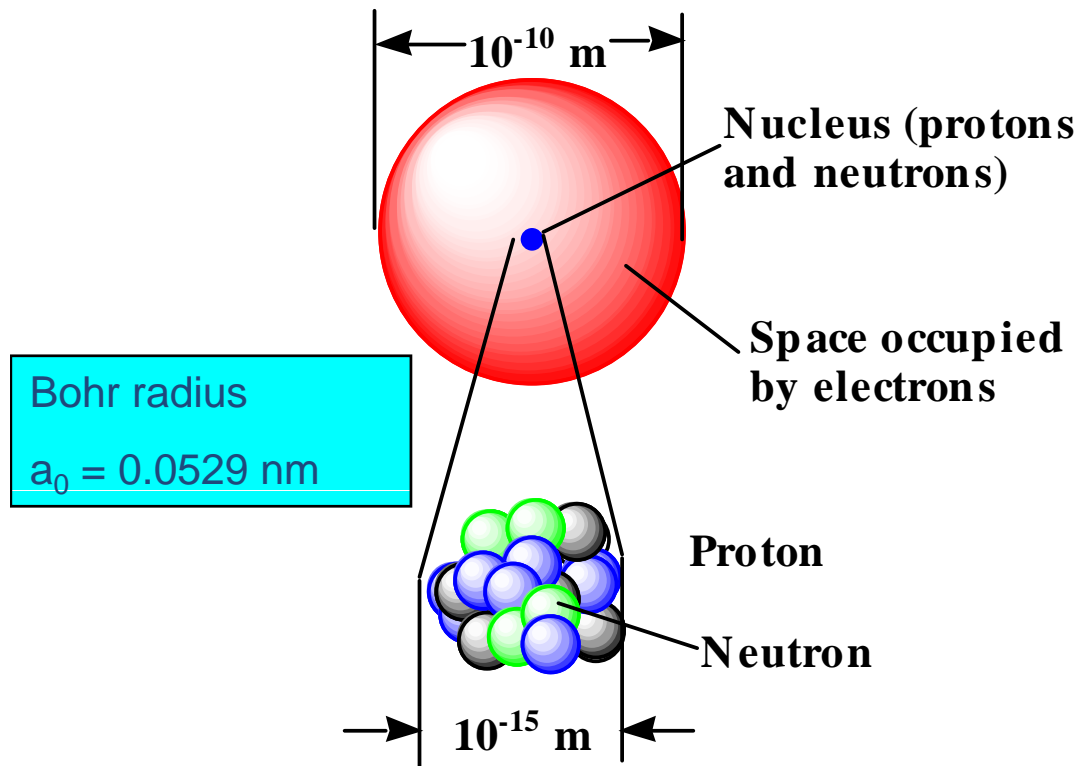


In nature's infinite book of secrecy

## **2. MATERIALS' FOUNDATIONS**

# Atomic Structure

	Proton	Neutron	Electron
Charge	$+1.60 \times 10^{-19} \text{ C}$	0	$-1.60 \times 10^{-19} \text{ C}$
Mass	$1.67 \times 10^{-27} \text{ kg}$	$1.67 \times 10^{-27} \text{ kg}$	$9.11 \times 10^{-31} \text{ kg}$



- Atomic number Z: number of protons in the nucleus
- Isotopes: same Z but different atomic weight
- Atomic mass unit (amu): 1/12 of  $^{12}\text{C}$
- One mole of material :  $6.02 \times 10^{23}$  atoms or molecules

# Quantum Mechanics: Electrons in Atoms

- Classical Mechanics vs. Quantum Mechanics: Schrödinger Equation  $H\Psi = E\Psi$   $\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} \{E - V(x)\} \psi$
- Wave-Particle duality de Broglie equation:  $\lambda = \frac{h}{p}$ , where  $h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s}$   $\psi = e^{ikx} = \cos kx + i \sin kx$

**Table 2.1** Summary of quantum numbers of electrons in atoms.

Name	Symbol	Permitted values	Property
Principal	$n$	Positive integers (1, 2, 3, ...)	Orbital energy (size)
Angular momentum	$l$	Integers from 0 to $n - 1$	Orbital shape (the $l$ values 0, 1, 2 and 3 correspond to s, p, d and f orbitals, respectively)
Magnetic	$m_l$	Integers from $-l$ to 0 to $+l$	Orbital orientation
Spin	$m_s$	$+\frac{1}{2}$ or $-\frac{1}{2}$	Direction of electron spin

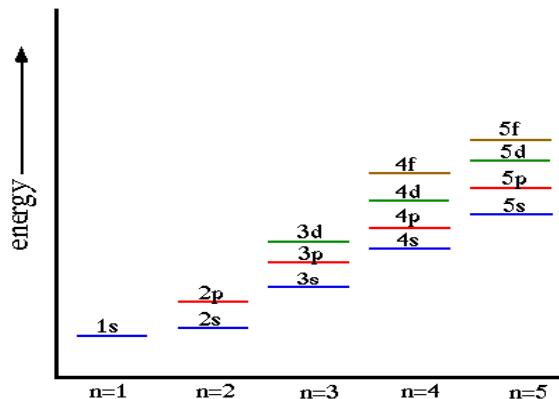
- Energy of subshells with different  $m_l$  (and also  $m_s$ ) gets splitted when a magnetic field is applied.
- Each electron in an atom has a unique set of quantum numbers: Pauli exclusion principle

