Nem-kovalens kölcsönhatások

Intermolekuláris
Intermolekuláris

Fizikai tulajdonságok, pl. forráspont, oldhatóság, stb.
Biológia: makromolekulák alakja; kölcsönhatások, gyógyszerhatás, stb.

Típusai:

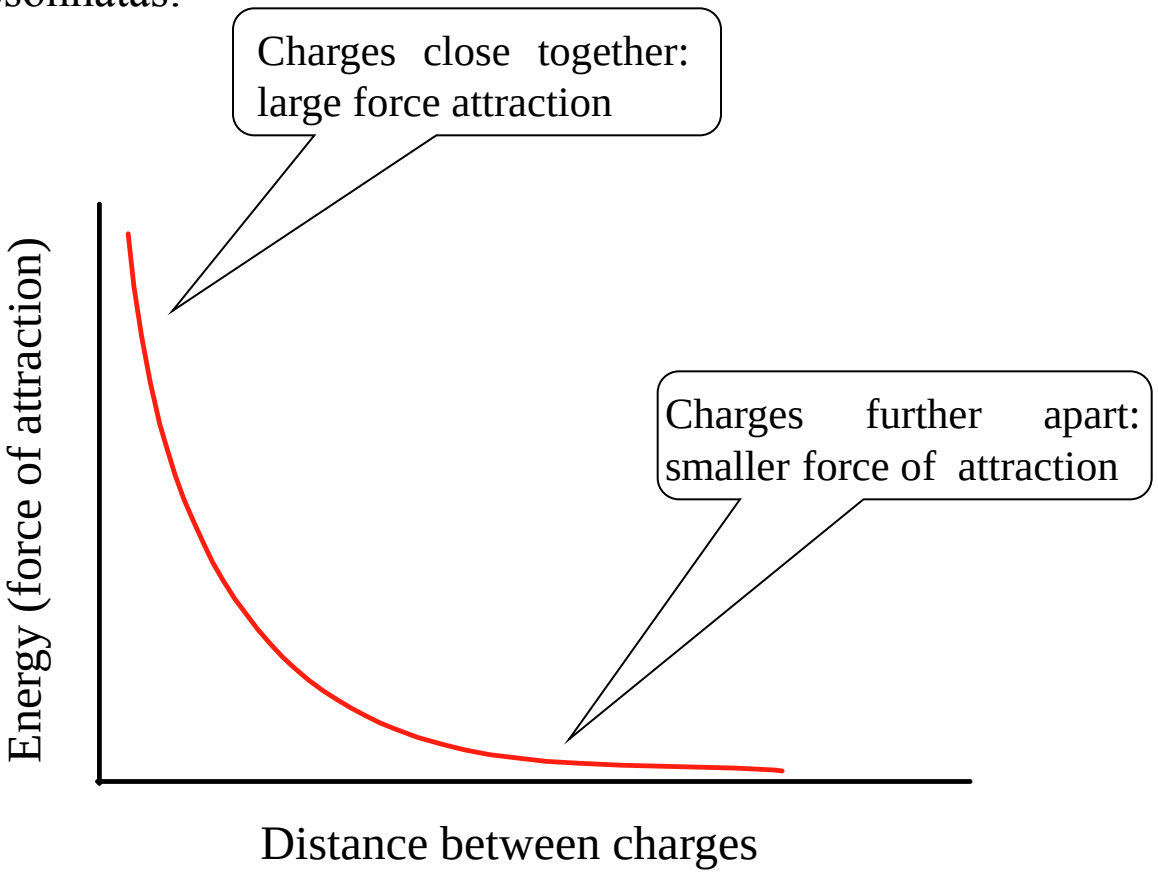
i) diszperziós kölcsönhatás
ii) állandó dipólusok közötti (dipoláris) kölcsönhatás
iii) hidrogén-híd
iv) ionos kölcsönhatás
v) hidrofób kölcsönhatás

i-iv: elektrosztatikus jellegű

A comparison of the typical energies of a range of physical interactions

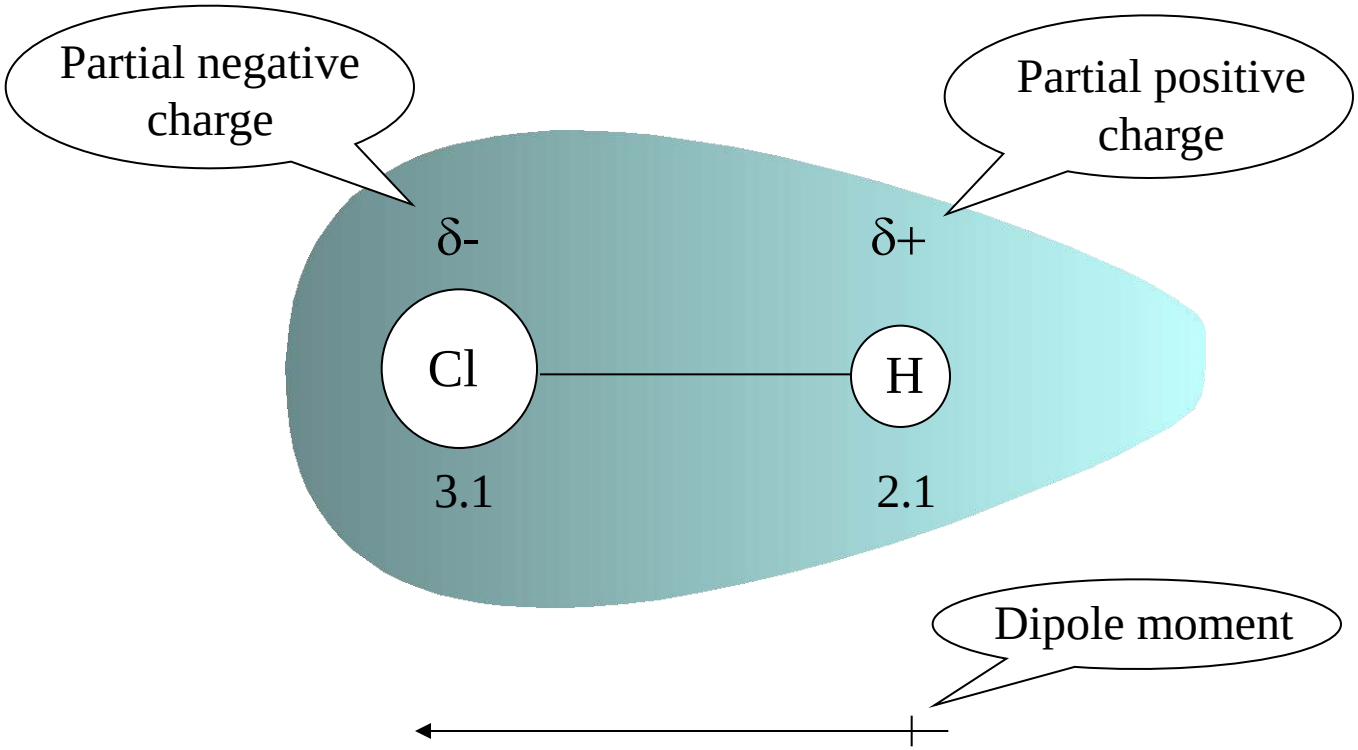
Interaction type	**Typical energy (kJ mol^{-1})**
Covalent bond	150-1000
Ionic bond	250
Dispersion force	2
Dipole-dipole interaction	2
Hydrogen bond	20

elektrosztatikus kölcsönhatás:
Coulomb potenciál



The force of attraction that exists between two opposite charges varies as the distance between the charges increases. The force of attraction decreases rapidly as the distance between the charges increases.

