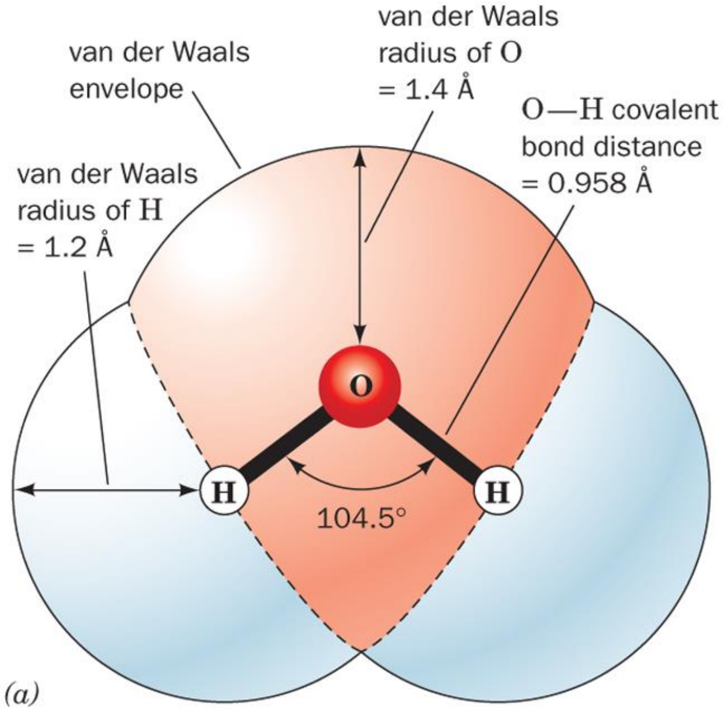
Introduction to Biochemistry

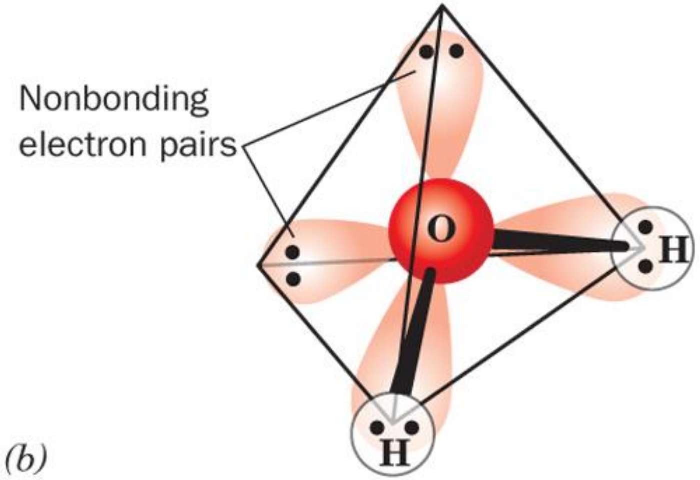
Part 1: Physical and Chemical Properties of Water

Dr. Matthew Lafrenière

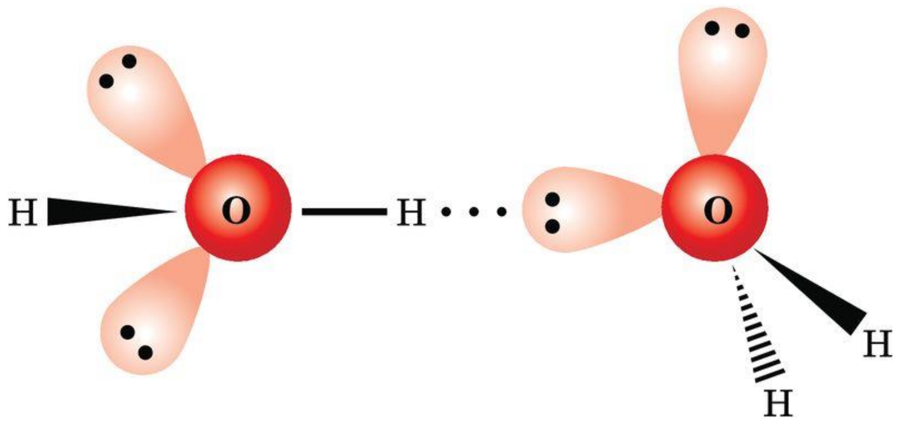
21 May 2019

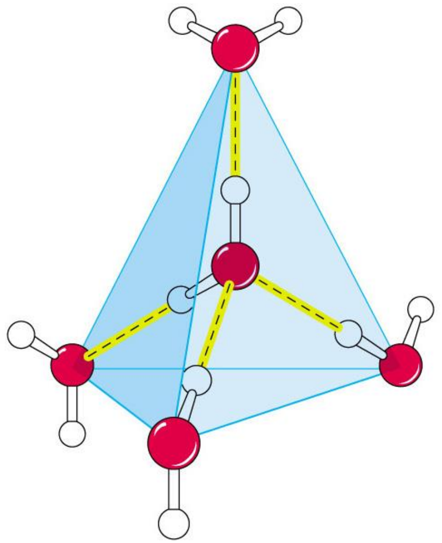
The Properties of Water

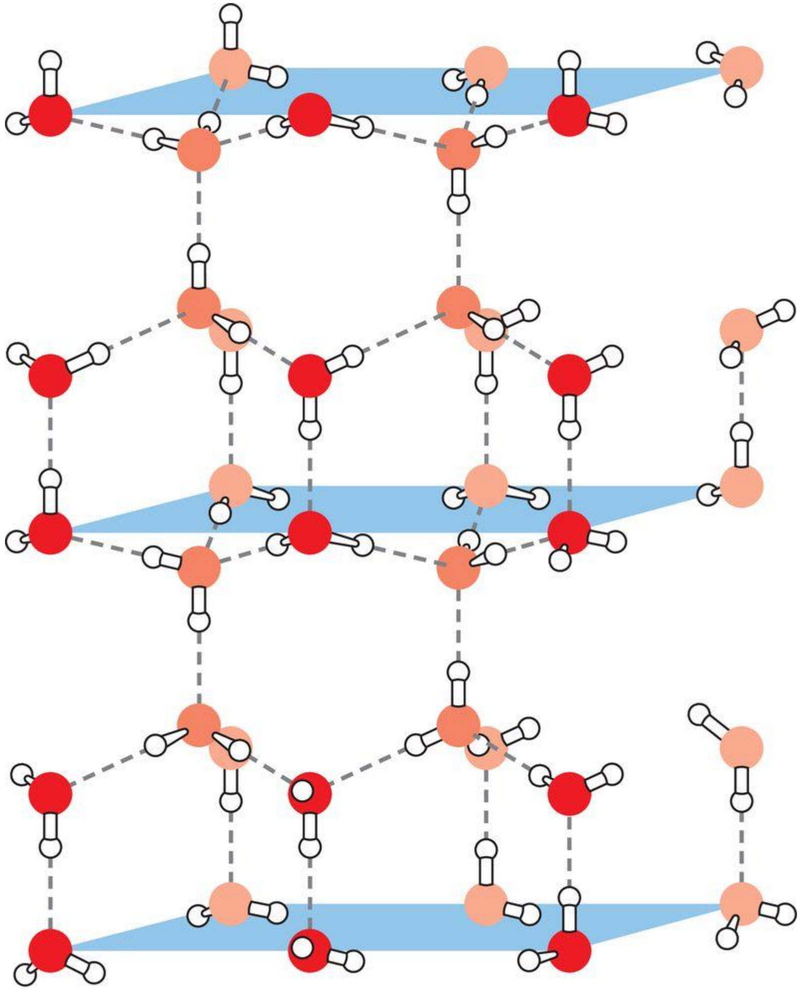




The Properties of Water



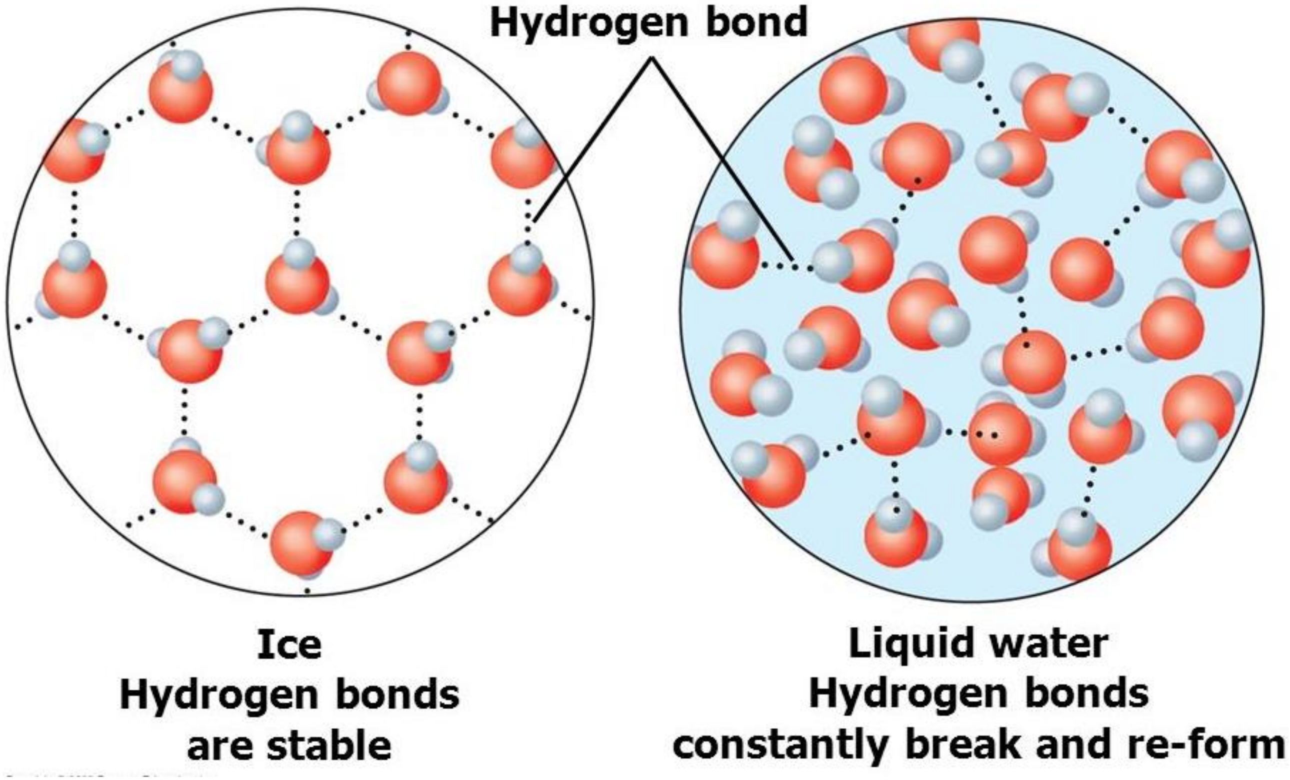




After Liu, K., Cruzan, J.D., and Saykally, R.J., Science 271, 929 (1996).

The Properties of Water

- Given the structure of water and its ability to form hydrogen bonds (on the previous slide), there are a few additional properties of water:



- Hydrogen bonding is the principle cause of all of these properties!

