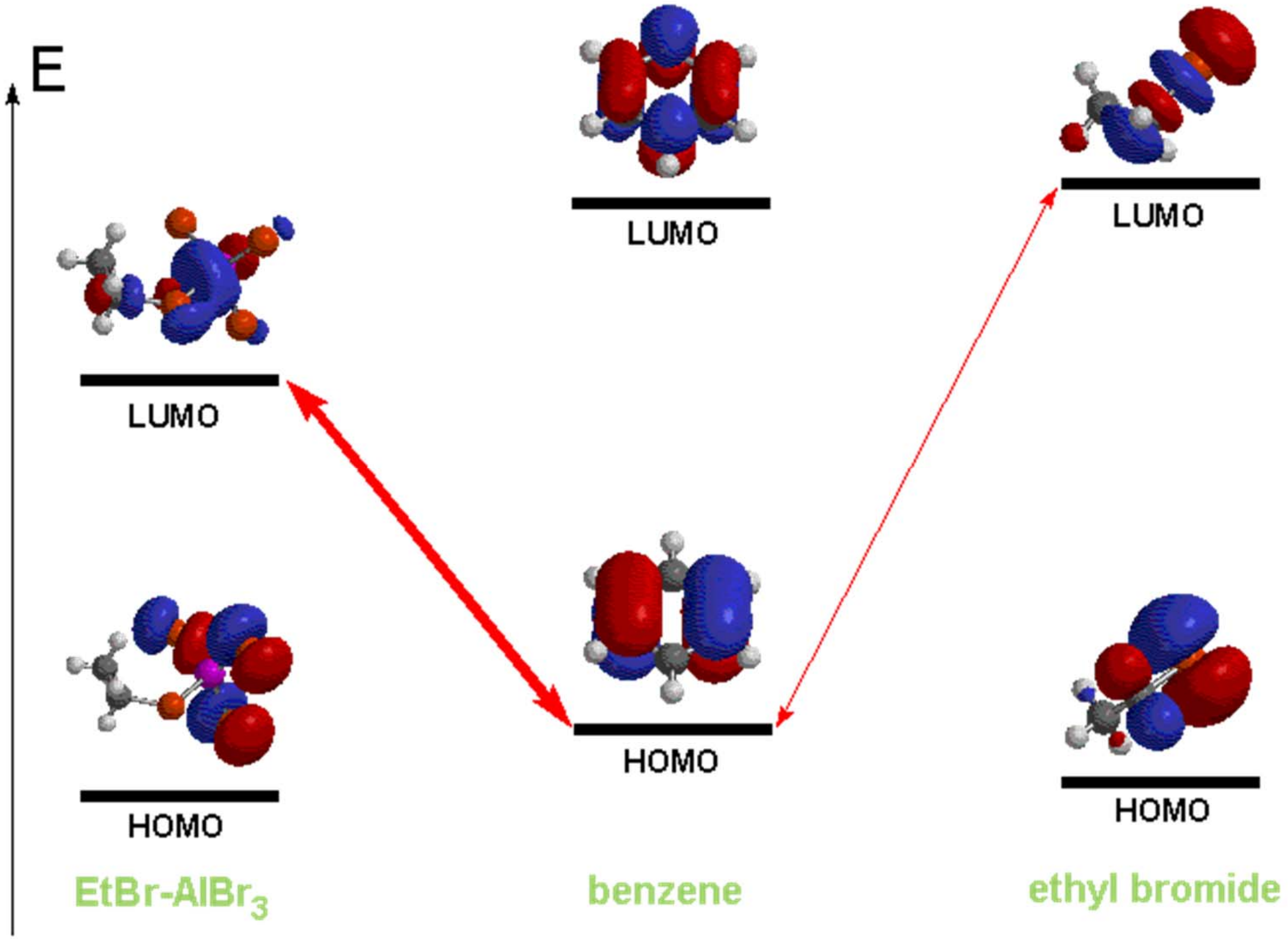
AO

coefficient of AO_{μ} in MO_i

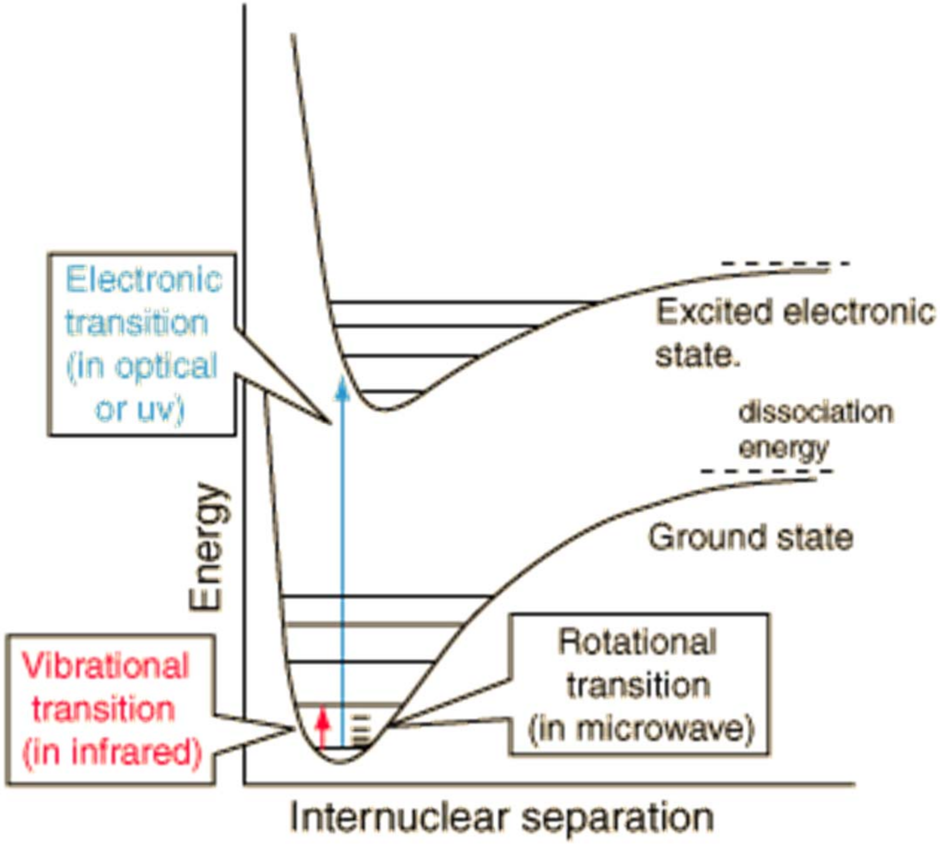


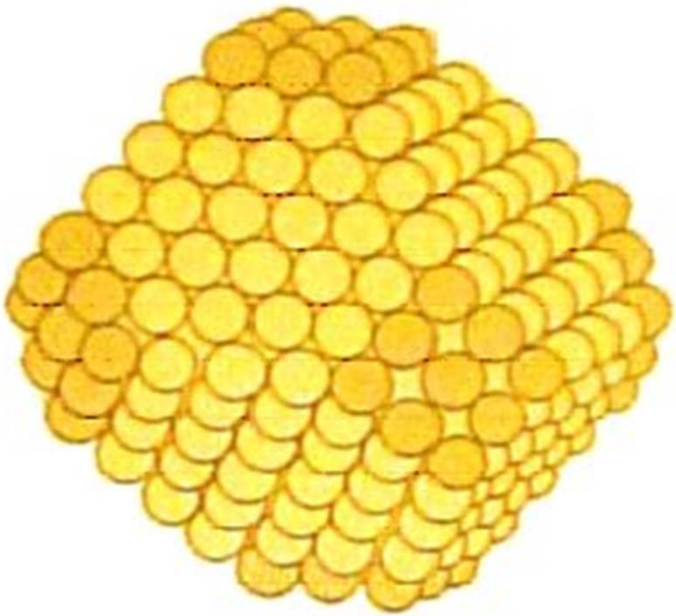
Oxygen





E
LUMO
LUMO
LUMO
HOMO
HOMO
HOMO
EtBr-AlBr3
benzene
ethyl bromide


Electronic transition (in optical or uv)
Excited electronic state.
dissociation energy
Ground state
Energy
Vibrational transition (in infrared)
Rotational transition (in microwave)
Internuclear separation



GOLD CUBOCTAHAL CLUSTER

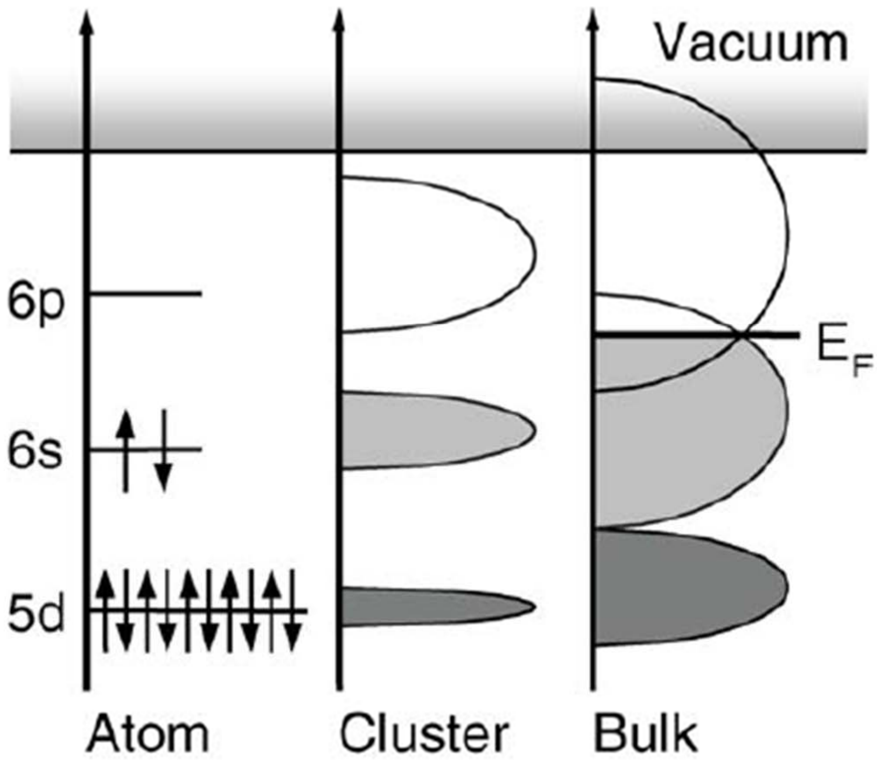


Figure 5 Energy diagram describing a generic Bloch-Wilson MIT in clusters (with specific reference to the energy levels of mercury). For sufficiently large clusters, the *s-p* band gap closes with increasing cluster size (shaded areas represent energy range with occupied electron levels). Overlap leads to a "continuous" DOS at E_F and to an Insulator to Metal transition.

