Entropic Costs

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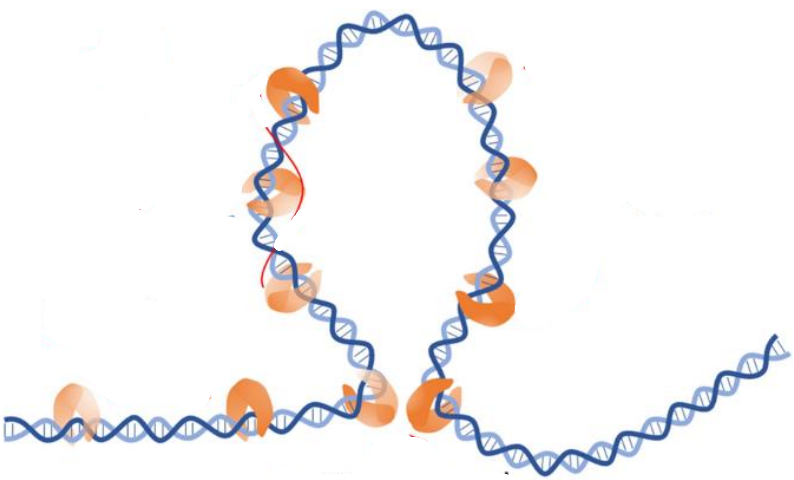
Suppose there were 2 types of binding sites on the strand:

$$S = k_B \ln(\Omega)$$

Protein binding sites on DNA:



Representative image from:
Park et al., J. Korean. Phys. Soc., **78**, 408–426 (2021): review

Entropy of composite systems:

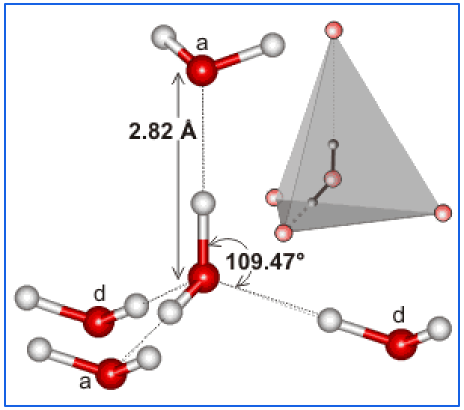
For the composite system,

$$\Omega_{(total)} = \Omega_1 \times \Omega_2$$

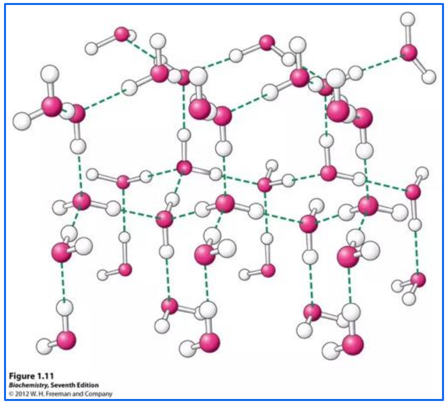
$$S_{tot} = k_B \ln \underline{\Omega} = \underline{S_1} + \underline{S_2}$$

