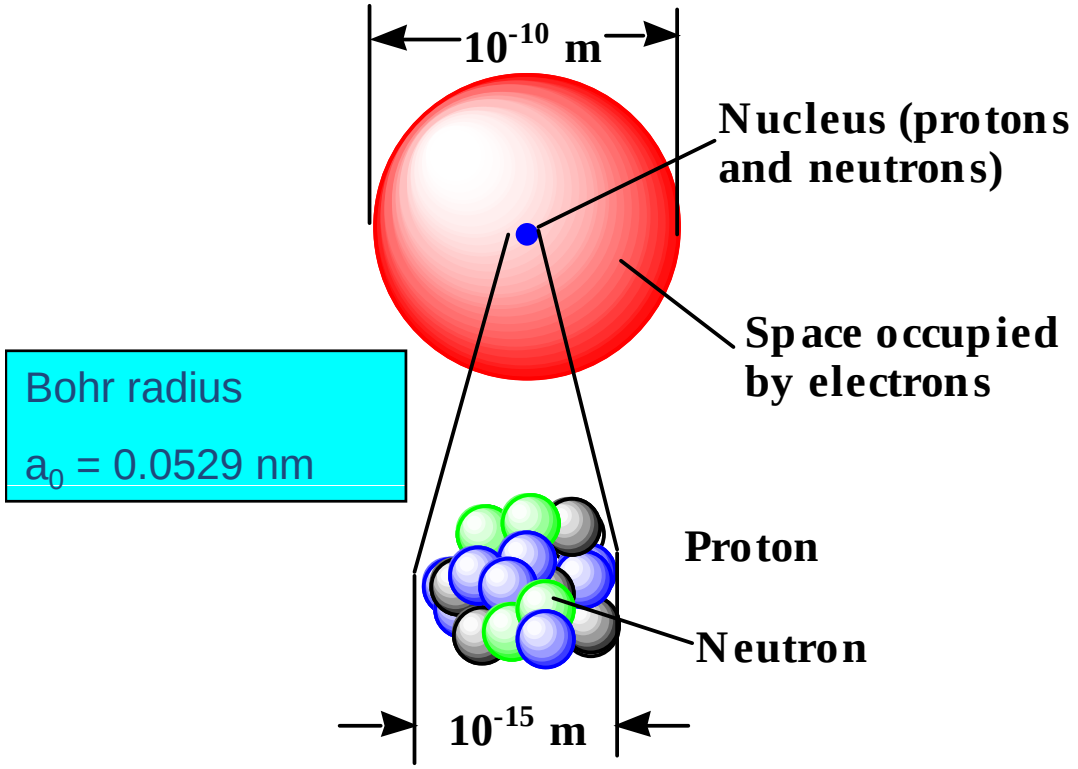
In nature’s infinite book of secrecy

2. MATERIALS’ FOUNDATIONS

Atomic Structure

	Proton	Neutron	Electron
Charge	+1.60 x 10^{-19} C	0	-1.60 x 10^{-19} C
Mass	1.67 x 10^{-27} kg	1.67 x 10^{-27} kg	9.11 x 10^{-31} 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}C
- One mole of material : 6.02 x 10^{23} atoms or molecules

Quantum Mechanics: Electrons in Atoms

- Classical Mechanics vs. Quantum Mechanics: $\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\{E - V(x)\}\psi$

  $\psi = e^{ikx} = \cos kx + i \sin kx$

  Schrödinger Equation $H\Psi = E\Psi$
- Wave-Particle duality $\lambda = \frac{h}{p}$

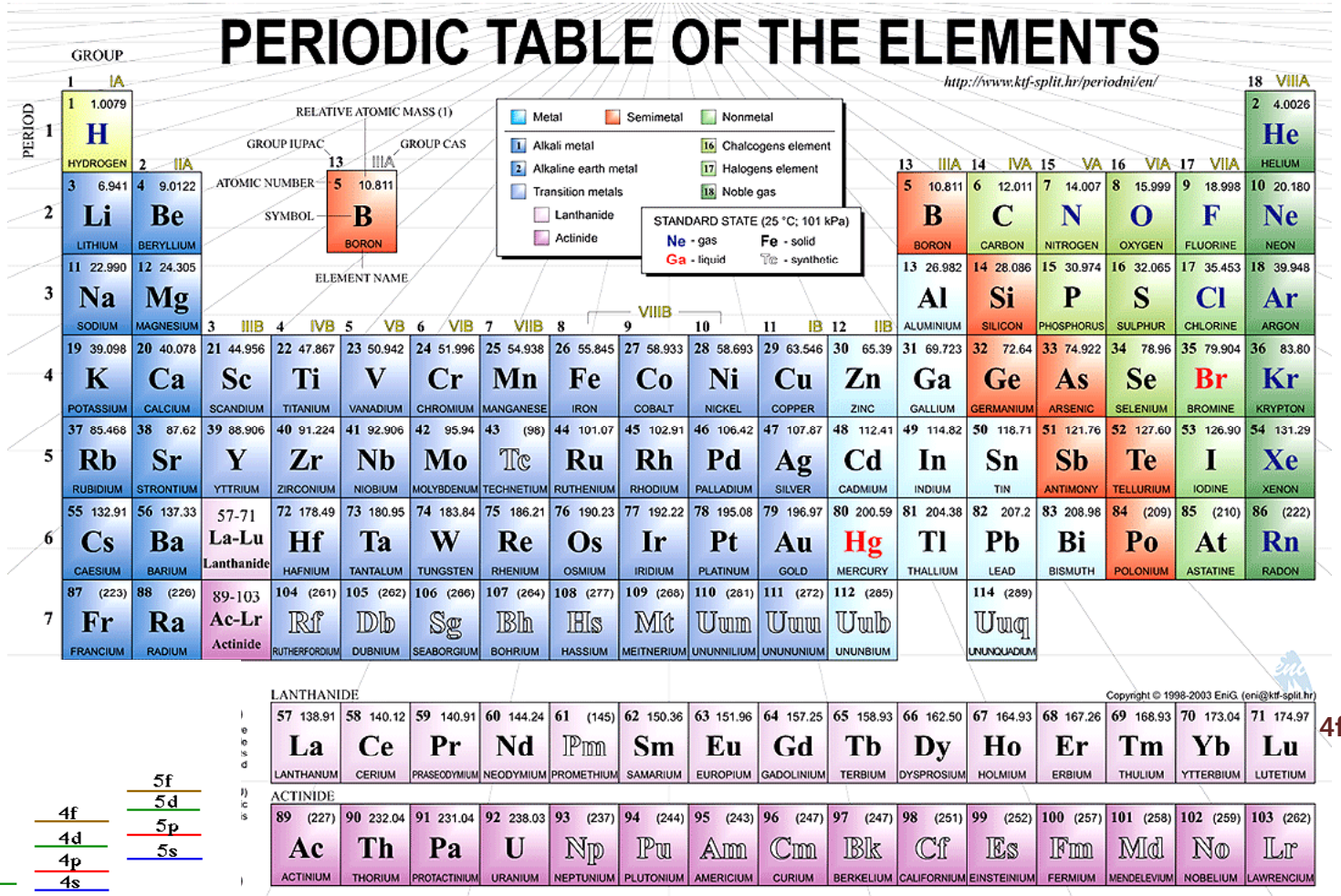
  de Broglie equation: , where $\mathrm{h} = 6.626 \times 10^{-34}\ \mathrm{J \cdot s}$

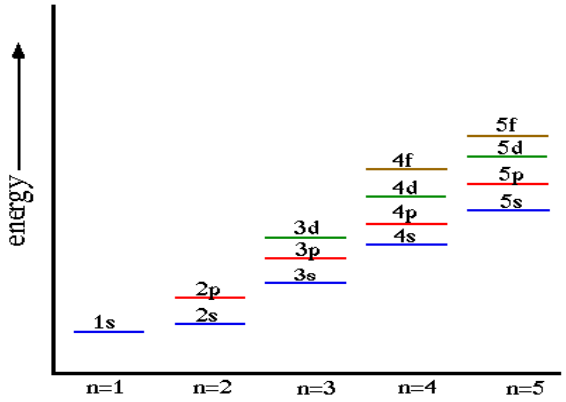
Table 2.1 Summary of quantum numbers of electrons in atoms.

