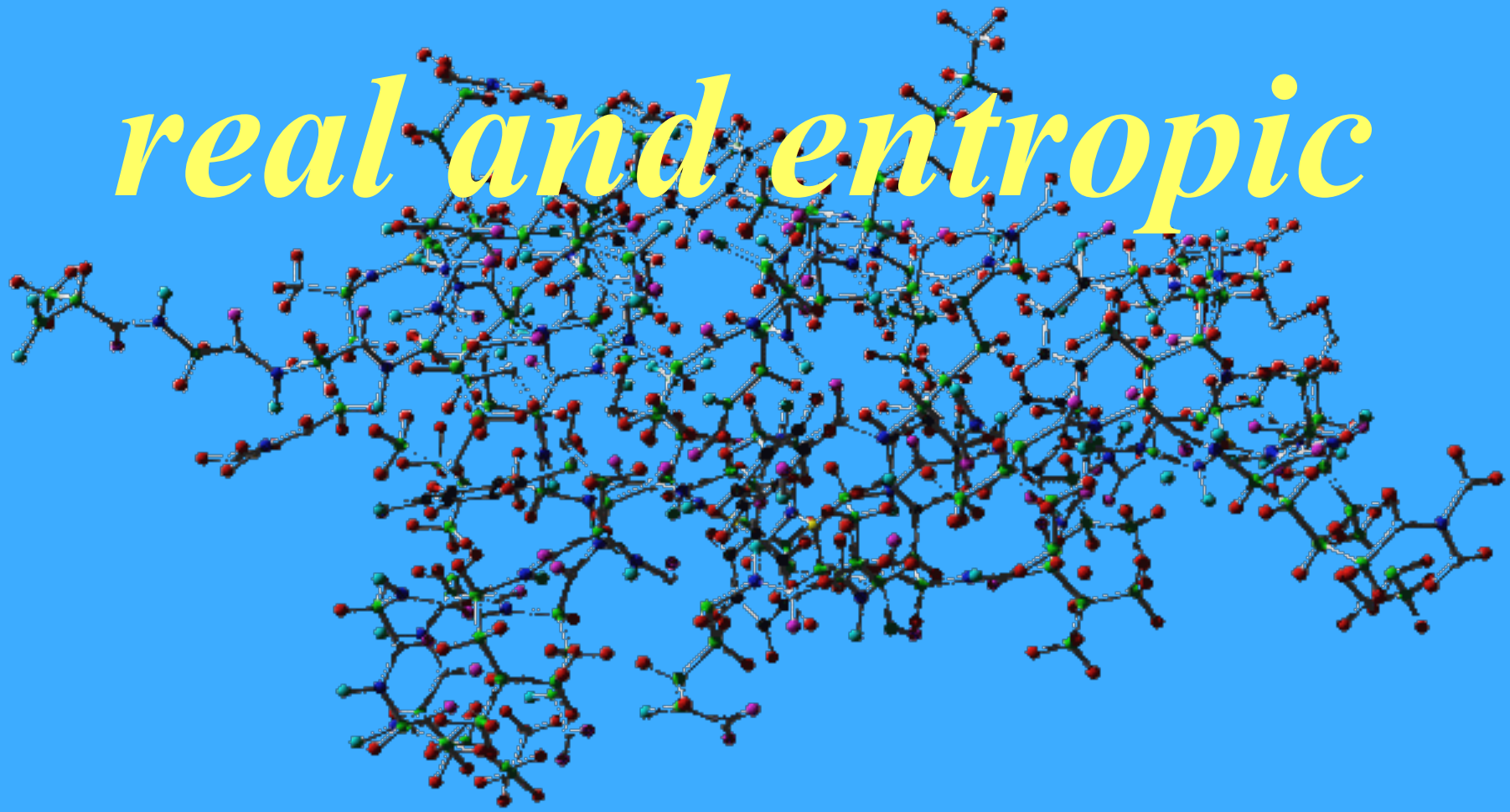
Interactions real and entropic



$$\Delta G = \Delta H - T\Delta S$$

Biological macromolecules are stabilized by physical interactions:

Bond energy (interaction energy) is the work required to bring the two atoms (objects) from infinite distance to the length of the bond.

Always has a negative value!

Strong ***Weak***

-200 - -800 kJ/mol (-50 - -200 kcal/mol)

Covalent bonds

-40 - -400 kJ/mol (-10 - -100 kcal/mol)