The Solvent Properties of Water

- The most valuable property of water is its ability to dissolve "like" molecules (water is considered a **universal solvent** – the ability to dissolve or dissociate compounds)
  - This is due to water's ability to form hydrogen bonds with polar and charge molecules (ions and hydrophilic solvents dissolve readily in aqueous environments)

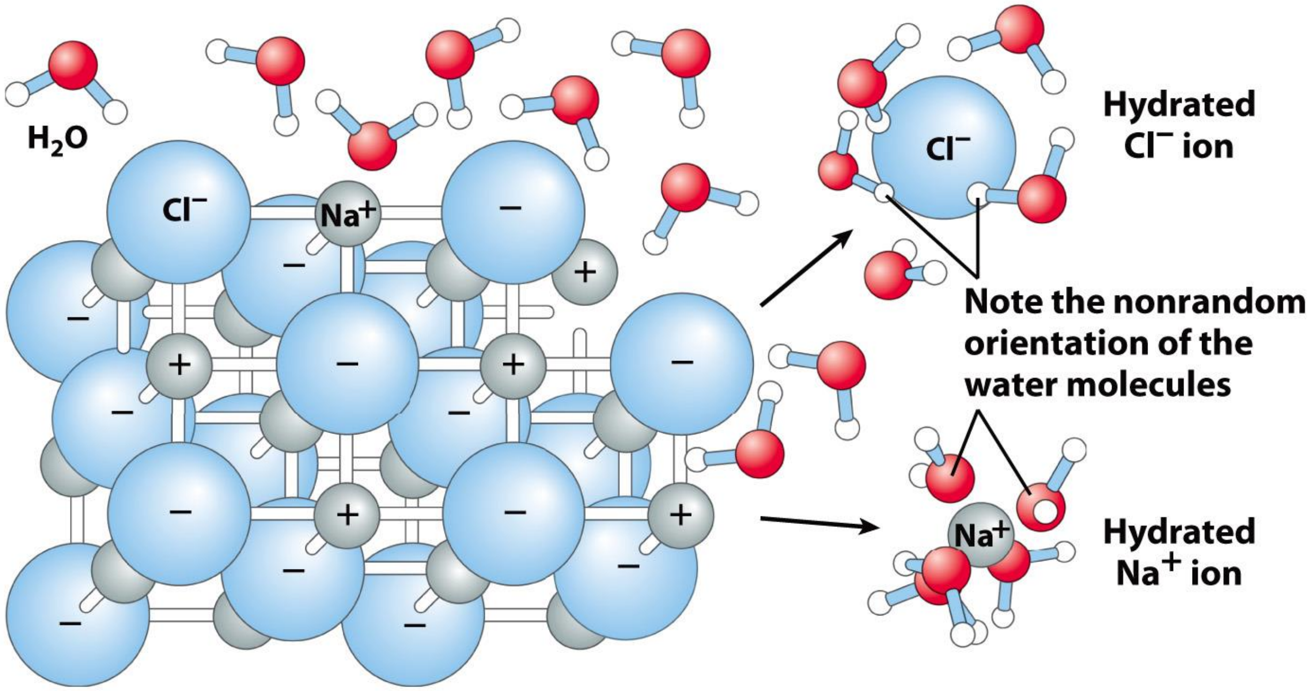


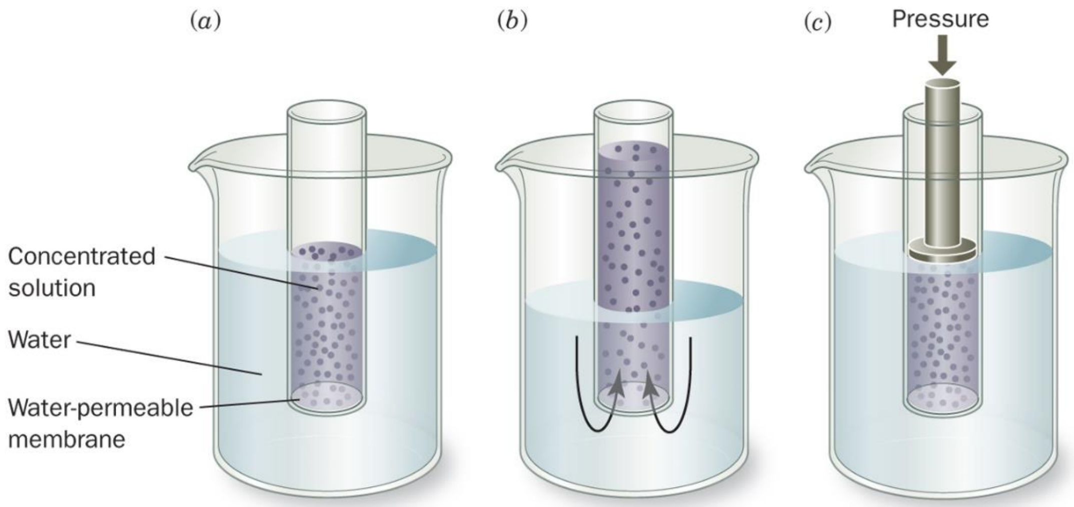
Figure 2-6
Lehninger Principles of Biochemistry, Seventh Edition

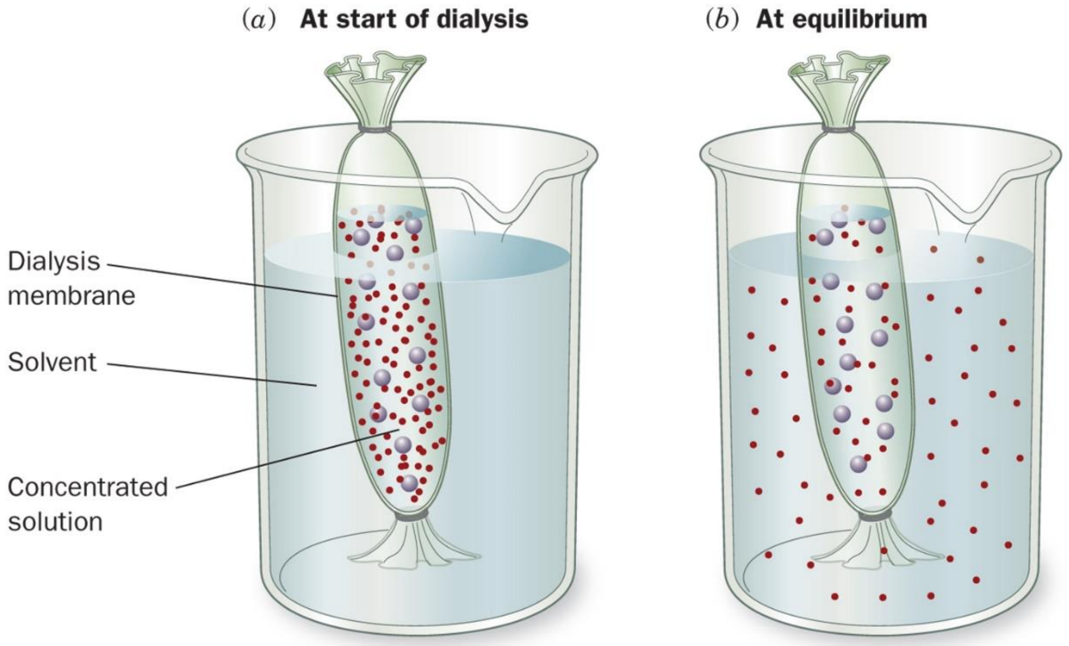
Solvent	**dielectric constant**
hexane	1.9
benzene	2.3
diethyl ether	4.3
$CHCl_3$	5.1
acetone	21.4
Ethanol	24
methanol	33
H_2O	80
HCN	116

http://riessayrggg.riverbendrestoration.us/water-as-a-universal-solvent.html

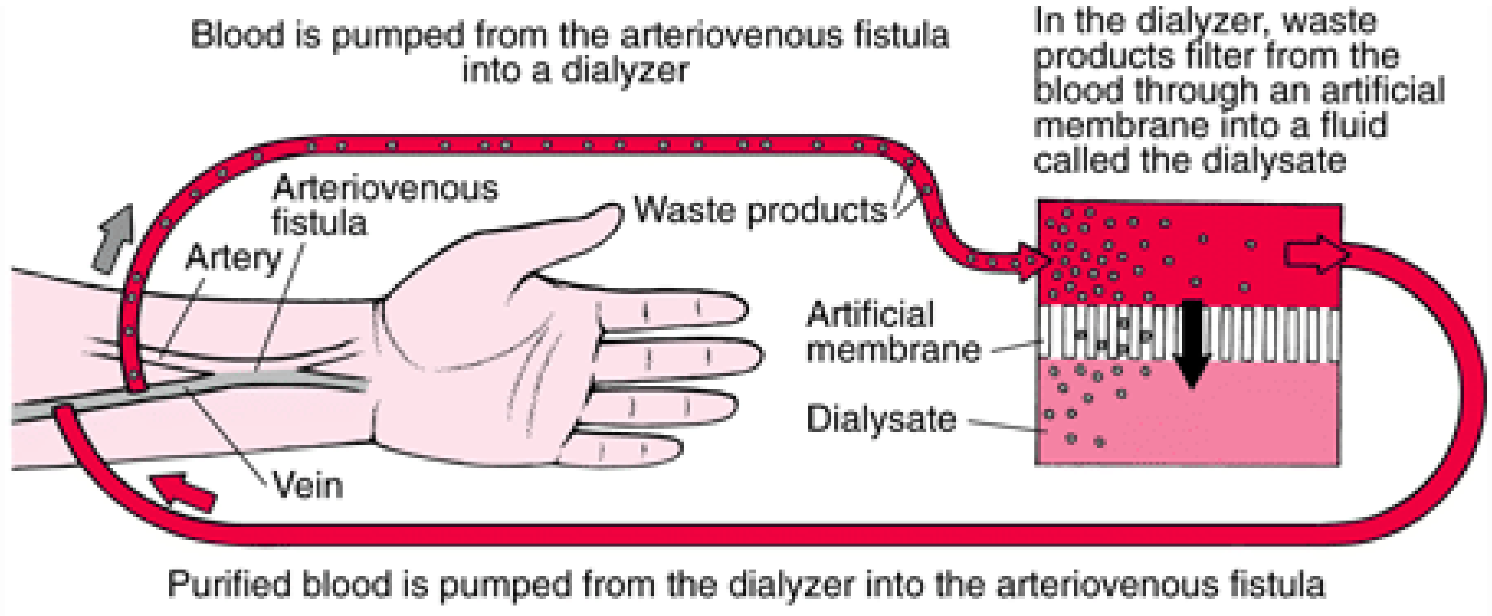
The Solvent Properties of Water

- In addition to the properties outlined in the previous slides about water, we need to also discuss **osmosis** and **diffusion**.
  - **Osmosis:** the movement of water form high to low concentration
  - **Diffusion:** the movement of solute





Osmosis in The Clinic

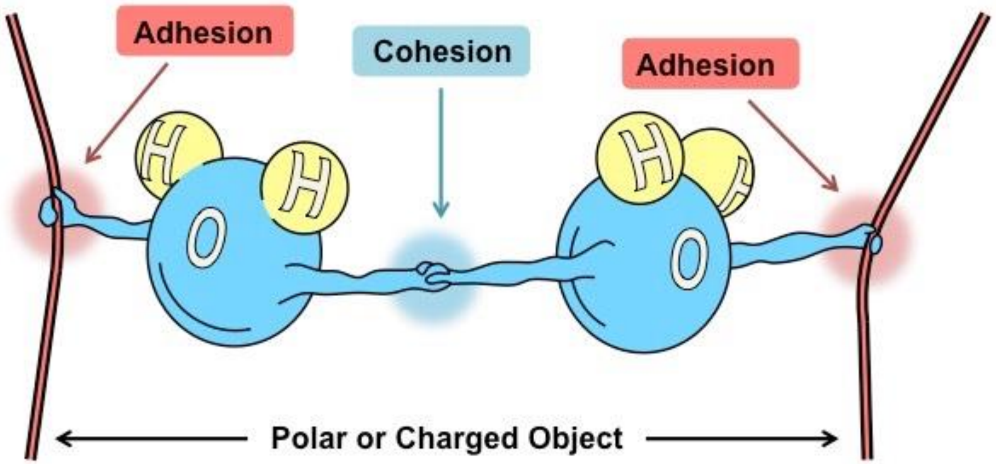


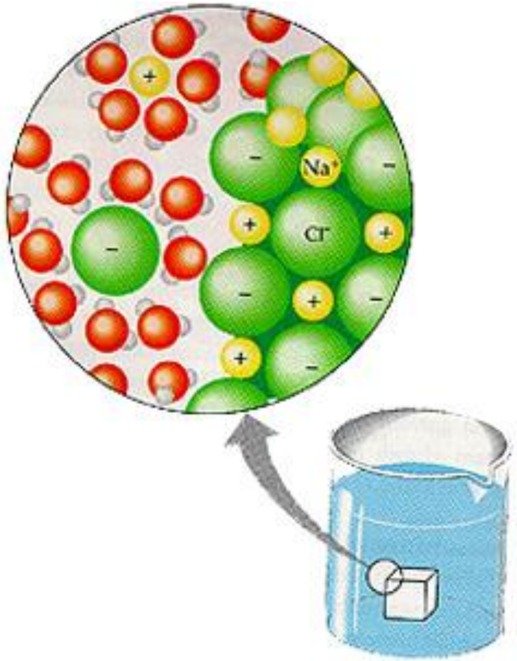
Hemodialysis

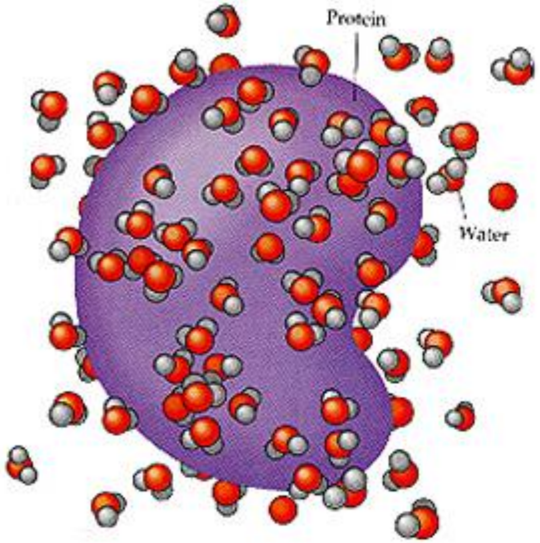
https://www.merckmanuals.com/en-ca/home/kidney-and-urinary-tract-disorders/dialysis/dialysis

