- Reading
- Today: pp 87-90
- Thur: pp 101-104
- Fri. pp 104(bottom)-107

Practice Problem for Problem S4 of homework #2

Remember that if we ***choose*** property A to be a function of B and C, i.e., = A(B,C), this is ***equivalent*** to saying what?:

$$dA = \left(\frac{\partial A}{\partial B}\right)_C dB + \left(\frac{\partial A}{\partial C}\right)_B dC$$

for any state function.

Practice Problem like homework S4

Picking some letters randomly from the alphabet,

A =A(B,C); **dA=D dB +E dC** i.e., variables are B and C

and **D** and **E** are slopes (= partial derivatives)

This means ***automatically*** (no thought required) that

$$dA = \left(\frac{\partial A}{\partial B}\right)_C dB + \left(\frac{\partial A}{\partial C}\right)_B dC$$

Then it follows that: $\left(\frac{\partial A}{\partial B}\right)_C = D$ and $\left(\frac{\partial A}{\partial C}\right)_B = E$

and James Clerk Maxwell showed that $\left(\frac{\partial D}{\partial C}\right)_B = \left(\frac{\partial E}{\partial B}\right)_C$

The B slope (i.e., D) changes with C *exactly* as the C slope)(i.e., E) changes with B

a. Weak Non-Covalent "Reactions"

essential for the ***DYNAMICS*** of life processes

1. Ionic (in solution or biopolymers),
2. "hydrogen bonding",
3. hydrophobic (not) bonding
4. London dispersion forces

   (universally present)

b. proteins: what are they?

and what do they do?

All of chemistry is built from Coulomb's Law: The very strong attraction of opposite charges and repulsion of like charges.

TABLE 3.1 Enthalpies of Noncovalent Bonds and Interactions*

Reaction	Characteristic interaction	$\Delta_r H^\circ$ (kj mol^{-1})
$Na^+(g) + Cl^-(g) \rightarrow NaCl(s)$	Ionic	−785
$NaCl(s) + \infty H_2O(l) \rightarrow Na^+(aq) + Cl^-(aq)$	Ionic and ion–dipole	4
Argon(*g*) → Argon(*s*)	London	−8
n-Butane(*g*) → *n*-Butane(*l*)	London–van der Waals	−20
Acetone(*g*) → Acetone(*l*)	London–van der Waals	−30

van der Waals: a ***mixture*** of London and permanent dipole-dipole interactions

Coulombic Terms (electrostatic)

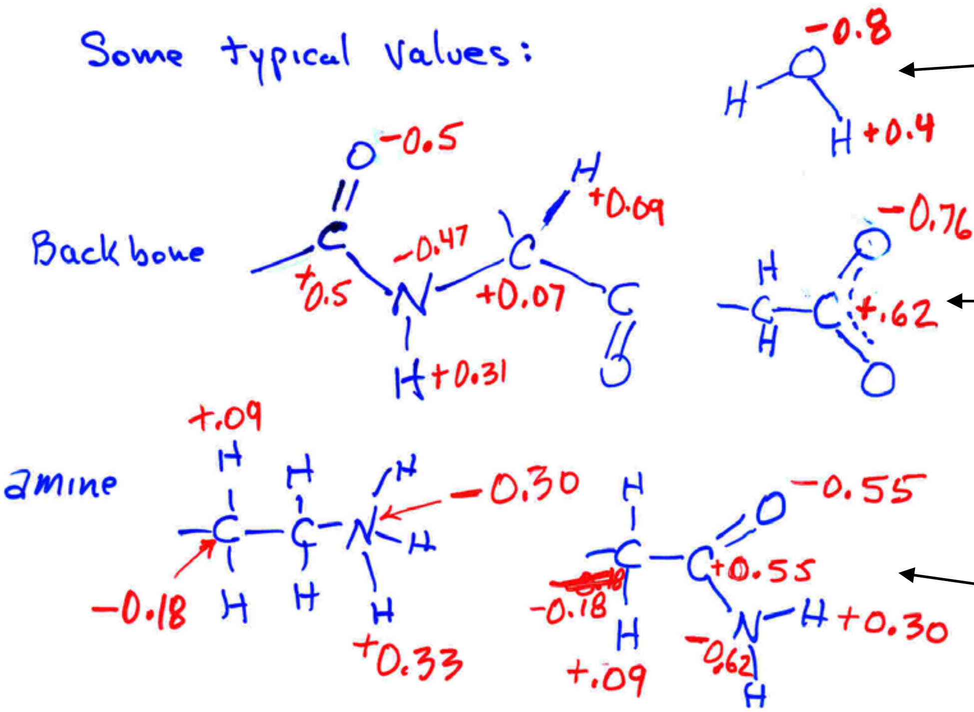
$$(V_{Coul})_{ij} = \frac{q_i q_j}{r_{ij}} (9 \times 10^9) \text{ Joules}$$

for q in coulombs
r_{ij} in meters.

$= $ **1328 kJ/mol** per $\frac{e^2}{Å}$

Atoms are treated as point charges and point masses.

Some typical values:



Hydrogen bonding is almost all *electrostatic* attraction of partial charges. It is strong because of ***smallness of H;***

H gets closer than any other atom!

