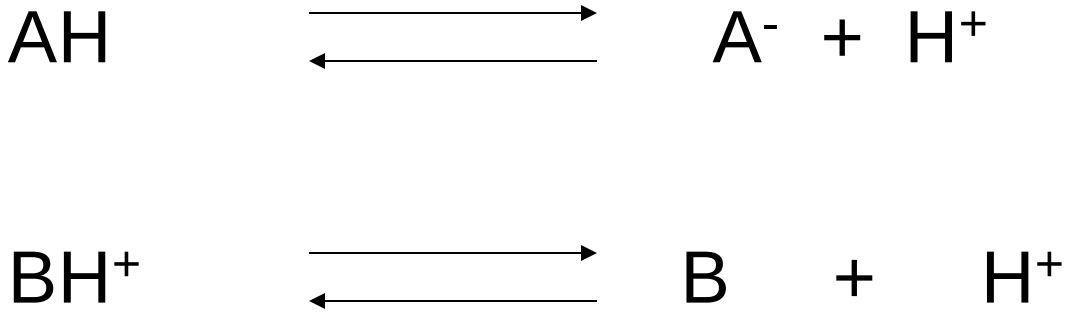
Solutions and Water Structure

- Properties of solutions
- Water microstructure
- Solute microstructure
  - Ionic solutes
  - Polar solutes
  - Nonpolar solutes (the hydrophobic effect)

