November 21, 2005
Global Focus on Knowledge 2005
Science of Matter

Global Focus on Knowledge 2005
Science of Matter

Science of Materials
―Origin and Application―

Lecture 6~9

Characteristics of Matter

The University of Tokyo,
The Institute For Solid State Physics

Yasuhiro Iye

Lecture Outlook

Lecture 1 Dr. Masatoshi Koshiba "The Creation of Matter"

Lecture 2-5 Dr. Katsuhiko Sato
"The Birth of Matter- Elementary Particles, Atoms, and the Universe"

Lecture 6-9 Dr. Iye Yasuhiro "Characteristics of Matter"

- **Lecture 6 What is Solid-state Physics?**
- **Lecture 7 Quantum Mechanics and Artificial Materials- High-tech and the State-of-the- art Physics**
- **Lecture 8 Atom Control and Quantum Control -- Nano-science and Quantum Information**
- Lecture 9 Diverse Matter and Physical Properties

Lecture 10-13 Dr. Hiroshi Komiyama " The Production and Application of Matter"

November 21, 2005
University Lecture
Science of Matter

Lecture 6 What is Condensed Matter Physics?

Lecture 7 Quantum Mechanics and Artificial Materials
-- High-tech and the State-of-the-art Physics

Lecture 8 Atom Control and Quantum Control
--Nano-science and Quantum Information

Lecture 9 Diverse Matter and Physical Properties

**The University of Tokyo,
The Institute For Solid State Physics**

Yasuhiro Iye

Today’s Topics

- Stories about size and extent
- Modern civilization and physics
- Condensed matter physics is the field of physics,
- Quantum mechanics and atomic structure
- Existing forms of matter
- Agglutination mechanism and crystal structure of atoms.

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Macroscopic Scale

End of Universe

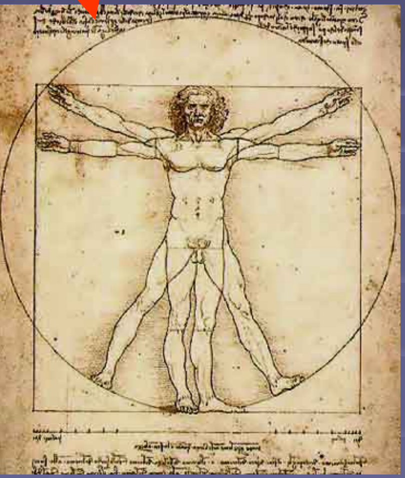
1 m | 10^3 m | 10^6 m | 10^{12}m | 10^{18}m | 10^{24}m

1km

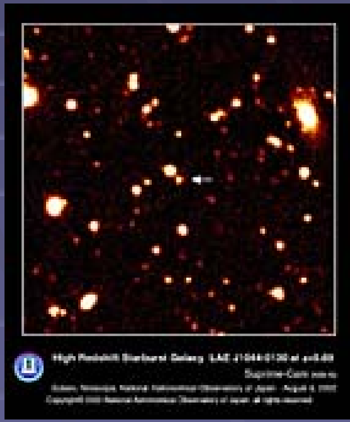
1000 km

1 cosmological unit

1 light year



12800km



出典:http://www.solarviews.com/eng/homepage.htm

Microscopic Scale

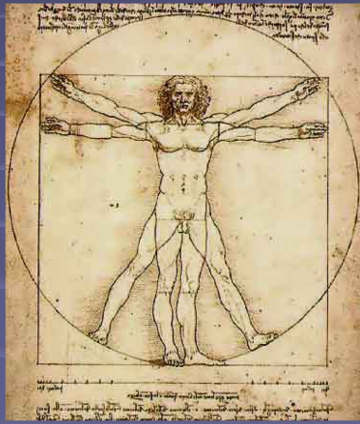
10^{-12} m | 10^{-9} m | 10^{-6} m | 10^{-3} m | 1 m

1 pm
Picometer

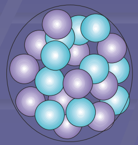
1 nm
Nanometer

1 μm
Micrometer (Micron)

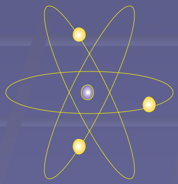
1 mm
Millimeter



Size of atomic nucleus



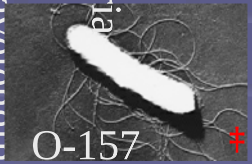
Size of atom



Virus

Wavelength of visible light

Bacteria



Needle hole and human hair

10^{-35}m
Planck scale

10^{-32}m
The grand unified scale

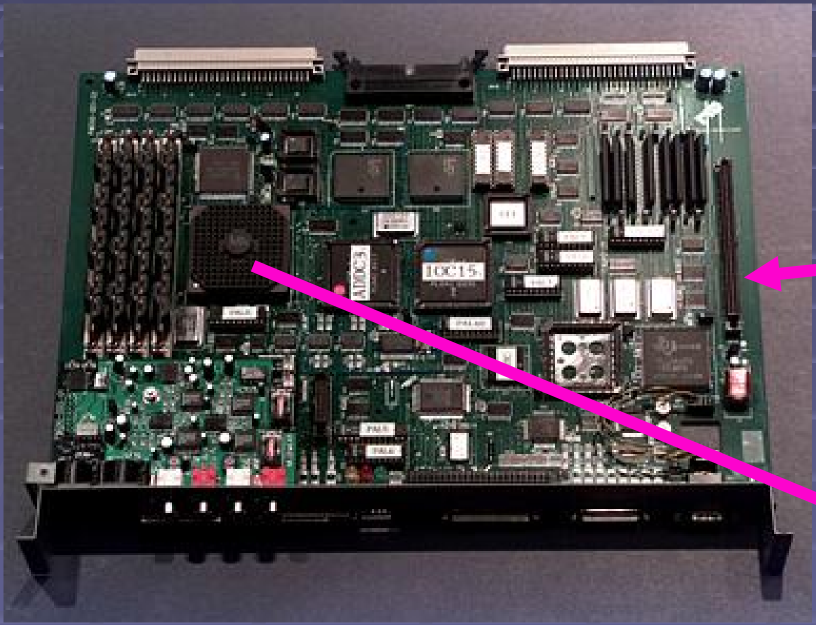
10^{-21}m

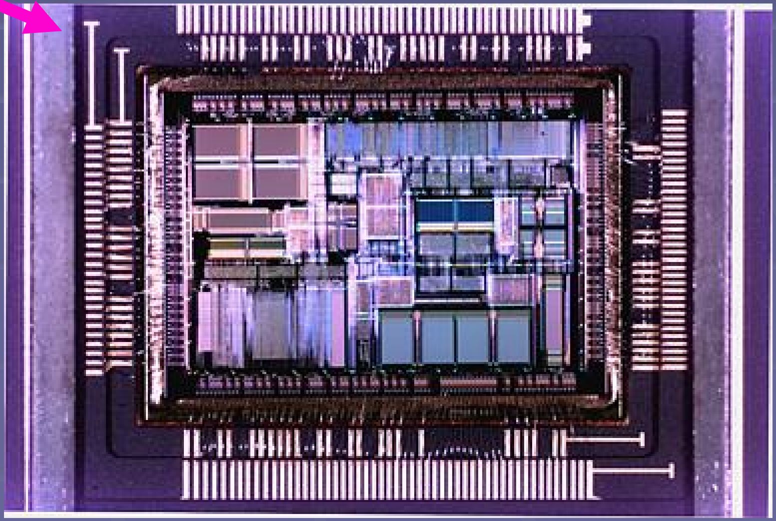
10^{-18}m
Electroweak unification scale

Modern Civilization and Physics

Computer

Personal computer





Behavior of electrons in semiconductors:

Condensed matter physics is based on quantum mechanics.

Memory Storage

Magnetic hard disk

Recording digital information as magnetizing directions of magnetic substances.

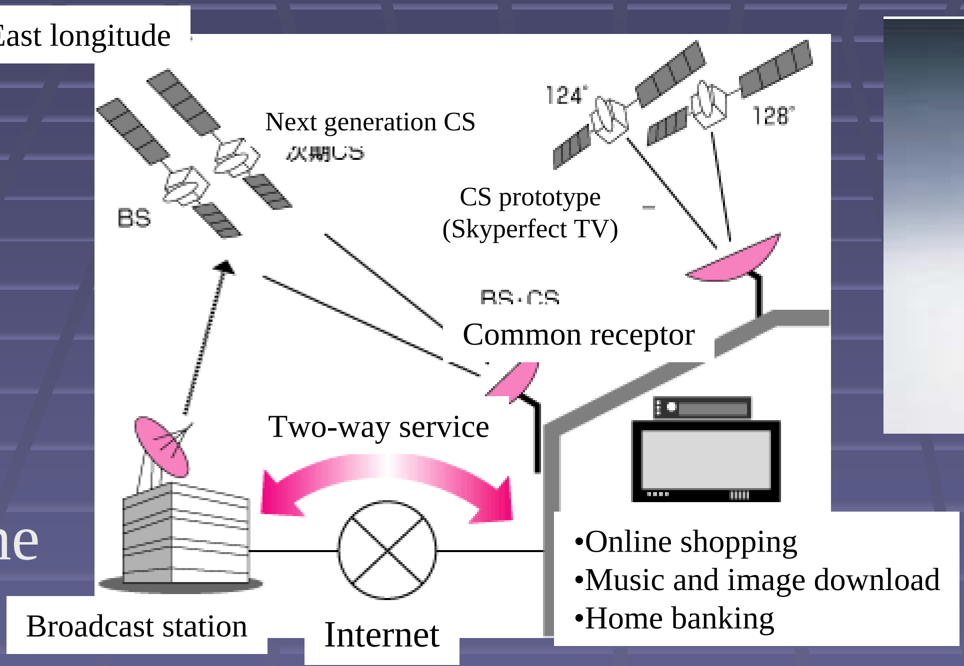
CD-ROM/DVD

Using laser reflection differences against irregularities on the recording surface.

Semiconductor memory
Flash memory
Ferroelectric memory

Radio (High Frequency) and Optical Communication

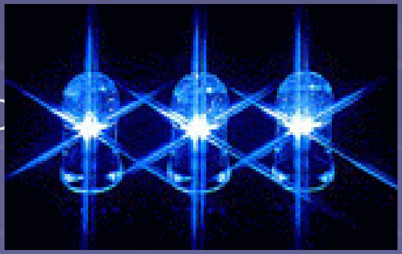
Mobile phone



Satellite communicatio
Satellite broadcasting

Optical fiber

High mobility transistor
HEMT



Luminescent diode
Semiconductor laser

GPS (Global Positioning System) Navigation

24 stationary satellites have been launched.

These satellites trace the location of the target by triangulation.

Accurate timing is essential. An atomic clock is deployed in satellites.

