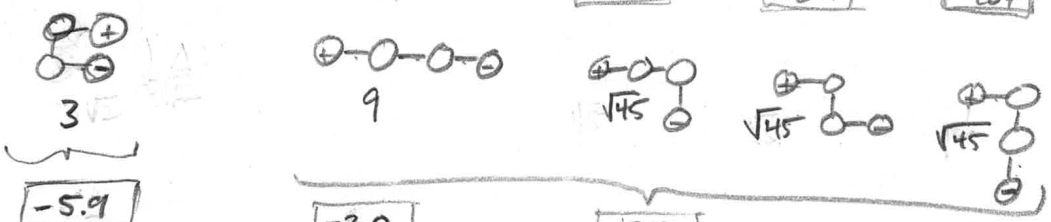
GOAL: MAP MICROSCOPIC CHEMISTRY TO MESOSCOPIC BIOLOGY

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

ΔH: DIFF INTERACT

ΔS: DIFF IN DEGENERACY

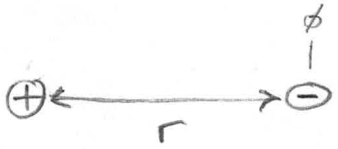
VACUUM: $\boxed{-463\ kJ/mol}$ | $\boxed{-154}$ | $\boxed{-207}$ | $\boxed{+207}$ | $\boxed{-207}$



H_2O: $\boxed{-5.9}$ | $\boxed{-2.0}$ | $\boxed{-2.6}$

HOW DO WE CALCULATE ΔS? COUNT

ΔH? FORCEFIELD.



$$F = \frac{-kq_1q_2}{r^2} \qquad \epsilon = \int \frac{-kq_1q_2}{r^2}\,dr$$

$$k = 1389\ \frac{kJ}{mol \cdot \text{Å}} \qquad = -kq_1q_2 \int \frac{1}{r^2}\,dr$$

$q \in \{+1, +2, -1, \ldots 3\}$ $\qquad = \frac{kq_1q_2}{r} + c \Big|_{\infty}^{r}$

BOUNDARY CONDITION: AS $r \to \infty$, $\epsilon \to \phi$

$$\epsilon = \phi + c \therefore c = \phi$$

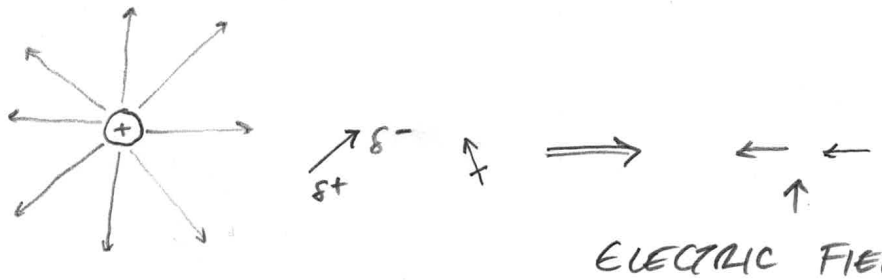
$$\epsilon = \frac{kq_1q_2}{r}$$

$RT = 0.008314 \times 298 = 2.42$

$$\Delta G = -RT \ln\left[\frac{e^{-463/RT}}{e^{-154/RT} + 3e^{-207/RT}}\right]$$

$\boxed{= -253\ kJ/mol}$ VACUUM $\Rightarrow$ $\boxed{-0.1\ kJ/mol}$ H_2O

BUT THAT ASSUMED A VACUUM...



ELECTRIC FIELDS <u>POLARIZE</u> MATERIALS. THIS ATTENUATES THE FIELD (WEAKENS INTERACTIONS)

POLARIZABILITY CAPTURED BY DIELECTRIC CONSTANT ε.
- ASSUMES "BULK", ISOTROPIC MATERIAL.

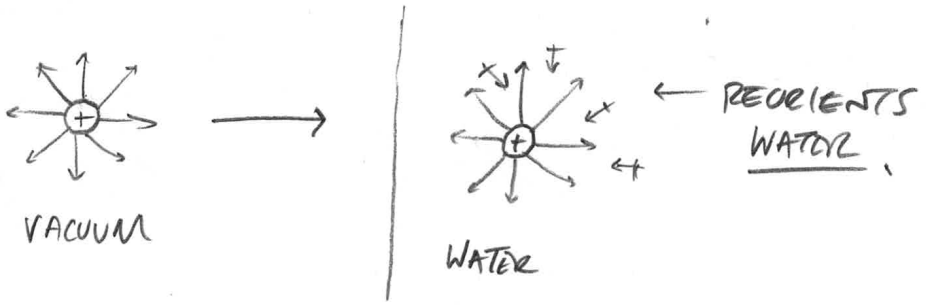
$$E = \frac{k q_1 q_2}{r \varepsilon}$$

ε	MATERIAL
1	VACUUM
2-4	OIL, DEHYDRATED PROTEIN
78.5	H_2O

CAN HAVE A HUGE EFFECT:

-117 kJ/mol (VACUUM) $\longrightarrow$ $+1.6$ kJ/mol (H_2O)

<u>SELF ENERGY</u>:



$$\Delta G_{TRANSFER} = \frac{k q^2}{r_{ion}} \left(\frac{1}{\varepsilon_{H_2O}} - \frac{1}{1} \right)$$

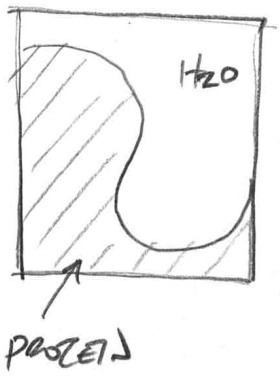
<u>EXERCISE</u>:

$r_{ion} = 1$ Å WATER → MIDDLE OF BILAYER.

$q = +1$

$$\frac{1389 \cdot 1^2}{1} \left(\frac{1}{4} - \frac{1}{78.5} \right) = 330 \text{ kJ/mol}$$ (A LOT!)

PROBLEM: BIOMOLECULES HAVE SHAPE.



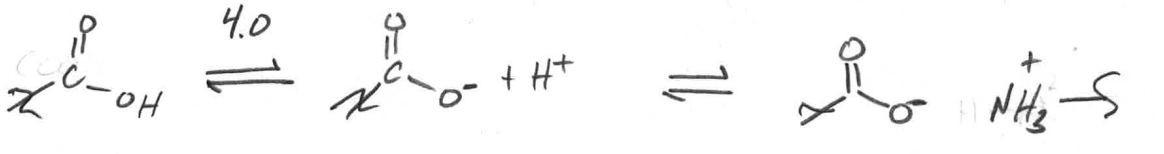
$$\nabla^2\psi(\vec{x}) = \frac{-\alpha [I]\left(e^{-\psi(\vec{x})/kT} - e^{\psi(\vec{x})/kT}\right)}{\varepsilon(\vec{x})}$$

POISSON-BOLTZMANN EQUATION.

$\psi(\vec{x})$ POTENTIAL

$\vec{x}$ POSITION IN SPACE

YOU CAN MEASURE STRENGTH OF AN INTERACTION BY ΔpK_a.



pKa OF ASP WILL GO DOWN