

From the atomic
structure to the
macrostructure

Research methods

Atomic and molecular level material study methods allow us to „get an insight” into the matter

- microscopy methods: scanning , transmission electron , optical microscopy
- diffraction methods: X-ray, neutron, electron
- NMR – nuclear magnetic resonance spectroscopy
- mass spectroscopy
- IR, UV spectroscopy
- chemical analytical methods (Chromatography, adsorption, emission methods, thermogravimetry, electrolysis, nuclear activation etc. etc.)

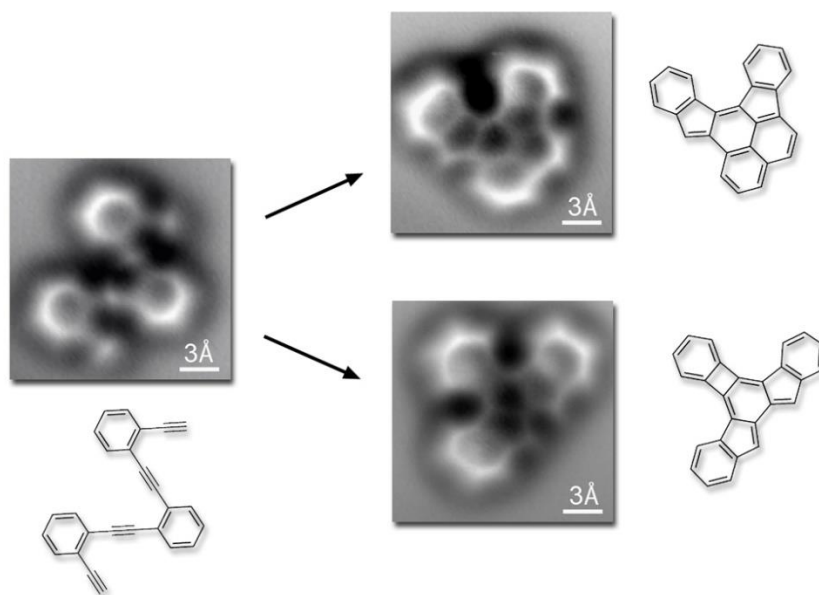
From the atomic structure to the macro structure

First image of an atomic chain taken by scanning electron microscope (polymer chain with Thorium atoms on it)



From the atomic structure to the macro structure

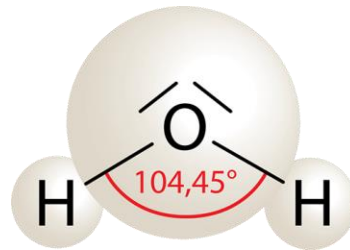
High resolution image of a molecule as it breaks.



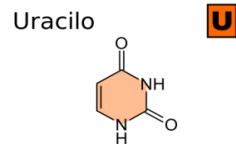
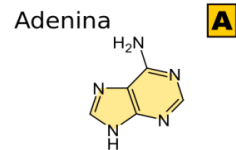
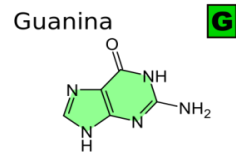
From the atomic structure to the macro structure

Molecular structure of materials

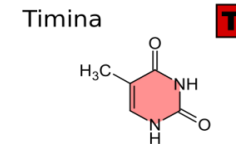
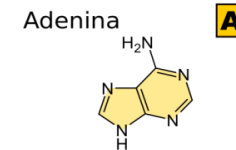
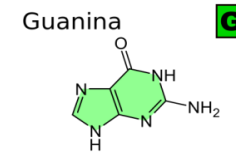
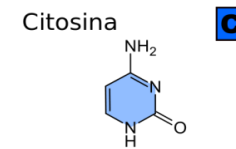
Water



From the atomic structure to the macro structure



Bases
del ARN

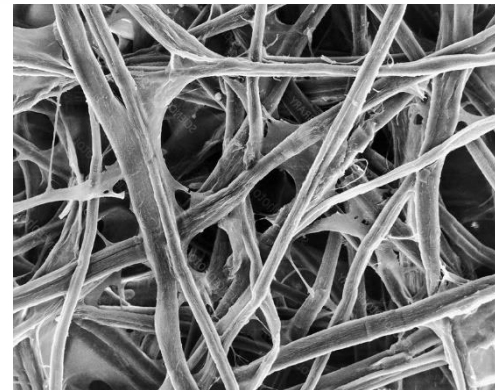
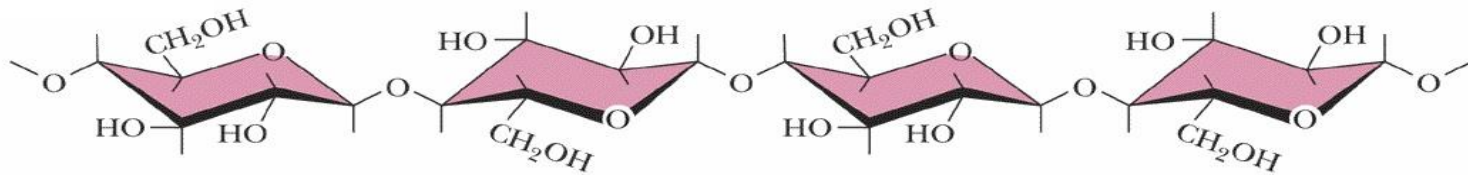


Bases
del ADN

From the atomic structure to the macro structure

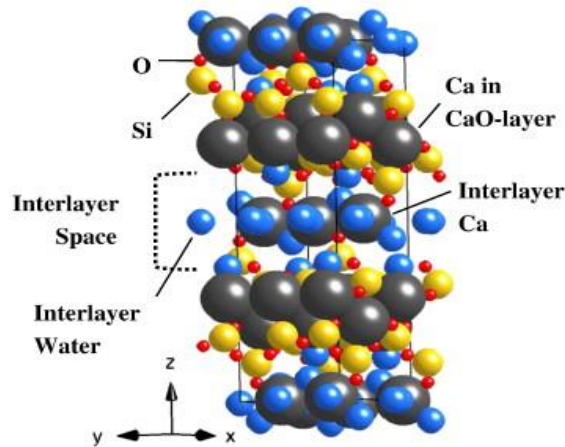
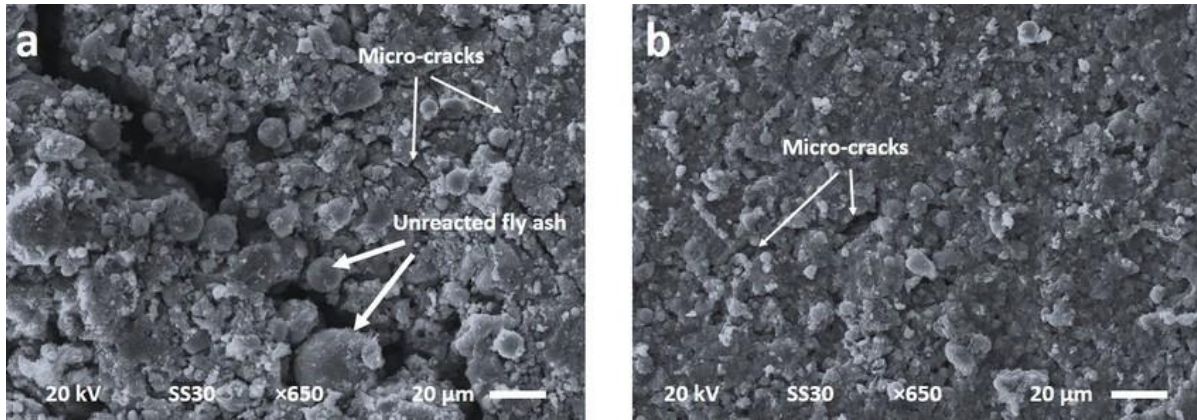
Molecular structure of organic materials