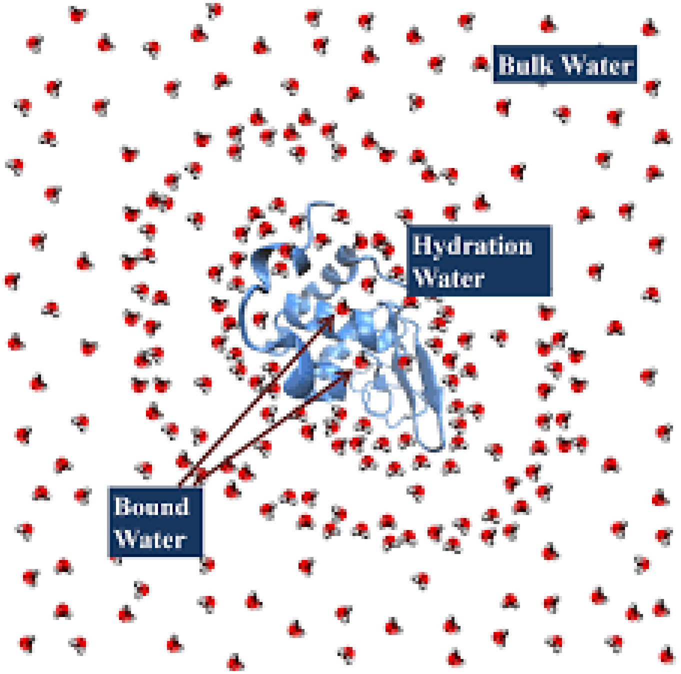
The Properties of Water

- Given the polarity of water, water has both cohesive and adhesive properties:
  - **Adhesion:** The ability of a substance to stick to an “unlike” substance
  - **Cohesion:** The various intermolecular forces that hold solids and liquids together (consider **surface tension**)









https://prezi.com/nwg988l0knjs/properties-of-water; http://www.bio.miami.edu/dana/226/226F08_9print.html; http://people.du.ac.in/~pbiswas/research.html

Intermolecular Forces: Biomolecular Shapes & Interactions

- The shapes and interactions of biomolecules (DNA, RNA, and proteins) are determined not only by the properties of water discussed on the previous slides but also intermolecular forces.

- Below is an a key point to consider in biochemistry (and this is linked to the structure/function paradigm in biochemistry):

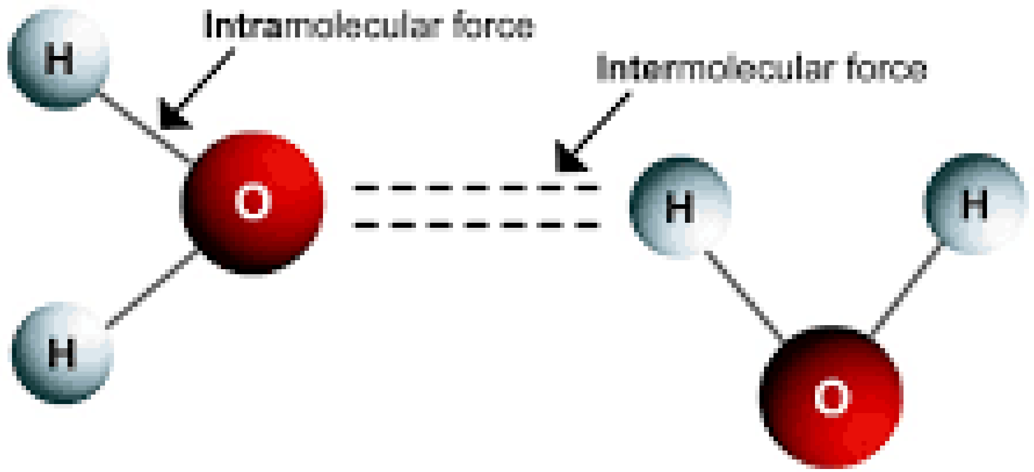


TABLE 2-1 Bond Energies in Biomolecules

Type of Bond	Example	Typical Bond Energy ($kJ \cdot mol^{-1}$)
Covalent	O—H	460
	C—H	414
	C—C	348
Noncovalent		
Ionic interaction	$—COO^{-} \cdots {}^{+}H_3N—$	86
van der Waals forces		
Hydrogen bond	$—O—H \cdots O<$	20
Dipole–dipole interaction	$>C=O \cdots >C=O$	9.3
London dispersion forces	$—CH_2—H \cdots H—CH_2—$	0.3

https://slideplayer.com/slide/8733835/

Intermolecular Forces: Ionic Interactions

- **Electrostatic interactions:** the attractive or repulsive forces between charges

Intermolecular Forces: Hydrogen Bonding

- **Hydrogen bonding:** An electrostatic attraction between the lone-pair of election on an atom and the hydrogen atom on another molecule (which is covalently bound to the a more electronegative atom).

Intermolecular Forces: Hydrogen Bonding

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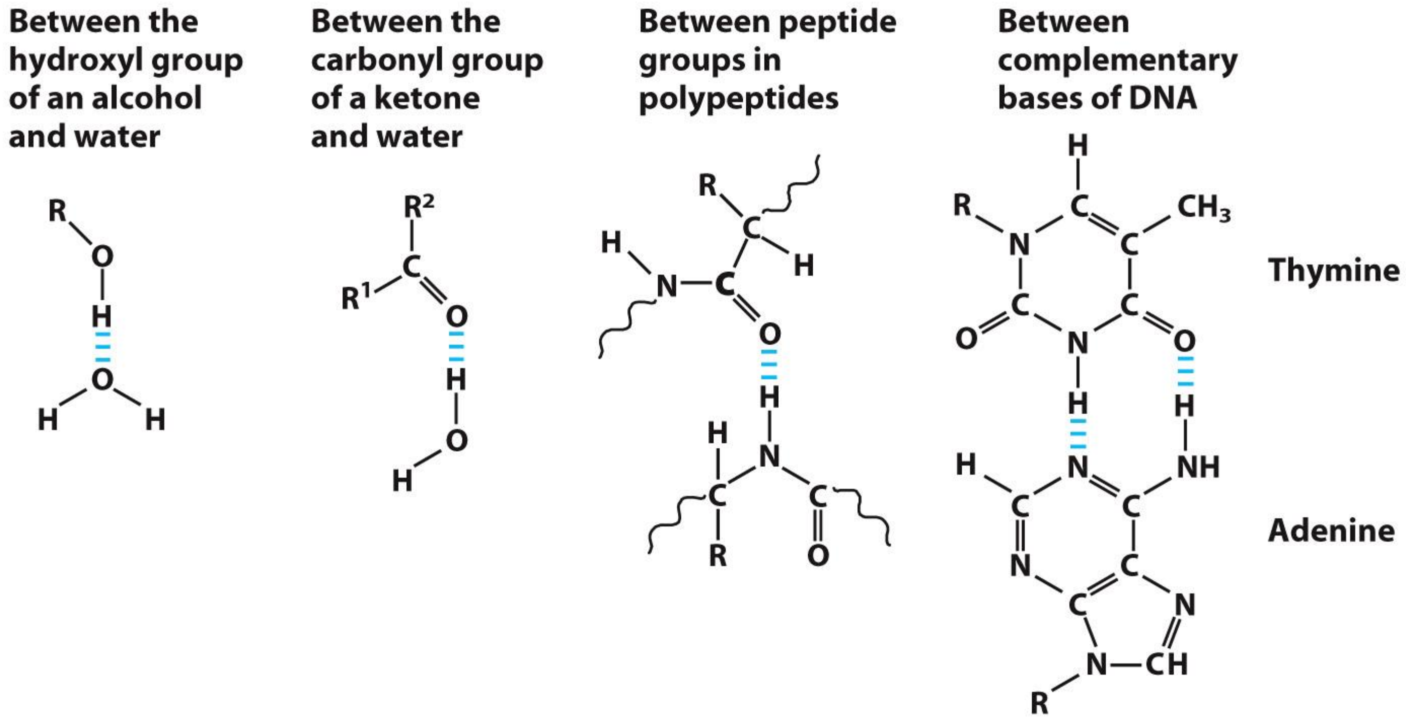


Figure 2-4
Lehninger Principles of Biochemistry, Seventh Edition

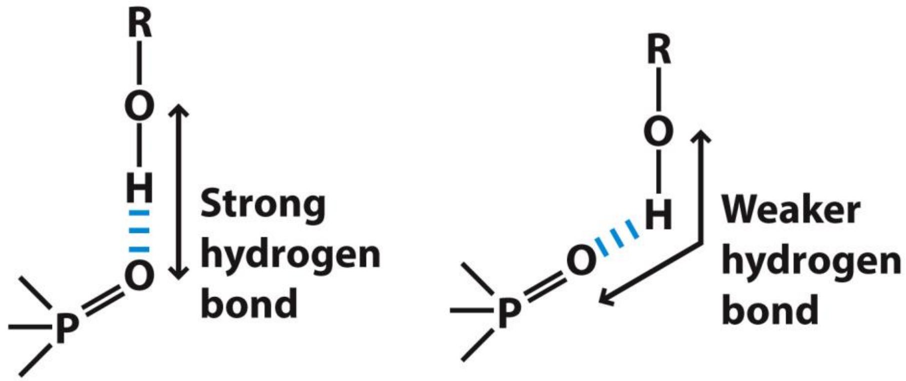
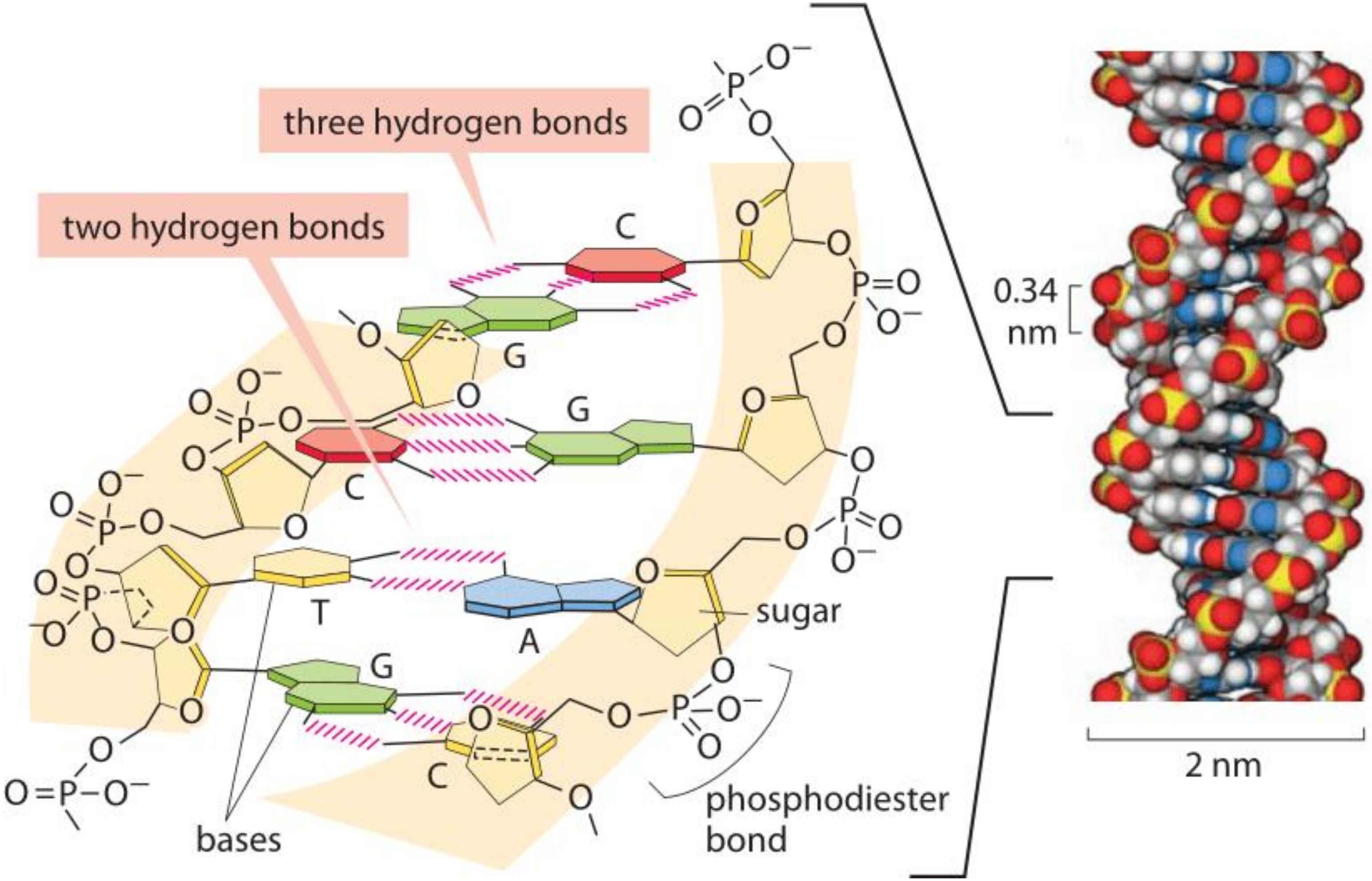


Figure 2-5
Lehninger Principles of Biochemistry, Seventh Edition

Intermolecular Forces: Hydrogen Bonding

- **Hydrogen bonding:** An electrostatic attraction between the lone-pair of election on an atom and the hydrogen atom on another molecule (which is covalently bound to the a more electronegative atom).