# Orbital Filling : Periodic Table

**PERIODIC TABLE OF THE ELEMENTS**

<http://www.ktf-split.hr/periodni/en/>

PERIOD	GROUP I IA	GROUP IIA	GROUP IIIA	GROUP IVA	GROUP VA	GROUP VIA	GROUP VIIA	GROUP VIIIA										
1	1.0079 <b>H</b> HYDROGEN							2 4.0026 <b>He</b> HELIUM										
2	3 6.941 <b>Li</b> LITHIUM	4 9.0122 <b>Be</b> BERYLLIUM						10 20.180 <b>Ne</b> NEON										
3	11 22.990 <b>Na</b> SODIUM	12 24.305 <b>Mg</b> MAGNESIUM						18 39.948 <b>Ar</b> ARGON										
4	19 39.098 <b>K</b> POTASSIUM	20 40.078 <b>Ca</b> CALCIUM	21 44.956 <b>Sc</b> SCANDIUM	22 47.867 <b>Ti</b> TITANIUM	23 50.942 <b>V</b> VANADIUM	24 51.996 <b>Cr</b> CHROMIUM	25 54.938 <b>Mn</b> MANGANESE	26 55.845 <b>Fe</b> IRON	27 58.933 <b>Co</b> COBALT	28 58.693 <b>Ni</b> NICKEL	29 63.546 <b>Cu</b> COPPER	30 65.39 <b>Zn</b> ZINC	31 69.723 <b>Ga</b> GALLIUM	32 72.64 <b>Ge</b> GERMANIUM	33 74.922 <b>As</b> ARSENIC	34 78.96 <b>Se</b> SELENIUM	35 79.904 <b>Br</b> BROMINE	36 83.80 <b>Kr</b> KRYPTON
5	37 85.468 <b>Rb</b> RUBIDIUM	38 87.62 <b>Sr</b> STRONTIUM	39 88.906 <b>Y</b> YTTRIUM	40 91.224 <b>Zr</b> ZIRCONIUM	41 92.906 <b>Nb</b> NIOBIUM	42 95.94 <b>Mo</b> MOLYBDENUM	43 (98) <b>Tc</b> TECHNETIUM	44 101.07 <b>Ru</b> RUTHENIUM	45 102.91 <b>Rh</b> RHODIUM	46 106.42 <b>Pd</b> PALLADIUM	47 107.87 <b>Ag</b> SILVER	48 112.41 <b>Cd</b> CADMIUM	49 114.82 <b>In</b> INDIUM	50 118.71 <b>Sn</b> TIN	51 121.76 <b>Sb</b> ANTIMONY	52 127.60 <b>Te</b> TELLURIUM	53 126.90 <b>I</b> IODINE	54 131.29 <b>Xe</b> XENON
6	55 132.91 <b>Cs</b> CAESIUM	56 137.33 <b>Ba</b> BARIUM	57-71 <b>La-Lu</b> Lanthanide	72 178.49 <b>Hf</b> HAFNIUM	73 180.95 <b>Ta</b> TANTALUM	74 183.84 <b>W</b> TUNGSTEN	75 186.21 <b>Re</b> RHENIUM	76 190.23 <b>Os</b> OSMIUM	77 192.22 <b>Ir</b> IRIDIUM	78 195.08 <b>Pt</b> PLATINUM	79 196.97 <b>Au</b> GOLD	80 200.59 <b>Hg</b> MERCURY	81 204.38 <b>Tl</b> THALLIUM	82 207.2 <b>Pb</b> LEAD	83 208.98 <b>Bi</b> BISMUTH	84 (209) <b>Po</b> POLONIUM	85 (210) <b>At</b> ASTATINE	86 (222) <b>Rn</b> RADON
7	87 (223) <b>Fr</b> FRANCIUM	88 (226) <b>Ra</b> RADIUM	89-103 <b>Ac-Lr</b> Actinide	104 (261) <b>Rf</b> RUTHERFORDIUM	105 (262) <b>Db</b> DUBNIUM	106 (266) <b>Sg</b> SEABORGIUM	107 (264) <b>Bh</b> BOHRIUM	108 (277) <b>Hs</b> HASSIUM	109 (268) <b>Mt</b> MEITNERIUM	110 (281) <b>Uun</b> UNUNNIUM	111 (272) <b>Uuu</b> UNUNUNIUM	112 (285) <b>Uub</b> UNUNBIUM	114 (289) <b>Uuq</b> UNUNQUADIUM					

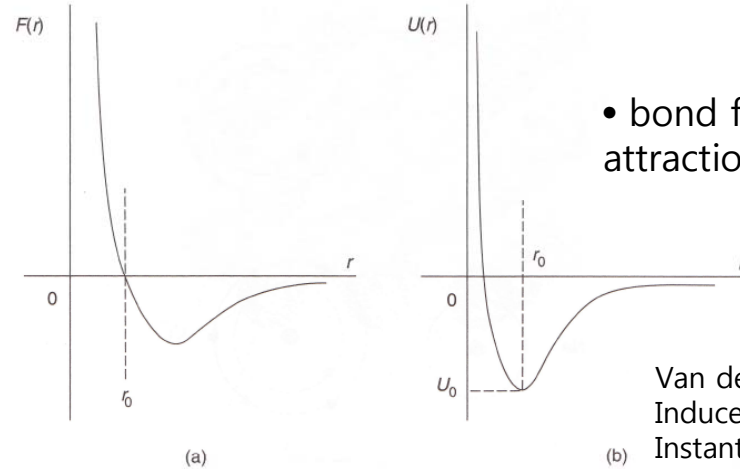
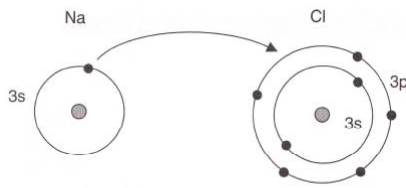


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LANTHANIDE														
57 138.91 <b>La</b> LANTHANUM	58 140.12 <b>Ce</b> CERIUM	59 140.91 <b>Pr</b> PRASEODYMIUM	60 144.24 <b>Nd</b> NEODYMIUM	61 (145) <b>Pm</b> PROMETHIUM	62 150.36 <b>Sm</b> SAMARIUM	63 151.96 <b>Eu</b> EUROPIUM	64 157.25 <b>Gd</b> GADOLINIUM	65 158.93 <b>Tb</b> TERBIUM	66 162.50 <b>Dy</b> DYSPROSIUM	67 164.93 <b>Ho</b> HOLMIUM	68 167.26 <b>Er</b> ERBIUM	69 168.93 <b>Tm</b> THULIUM	70 173.04 <b>Yb</b> YTTERIUM	71 174.97 <b>Lu</b> LUTETIUM
ACTINIDE														
89 (227) <b>Ac</b> ACTINIUM	90 232.04 <b>Th</b> THORIUM	91 231.04 <b>Pa</b> PROTACTINIUM	92 238.03 <b>U</b> URANIUM	93 (237) <b>Np</b> NEPTUNIUM	94 (244) <b>Pu</b> PLUTONIUM	95 (243) <b>Am</b> AMERICIUM	96 (247) <b>Cm</b> CURIUM	97 (247) <b>Bk</b> BERKELIUM	98 (251) <b>Cf</b> CALIFORNIUM	99 (252) <b>Es</b> EINSTEINIUM	100 (257) <b>Fm</b> FERMIUM	101 (258) <b>Md</b> MENDELEVIUM	102 (259) <b>No</b> NOBELIUM	103 (262) <b>Lr</b> LAWRENCIUM

- Hund's rule: When equal energy orbitals are available, electrons enter singly with parallel spin.

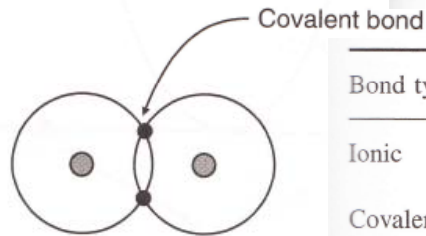
# Chemical Bonding



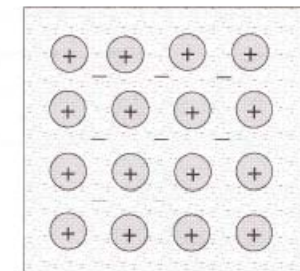
- bond formation driven by electrical attraction and repulsion

Van der Waals:  
 Induced dipole – induced dipole (dispersion force)  
 Instantaneous dipole-induced dipole (London force)

**Figure 2.6** (a) Interaction force  $F(r)$  between two atoms as a function of their interatomic separation  $r$ . (b) Potential energy  $U(r)$  as a function of interatomic separation  $r$ . The equilibrium separation is  $r_0$ .

