Special Properties of Water

class – 22 (16.11.24)

LS2103 (Autumn 2024)

IISER Kolkata

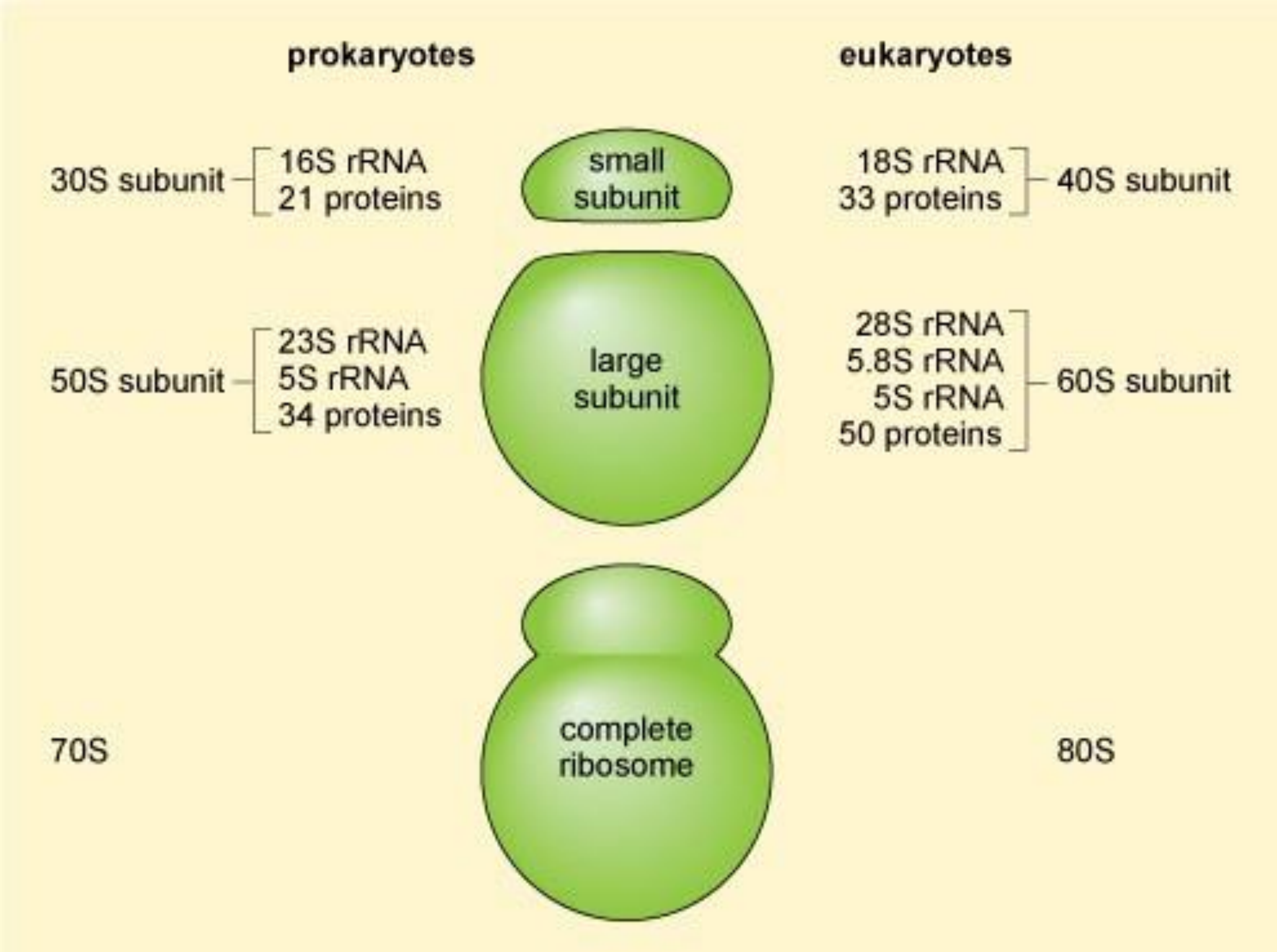
Dr. Neelanjana Sengupta

Associate Professor

Dept. of Biological Sciences, IISER Kolkata

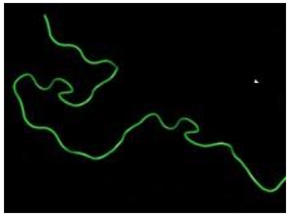
https://www.iiserkol.ac.in/~n.sengupta/

Ribosome subunits

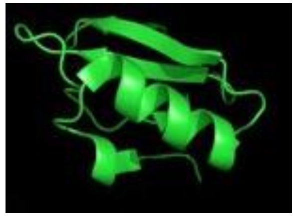


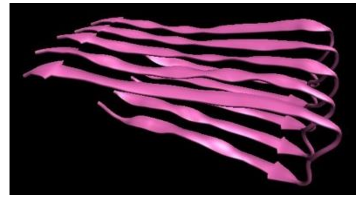
Svedberg units are non additive – why?