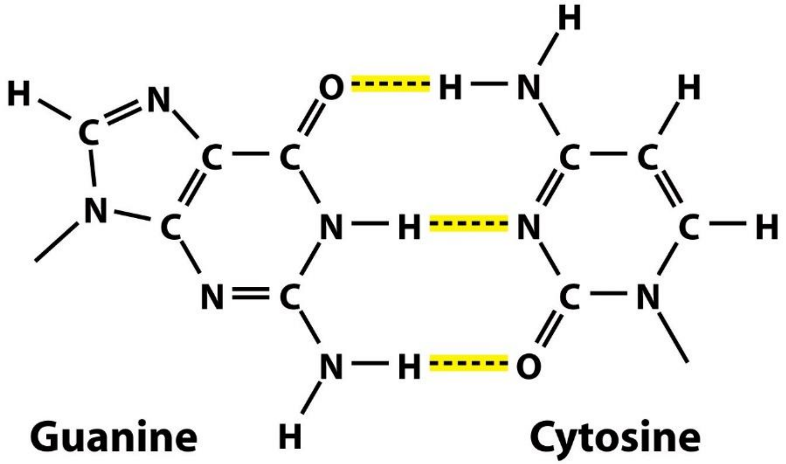


Figure 2-11 Principles of Biochemistry, 4/e
© 2006 Pearson Prentice Hall, Inc.

http://book.bionumbers.org/what-is-the-energy-of-a-hydrogen-bond/

Intermolecular Forces: Hydrogen Bonding

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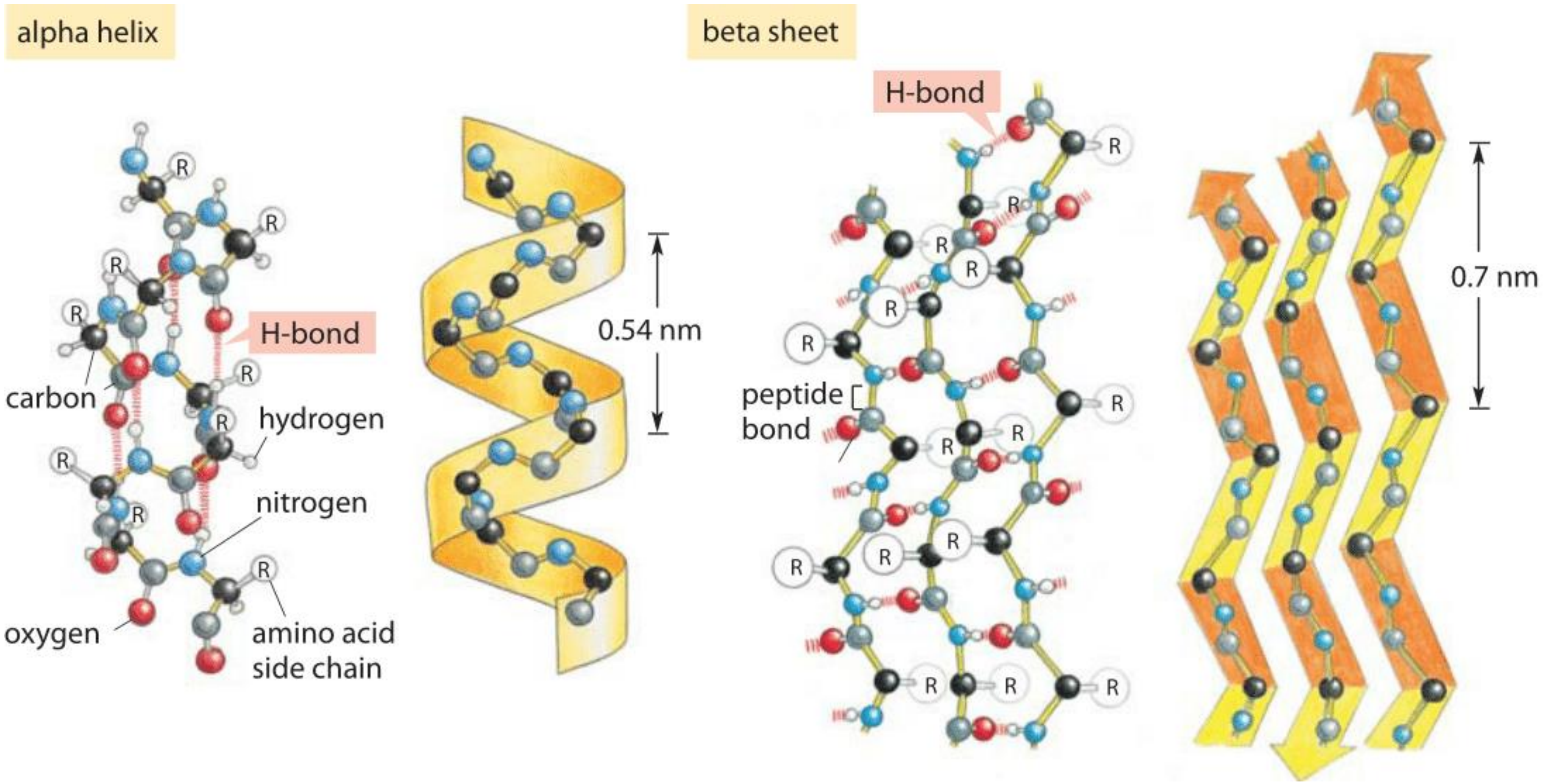
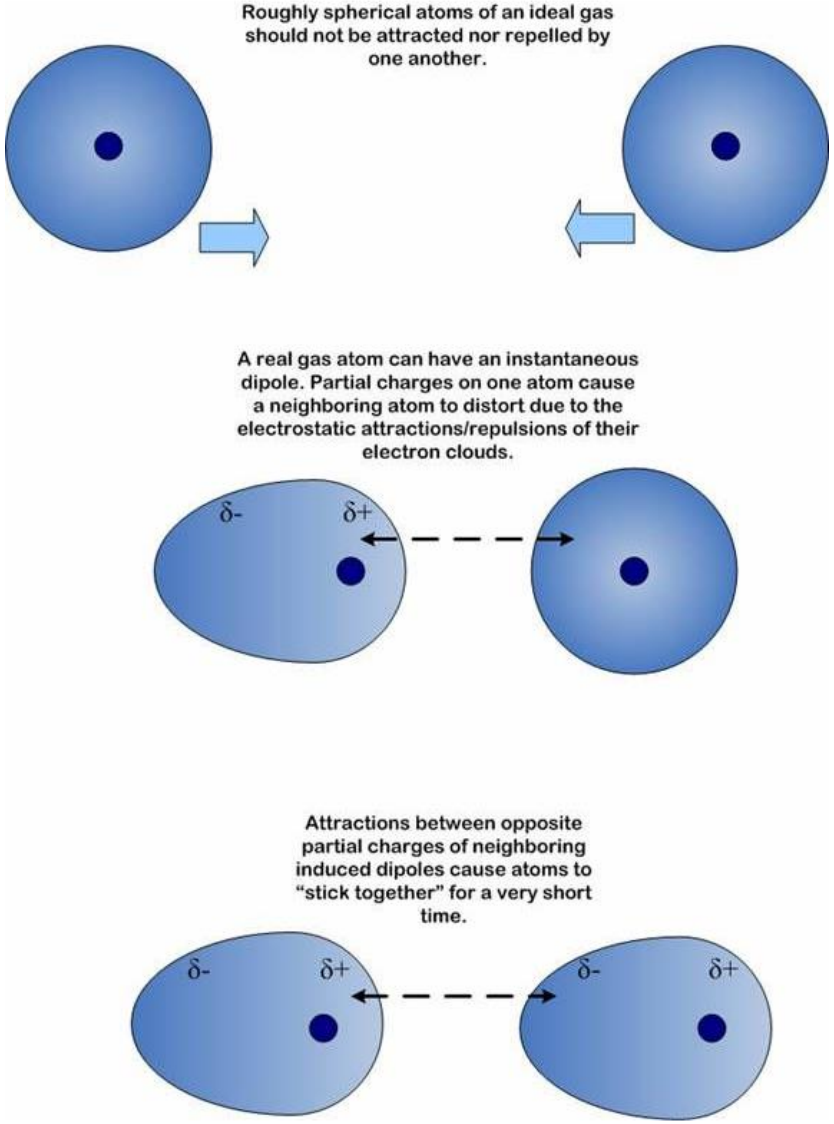


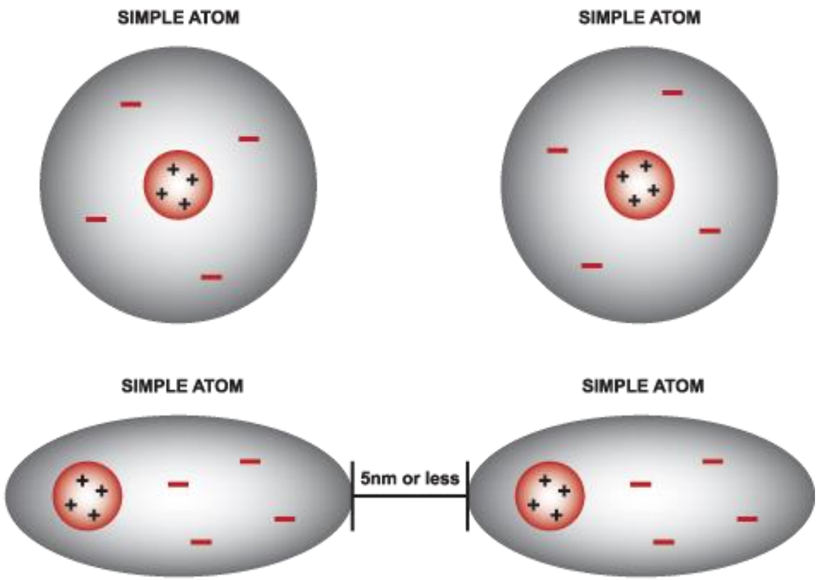
http://book.bionumbers.org/what-is-the-energy-of-a-hydrogen-bond/

Intermolecular Forces: Van der Waals interactions

- **Van der Waals:** Attractive force exists between any pair of electrons – even those which have no permanent dipole moments.