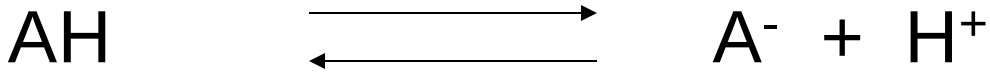
$$pH = -\log_{10}[H^+]$$

Acid base equilibria



$$pK = -\log_{10}\left[\frac{[A^-][H^+]}{[AH]}\right]$$

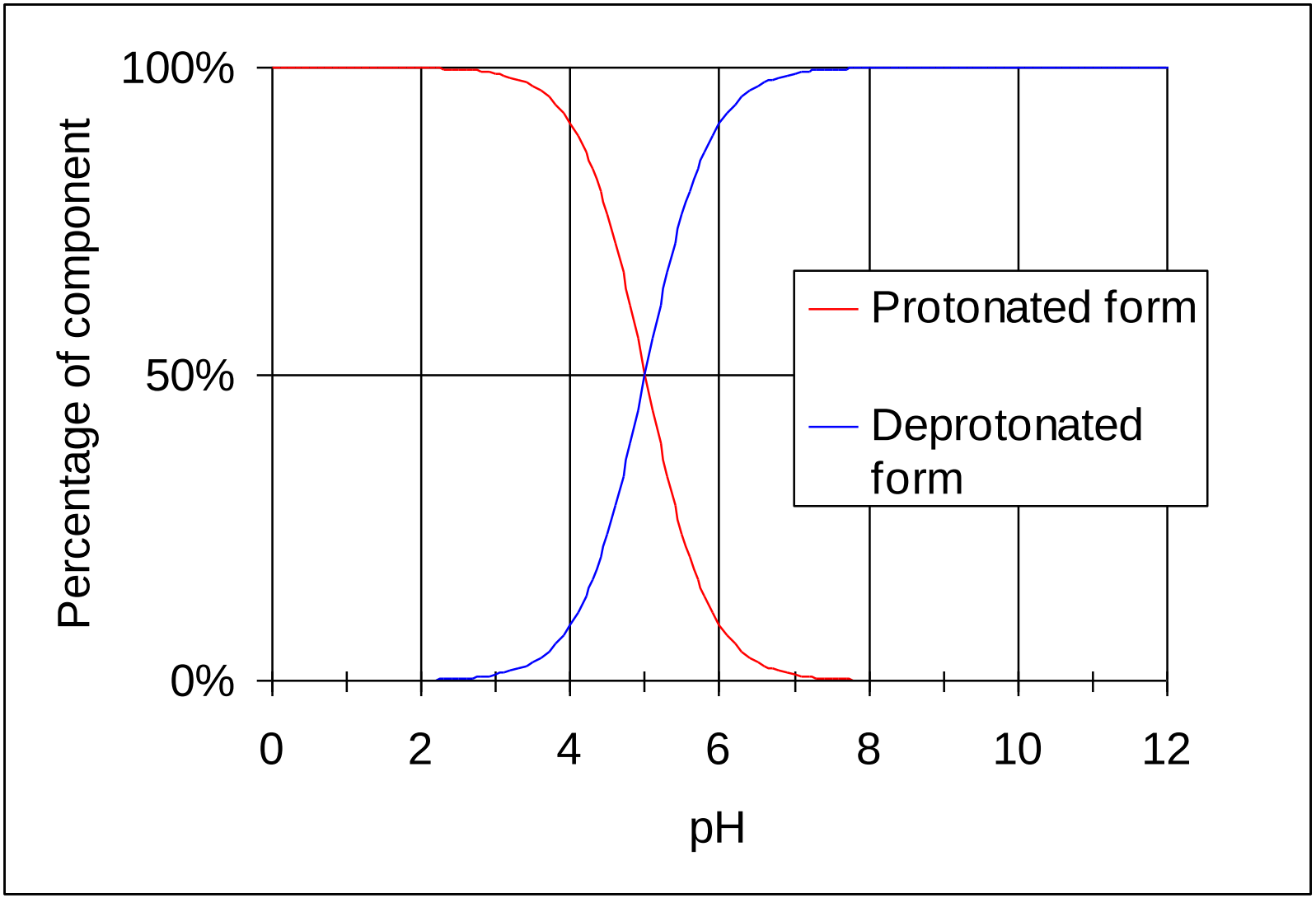
Henderson Hasselbach



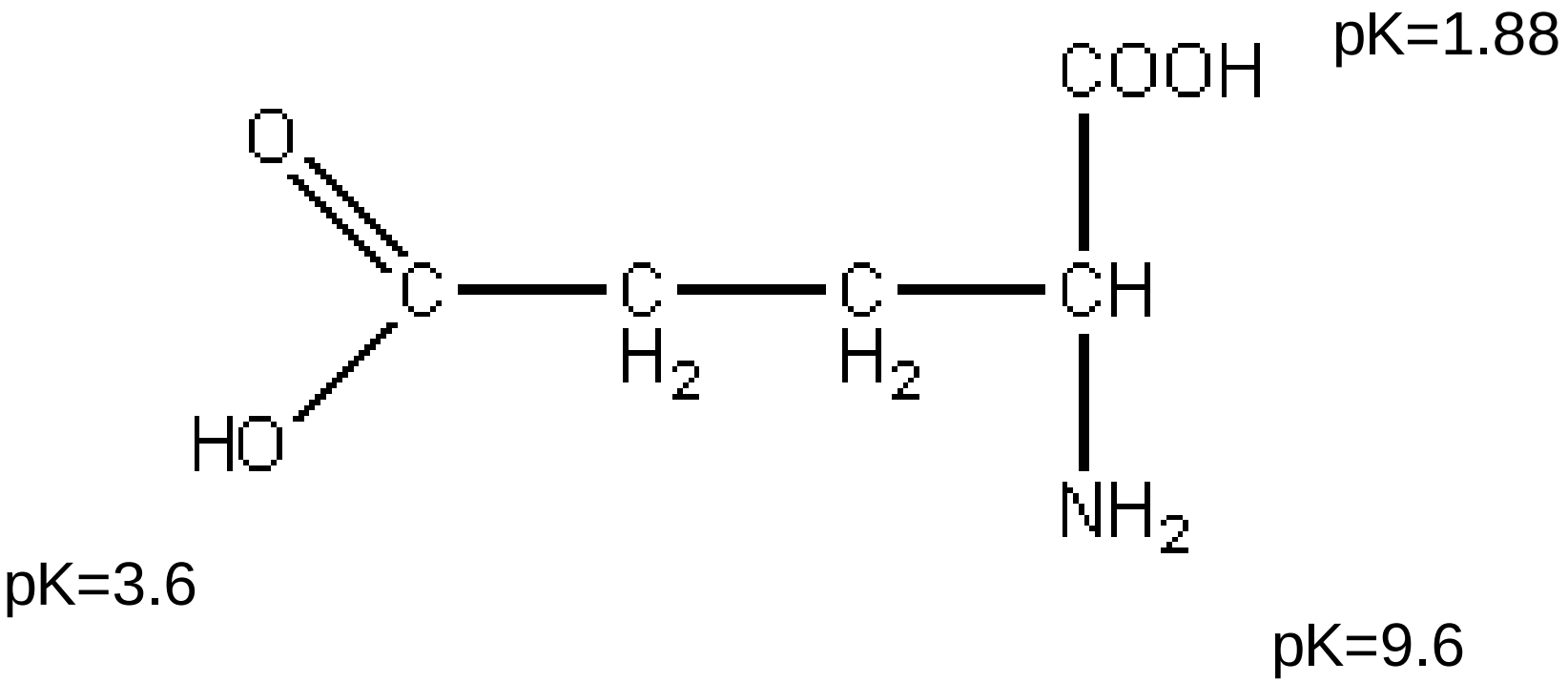
$$K = \left[\frac{[A^-][H^+]}{[AH]} \right] = \frac{[A^-]}{[AH]} \times [H^+]$$