Water

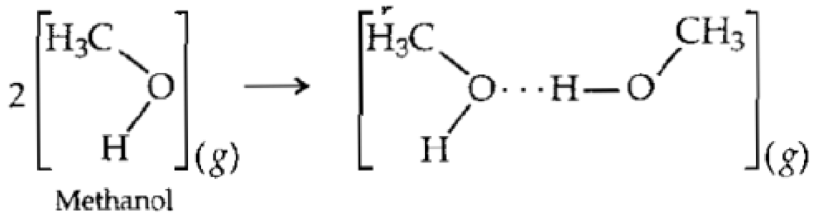
Glu or Asp

Gln or Asn

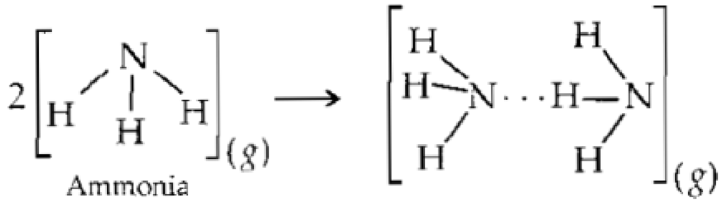
Hydrogen Bonding

Hydrogen bonding is almost all _electrostatic attraction_ of partial charges. It is strong because of _smallness_ of H

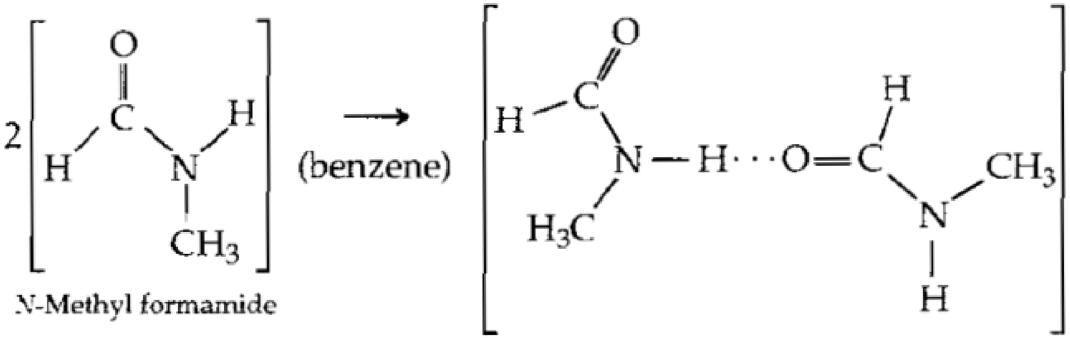
GAS PHASE



Hydrogen bond (g) −20

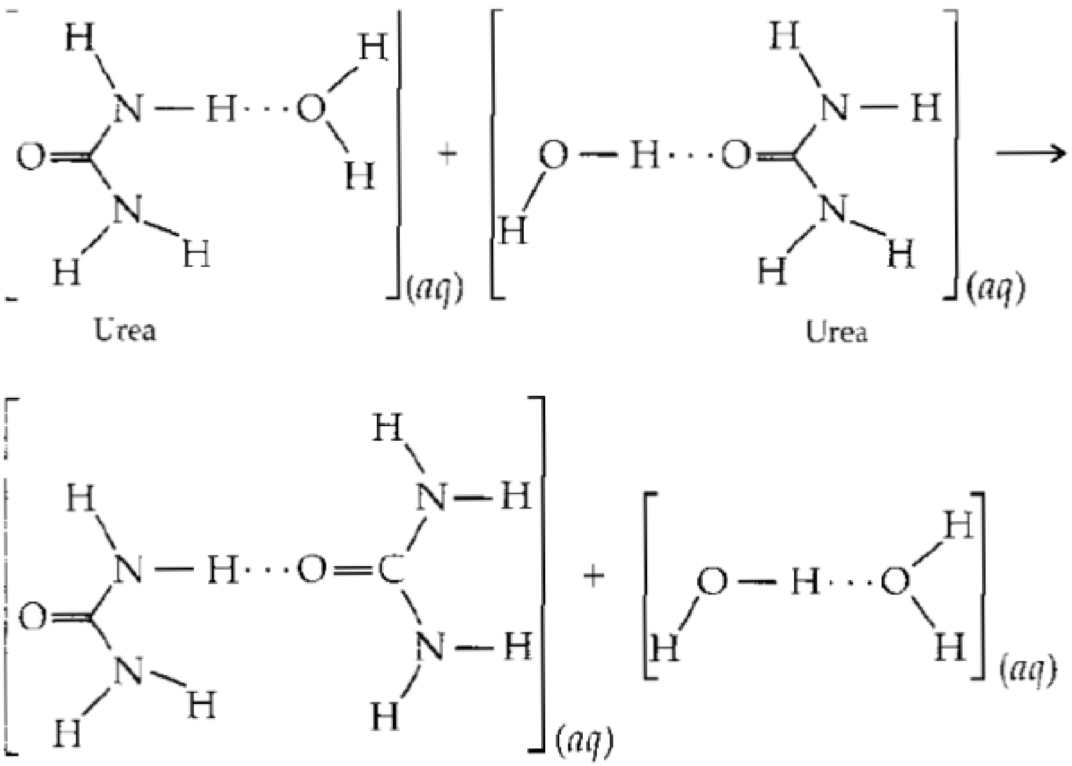


Hydrogen bond (g) −15



Hydrogen bond (benzene) −15

IN WATER



(reaction scheme above)	Hydrogen bond (aqueous)	−5
$C_3H_6(l) + \propto H_2O(l) \rightarrow C_3H_6(aq)$	Hydrophobic	−10
$\text{Benzene}(l) + \propto H_2O(l) \rightarrow \text{benzene}(aq)$	Hydrophobic	0

London dispersion forces

Quantum behavior and ***ALWAYS PRESENT***
regardless of what other label is given to a force