Ionic interactions

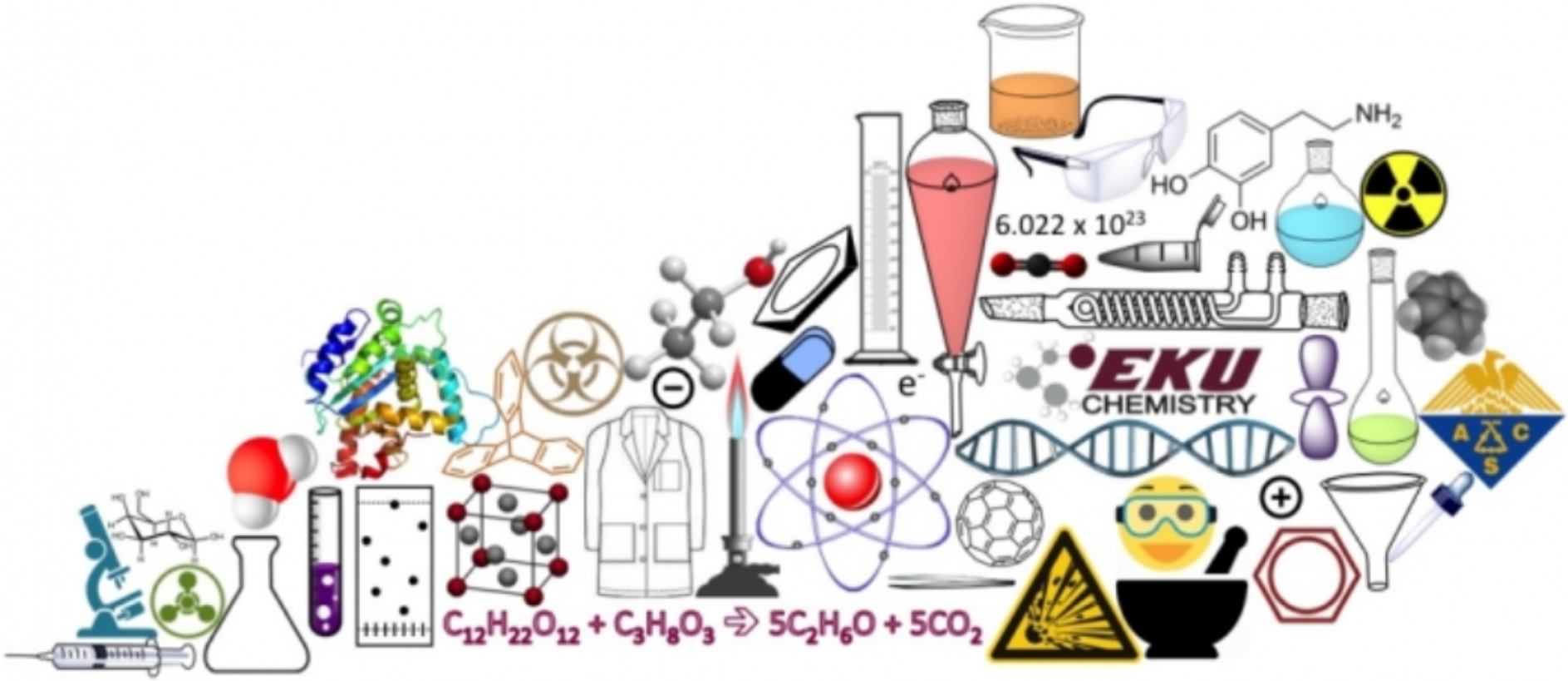
Ion-dipole interactions

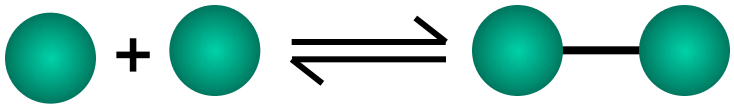
Hydrogen bonds

Van der Waals interactions

Hydrophobic effect

Chemistry


6.022 x 10^23
NH2
HO
OH
e-
EKU
CHEMISTRY
A C S
C12H22O12 + C3H8O3 ⇨ 5C2H6O + 5CO2

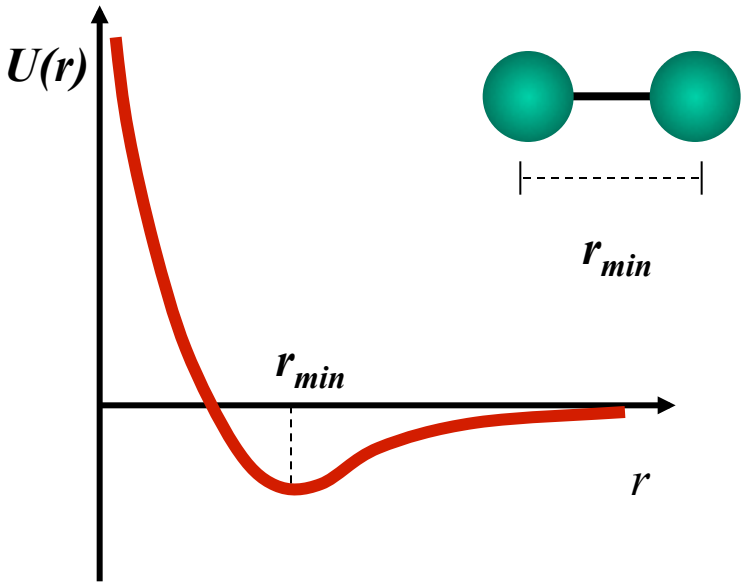


Atoms

Diatomic molecule (+ heat)

Bio-polymers are held together by covalent bonds between subunits.

Lennard-Jones Potential

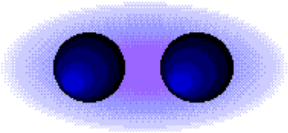


Bond formed due to presence of a stable minimum in the interaction potential energy

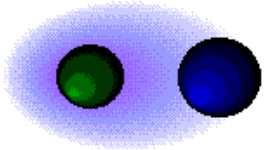
-200 to -800 kJ/mol
-50 to -200 kcal/mol

A covalent bond is formed between the two non-metals which share a pair of valance electrons so that each obtains a filled valence shell.

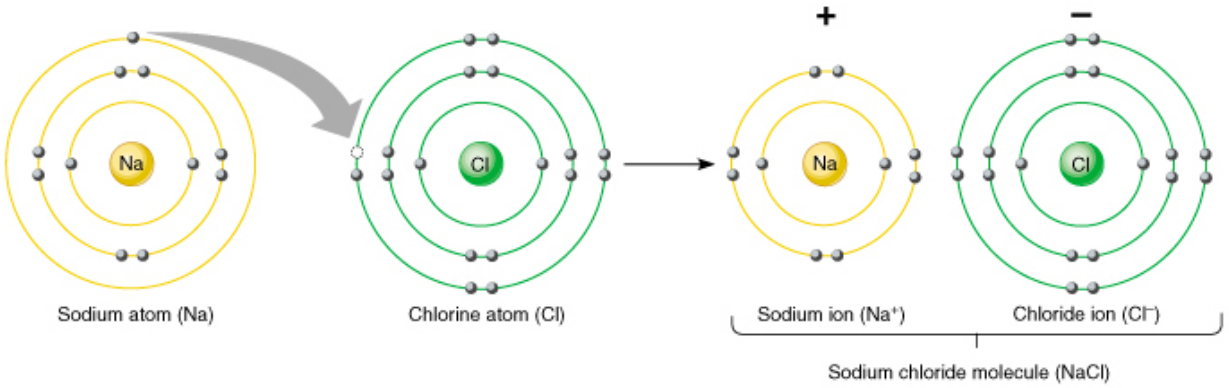
A non-polar covalent bond



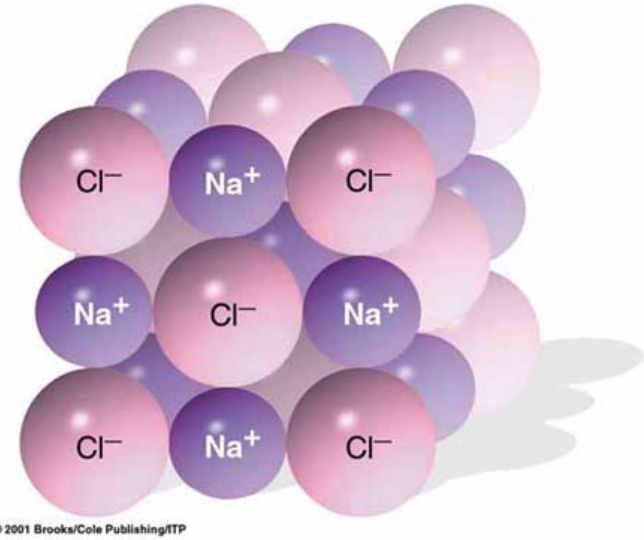
A polar covalent bond

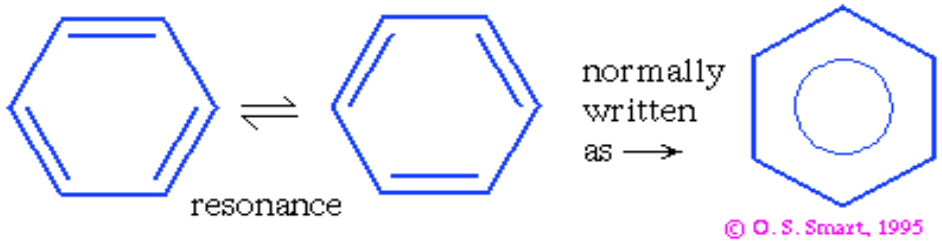


Ionic bonds



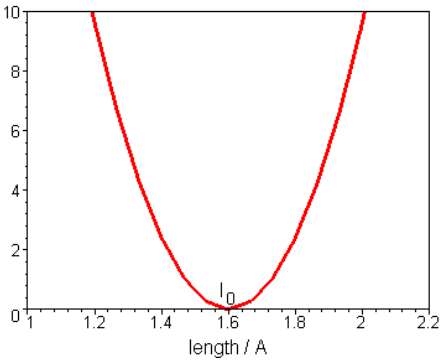
- The valence electrons interact and the metal transfers its valence electrons to the non-metal.

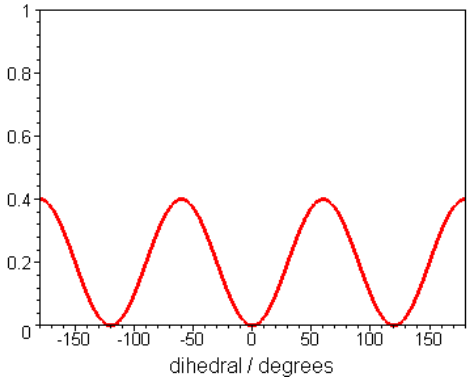




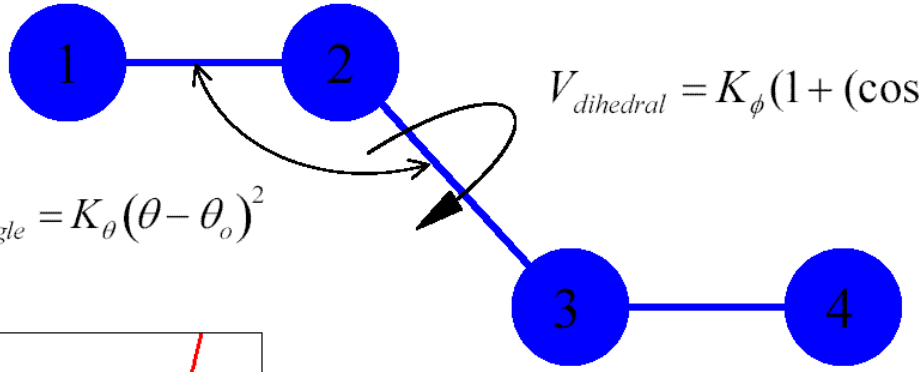
- ***Delocaltzed bonding*** – a resonance hybrid between alternate structures e.g., benzene

Bonding potential (covalent bonds)