$$pK = pH - \log_{10} \frac{[A^-]}{[AH]}$$

$$AH \rightleftharpoons A^- + H^+$$

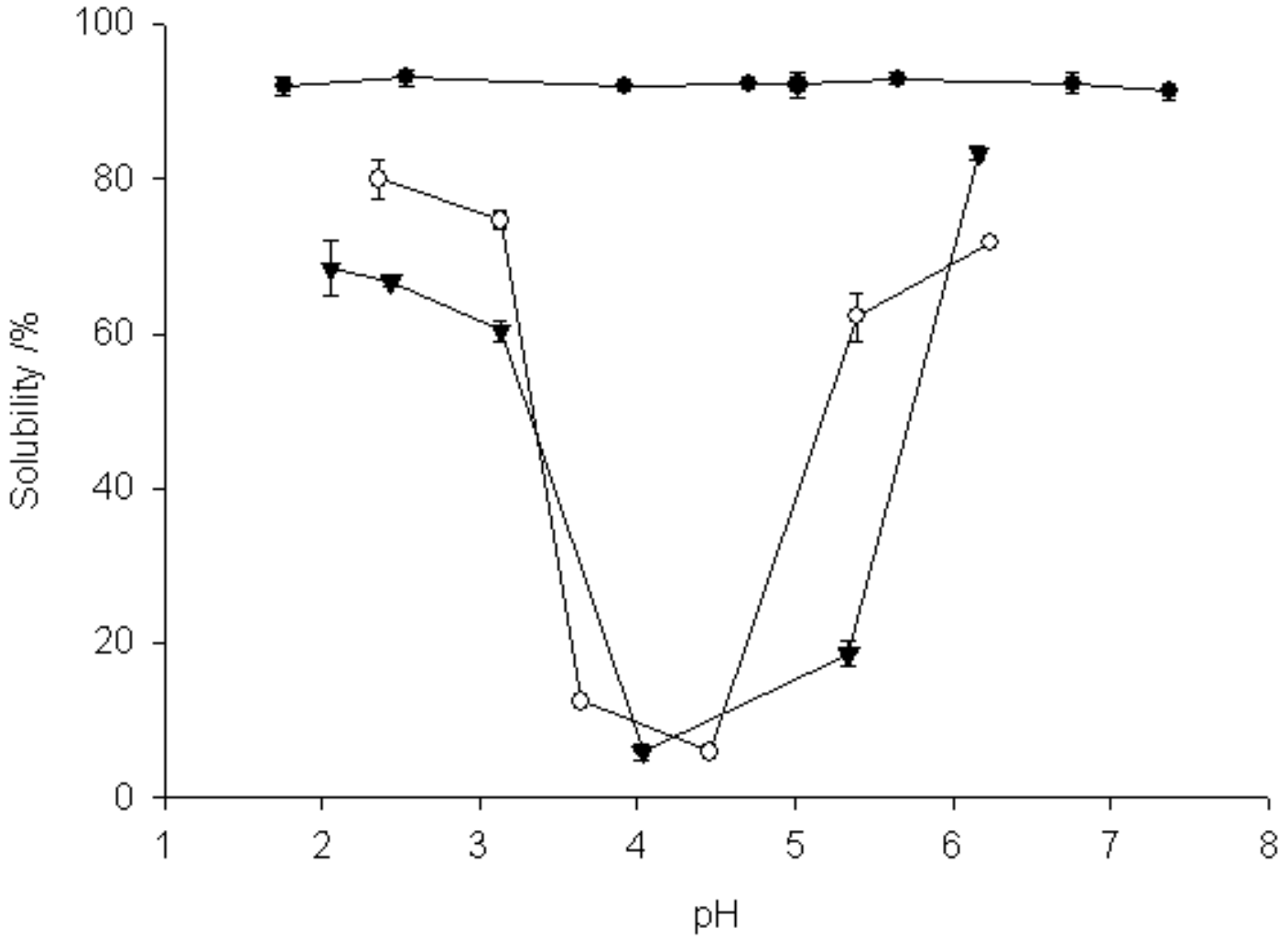


Monosodium glutamate



Monosodium glutamate (MSG) is a flavor enhancer. It is most active over the pH range 6-8 and decreases at lower values.