Kötés polarizáció: poláris kötés, permanens dipólus

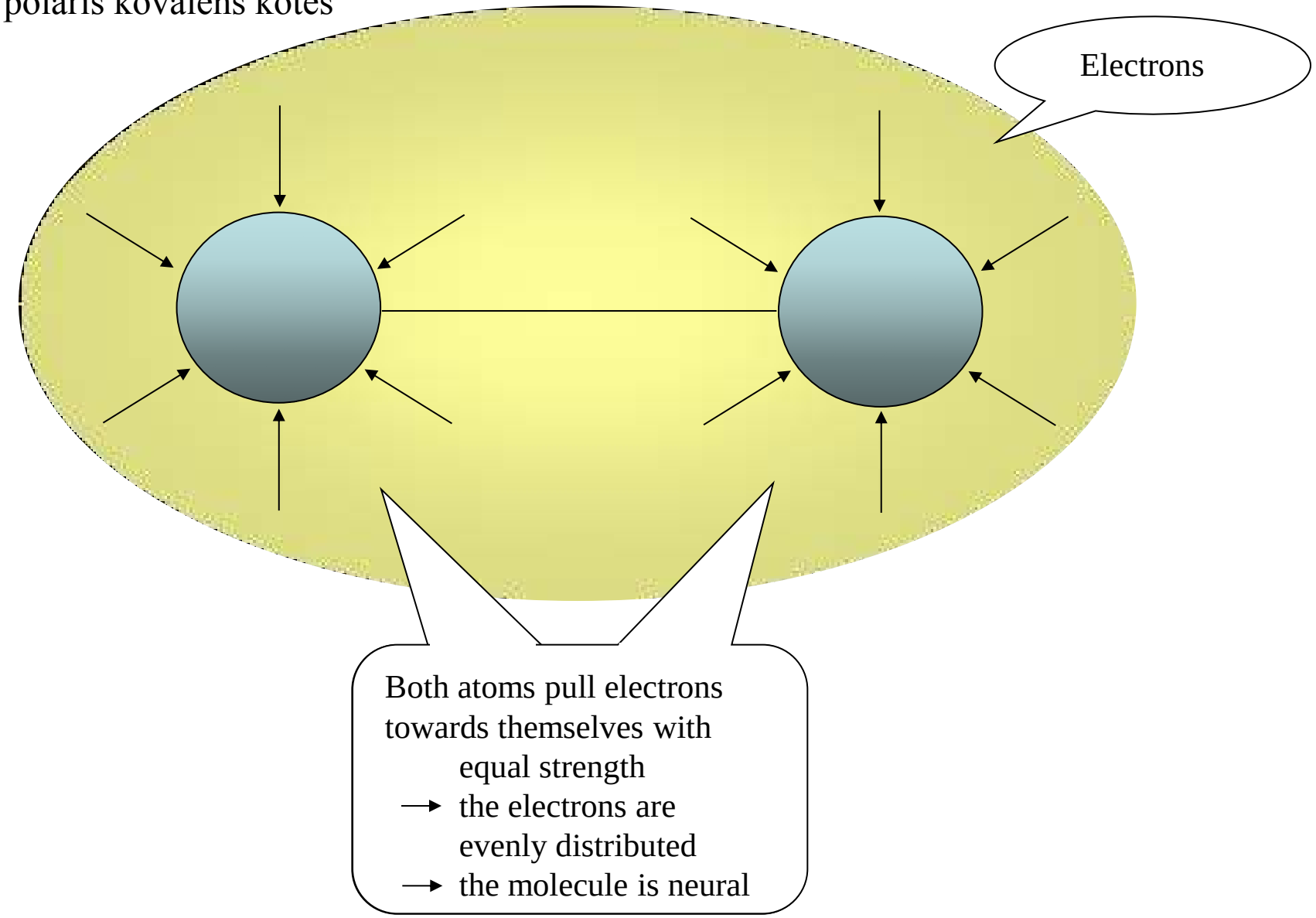


The relaive distribution of electrons in a molecule of hydrogen chloride, HCl.
The distribution of electrons is skewed towards the highly electronegative chlorine atom.

Nem-poláris kovalens kötés

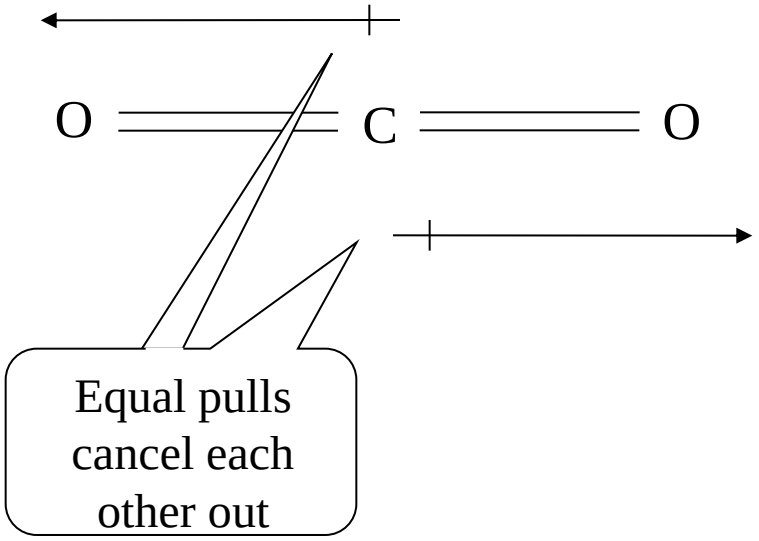
Poláris kötés nem-poláris molekulában

Nem poláris kovalens kötés



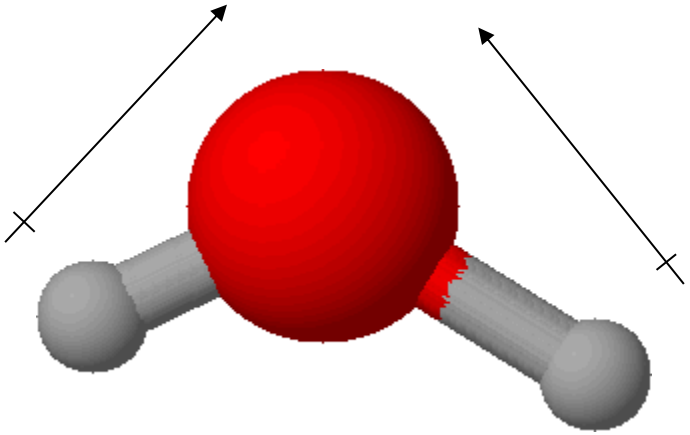
When two atoms of the same element are joined by covalent bond, electrons are shared equally between the two atoms. The resulting molecule is non-polar.

Nem-poláris molekula



A molecule of carbon dioxide features two polarized bonds. However, the two bonds exert equal ‘pulls’ in opposite directions and cancel each other out. So carbon dioxide is a non-polar molcule.

Poláris molekula



A water molecule features two polarized bonds. Water is a non-symmetrical molecule: the dipole moments do not ‘pull’ in equal and opposite directions, so they do not cancel each other out. Therefore, water is a polar molecule.

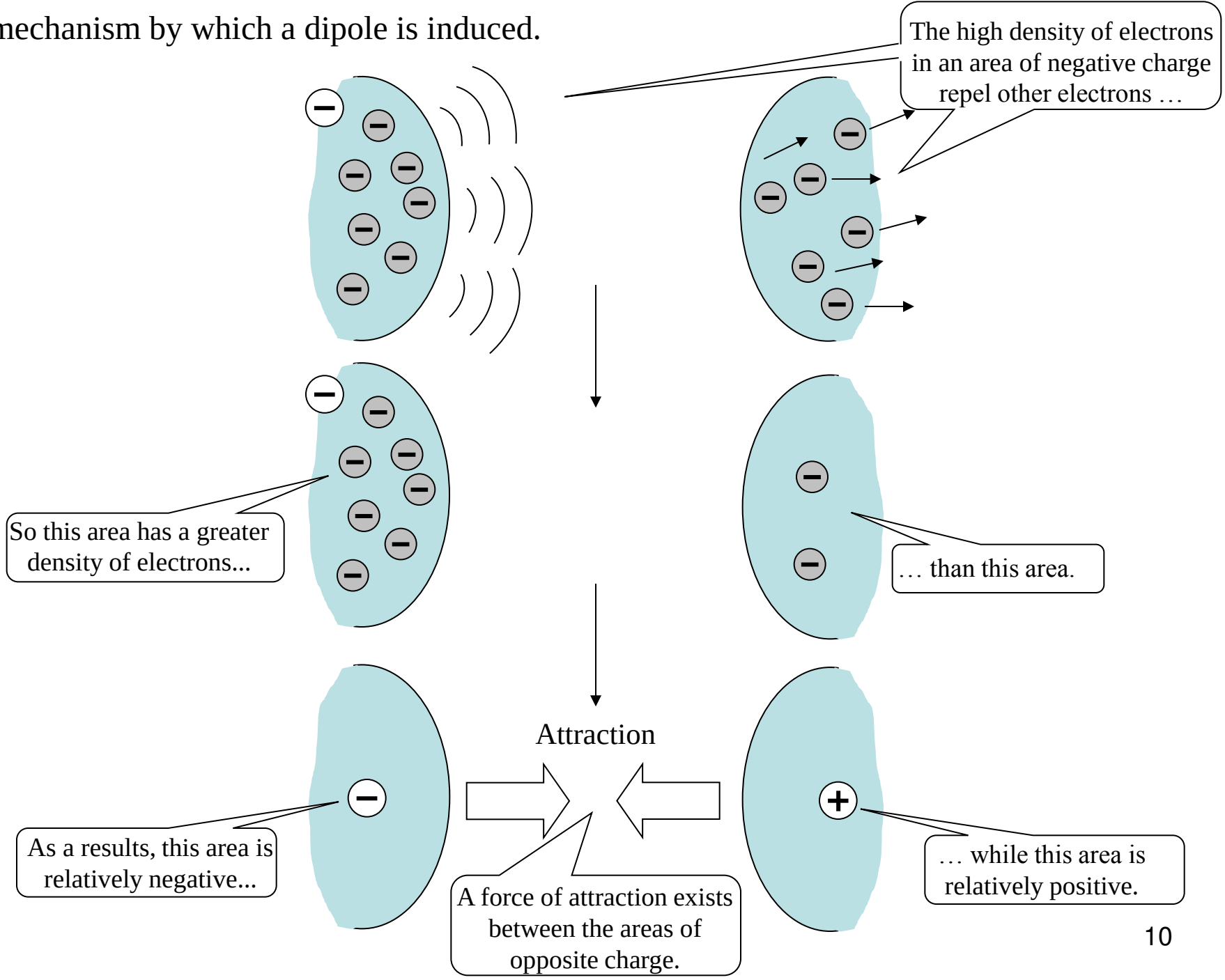
Diszperziós kölcsönhatások

i) átmenetileg lépnek fel (10^{-16} s)
ii) nagyon gyenge kölcsönhatások
iii) nagyon rövid a hatótávolságuk