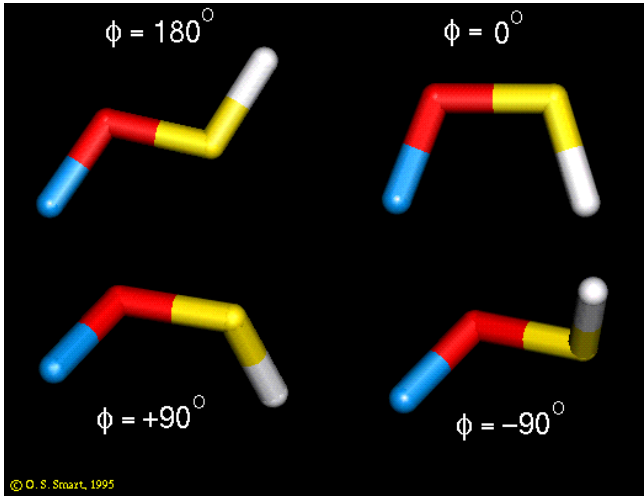


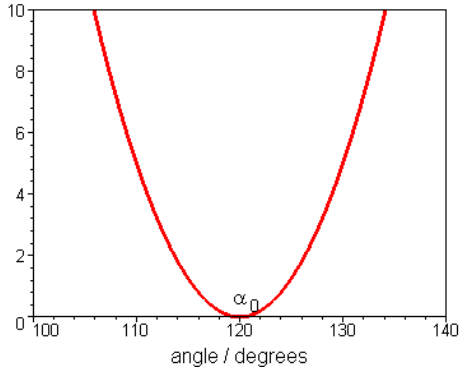
$$V_{bond} = K_b(b - b_o)^2$$



$$V_{dihedral} = K_\phi(1 + (\cos n\phi - \delta))$$

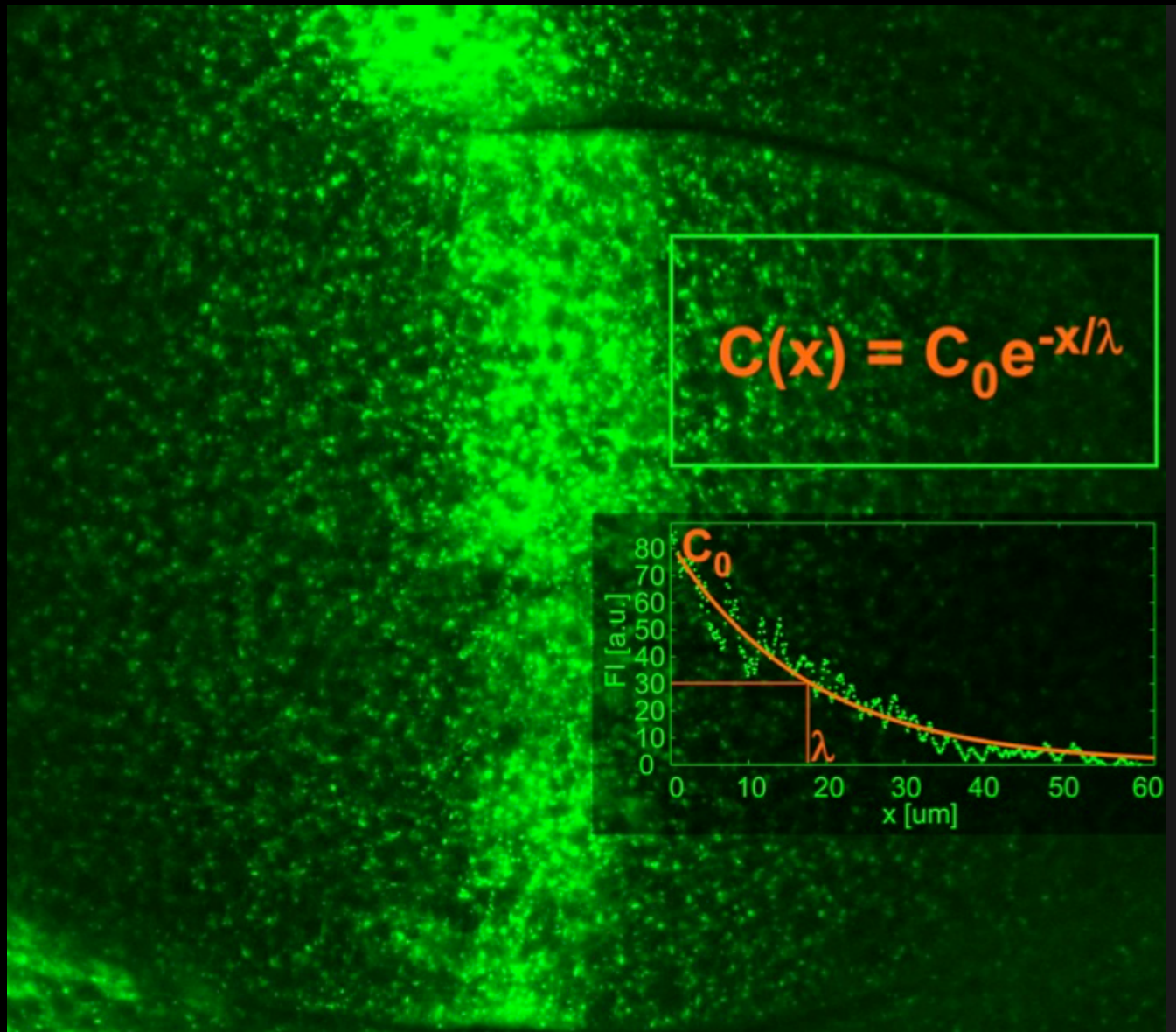
$$V_{angle} = K_\theta(\theta - \theta_o)^2$$





$V_{bonding}$ is big, but $\Delta V_{bonding}$ between conformations is not so big → $V_{nonbonding}$ is what counts most in biological system

Biophysics


$C(x) = C_0 e^{-x/\lambda}$
C_0
λ
Fl [a.u]
0
10
20
30
40
50
60
70
80
0
10
20
30
40
50
60
x [um]

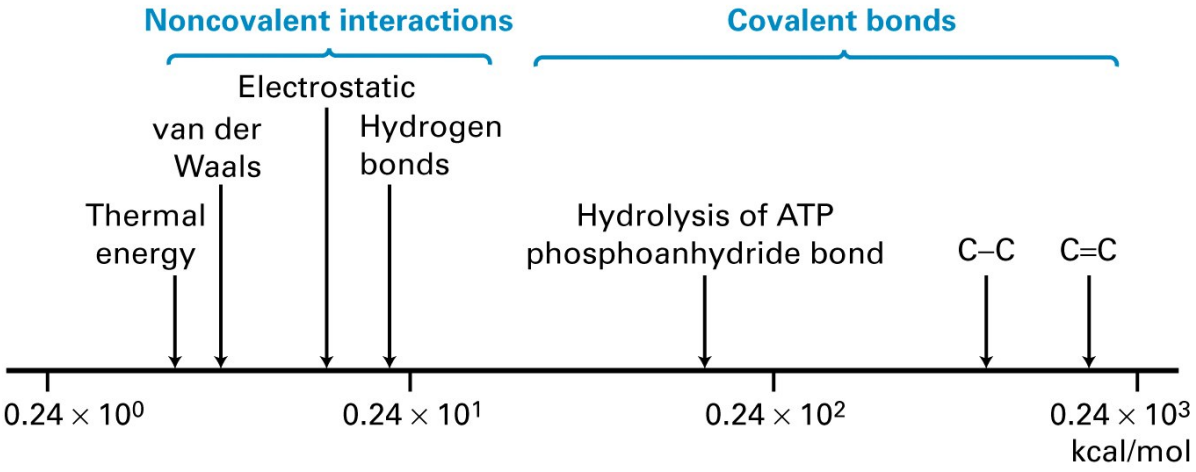
Intra- and Inter-molecular interactions is what biology is all about.