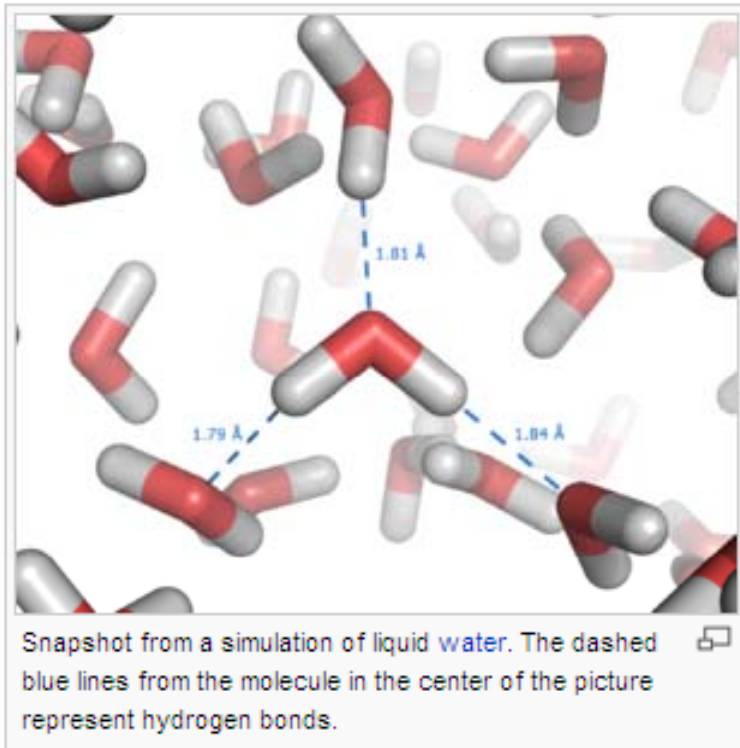


Bond type	Examples	Bond energy (eV per atom)	Melting temperature (°C)
Ionic	NaCl	3.3	801
	MgO	5.2	2852
Covalent	Si	4.0	1410
	C (diamond)	7.4	3550
Metallic	Cu	3.1	1083
	Al	3.4	660
Van der Waals	Ar	0.08	-189
	Cl <sub>2</sub>	0.32	-101
Hydrogen	H <sub>2</sub> O	0.52	0
	NH <sub>3</sub>	0.36	-78



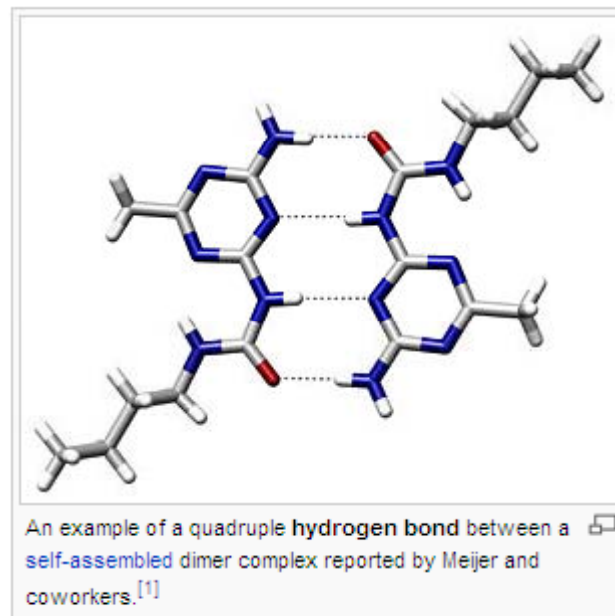
- 1 eV : energy acquired by one electron accelerated in the potential difference of 1 V. (=1.60 x 10<sup>-19</sup> J)

# Hydrogen Bonding



Supramolecular Chemistry  
Self-assembly  
Bottom-up nanofabrication

- $\text{F—H}\cdots\text{F}$  (155 kJ/mol or 40 kcal/mol)
- $\text{O—H}\cdots\text{N}$  (29 kJ/mol or 6.9 kcal/mol)
- $\text{O—H}\cdots\text{O}$  (21 kJ/mol or 5.0 kcal/mol)
- $\text{N—H}\cdots\text{N}$  (13 kJ/mol or 3.1 kcal/mol)
- $\text{N—H}\cdots\text{O}$  (8 kJ/mol or 1.9 kcal/mol)
- $\text{HO—H}\cdots\text{OH}_3^+$  (18 kJ/mol or 4.3 kcal/mol)



Source:  
*Wikipedia*

# Carbon Atom Hybridization for Bond Formation

- Why hybridization? :  
Energy pay-back

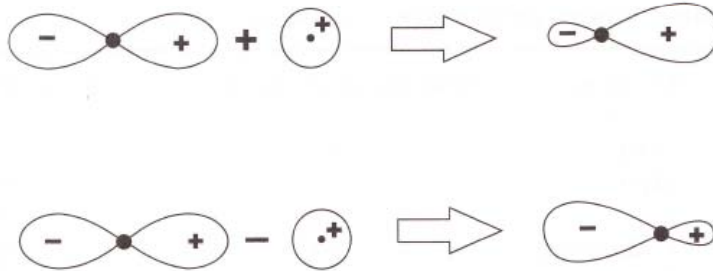


Figure 2.16

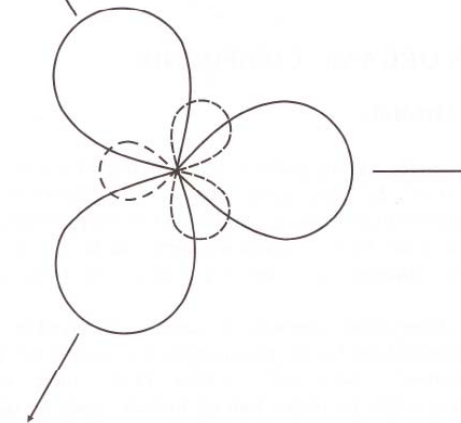


Figure 2.17 Three  $sp^2$  hybridized orbitals.

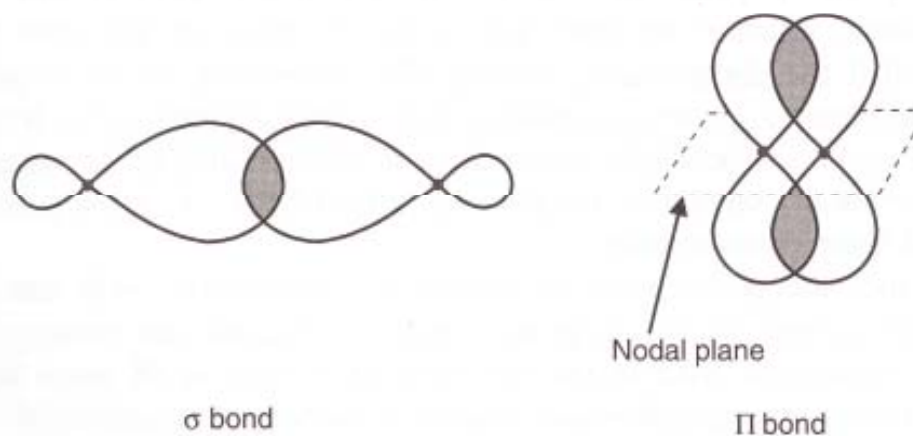
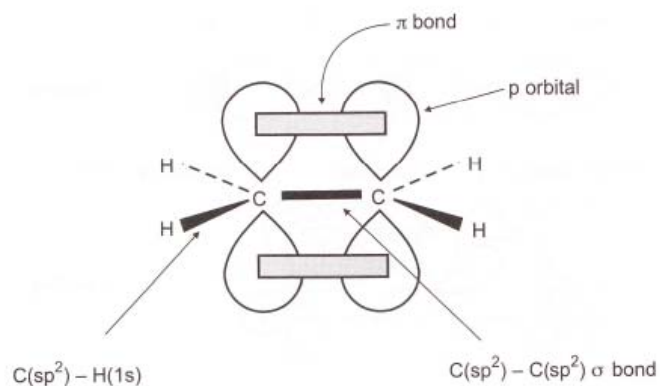


Figure 2.25  $\sigma$ - and  $\pi$ -bonds.