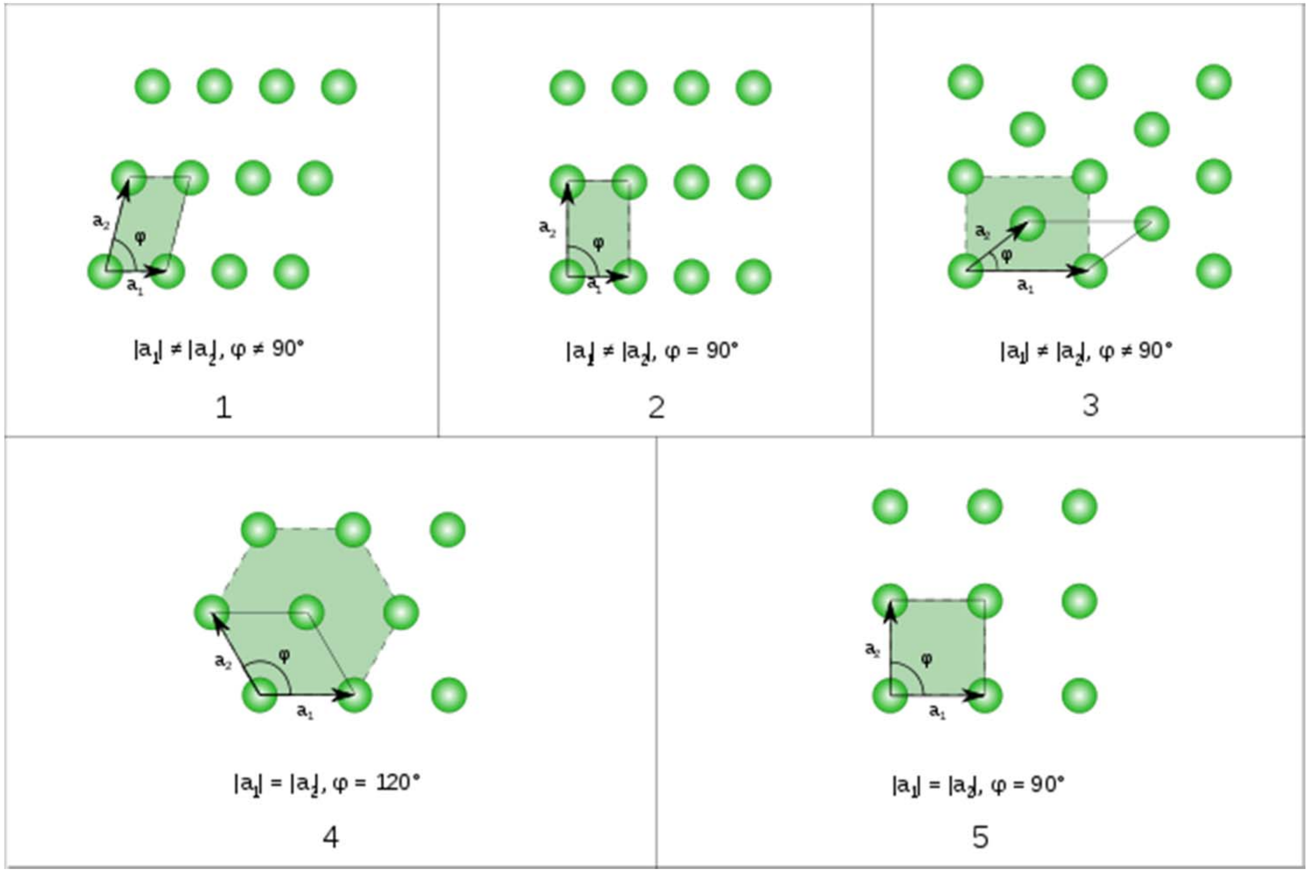
Bloch wave

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

A **Bloch wave** or **Bloch state**, named after Felix Bloch, is the wavefunction of a particle (usually, an electron) placed in a periodic potential.

$$\epsilon n(\mathbf{k}) = \epsilon n(\mathbf{k} + \mathbf{K}),$$

The five fundamental two-dimensional Bravais lattices



Unit Cell

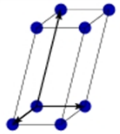
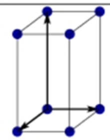
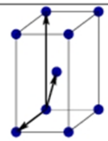
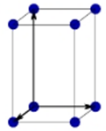
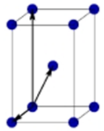
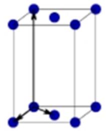
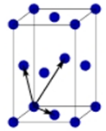
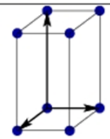
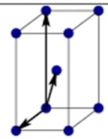
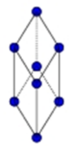
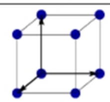
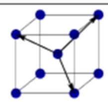
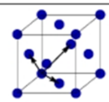
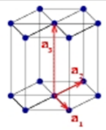
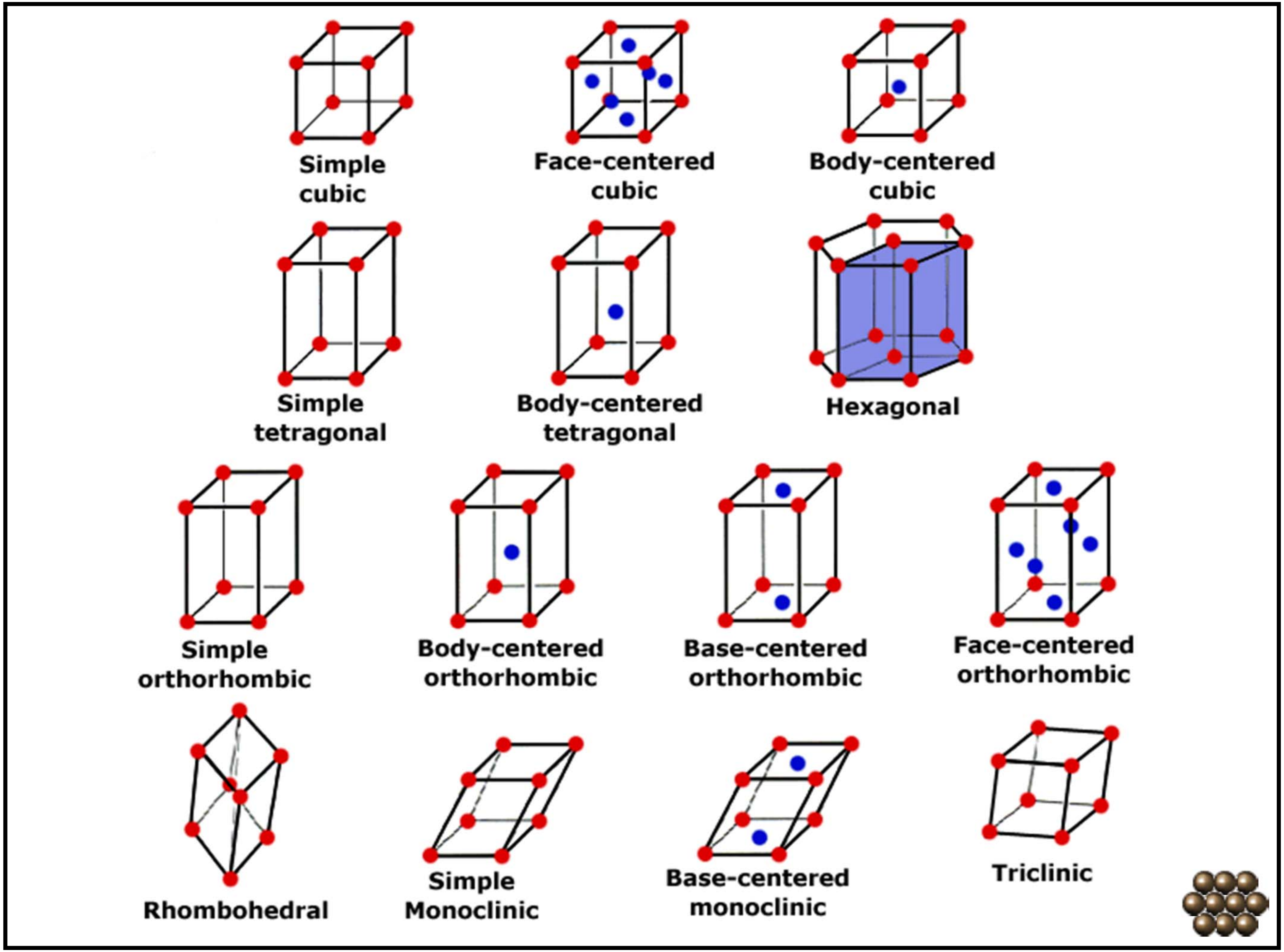
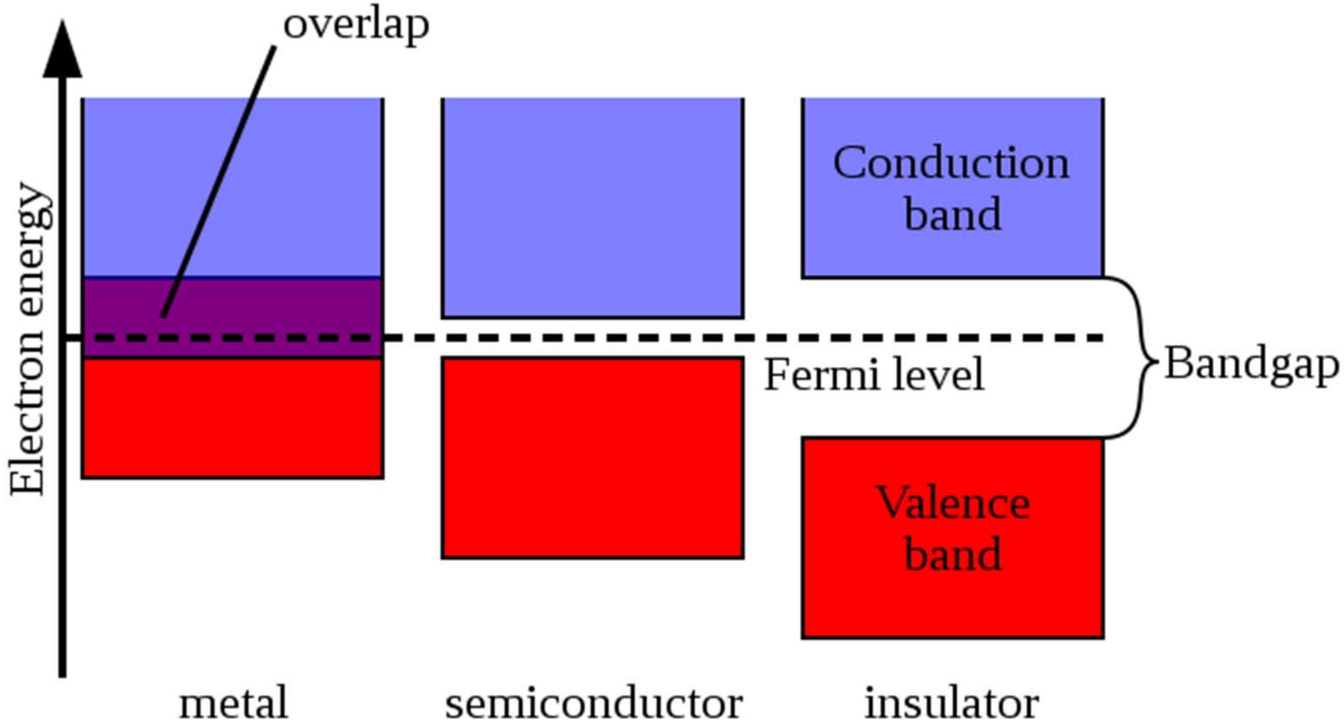
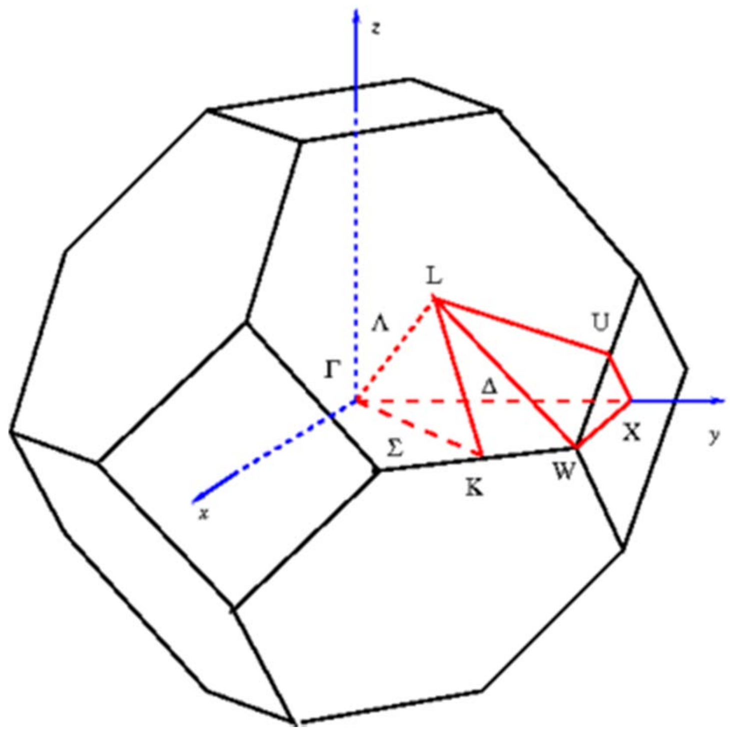
Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