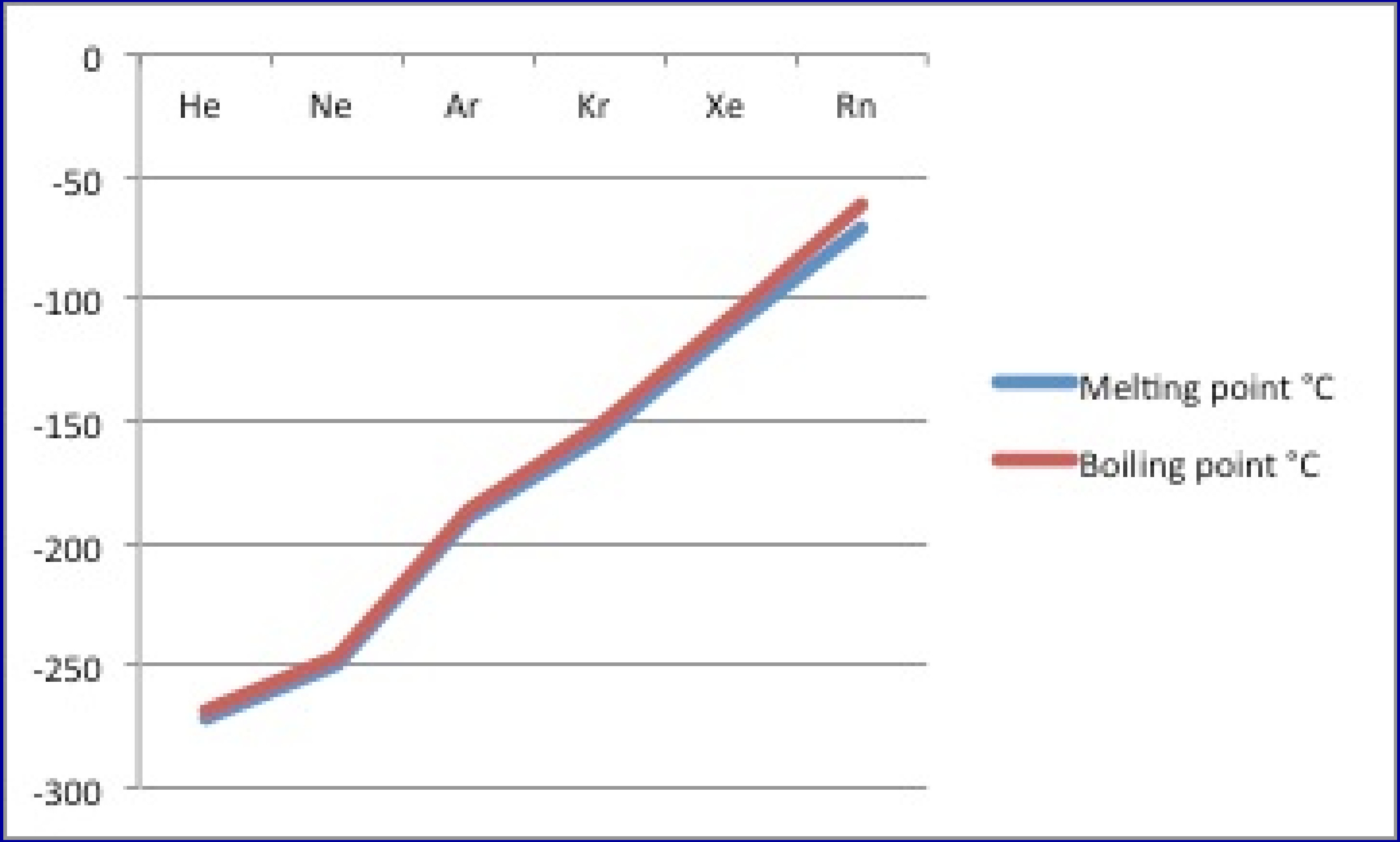
Electrons in atoms act like **particles**, although the orbital picture makes them seem like spherical clouds with no dipole.

Particle behavior means *helium* atoms have **large f*luctuating* *dipoles.***

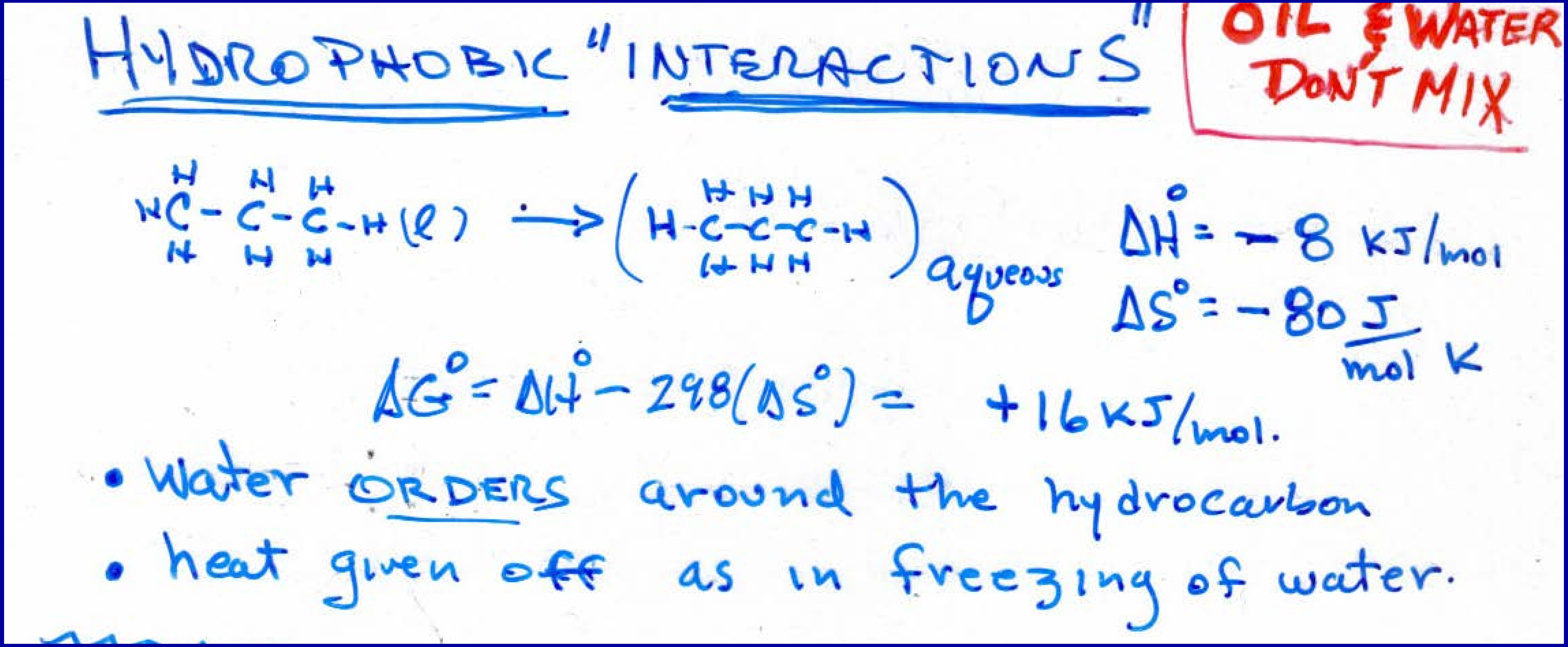
Two helium atoms side by side attract because the **fluctuations are correlated to reduce electron repulsion** between the atoms.