Cellulose



<https://www.sciencephoto.com/media/874491/view/cellulose-fibres-print-paper-sem>

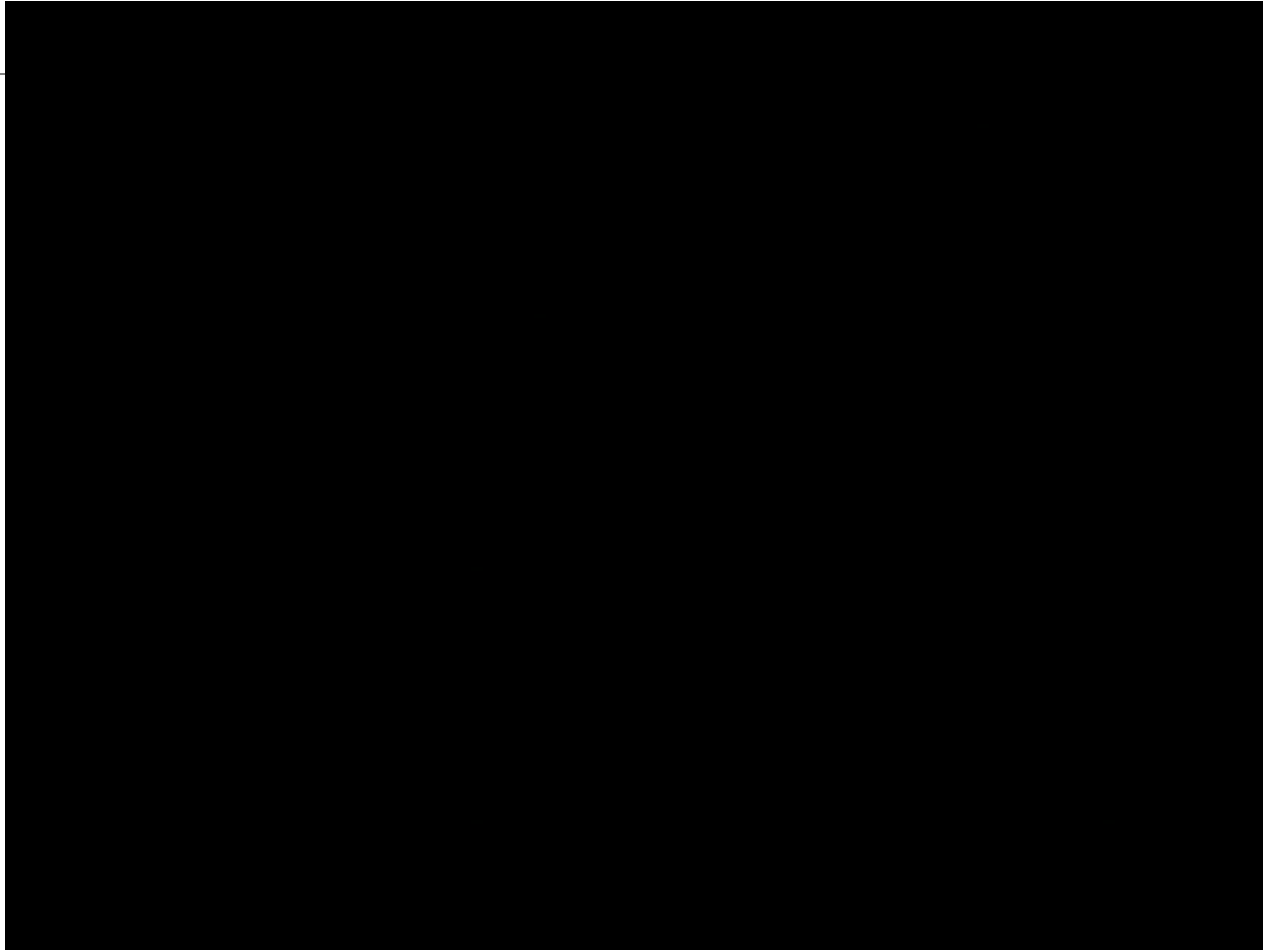
From the atomic structure to the macro structure



C-S-H

https://www.researchgate.net/figure/SEM-images-of-hydrated-cement-paste-for-a-cement-made-with-raw-materials-milled_fig5_309825572

<https://www.youtube.com/watch?v=Nx90iE6wmig>



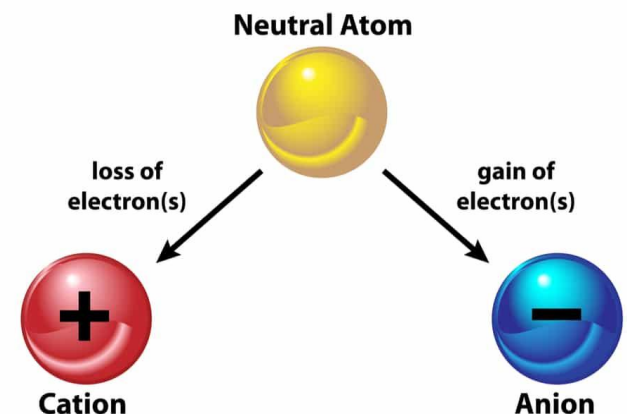
Chemical bond

- chemical bond: is an **attraction** between atoms, ions, molecules
- enables the formation of compounds
- the result of the **different type of attractions** between **valence electrons** of the atoms is the condensed matter
- valence electron: outer shell of an atom (1-8 for the main groups of the periodic table, 3-12 for the transition metals)

- types of attraction**:
 - electrostatic type
 - sharing of electrons
 - dipole-dipole interaction, Van der Waals type bonding

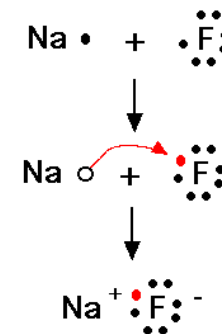
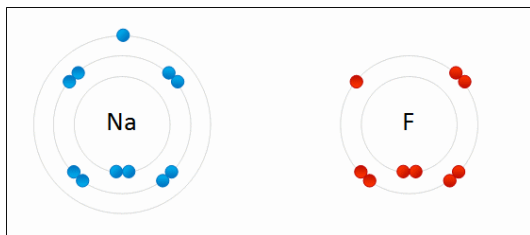
Ionic bonding

- ❑ **electrostatic** interaction between anions and cations
- ❑ **ion**: is an atom or molecule that has a net electrical charge
- ❑ A **cation** is a positively charged ion, with fewer electrons than protons, while an **anion** is negatively charged, with more electrons than protons.
- ❑ Because of their opposite electric charges, cations and anions attract each other and readily form ionic compounds



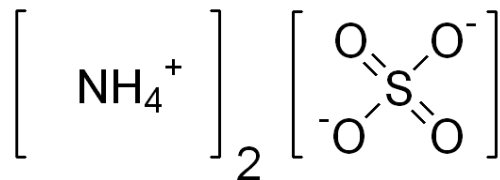
Ionic bonding

- electrostatic interaction between anions and cations
- **simple:** metal – non-metal ions