Table 1.1: Bravais lattices in three-dimensions.

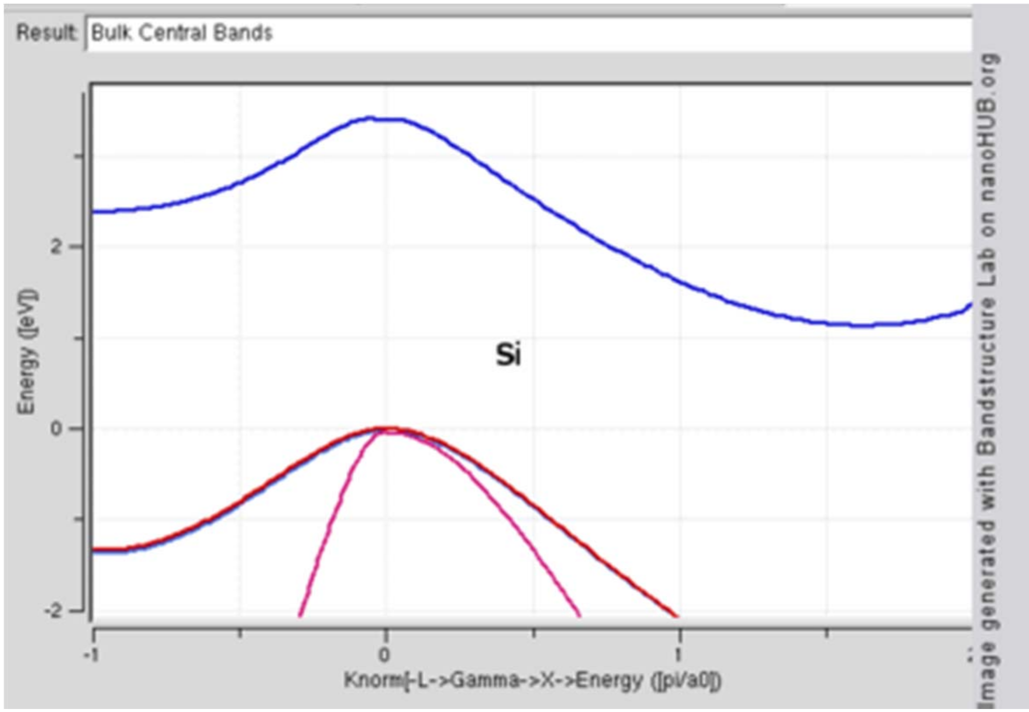

Simple cubic
Face-centered cubic
Body-centered cubic
Simple tetragonal
Body-centered tetragonal
Hexagonal
Simple orthorhombic
Body-centered orthorhombic
Base-centered orthorhombic
Face-centered orthorhombic
Rhombohedral
Simple Monoclinic
Base-centered monoclinic
Triclinic


overlap
Electron energy
Conduction band
Fermi level
Bandgap
Valence band
metal
semiconductor
insulator

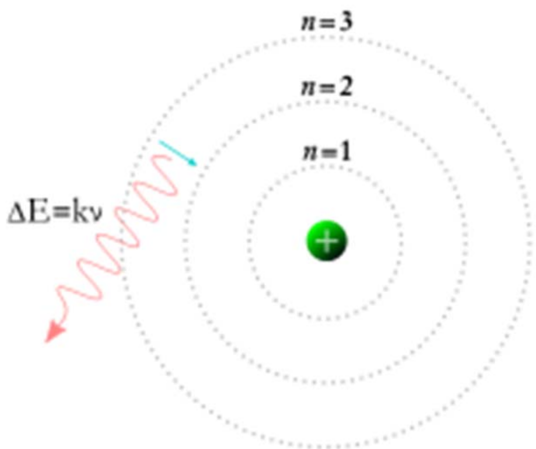
First Brillouin zone of FCC lattice showing symmetry labels