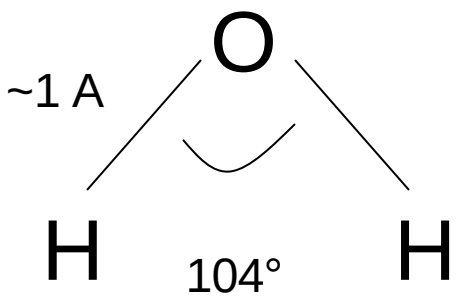
Soy protein solubility

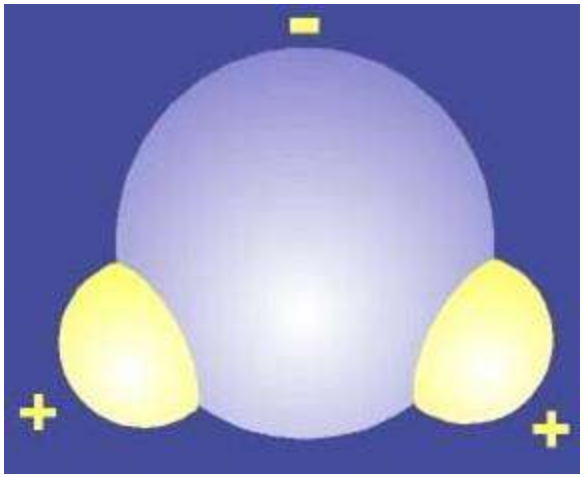


Water Structure

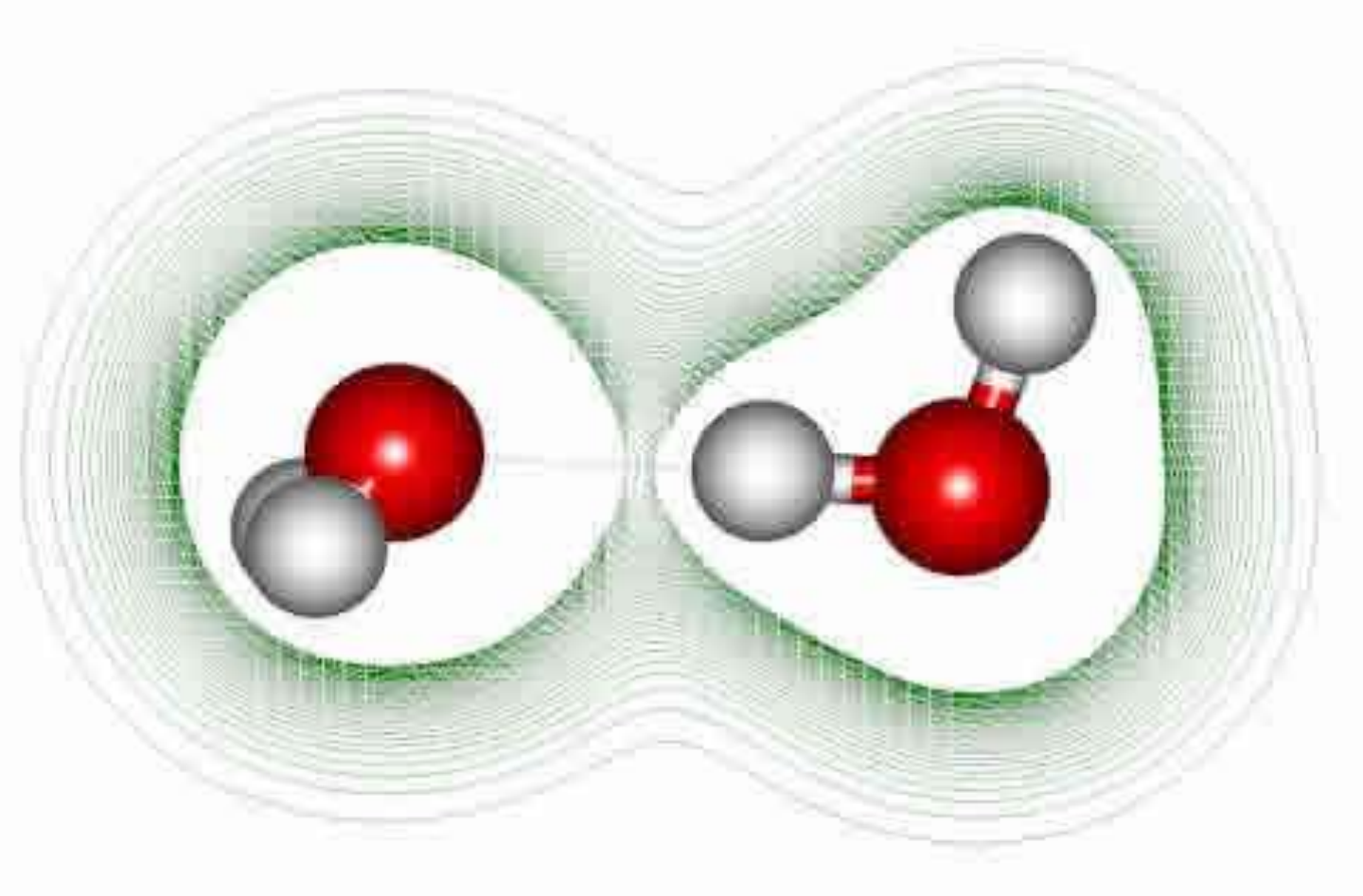
- Molecular structure
- Supramolecular structure
- Solutes
  - Ionic
  - Polar
  - Nonpolar (the hydrophobic effect)

Water Molecular Structure





The Hydrogen Bond



(http://www.martin.chaplin.btinternet.co.uk/molecule.html)