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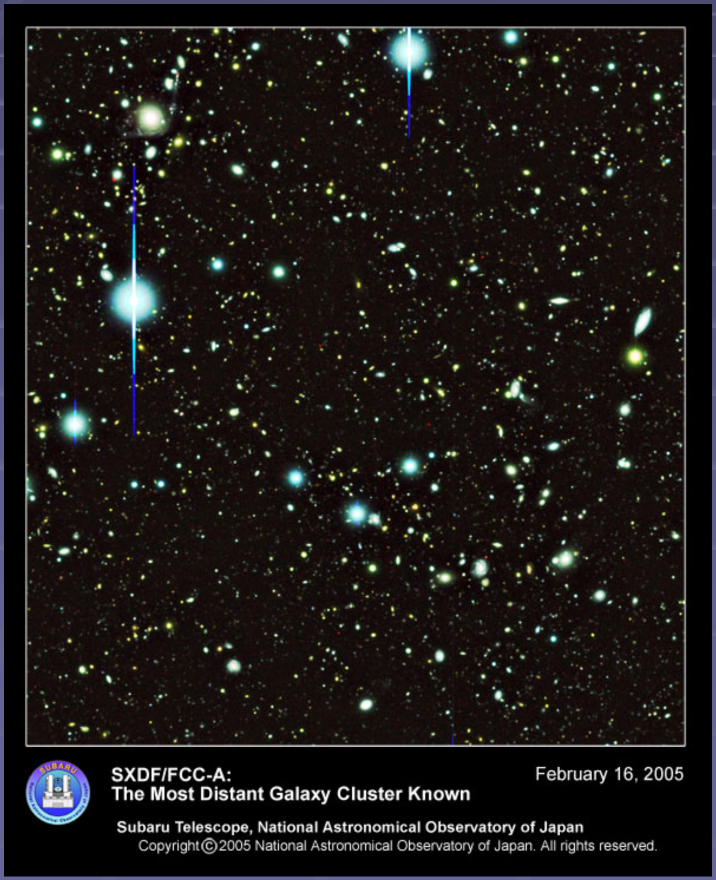
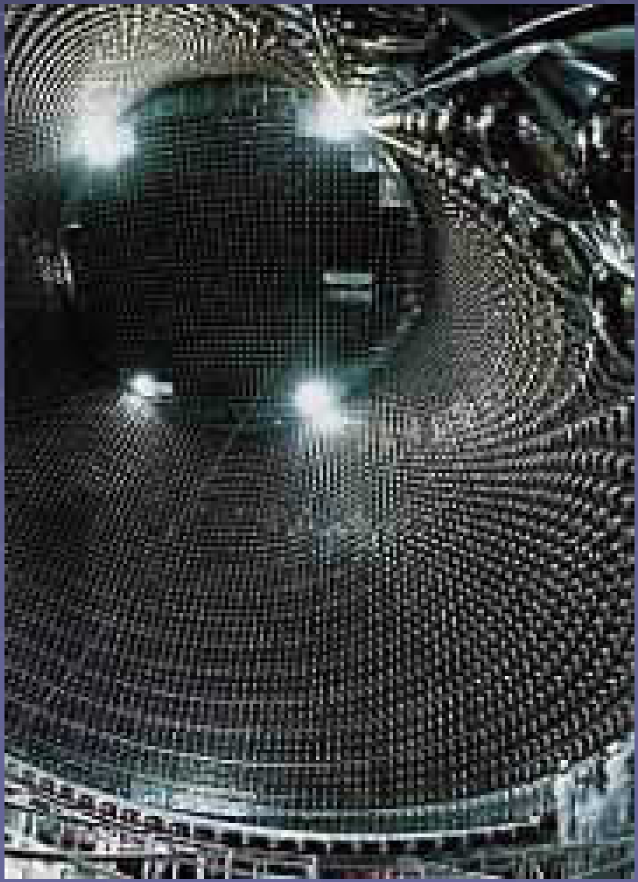
In order to achieve satisfactory functioning of GPS, correction for general and special relativity is required.

In Elementary Particle and Cosmology Research

Subaru telescope
CCD cameras



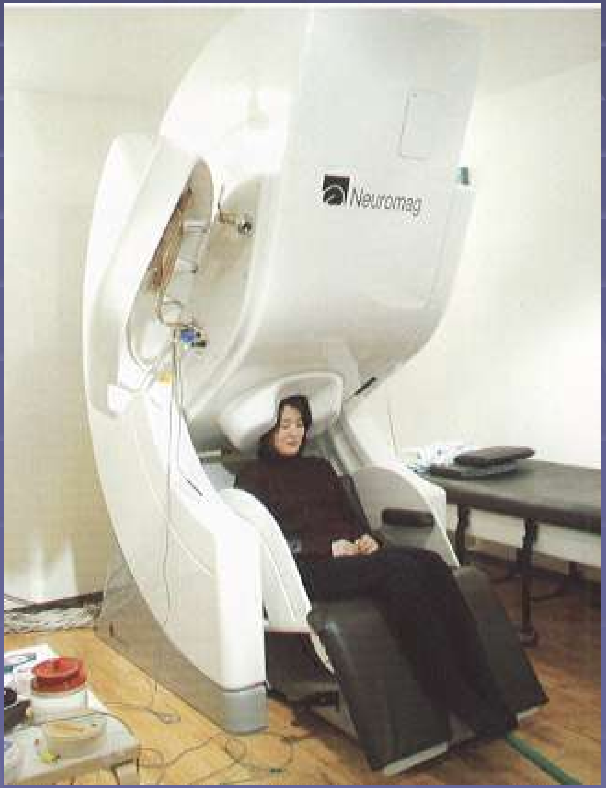
Super Kamiokande
Photomultiplier tubes



In State-of-the-art Medical Service

MRI (Magnetic Resonance Imaging)

MEG (magnetoencephalogram) and SQUID (superconducting quantum interference device) detect weak magnetic signals.



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In Everyday Life

- Liquid crystals, e.g., displays.
- High strength fibers, e.g., for tennis rackets.
- Gels, e.g., paper diapers.
- Fuel cells
- Solar power generation
- Photo-catalysts
- …..

Condensed Matter Physics is the Field of Physics

Matter and Materials

Matter: A substance that occupies space-time.

Material: The substance of which something is composed.

Solid State Physics

Condensed Matter Physics

Materials Science

Materials Engineering

The Notion of Condensed Matter Physics

It is intellectual curiosity that drives us to want to learn more about the properties of matter and their correlation with the foundation of physics.

⇒ The viewpoint of matter is organized.

We further understand and utilize matter to cultivate and control useful functions.

⇒ Applied physics

Curiosity-Driven Research

Mission-Oriented Research

The Notion of Condensed Matter Physics

It is a game of catch of the concepts between condensed matter physics and elementary particle and nuclear physics.

Phase transition: Spontaneous symmetry breaking.

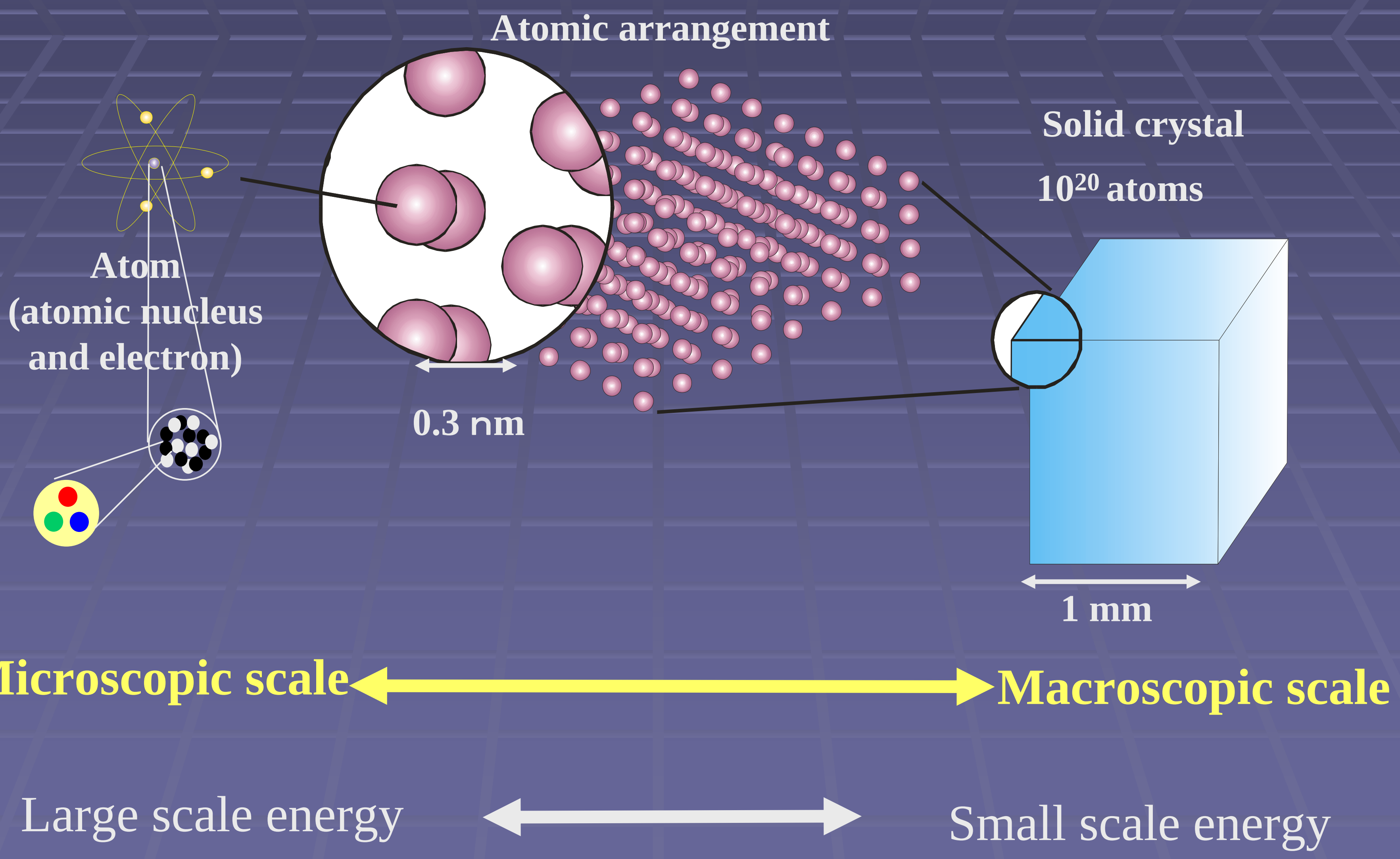
Nambu-Goldstone mode

Asymptotic freedom,

topological excitation, and quantum phase.

……….

The Hierarchical Structure of the Physical World



Condensed Matter Physics

- The field of study that deals with the diverse physical properties of matter based on the understanding of physical principles.
- Characteristics
  - Experimental (⇔Astrophysics and planetary geophysics)
  - Small science (⇔Big science)
  - Chemistry, applied physics, … , and life science?
- Confirmation
  - Comparison between experiments and theory
  - Hypothesis and demonstration, i.e., a game of catch.
- Useful properties ⇒ application
- Construction of matter viewpoint.

The World View of Physics

Reductionism

The behaviors of a system that belong to a particular hierarchy can be explained by more-simply-reduced hierarchy of principles.

The fundamental constituent of all force ⇒ The ultimate theory

Emergent properties

Interaction of many-body systems: phase transition.

E.g., superconductivity and the life process.

More is different.