Weak Interactions are additive

Weak interactions are dynamic

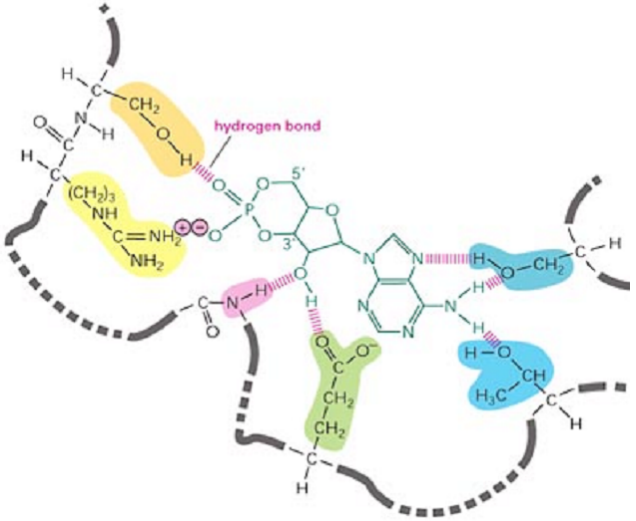
(interactions form, break, re-form constantly)

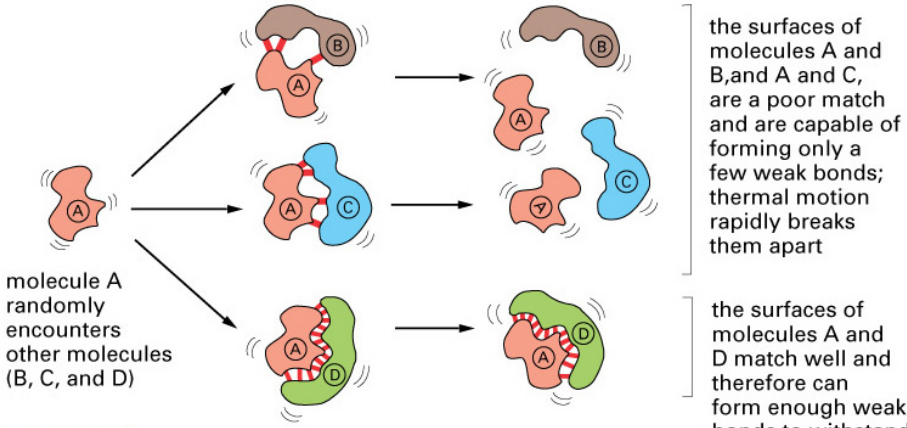
Interaction type	Range	Directional	Energy (kJ/mol)	Energy (k_BT)
Covalent	very short	yes	100 - 900	40 - 360
Hydrogen bond	very short	yes	10 - 40	4 - 16
Charge-charge	$\propto r^{-1}$	no	503	200
Charge-dipole	$\propto r^{-2}$	yes	97	39
Dipole-dipole	$\propto r^{-3}$	yes	19	7.5
van der Waals	$\propto r^{-6}$	no	0.5 - 5	0.2 - 2

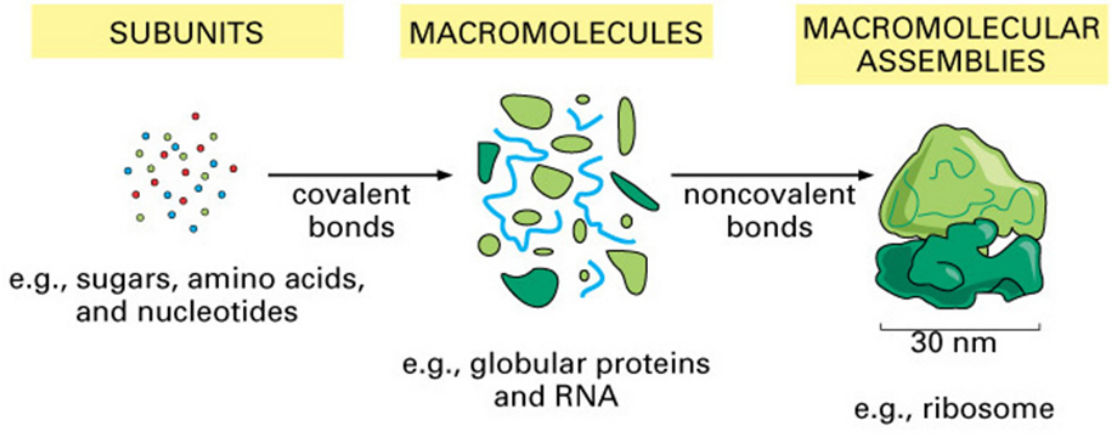


Weak interactions

- *They determine the shape of macromolecules*
- *They produce reversible self-assembly of presynthesized subunits into specific structures*
- *They determine the specificity of most molecular interactions*
- *Molecules or supramolecular aggregates changes upon environmental changes which affect the strengths of weak bonds*

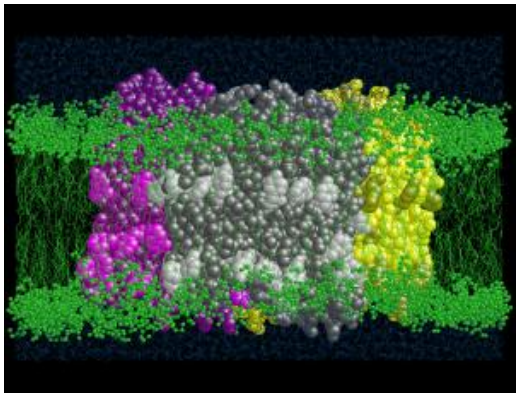






Energy of macromolecules and aggregates

There are two types of interactions



$$V = \sum_{i<j} \frac{q_i q_j}{4\pi\varepsilon_0 r_{i,j}} + \sum_{i<j} \left(\frac{A_{i,j}}{r_{i,j}^{12}} - \frac{B_{i,j}}{r_{i,j}^{6}} \right) +$$