Biological "solvent" is predominantly water

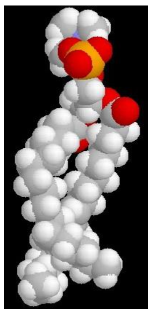


polypeptides

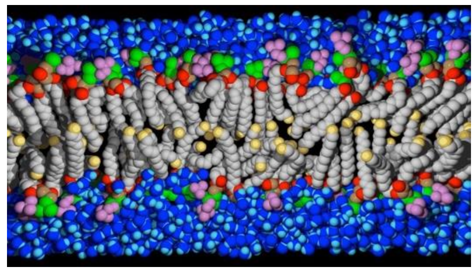




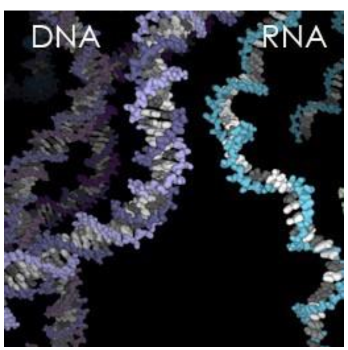
protein structures



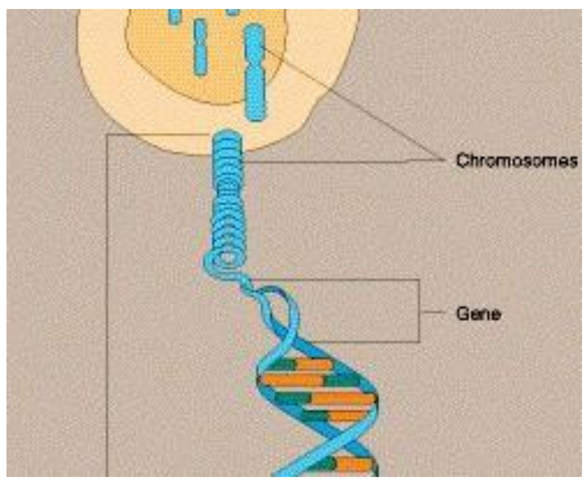
phospholipids

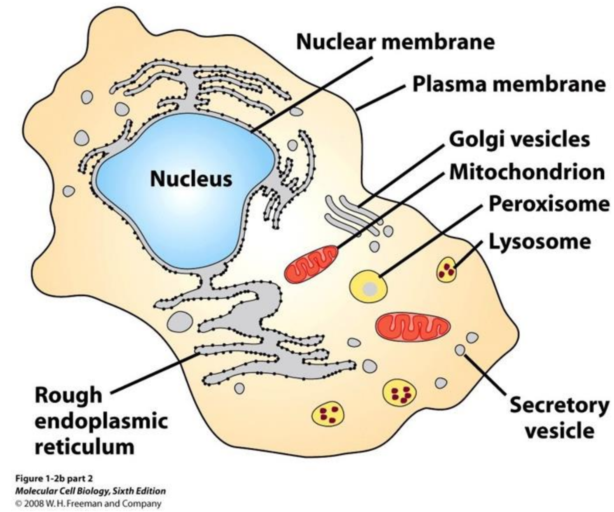


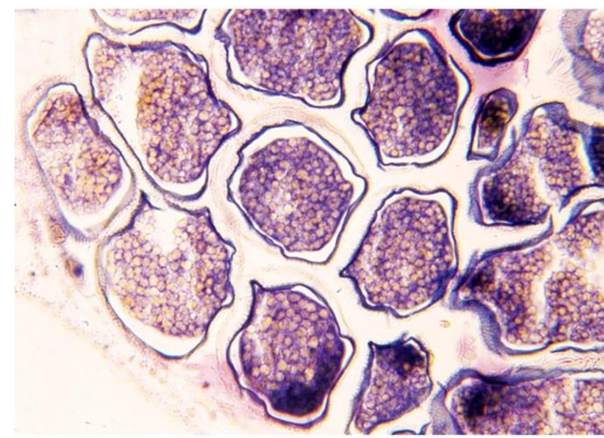
membranes



nucleic acids

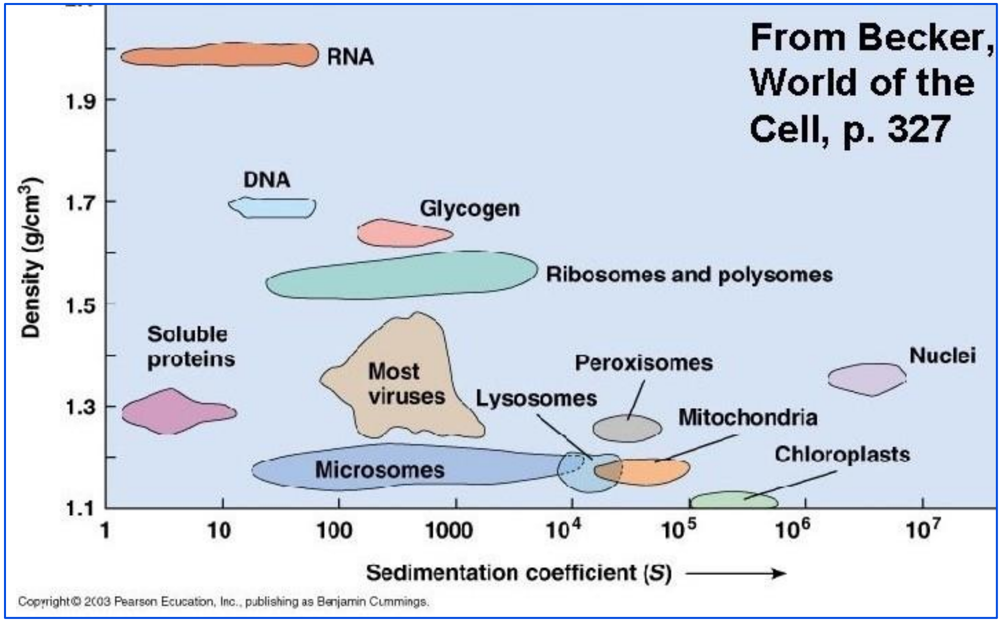


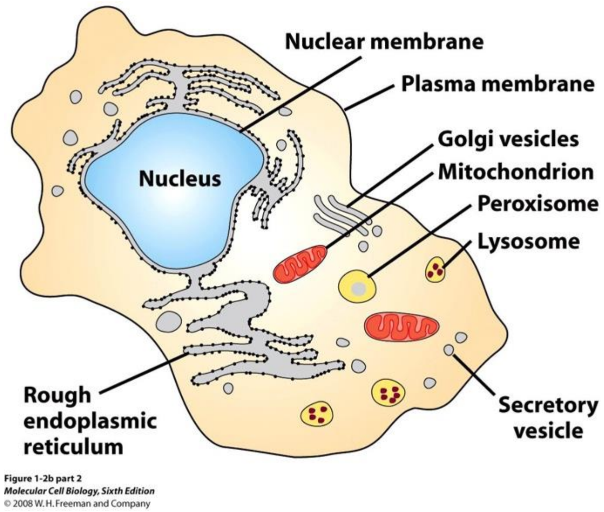


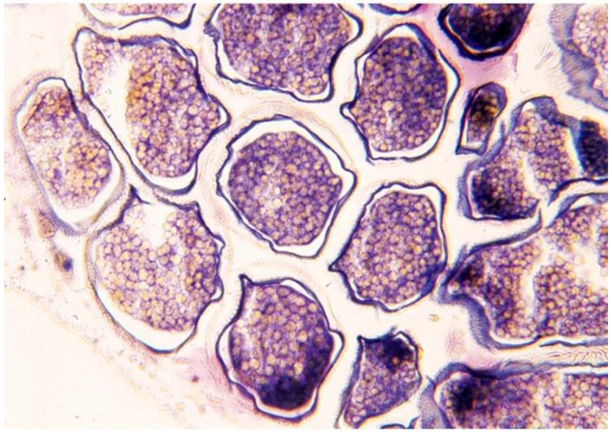