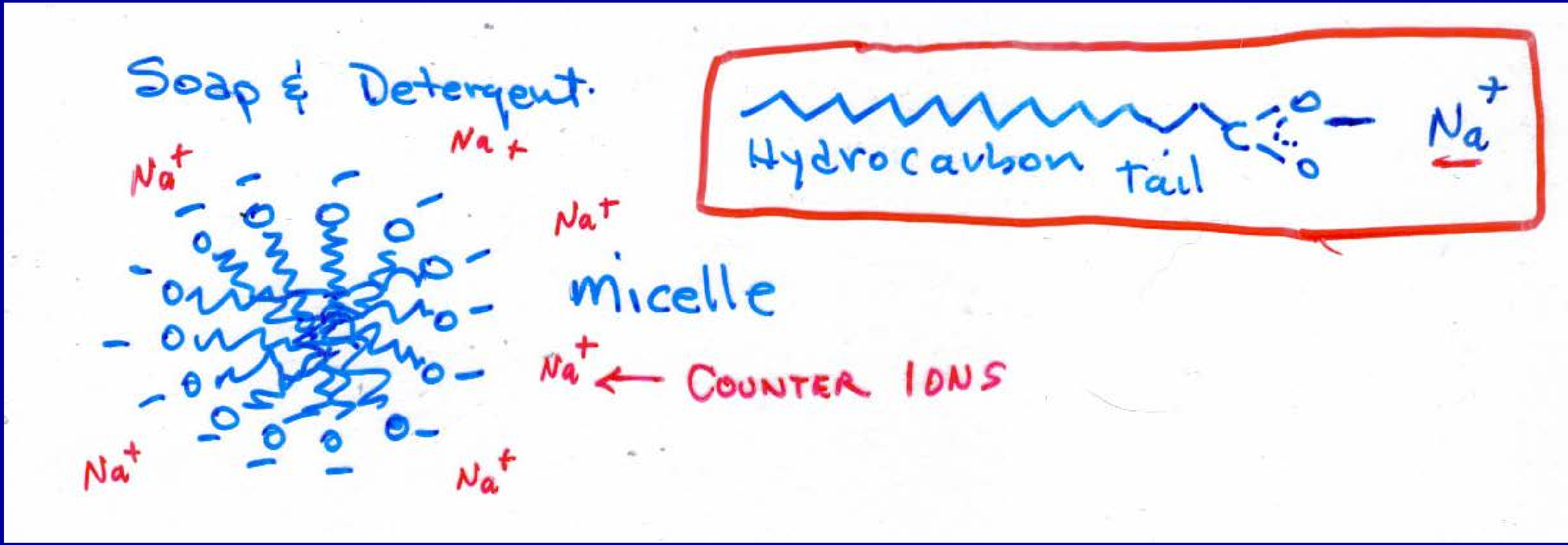
instantaneous dipole- induced dipole

+	-		-	+
-	+	***or***	+	-


0
-50
-100
-150
-200
-250
-300
He
Ne
Ar
Kr
Xe
Rn
Melting point °C
Boiling point °C

Hydrophobic "bonding", "interactions", are actually ***thermodynamic reactions*** that involve all the forces we have introduced.

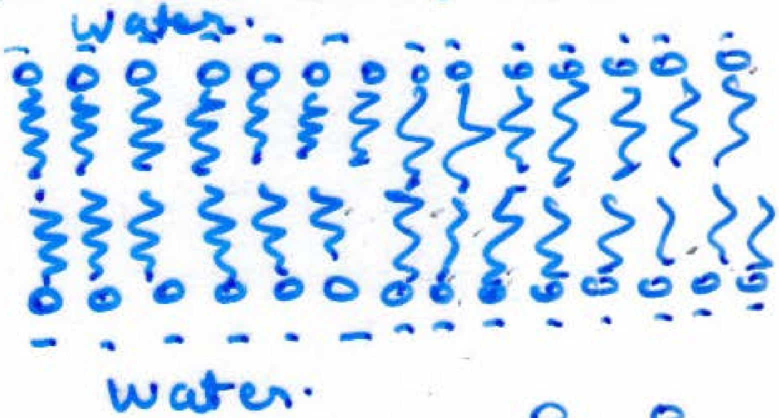




Soap & Detergent.
Hydrocarbon tail
C
O
O
Na+
micelle
Na+
Na+ ← COUNTER IONS

BIOLOGICAL SOAPS = LIPIDS = FATS.

