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PHYS3009: Force and Function at the Nanoscale
Week 27 – 9:00am Friday – 24 March 2023

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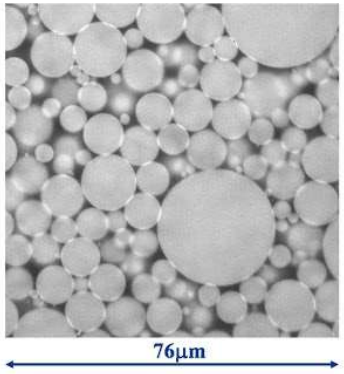
Self-assembly - Micelles

Force & function at the nanoscale

Mayonnaise

Oil and water will separate out in order to minimise the interfacial energy cost associated with the interface between the two materials.

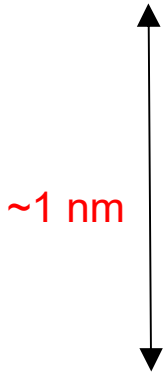
However, Mayonnaise is mostly oil and water yet it does not separate out. Why?

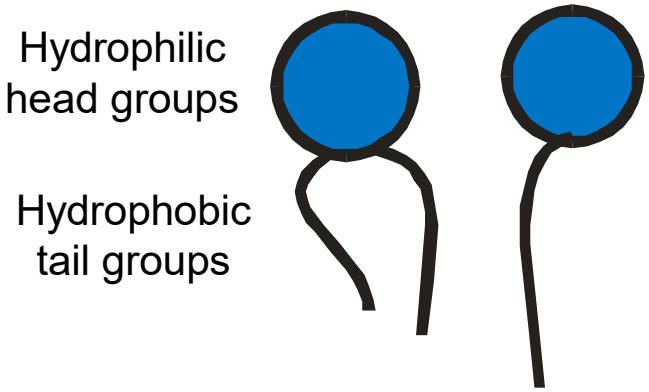


Some of the molecules contained in egg can stabilise the droplets of oil and prevent them from coalescing. These molecules sit at the interface between the two liquids.

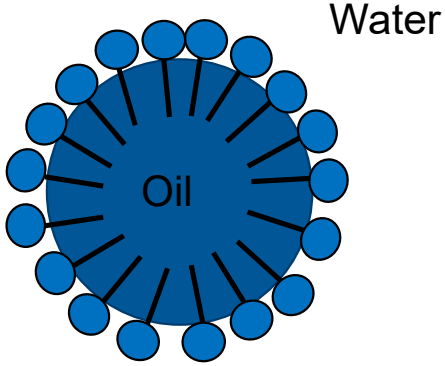
Amphiphilic molecules

Amphiphiles are molecules which have a water soluble head group and a hydrophobic tail group





When amphiphiles sit at the interface between the water and oil these 2 liquids do not come into contact as much, which can reduce or eliminate the energy cost of the interface.



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16.1 - Problem: Why do we use soap?!

Soap is full of amphiphiles. When you wash you dissolve soap in the water.

Assume that a piece of dirt is hydrophobic and that the surface is relatively hydrophilic.

Think about the interfacial energies and explain why soap helps to pull the dirt away from the surface.

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“Micellar Technology”

REDKEN 5TH AVENUE NYC

PRODUCTS HAIRCOLOR MEN'S LOOKBOOK HAIR STYLING BLOG HAIR DIAGNOSTIC TOOL REDKENPRO

HAIRCARE

WHAT IS MICELLAR SHAMPOO AND WHAT ARE THE BENEFITS?

APRIL 12, 2017

Tags : haircare

It’s no secret that beauty fanatics can’t stop raving about the benefits of micellar water. Whether it’s for removing waterproof makeup or used as a quick way to refresh the skin, these gentle cleansers can seemingly do it all. However, micellar waters are no longer exclusive to your skincare. This latest haircare innovation brings the power of micelles into your shower.