Entropy is additive

Hydrophobicity: **entropic cost** of solvation

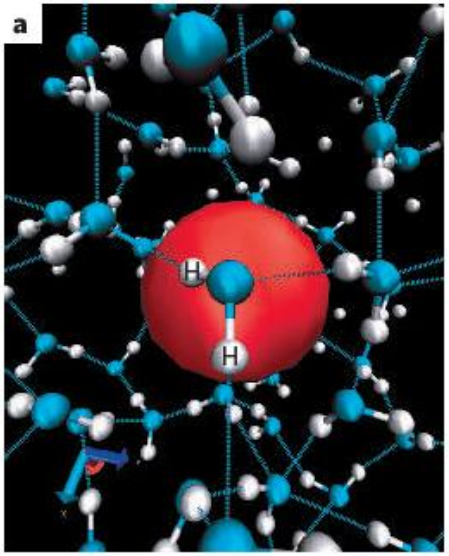


H_2O form tetrahedral structure



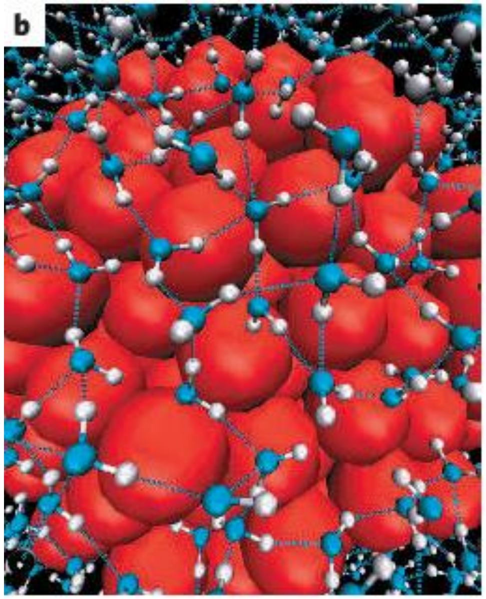
Network of hydrogen bonded molecules

Small (water unfriendly) solute

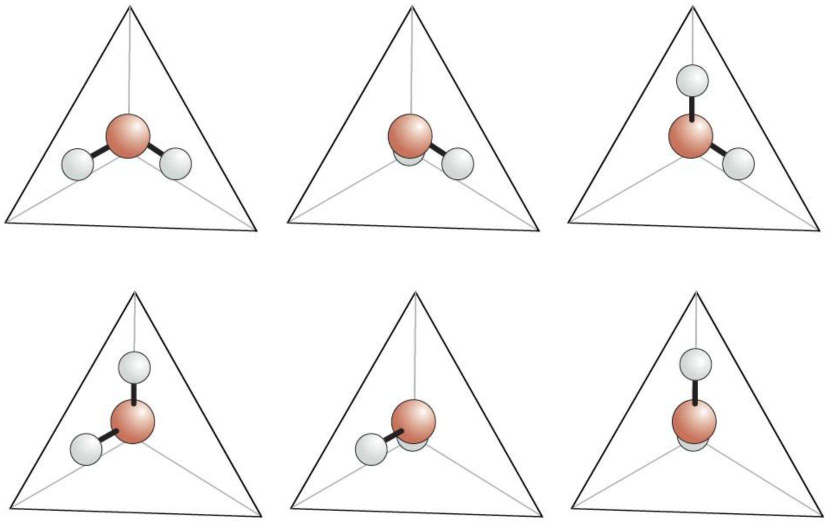


VS.