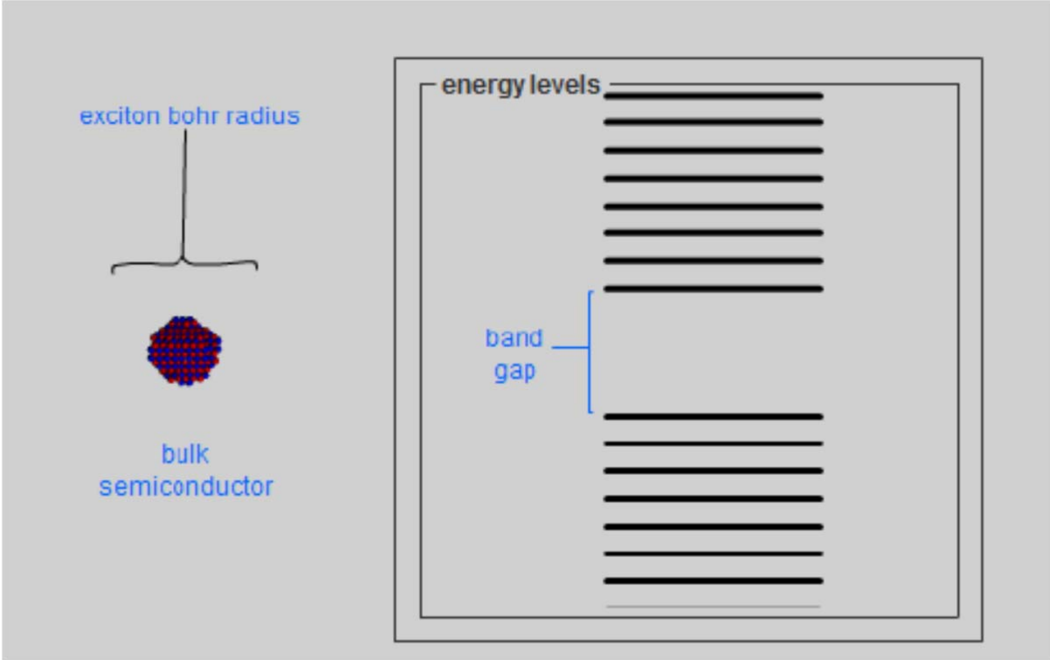


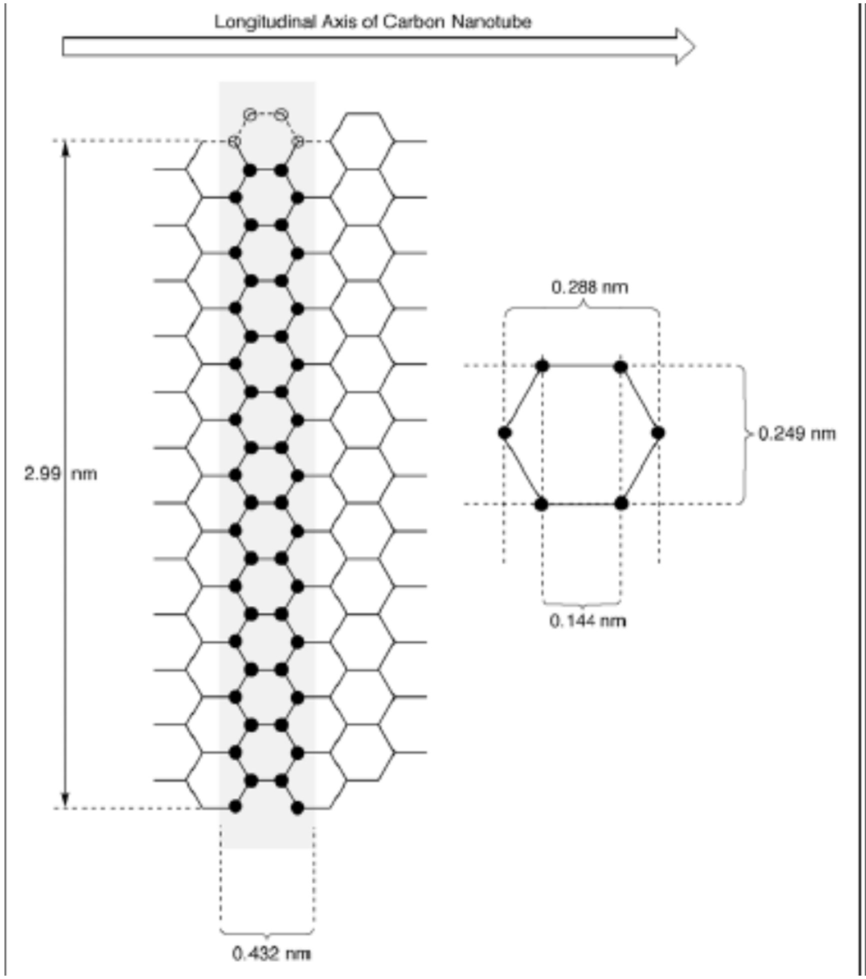
Band Structures



Bohr Exciton Radius







$2a = 0.144 \text{ nm}$

$a = 0.072 \text{ nm}$

$(Altitude)^2 = a^2 + 2a^2 = a\sqrt{3}$

$\text{Minimal diameter} = 2 \cdot a\sqrt{3} = 2 \cdot (0.072)\text{nm} \cdot \sqrt{3}$

$= \mathbf{0.249\ nm}$

Circumference or Perimeter, $p = 12 \cdot 0.249 \text{ nm} = \mathbf{2.988\ nm}$

$$p = \pi d; \text{ the } d = \frac{p}{\pi} = \frac{2.988\text{nm}}{\pi} = \mathbf{0.951\ nm}$$

$$m = \left(\frac{12.011\text{g}}{\text{mol}}\right)\left(\frac{1 \text{ mol}}{6.022x10^{23} \text{ atoms}}\right)48 \text{ atoms} = \mathbf{9.573x10^{-22}g}$$

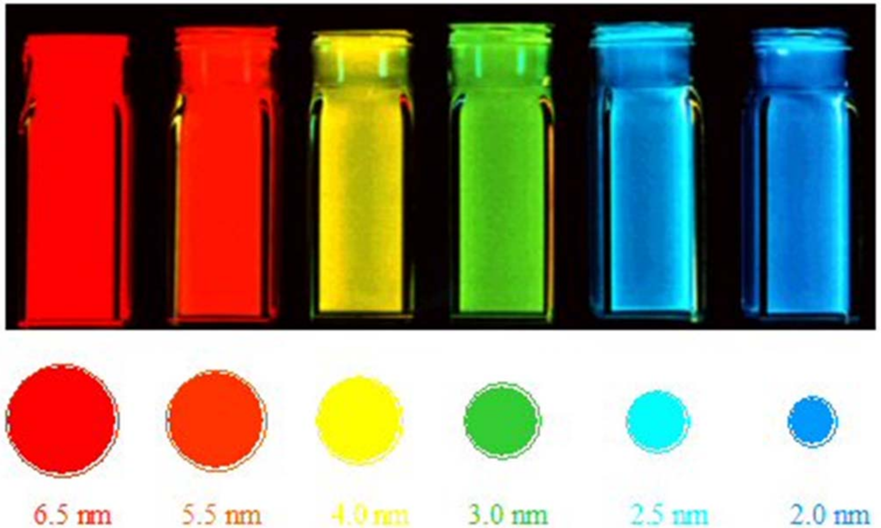
$$V_{unit\ cell} = 0.432\text{nm} \cdot \pi r^2 = 0.432\text{nm} \cdot \pi \cdot \left(\frac{0.951\text{nm}}{2}\right)^2 = \mathbf{0.307\ nm^3}$$

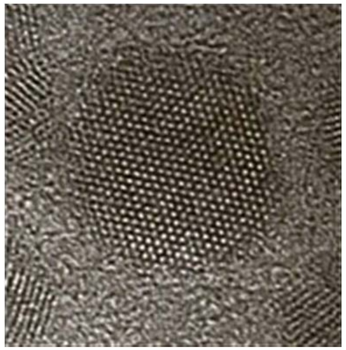
$$0.307\text{nm}^3\left(\frac{\text{cm}}{10^7\text{nm}}\right)^3 = \mathbf{3.07x10^{-22}\ cm^3}$$

$$\rho = \frac{\text{g}}{\text{cm}^3} = \frac{9.573x10^{-22}\text{g}}{3.07x10^{-22}\text{ cm}^3} = \mathbf{3.12\ g \cdot cm^3}$$

$$S_{Unit-cell} = \frac{p \cdot W}{m} = \frac{2.99\text{nm} \cdot 0.432\text{nm}}{9.573x10^{-22}g}\left(\frac{\text{m}}{10^9\text{nm}}\right)^2 = \mathbf{1.35x10^3\ m^2 \cdot g^{-1}}$$

CdSe





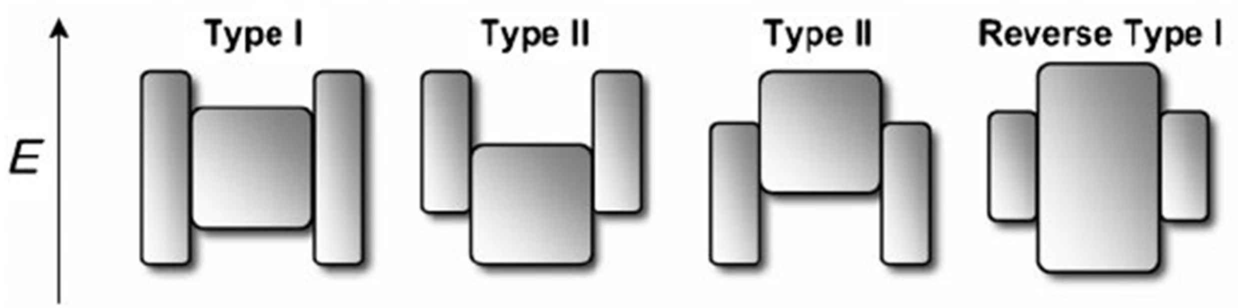
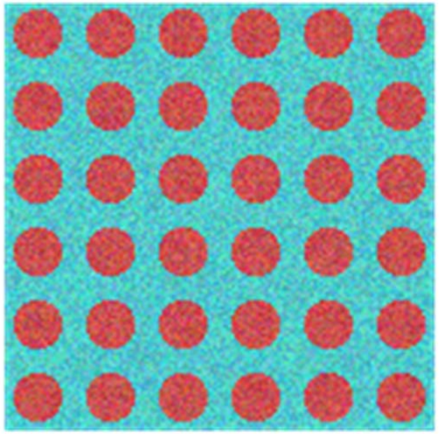
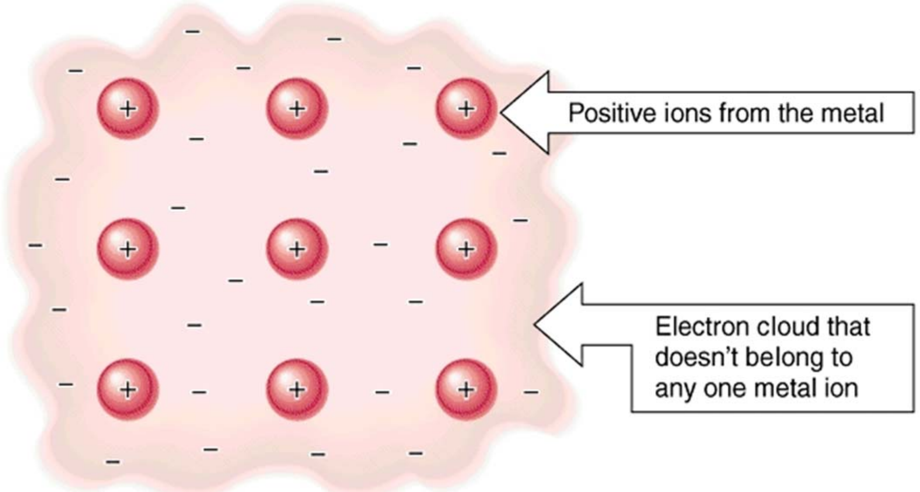


Figure 1. Schematic representation of the energy-level alignment in different core/shell systems realized with semiconductor NCs to date. The upper and lower edges of the rectangles correspond to the positions of the conduction- and valence-band edge of the core (center) and shell materials, respectively.