Sodium Fluoride

- **complex:** between molecular ions



Ionic bonding

RESUME

- electrostatic** type interaction between atoms, that become positively or negatively charged
- the bonding electron is **transferred**
- ionic bonds are **strong** (and thus ionic substances require high temperatures to melt) but also **brittle**, since the forces between ions are short-range and do not easily bridge cracks and fractures. This type of bond gives rise to the physical characteristics of crystals of classic mineral salts, such as table salt

Ionic solids

- their **melting and boiling point** is inversely proportional to the distance between the ions
- solid** state at room temperature
- high brittleness** (because of the electrostatic force between the similarly charged ions)
- bad electric conductors** (the charges are fixed, they don't change their place)
- their solution is good conductor
- generally they are colorless



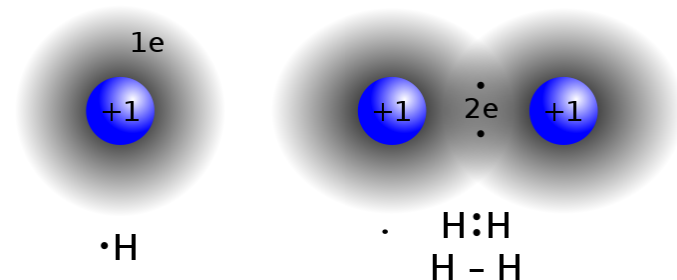
NaCl



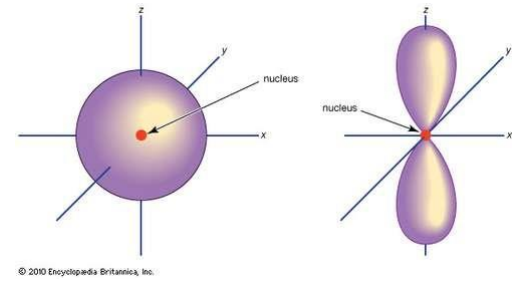
$(\text{NH}_4)_2\text{SO}_4$

Covalent bonding

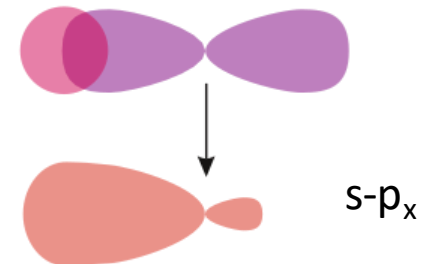
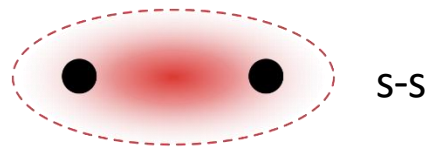
- ❑ in order to achieve a stable electron configuration an atom can **share electrons** with another atom (stable **balance of attractive and repulsive forces** between atoms)
- ❑ covalency is greatest between atoms of similar electronegativities
- ❑ covalent bonding is formed between **same elements or different elements**, but with comparable electronegativity
- ❑ delocalized electrons: electrons that take part in the covalent bonding, sharing more than two electrons



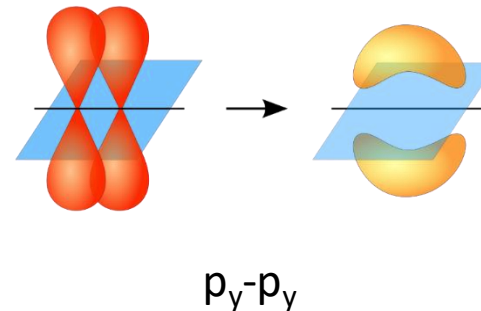
Covalent bonding



- types of covalent bonds
 - **σ -bonding**: head-on overlapping of the orbitals
 - **strong bond**
 - typical to single bonds



- **π -bonding**: parallel overlapping
- **less strong** than σ -bonding
- typical to double and triple bonds in organic materials



Covalent network solids

RESUME

- strong
- bad electric and thermal conductors
- high melting point
- non-soluble in water nor in organic-solvents



diamond



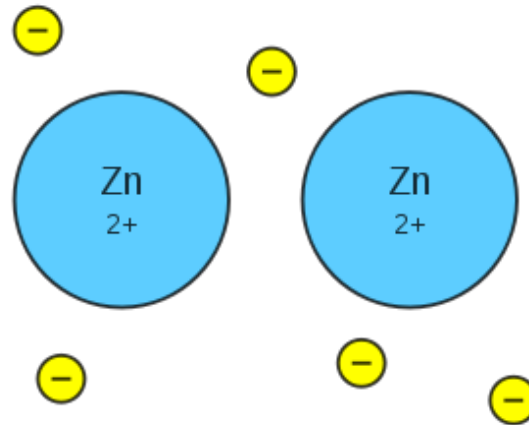
quartz



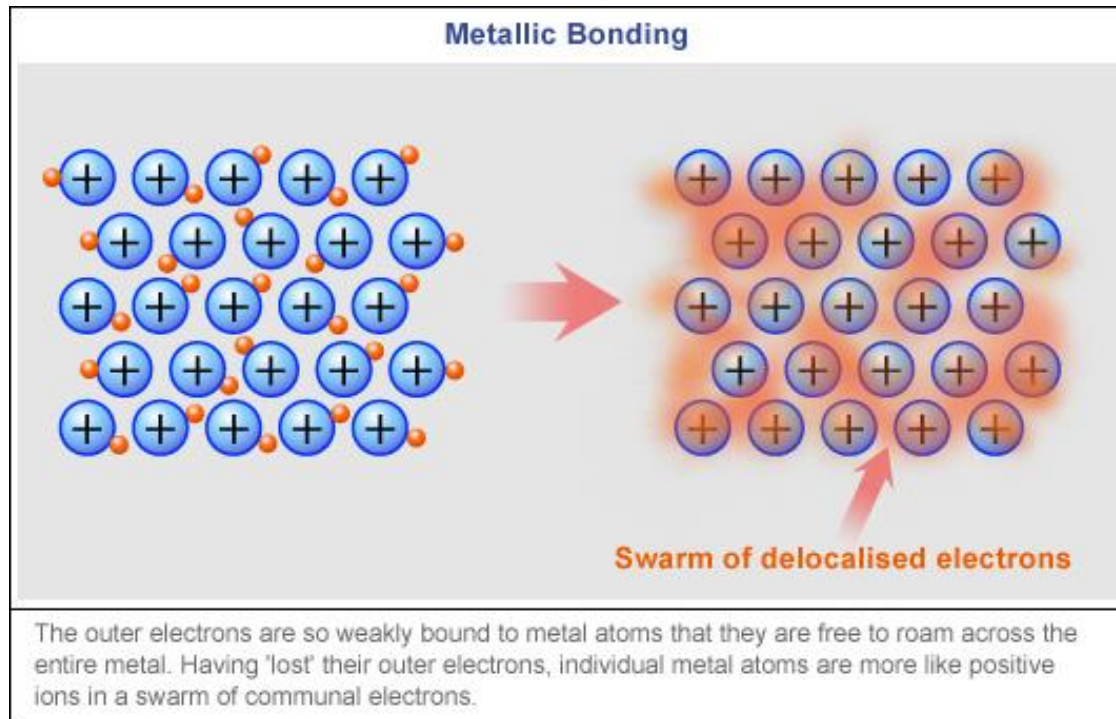
sphalerite

Metallic bonding

- ❑ metal-to-metal bonding: **electrostatic** attractive force between conduction electrons and positively charged metal ions
- ❑ conduction electrons: delocalized electron's cloud, belong „commonly” to each metallic ion