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

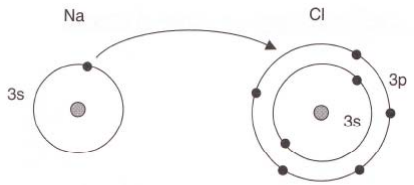
Orbital Filling : Periodic Table





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

Chemical Bonding



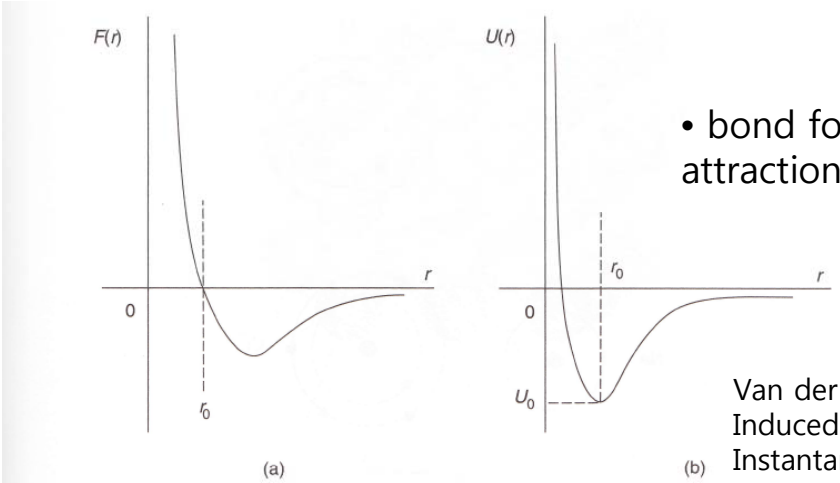
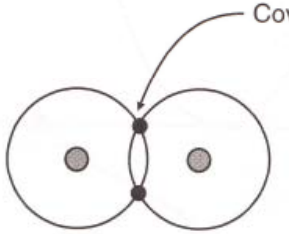


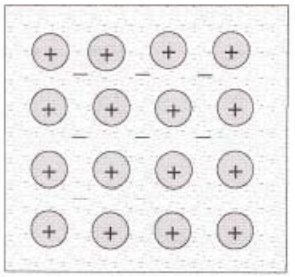
Figure 2.6 (a) Interaction force $F(r)$ between two atoms as a function of their interatomic separation r. (b) Potential energy $U(r)$ as a function of interatomic separation r. The equilibrium separation is r_0.

- bond formation driven by electrical attraction and repulsion

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

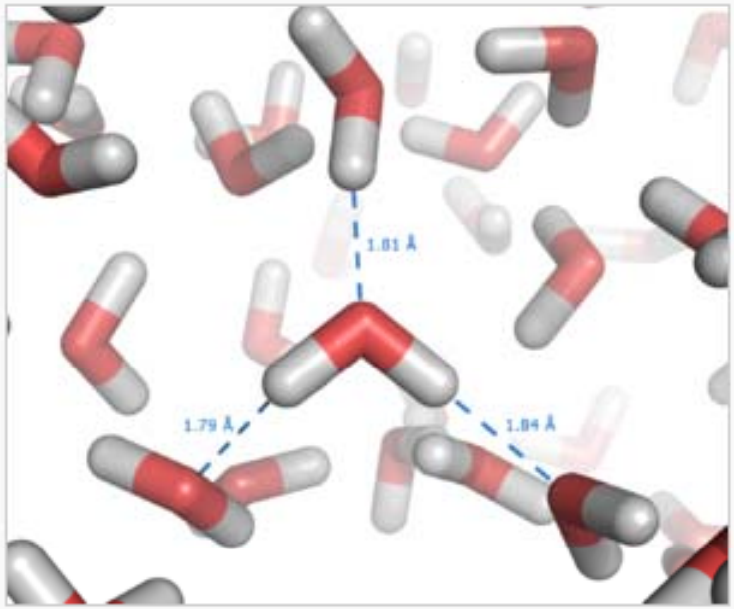


Bond type	Examples	Bond energy (eV per atom)	Melting temperature (°C)
Ionic	NaCl	3.3	801
	MgO	5.2	2852
Covalent	Si	4.0	1410
	C (diamond)	7.4	3550
Metallic	Cu	3.1	1083
	Al	3.4	660
Van der Waals	Ar	0.08	−189
	Cl_2	0.32	−101
Hydrogen	H_2O	0.52	0
	NH_3	0.36	−78



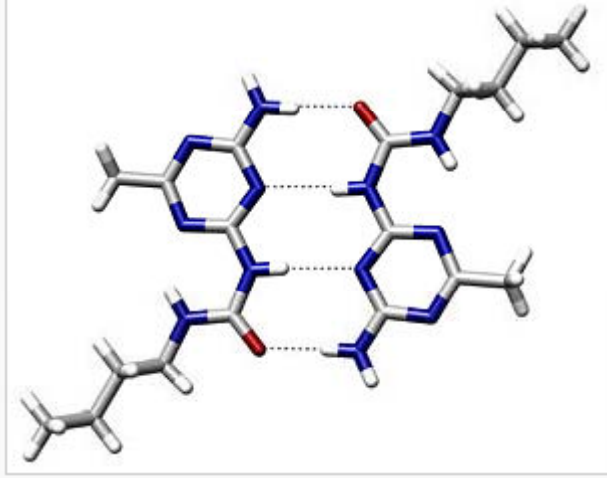
- 1 eV : energy acquired by one electron accelerated in the potential difference of 1 V. (=1.60 x 10^{-19} J)

Hydrogen Bonding



Snapshot from a simulation of liquid water. The dashed blue lines from the molecule in the center of the picture represent hydrogen bonds.