Electron Sea

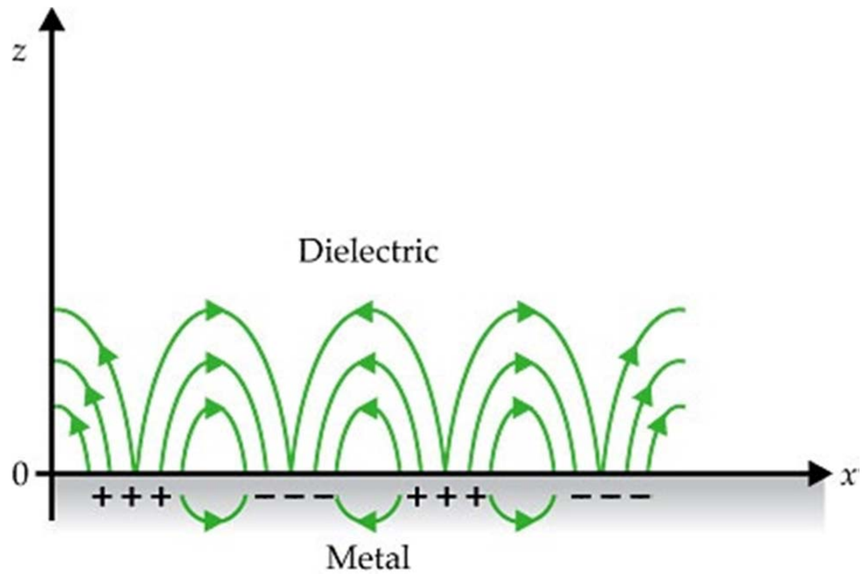




$$m \frac{d^2 \delta x}{dt^2} = e\, E_x = -m {\omega_p}^2\, \delta x,$$

$${\omega_p}^2 = \frac{n\, e^2}{\epsilon_0\, m},$$

Surface Plasmonon



$$\varepsilon_m = 1 - \frac{\omega_p^2}{\omega^2}$$

TiO_2

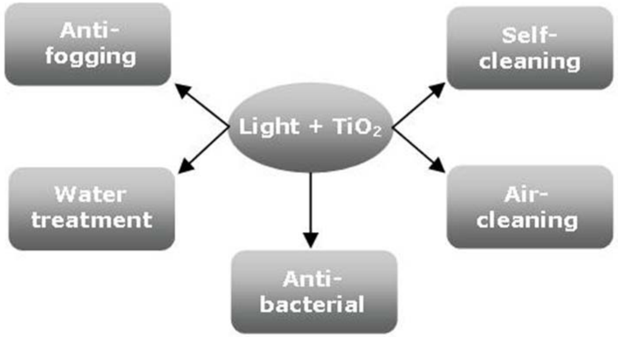
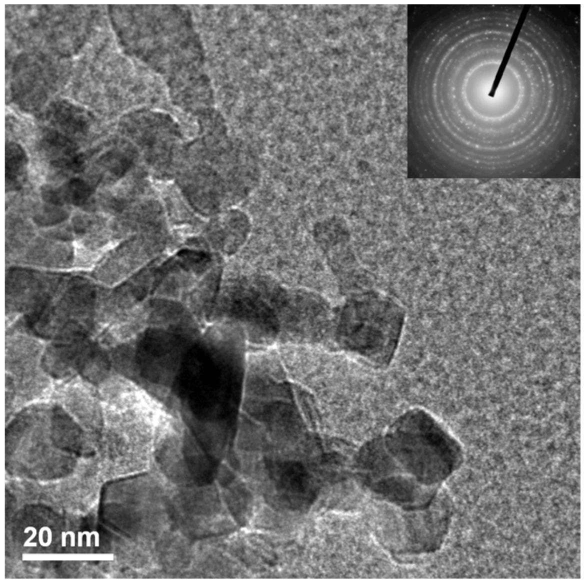
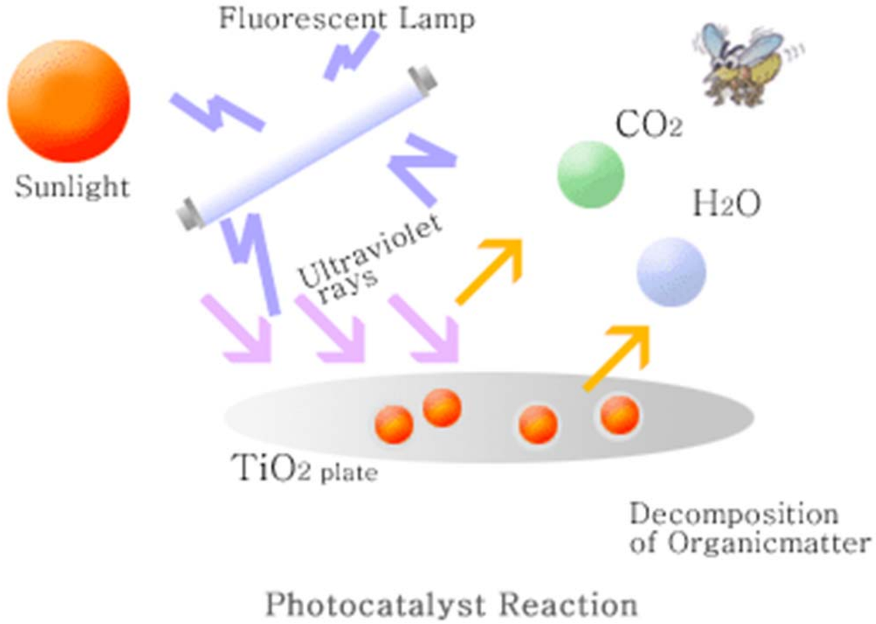
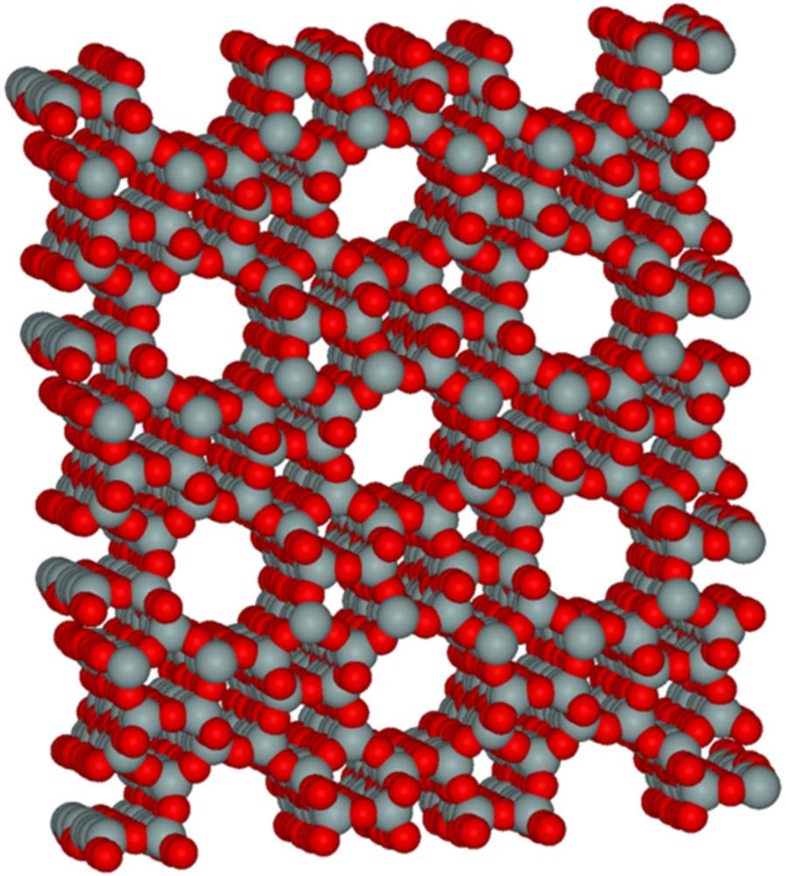


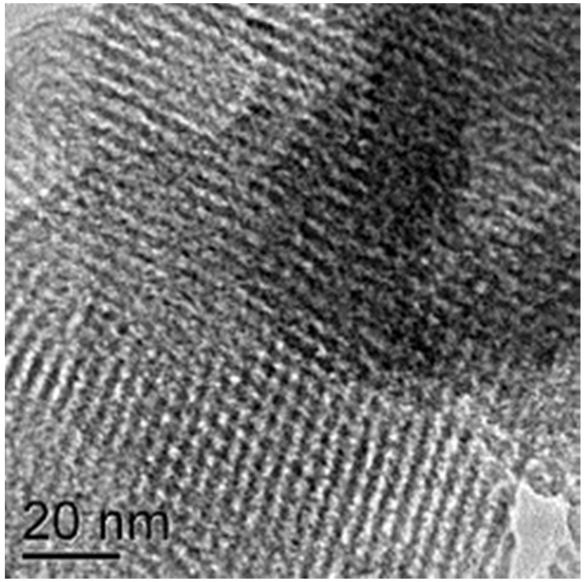
Figure 1. Major areas of activity in titanium dioxide photocatalysis