Metallic bonding

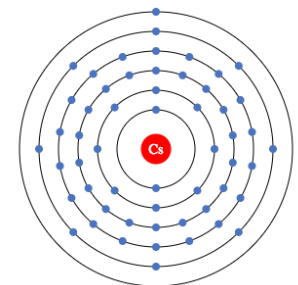


Metallic bonding

RESUME

- ❑ a crystal of a metal **represents a single molecule** over which all conduction electrons are **delocalized** in all three dimensions
- ❑ metallic bonding is mostly **non-polar**, because even in alloys there is little difference among the electronegativities
- ❑ the delocalization is most pronounced for s- and p-electrons
- ❑ delocalization for caesium it is so strong that the electrons are virtually free from the caesium atoms to form a gas constrained only by the surface of the metal

55: Cesium



[Xe] 6s1

[2, 8, 18, 18, 8, 1]

Metallic solids

- metallic bonding, **free electrons**
- good electric and thermal conductors**
- moderately elastic, those with **fcc lattice are well workable**, those with **bcc lattice can be easily cut**, the **hexagonal lattice metals are more rigid**
- the **melting point increases with the strength of the metallic bonding**
- soluble only in their own solvents (metallic solutions)

silver



iron

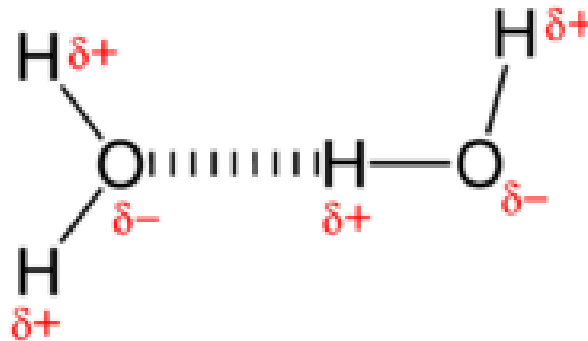


magnesium



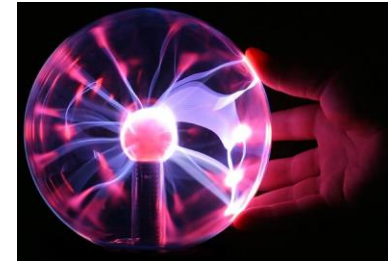
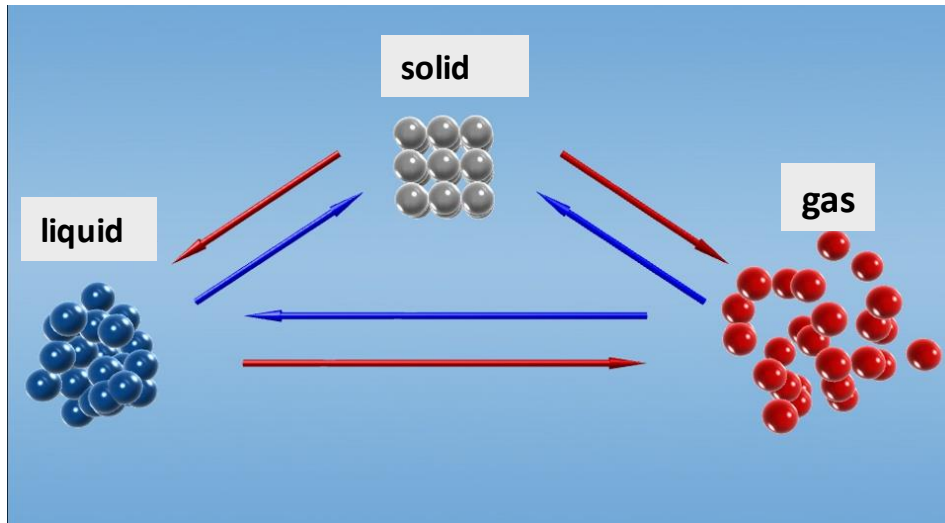
Weak bonding

- intermolecular bonding: weaker than the covalent and ionic bonding
- for example: **hydrogen bond**: attraction between the lone pair of an electronegative atom and a H atom (bonded to N, O, F)



From the atomic structure to the macro structure

Ordered structure – disordered structure



plasma

Solid state materials

General characteristics

- Solids are characterized by
 - structural rigidity**
 - resistance to changes of shape or volume**
 - the atoms of a solid are **tightly bound** to each other in a regular (crystalline) or irregular (amorphous) way
- Material science** is concerned with the physical and chemical characteristics of the (solid) materials
- Main classes of the solid state materials:
 - amorphous
 - crystalline

Classes of solid state materials

Crystalline structure

Amorphous structure

Classes of solid state materials

Crystalline structure

- long range atomic order
- regular structure
- symmetrical crystal lattice
- definite physical characteristics
- good conducting properties
- chemical and physical characteristics depending on orientation
- single crystals or polycrystals

Amorphous structure

- short range atomic order
- non-regular structure
- similar to high-viscosity liquid structure (no symmetry)
- without definite melting point
- good insulating characteristics
- no orientation
- high strength
- good corrosion and abrasion resistance