Hair 101: How T
Choose the Be
Shampoo For
Hair

Hair 101: How T
The Best Brush
Your Hair Type

Quiz: How To C
The Right Hairc
Routine For Yo
Lifestyle

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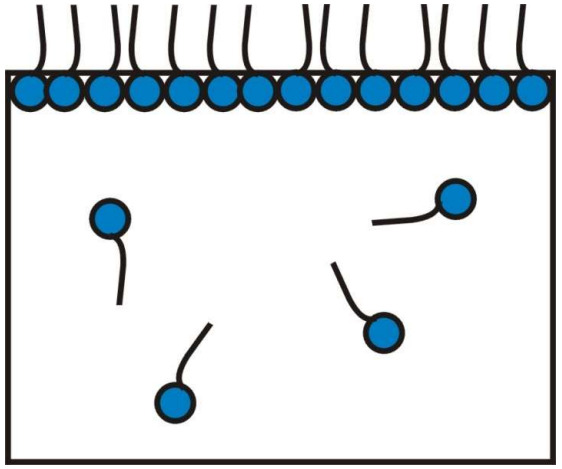
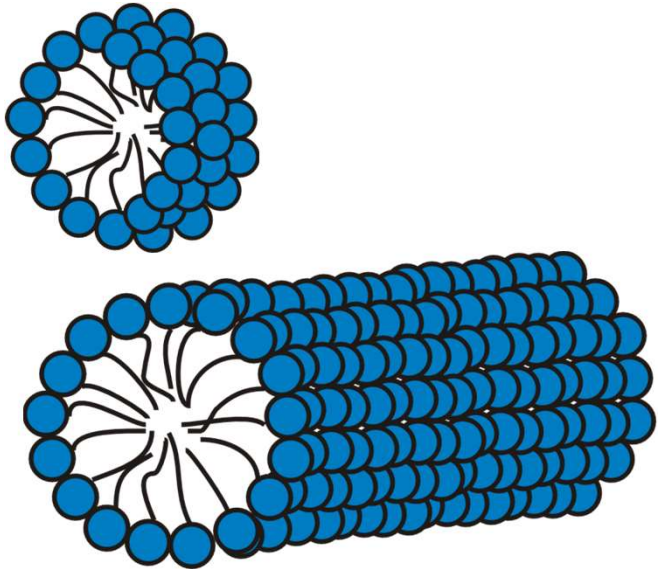
The critical micelle concentration

When amphiphilic molecules are added to just water, they will disperse and some will migrate to the surface to reduce the unfavourable contact between the hydrocarbon tails and the water. The molecules exist as monomers





At a concentration called the **critical micelle concentration** aggregates (or micelles) start to form in such a way that the hydrophobic tails become shielded from the aqueous environment

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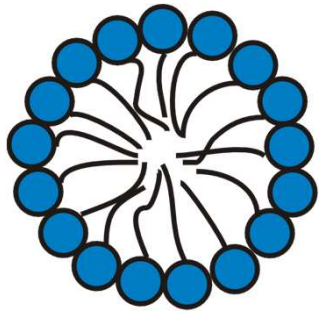
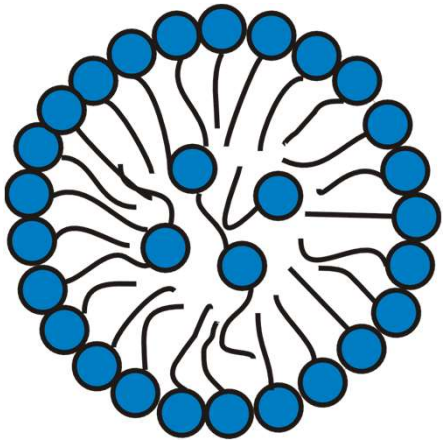
The structure of a micelle

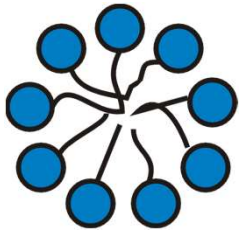
The free energy per molecule of amphiphiles in a micelle has a minimum at a specific aggregation number.