(P.W.Anderson)

What Condensed Matter Physics Is Concerned With

Solid bodies (monocrystals and polycrystals).
Disturbed crystals (impure and defective types).
Amorphous, glass, liquids, and quasi-crystals.
Fine particles and cluster.
Surface and interface.
Artificial crystals (superlattice) and nano-structures.
Soft matter (polymers, liquid crystals, and gels).
Atomic gases (Bose condensate)

Properties of Matter

- Structural properties (Crystal structure and the disturbance)
  - Solid, liquid, and glass.
- Mechanical properties (Compressibility, elasticity modulus, and plasticity)
  - Diamonds and iron and steel are hard while gold is soft. Glass is hard but brittle.
- Thermal properties (Melting point, boiling point, specific heat, and thermal conductivity)
  - Copper has high thermal conductivity while stainless steel has low thermal conductivity.

Properties of Matter

- Electrical properties (Electric conductivity, dielectric constant, and superconductivity)
  - Metal, insulators, and semiconductors
  - Ferroelectrics
  - Superconductors
- Magnetic properties (Susceptibility and magnetization)
  - Ferromagnetic body: How does iron become magnetized?
- Optical properties (Optical spectrum, transmittance, and reflectivity)
  - The color of gemstones and metallic luster
  - Luminescence (light-emitting diodes and semiconductor lasers

Matter and the Physical Environment

The environment, outer field, and perturbation where matter is placed.

- Temperature
- Pressure and stress
- Electric field
- Magnetic field
- Interaction with light (electromagnetic waves)
- Sample sizes

Quantum Mechanics and Atomic Structure

Major Players in Condensed Matter Physics

The players (“Elementary” particles)

$$e = 1.60 \times 10^{-19}\ \mathrm{C}$$

$$m_e = 0.91 \times 10^{-30}\ \mathrm{kg}$$

- Electrons
- Atomic Nucleus (protons + neutrons)

$$m_p \approx m_n \approx 1840\, m_e$$

- Atoms and molecules
- Ion

The forces that act among “elementary” particles: electromagnetic interaction.

Light (electromagnetic wave) $h\nu$ photon. $h = 6.62 \times 10^{-34}\ \mathrm{J \cdot s}$

Energy Scale

Kinetic energy

$$\frac{1}{2}mv^2$$

Energy unit: Joules

$$\mathrm{J} = \mathrm{kg\,m^2/s^2}$$

Electron volts

$$e = 1.6\times10^{-19}\,\mathrm{C}$$

$$1\,\mathrm{eV} = 1.6\times10^{-19}\,\mathrm{J}$$

Planck constant is

$$h = 6.62\times10^{-34}\,\mathrm{J\cdot s}$$

$$= 4.13\times10^{-15}\,\mathrm{eV\cdot s}$$

The oscillation frequency, wave number, wavelength of the photon with energy $1\,\mathrm{eV}$.

$$h\nu = 1\,\mathrm{eV} \quad \leftrightarrow \quad \nu = 2.42\times10^{14}\ \mathrm{Hz}$$

$$\leftrightarrow \quad \frac{\nu}{c} = 8070\ \mathrm{cm^{-1}} \quad \leftrightarrow \quad \lambda = 1240\ \mathrm{nm}$$

Quantum Mechanics

Wave function $\psi(x, y, z)$

Probability distribution of particles

$$\left|\psi(x, y, z)\right|^2$$

Schroedinger's equation

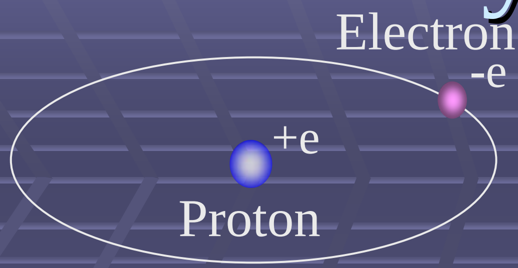
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(x, y, z) = E\,\psi(x, y, z)$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

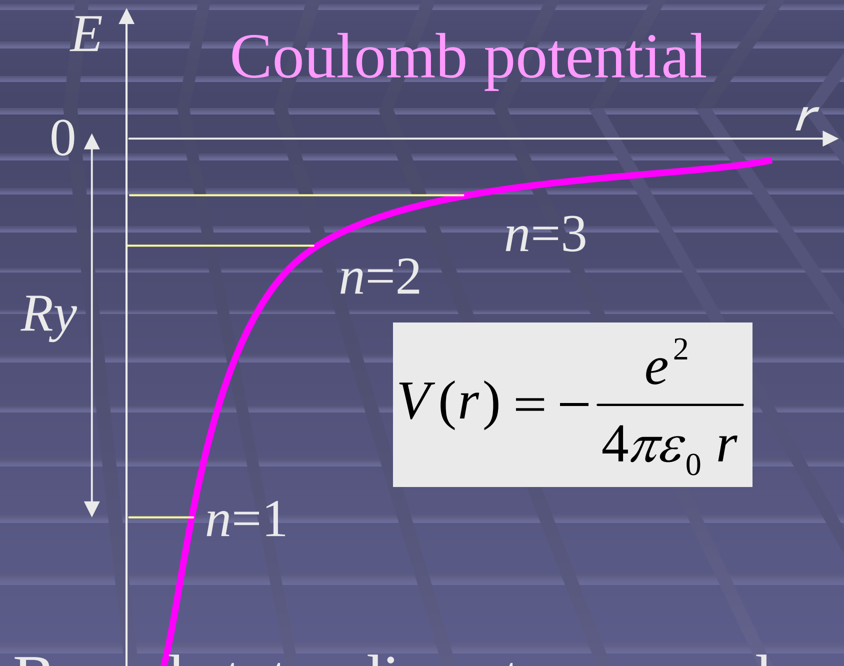
$$\hbar = \frac{h}{2\pi} = 1.05 \times 10^{-34}\ \mathrm{J \cdot s}$$

Energy level E

Hydrogen Atoms



$$\left[-\frac{\hbar^2}{2m}\nabla^2-\frac{e^2}{4\pi\varepsilon_0 r}\right]\psi(r)=E\psi(r)$$



$$V(r)=-\frac{e^2}{4\pi\varepsilon_0\, r}$$

Bound state: discrete energy level

Bohr radius

$$a_0=\frac{4\pi\varepsilon_0\hbar^2}{me^2}=0.053\text{nm}$$

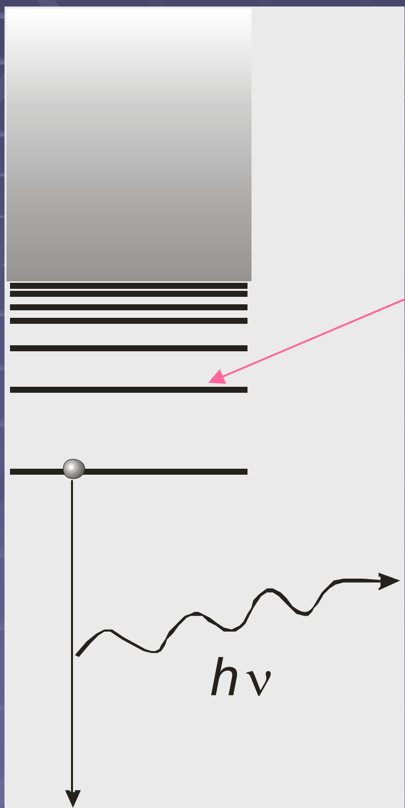
Rydberg constant

$$Ry=\left(\frac{1}{4\pi\varepsilon_0}\right)^2\frac{me^4}{2\hbar^2}=13.6\,\text{eV}$$

$$E_n=-\frac{1}{n^2}Ry$$

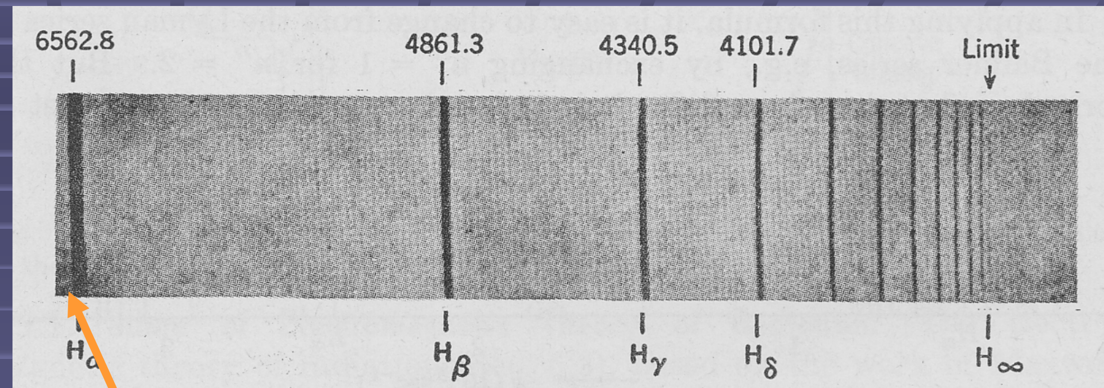
$$\langle r\rangle_n=n^2a_0$$

Spectrum of Hydrogen Atoms



$$E_n = -\frac{Ry}{n^2}$$

$$h\nu = E_n - E_m = Ry\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$



Balmer series(m=2)

$$E_n - E_m = Ry\left(\frac{1}{2^2} - \frac{1}{3^2}\right) = \frac{5}{36} Ry = 1.89\,\text{eV}$$

$$\nu = 4.55 \times 10^{14}\ \text{Hz}$$

$$\lambda = 659\,\text{nm}$$

Energy Level of Hydrogen Atoms

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(x,y,z) = \varepsilon\psi(x,y,z)$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Spherically symmetry potential