- F—H···:F (155 kJ/mol or 40 kcal/mol)
- O—H···:N (29 kJ/mol or 6.9 kcal/mol)
- O—H···:O (21 kJ/mol or 5.0 kcal/mol)
- N—H···:N (13 kJ/mol or 3.1 kcal/mol)
- N—H···:O (8 kJ/mol or 1.9 kcal/mol)
- HO—H···:OH_3^+ (18 kJ/mol or 4.3 kcal/mol)



An example of a quadruple **hydrogen bond** between a self-assembled dimer complex reported by Meijer and coworkers.[1]

Supramolecular Chemistry
Self-assembly
Bottom-up nanofabrication

Source: Wikipedia

Carbon Atom Hybridization for Bond Formation

- Why hybridization? :
  Energy pay-back

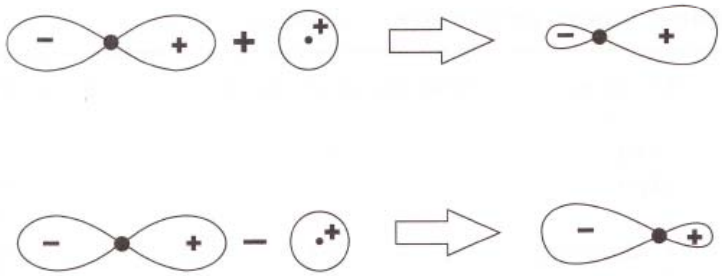


Figure 2.16

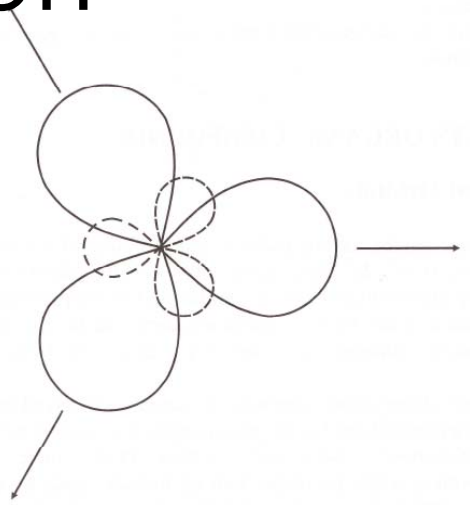


Figure 2.17 Three sp^2 hybridized orbitals.

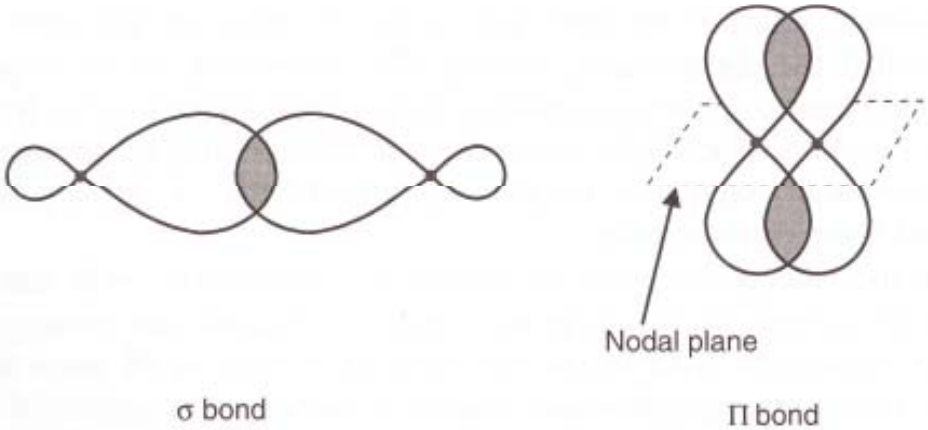


Figure 2.25 σ- and π-bonds.

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_3CH_3	$C(sp^3)$–$C(sp^3)$	3.83	0.154
	$C(sp^3)$–H(1s)	4.26	0.110
Ethylene, $H_2C{=}CH_2$	$C(sp^2)$=$C(sp^2)$	6.61	0.133
	$C(sp^2)$–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

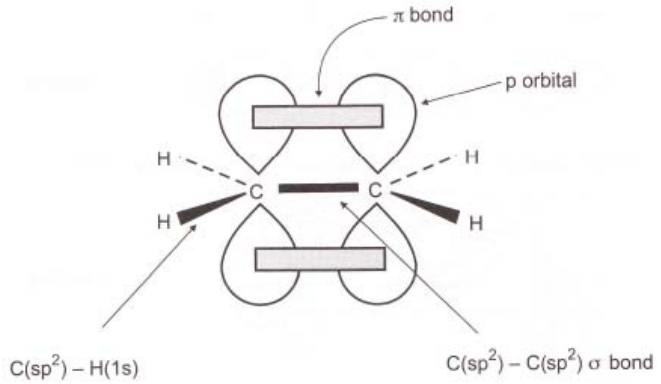
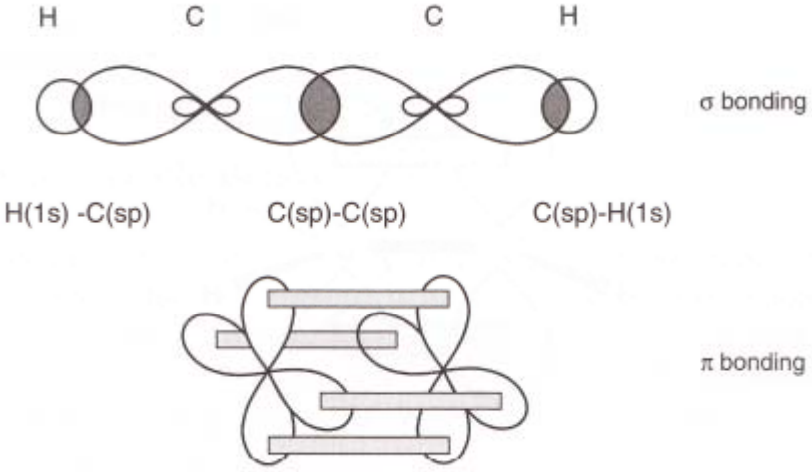
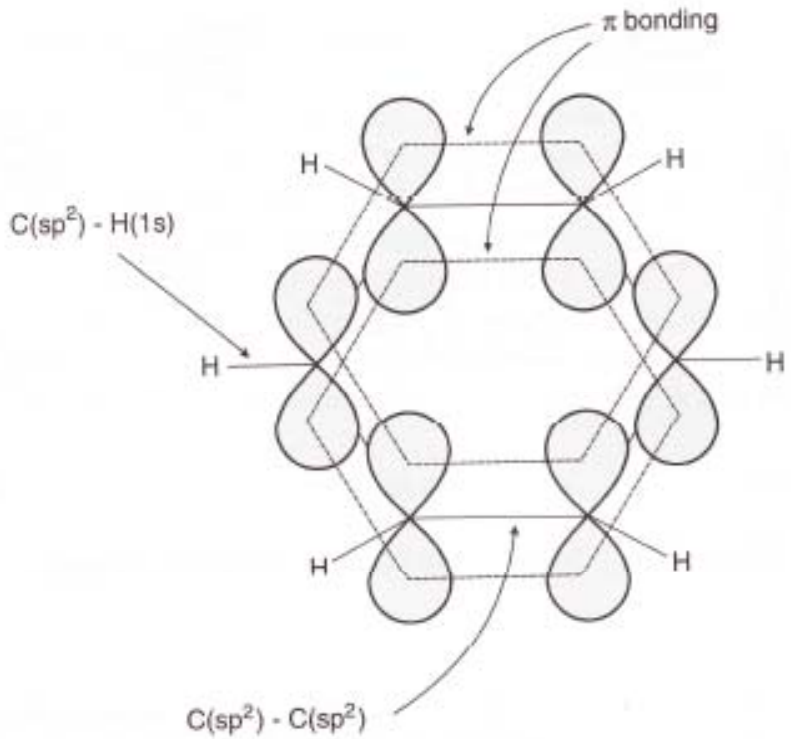
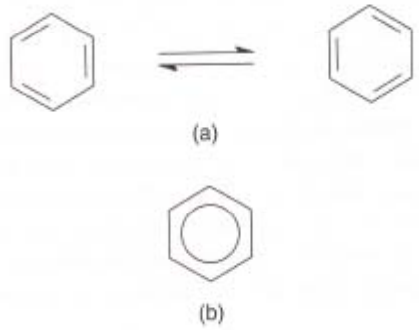


Figure 2.26 σ- and π-bonding in ethylene, $CH_2{=}CH_2$.