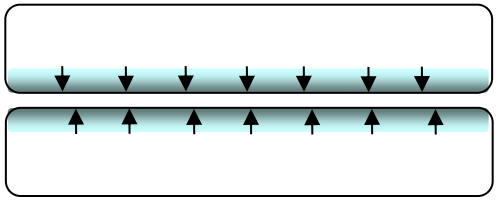
- a molekulaalak és méret befolyásolja

- különösen fontosak biológiai rendszerekben

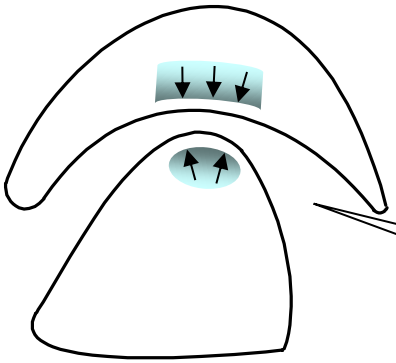
The mechanism by which a dipole is induced.



Planar



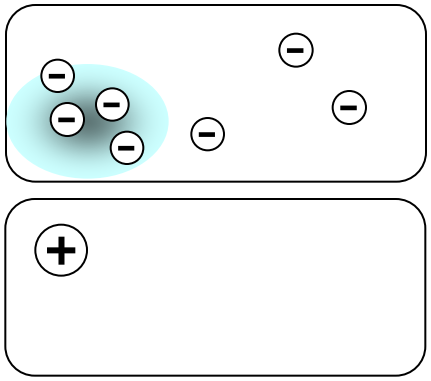
Many points of close association
→ stronger dispersion forces



Irregular

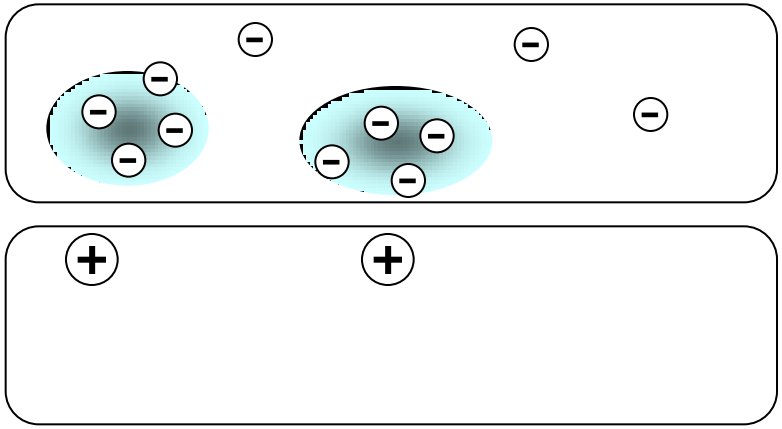
Few points of close association
→ weaker dispersion forces

Planar molecules are able to associate closely with one another, allowing extensive dispersion forces to occur. By contrast, irregularly shaped molecules cannot associate so closely, so less extensive dispersion forces can occur.



Small molecules

→ few electrons
→ limited opportunities
for induced dipoles

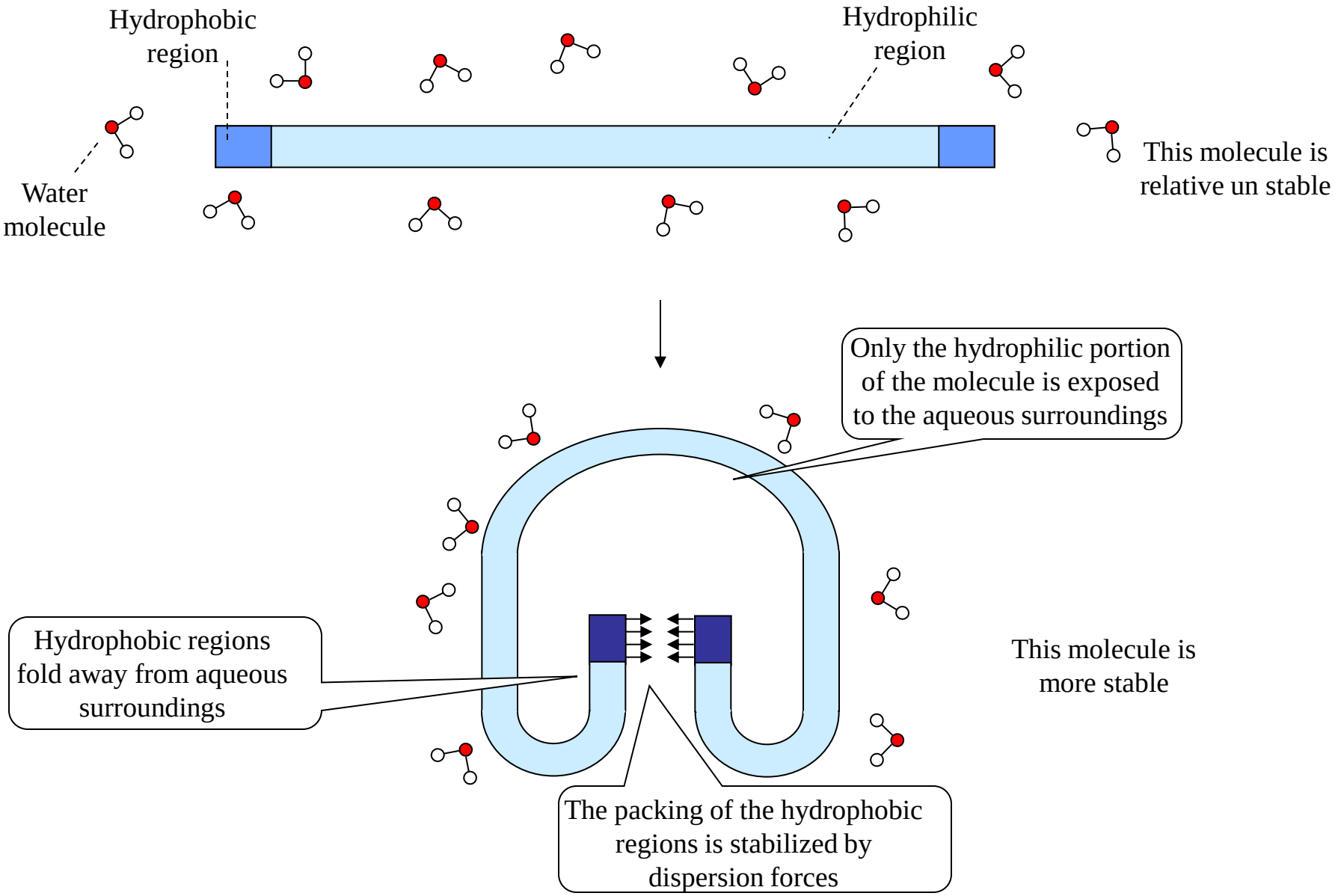


Larger molecules

→ more electrons
→ more opportunities
for induced dipoles

Large molecules, with a large number of electrons and more opportunities for induced dipoles to arise, experience greater dispersion forces than smaller molecules, which possess fewer electrons and experience fewer induced dipoles.

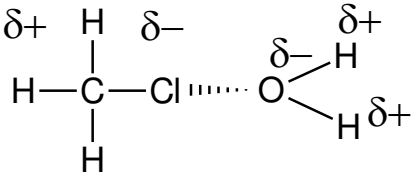
Hidrofób és diszperziós kölcsönhatások biológiai rendszerekben



The folding of a polypeptide possessing hydrophobic and hydrophilic portions. The darker hydrophobic portions fold away from the aqueous surroundings; this arrangement is stabilized by dispersion forces which operate between the tightly packed hydrophobic portions.

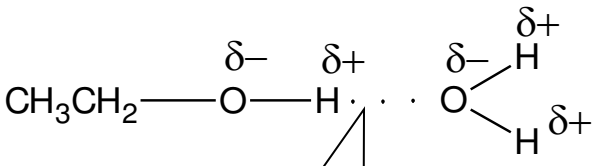
Miért hidrofób jellegűek a nem-poláris molekulák?