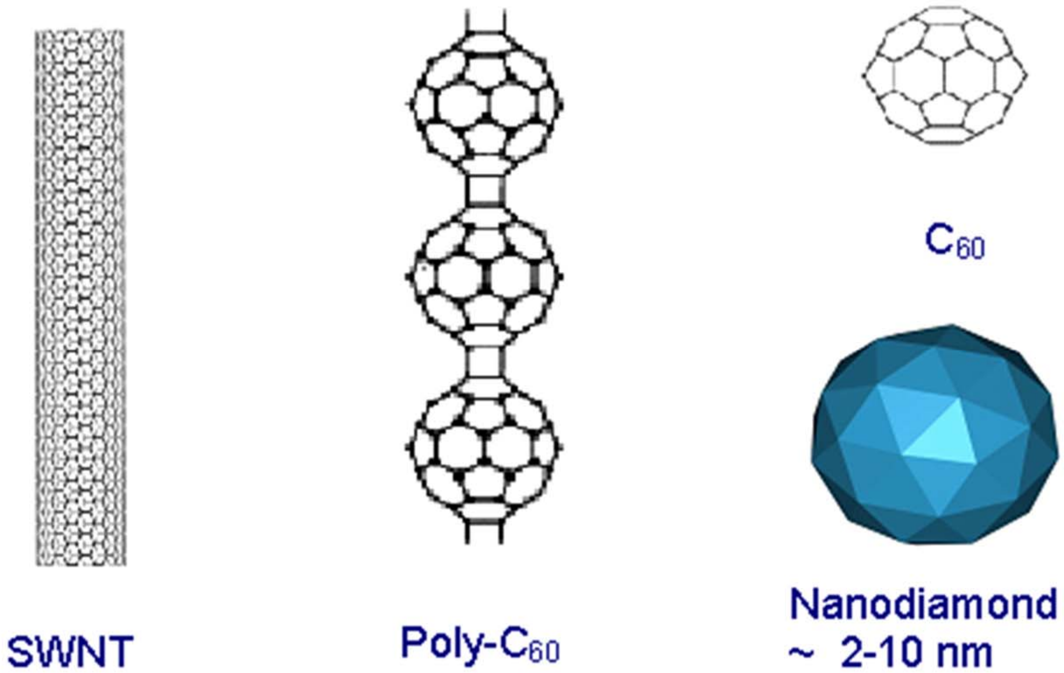


Zeolite

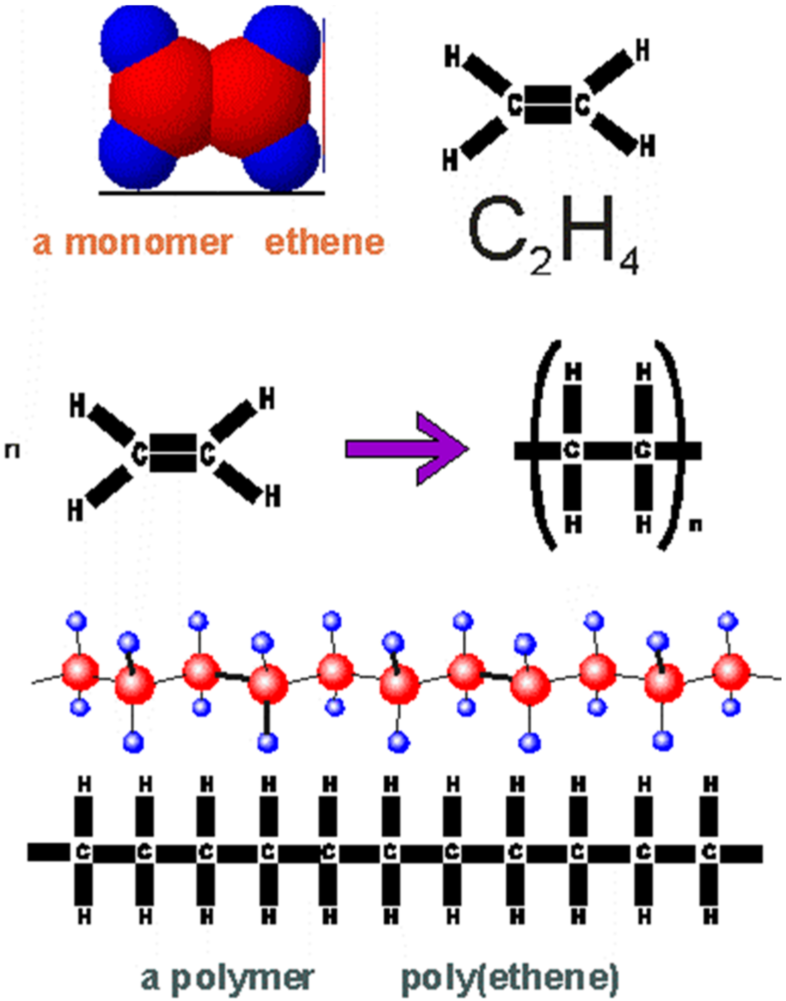




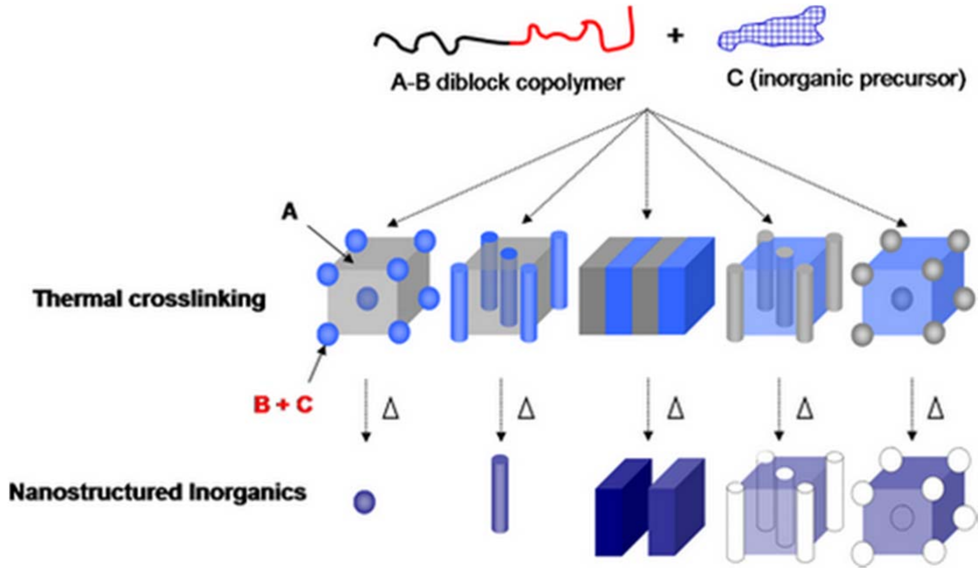
Carbon



Polymer

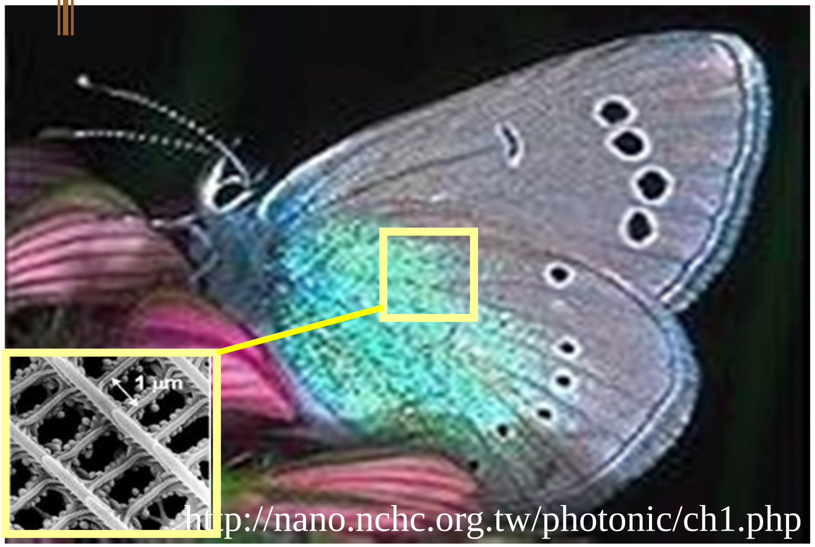


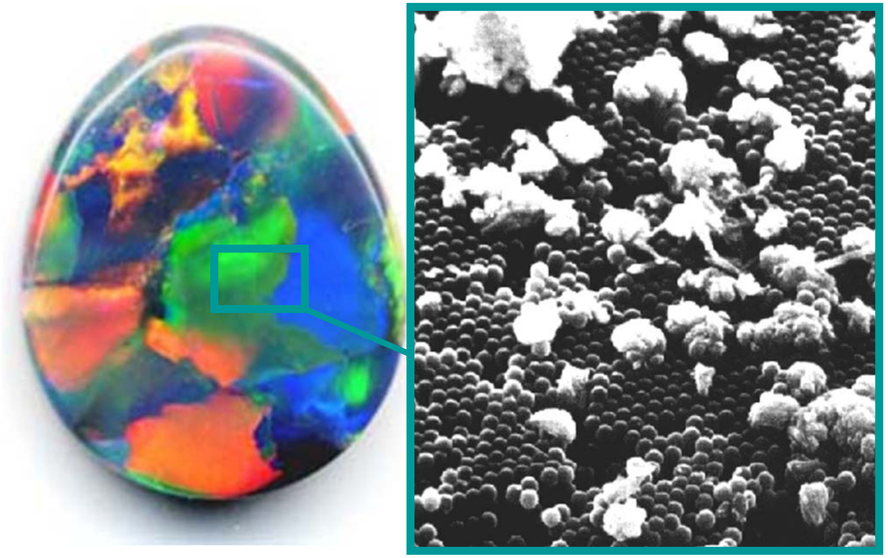
a monomer
ethene
C_2H_4
n
a polymer
poly(ethene)