$$\nabla^2 \equiv \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

$$Y_l^m(\theta,\phi) \propto P_l^{|m|}(\cos\theta)\exp(im\phi)$$

Angular momentum quantum number

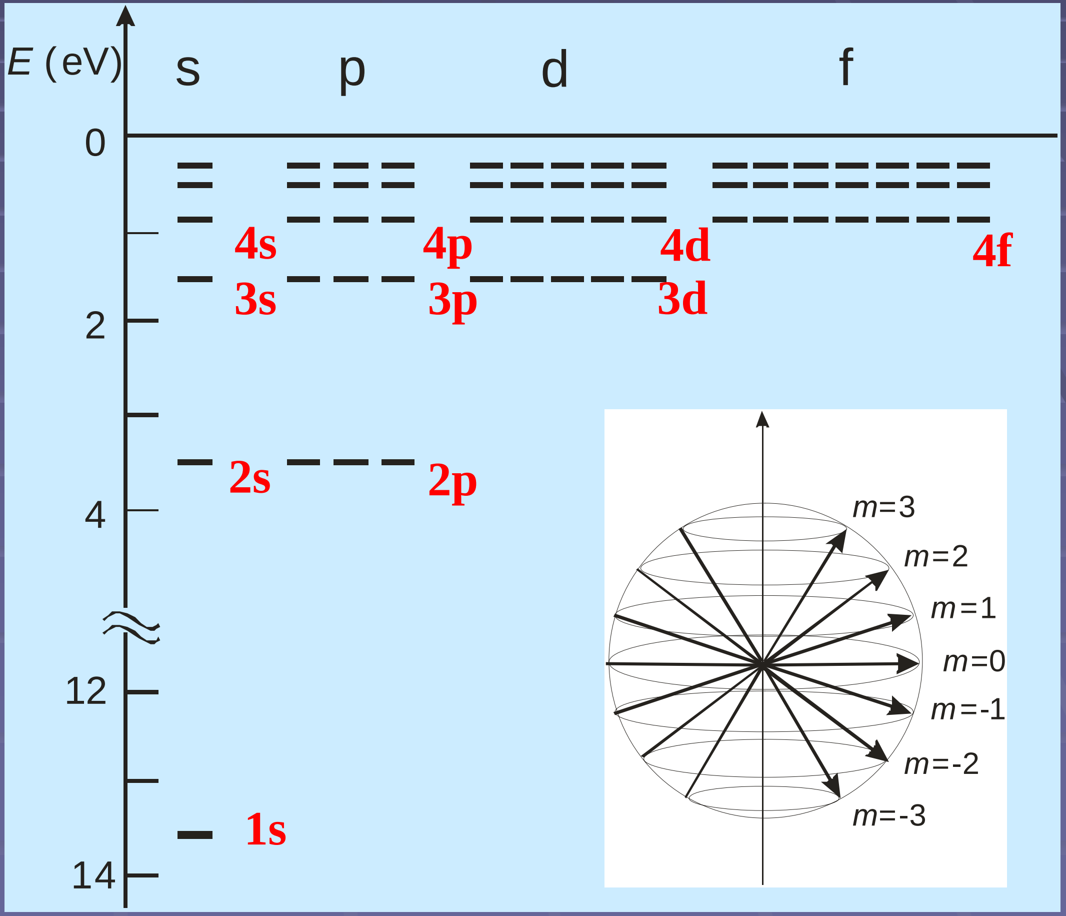
$$l = 0, 1, 2, \cdots$$

$$m = -l, \cdots, l-1, l \qquad (2l+1)$$

Principle quantum number $n = l, l+1, \cdots$

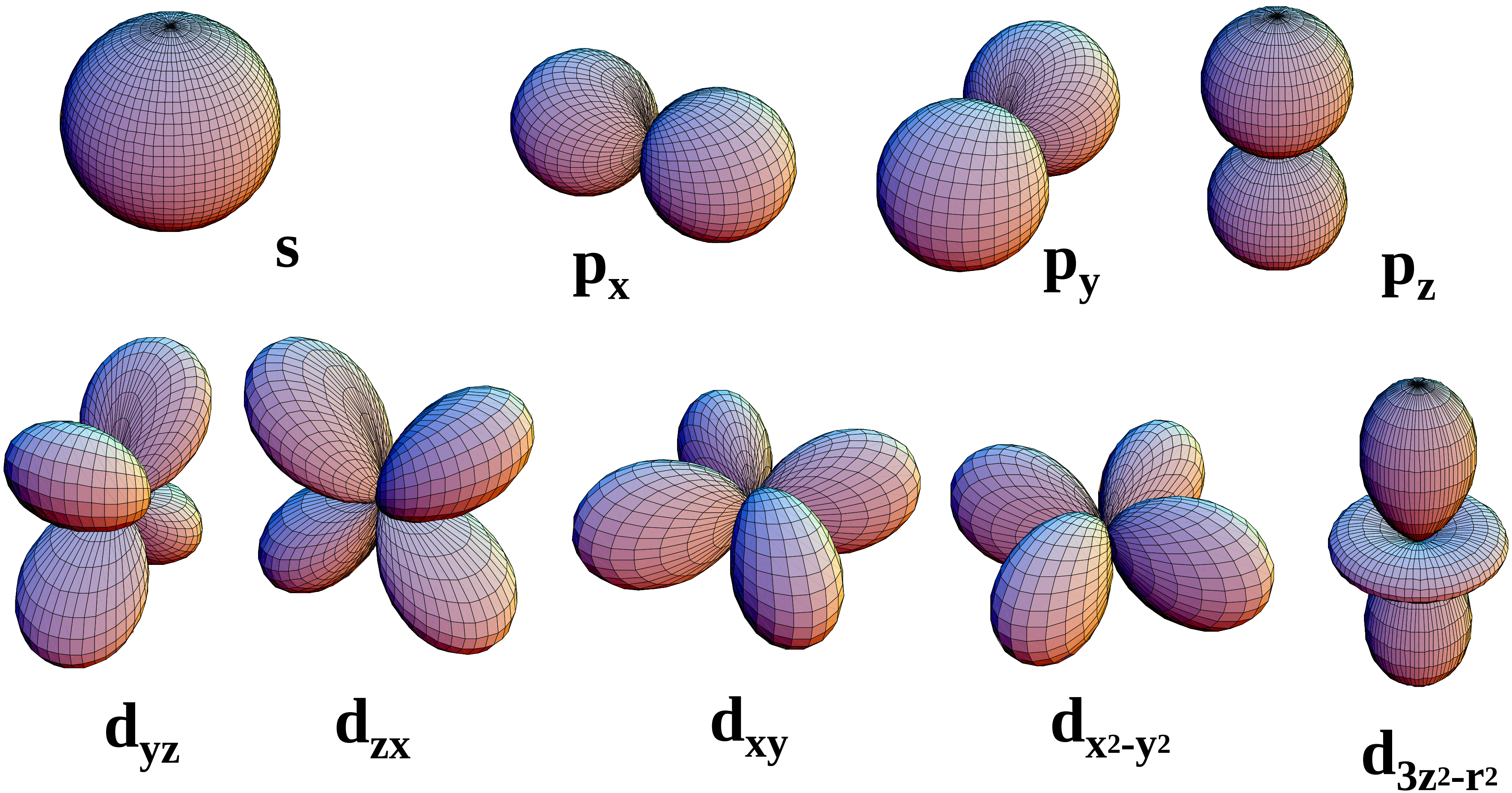
Spin quantum number $\sigma = \pm 1$

$$n, l, m, \sigma$$



Angles in the Atomic Wavefunction

$$Y_l^m(\theta,\phi) \propto P_l^{|m|}(\cos\theta)\exp(im\phi)$$

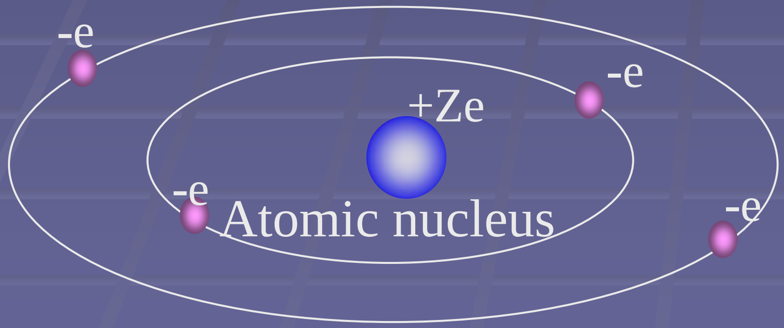


Electron Energy Level of Atoms

Many-electron atoms:

Atomic nuclei that possess electric charges +Ze and Z electrons.

Electrons received at the energy level are assigned by the fermions ⇒ (n, l, m, σ)

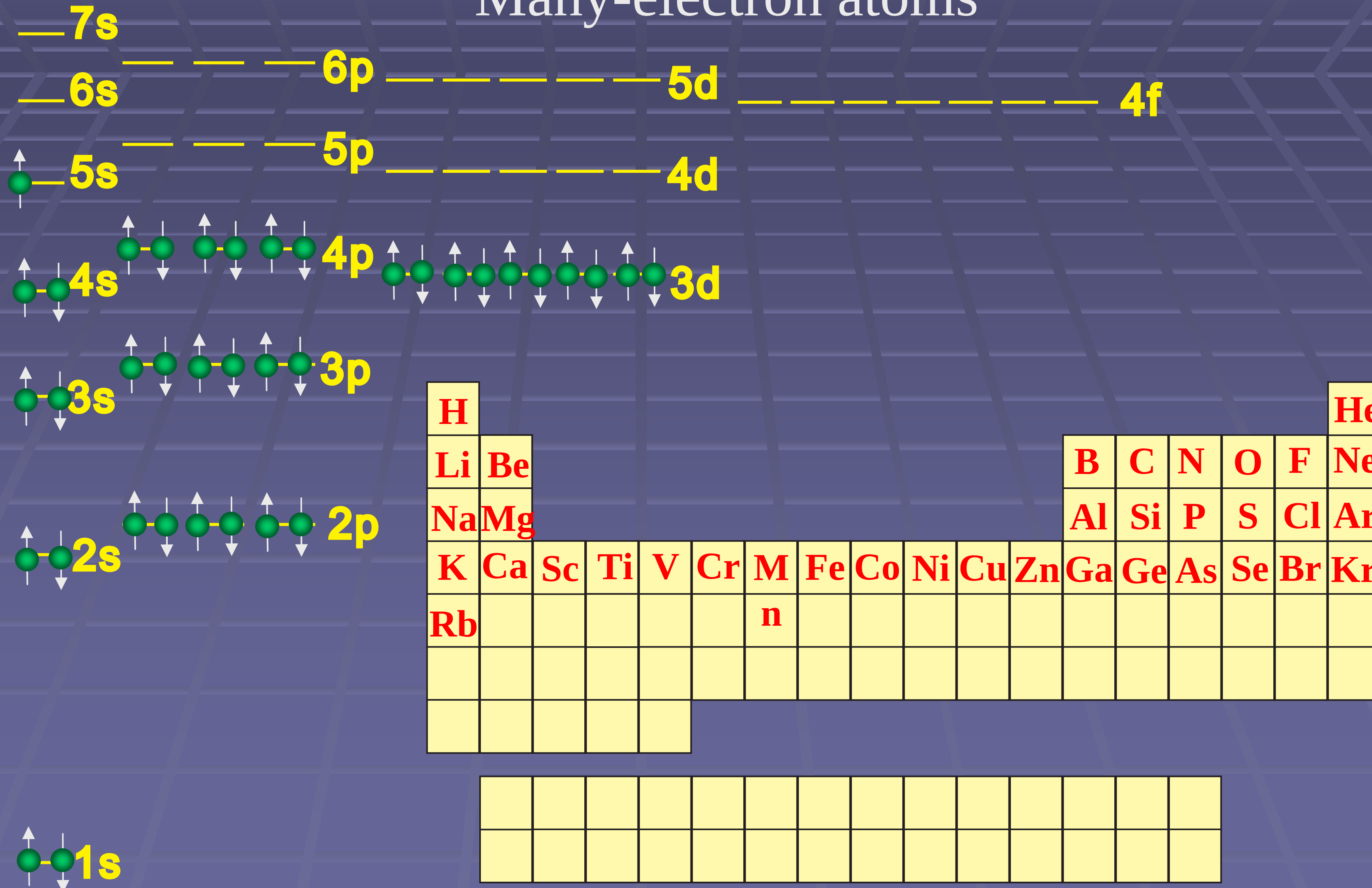


Na： Z=11

$$\mathrm{Na}:(1s)^2(2s)^2(2p)^6(3s)^1$$

Method of Filling the Electron Energy Level

Many-electron atoms



Electron Energy Level in Atoms

Each electron is received at the energy level that are assigned by the fermions ⇒ $(\boldsymbol{n, l, m, \sigma})$

The shell structure assigned by the value of ***n***

n=1 2×1 = 2
n=2 2×(1+3) = 8
n=3 2×(1+3+5) =18

The number of atoms with completely occupied shells 2, 10, 18, 36･･･are energy stable.