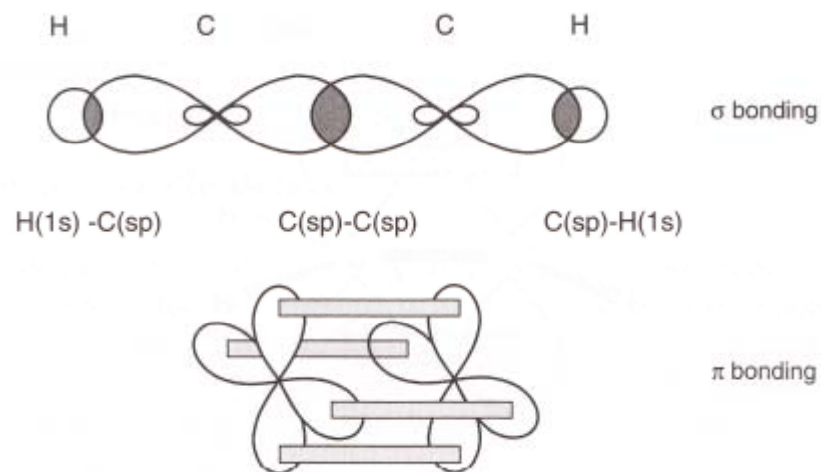
# Double and Triple Bonds

**Table 2.5** Comparison of carbon-carbon and carbon-hydrogen bonds in ethane, ethylene and acetylene.

Molecule	Bond	Bond strength (eV)	Bond length (nm)
Ethane, CH <sub>3</sub> CH <sub>3</sub>	C(sp <sup>3</sup> )-C(sp <sup>3</sup> )	3.83	0.154
	C(sp <sup>3</sup> )-H(1s)	4.26	0.110
Ethylene, H <sub>2</sub> C=CH <sub>2</sub>	C(sp <sup>2</sup> )=C(sp <sup>2</sup> )	6.61	0.133
	C(sp <sup>2</sup> )-H(1s)	4.48	0.108
Acetylene, HC≡CH	C(sp)≡C(sp)	8.70	0.120
	C(sp)-H(1s)	5.43	0.106

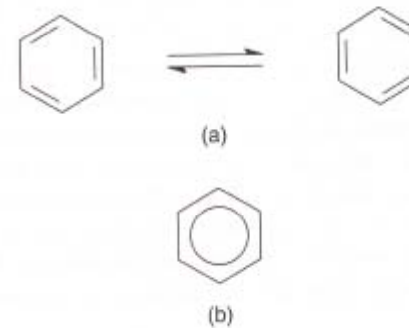
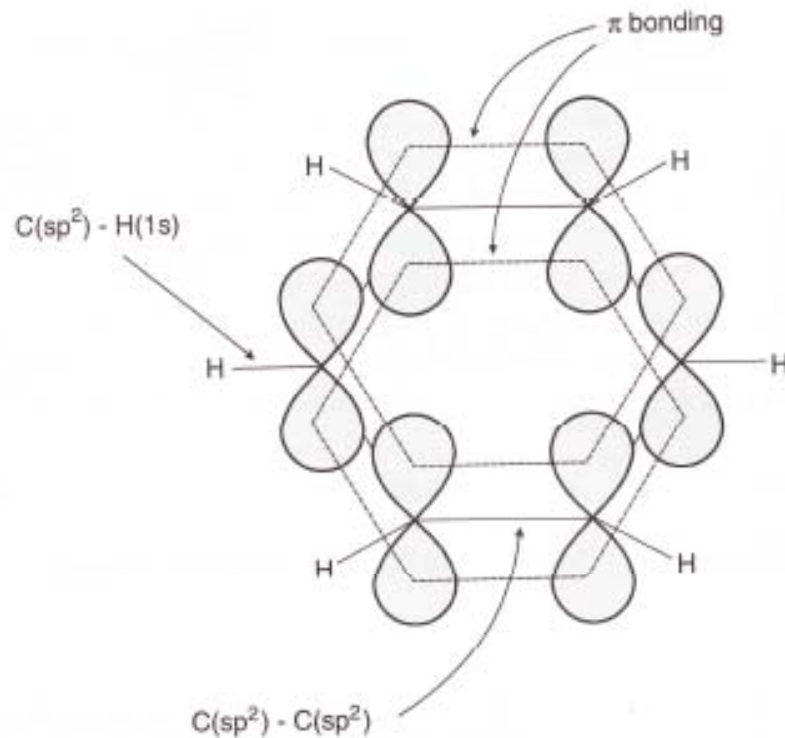


**Figure 2.26**  $\sigma$ - and  $\pi$ -bonding in ethylene, CH<sub>2</sub>=CH<sub>2</sub>.





# Benzene: Aromatic Molecule



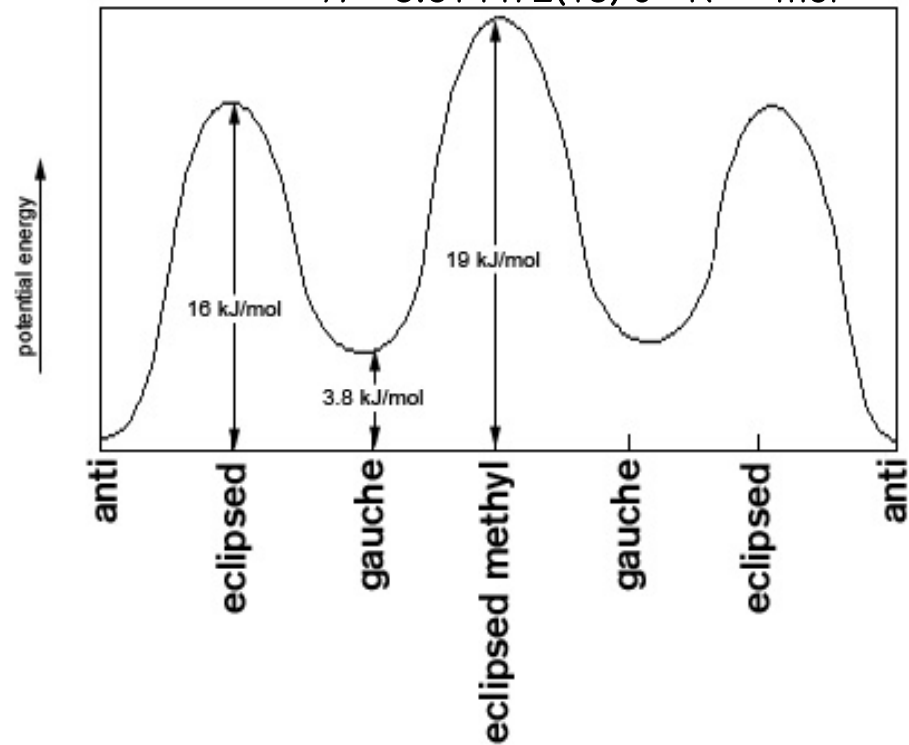
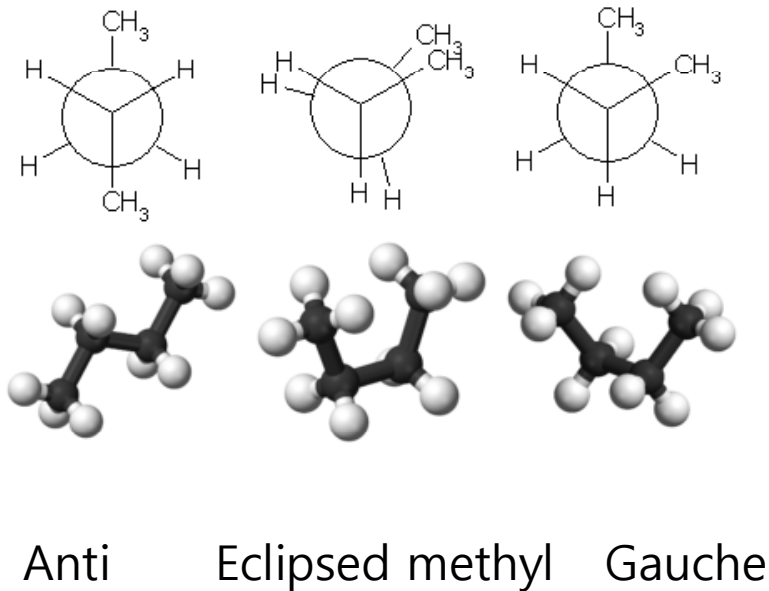
- C-C length: 0.140 nm  
Intermediate btw single and double bond