Cells and Tissues

Biological "solvent" is predominantly water





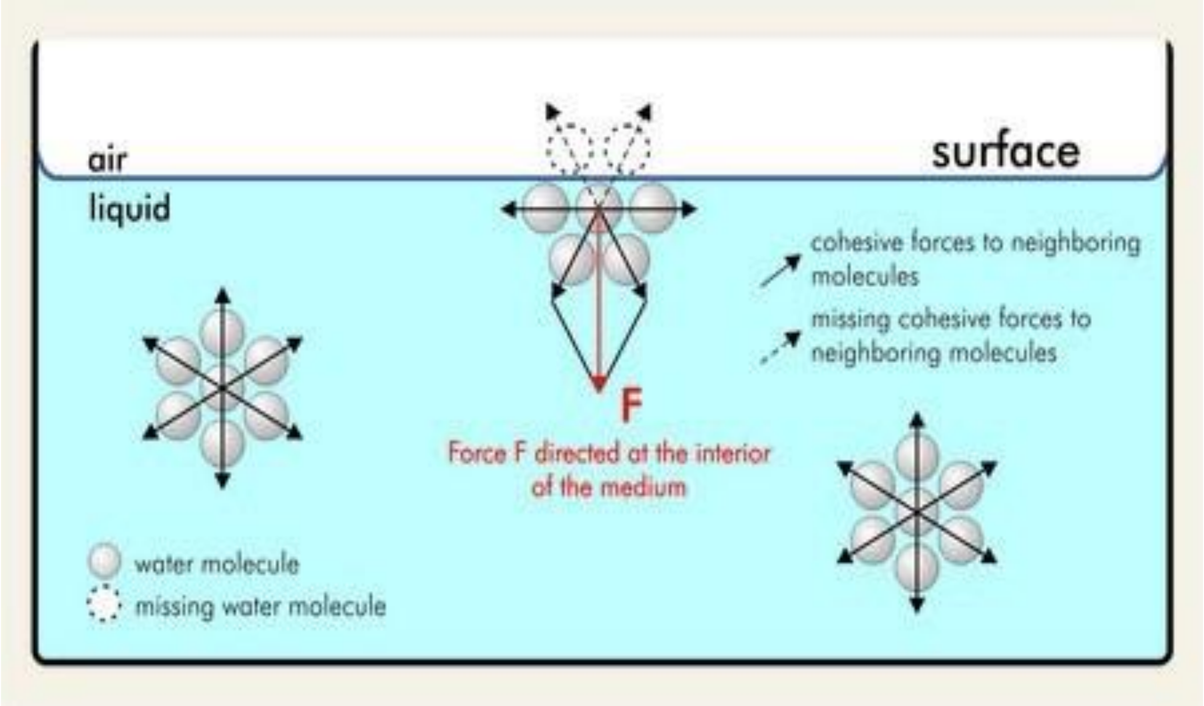


Cells and Tissues

Biological "solvent" is predominantly water

Surface Tension: Attraction of surface particles to the (inner) bulk that resists external force

Units / Dimensions: Energy per unit area, or, Force per unit length

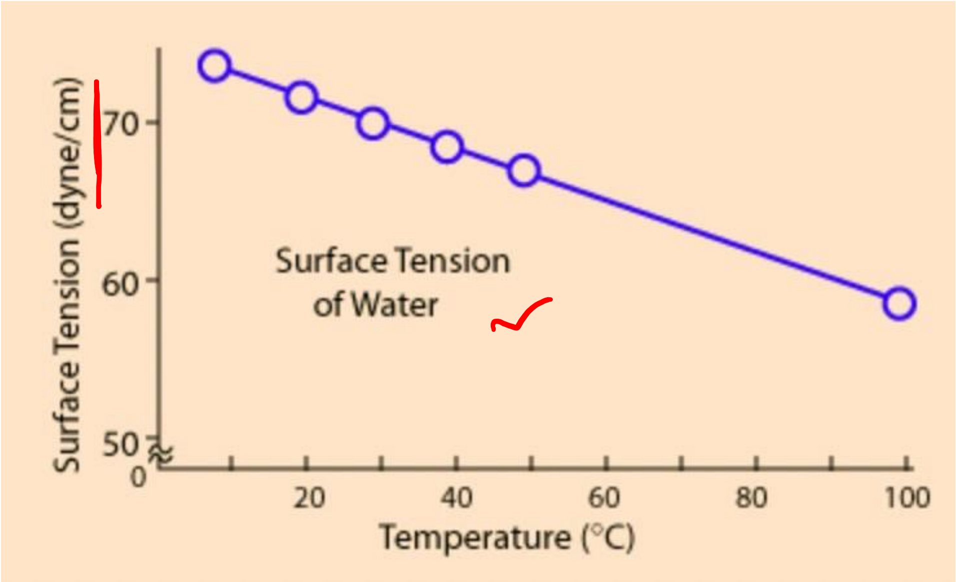


https://www.sita-process.com/information-service/process-parameter-surface-tension/overview/