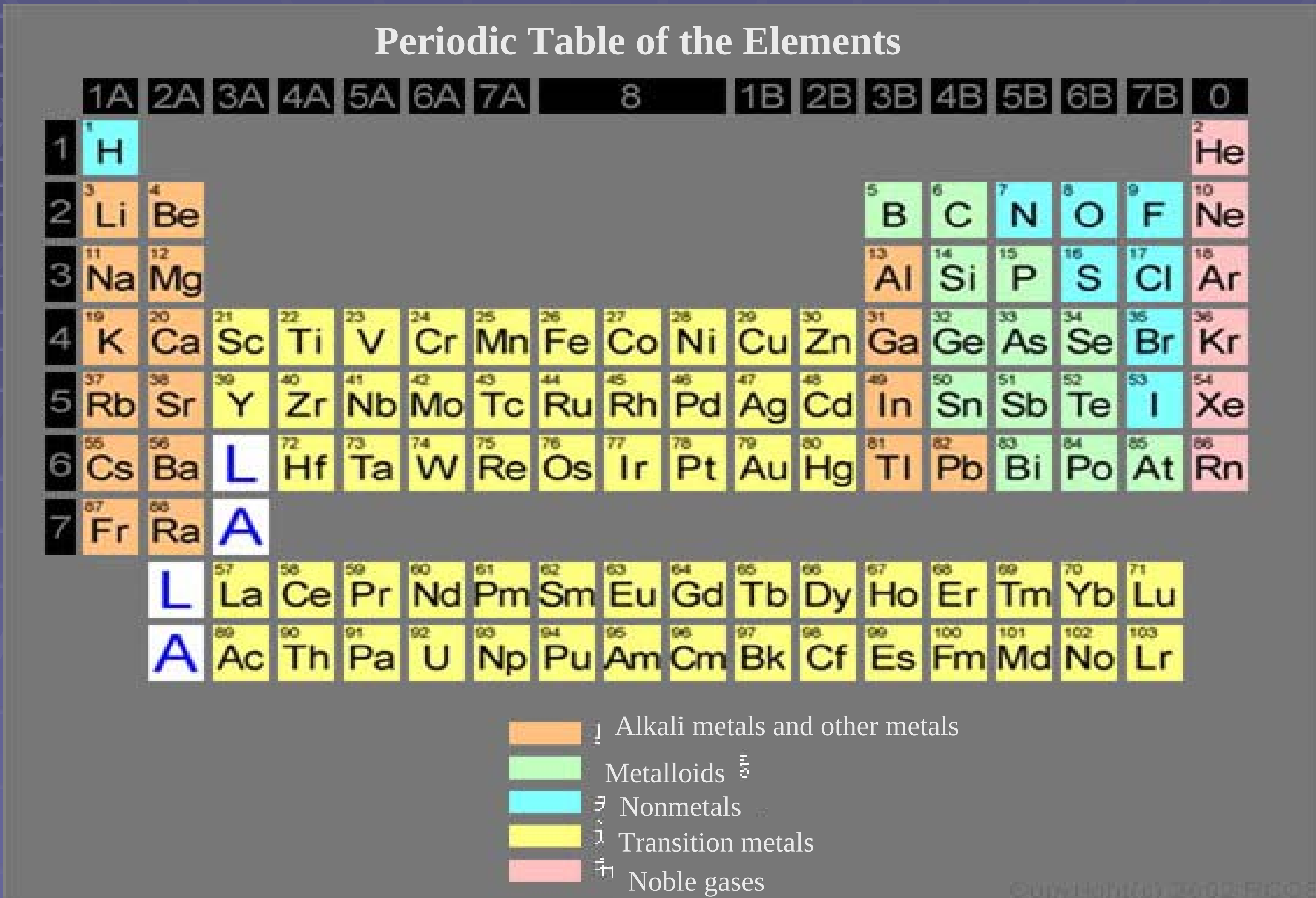
Noble gas (inert gas) atom:
He, Ne, Ar, Kr, and Xe.

Electron Energy Level in Atoms

Electrons in the outermost shell are the most important in affecting the physical properties of matter because the electrons can be dropped into lower orbits. ⇒ Valence electrons

The atoms that have similar electron configuration in the outermost shells represent similar chemical properties.⇒ Periodic table of the elements

Periodic Table of the Elements



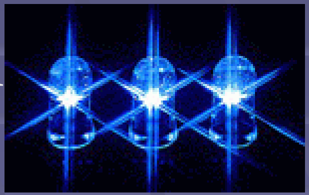
Electron Energy Level in Atoms

Although, there is greater coulombic attraction involved with the atoms of greater *Z*, there will also be a greater number of electrons around the atoms thus, the electron energy of the outermost shell will be obtained as approximately a few eV energy level.

The energy scale of condensed matter physics is between a few eV and meV.

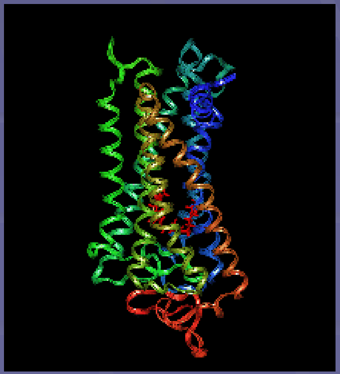
Dry battery is 1.5V.

Electromotive force due to the exchange of atom



Laser pointer　Two dry batteries 3V

Red light　～1.5eV, Green light　～2.5eV



Rhodopsin: the light receptor protein in the retina.　Has an energy level equivalent to that of visible light.

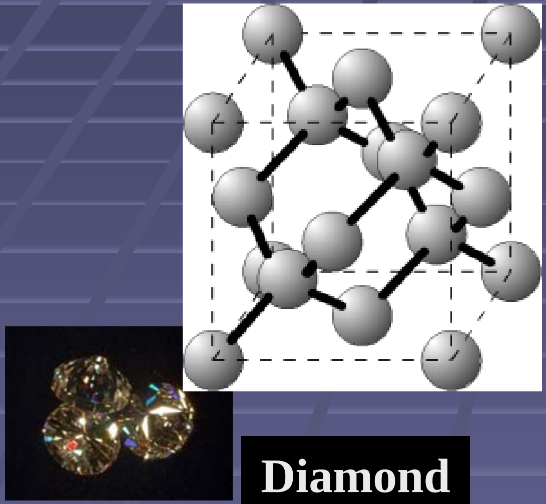
Existing Forms of Matter

Types of Matter

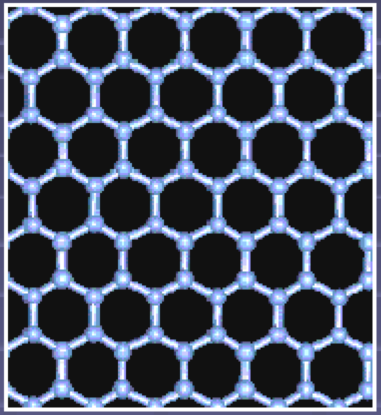
There are roughly 100 types of single-elements.
(Carbon, for example, has many different existing forms.)

Seven Types of Carbon

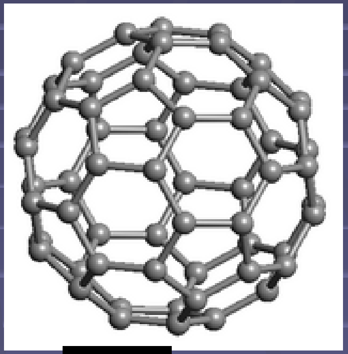
Carbon atoms can form a variety of materials.



Diamond

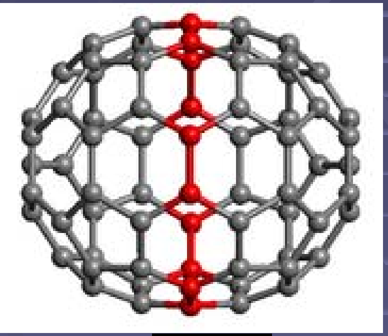


Graphite

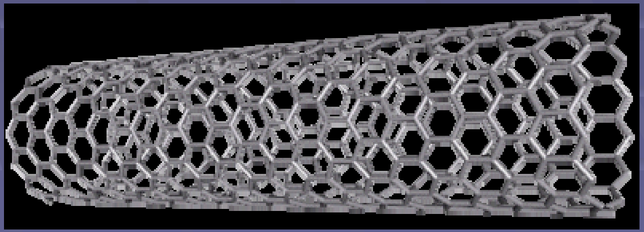


C_{60}

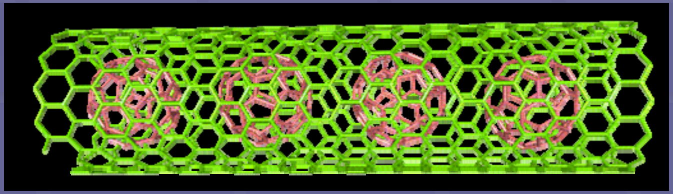
fullerene



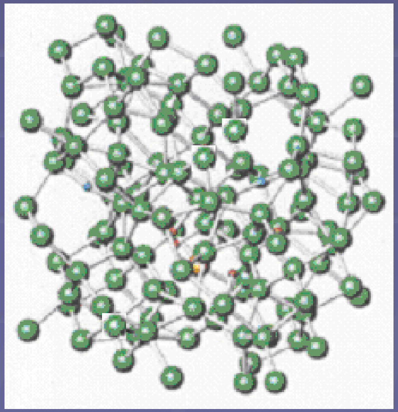
C_{70}



Carbon nanotubes



Carbon peapod



Amorphous carbon

Types of Matter

There are roughly 100 types of single-elements.
(Carbon, for example, has many different existing forms.)

There are variety of the combinations when compound such as NaCl and the alloy such as $Pb_{1-x}Sn_x$ are considered.

When three-dimension compounds and four-dimension compounds, and more,… are further considered, then there would be an infinite possibility for various types of matter⇒ search and development of matter and materials.