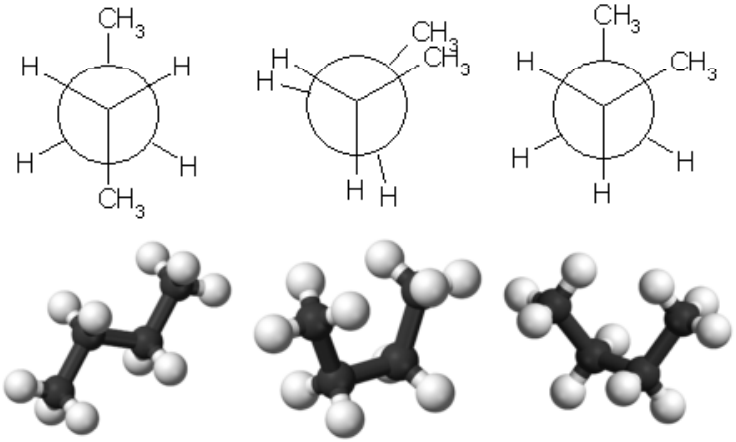
Benzene: Aromatic Molecule





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

Conformation

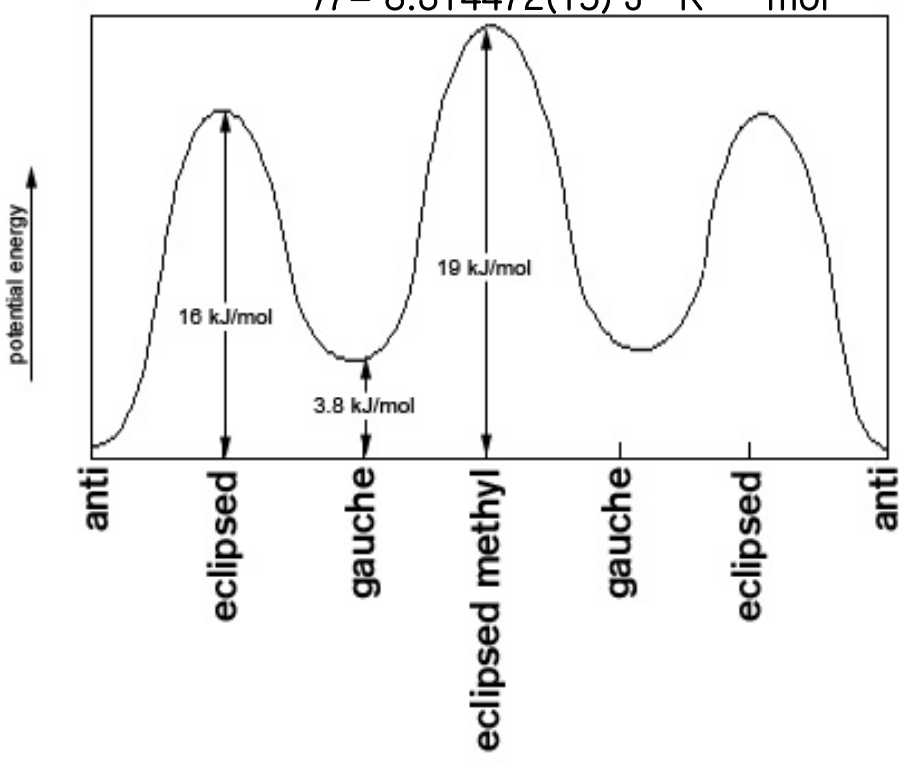


Anti Eclipsed methyl Gauche

The population of different conformers follows a Boltzmann distribution:

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

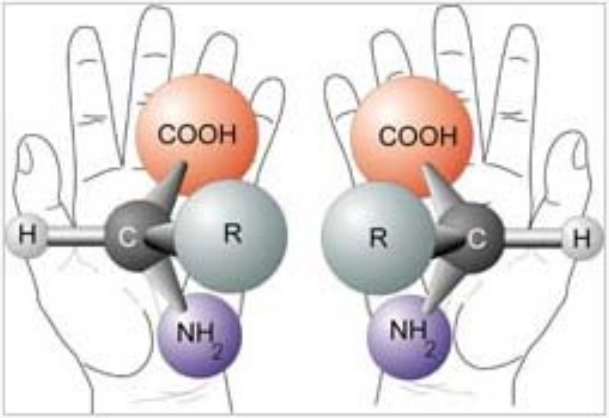
R = 8.314472(15) J · K^{-1} · mol^{-1}



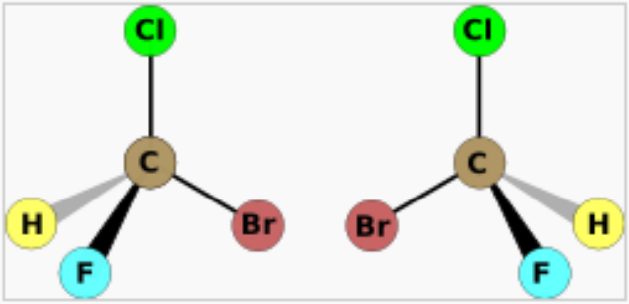
conformer potentials of butane about central C-C bond

Source: Wikipedia

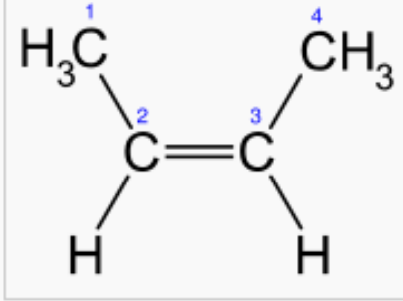
Configuration: Stereo Isomer



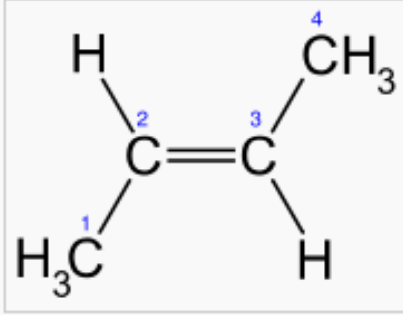
Two enantiomers of a generic amino acid



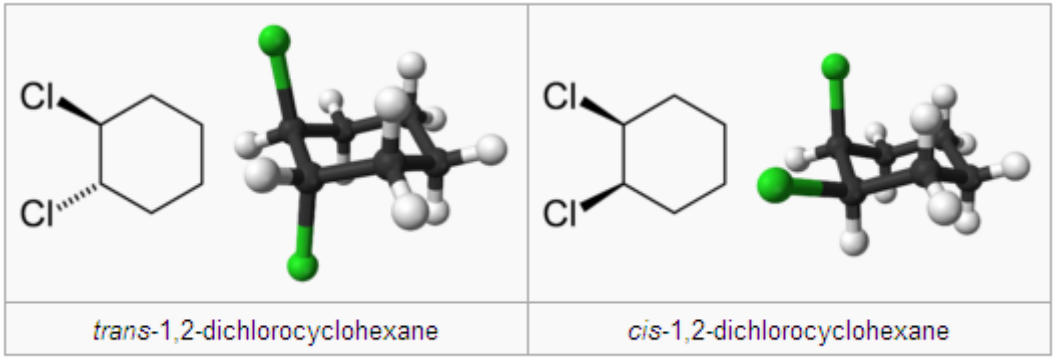
The two enantiomers of bromochlorofluoromethane