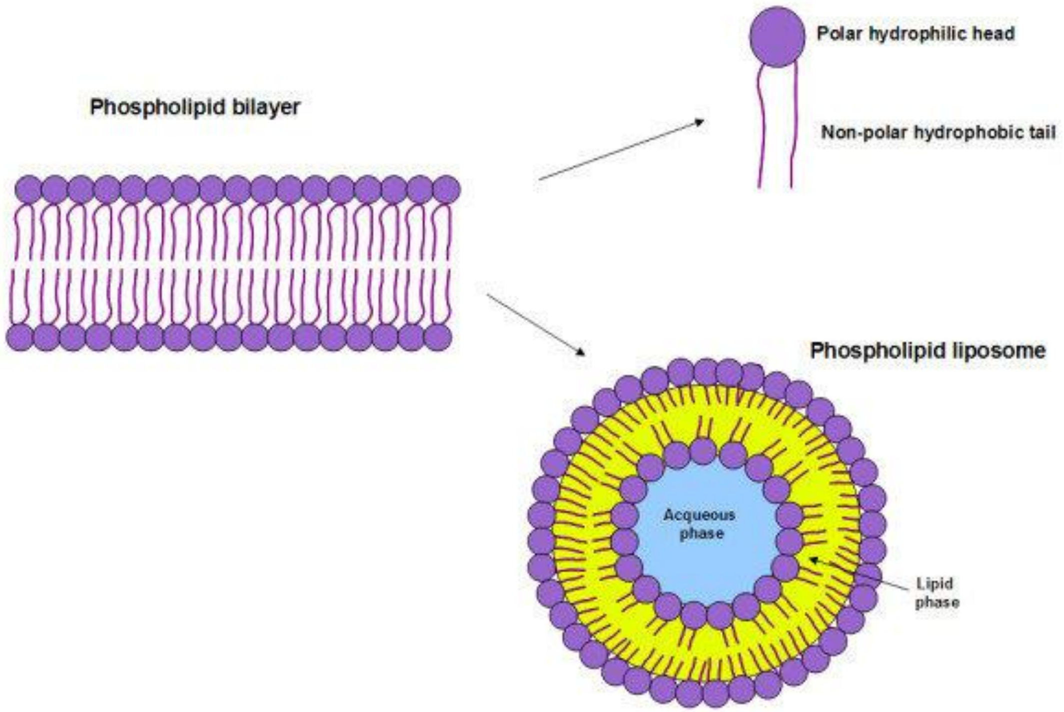
Fritz London (1990-1954)

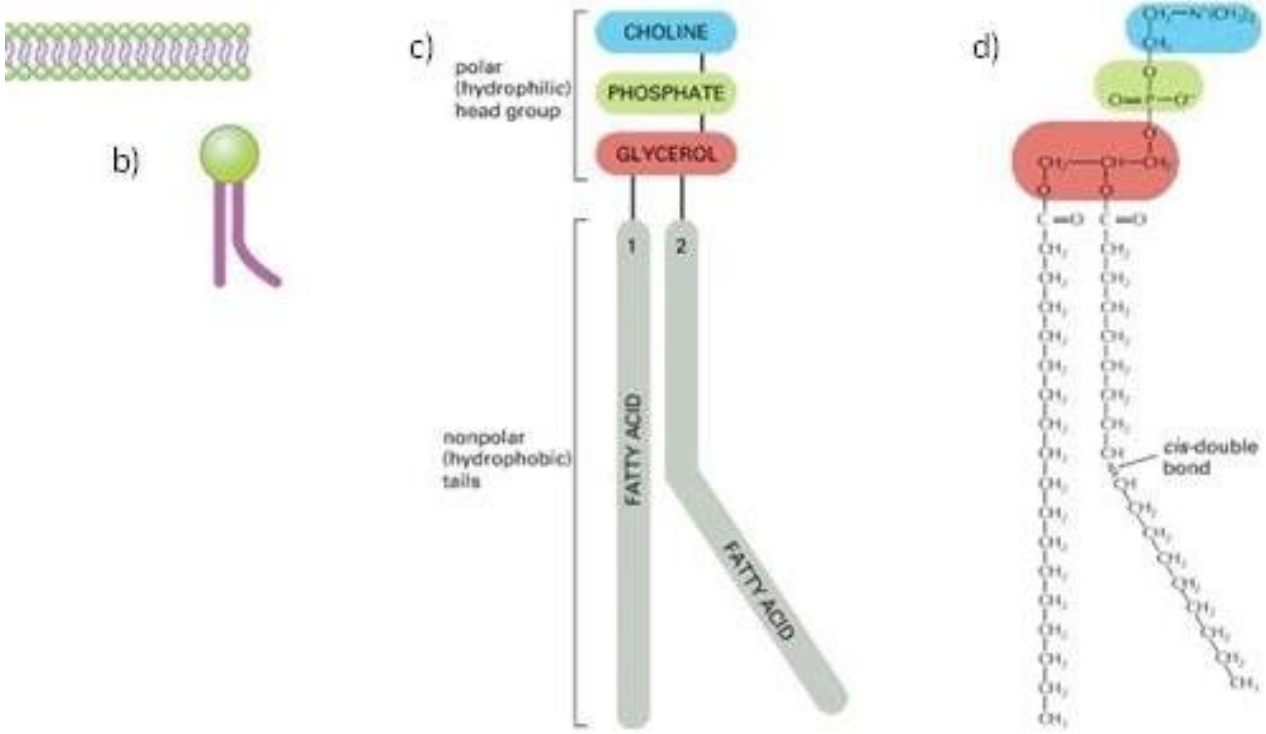




https://www.zmescience.com/science/physics/direct-measurement-of-van-der-waals-force-made-for-the-first-time/

Intermolecular Forces: Van der Waals interactions





https://www.researchgate.net/figure/a-The-typical-plasma-membrane-is-a-phospholipid-bilayer-b-A-single-phospholipid_fig1_281556431; https://www.researchgate.net/figure/Phospholipid-bilayer-composed-of-hydrophobic-non-polar-tails-and-hydrophilic-polar-heads_fig1_51980719

Intermolecular Forces are Important in Biochemistry

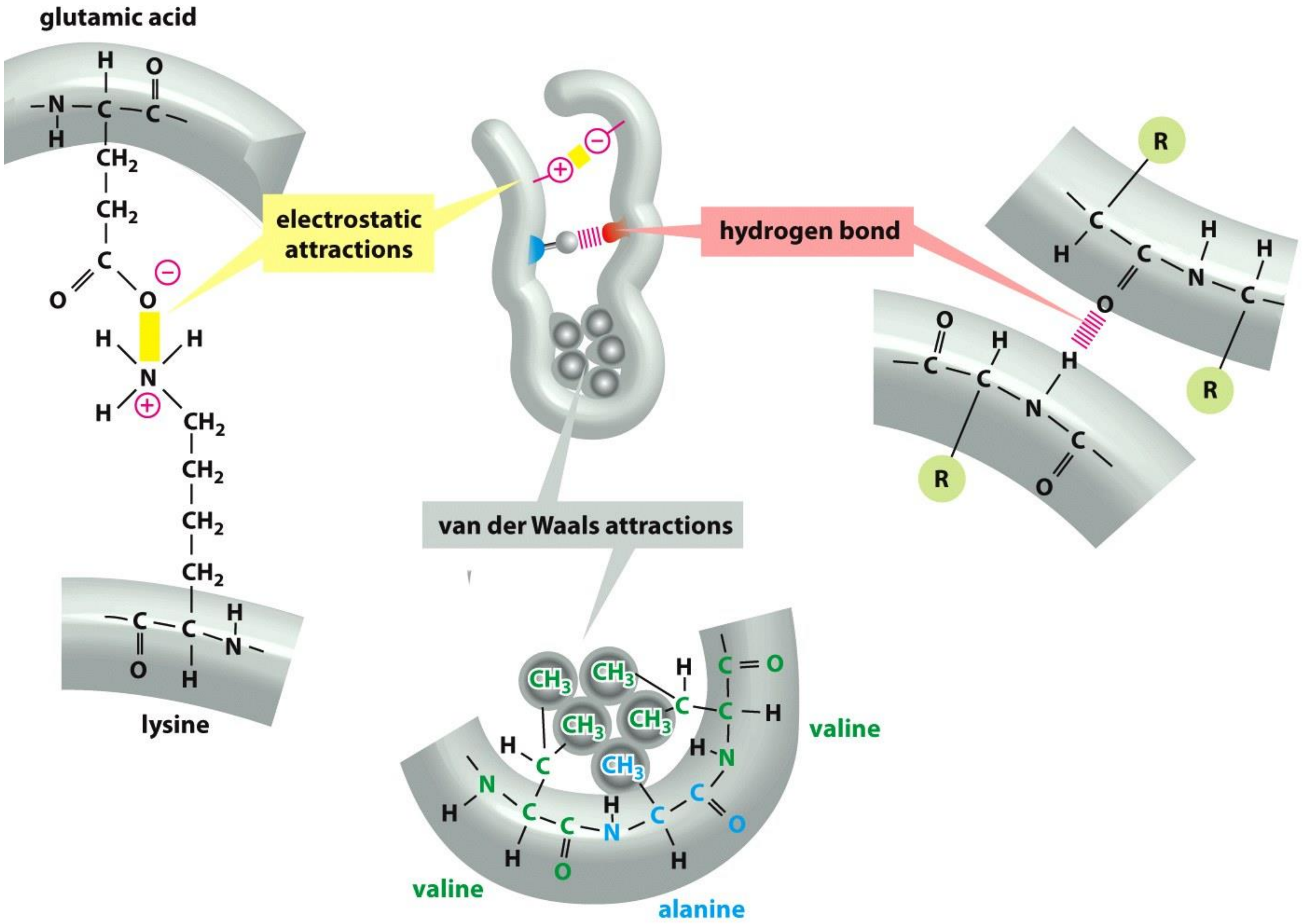
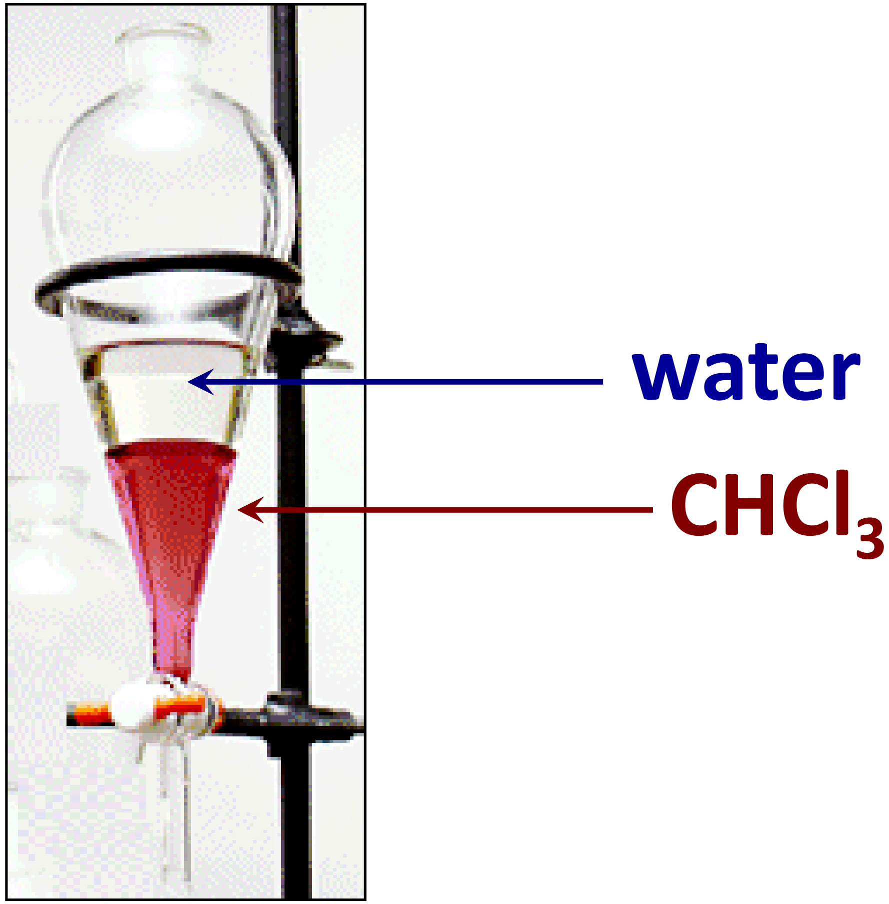
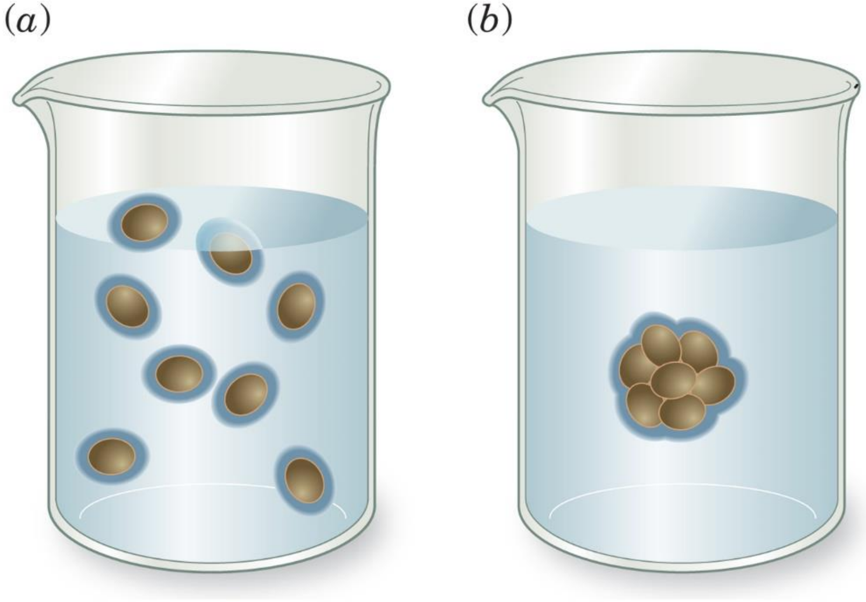


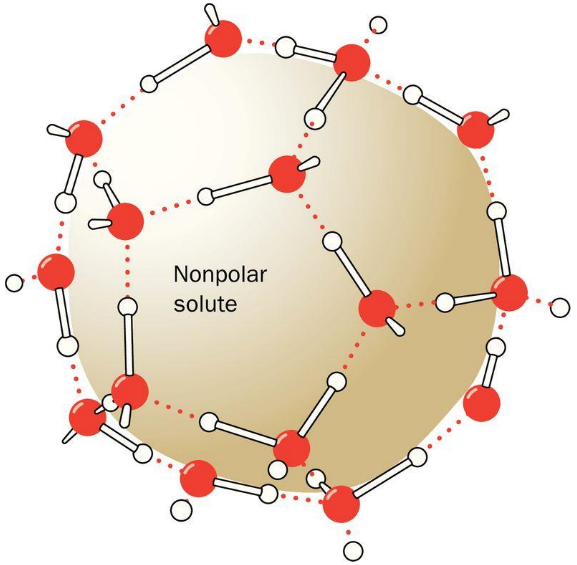
Figure 4-4 Essential Cell Biology 3/e (© Garland Science 2010)

Hydrophobic Interactions in Biochemistry

- **Hydrophobic interactions:** the tendency of non-polar substances to aggregate in polar solvents in order to exclude water.