Chloromethane: polar

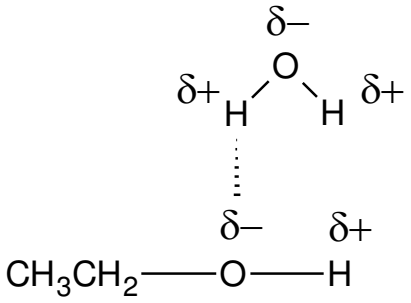


Dipolar interaction

Ethanol: polar

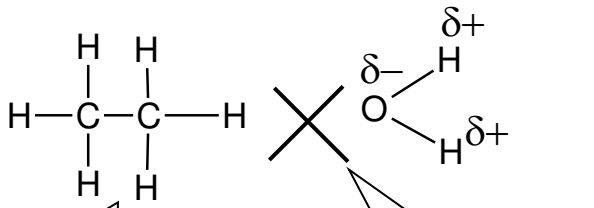


or



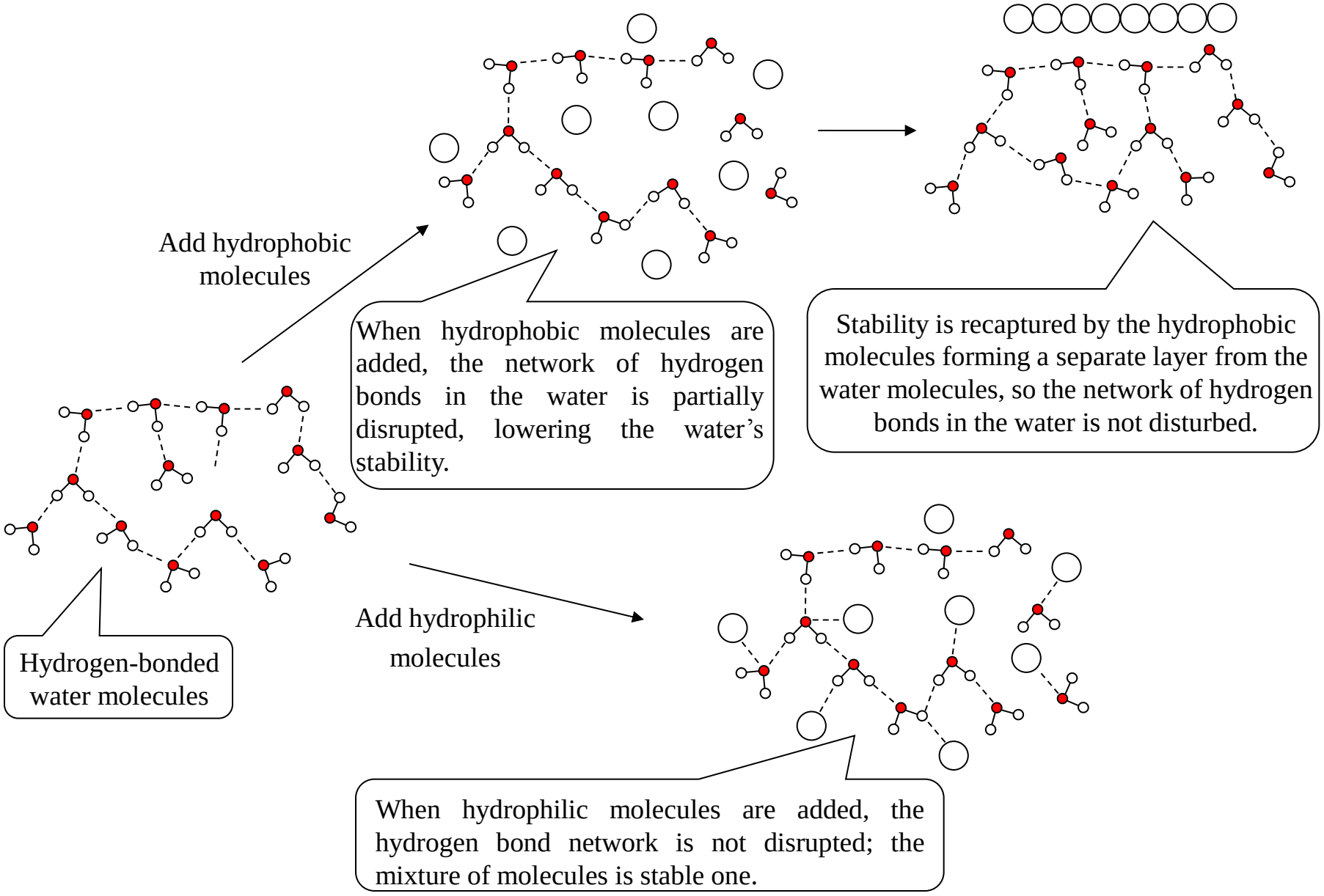
Dipolar interaction

Ethane: non-polar



Can only participate in dispersion forces; inadequate for interaction with water

For a molecule to be water-solube it must be able to participate in dipolar interactions or hydrogen bonds with water. Polar molecules can participate in dipolar interactions (and, in some cases, hydrogen bonds) and so are water-soluble: they are hydrophilic. By contrast, non-polar molecules cannot participate in dipolar interactions or hydrogen bonds, and so are not water-soluble; they are hydrophobic.



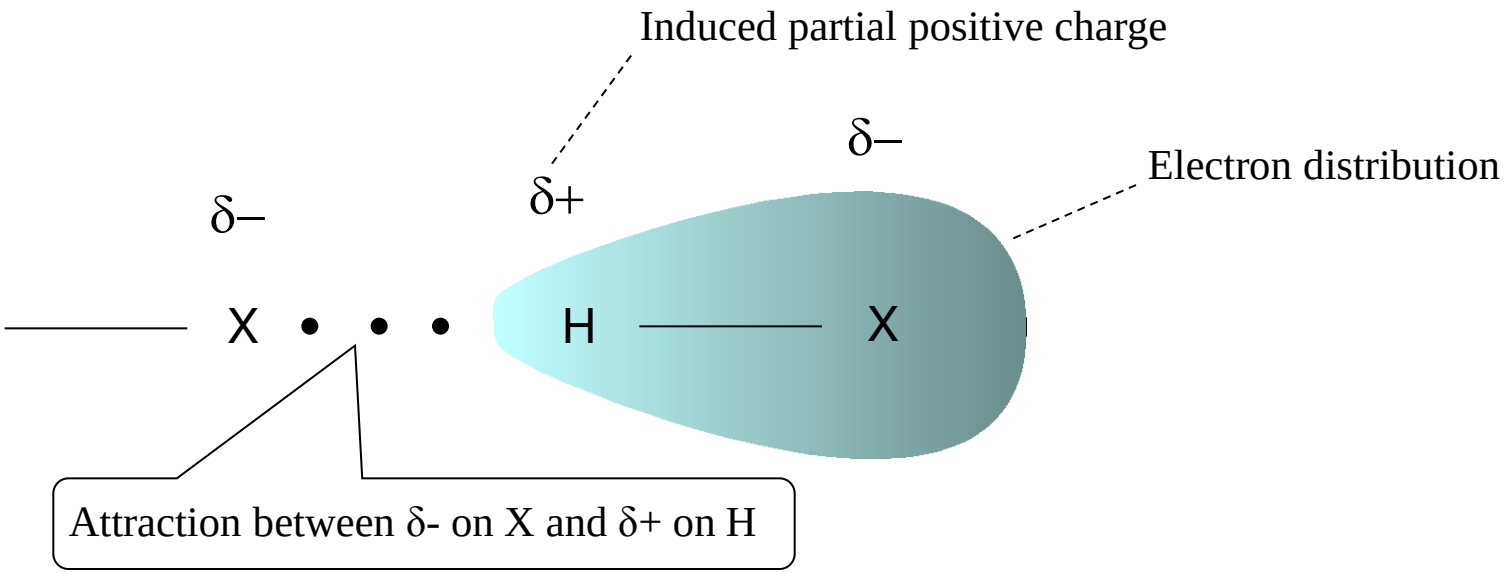
Hydrophobic molecules disrupt the network of hydrogen bonds that exist in water. Consequently hydrophobic molecules partition to form a separate layer (just like oil forms a separate layer which floats on water). Hydrophilic molecules can integrate into a network of hydrogen bonds, and so can mix fully with water.

A dipoláris kölcsönhatások állandó dipólusok között hosszu élettartamúak!

Hidrogén kötés

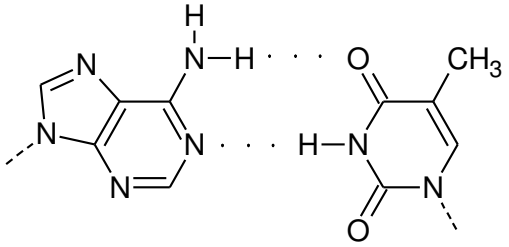
akceptor: oxigén, fluor, nitrogén magános elektronpár
donor: H-fluor, H-oxigén, H-nitrogén

Jelentősége:
biológiai rendszerekben (pl. fehérjeszerkezet; nukletid bázispárok)
oldhatóság
stb.