Biological "solvent" is predominantly water

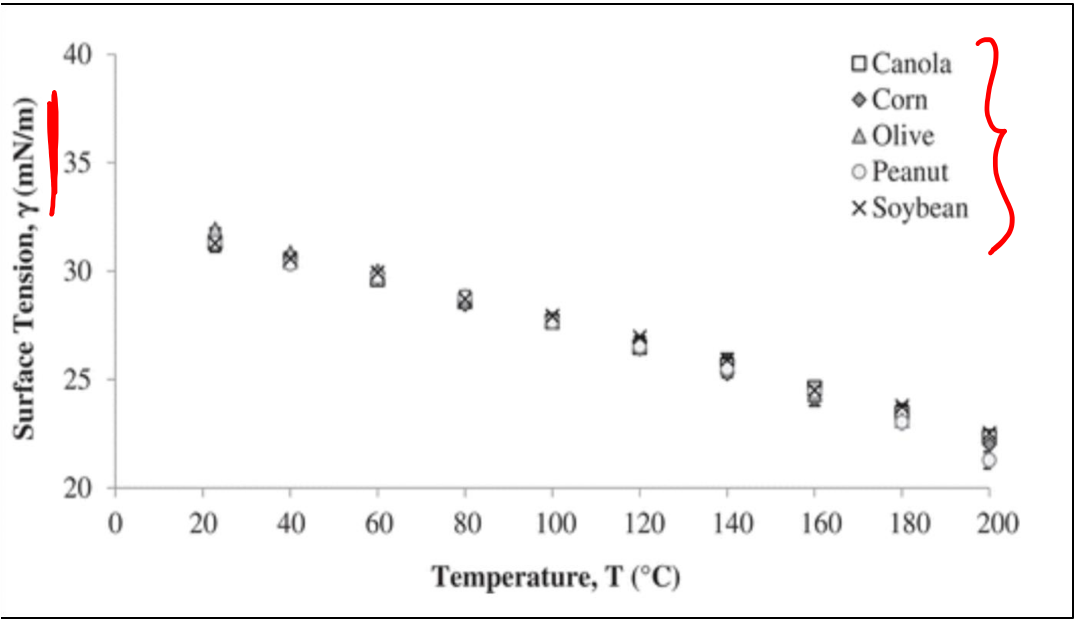
Comparison with other liquids

- Water has higher surface tension than other common solvents



http://hyperphysics.phy-astr.gsu.edu/hbase/surten.html

Sahasrabudhe et al., Int. J. Food. Prop., 2017

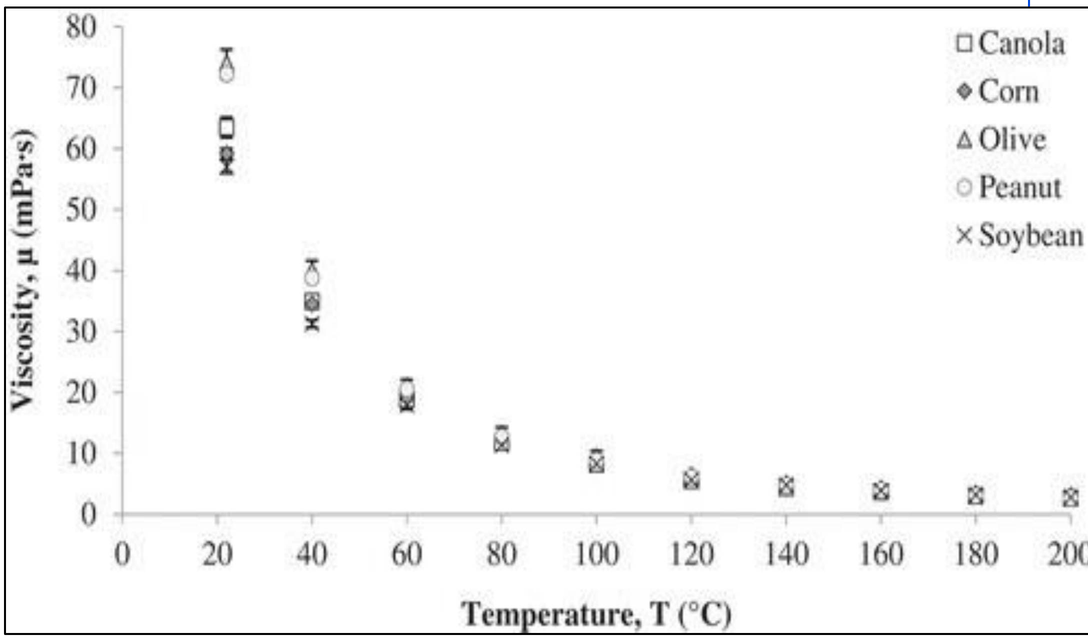


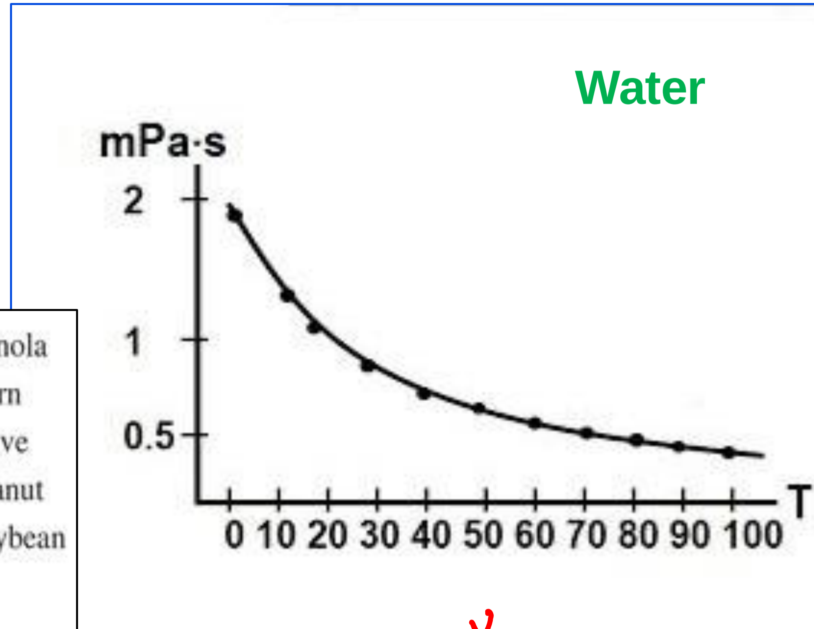
Biological "solvent" is predominantly water

