Model Studies on self-assembly of amphiphilic macromolecules with solvent exposed hydrophobic moieties

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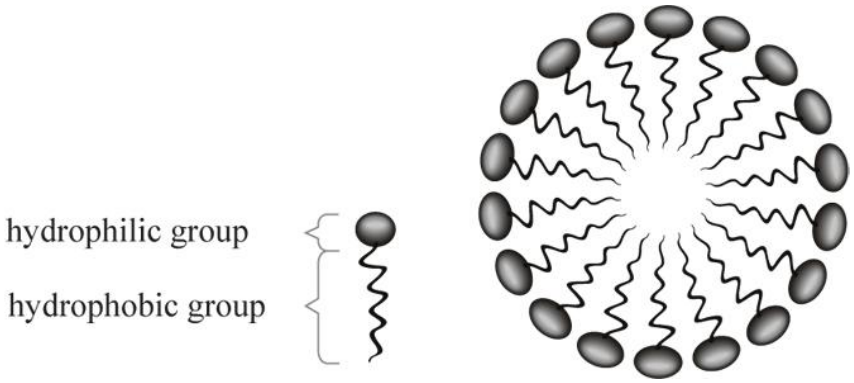
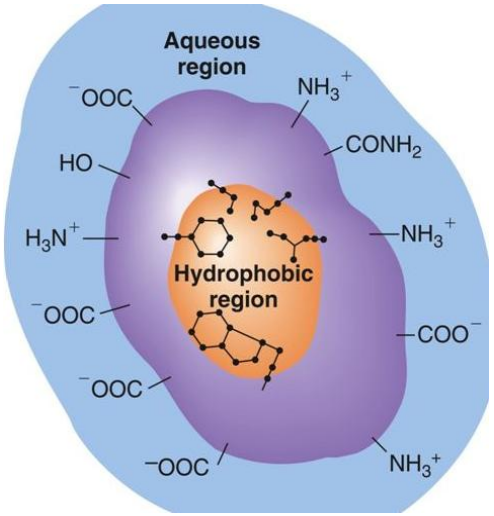
Self assembly

❑ Amphiphilic molecules self-assemble typically at nanometer (nm) length scale to expose their hydrophilic parts and hide in the hydrophobic parts

❑ Surfactant



❑ Proteins; amphiphilic molecule, structurally complex



Reverse situation: hydrophobic parts exposed either by design or physiological reasons

Mis-folding: macro-molecular assemblies

- **bio-compatibility**
- **diseases**

Background

❑Coarse grained model for self-assembly in macromolecules:

- balance between short-ranged depletion mediated attraction and long ranged electrostatic repulsion;
- applied to lysozyme clusters

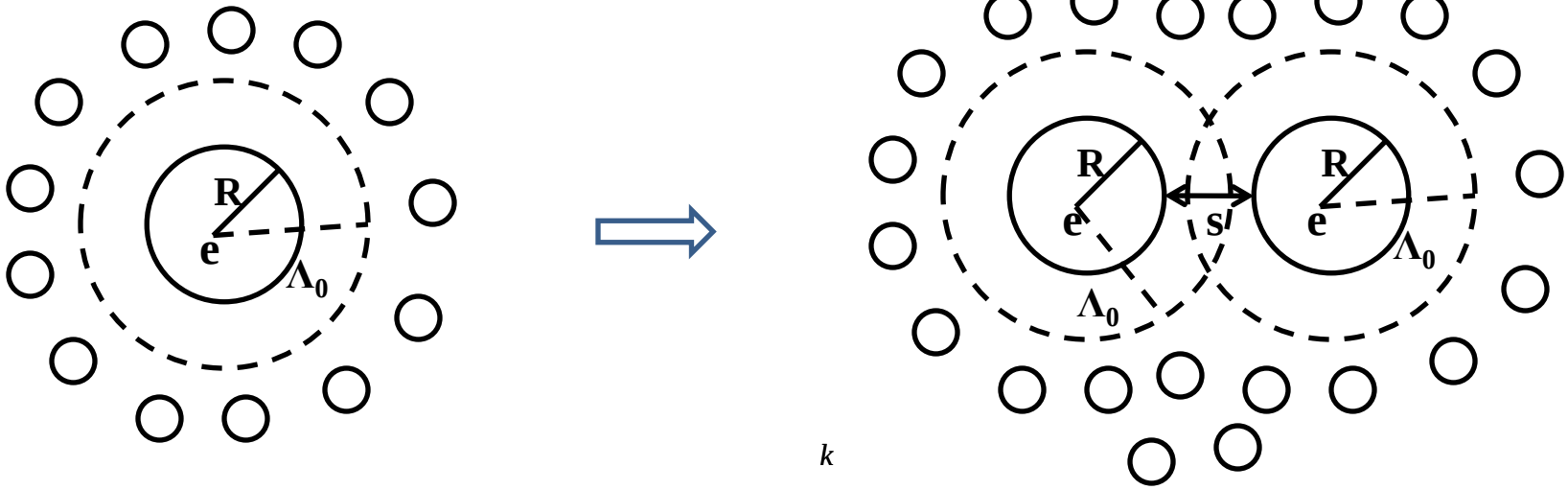
❑Studies on Mis-folded proteins (amyloids):