Cis-2-butene



Trans-2-butene

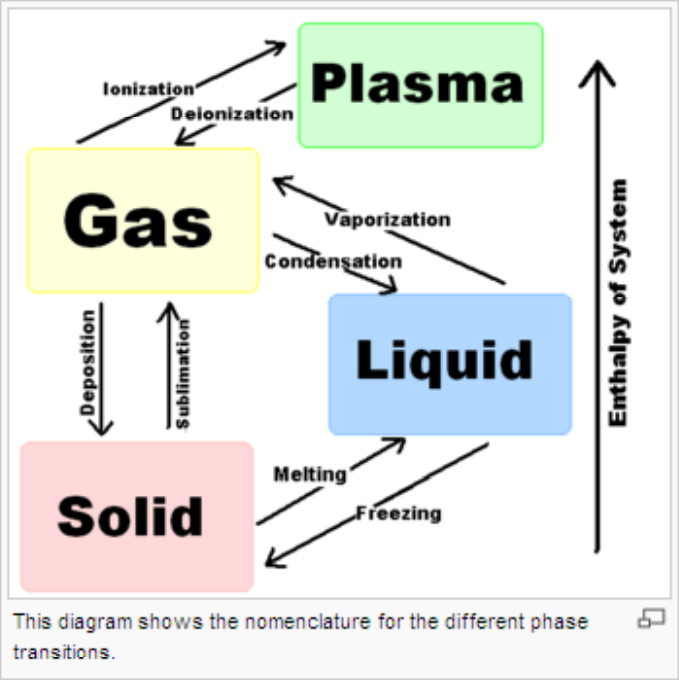


trans-1,2-dichlorocyclohexane | *cis*-1,2-dichlorocyclohexane

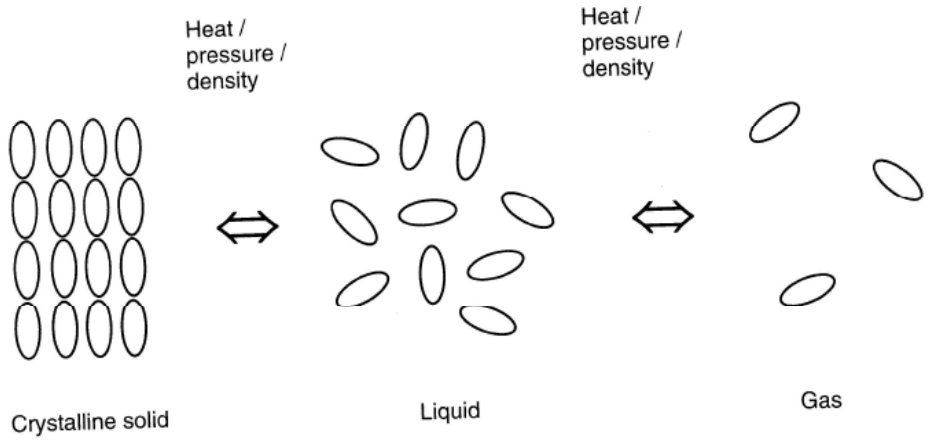
- Chirality
- Enantiomer
- Optical Isomer
- Bio Systems

Source: Wikipedia

States of Matter



This diagram shows the nomenclature for the different phase transitions.



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

Phase Changes and Thermodynamic Equilibrium

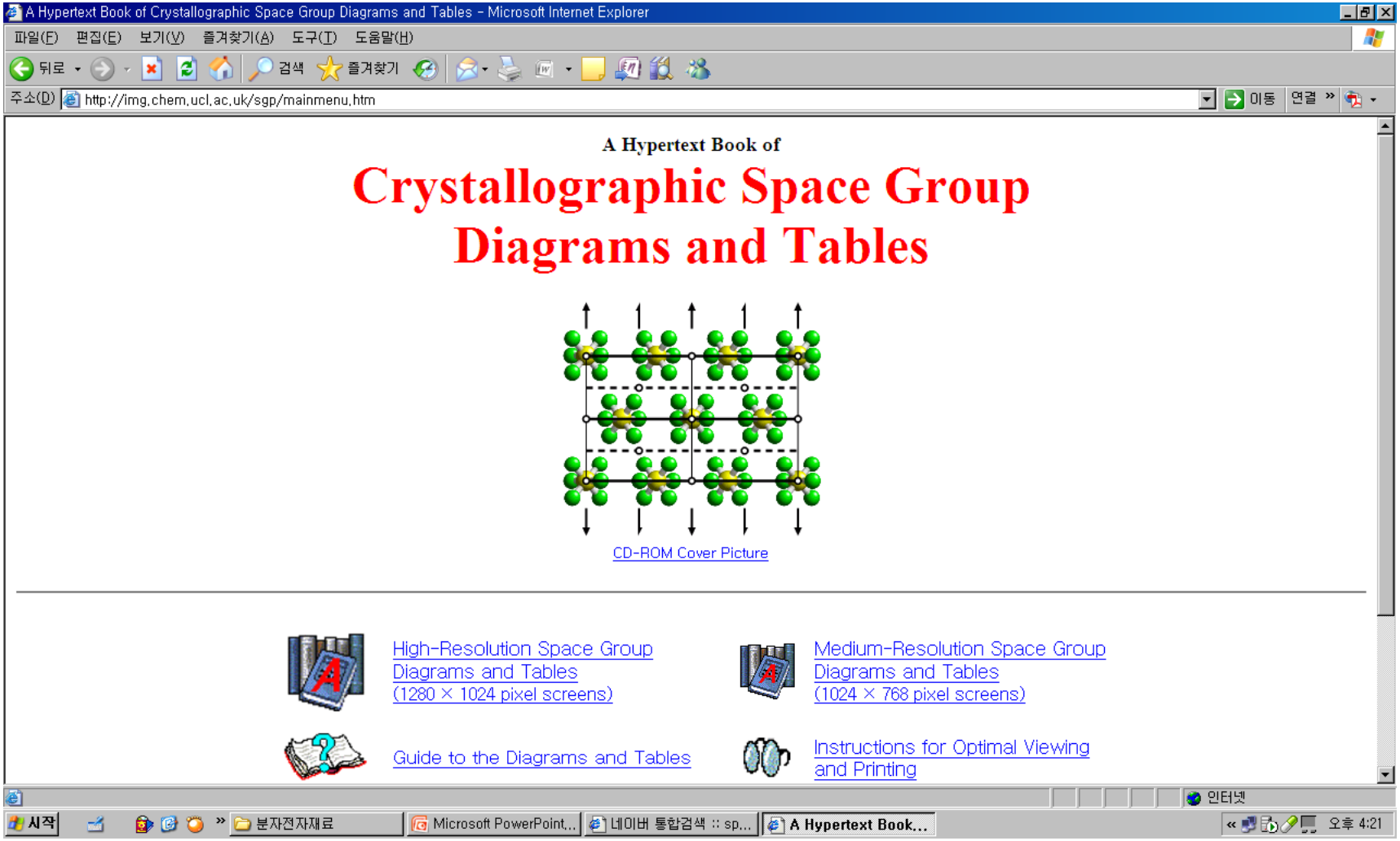
- Thermodynamic equilibrium after long while: free energy is minimized
- Constant V system: Helmholtz free energy
  F=U-TS
- Constant P system: Gibbs Free energy
  G=H-TS=U+PV-TS,
  H: enthalpy or latent heat of transformation
  S=H/T: measure of a disorder of a thermodynamic system
  At low temp H contributes 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
Total	32	14	230