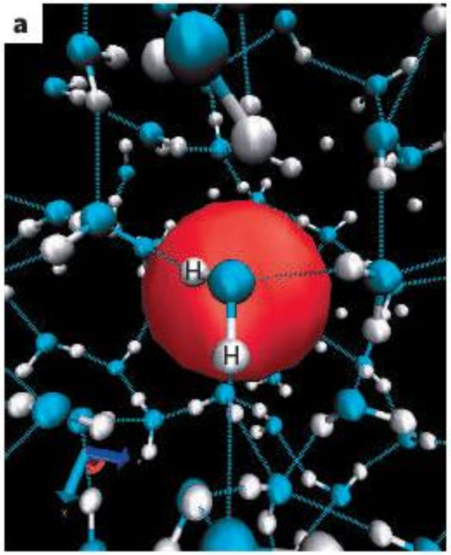
Large solute



Approximating the entropic cost



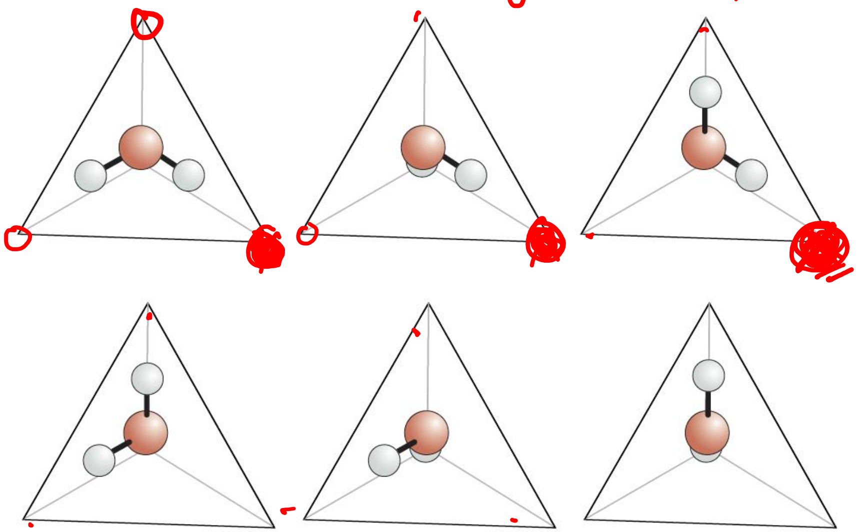
6 possible molecular orientations



Approximating the entropic cost of hydrophobic solvation

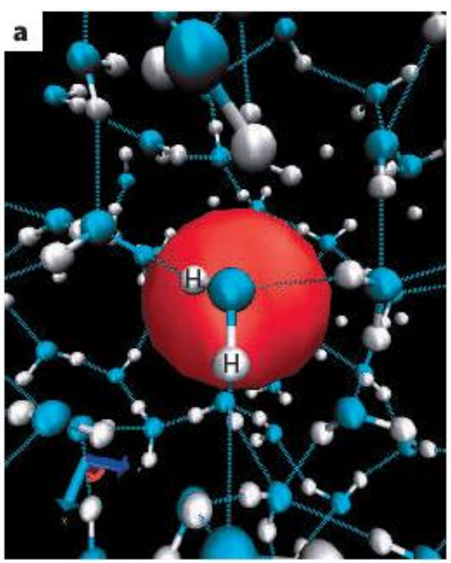
● → an original H_2O partner

⊗ → occupied by a hydrophobic molecule (entity)