Crystalline materials

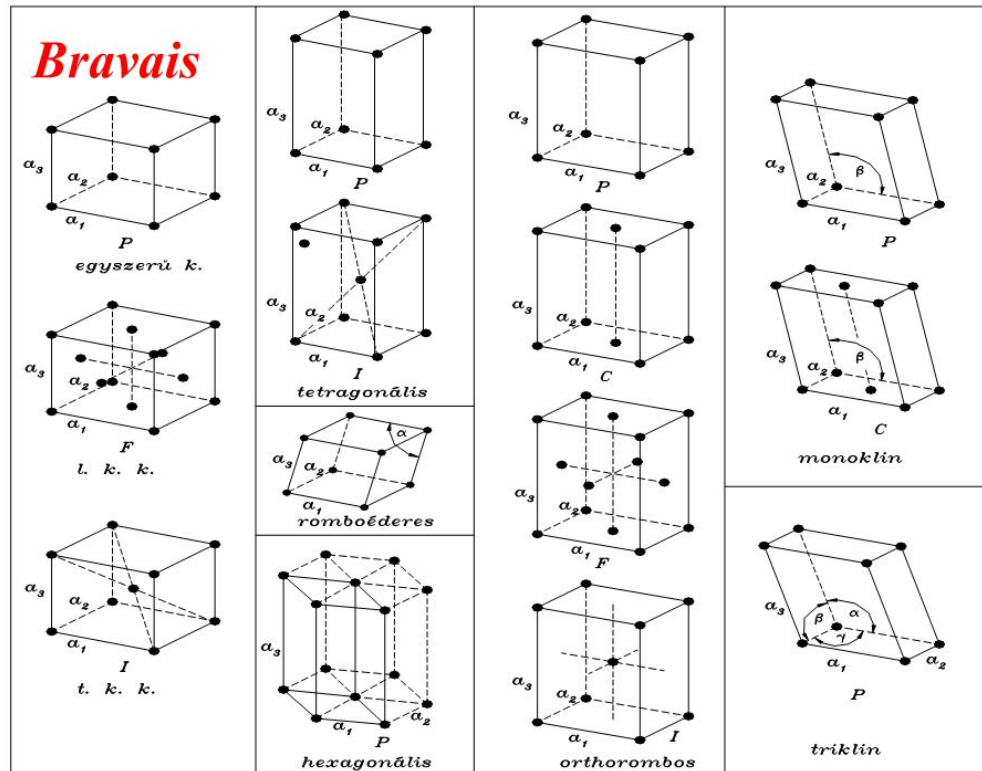
Bravais lattice cells



quartz



halite



Amorphous materials



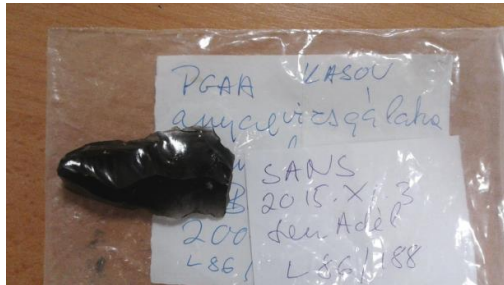
beeswax



bitumen



glass

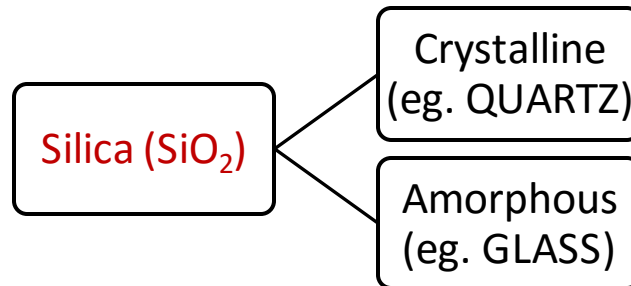


obsidian

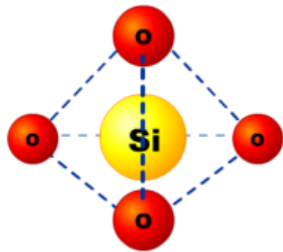


amber

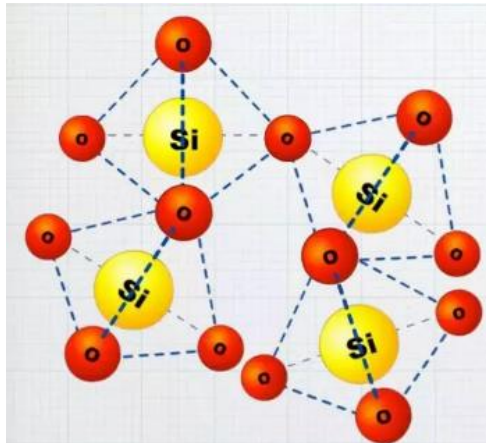
Amorphous structure



Basic building block of both:
silicon tetrahedra $[\text{SiO}_4]^{4-}$

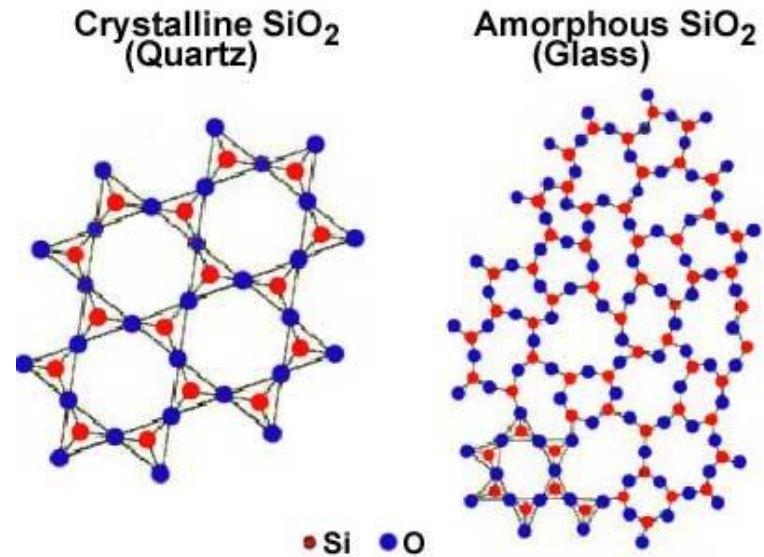
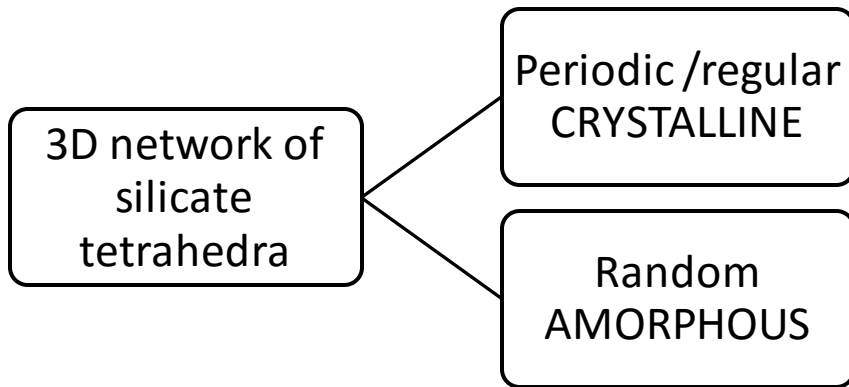


3D network of corner sharing tetrahedra



$4 \times \frac{1}{2} \text{O} = 2$
oxygen/tetrahedra

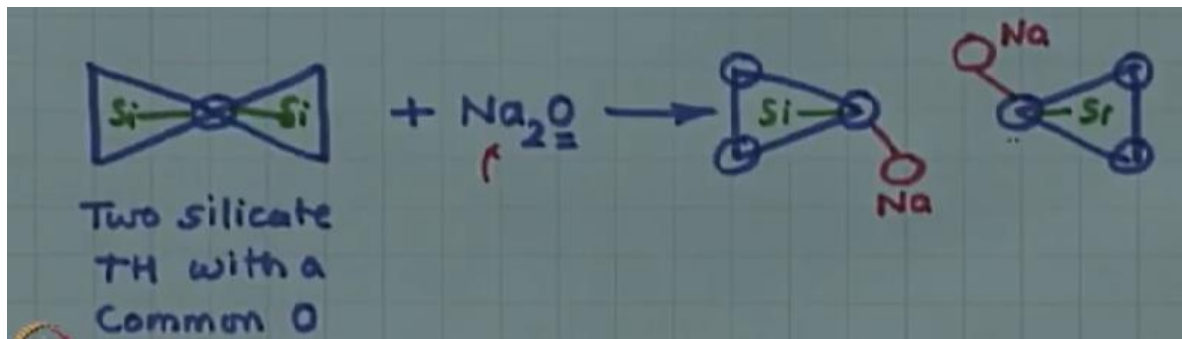
Amorphous structure



Amorphous structure

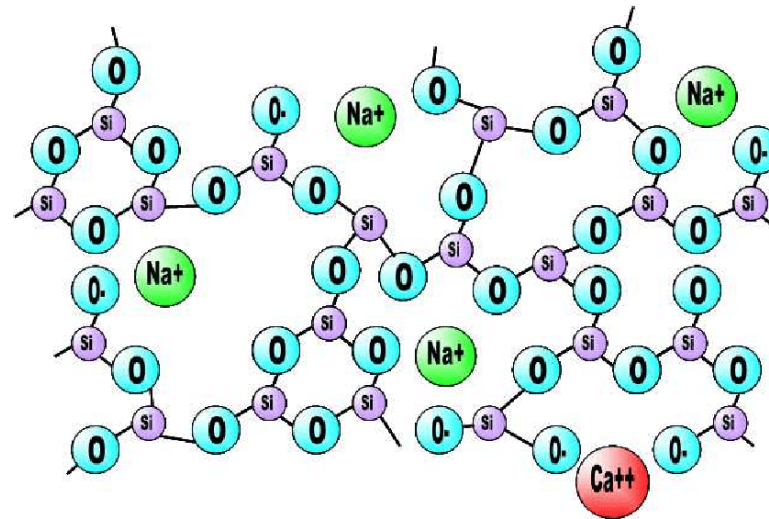
- Si – O bonds are strong primary bonds
- strong glass – fused silica glass
- high melting point