Link Site for Crystallographic Space Group Info

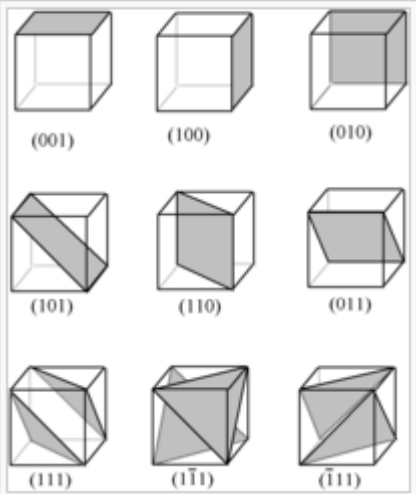


Miller Indices

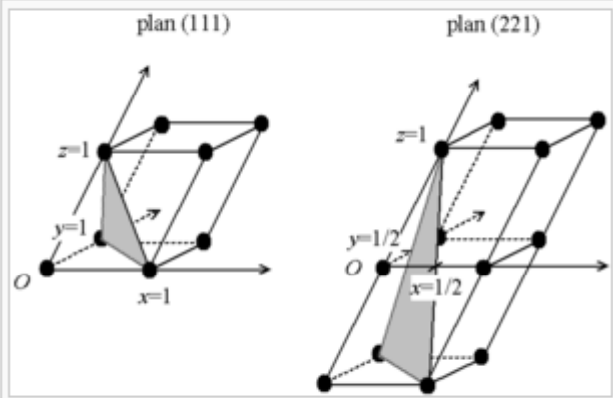
Miller indices are a notation system in crystallography for planes and directions in crystal (Bravais) lattices.

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.[1] $[\ell mn]$, with square instead of round brackets, denotes a direction in the basis of the direct lattice vectors instead of the reciprocal lattice. The notation $\{\ell mn\}$ denotes all planes that are equivalent to (ℓmn) by the symmetry of the crystal. Similarly, the notation $\langle \ell mn \rangle$ denotes all directions that are equivalent to $[\ell mn]$ by symmetry.



Planes with different Miller indices in cubic crystals



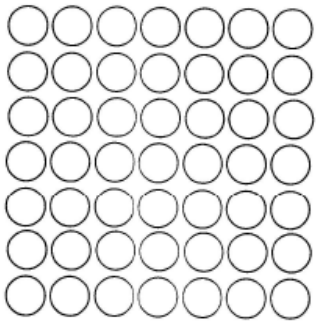
Examples of determining indices for a plane using intercepts with axes; left (111), right (221).

Source: Wikipedia

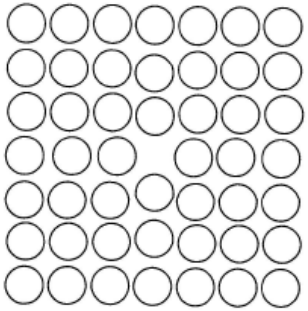
Distance btw (hkl) planes are given for cubic system

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

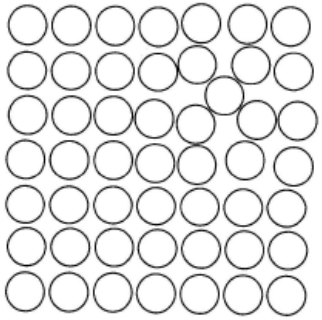
Point Defects / Line Defects



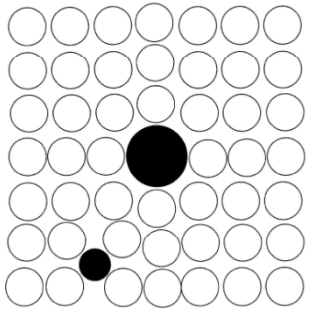
Defect free



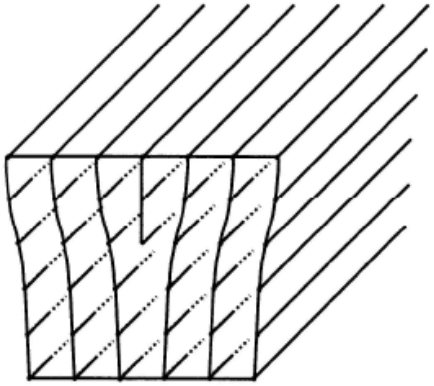
Vacancy defect
(Schottky defect)



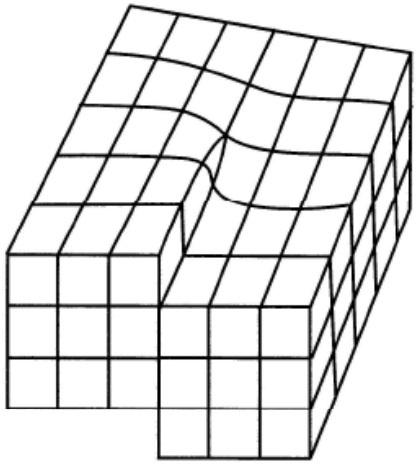
Interstitial defect
(Frenkel defect)