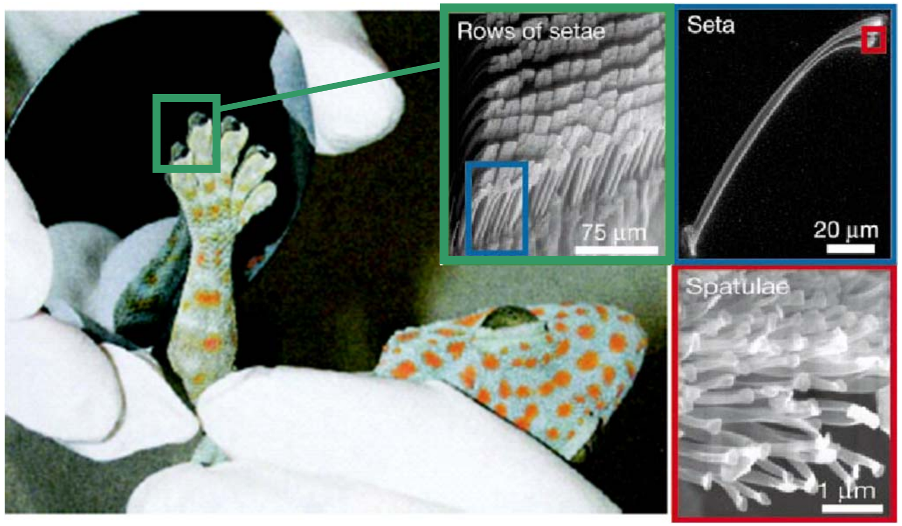


+
A-B diblock copolymer
C (inorganic precursor)
A
Thermal crosslinking
B + C
Δ
Nanostructured Inorganics

Nature Materials



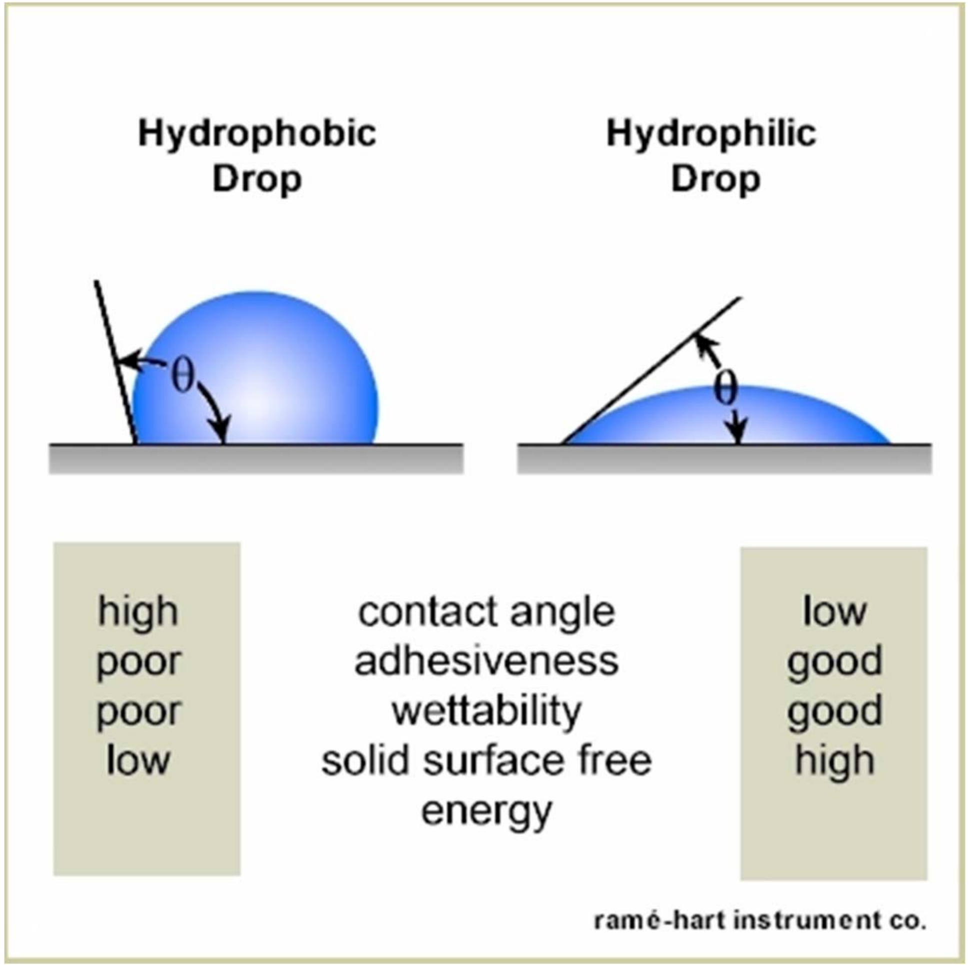




Surface Energy

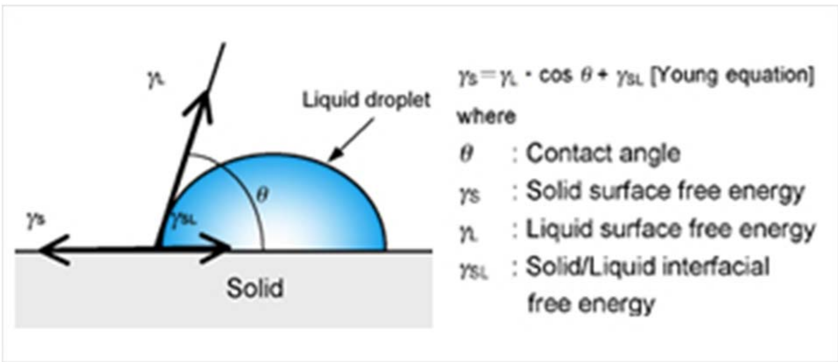
One face surface energy: γ
27 cube: 27 x 6 γ
3 x 9 cube line: 114 γ
3 x (3x3) square: 90 γ
3 x 3 x 3 cube: 54 γ

Contact Angle



Young's Equation

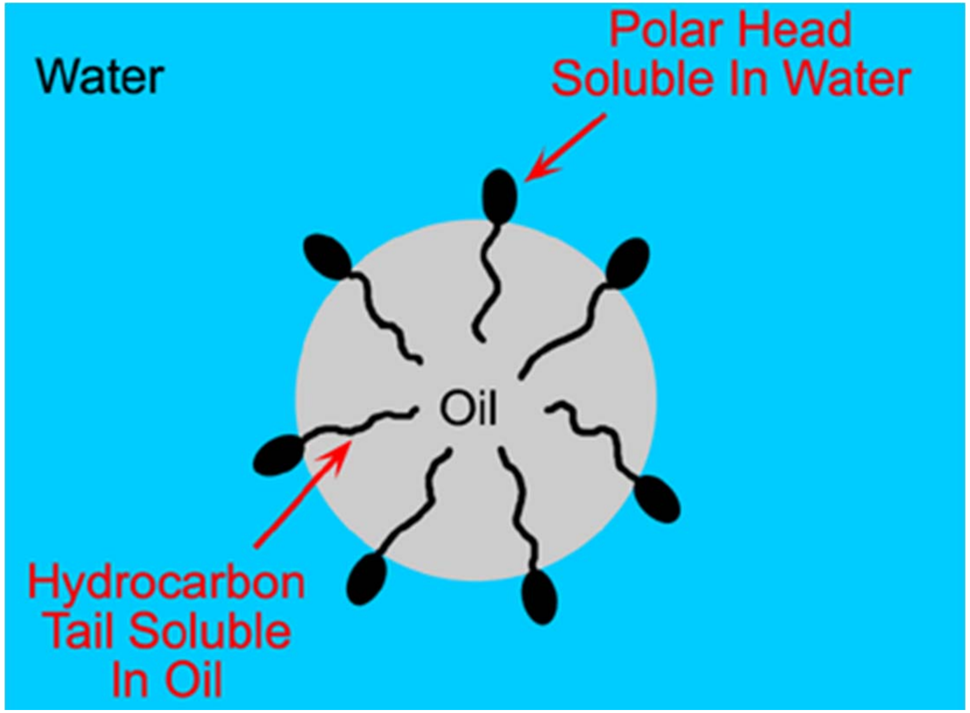
$$\gamma_{SL} + \gamma_{LV} \cos \theta_c = \gamma_{SV}$$



Surface Energy Minimization

- Surfactants
- DLVO
- Polymeric
- Nucleation
- Ostwald Ripening
- Sintering
- Restructure