FORM BILAYERS = MEMBRANES.

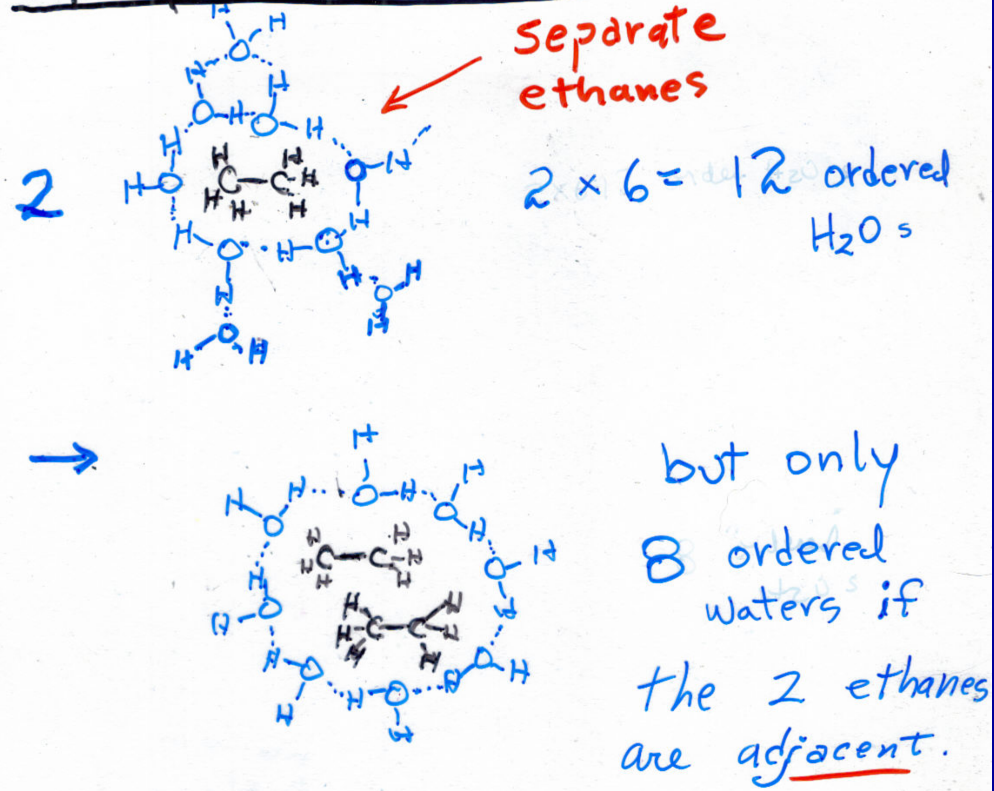


AND VESICLES

(for transporting.)

e.g. neural transmitters)

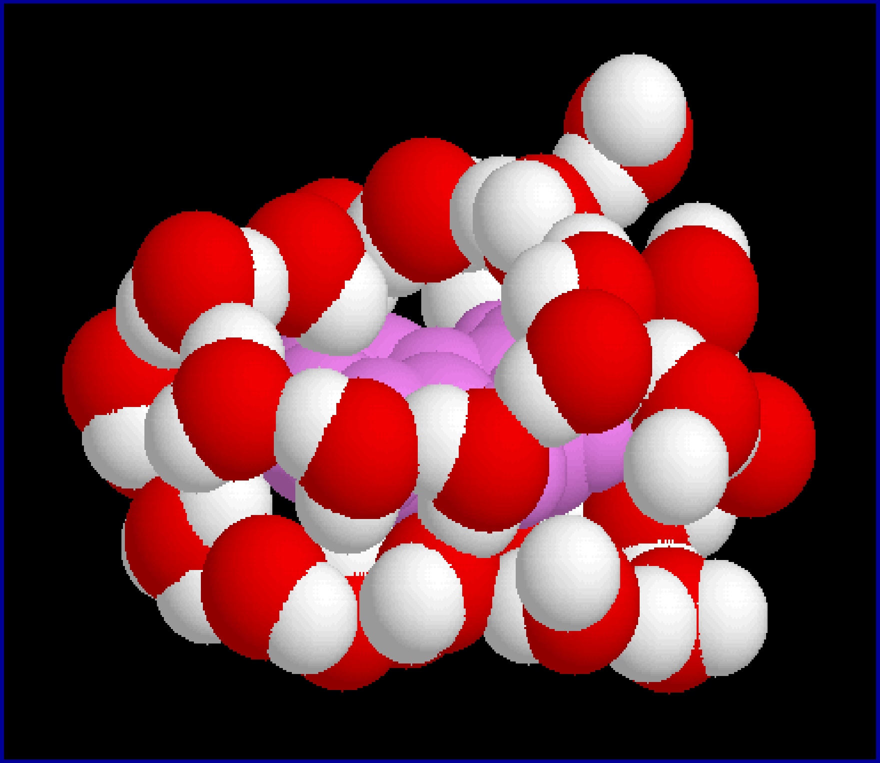
Hydrophobic "Interaction"