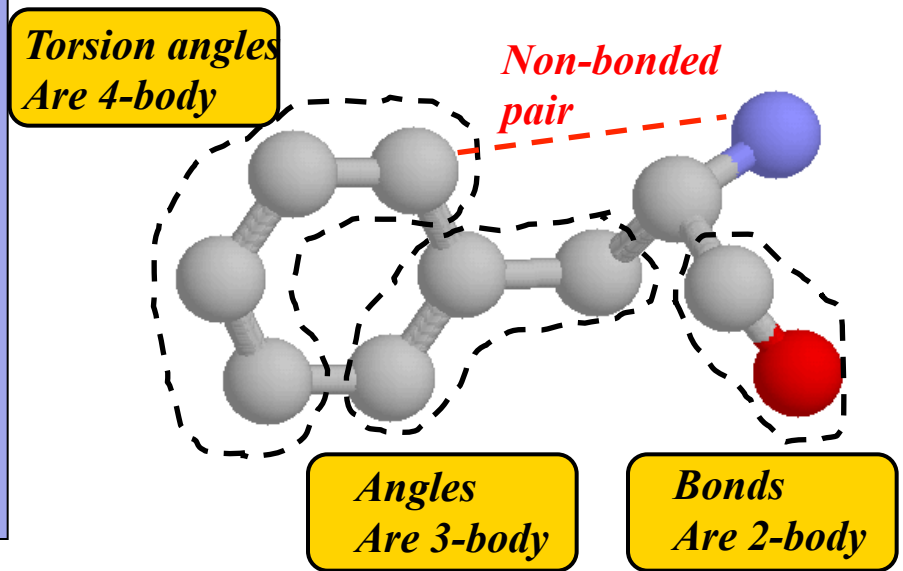
- noncovalent

$$+ \sum_{bonds} \frac{1}{2} k_{i,j}^{b} \left(r_{i,j} - b_{i,j}^{0} \right)^2$$

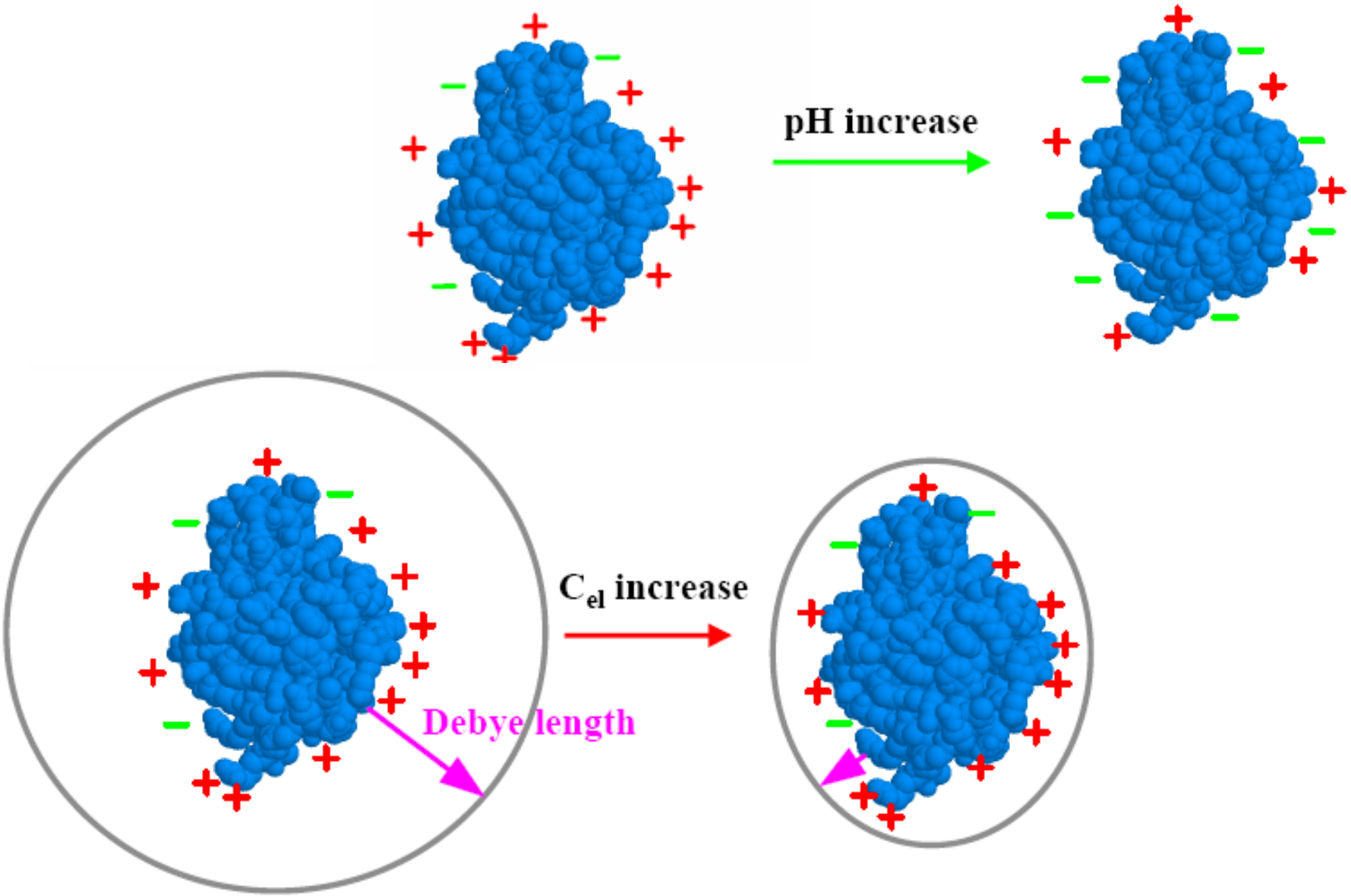
$$+ \sum_{angels} \frac{1}{2} k_{i,j,k}^{\theta} \left(\theta_{i,j,k} - \theta_{i,j,k}^{0} \right)^2 +$$

$$+ \sum_{dihedrals} k^{\phi} (1 + \cos(n(\phi - \phi^0)))$$

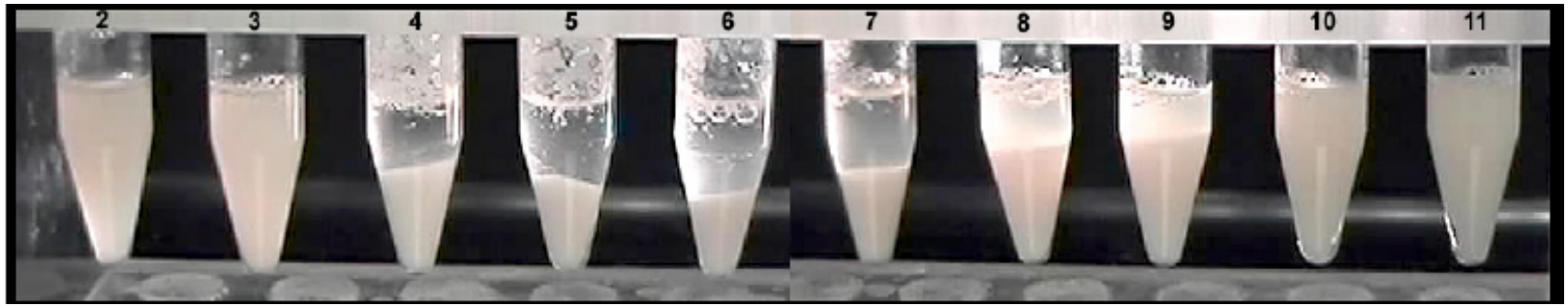
- covalent

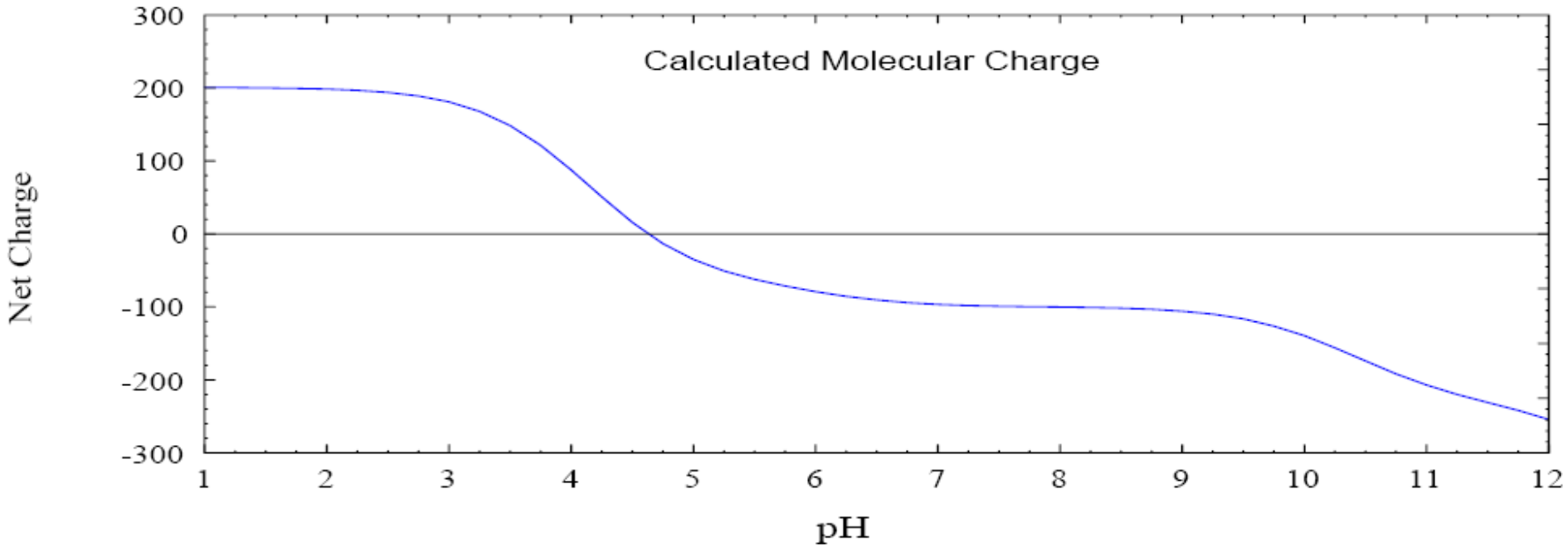


The two basic parameters affecting maacromolecule interactions



Correspondence between charge and precipitation equilibria - soy protein.