# Conformation

The population of different conformers follows a Boltzmann distribution:

$$\frac{N_i}{N_j} = \frac{g_i}{g_j} \exp\left(\frac{-(E_i - E_j)}{RT}\right)$$

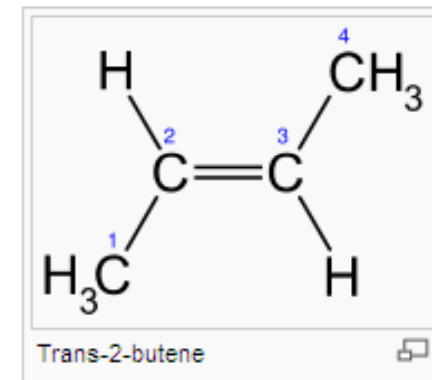
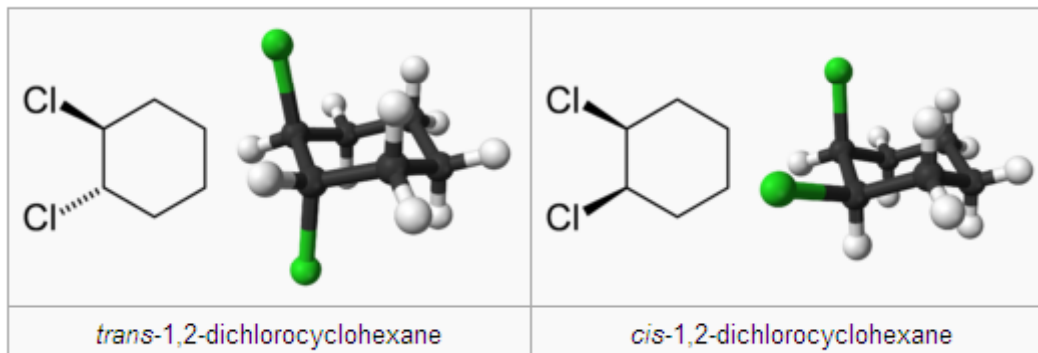
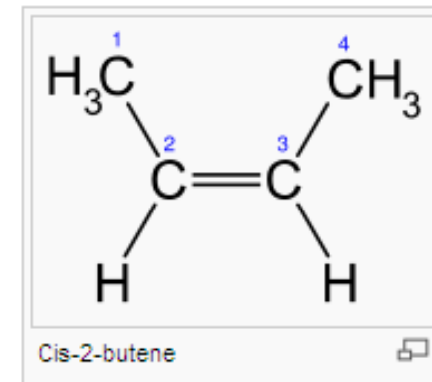
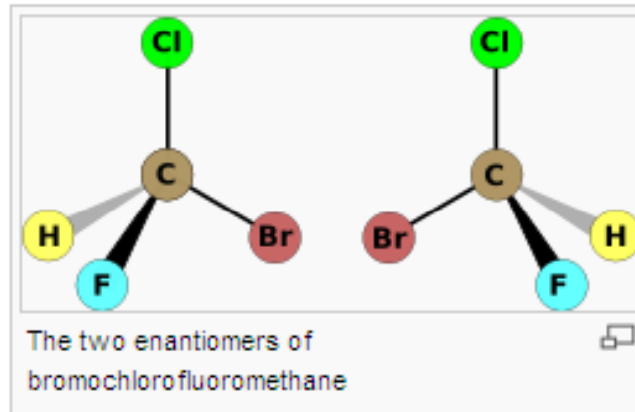
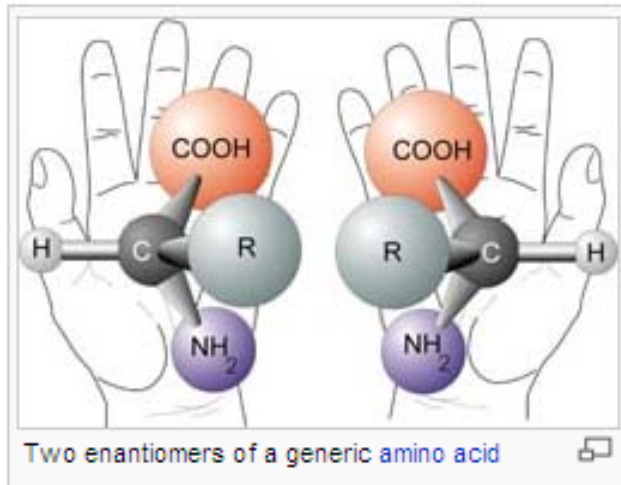
$$R = 8.314472(15) \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$



conformer potentials of butane about central C-C bond

Source: Wikipedia

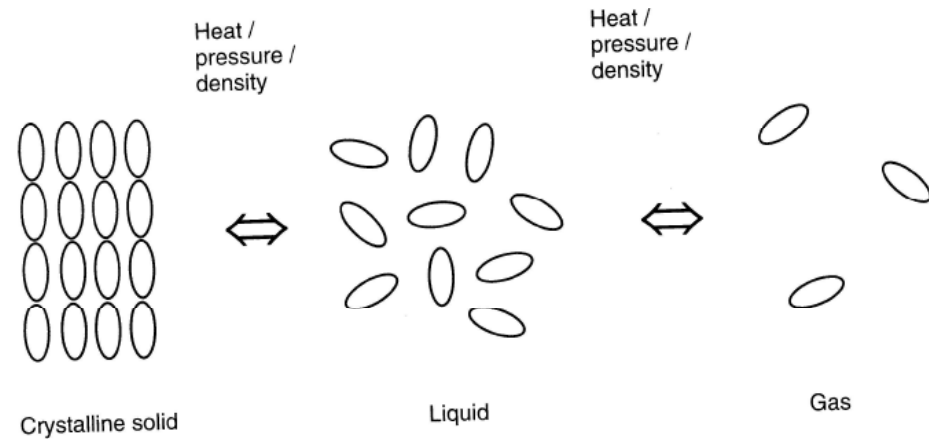
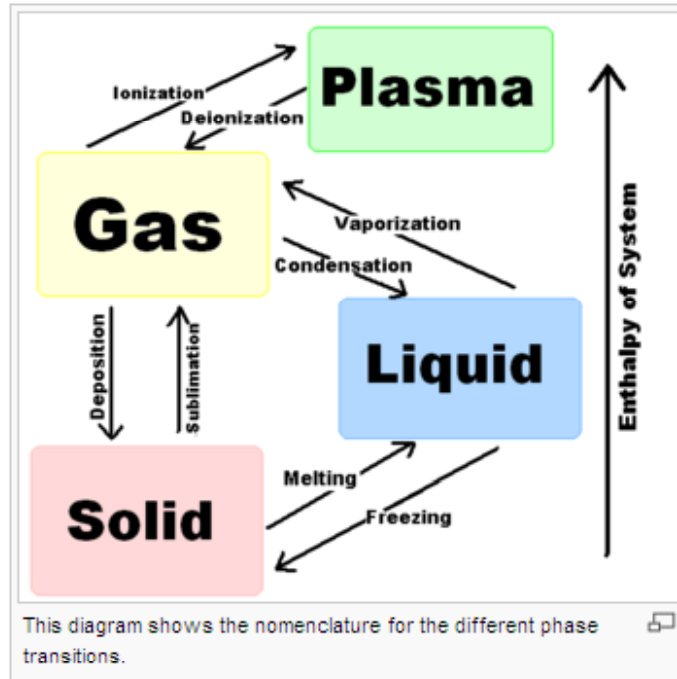
# Configuration: Stereo Isomer