- cluster size depending on stretch of hydrophobic parts,
- pH and salt-concentration ;
- Temperature: maximum cluster size at an intermediate temperature

Objective

To understand: balance of forces to stabilize nm sized clusters of macromolecules with exposed hydrophobic parts

Model System



k

Attractive potential

$$V_A(s) = -\alpha[s(1 - (\Lambda_0/R)^2) - s^2/2R]$$

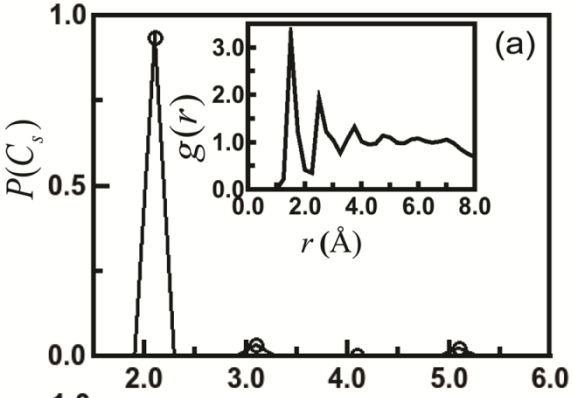
$$\alpha = 8\pi\gamma\Lambda_0$$

γ: surface tension

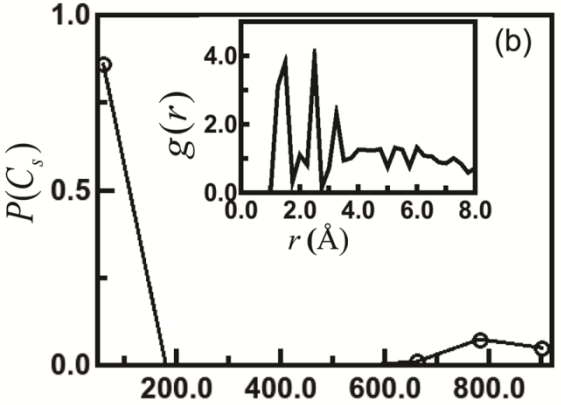
Electrostatic screened repulsion between charges at centre: Debye screening length , $1/\kappa$