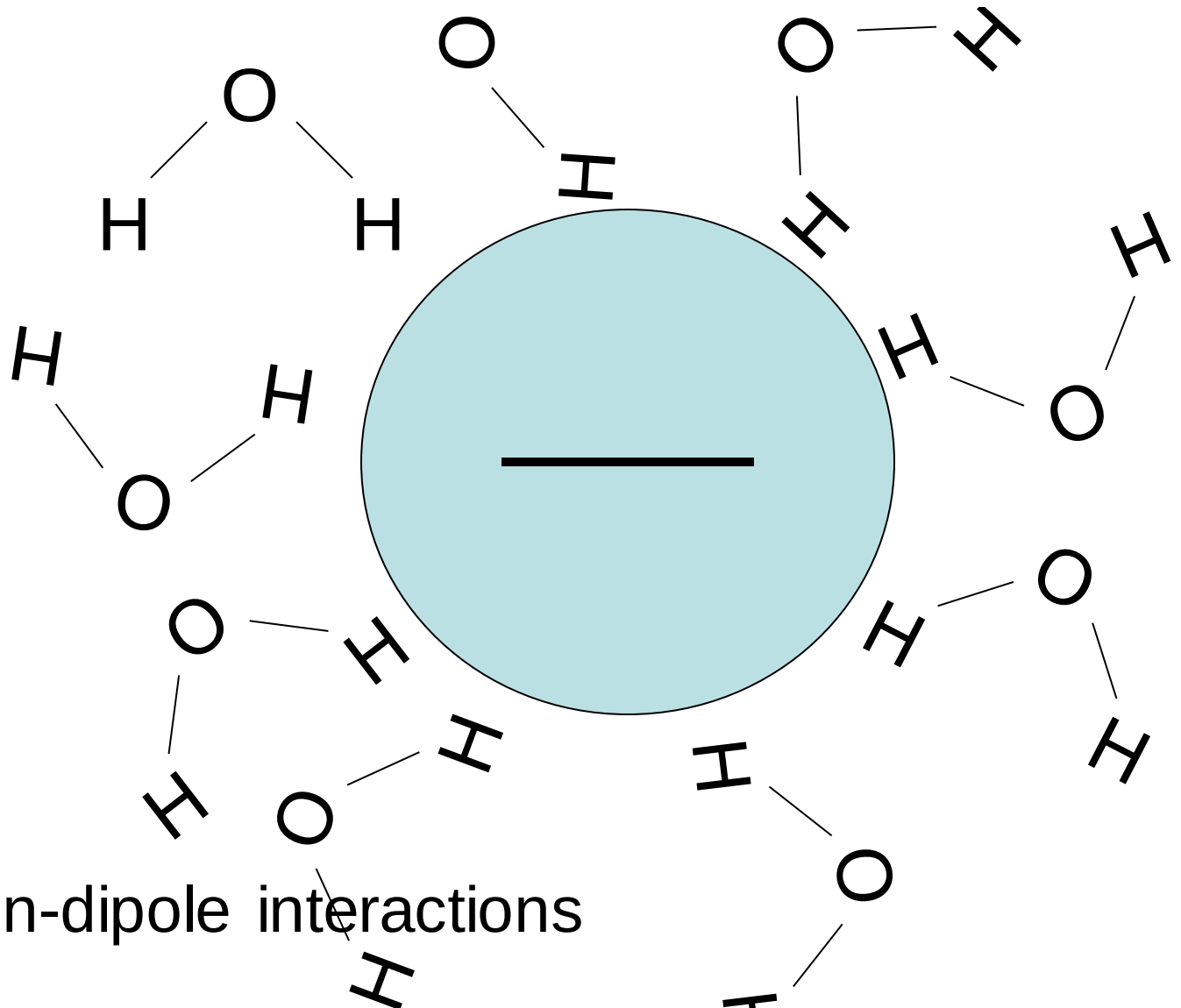
Tetrahedral Structure of Water

- The lone pairs and bonding electrons repel one another
- The OH bonds are highly polarized
- Strong H-bonds (~10% of covalent bond)
- Each water molecule can hydrogen bond to two neighbors allowing the formation of an extensive 3D structure
- http://wps.prenhall.com/wps/media/objects/439/449969/Media_Portfolio/Chapter_08/FG08_13.JPG

Supramolecular Structure of Water

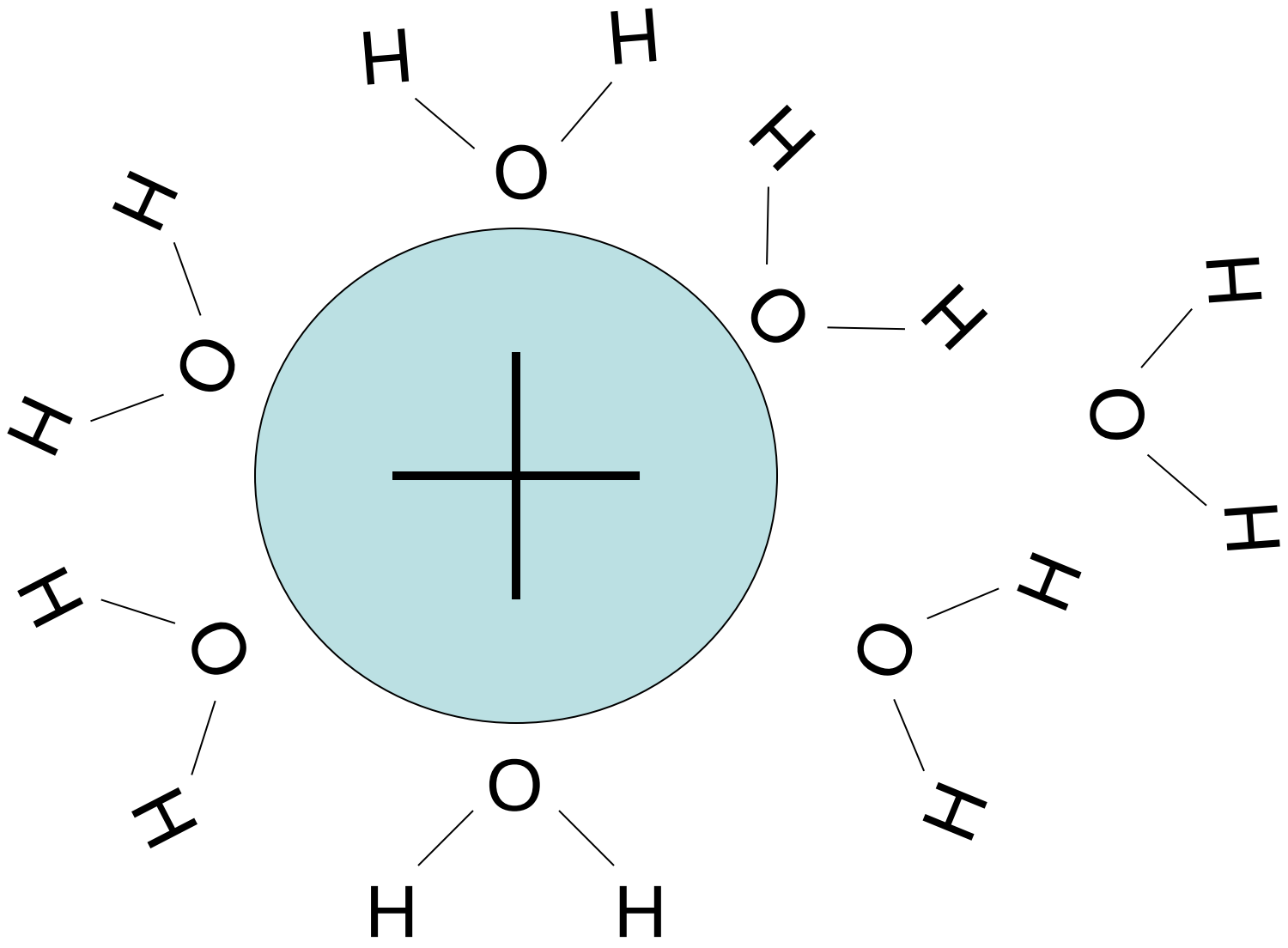
- Water is highly hydrogen bonded (only about 15% of H-bonds break on melting ice)
- The bonds form and break dynamically
- Strong affinity of water for itself
- High specific heat (to warm water must break some H-bonds)