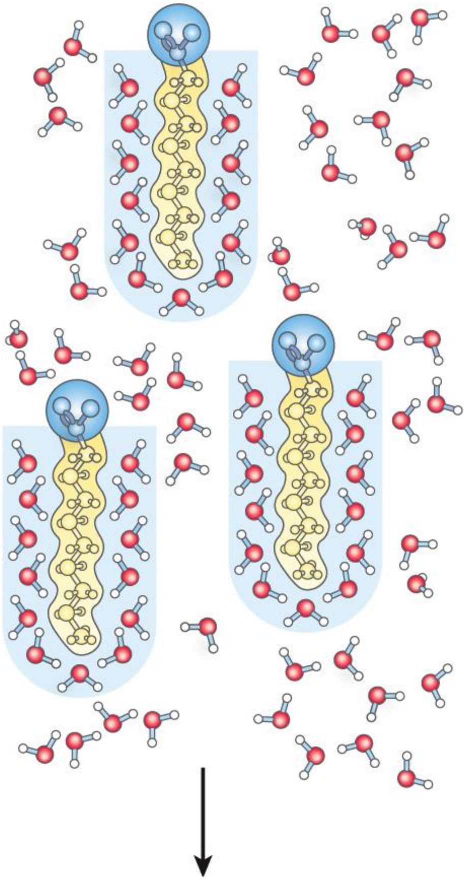




Hydrophobic Interactions in Biochemistry: A Thermodynamic Explanation

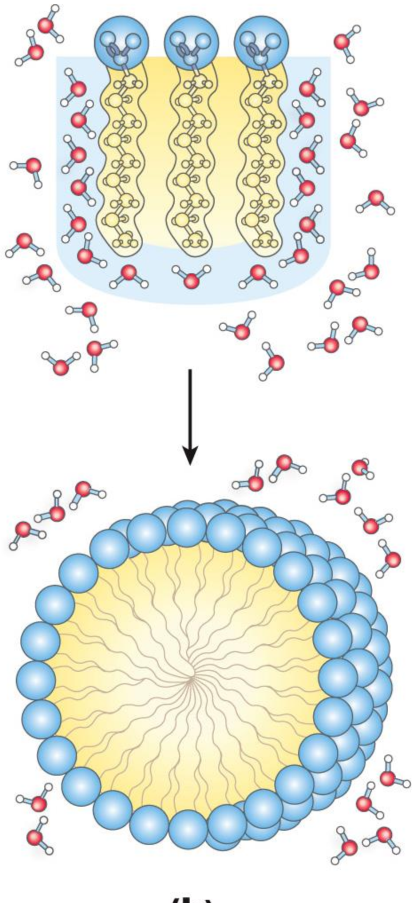
- How can we explain the observation that non-polar oil droplets (or other non-polar residues) tend to “clump” together to exclude water?

Hydrophobic Interactions in Biochemistry: The Micelle



Dispersion of lipids in H_2O

Each lipid molecule forces surrounding H_2O molecules to become highly ordered.



Clusters of lipid molecules

Only lipid portions at the edge of the cluster force the ordering of water. Fewer H_2O molecules are ordered, and entropy is increased.

Micelles

All hydrophobic groups are sequestered from water; ordered shell of H_2O molecules is minimized, and entropy is further increased.

(b)

Hydrophobic Interactions in Biochemistry: Protein-Enzyme Interactions

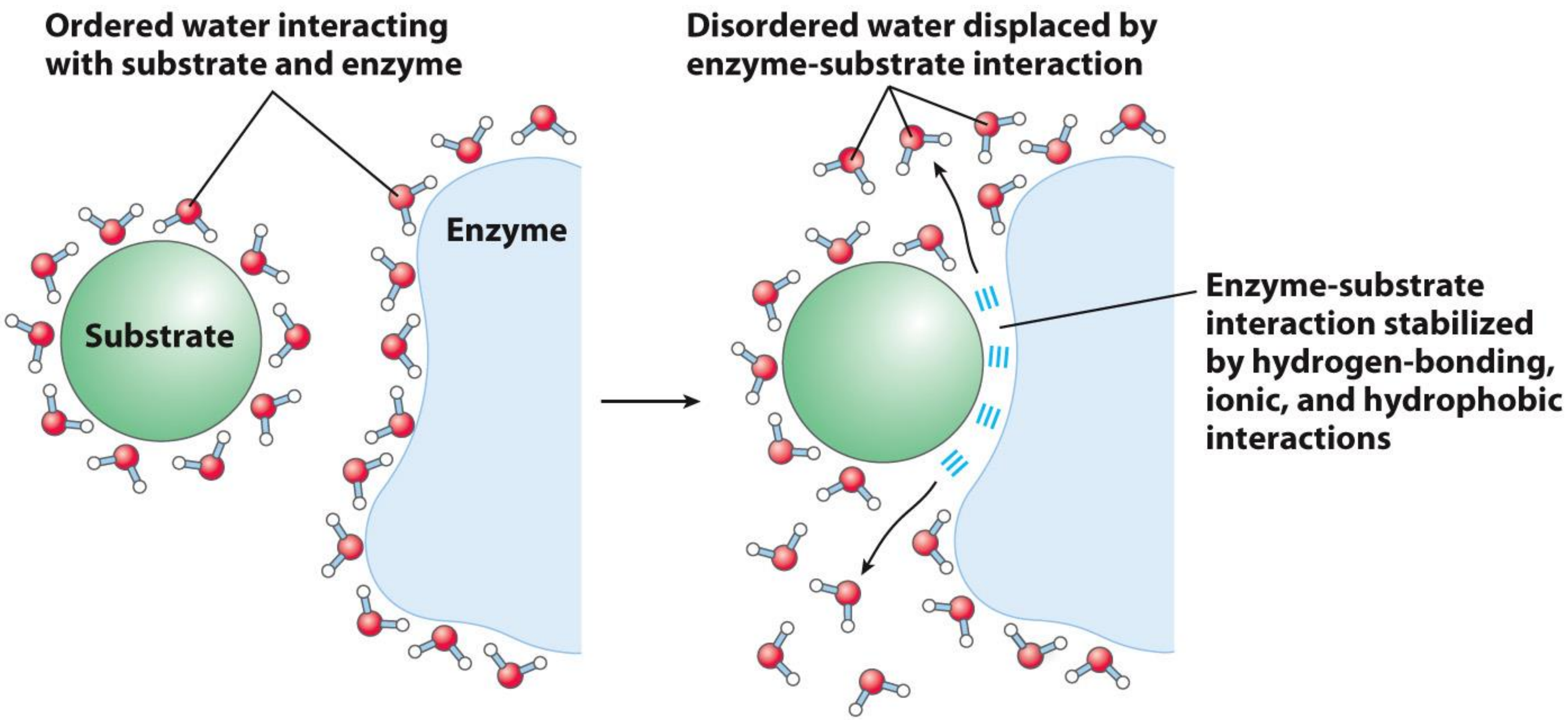


Figure 2-8
Lehninger Principles of Biochemistry, Seventh Edition

Acid-Base Chemistry

- The maintenance (homeostasis) of internal ionic concentration, including pH, is critical for the structure and function of biomolecules.
- **Bronsted Acid:** Proton donor
- **Bronsted base:** Proton acceptor
- **Strong acid (strong base):** nearly completely dissociates (or associates) in solution.
- **Weak acid (weak base):** dissociates (associates) partially, resulting in a measureable equilibrium between the acid (base) and conjugate base (conjugate acid):

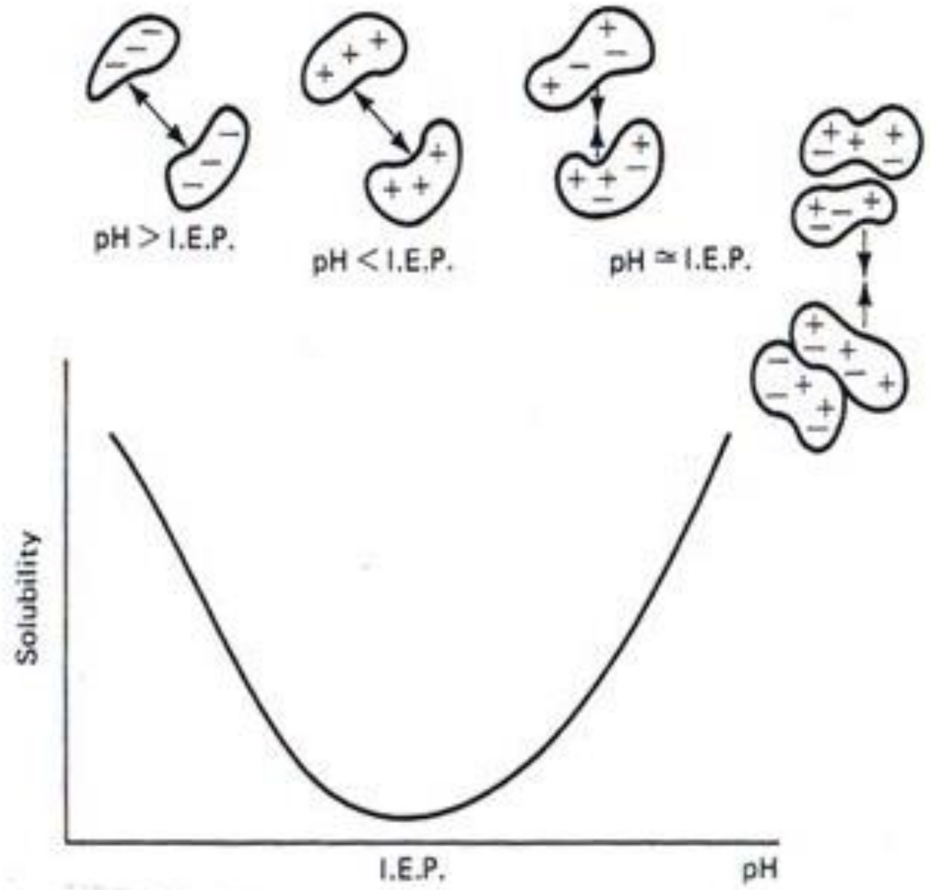


Figure 4.3. Solubility of a globulin-type protein close to its isoelectric point (IEP).

https://slideplayer.com/slide/10252764/

Acid-Base Chemistry: Water Ionization

- Important to note that water can ionize:

- The equilibrium constant for water ionization is:

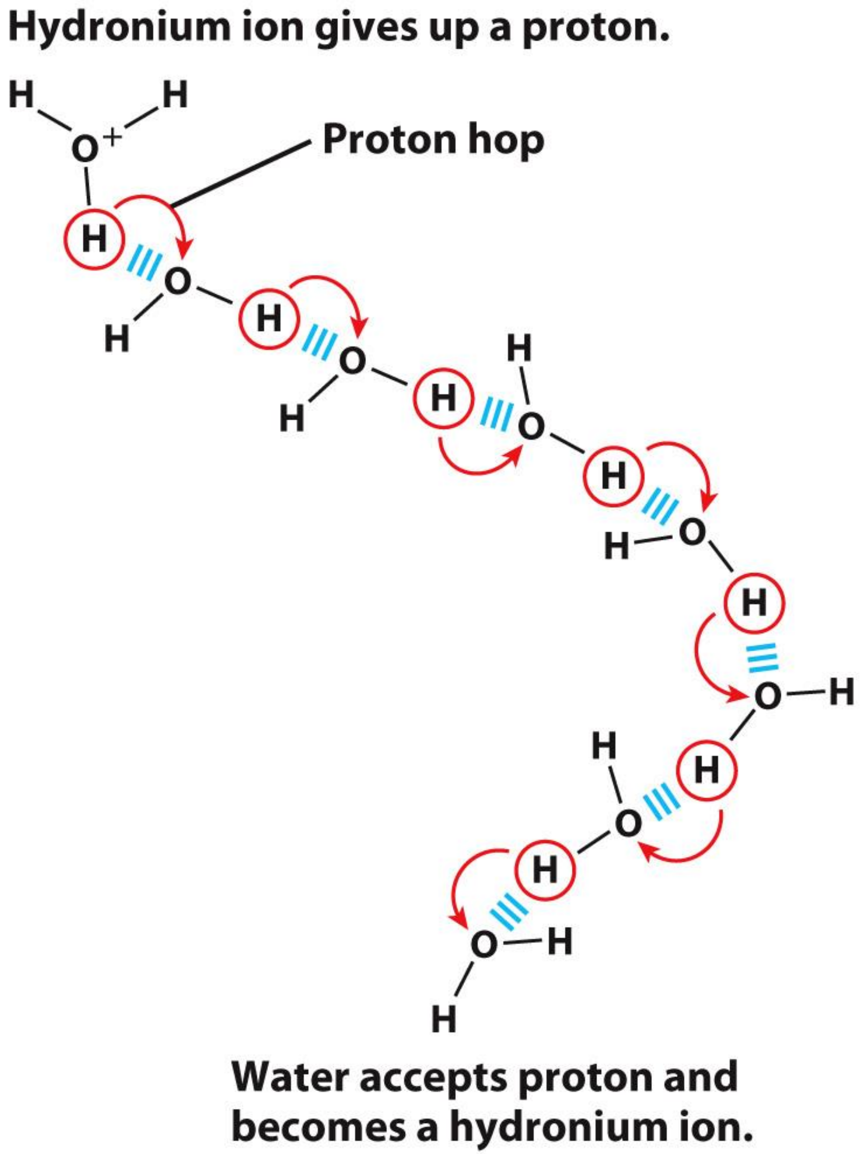
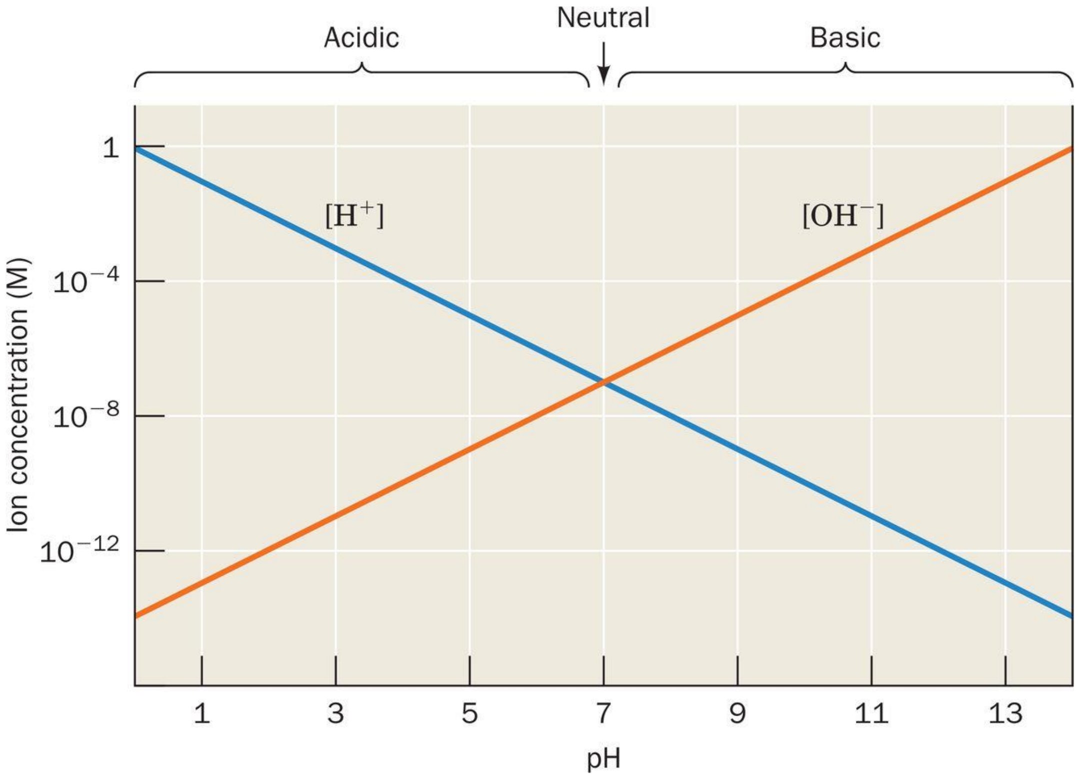


Figure 2-14
Lehninger Principles of Biochemistry, Seventh Edition

Acid-Base Chemistry: The pH Scale



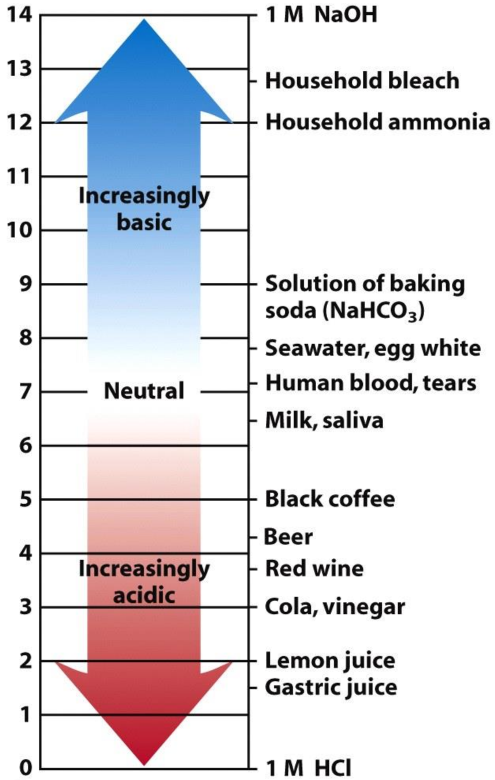
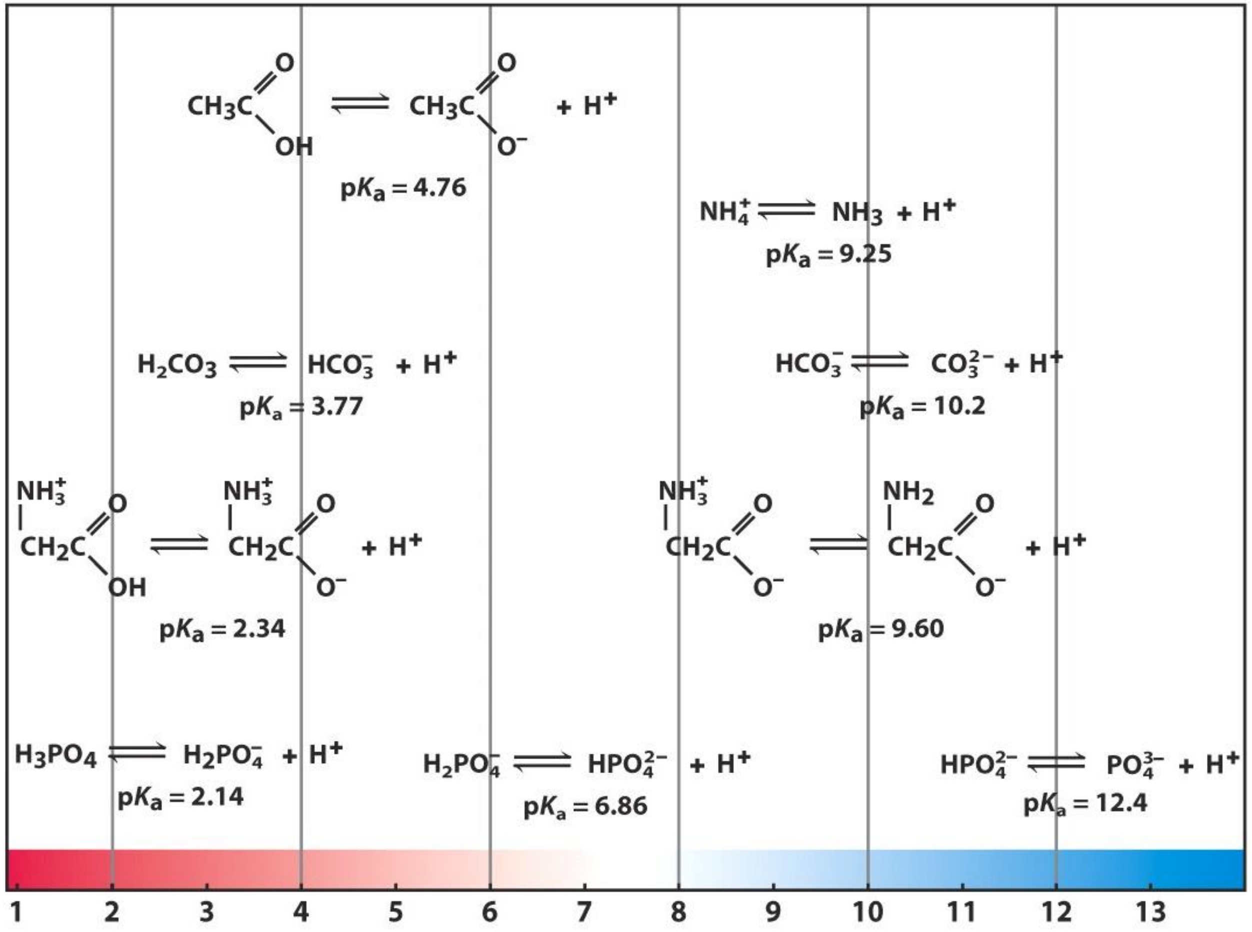


Figure 2-14
Lehninger Principles of Biochemistry, Fifth Edition

Acid-Base Chemistry: Biological Acids & Bases

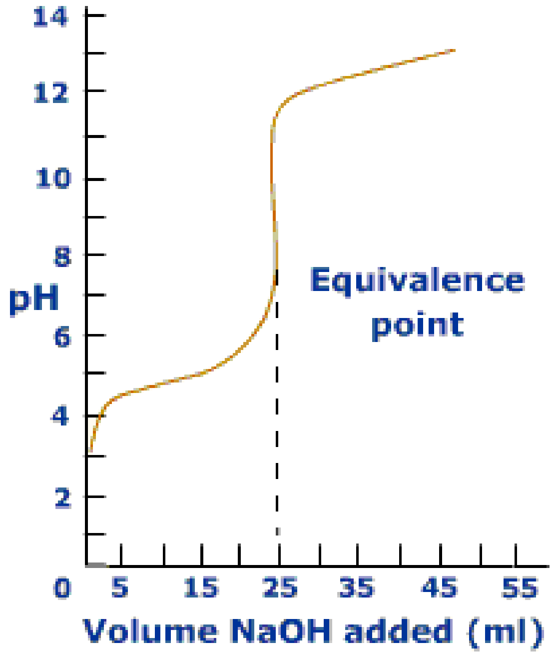
- Weak acids and weak bases are key for maintaining environmental pH in the face of changing protonation states of biomolecules



- Note that a larger Ka (a smaller pKa) is representative of a stronger acid.

Acid-Base Chemistry: The Relationship Between pH and pKa

- **Henderson-Hasselbalch equation:** Quantitative relationship between the pH of a solution and the ratio of the concentration of the deprotonated to protonated form of an ionizable group.