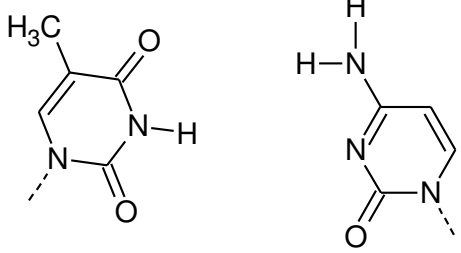


X must be O, N, or F

The formation of a hydrogen bond. A hydrogen bond forms between an electronegative atom (O, N, or F), and a hydrogen atom which is itself bonded to an atom of O, N, or F.

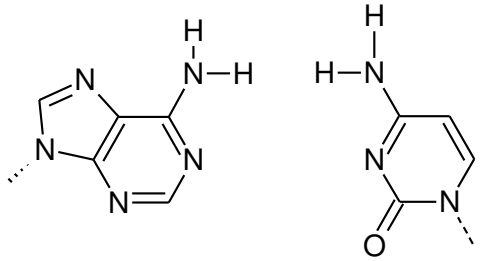


Adenine Thymine ✓



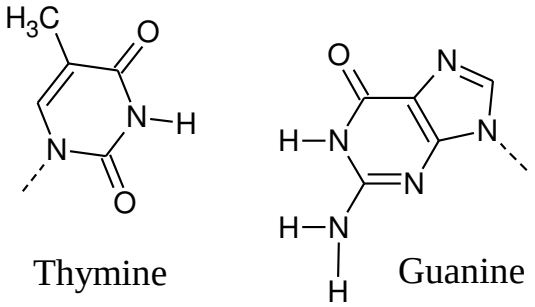
Thymine Cytosine X

Two pyrimidines together are too small to enable complementary strands to form a double helix



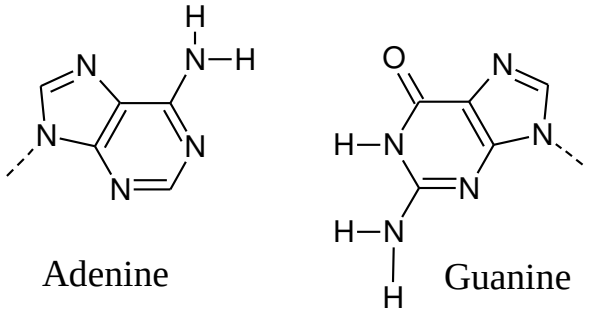
Adenine Cytosine X

Cannot form adequate hydrogen bonds for stable interaction



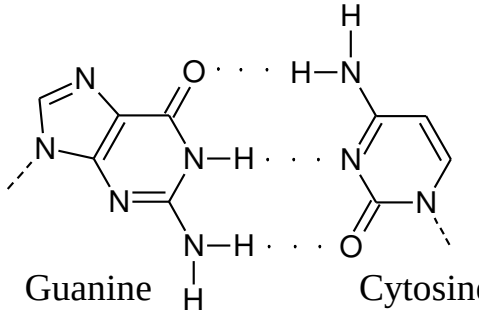
Thymine Guanine X

Cannot form adequate hydrogen bonds for stable interaction



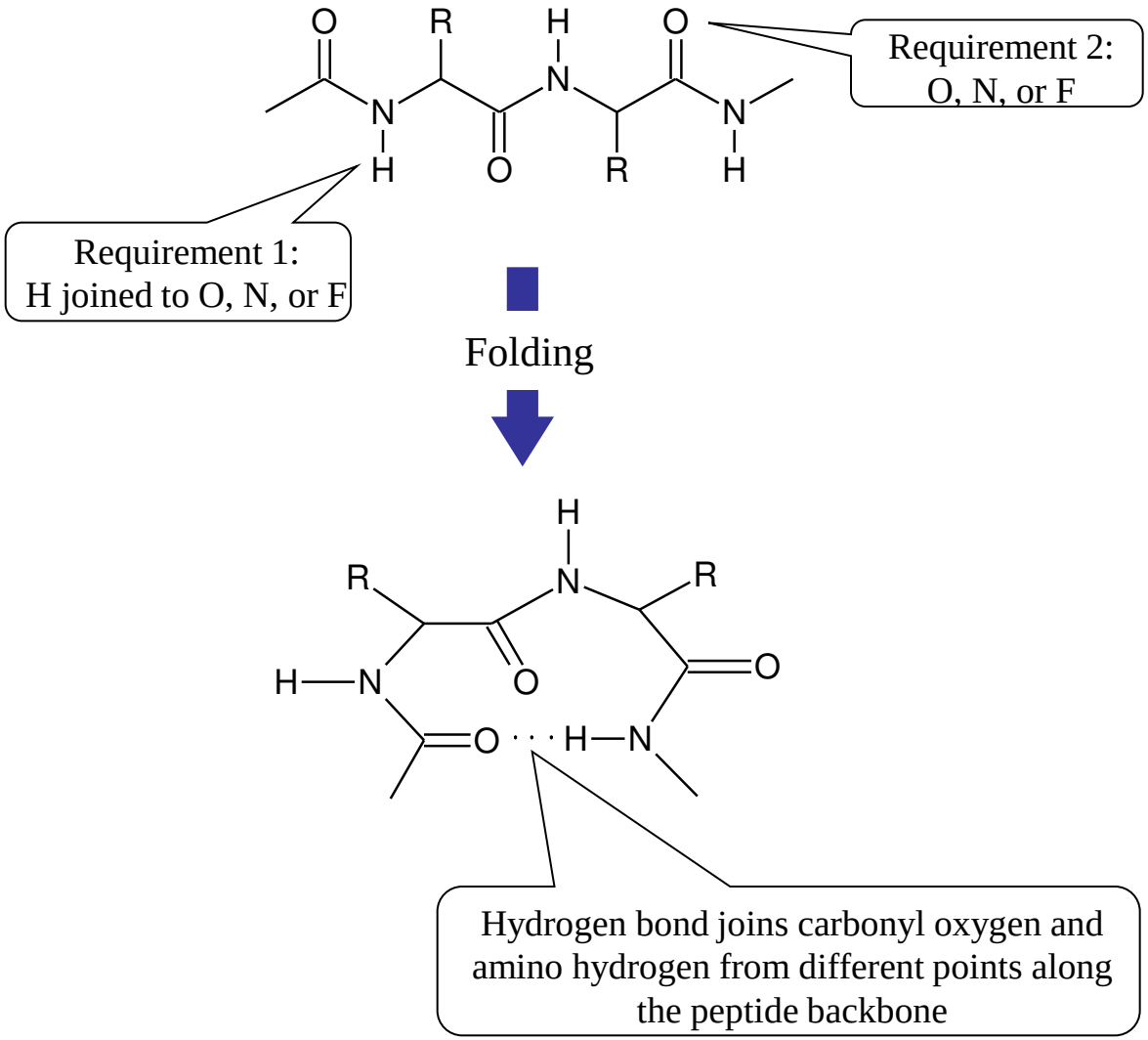
Adenine Guanine X

Two purines together are too bulky to enable complementary strands to form a double helix