Ionic Solutes



- Ion-dipole interactions

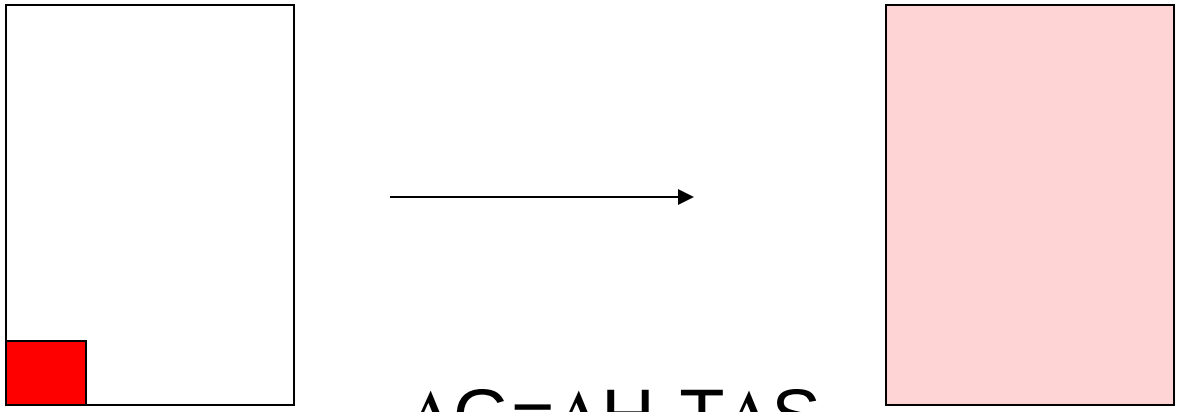
Ionic Solutes



Polar Solutes

- Hydrogen bonds
- Dipole-dipole attractions

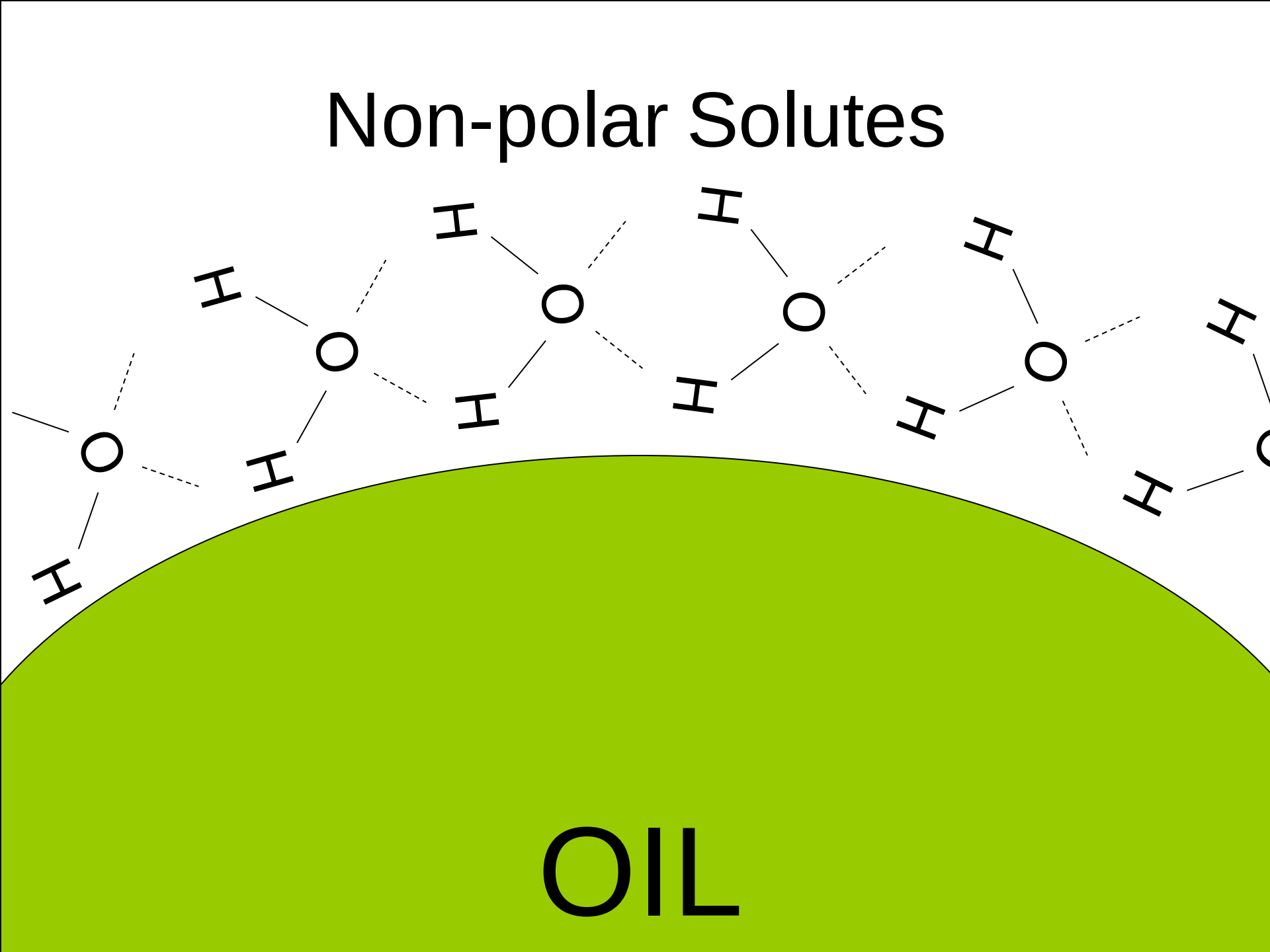
Thermodynamics of Binding



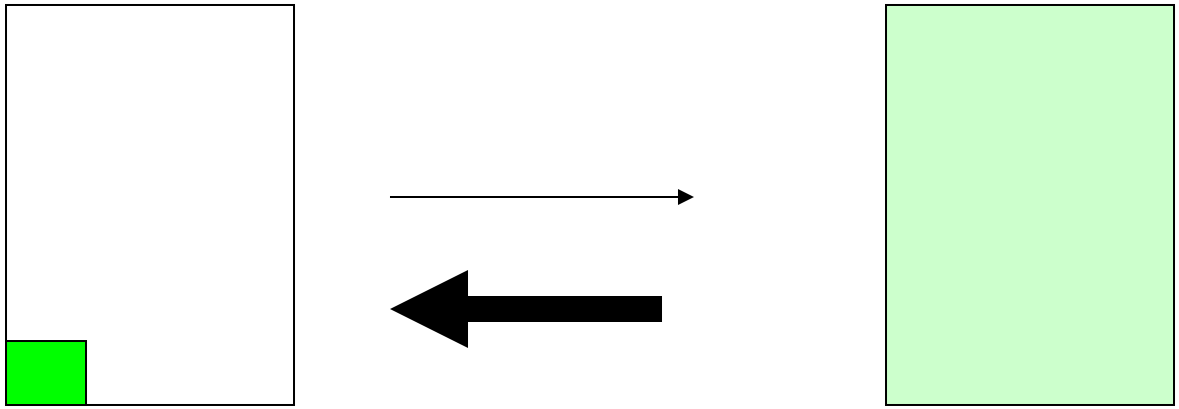
$\Delta G = \Delta H - T\Delta S$

- Entropy cost to solvent ($\Delta S < 0$, $-T\Delta S > 0$)