We hope to design and create the particular matter that we want ⇒ Material design (computational material science)

Existing Forms of Matter

Interacting many-particle system

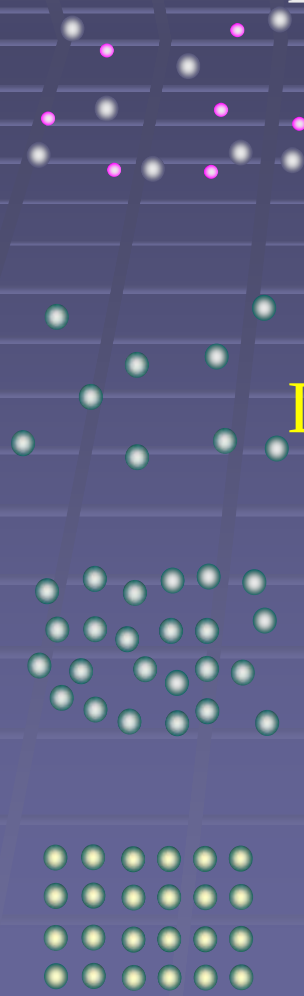
Temperature

Plasma

Vapor

Liquid

Solid



Energy versus entropy

Disordered state

Phase transition

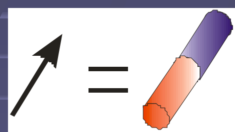
Ordered state

Greatest possible freedom

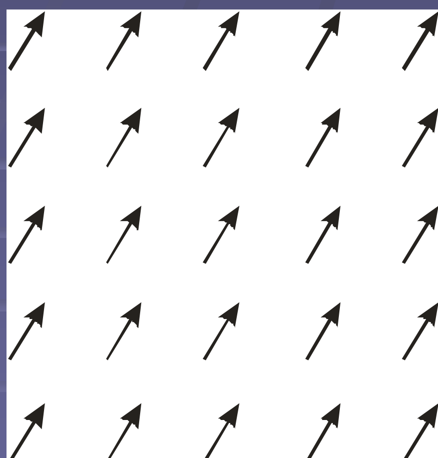
Lowest possible energy

Phase Transition

Spin：magnetic momentum (micro-magnet)



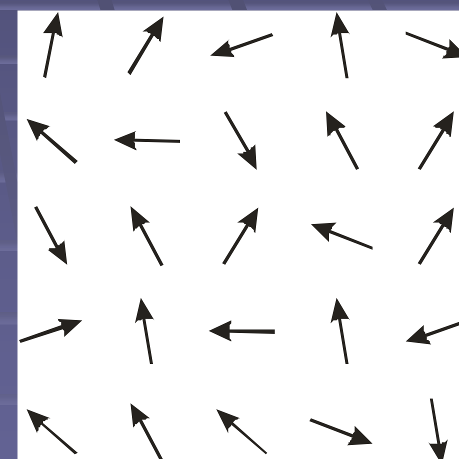
The spins will try to be parallel or antiparallel.



$T = 0$

Absolute zero point：ferromagnetic phase.
Ordered state

Under high temperatures, the spins tend to direction randomly.



$T > T_c$

High temperature：paramagnetic phase.
Disordered state

Energy and Entropy

The lowest energy state (ground state) can be obtained under the absolute zero point.

The crystal state where atoms are orderly aligned.
The magnetic ordering state where a moment is lined in order.

Under a finite temperature ($T > 0$), the condition of the state is determined by the balance between energy E and entropy S .

Free energy ($F = E\text{-}TS$) is the lowest state.

$$F = E - TS$$

The phase transition from the ordered state to the disordered state occurs at a particular temperature (critical temperature).

Solid ⇔ Liquid
(Anti)Ferromagnetic phase ⇔ Paramagnetic phase

Thermal Energy

Temperature T

$$k_B = 1.38 \times 10^{-23}\ \mathrm{J/K}$$

Boltzmann constant

Thermal energy $k_B T$

$$k_B T = 1\ \mathrm{eV} \quad \leftrightarrow \quad T = 11600\ \mathrm{K}$$

Room temperature $T = 300\ \mathrm{K} \quad \leftrightarrow \quad k_B T = 25\ \mathrm{meV}$

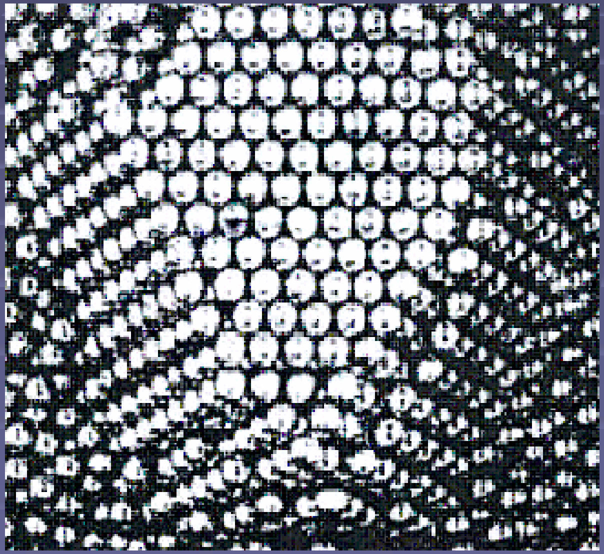
The Agglutination Mechanism and the Crystal Structure of Atoms

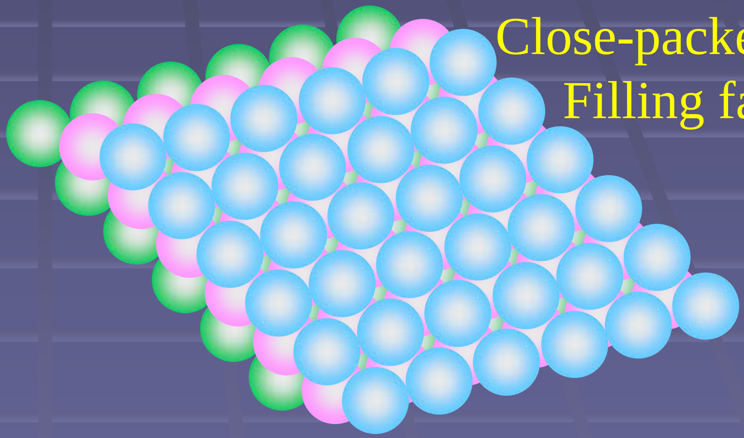
Crystal Structure

What types of atomic arrangement would have the lowest energy?

What happens when a box is occupied with many rigid spheres?

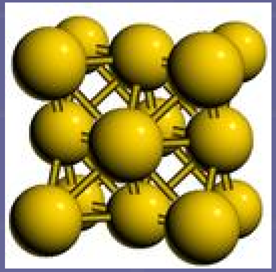
Packing problem



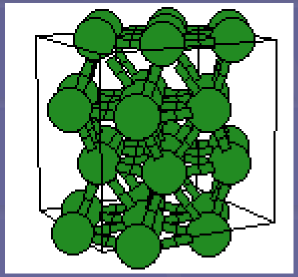


Close-packed structure
Filling factor 74%

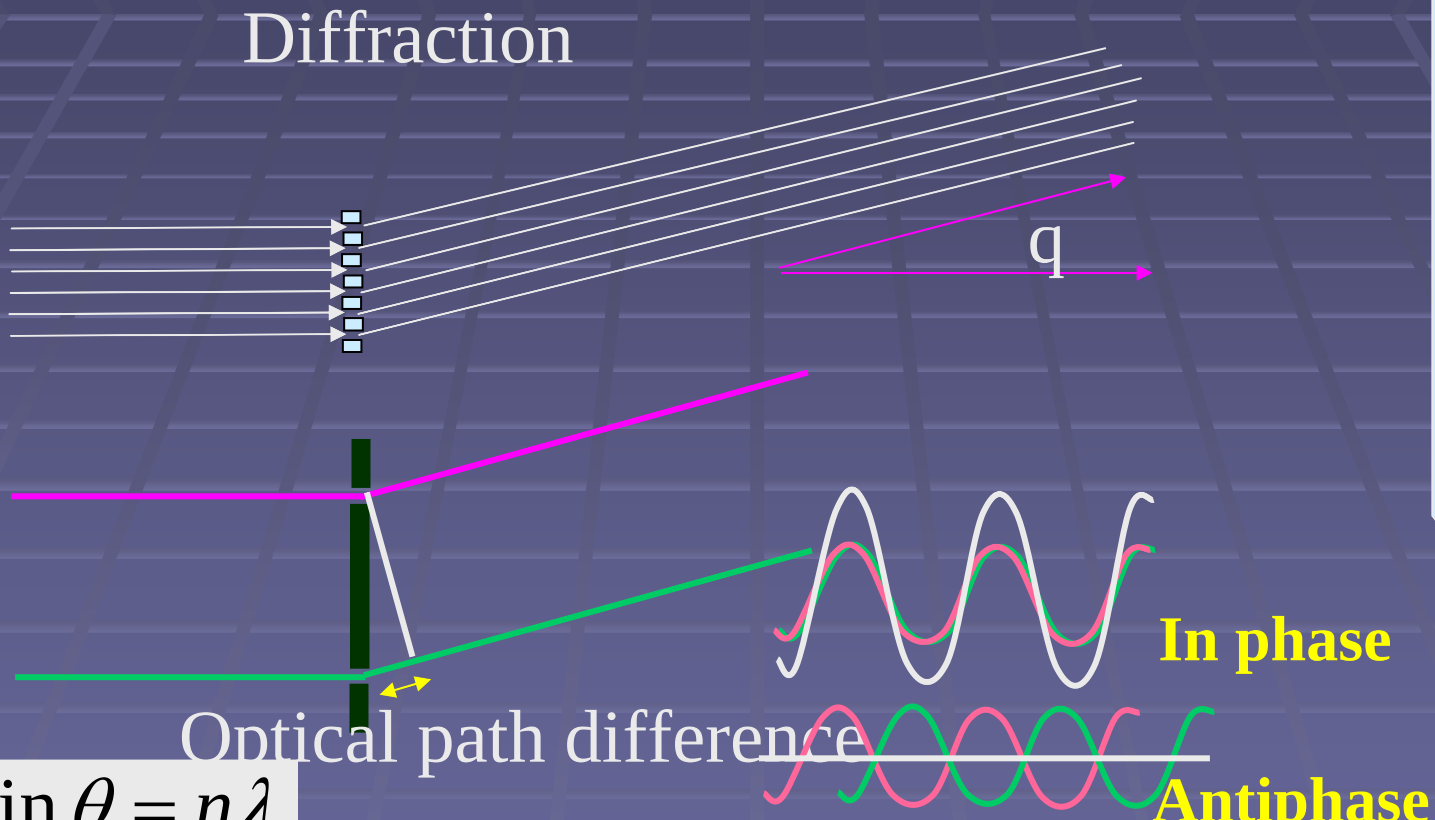
Face-centered cubic lattice (fcc)

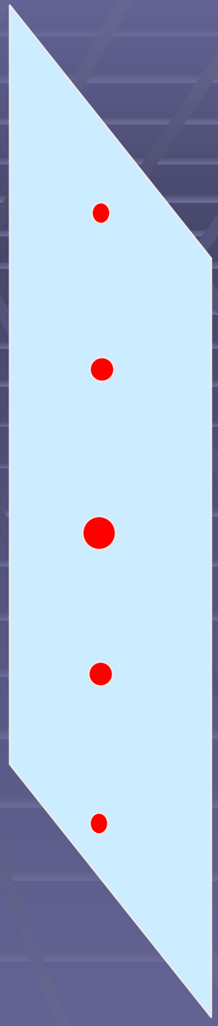


Hexagonal close-packed lattice (hcp)



How Do We Study the Periodic Order of Atoms?