Comparison with other liquids

Dynamic viscosity (η):

Sahasrabudhe et al., Int. J. Food. Prop., 2017

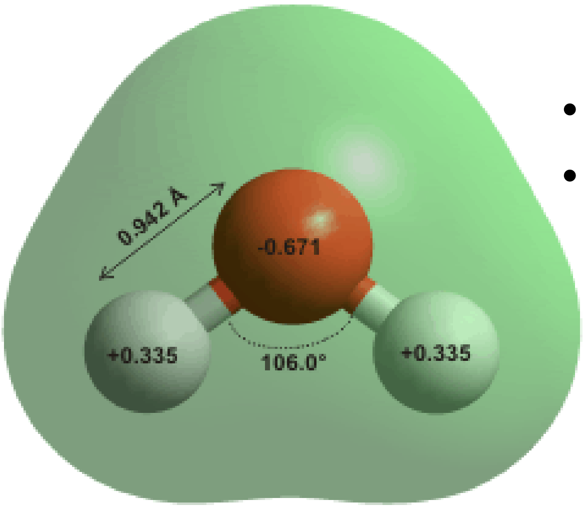




T(°C)	γ $\cancel{\mu}$(mPa·s)
0	~1.8
10	1.308
20	1.002
30	0.7978
40	0.6531
50	0.5471
60	0.4658
70	0.4044
80	0.3550
90	0.3150
100	0.2822

- Water has **higher surface tension** than other common solvents
- Water has **lower viscosity** than other common solvents

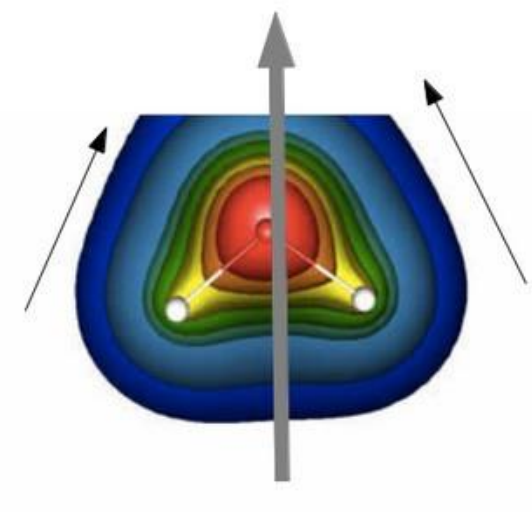
The molecular picture of water

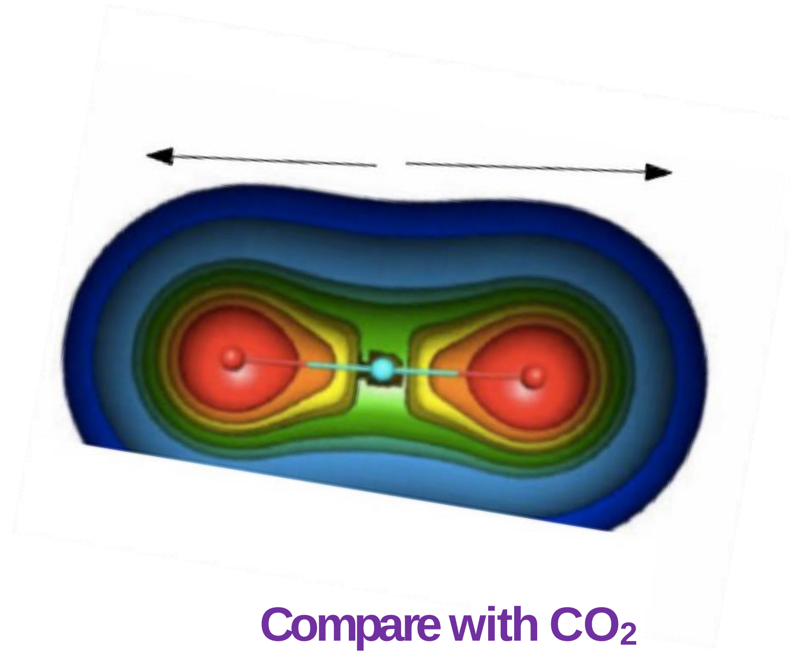


What is ‘special’?

- Two lone pairs of electrons at the oxygen atom
- Resulting shape: Bent structure and **net dipole moment** (~1.84 Debye)

dipole moment





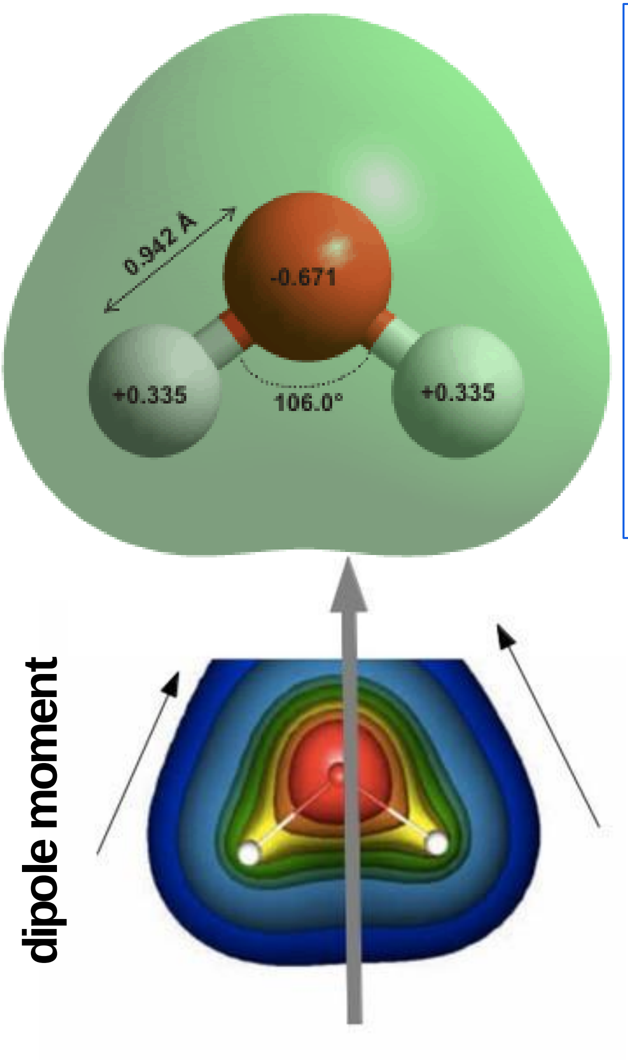
Compare with CO_2
(no net dipole moment)