- Chirality
- Enantiomer
- Optical Isomer
- Bio Systems

*Source: Wikipedia*

# States of Matter



- Solid, liquid, gas, plasma, liquid crystal
- Crystal: long-range translational and orientational orders
- Liquid, gas: fluidity
- Gas: easy compression, Liquid: incompressible
- Properties: isotropic, anisotropic

# Phase Changes and Thermodynamic Equilibrium

- Thermodynamic equilibrium after long while: free energy is minimized
- Constant V system: Helmholtz free energy  
 $F=U-TS$
- Constant P system: Gibbs Free energy  
 $G=H-TS=U+PV-TS,$   
H: enthalpy or latent heat of transformation  
S=H/T: measure of a disorder of a thermodynamic system  
At low temp H contributes more to G (thus solid), however S gets more influential at higher temp stabilizing the fluid phase preferentially.
- Phase transition:  $dG=0, \Delta H-T\Delta S=0$
- **First order transition** : includes latent heat ( $\Delta H=T\Delta S$ )  
g(=G/n) is continuous, but the first derivative( $\partial G/\partial T=S$ ) is discontinuous
- **Second order transition**: ( $\Delta H=0$ )  
Second derivative of G is discontinuous  
Molar specific volume does not change

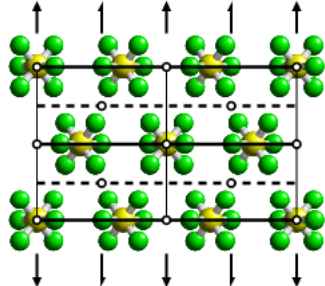
# Crystal System, Bravais Lattice, Point Group, Space Group

- Crystal System (7): Geometry of the unit cell
- Bravais Lattice (14): Associated lattice points (P, C, F, I)
- Crystallographic Point Group –Crystal Class (32): set of non-translational symmmetries that leave a point in acrystal fixed
- Space Group (230): translational symmetries added to the symmetries of the point group

Crystal system	No. of point groups	No. of bravais lattices	No. of space groups
Triclinic	2	1	2
Monoclinic	3	2	13
Orthorhombic	3	4	59
Tetragonal	7	2	68
Rhombohedral	5	1	25
Hexagonal	7	1	27
Cubic	5	3	36
<b>Total</b>	<b>32</b>	<b>14</b>	<b>230</b>





# Link Site for Crystallographic Space Group Info

A Hypertext Book of  
**Crystallographic Space Group  
Diagrams and Tables**



[CD-ROM Cover Picture](#)

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	<a href="#">High-Resolution Space Group Diagrams and Tables (1280 × 1024 pixel screens)</a>		<a href="#">Medium-Resolution Space Group Diagrams and Tables (1024 × 768 pixel screens)</a>
	<a href="#">Guide to the Diagrams and Tables</a>		<a href="#">Instructions for Optimal Viewing and Printing</a>

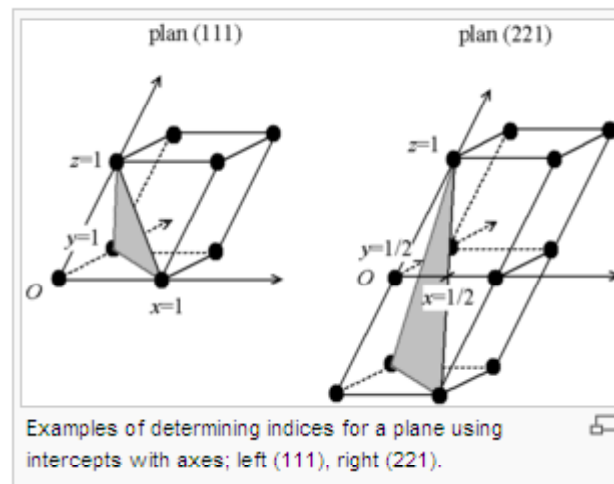
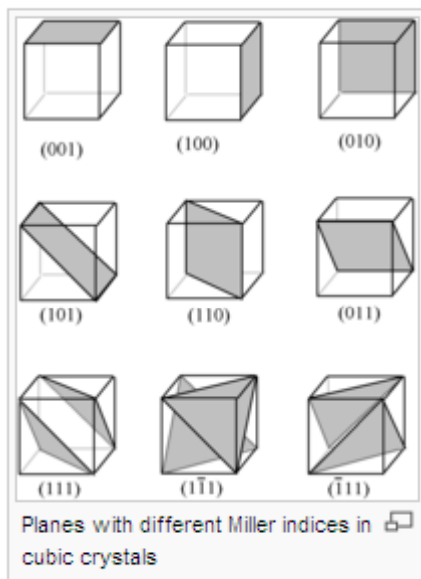
시작 | 인터넷 | 오후 4:21

# Miller Indices

**Miller indices** are a notation system in crystallography for planes and directions in crystal (Bravais) lattices.

In particular, a family of lattice planes is determined by three integers  $l$ ,  $m$ , and  $n$ , the *Miller indices*. They are written  $(lmn)$  and denote planes orthogonal to a direction  $(l, m, n)$  in the basis of the reciprocal lattice vectors. By convention, negative integers are written with a bar, as in  $\bar{3}$  for  $-3$ . The integers are usually written in lowest terms, i.e. their greatest common divisor should be 1.

There are also several related notations.<sup>[1]</sup>  $[lmn]$ , with square instead of round brackets, denotes a direction in the basis of the direct lattice vectors instead of the reciprocal lattice. The notation  $\{lmn\}$  denotes all planes that are equivalent to  $(lmn)$  by the symmetry of the crystal. Similarly, the notation  $\langle lmn \rangle$  denotes all directions that are equivalent to  $[lmn]$  by symmetry.



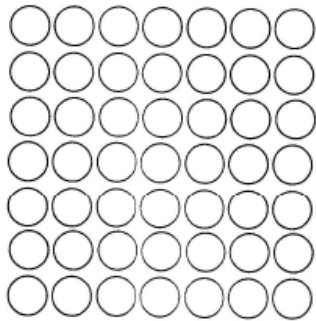
Distance btw (hkl) planes are given for cubic system

$$d_{hkl} = \frac{a_0}{\sqrt{(h^2 + k^2 + l^2)}}$$

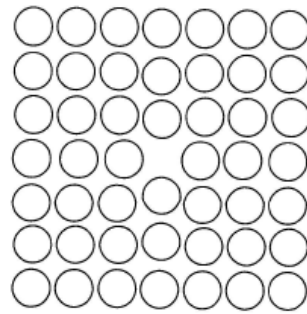
Source: Wikipedia



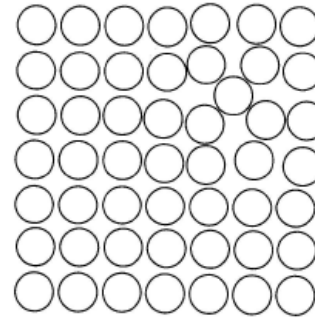
# Point Defects / Line Defects



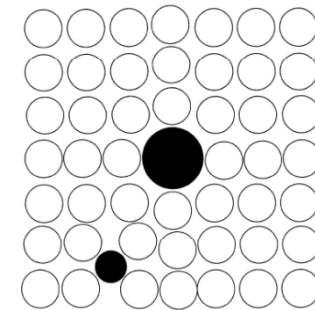
Defect free



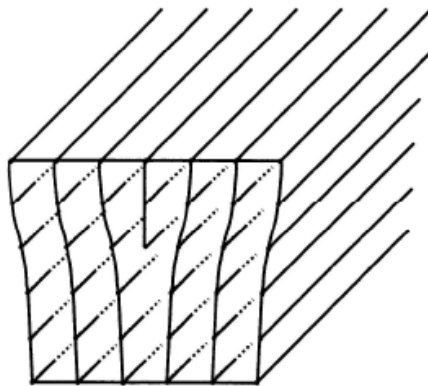
Vacancy defect  
(Schottky defect)