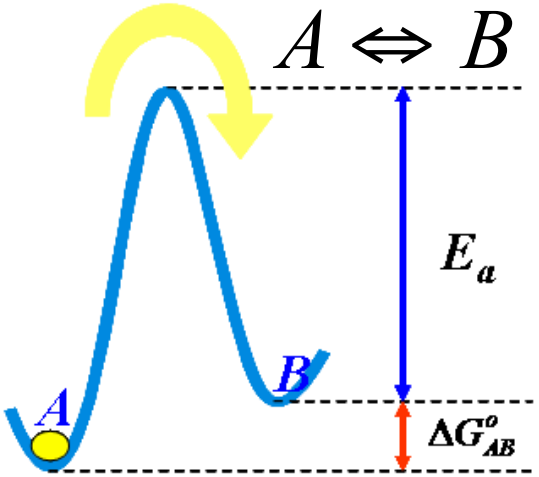


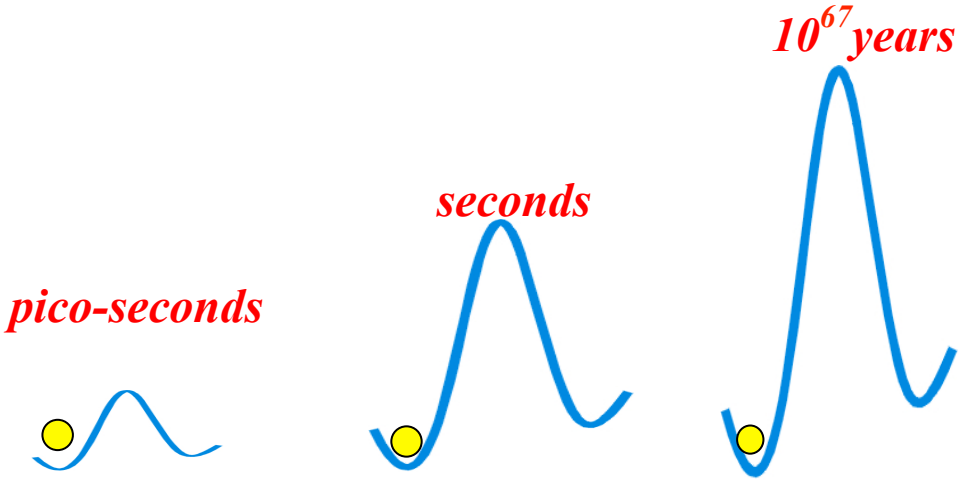
Biology works within kT

1kT = 0.62 kcal/mole (at T=300K)

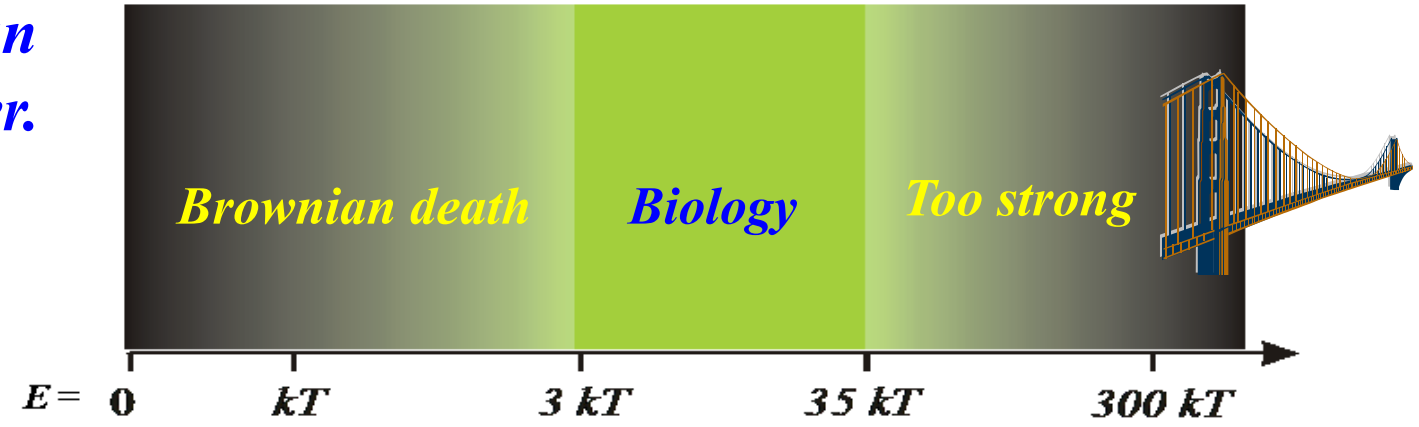
At equilibrium

$$K_{A \leftrightarrow B} = \frac{[B]}{[A]} = e^{-\frac{\Delta G^{o}_{A \leftrightarrow B}}{k_B T}}$$



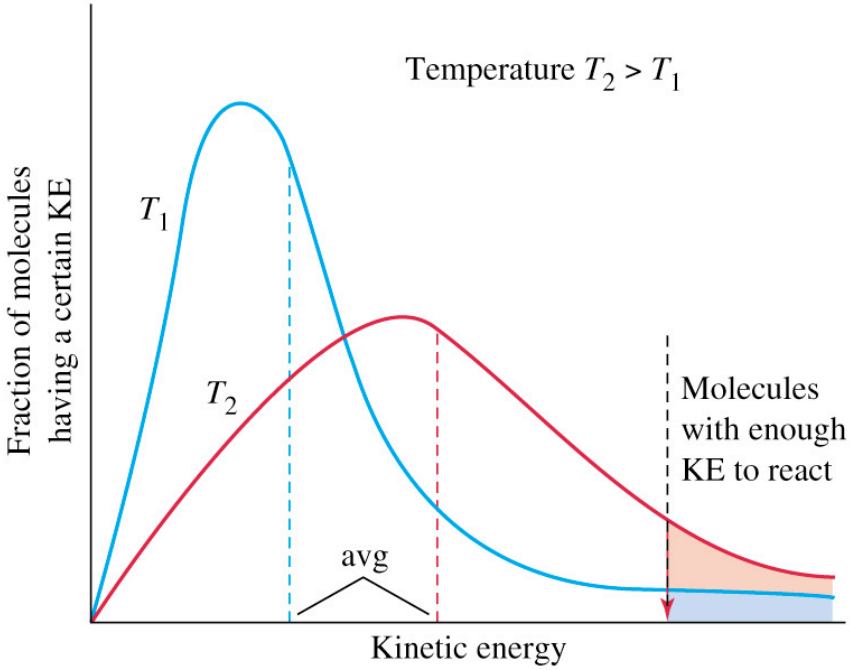


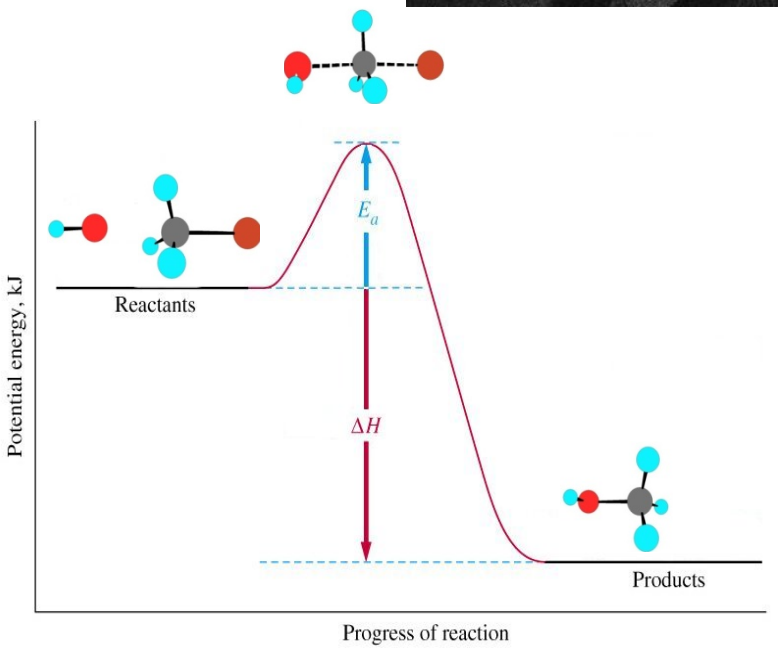
The time it will take for Brownian motion to overcome an energy barrier.



Energetics of transition state theory

Svante Arrhenius (Nobel Prize, 1903).