- reduce the melting point: ADDITIVES
 - eg. soda-lime glass: Na_2O is added (network modifier)



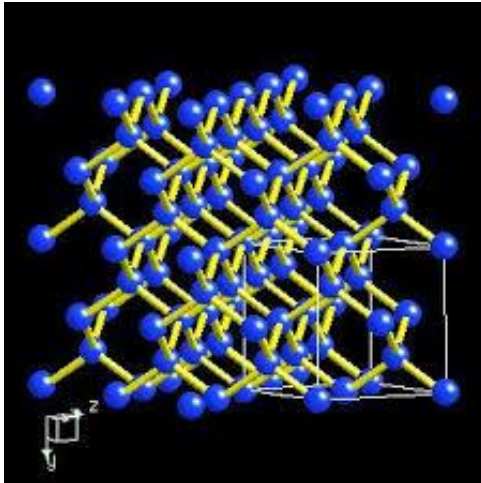
Amorphous structure

Soda-lime glass (sodium carbonate, lime, magnesium-oxide, aluminum-oxide)



Crystalline structure

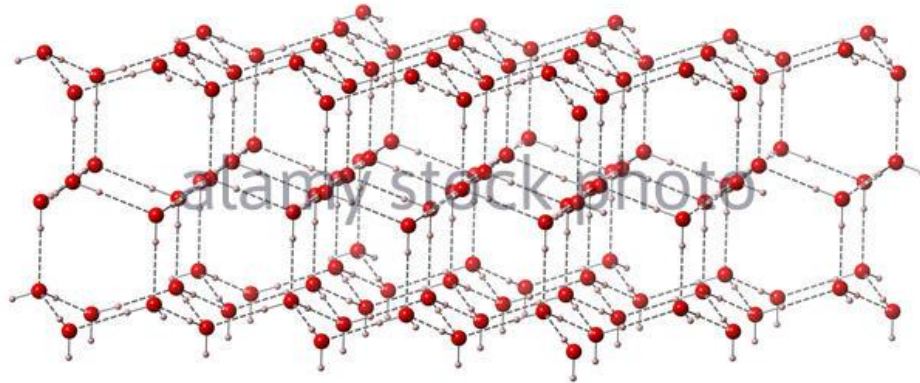
- ❑ **ordered arrangement** of atoms, ions, molecules in 3D
- ❑ smallest repeating group is called **unit cell**
- ❑ entire 3D structure is called **crystalline lattice**, formed by the **translation** of the unit cell



silica crystal
structure

Crystalline structure

- ❑ **ordered arrangement** of atoms, ions, molecules in 3D
- ❑ smallest repeating group is called **unit cell**
- ❑ entire 3D structure is called **crystalline lattice**, formed by the **translation** of the unit cell



ice 3D crystal
structure

Crystalline structure

- ❑ Discrete points are **atoms, ions, or molecules** of solid matter and define a ***crystalline arrangement***
- ❑ A **crystal** is made up of a periodic arrangement of one or more atoms (the *basis*) repeated at each lattice point
- ❑ In crystallography the crystalline type materials are ordered into groups according to the so called **Bravais lattice**
- ❑ **Bravais lattice:** is an infinite array of discrete points in three dimensional space generated by a set of translation. After such a translation the lattice becomes identical to itself Discrete points are **atoms, ions, or molecules** of solid matter and define a ***crystalline arrangement***

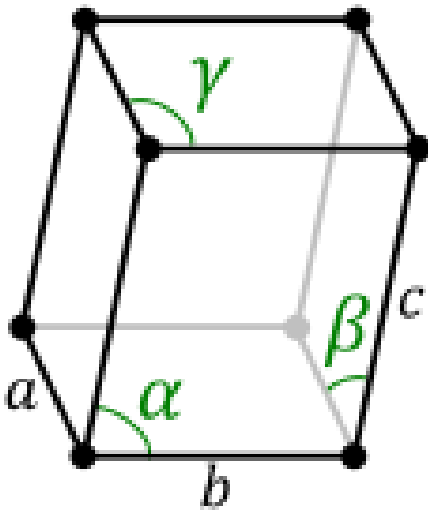
Bravais lattices

Crystal family	Lattice system	14 Bravais lattices				
		Primitive	Base-centered	Body-centered	Face-centered	Rhombohedrally-centered
triclinic						
		$\beta \neq 90^\circ$ $a \neq c$	$\beta \neq 90^\circ$ $a \neq c$			
monoclinic						
		$a \neq b \neq c$	$a \neq b \neq c$			
orthorhombic						
		$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$	
tetragonal						
		$a \neq c$		$a \neq c$		
hexagonal	rhombohedral					
	hexagonal					
cubic						



Triclinic

- a, b, c and α , β , γ

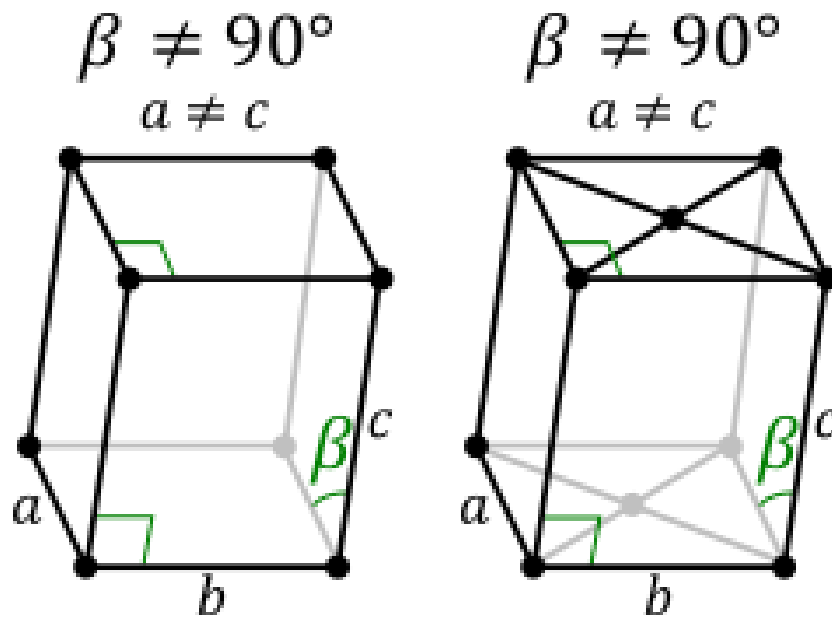


Microcline
(Argentina)