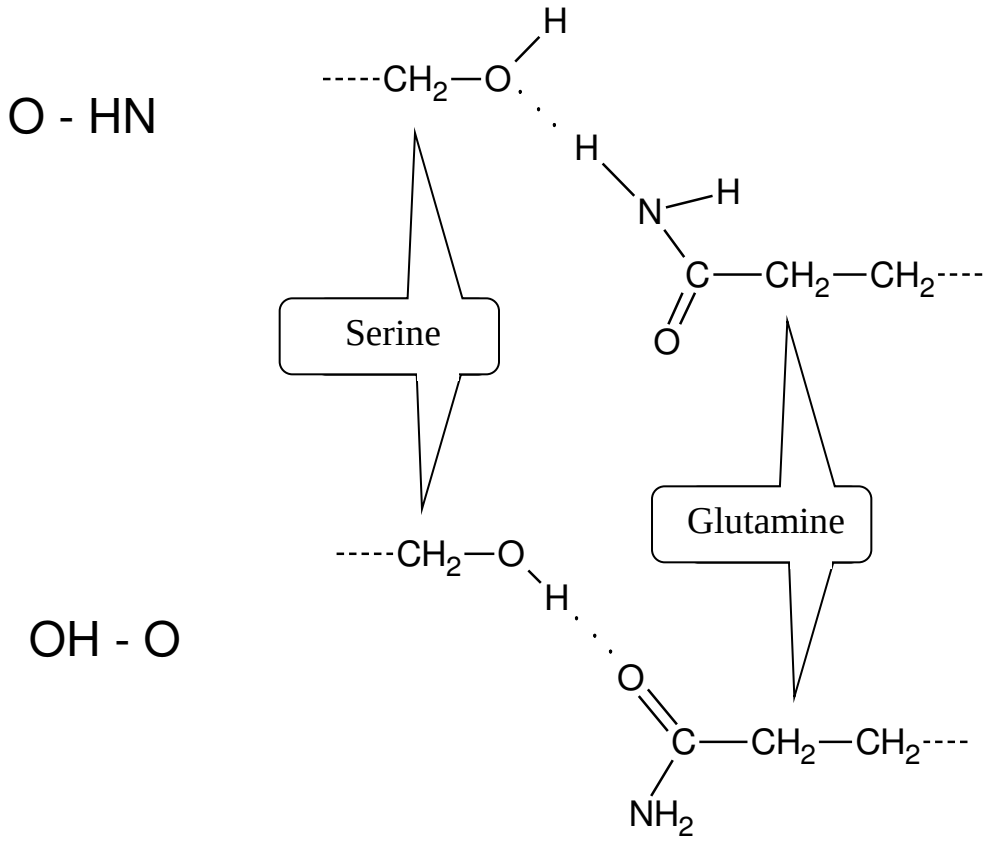


Guanine Cytosine ✓

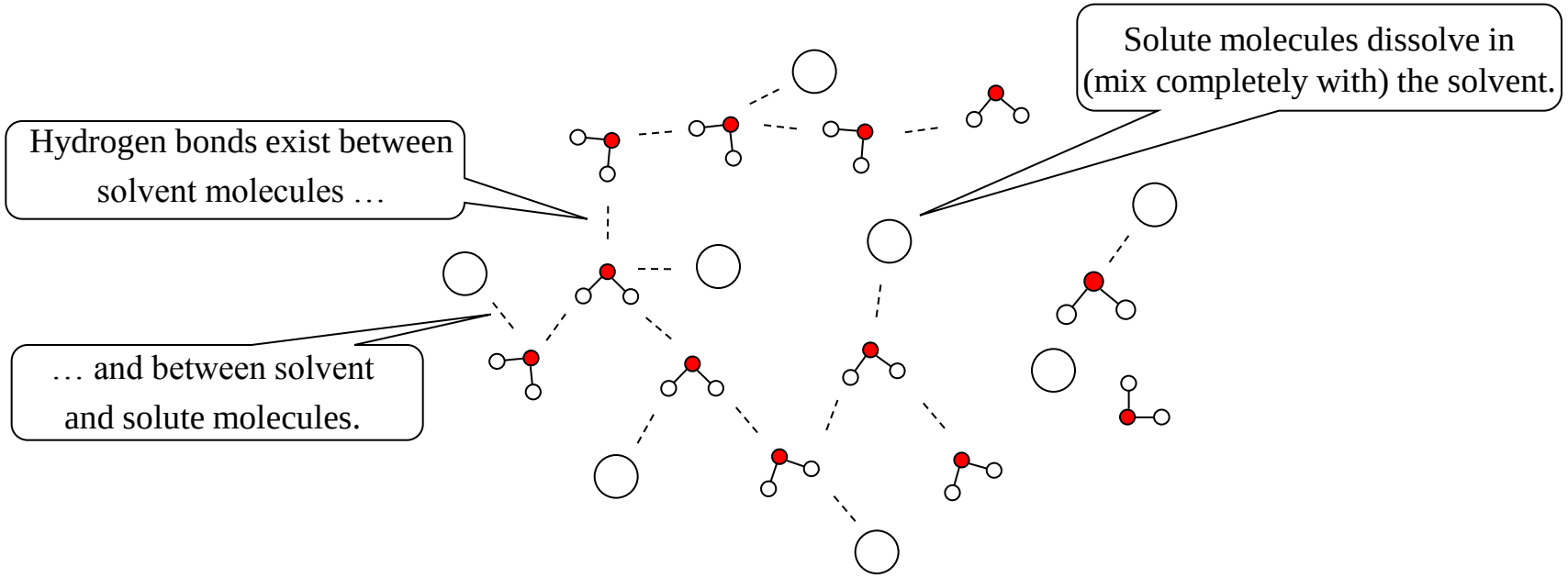
Hydrogen bonds only exist between two specific pairs of nucleotide bases: A and T, and C and G. Other base pairings are not possible.



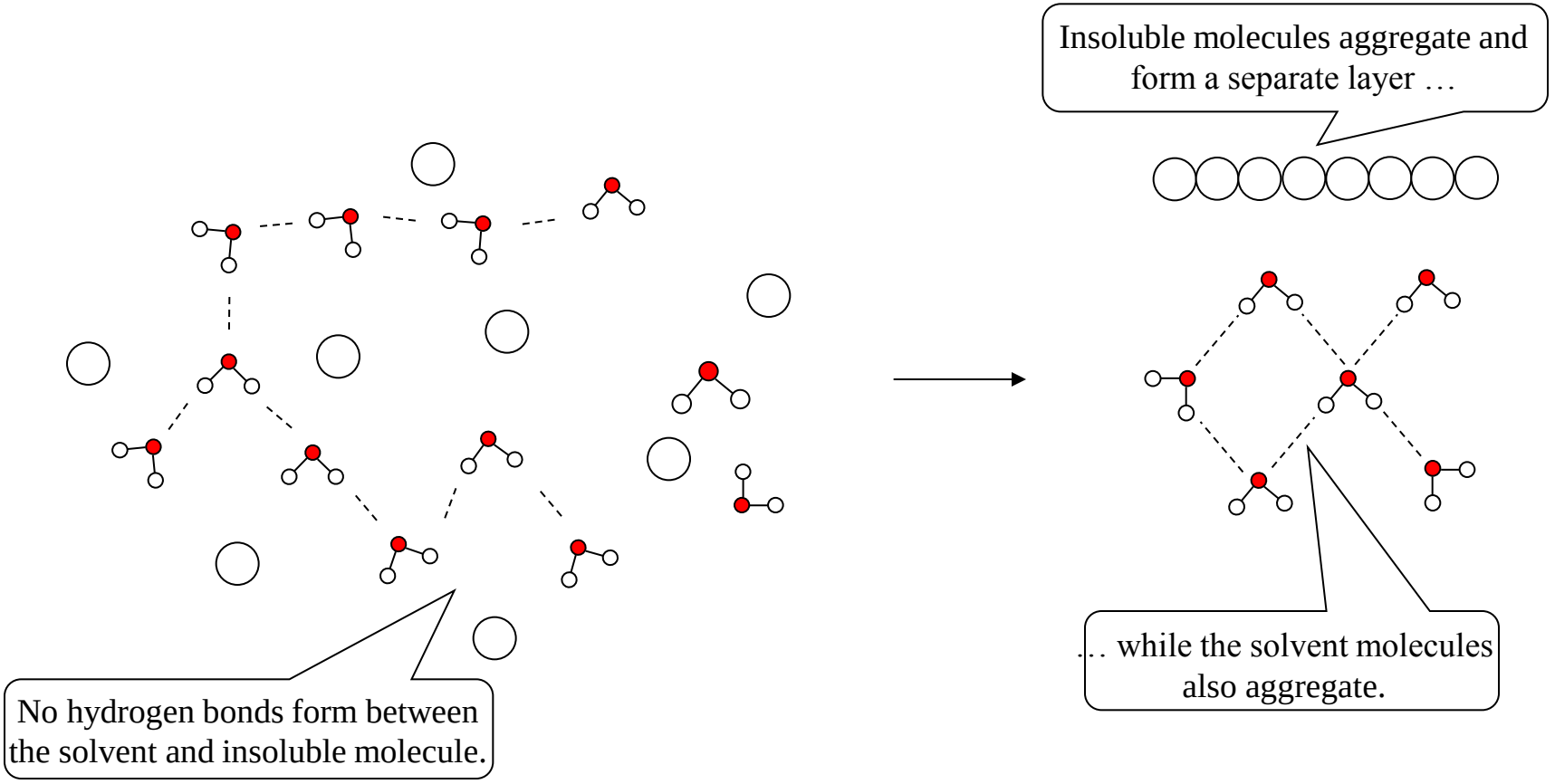
A polypeptide contains both the components necessary for hydrogen bond formation. Consequently, hydrogen bonds can form between different regions of a polypeptide chain, or between different polypeptide chains.