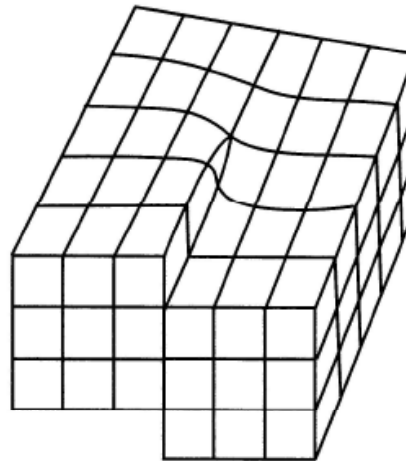
Interstitial defect  
(Frenkel defect)



Substitutional Impurity  
Interstitial Impurity



Edge dislocation

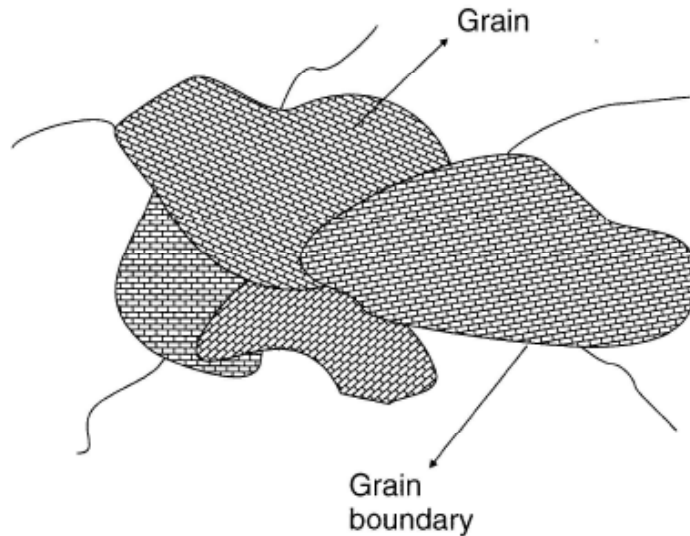


Screw dislocation

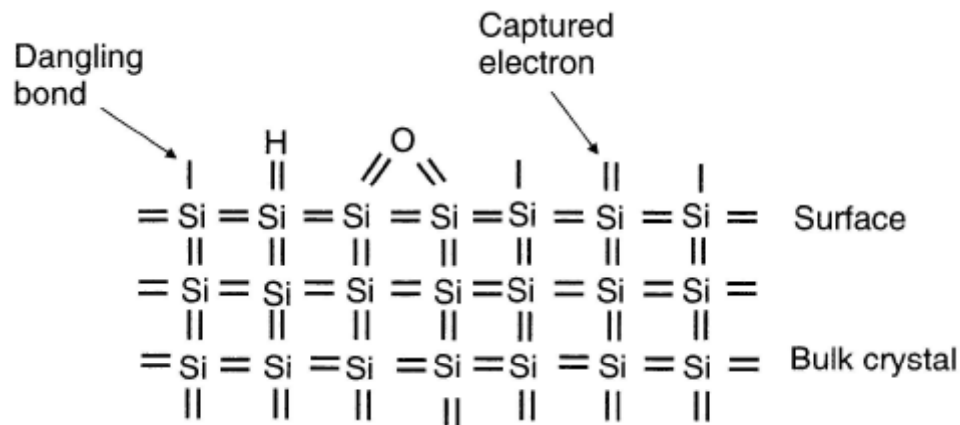
Dislocation density

- Si single crystal:  $<100 \text{ cm}^{-2}$
- Metallic crystal:  $>10^7 \text{ cm}^{-2}$

# Plane Defects, Surfaces



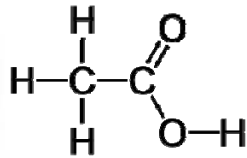
- Grain boundaries are more **chemically reactive** than the grain themselves and **impurity** atoms often preferentially segregate in these regions
- Interfacial and **grain boundary energies** exist due to different bonding environment
- **Stacking fault** is another plane defects



- Surface energy – Nanotechnology
- Physisorption:  $< 0.6$  eV adsorption energy
- Chemisorption:  $> 0.6$  eV (60 kJ/mol)

# Small Organic Molecules

Acetic acid



Vitamin C (Ascorbic acid)

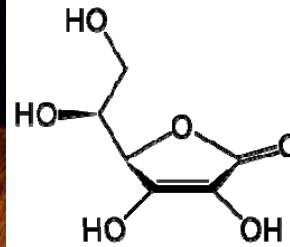
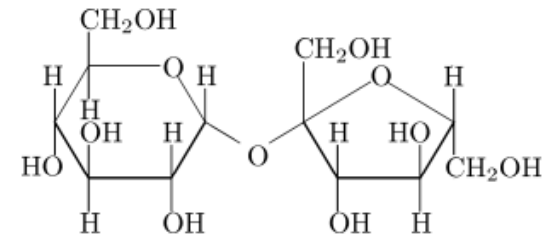
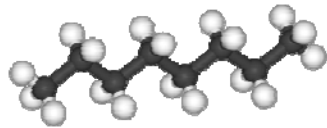


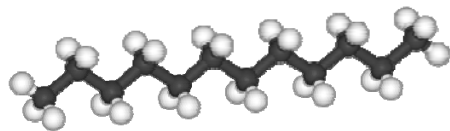
Table Sugar



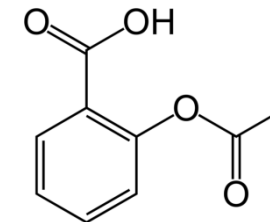
Gasoline : 5~9 C's



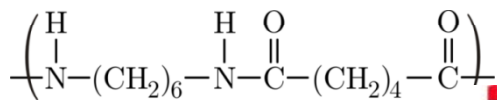
Diesel: ~12 C



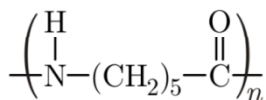
Aspirin (acetyl salicylate)



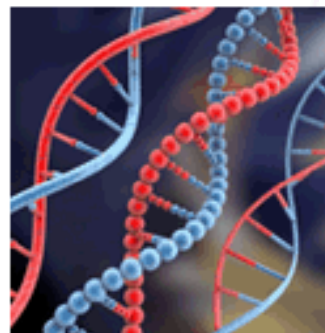
# Polymers



Nylon 66

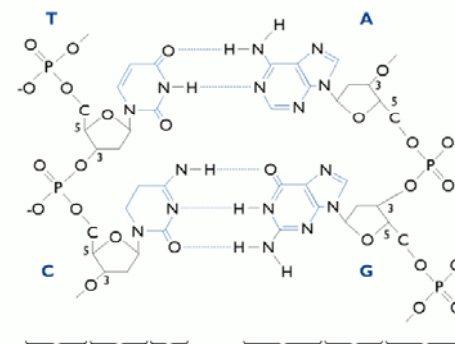
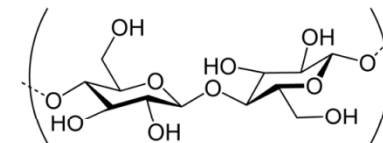