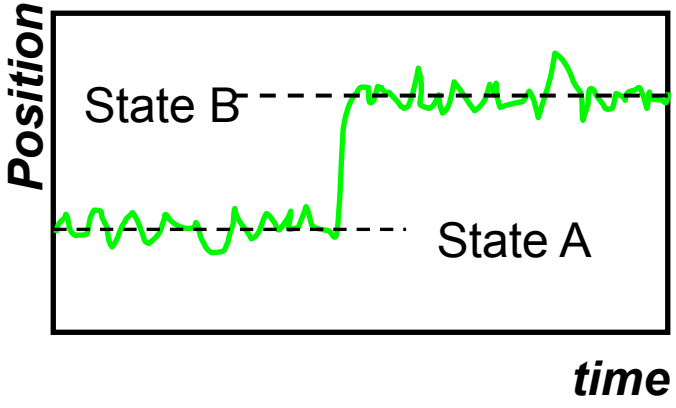


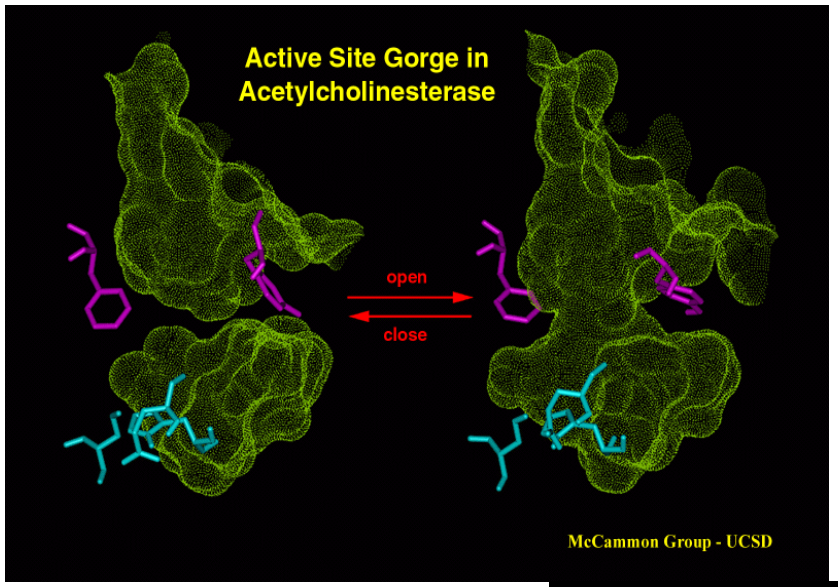


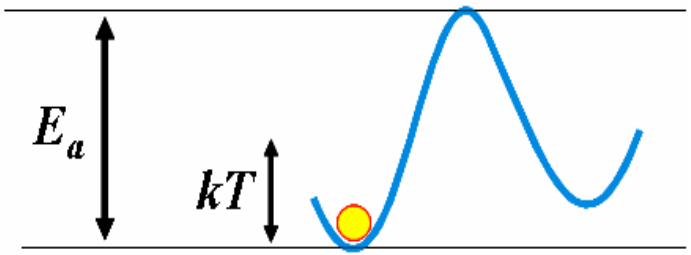
Thermal motion

- biomolecules are stable enough to make things work,

- allow the systems to play around in order to allow the evolution

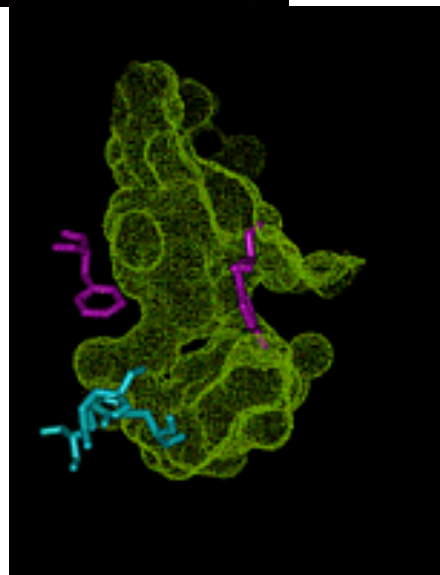






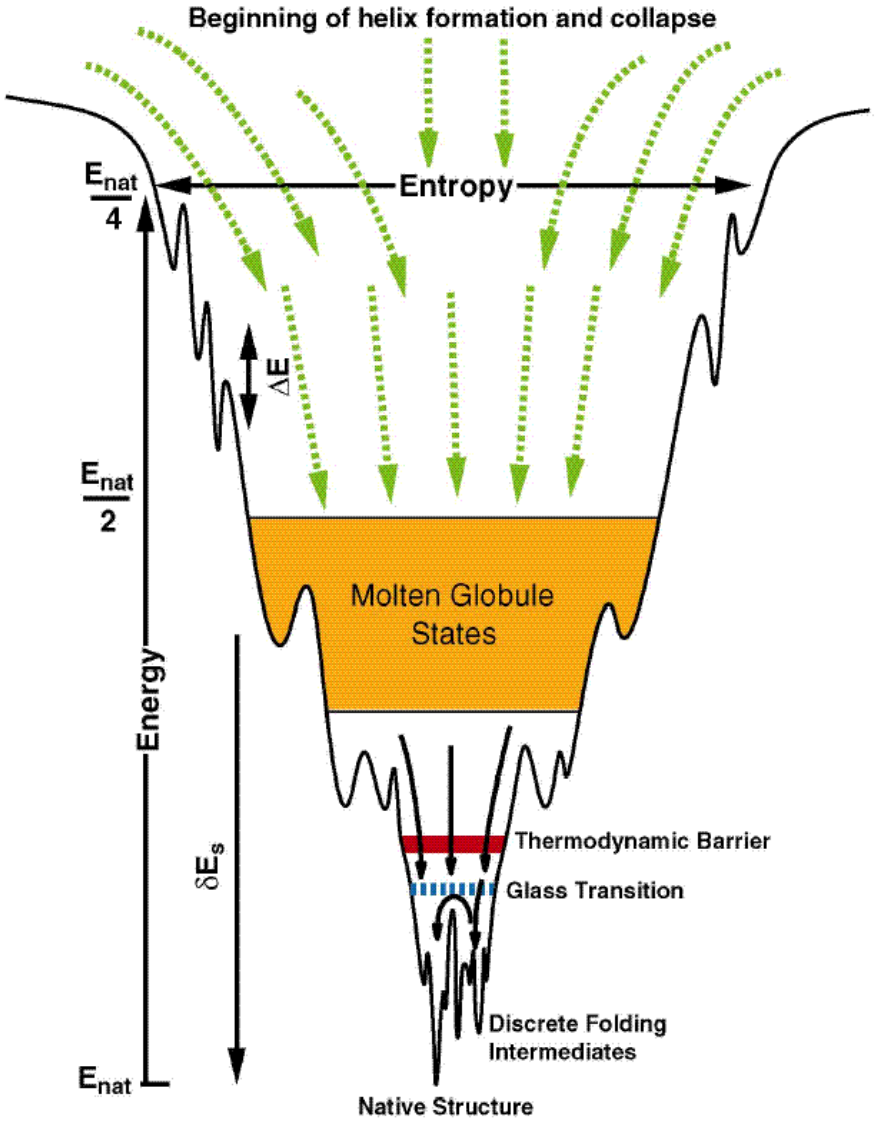
The average waiting time

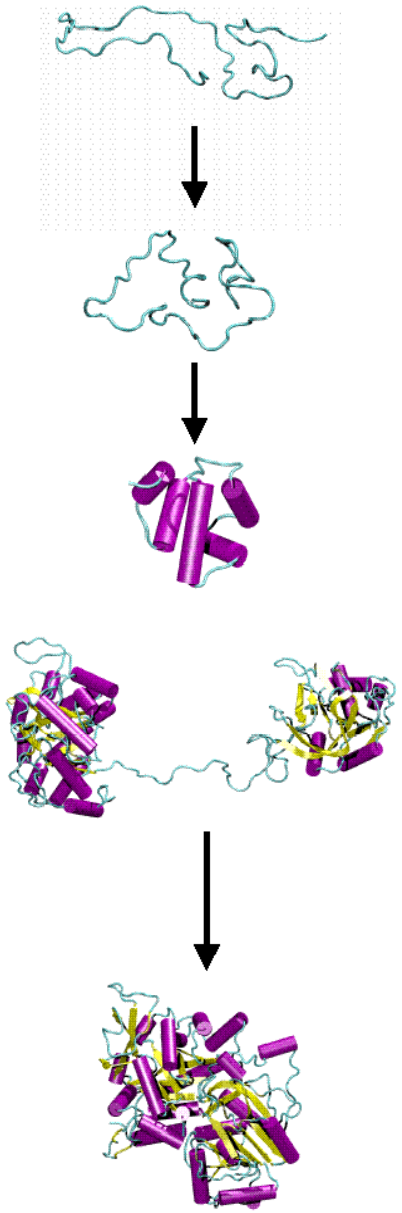
$$\tau_{A\to B} = Ce^{\frac{E_a}{kT}}$$



Conformation - surface outline or contour or 3-D orientation of chemical groups that are free to assume different positions in space without breaking any bonds.