Substitutional Impurity
Interstitial Impurity



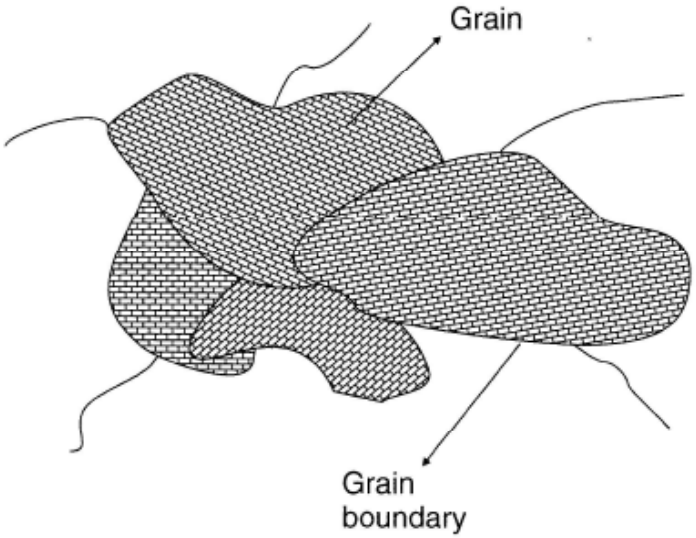
Edge dislocation



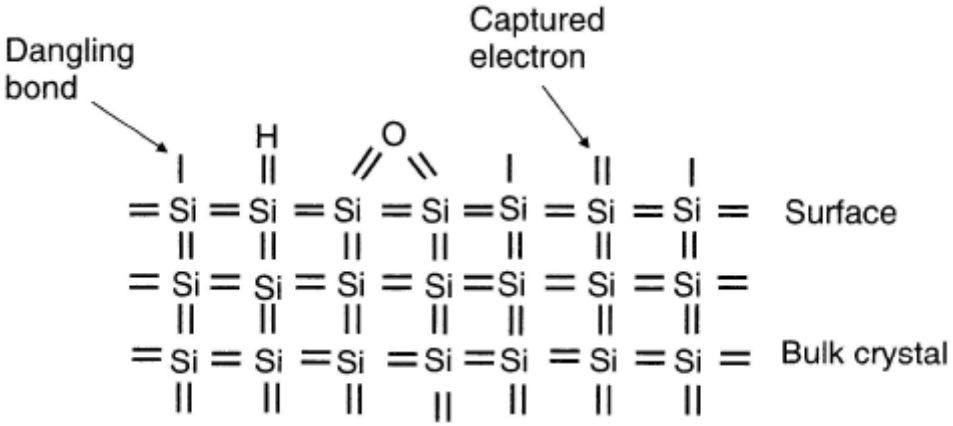
Screw dislocation

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

Plane Defects, Surfaces



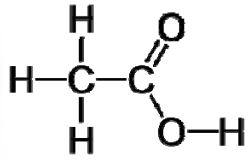
- Grain boundaries are more chemically reactive than the grain themselves and impurity atoms often preferentially segregate in these regions
- Interfacial and grain boundary energies exist due to different bonding environment
- Stacking fault is another plane defects



- 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)

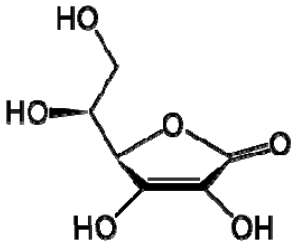
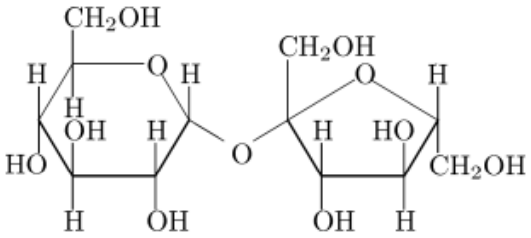
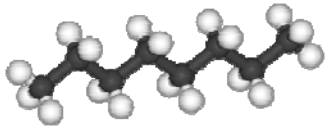


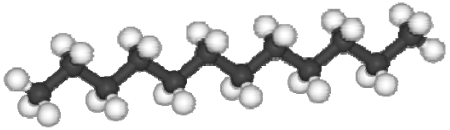
Table Sugar

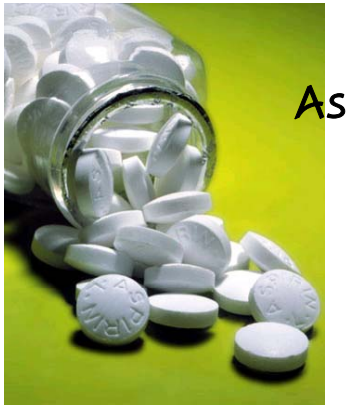


Gasoline : **5~9 C's**

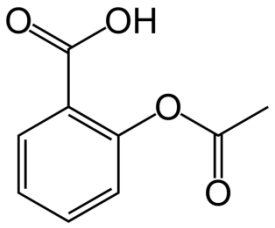


Diesel: ~12 C

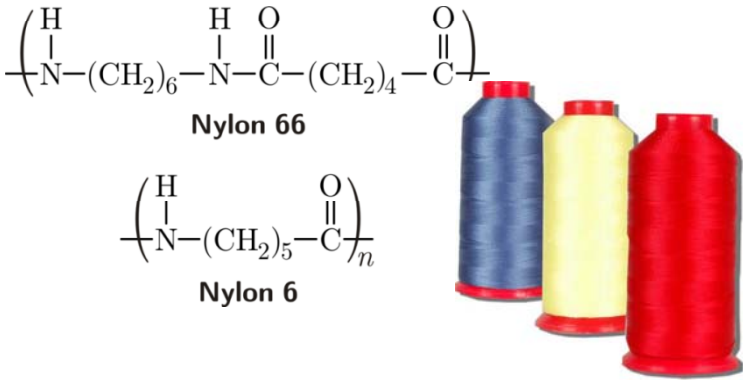




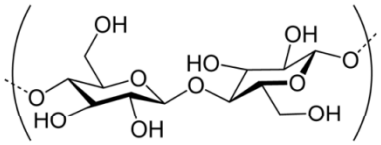
Aspirin (acetyl salicylate)



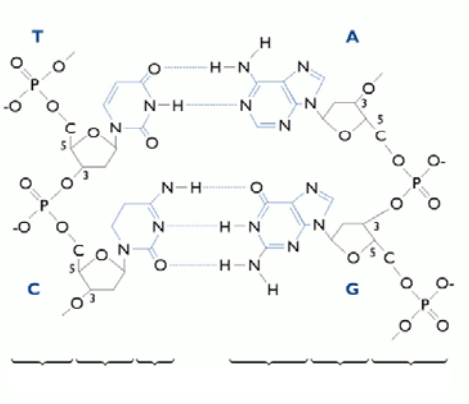
Polymers



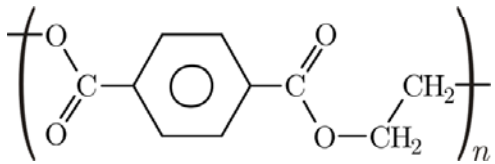
cellulose



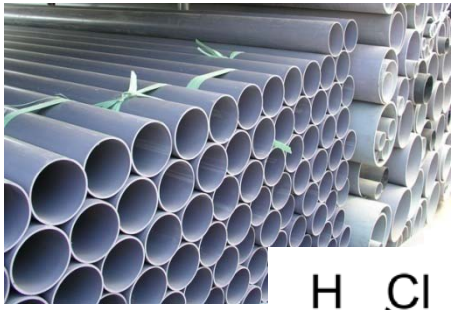
DNA

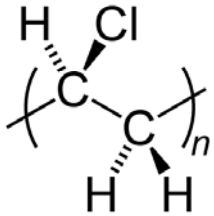


P.E.T(polyethylene terephthalate)

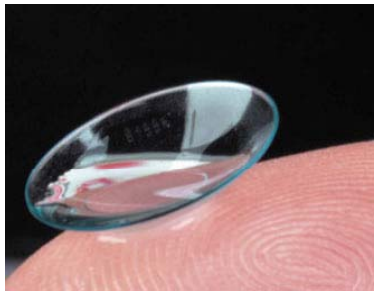


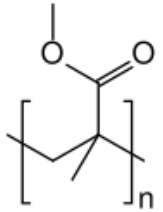
P.V.C(poly vinylchloride)