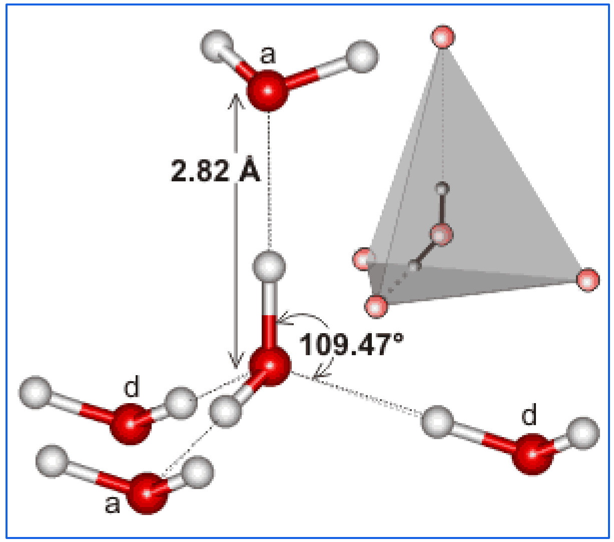
Results in **hydrogen bonded** and **tetrahedral** water network

Hydrogen bond (HB): A mainly electrostatic attraction between a H-atom covalently bonded to one electronegative atom ('HB donor'), and another electronegative atom ('HB acceptor').

- HBs are strongly "directional"

- They can "co-operate"





q = 1

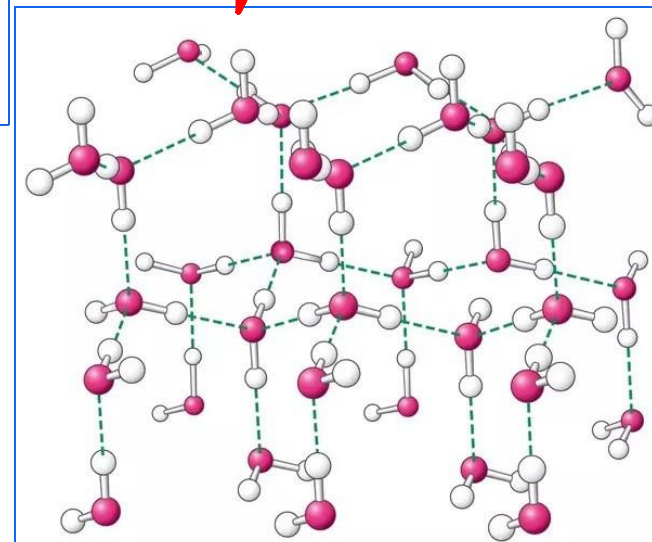
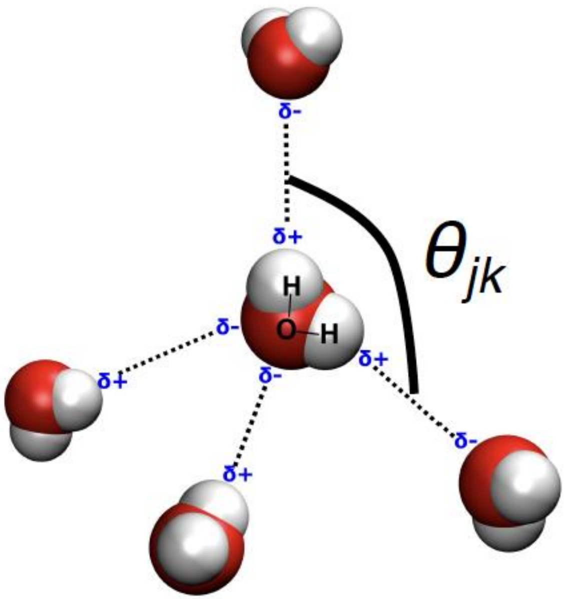


Figure 1.11
Biochemistry, Seventh Edition

Water tetrahedrality

Orientational Order Parameter:

$$q = 1 - \frac{3}{8}\sum_{j=1}^{3}\sum_{k=j+1}^{4}\left(\cos\theta_{jk} + \frac{1}{3}\right)^2$$