Surfactant



Water
Polar Head
Soluble In Water
Oil
Hydrocarbon
Tail Soluble
In Oil

DLVO Theory

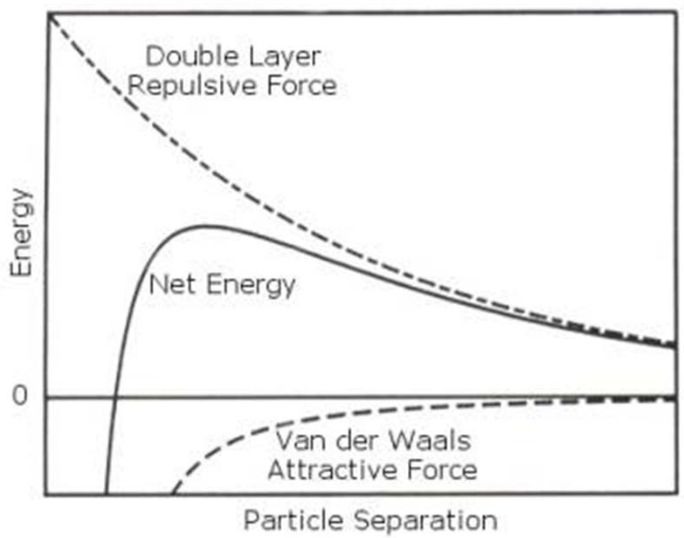
$$V_T = V_A + V_R + V_S$$

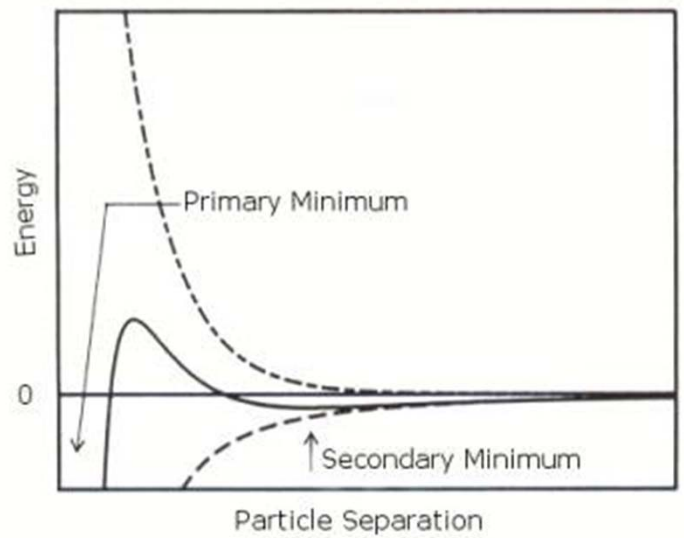
$$V_A = -A/(12\ \pi\ D^2)$$

A is the Hamaker constant and D is the particle separation

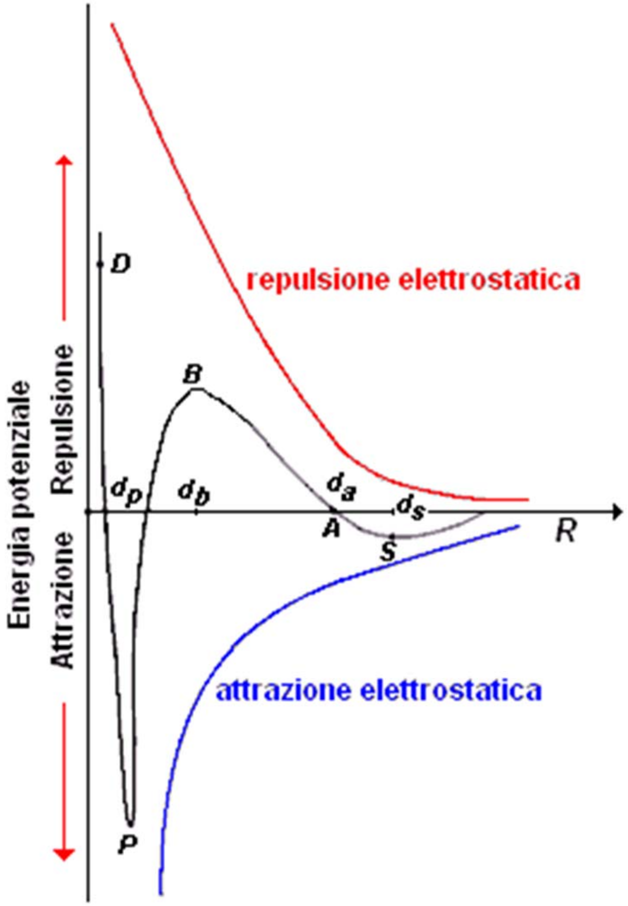
$$V_R = 2\ \pi\ \varepsilon\ a\ \xi^2 \exp(-\ \kappa D)$$

a is the particle radius, π is the solvent permeability,
κ is a function of the ionic composition and ξ is the zeta potential

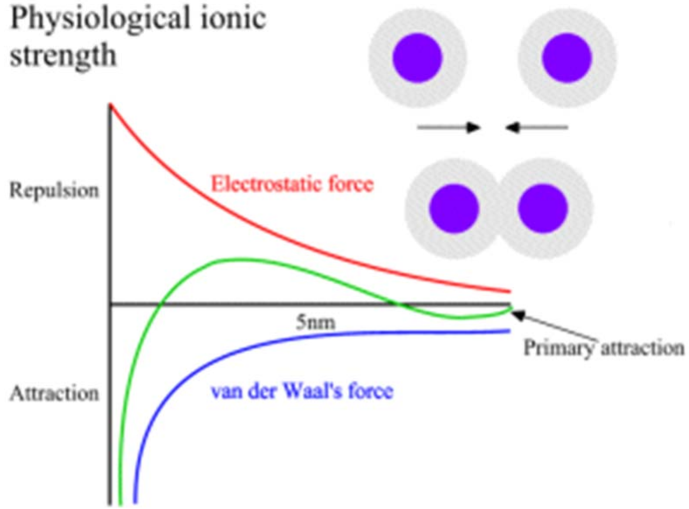

Double Layer
Repulsive Force
Energy
Net Energy
0
Van der Waals
Attractive Force
Particle Separation


Energy
Primary Minimum
0
Secondary Minimum
Particle Separation

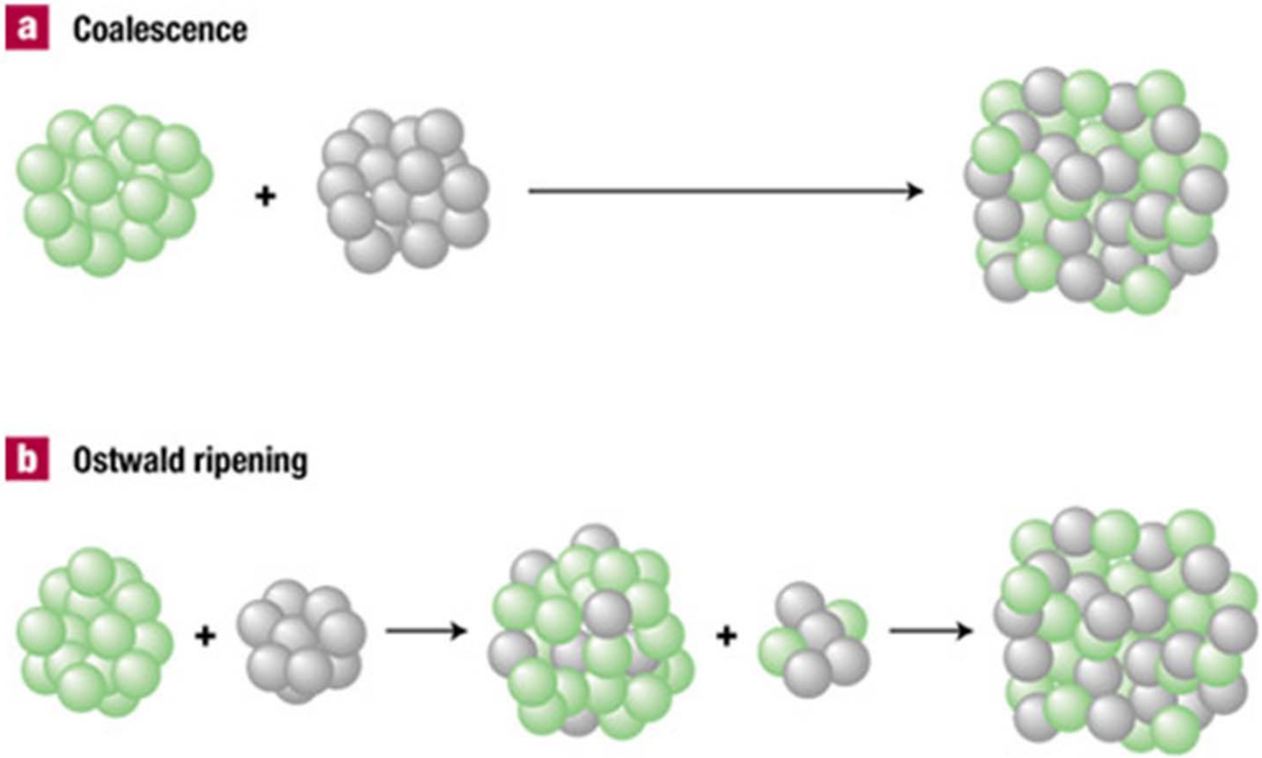
DLVO Theory



Energia potenziale
Repulsione
Attrazione
D
B
P
A
S
R
d_p
d_b
d_a
d_s
repulsione elettrostatica
attrazione elettrostatica



Physiological ionic strength
Repulsion
Attraction
Electrostatic force
van der Waal's force
5nm
Primary attraction



Two main mechanisms are shown here: **a**, coalescence sintering, and **b**, Ostwald ripening sintering. Coalescence sintering occurs when two clusters touch or collide and merge to form one bigger cluster. In contrast, Ostwald ripening sintering occurs by evaporation of atoms from one cluster, which then transfer to another. This is a dynamic process — both clusters exchange atoms, but the rate of loss from the smaller cluster is higher, because of the lower average coordination of atoms at the surface and their relative ease of removal. Thus big clusters get bigger at the expense of smaller clusters, which shrink and eventually disappear. The latter process is the usual form of sintering for metal clusters on a supported surface that are well spaced apart, although coalescence can occur for a high density of clusters. In general, the presence of the surface results in SMORS (surface-mediated Ostwald ripening sintering) in which material is transferred from one cluster to another by diffusion across the surface, and not through the gas phase.