$$\Omega_{original} = 6$$

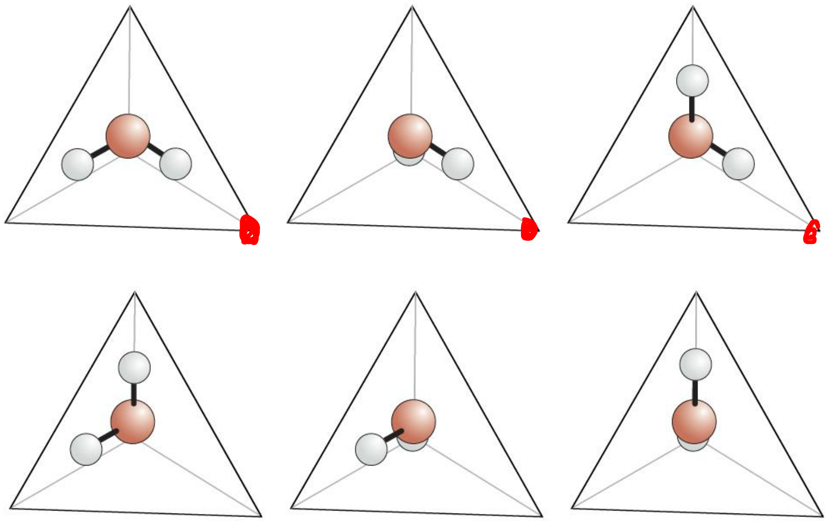
$$\Omega_{reduced} = 3$$



6 possible molecular orientations

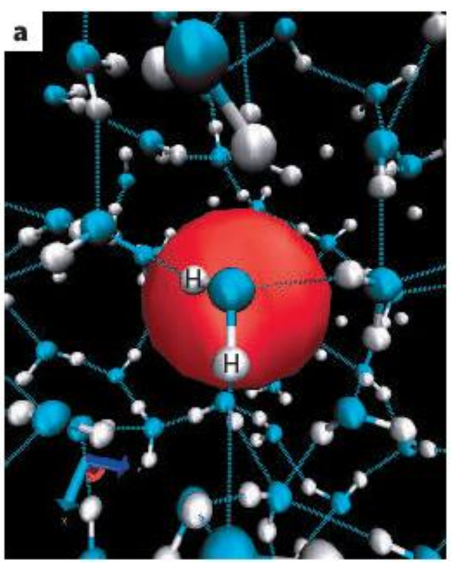
When one site is replaced,
3 orientations are lost.

Approximating the entropic cost of hydrophobic solvation



Water molecule orientations

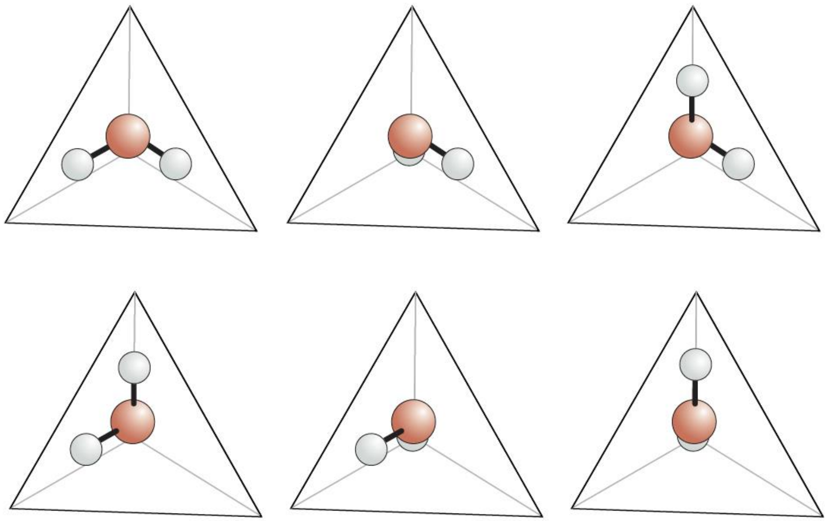
$$\Delta S_{hydrophobic} = S_{reduced} - S_{original} = -k_B \ln 2$$



When ‘n’ molecules lose one H-bonding partner,

$$\Delta S_{hydrophobic(n)} = -n k_B \ln 2$$

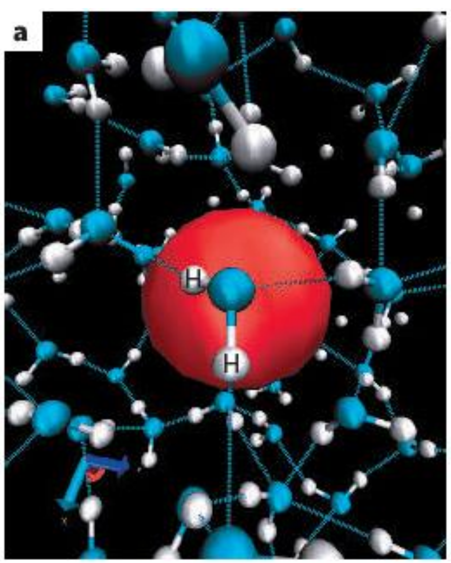
Approximating the entropic cost of hydrophobic solvation



If enthalpic (energetic) cost is insignificant,

$$\Delta G_{hydrophobic} = -T\Delta S_{hydrophobic}$$

$$= n k_B T \ln(2)$$

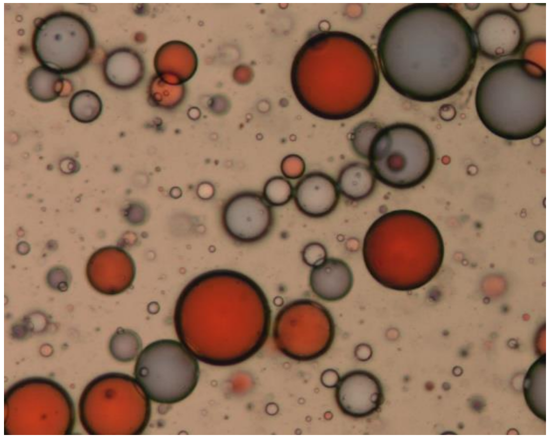


Now 'n' is proportional to the area (A) of hydrophobic solute, ie.