It is easy to see why this might be the case



Optimum size hydrocarbon tails pack in interior and are shielded from water by headgroups





Too small
Gaps between headgroups allow water to contact hydrophobic tails

Too big
Unfavourable interactions between headgroups and tail groups between molecules in micelle

Optimum headgroup area

There are two contributions to the optimum headgroup area

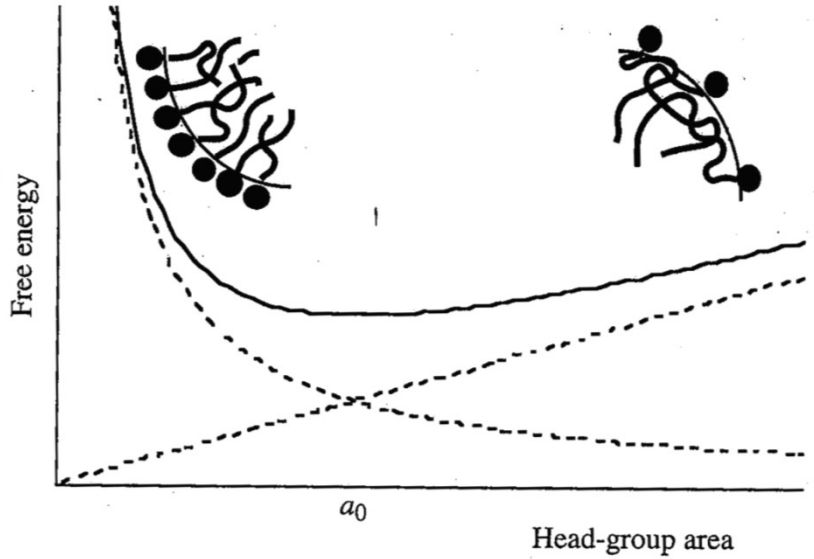
Electrostatic or steric effects

Repulsion between the head groups acts to force neighbouring molecules apart

Hydrophobic interactions

If the head groups are separated too much then hydrocarbon tails are exposed to water

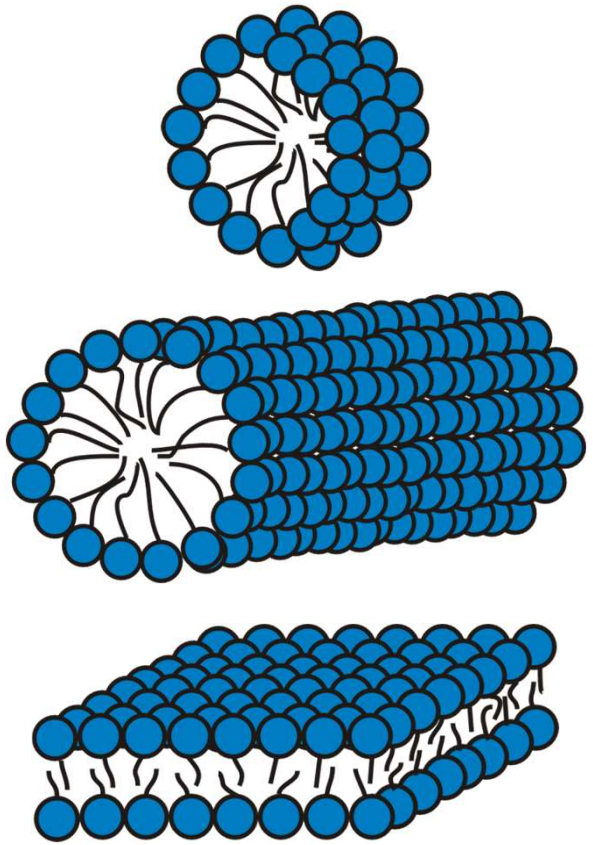
A balance between these interactions determines the optimum area that is occupied by each headgroup