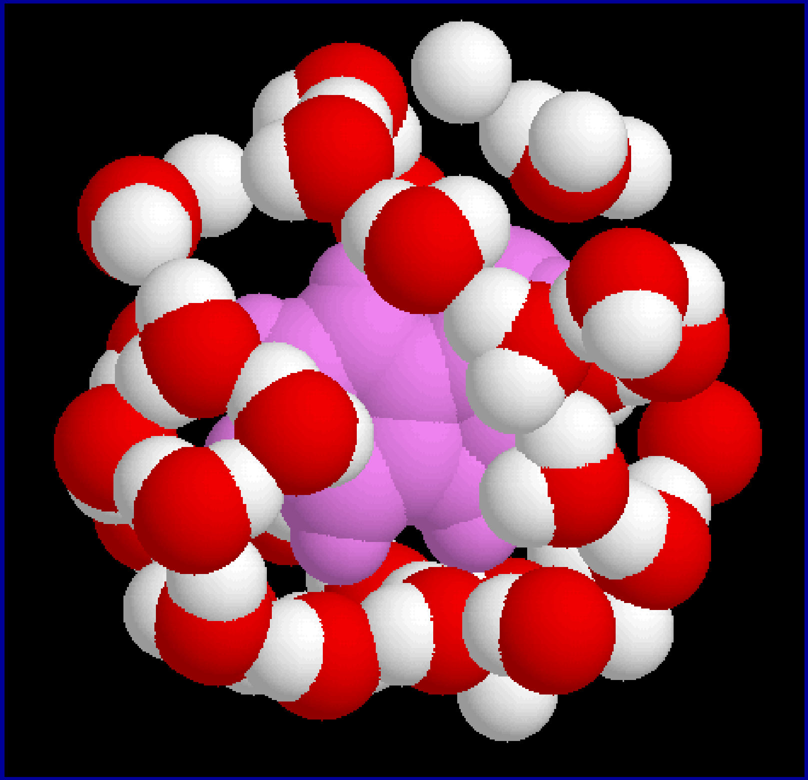


Note: **The London forces between water and ethane are ~same as between two ethanes.**
Total ordered water is reduced by association of ethanes.
The force is much the same as what causes water droplets in air to be spherical and makes them combine into larger drops, i.e., *surface tension.*
Reducing surface area is spontaneous.

Hydrophobic "Bonding"

AROMATIC RING IN WATER. Typical snapshot showing different views of the H-bonded chains formed by water within 4.0 Angstroms.





10 femtoseconds later

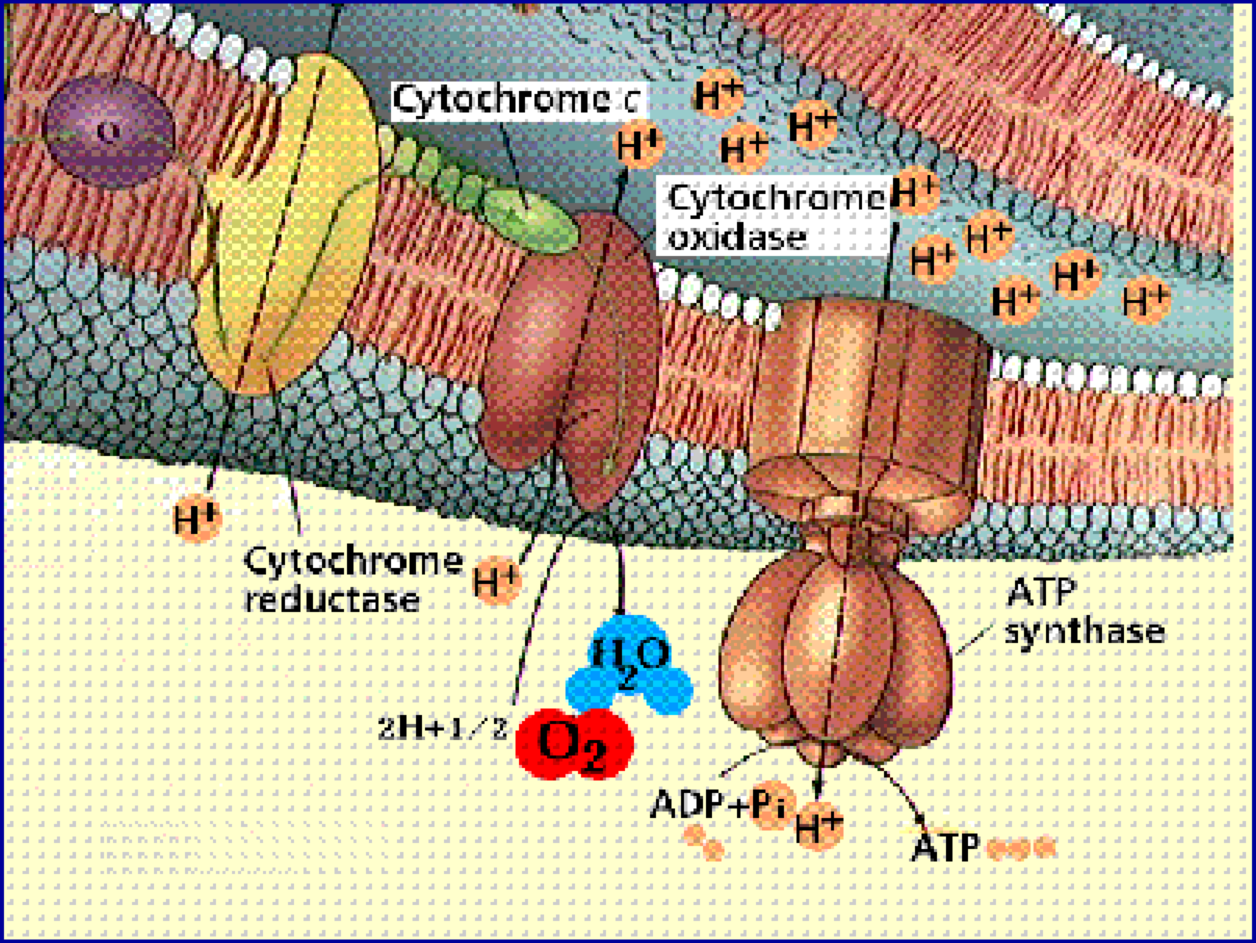
What are proteins and what do they do?