Monoclinic

Primitive and base centred

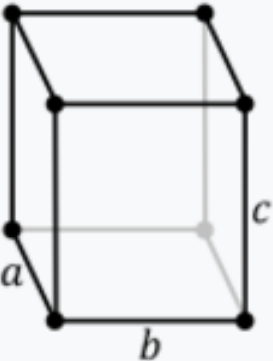
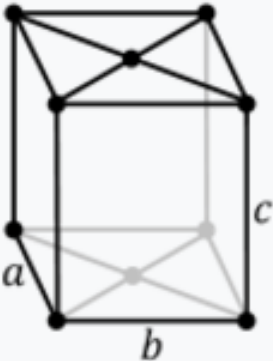
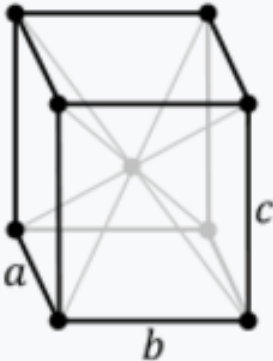
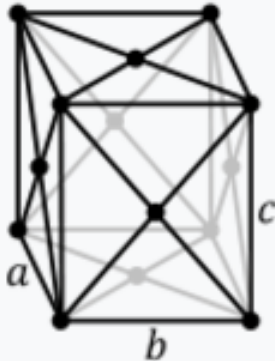
a, b, c and $90, \beta, 90$



Orthoclase
(Brazil)

Orthorhombic

a, b, c and $90, 90, 90$

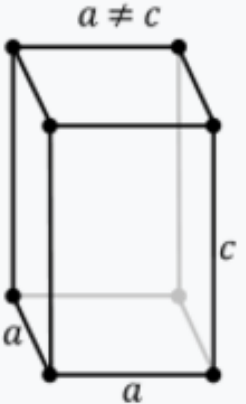
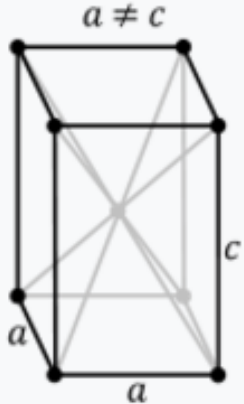
Primitive orthorhombic	Base-centered orthorhombic	Body-centered orthorhombic	Face-centered orthorhombic
$a \neq b \neq c$ 	$a \neq b \neq c$ 	$a \neq b \neq c$ 	$a \neq b \neq c$ 



Olivine – face-centred

Tetragonal

$a, a, c, 90, 90, 90$

Bravais lattice	Primitive tetragonal	Body-centered tetragonal
Unit cell		



Calcopyrite body-centred

Hexagonal

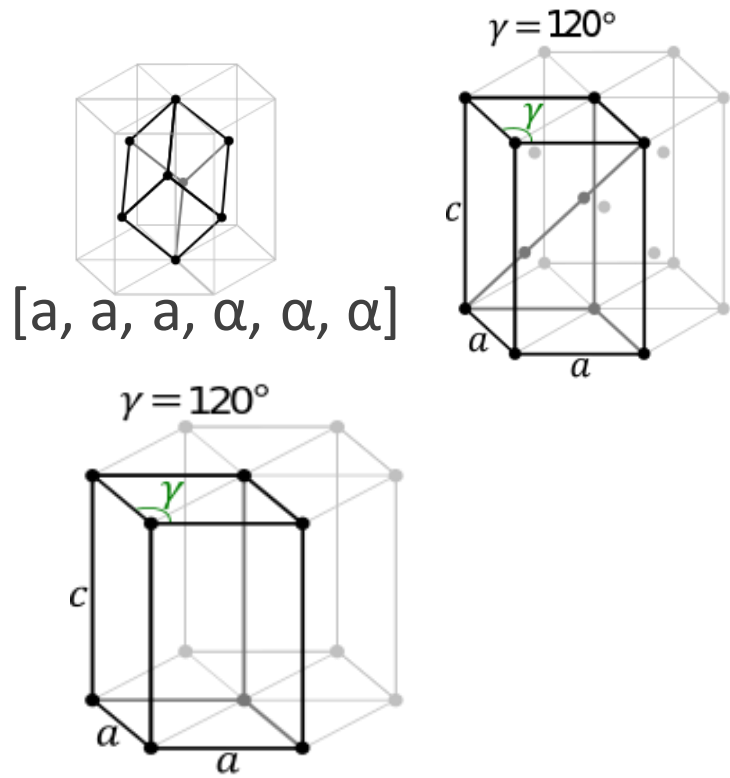
$a, a, c, 90, 90, 120$

quartz

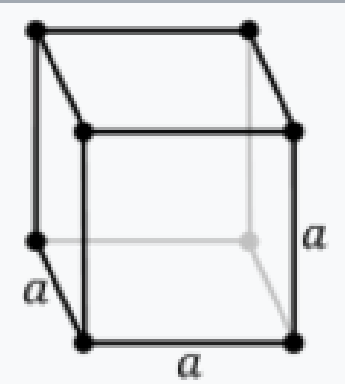
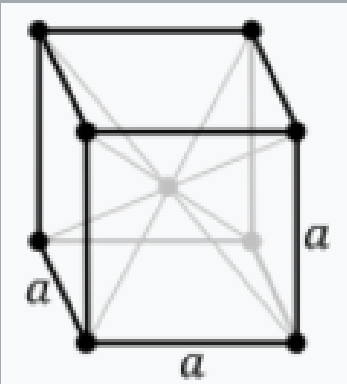
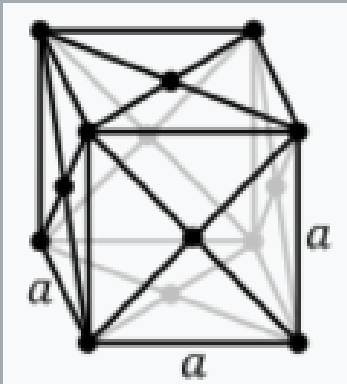


dolomite

hexagonal	rhombohedral
	hexagonal



Cubic

Bravais lattice	Primitive cubic	Body-centered cubic	Face-centered cubic
Unit cell			



pyrite

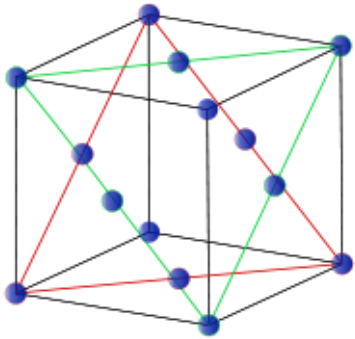


CsCl

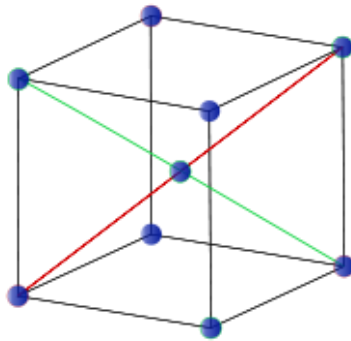


ZnS

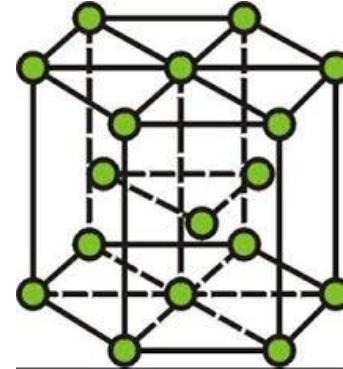
Covalent metallic bonding



silver



iron



magnesium



Allotropy

□ property of an element to exist in two or more forms, in the same physical state