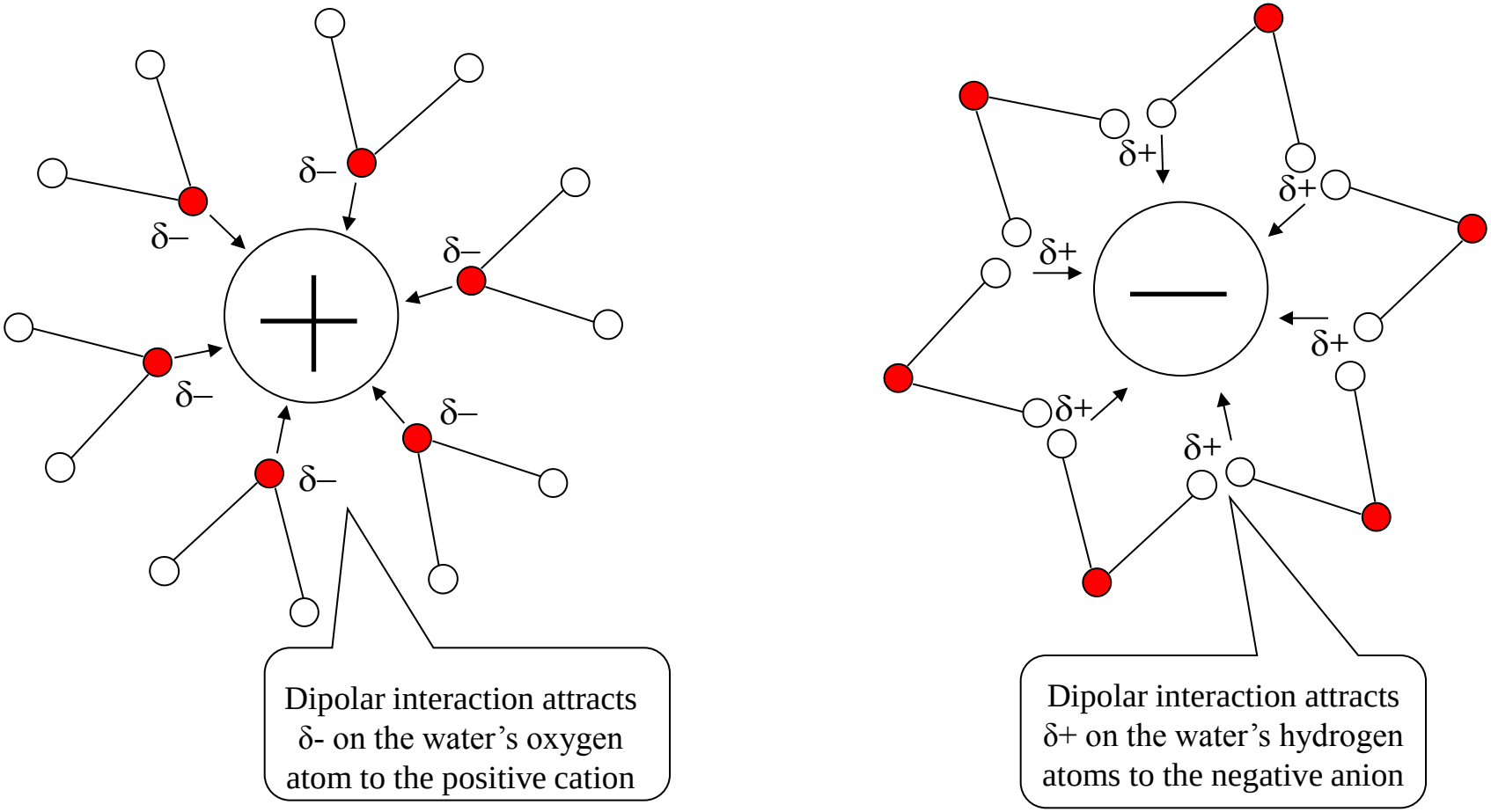
Two possible ways in which hydrogen bonds form between the side chains of the amino acids serine and glutamine.



Molecules of a water-soluble compound and molecules of water mingle freely with each other: the two types of molecule are able to mix completely.



If a compound is insoluble in water, its molecules cannot mix freely with molecules of water. Instead, the two types of molecule remain completely separate. Occasionally, a small amount of the solute dissolves, while the majority floats on top of the solution.

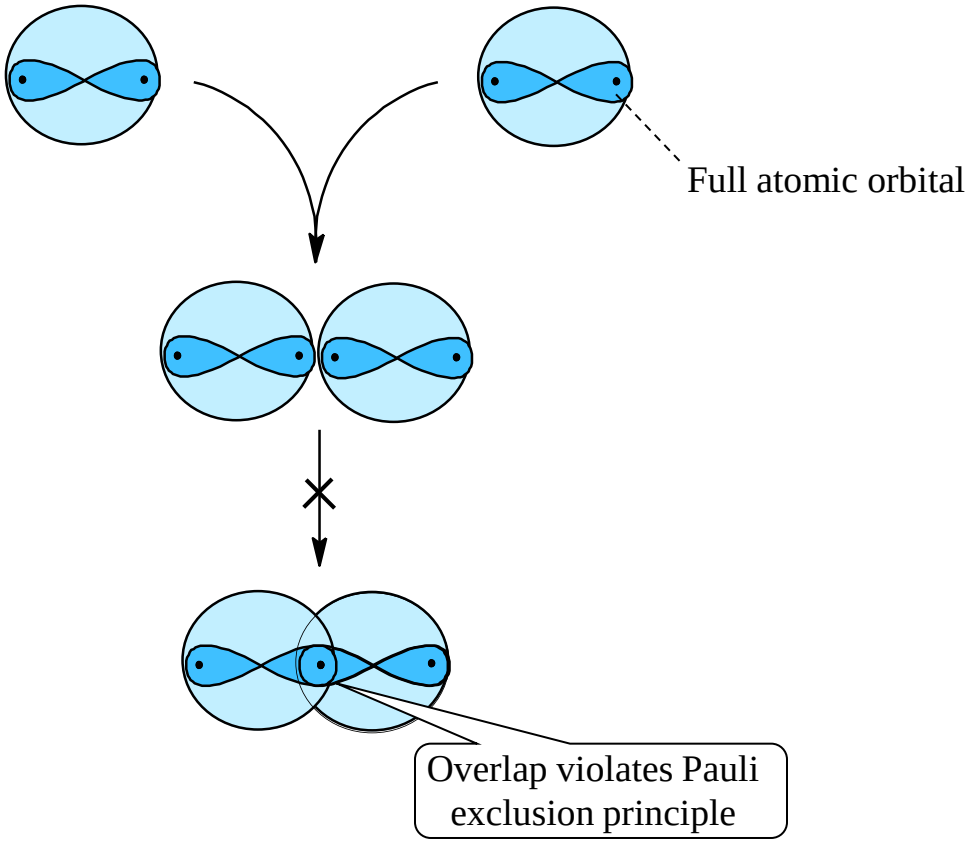


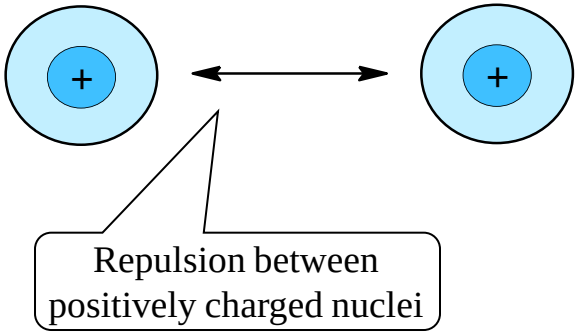
The hydration of ions by water molecules. The interaction of ions and water molecules is stabilized by dipolar interactions, which exist between the charge on the ion and the partial charge on the polar water molecule. The partial negative charge on a water molecule's oxygen atom is attracted to a cation's positive charge, while the partial positive charge on a water molecule's hydrogen atom is attracted to an anion's negative charge.

A nem-kovalens intermolekuláris kölcsönhatások:

van der Waals erők:
vonzó (pl. hidrogén-híd, hidrofób)
taszító (pl. betöltött orbitálok között)