The poetic answer:

"We now see that proteins are highly sophisticated molecular machines that process energy, matter, and information. Their beautiful molecular ballet is coming into view."

-Lubert Stryer

Biochemistry, 4th Ed.


Cytochrome c
H^+
Cytochrome
oxidase
H^+
Cytochrome
reductase
H_2O
2H+1/2
O_2
ATP
synthase
ADP+Pi
ATP

What do proteins do? **The list answer:**

(Gene == basic Protein)

but there are many forms of most basic proteins created by *post translationa*l processes

Mechanical support

Motion

Transport and storage

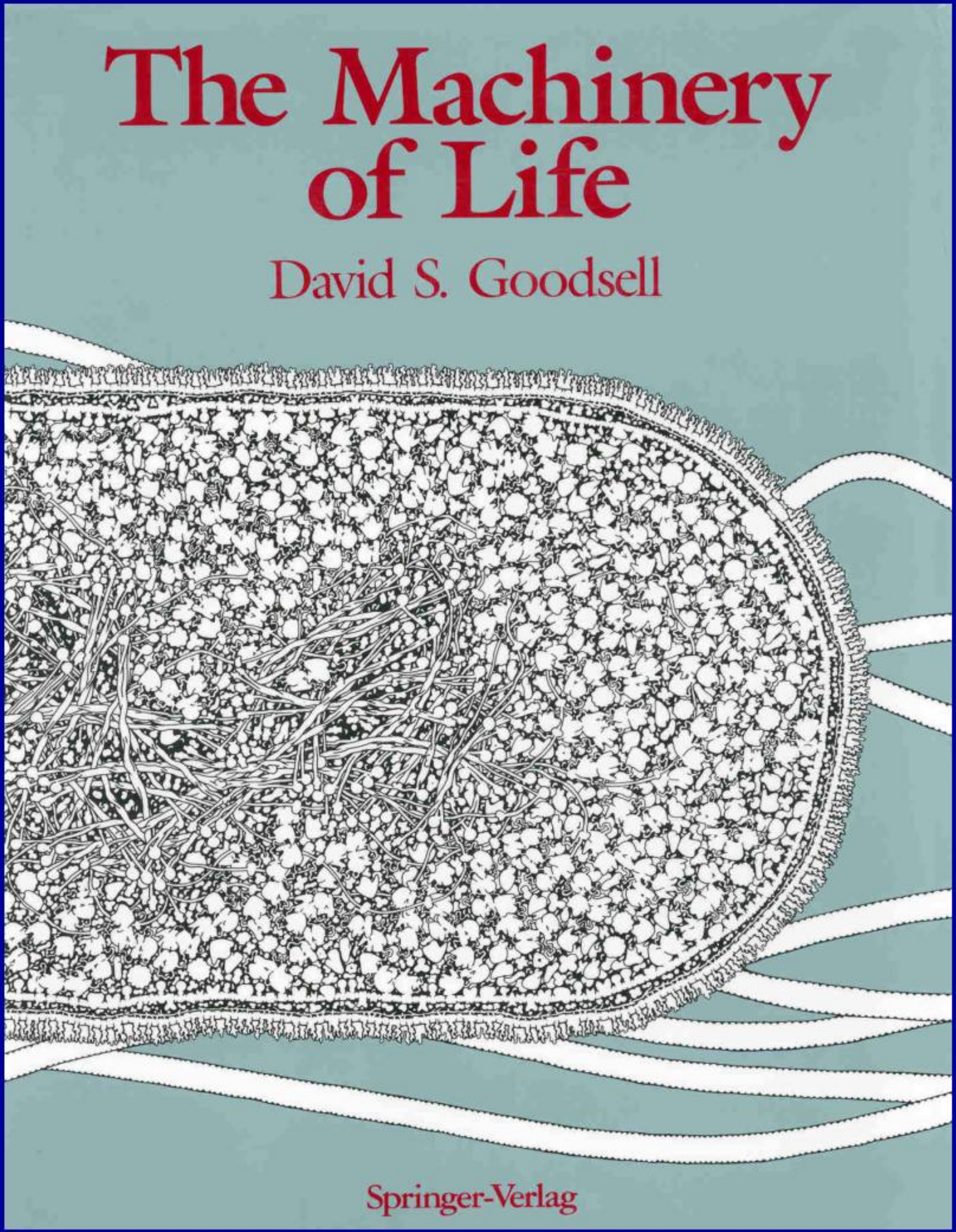
Immune protection

Signaling(nerve impulses, response to hormones, vision,……

Catalysis and recognition-- pervade most of the above

(in particular, hydrolysis of ATP and GTP provides the energy for switching and timing of the complex circuits)

and much,much more—yet to be discovered.