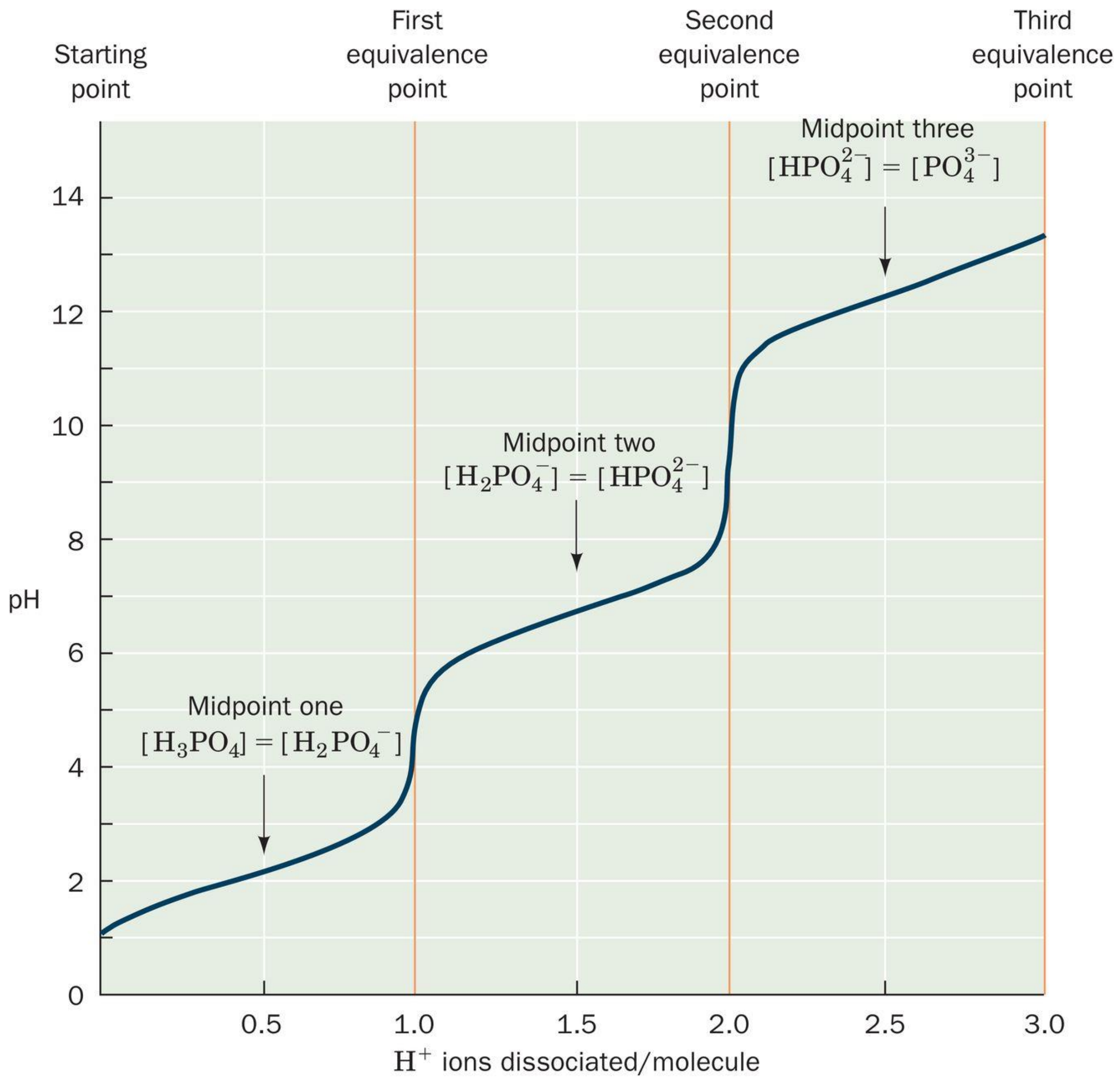
The pH titration curve of weak acid (CH_3COOH) and strong base (NaOH)

https://chem-guide.blogspot.com/2010/04/acid-base-titration.html

Acid-Base Chemistry: Monoprotic vs. Polyprotic Acids

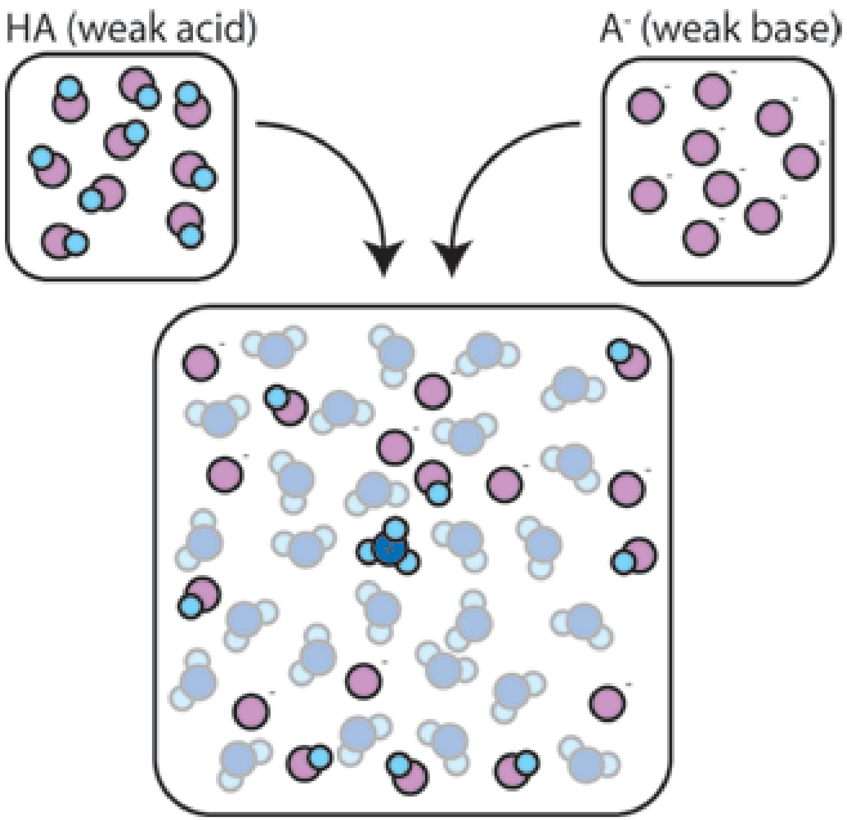
- A **monoprotic acid** has one ionizable hydrogen

- A **polyprotic acid** has more than one ionizable hydrogen



Acid-Base Chemistry: Buffers & How They Work

- **Buffers:** aqueous solutions that are able to resist small change in pH
- **A good buffer should be within 1 pH unit of the pKa of the acid.**
  - **Buffer capacity:** the moles of acid/base required to change pH by 1 unit



http://chemcollective.org/activities/tutorials/buffers/buffers3

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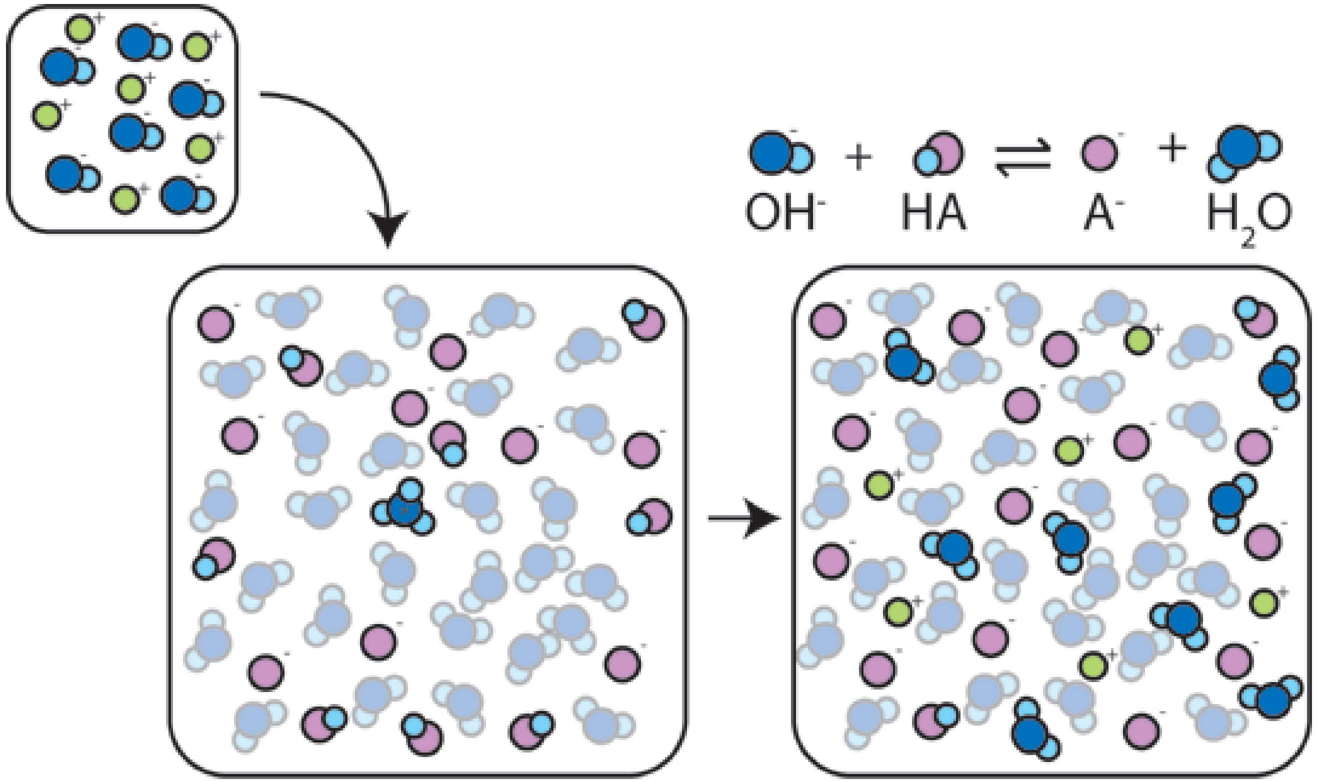

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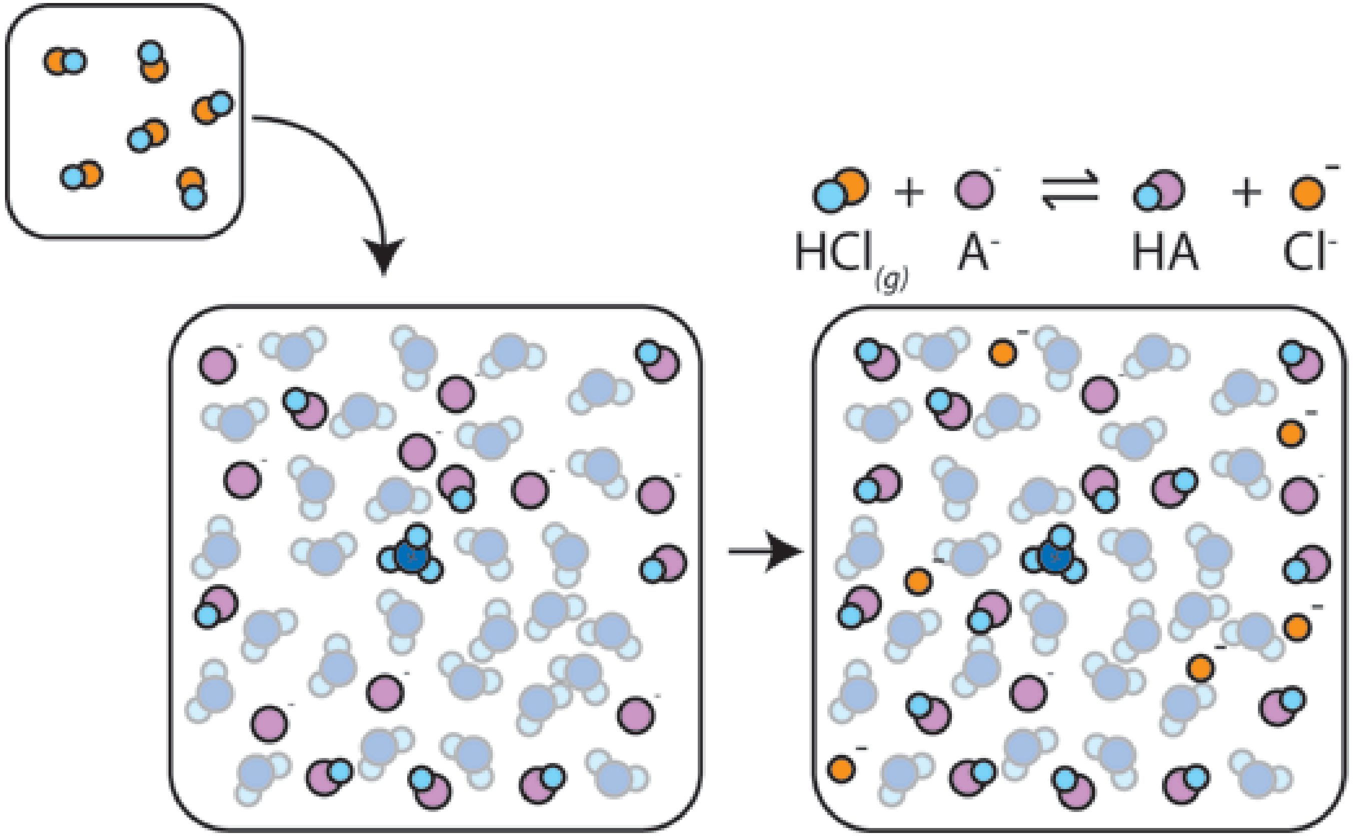

http://chemcollective.org/activities/tutorials/buffers/buffers3

To Prepare For Wednesday & Thursday's Class

Read

Chapter 8, all sections

Chapter 25, section 1 & 2

Practice

(1) Practice calculating pKa of weak acids/bases

(2) Practice calculating the pH of a buffer given concentations of acid and base

(3) Practice calculations of buffer capacity