- STRONG Enthalpy gain to solvent ($\Delta H < 0$)
- Net $\Delta G < 0$; reaction proceeds

Non-polar Solutes

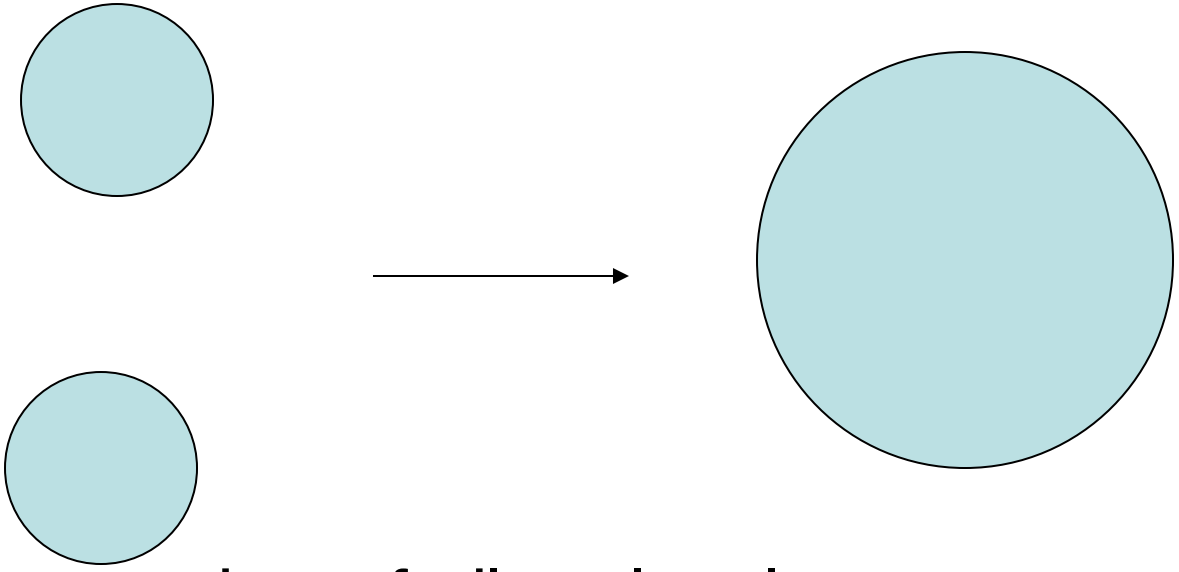


Non Polar Solutes



- Weak transcient dipole (Van der Waals attraction)
- Strong structuring of water into a hydrogen bonded clathrate cage – entropy cost