The folding of a mcacromolecule

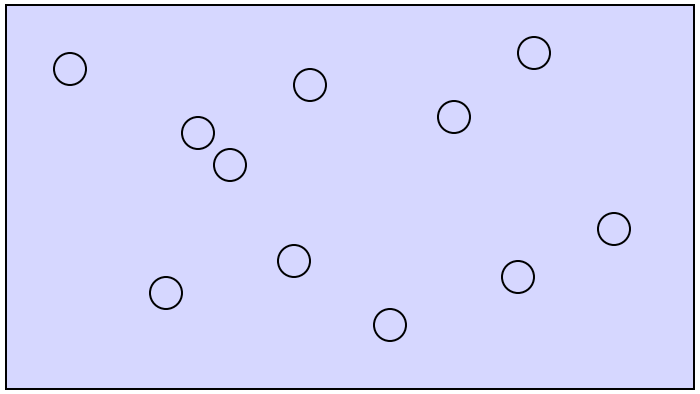


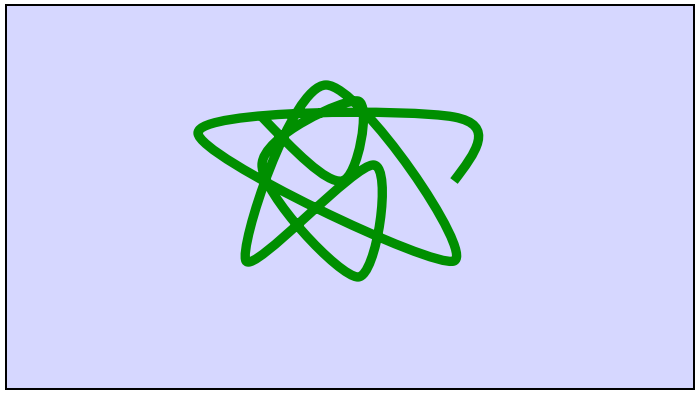


Entropic „Forces”

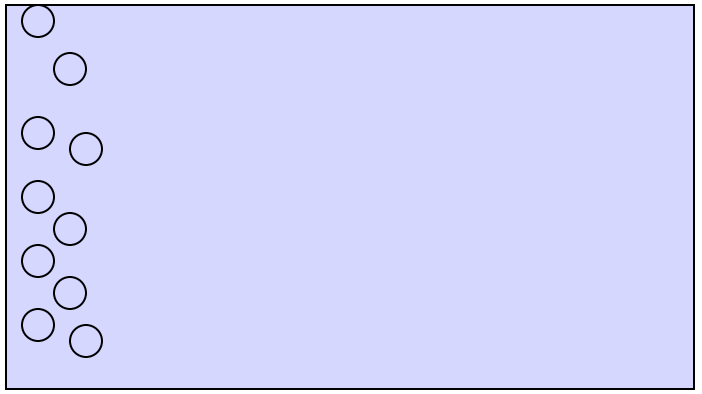
Disorder is Favorable

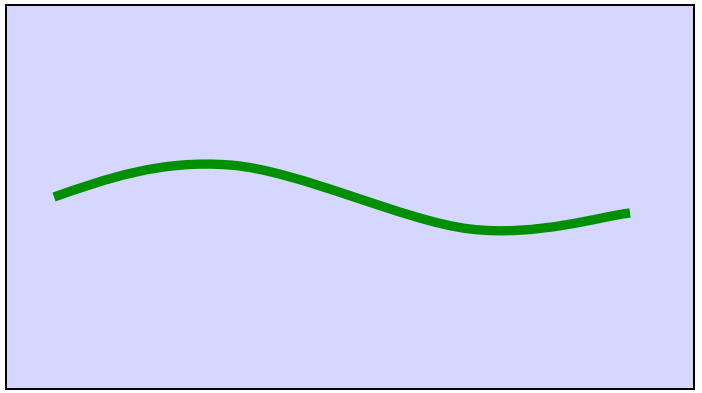
Probable

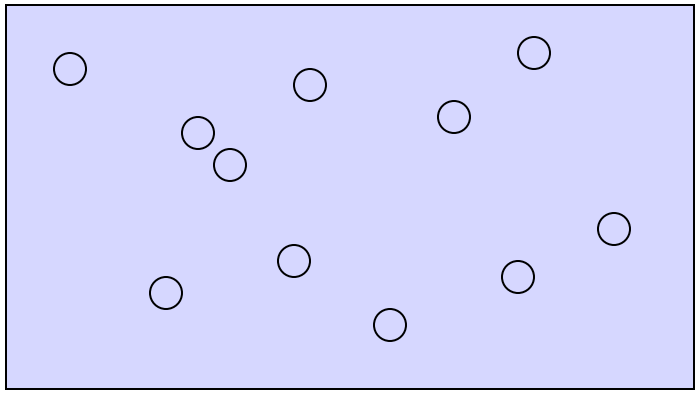
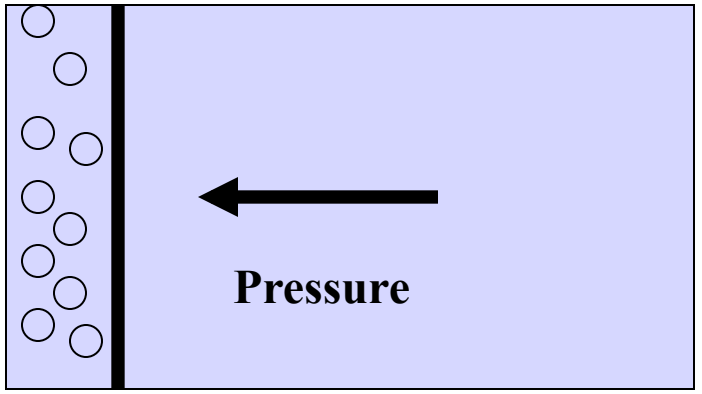
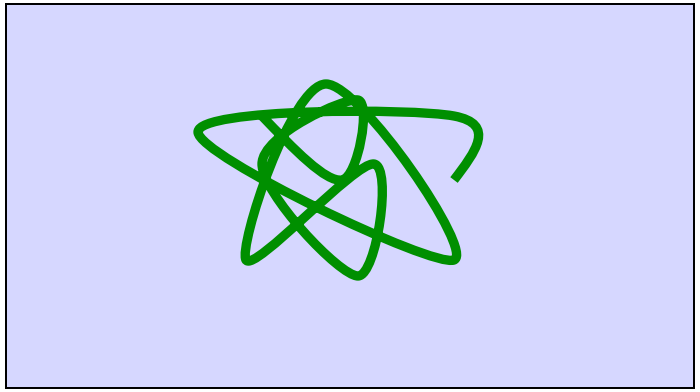
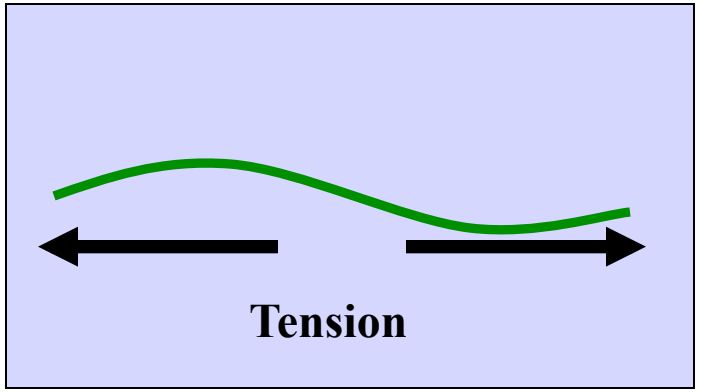




Improbable





The entropic forces can create a situation where two molecules will interact strongly, although there is not a direct "force" between them.

To create order 'work' must be done