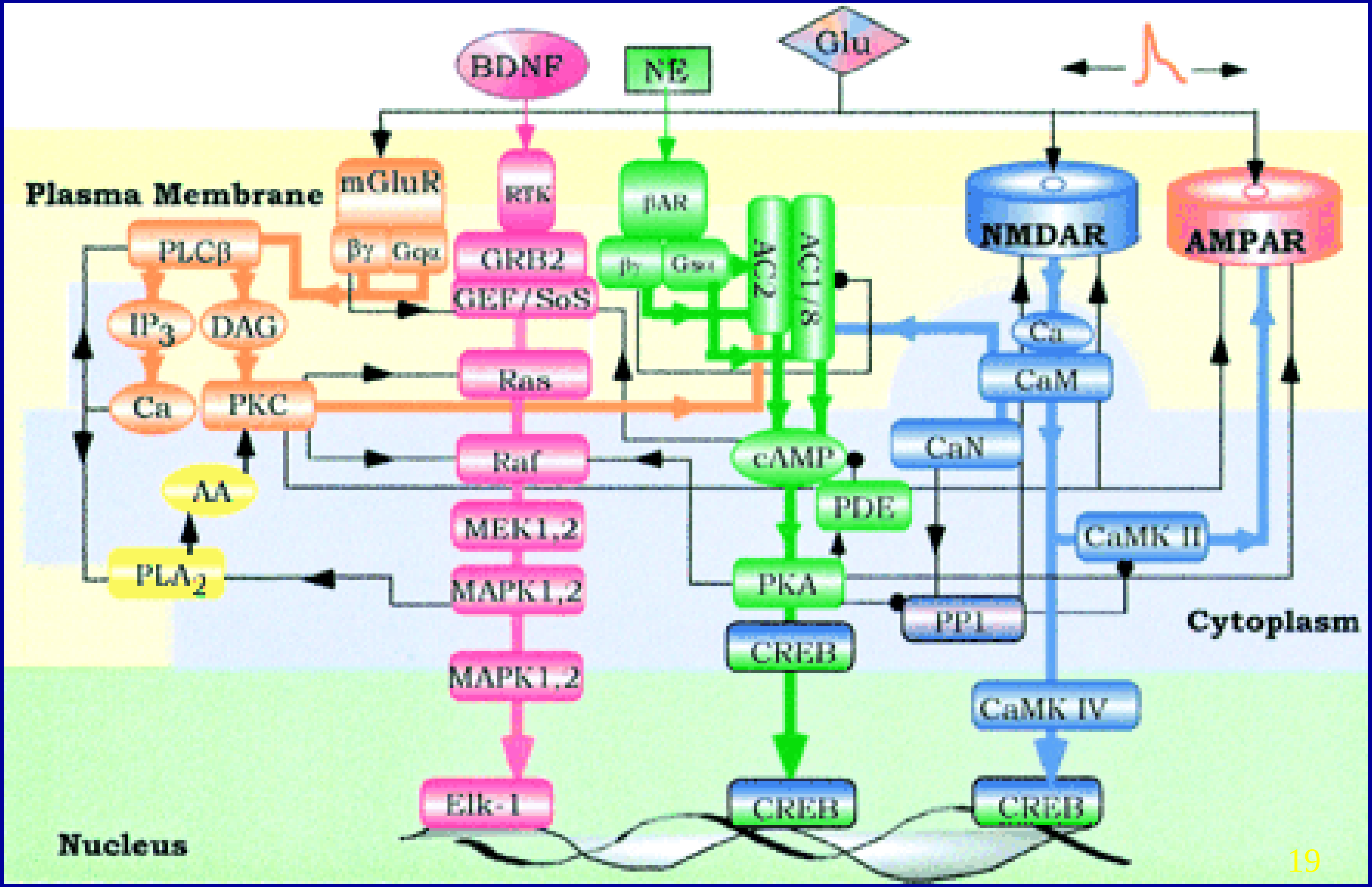
The visual answer

Ecoli Bacterium

Interacting Signaling Pathways

= ligands

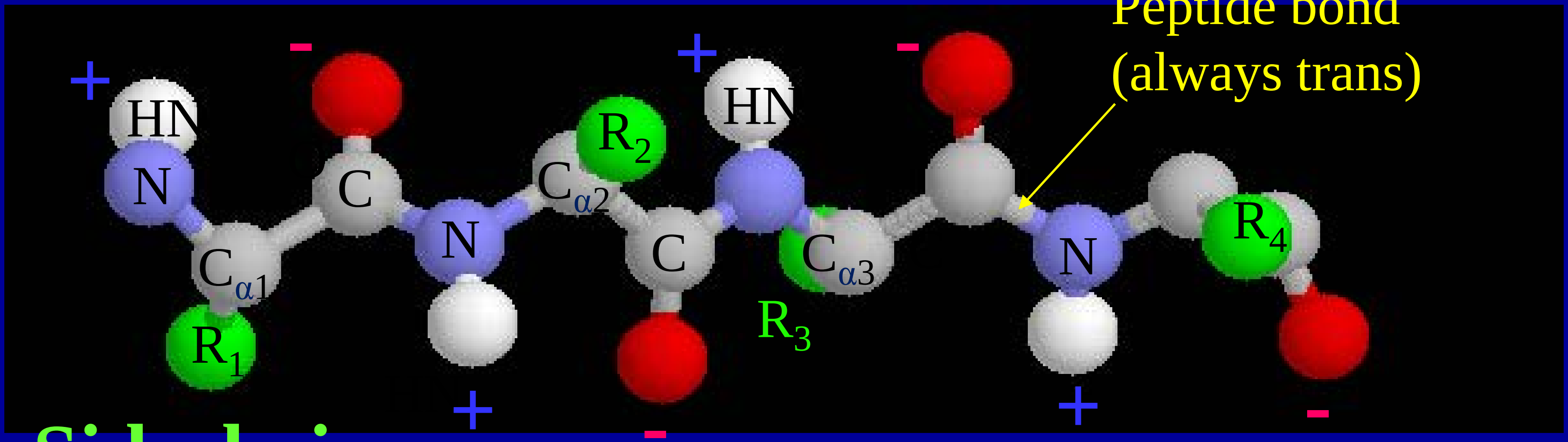
= PROTEINS



What are proteins? **The chemical answer**:

- Linear polymers of amino acids
- The sequence is from the genetic code
- ~100,000 proteins are responsible the life process

Backbone



Sidechains

H on each C_α not shown