q = 1 for perfect ice

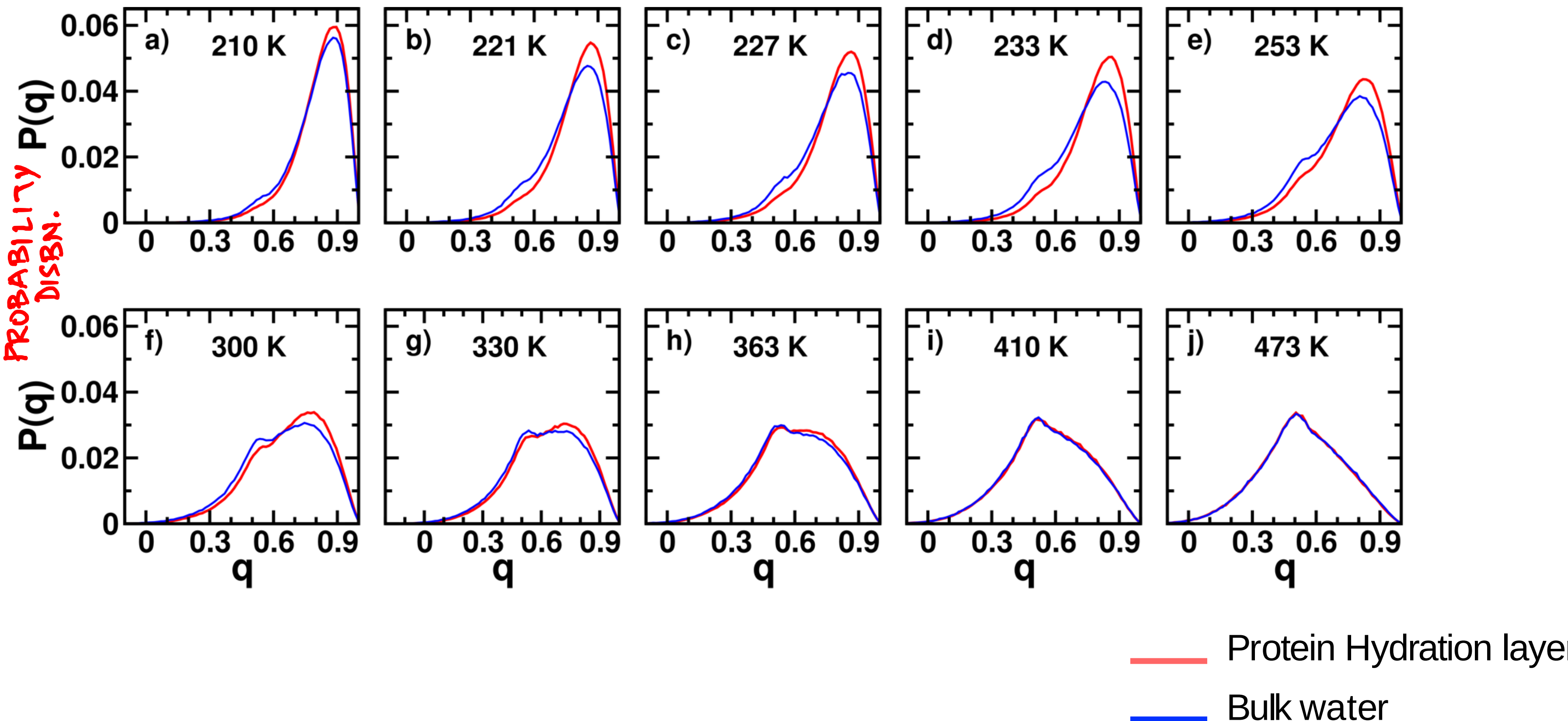
Errington and Debenedetti, Nature, 2001

https://www.nature.com/articles/35053024

Hydration(*) layer ordering
(results from computer simulations)

q = 1 for perfect ice

Ordering modified with temperature, and in presence of solute (biomolecule)

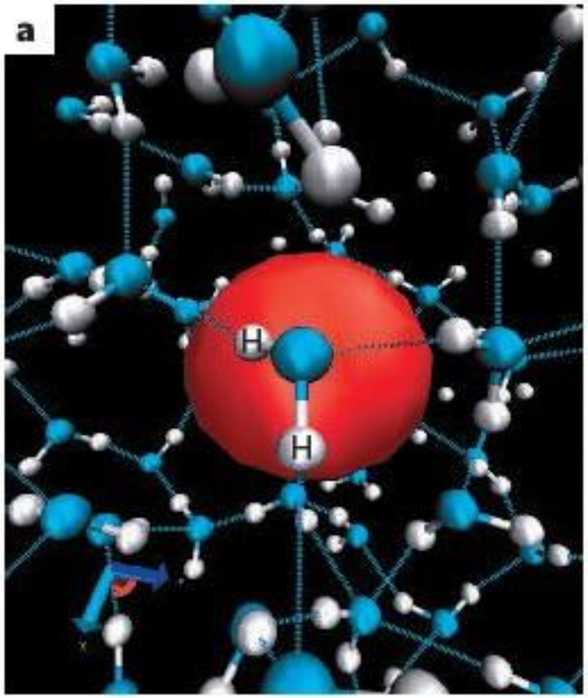


Errington and Debenedetti, Nature, 2001

https://www.nature.com/articles/35053024

Under "no perturbations", every H_2O will "make a break" H-Bonds

Molecular scale inspection with other H_2Os

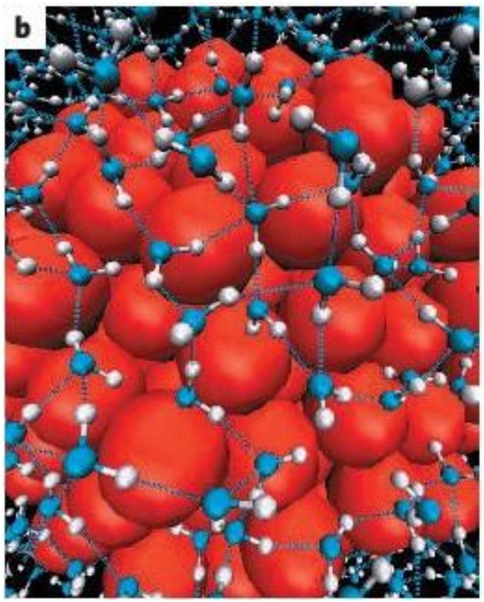


Chandler, Nature Reviews, **2005**, 437, 640

Solute radius comparable to H_2O

- Insignificant loss in H-bonds of nearby waters
- Marginal overall re-ordering of H-bonding network

Molecular scale inspection



Chandler, Nature Reviews, **2005**, 437, 640

Large solute (eg. protein)