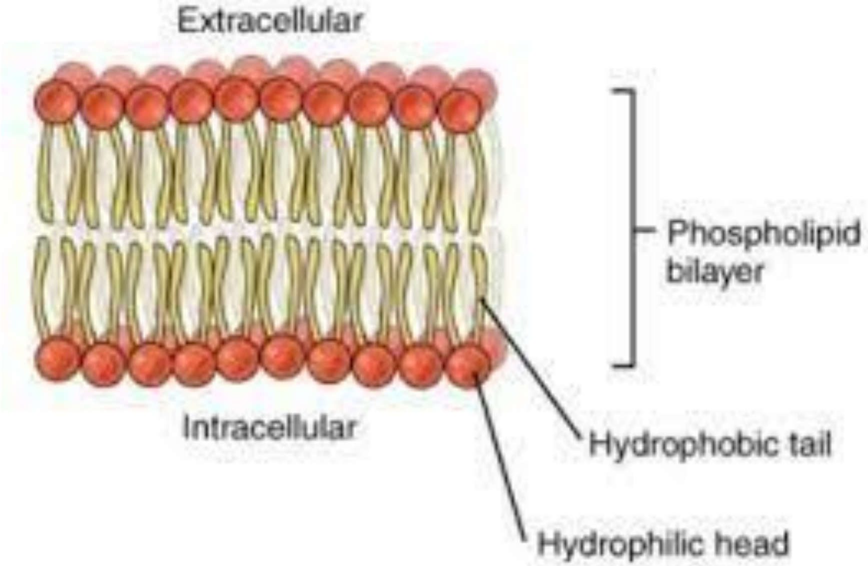
$$\Delta G_{hydrophobic} = (\text{cost per unit area}) \times A$$

What is the entropic cost of maintaining a hydrophobic surface?

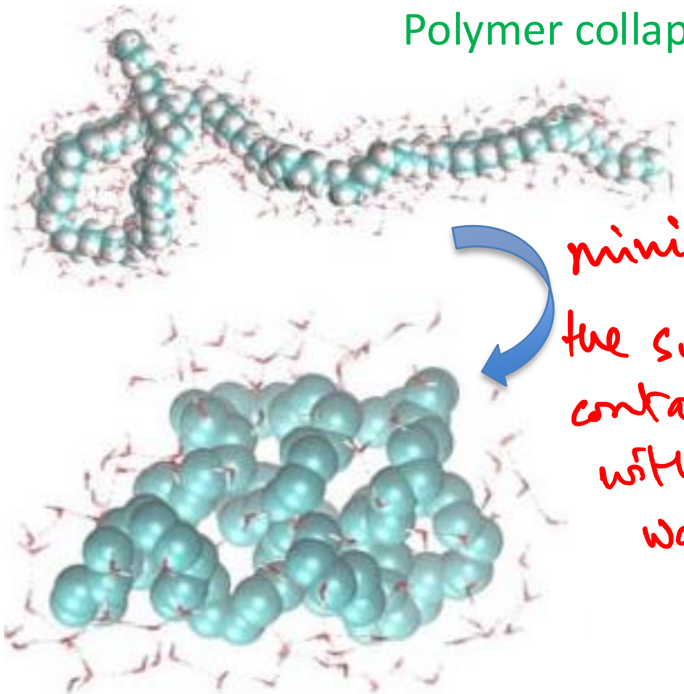
Oil droplets merging



Membrane bilayer formation



Polymer collapse



minimize the surface contact with water!

Protein folding (initial events)