□ Carbon

a. diamond

b. graphite

c. lonsdaleite

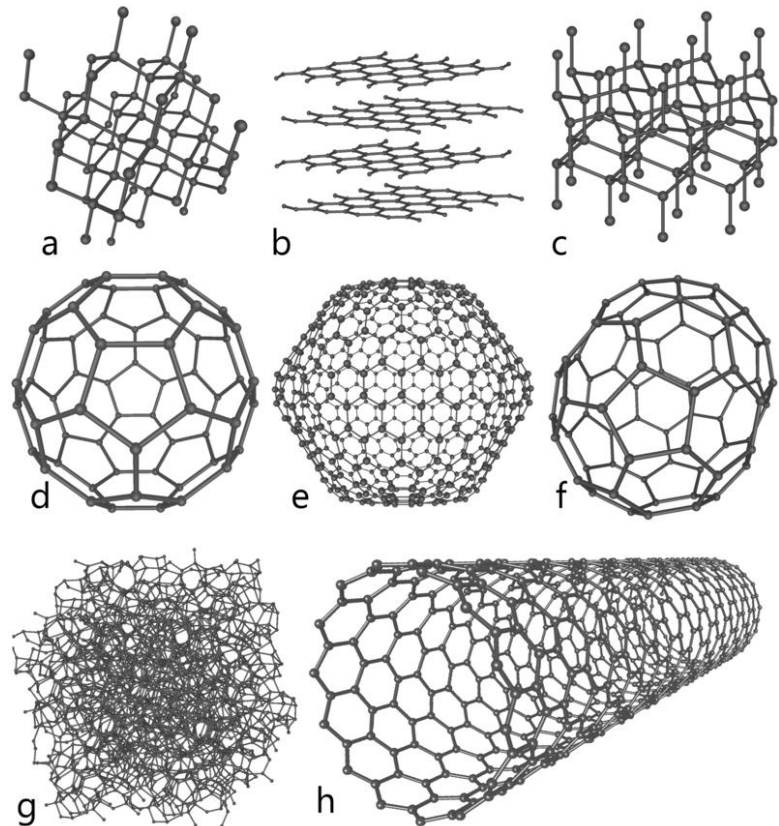
d. C₆₀ (Buckminster fullerene)

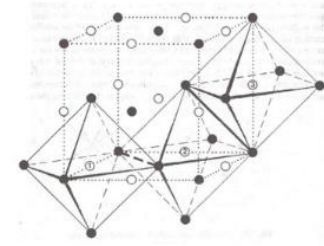
e. C₅₄₀ (Fullerite)

f. C₇₀

g. amorphous carbon

h. nanotube





Diamond

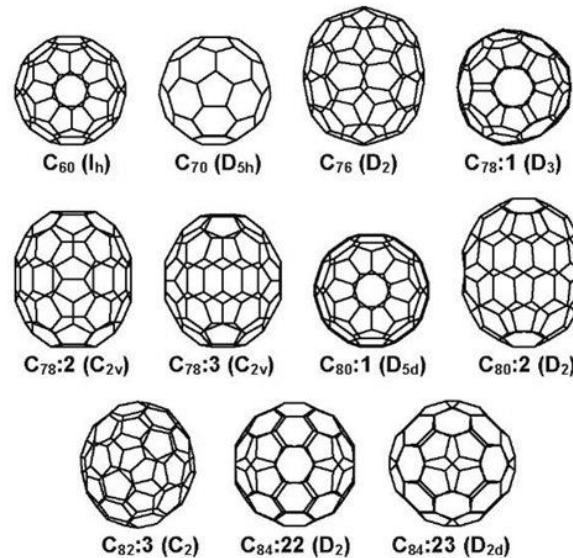
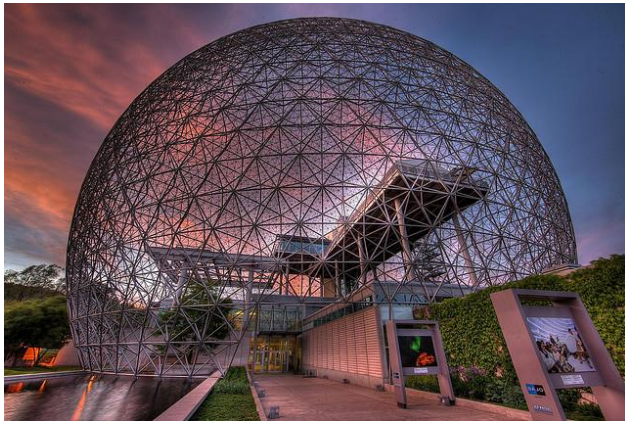
- Cubic
- Mohs hardness: **10**
- breaks easily** along the octahedral planed
- Density: 3,52 g/cm³
- Scatters and disperses the light
- At 720–1000 °C, in presence of oxigen burns to CO₂
- Resistant to chemicals, only the solution of the K₂Cr₂O₇ H₂SO₄ or the K₂CO₃ melt reacts with it



Buckminster fullerene

BUCKMINSTER FULLER – architect

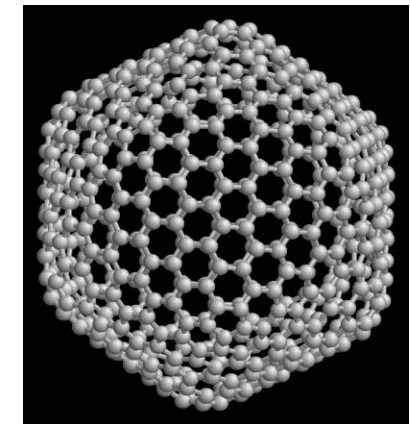
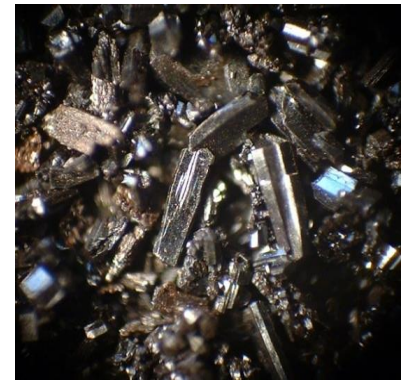
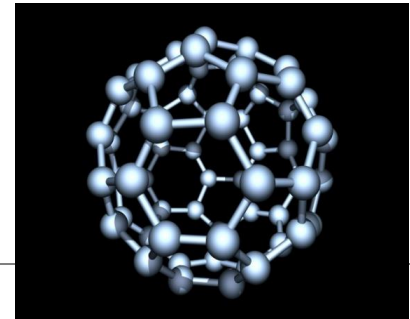
Fullerenes were discovered by Harold Kroto (University of Sussex), Robert Curl and Richard Smalley (Rice University) – 1996 – Nobel prize)

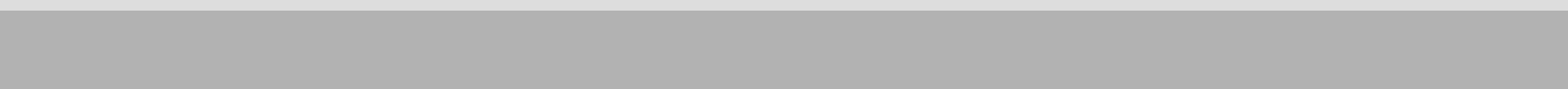


Fullerenes

Discovered in 1985

- formed by pentagons and hexagons
- C60: yellowish, C70 brown
- face-centred cubic crystal unit cells
- different hardness
- sensitive to water
- biologically active
- many functionalized form
- production: in laboratories and in industry with different methods





From the atomic structure to the macro characteristics