- No. of water H-bonds reduced significantly
- **Interface formed to minimize loss in H-bonds**
- Interface tends to move away from solute
- **Energetic cost of solvating the solute** (ie. forming the interface):

Assuming a spherical solute of radius 'R',

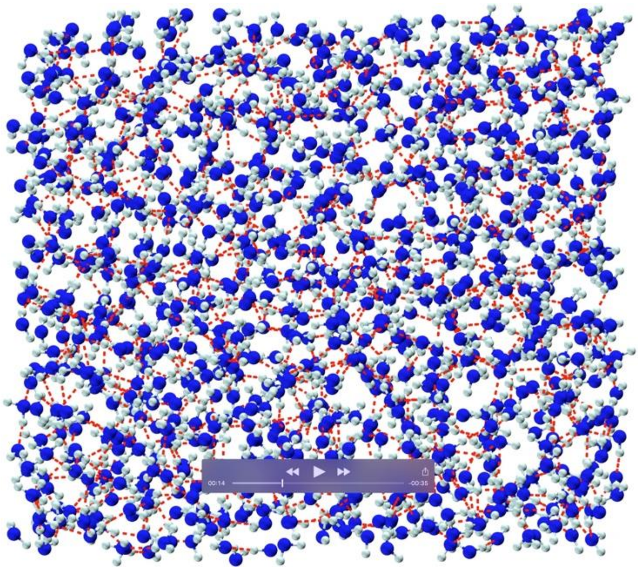
Free energy cost

$$\underline{\Delta G} \approx (4\pi R^2)\gamma$$

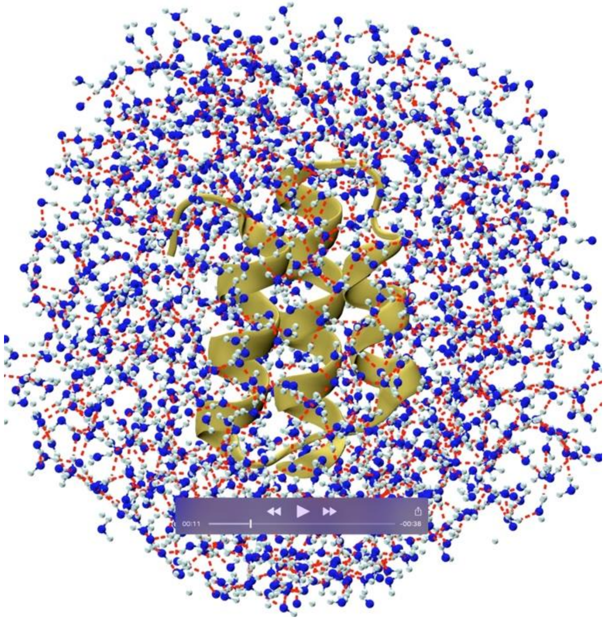
γ: Surface tension

Visualizing the H-bonded network (computer simulations)

Bulk water



Water close to a biomolecule
('hydration layer')

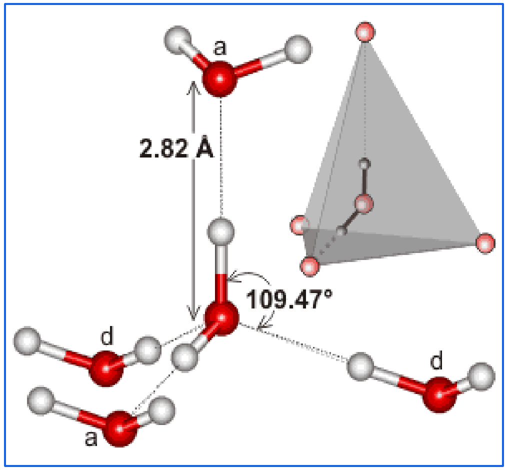


- Protein-water (P-W) H-bonds **compete with** water-water (W-W) H-bonds
- **Lifetimes and energetics** of P-W and W-W H-bonds may differ
- Water helps the protein achieve **functional flexibility**
- Water plays **thermodynamic role** in folding, enzyme-ligand binding, etc

Hydrogen bond (HB): A mainly electrostatic attraction between a H-atom covalently bonded to an electronegative atom ('HB donor'), and another electronegative atom ('HB acceptor').

Pure water: $E_{H\text{-}bond}$ ~ 5.6 kCal mol^{-1}, ie. ~ **9.7 RT at room temperature**

Prob. A Raman spectroscopy study showed that breakage of a single H-bond within pure water at room temperature (300 K) is commensurate with an **enthalpy increase of 1.9 kcal mol^{-1}, and an entropy increase of 2.4 k_B.**



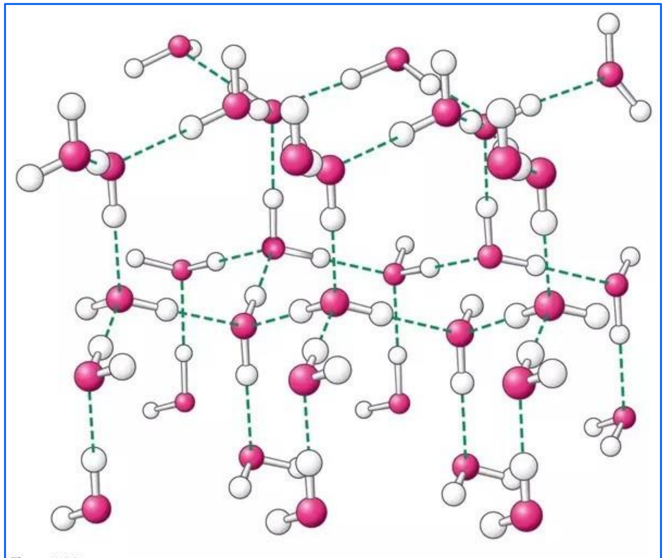


Figure 1.11
Biochemistry, Seventh Edition

- What is the **free energy cost** of breaking a single H-bond at room temperature?

Silverstein, Haymet & Dill, J. Am. Chem. Soc. 2000, 122, 8037-8041 https://doi.org/10.1021/ja000459t