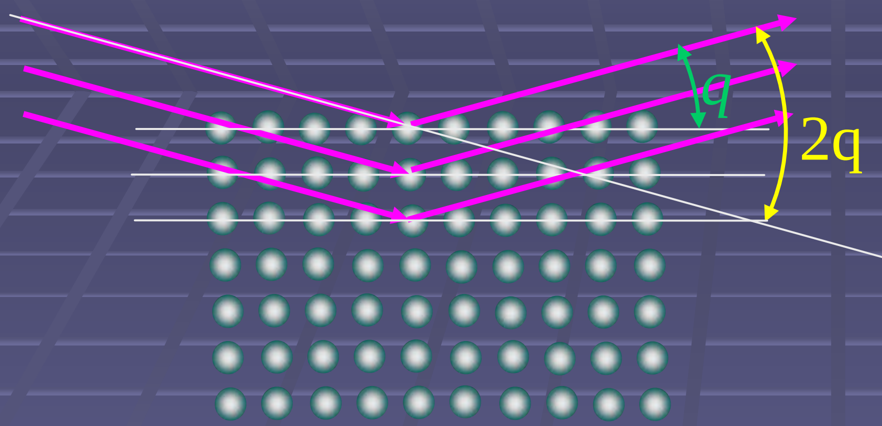
$$d \sin\theta = n\lambda$$

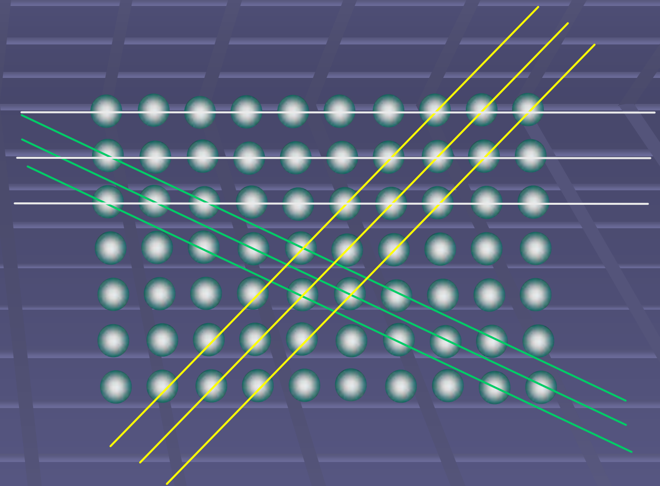
Interatomic space～0.3 nm ⇔ ～X-ray wavelength

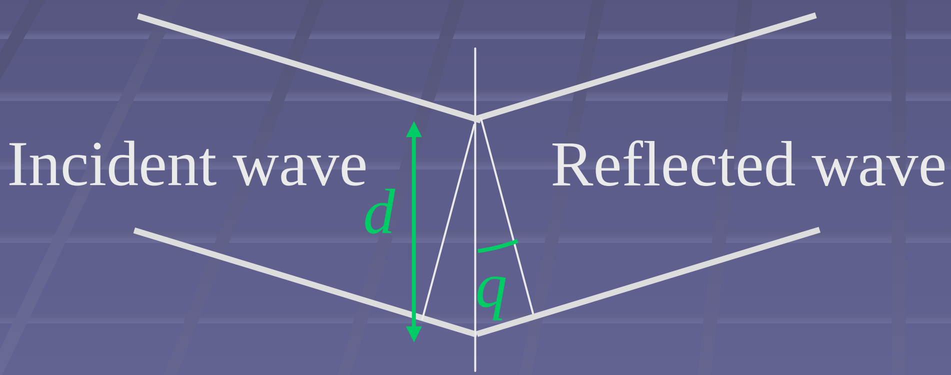
Electron beam and neutron beam diffractions are used.

Diffraction of light

Crystal Structure Analysis







$$2d \sin\theta = n\lambda$$

Bragg condition

Four-circle X-ray diffractometer

Atom Bonding Forces

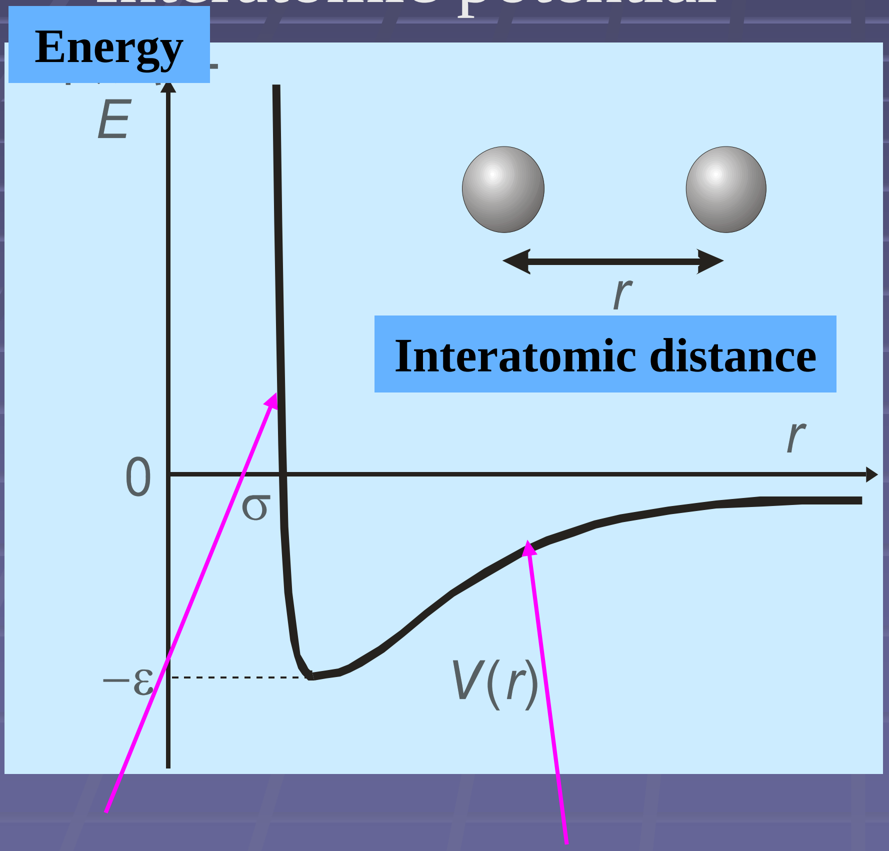
The attraction between atoms forms a condensed state (solid and liquid).

- Interatomic interaction
- Van der Waal bonding
- Ion bonding
- Covalent bonding
- Metallic bonding
- Hydrogen bonding

Various types of interatomic forces represent particular crystal structures

Noble Gas Crystal

Interatomic potential

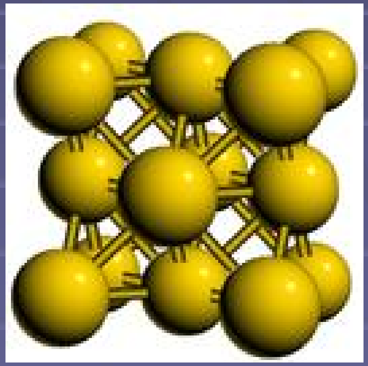


Rigid body repulsion

Van der Waal attraction

Ne, Ar、Kr, Xe

Close-packed structure
Face centered cubic lattice (fcc)

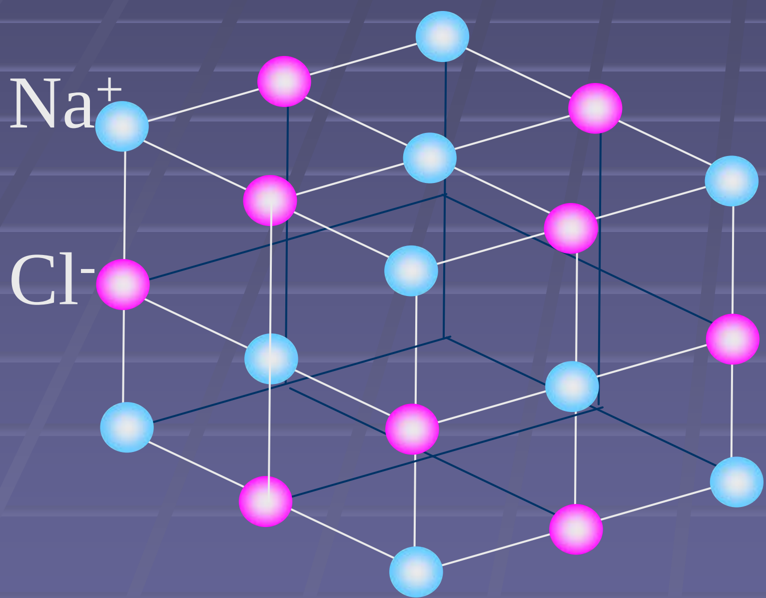


What about He？

Quantum liquid

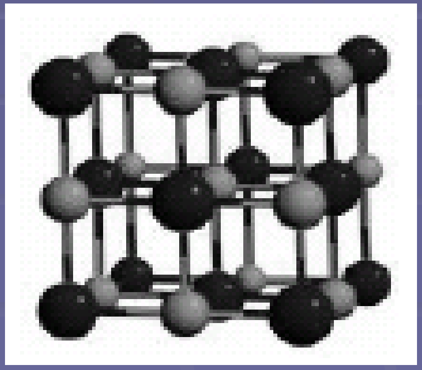
Ion Bonds

The coulombic attraction between cation and anion.

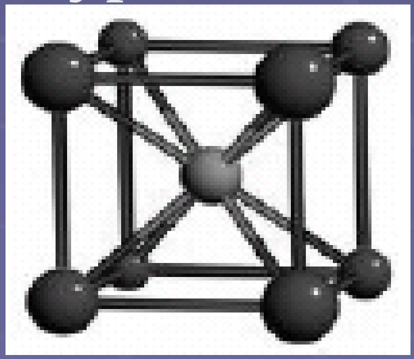


H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr

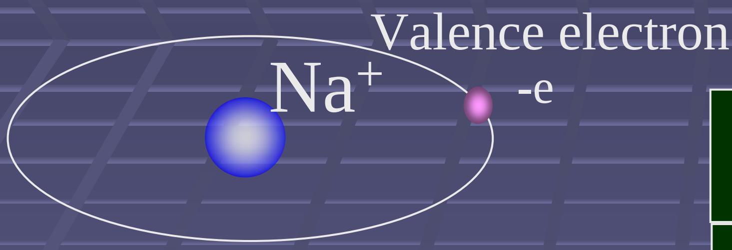
NaCl type



CsCl type

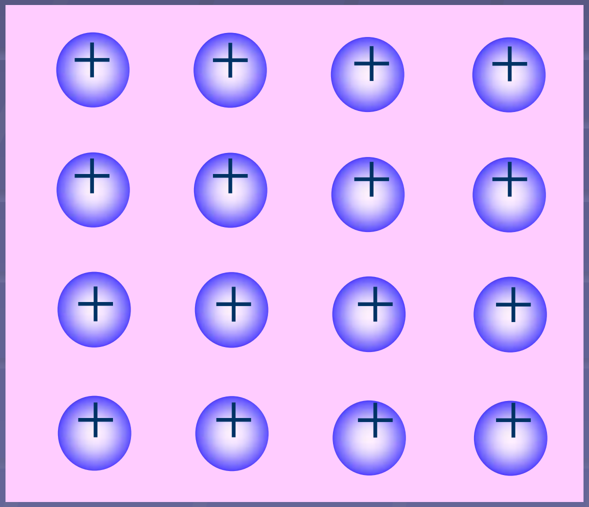


Metallic Bonds



$$Na : (1s)^2 (2s)^2 (2p)^6 (3s)^1$$

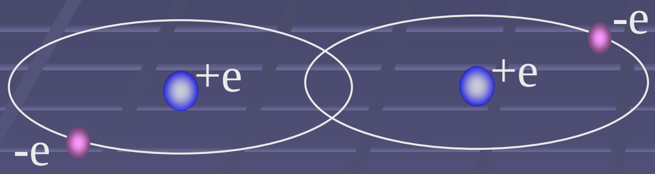
H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr



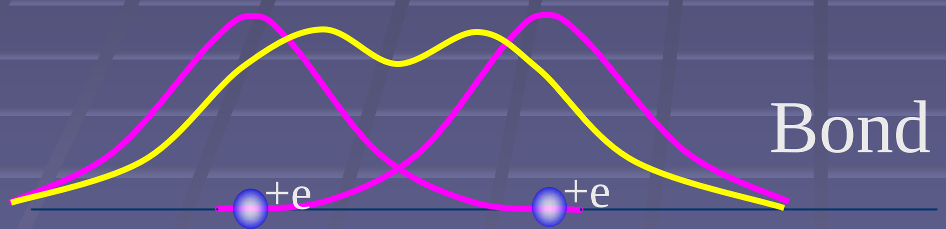
The cation is occupied in the negatively charged moving electron bed.