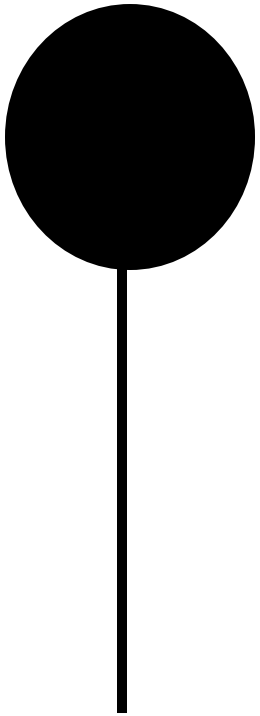
The Hydrophobic Effect



- Same number of oil molecules
- Less surface oil molecules
- Fewer order “clathrate cage” water molecules

$\Delta G<0$, droplets tend to merge

Small Molecule Surfactants

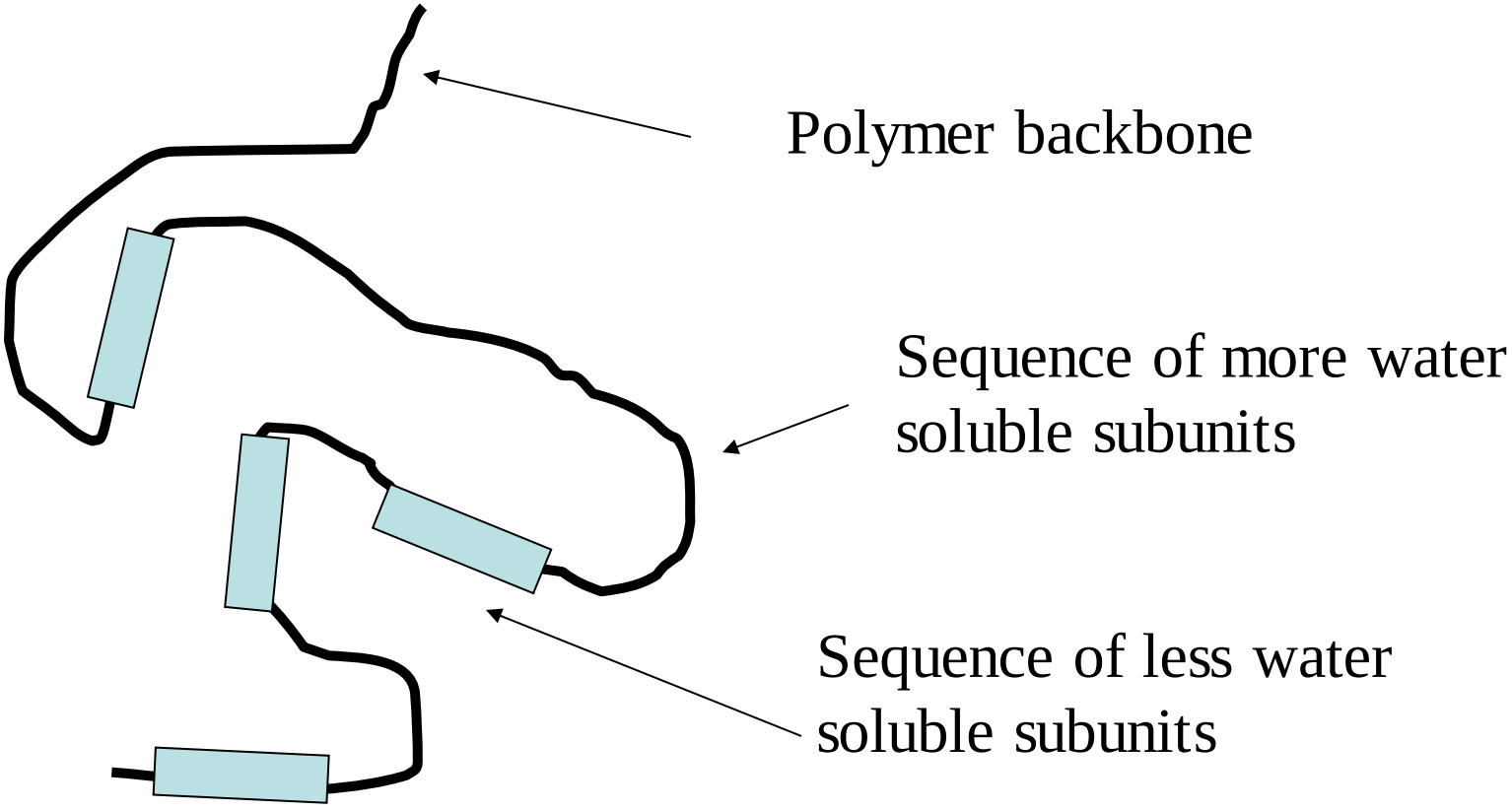


Hydrophilic head group (charged or polar)

Hydrophobic tail (non-polar)

- Micelles and membranes
- Surface activity

Amphiphilic Polymers



- Spontaneous folding
- Surface activity