J. Chakrabarti and Suman Dutta, Chemical Physics Letters, **620** (2015).

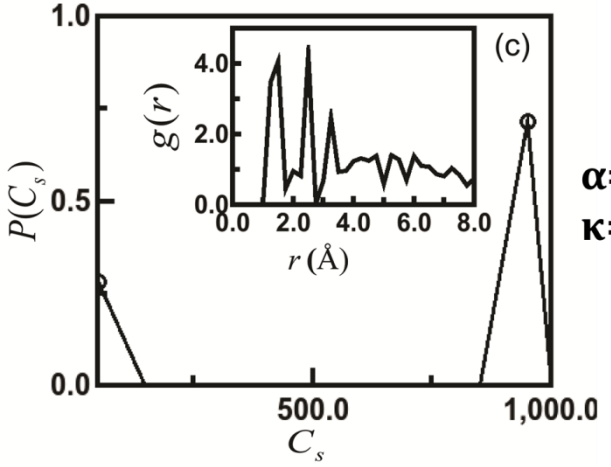
Monte-Carlo: Cluster size



α=3.0
κ=2.0

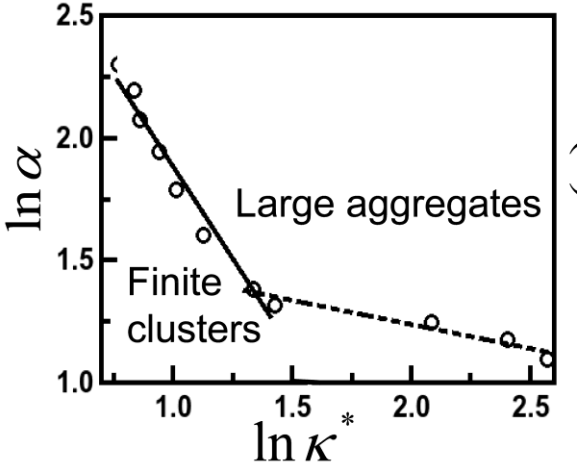


α=3.0
κ=6.0



α=3.0
κ=13.0

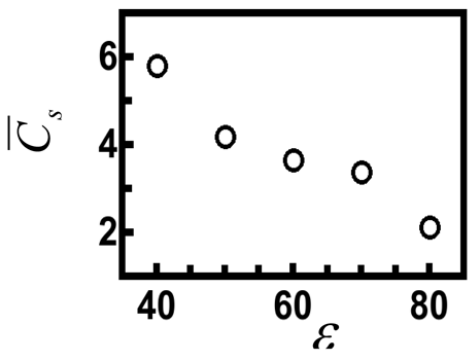
- Amorphous structure

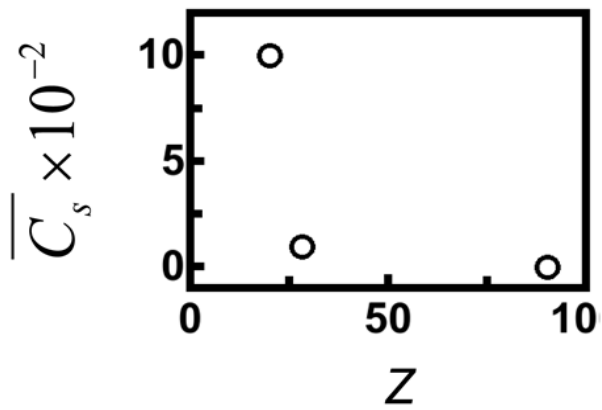


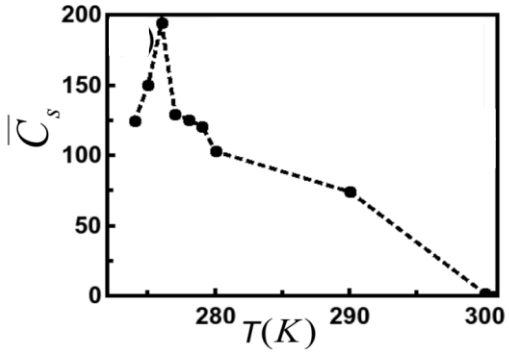
$$\alpha \sim \kappa^{-1.5}$$

Supported by mean spherical approximation

Cluster size

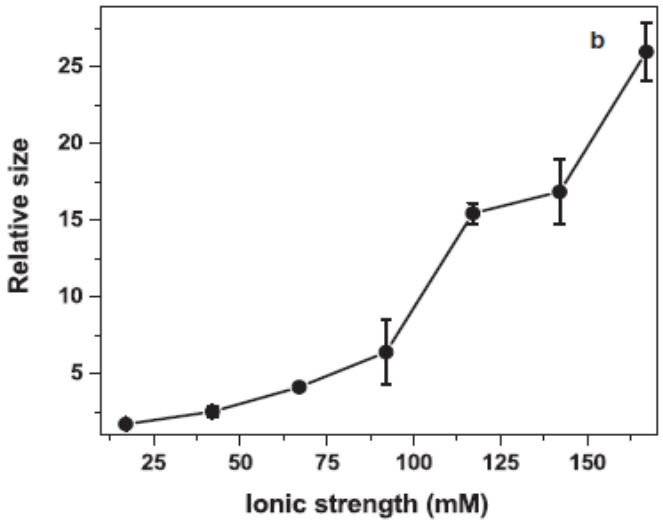


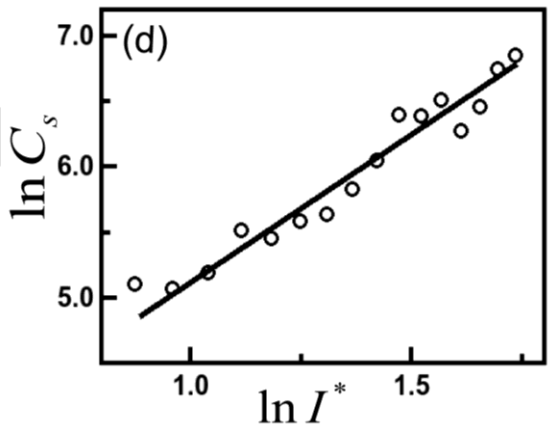




- Cluster size increases with decreasing polarity as well as for charge
- Cluster size shows non monotonic temperature dependence: decreasing surface tension and increasing compressibility with temperature

Comparing with experiments on amyloids





Conclusion: **Model for controlling macromolecular self-assembled structures**

Thank you