Covalent Bonds

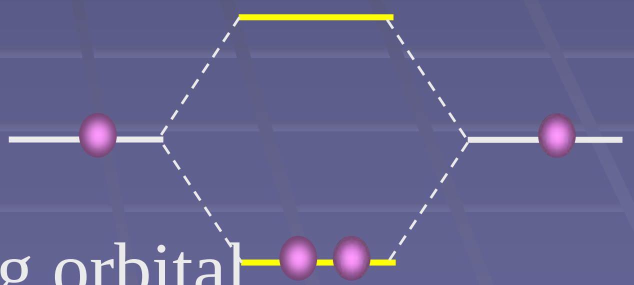
Hydrogen atom : H_2



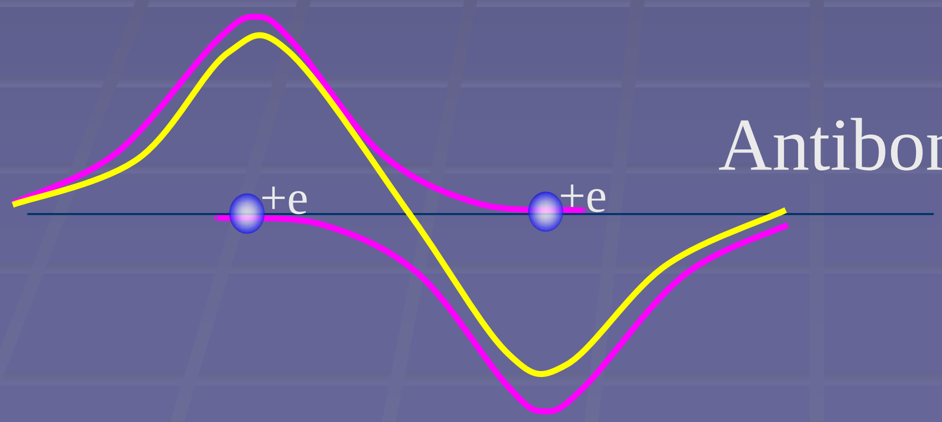
Molecular orbital



Bond orbital

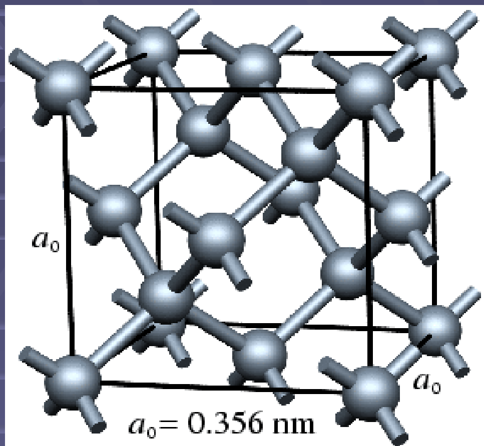


Antibonding orbital



Covalent Bonds

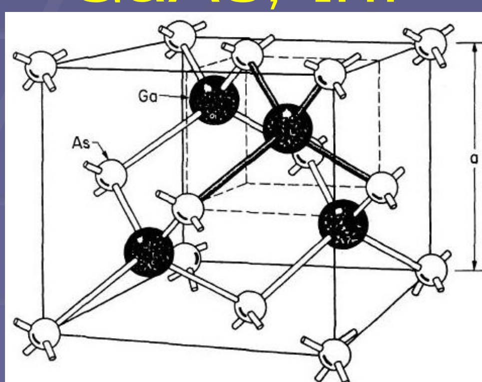
C, Si, Ge



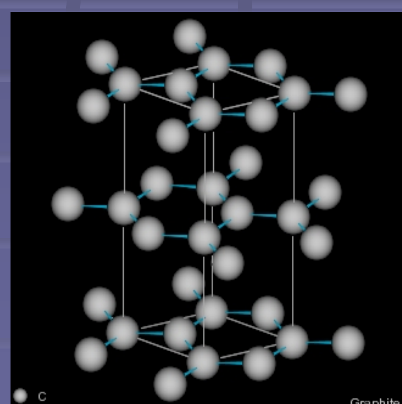
Diamond structure

H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr

GaAs, InP



Aphalerite structure



Graphite (black lead)

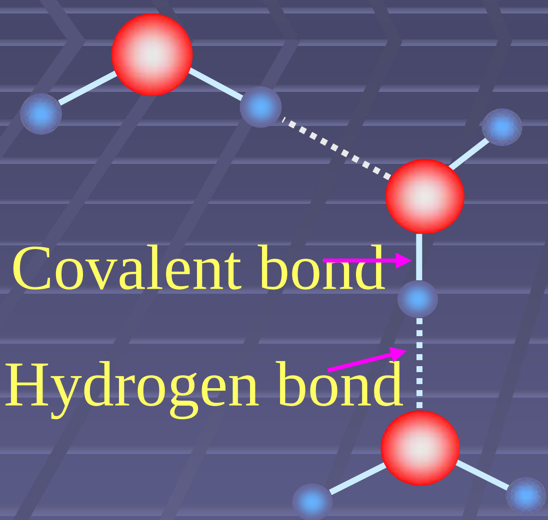
Lamellar crystal

Strong covalent bond is seen inside the layers, while weak Van der Waals bonding holds between the layers.

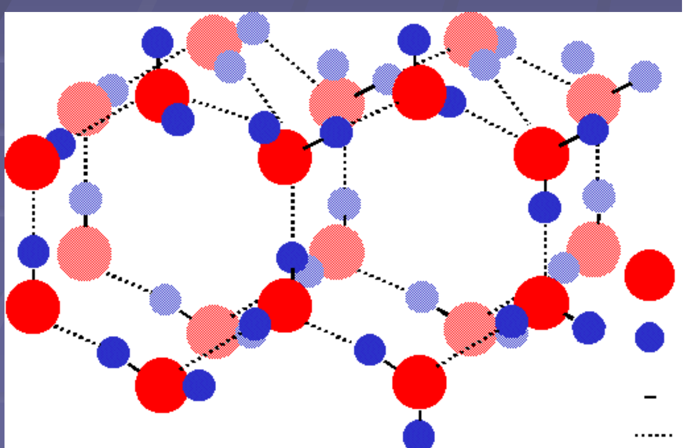
⇒ easy to split

Hydrogen Bonds

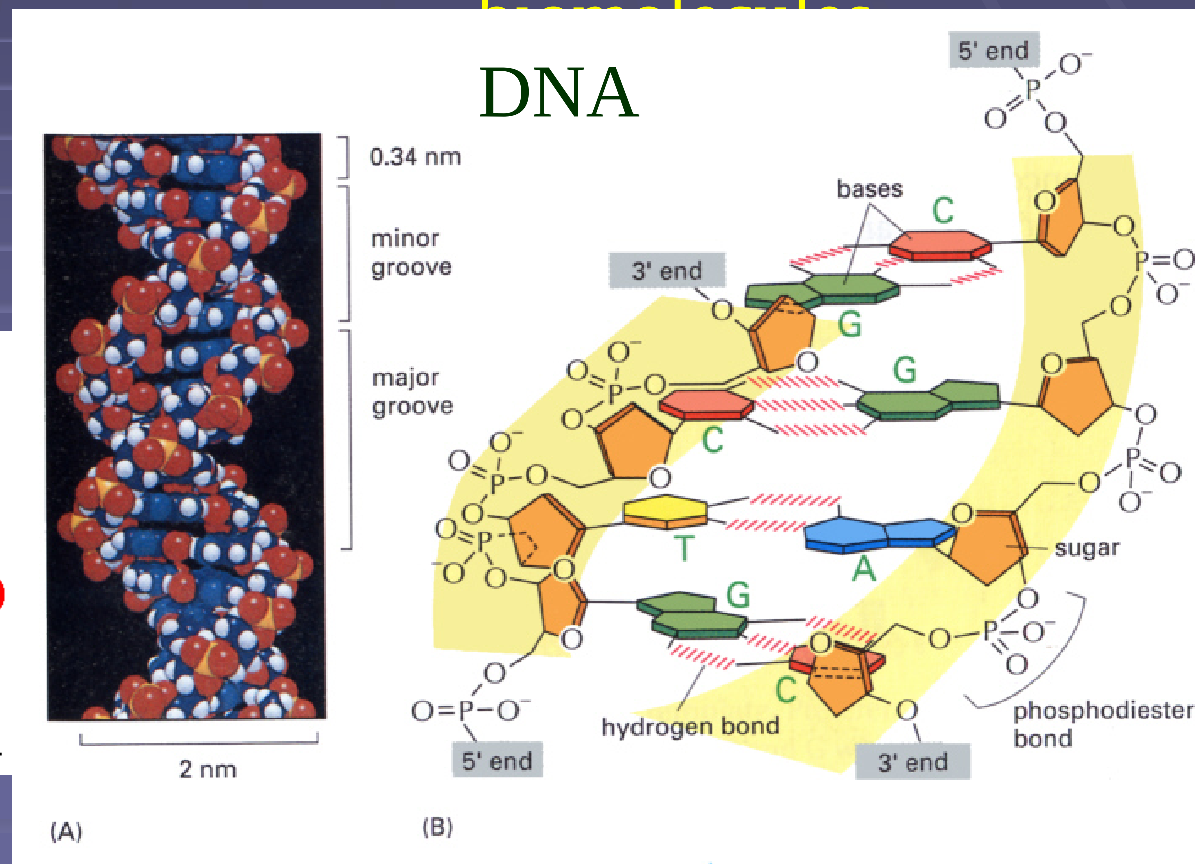
Water molecule



Hydrogen bonds play a very important role in



Ice crystal



Summary

- Stories about size and extent
- Modern civilization and physics
- Condensed matter physics; sub-field of physics
- Quantum mechanics and atomic structure
- Existing forms of matter
- Agglutination mechanism and crystal structure of atoms