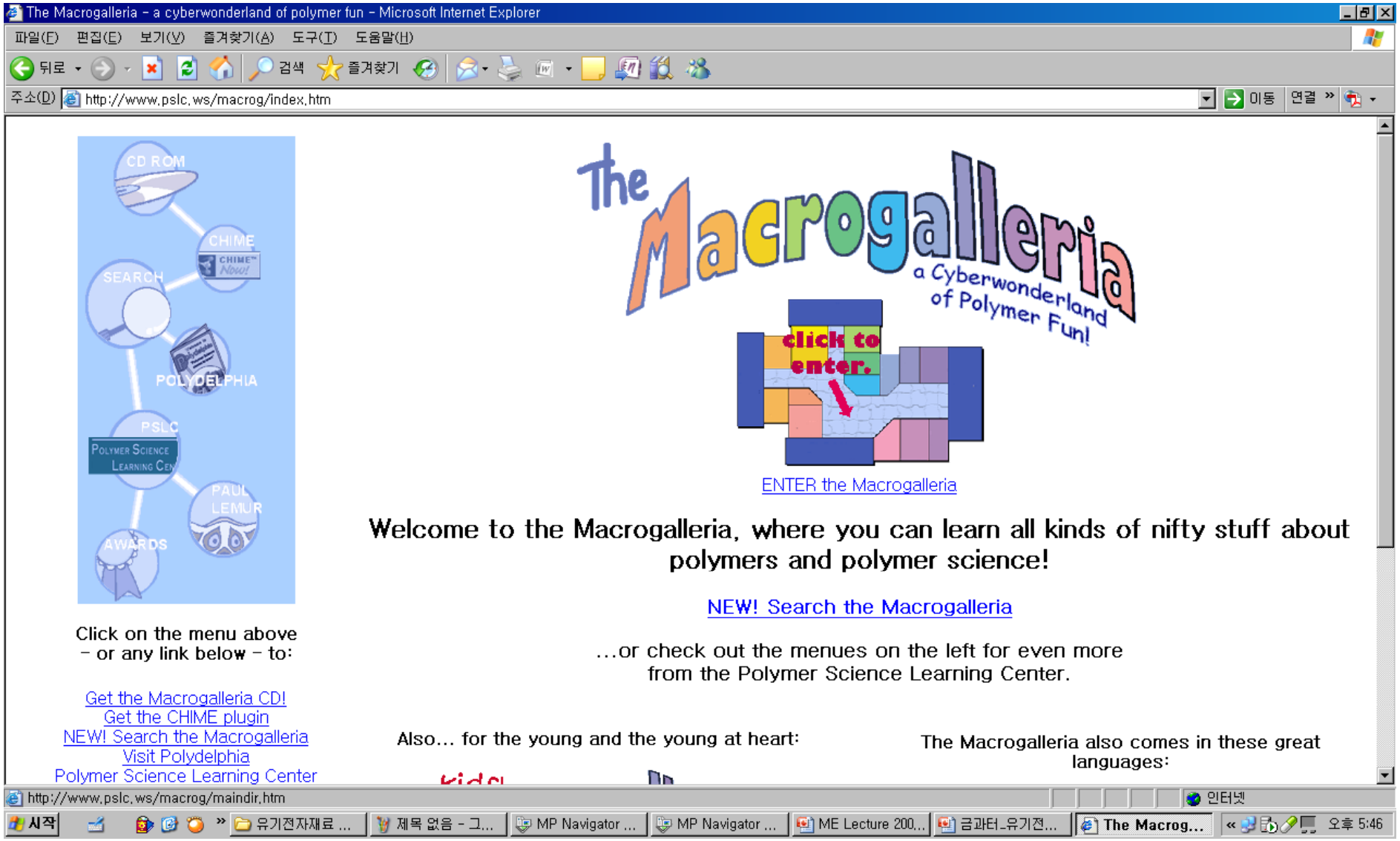
PMMA(poly methyl methacrylate)





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

Visiting Polymer World



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

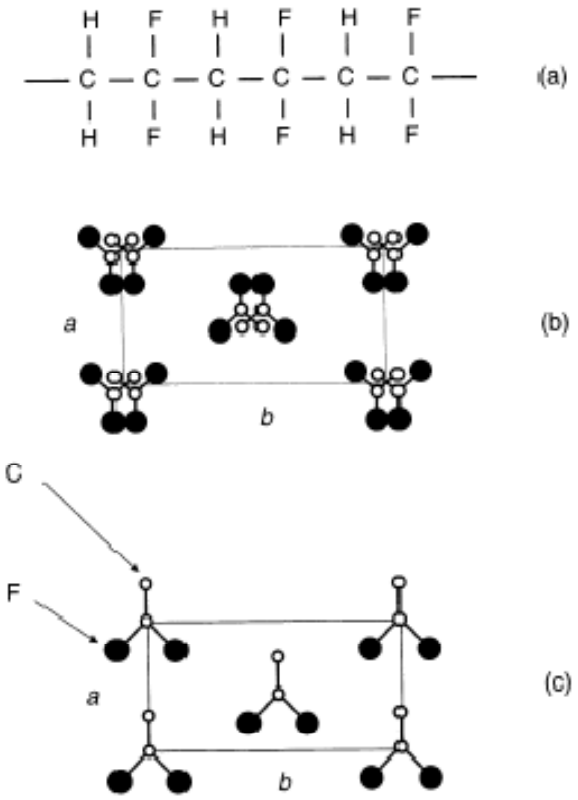
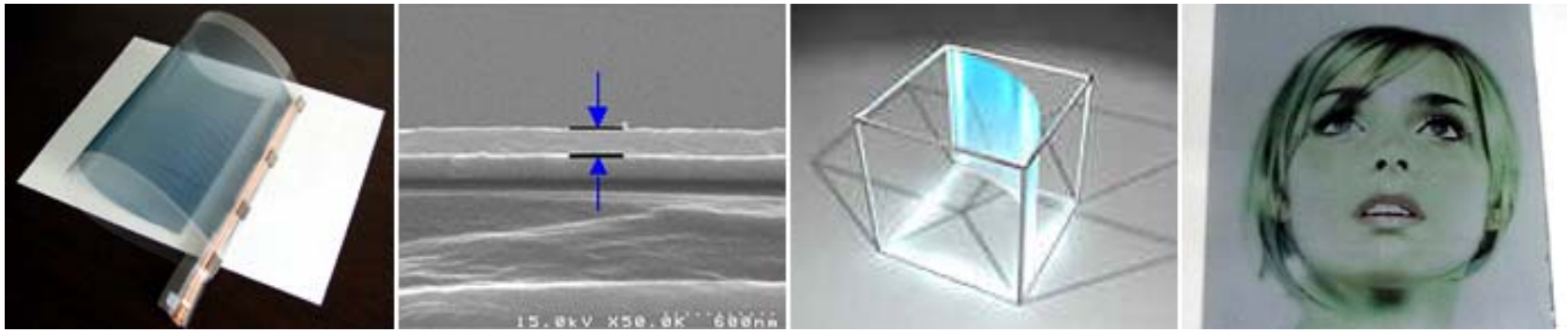


Figure 2.45 Structural forms of poly (vinylidene fluoride), PVDF. (a) Section of $(CH_2CF_2)_n$ chain; (b) α-phase; (c) β-phase. The projections of C atoms (small open circles) and F atoms (large full circles) on to the *ab* planes are shown. The H atoms have been omitted.



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

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