Nylon 6

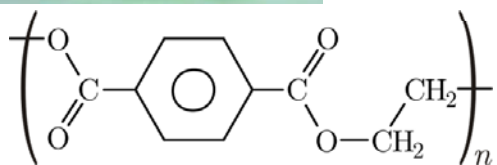


DNA

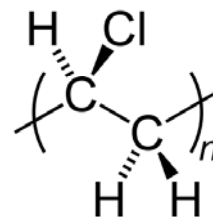
cellulose



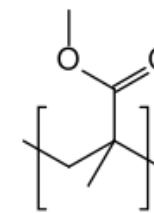
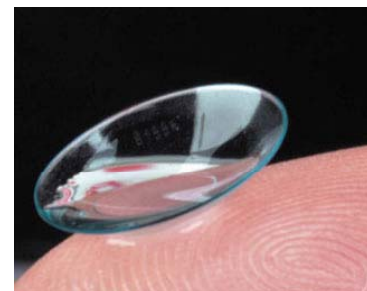
P.E.T(polyethylene terephthalate)



P.V.C(poly vinylchloride)



PMMA(poly methyl methacrylate)



<http://www.pslc.ws/macrog/index.htm>

# Visiting Polymer World

The Macrogalleria - a cyberwonderland of polymer fun - Microsoft Internet Explorer

주소(D) <http://www.pslc.ws/macrog/index.htm>

**The Macrogalleria**  
a Cyberwonderland of Polymer Fun!

click to enter.  
ENTER the Macrogalleria

Click on the menu above  
- or any link below - to:

[Get the Macrogalleria CD!](#)  
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[NEW! Search the Macrogalleria](#)  
[Visit Polydelphia](#)  
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Welcome to the Macrogalleria, where you can learn all kinds of nifty stuff about polymers and polymer science!

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...or check out the menus on the left for even more from the Polymer Science Learning Center.

Also... for the young and the young at heart:

The Macrogalleria also comes in these great languages:

주소(D) <http://www.pslc.ws/macrog/maindir.htm>

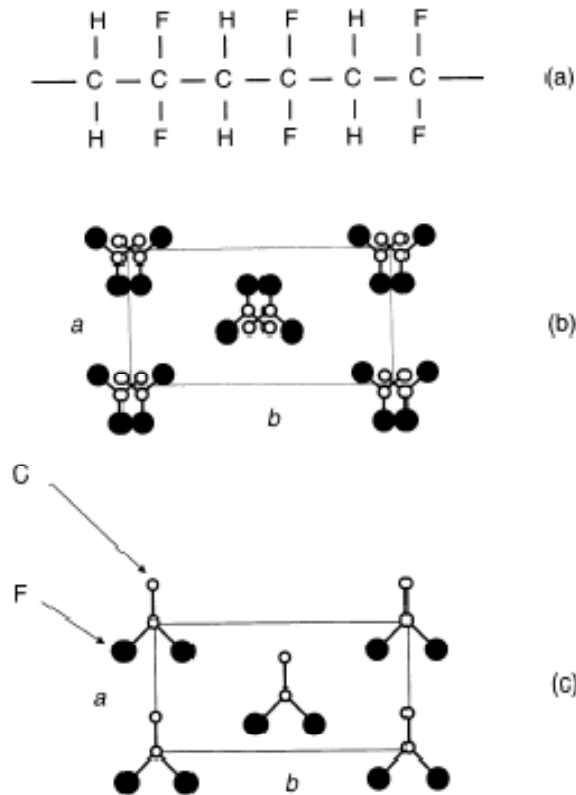
시작

MP Navigator ... MP Navigator ... ME Lecture 200... 금과터\_유기전... The Macrog... 오후 5:46

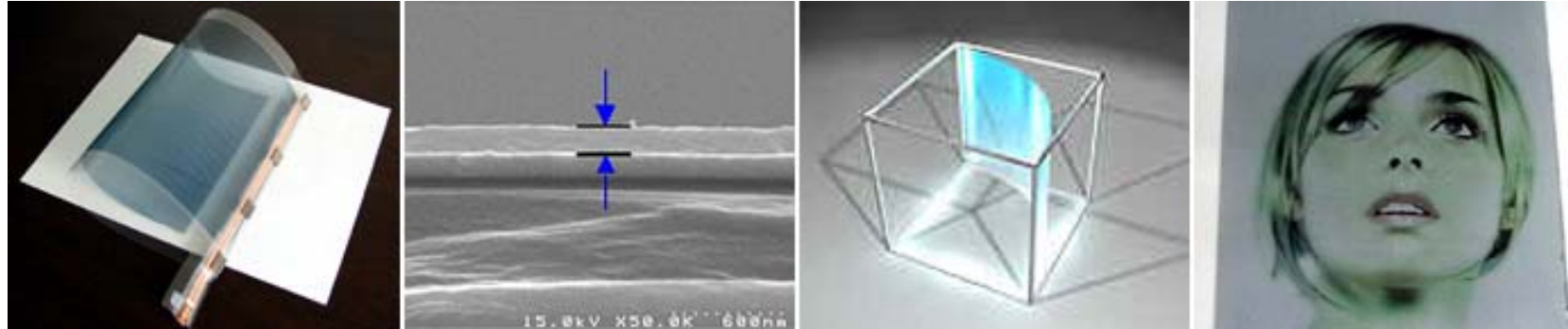
# Basic Concepts in Polymer Science

- Origin of polymer property (mechanical)
- Why does the polymerization proceed?
- Reaction mechanism (features) of radical and condensation polymerization
- Molecular weight and its distribution
- Homopolymer and copolymer
- Crystalline or amorphous morphologies
- Thermosets, thermoplastics, thermoelastomer
- Glass transition temperature and melting temperature
- Conjugated Polymers

# Polyvinylidene Fluoride : Ferroelectric polymer



**Figure 2.45** Structural forms of poly (vinylidene fluoride), PVDF. (a) Section of  $(\text{CH}_2\text{CF}_2)_n$  chain; (b)  $\alpha$ -phase; (c)  $\beta$ -phase. The projections of C atoms (small open circles) and F atoms (large full circles) on to the  $ab$  planes are shown. The H atoms have been omitted.



<http://transstudio.com/tm/2006/01/film-speaker.htm>

- Film Speaker is made of a piezoelectric coating bonded with PVDF (Poly Vinylidene Fluoride).
- TI has produced a speaker which is as thin as paper, transparent as glass, light as vinyl, and can be rolled up like tape. The speaker emits audio in all directions, and can be printed or painted with any image.



# Soft Matter: Emulsions, Foams and Gels

- **Colloid**: suspension in which the dispersed phase is so small (1-1000 nm) that gravitational forces are negligible and interactions are dominated by short-range forces such as van der Waals attraction and surface charges
- **Sol**: colloidal suspension of solid particle in a liquid
- **Aerosol** (fog, smoke): colloidal suspension of particles (liquid, solid) in a gas
- Dispersion, **Emulsion**: suspension of liquid droplet in liquid: surfactants are needed for stable emulsion
- **Foam**: a type of emulsion in which the inner phase is a gas.
- **Gel**: porous three-dimensionally interconnected solid network that expands in a stable fashion throughout a liquid medium

# Diffusion

- Whenever there is a concentration gradient of particles, there is a net diffusional motion of particles in the direction of decreasing concentration.
- Diffusivity (atom, molecule), Electrical conductivity (ions, electron, hole), Thermal conductivity (energy)
- Fick's first law

$$J = -D \frac{dC}{dx}$$