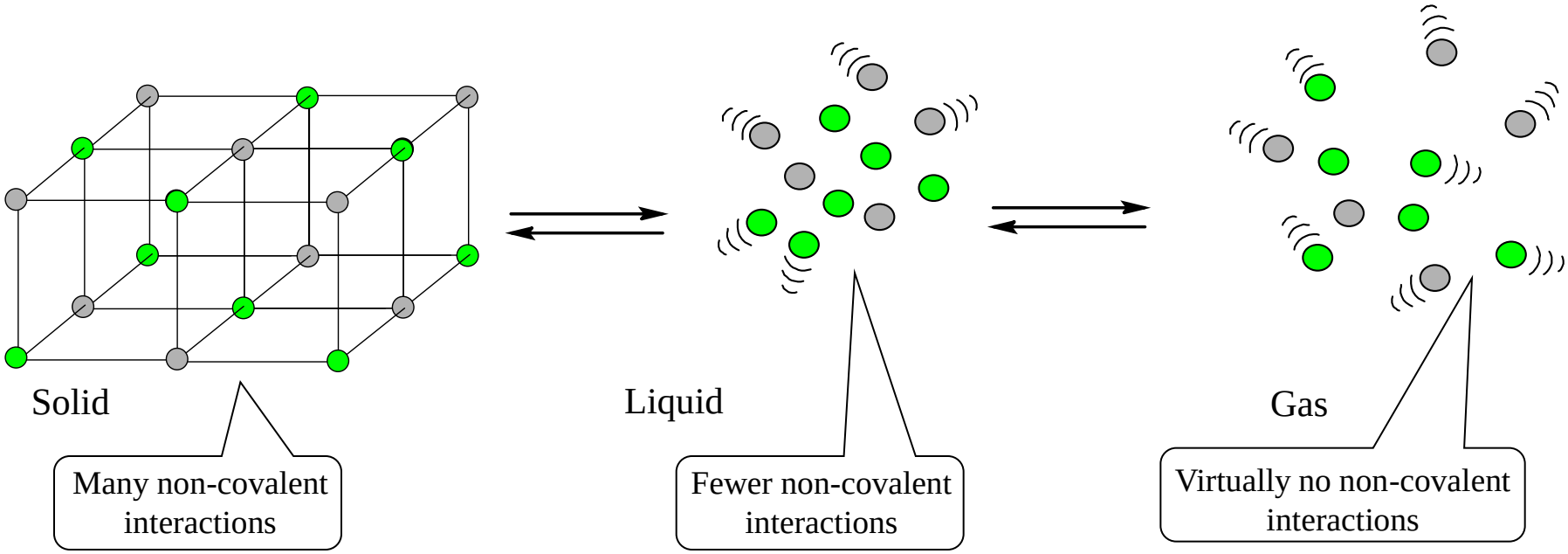
van der Waals erők: taszító is lehet





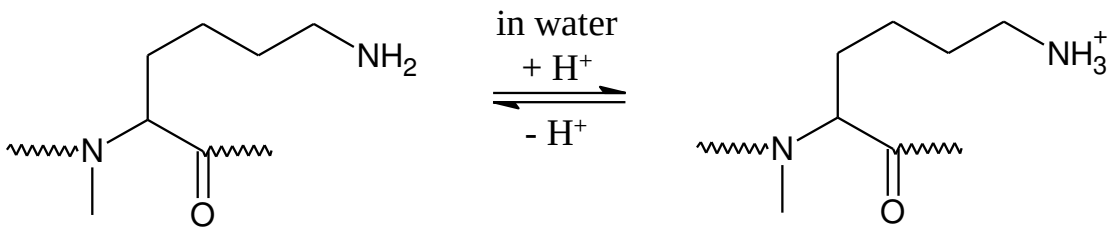
Two full atomic orbitals cannot overlap, as this would violate the Pauli exclusion principle (which states that an atomic orbital can contain a maximum of just two electrons). This limits how closely two atoms can interact. The nuclei of neighbouring atoms repel each other because they both carry like positive charges. This repulsion also limits how closely two atoms can interact.

Szilárd – folyadék - gáz



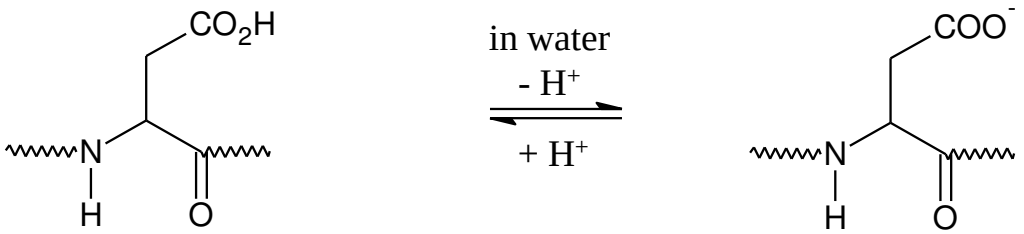
Molecular solids, liquids, and gases are characterized by the number of non-covalent forces that exist between their composite molecules.

Biológiai példák



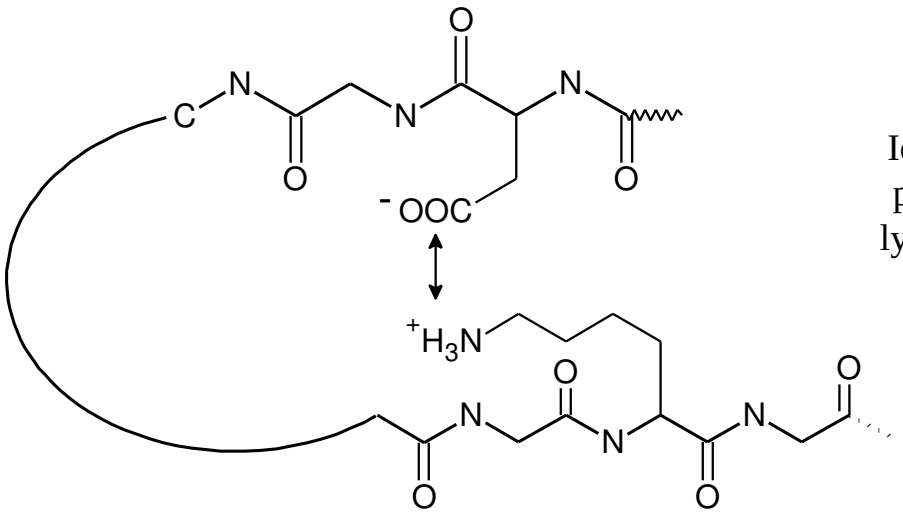
Lysine

Lysine gains a proton when dissolved in water, to form a positively charged side chain



Aspartic acid

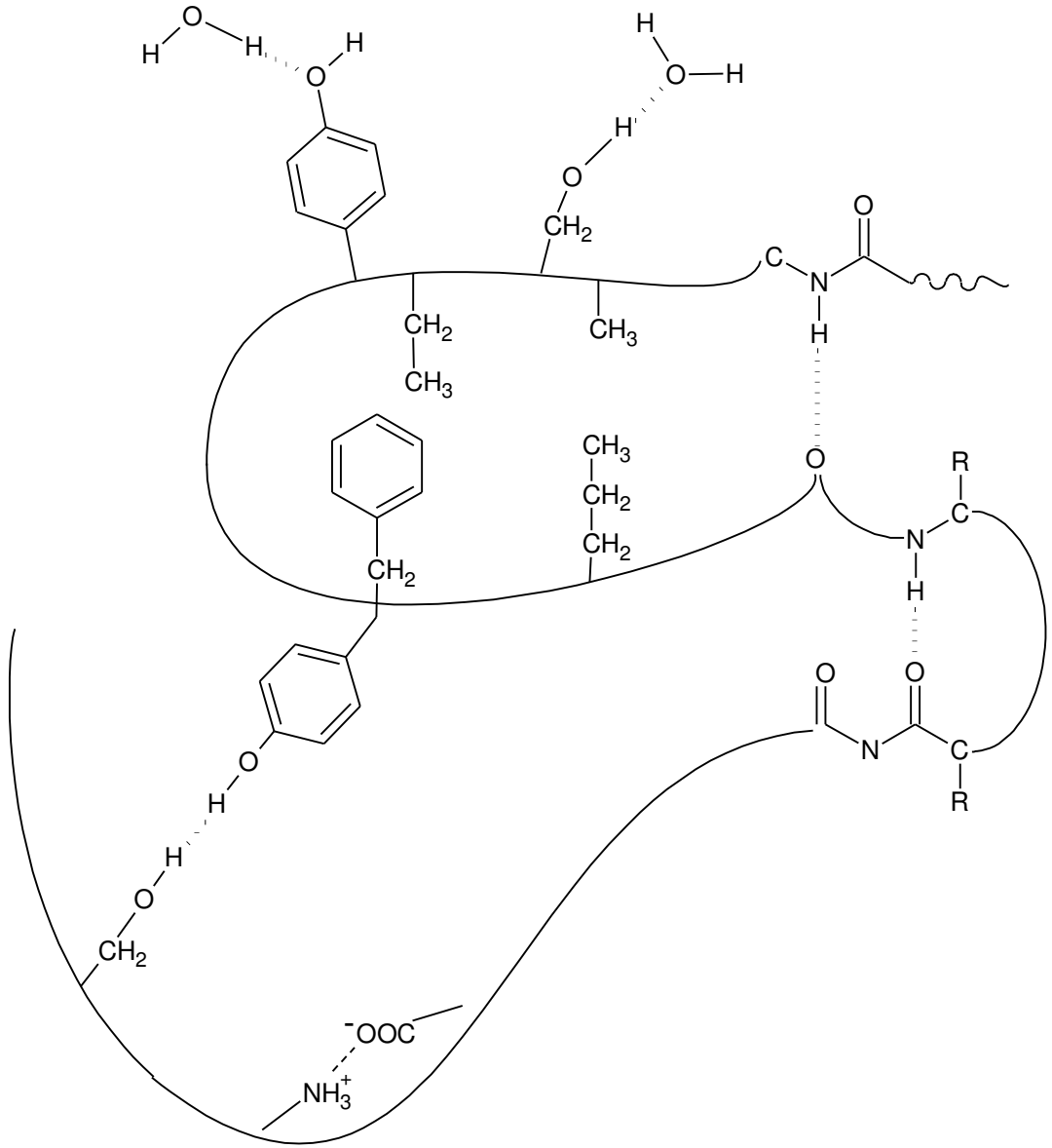
Aspartic acid loses a proton when dissolved in water, to a negatively charged side chain



Ionic forces operate between the positively charged side chain of lysine and the negatively charged side chain of aspartic acid

Polypeptide chain

Ionic forces can operate between a positively charged side chain of one amino acid and a negatively charged side chain of a different amino acid located elsewhere in a polypeptide chain



The various non-covalent forces that can operate in a biological molecule, such as a polypeptide.