16.2 - Factors influencing micelle shape

Amphiphiles are capable of forming different shaped micelles including spheres, cylinders and bi-layers

The fluid like nature of these molecules means that we can determine the shape of micelles by considering how the amphiphiles pack together

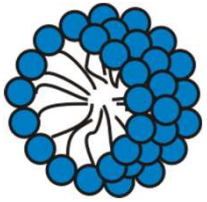


Amphiphile shapes

So the shape of micelles formed by amphiphiles is determined by a geometric packing parameter

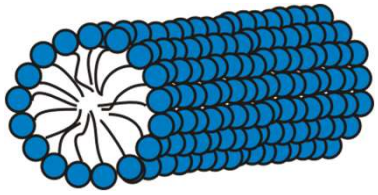
$$H = \frac{v}{l_c a_o}$$

$$H \leq \frac{1}{3}$$

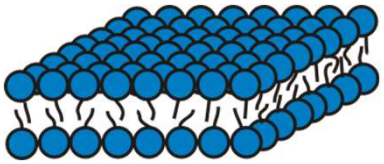


Small v
Large l_c and a_o

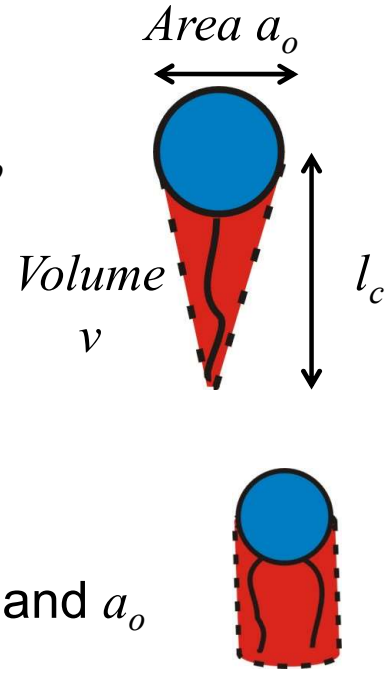
$$\frac{1}{3} < H \leq \frac{1}{2}$$



$$\frac{1}{2} < H \leq 1$$



Large v
Small l_c and a_o



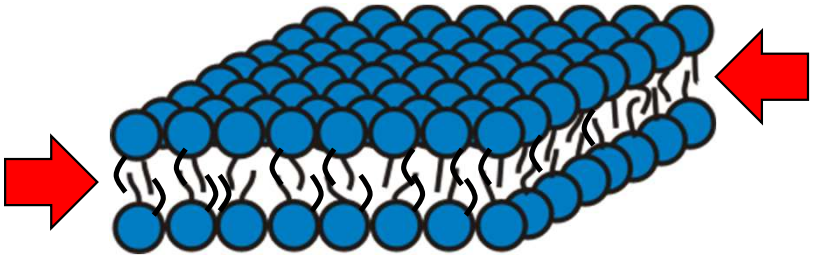
16.3 – What type of micelle is formed?

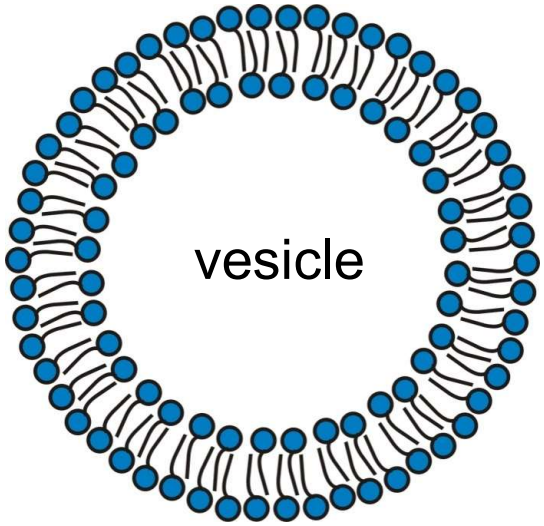
The volume of an amphiphilic molecule containing 10 carbon atoms is v= 0.296 nm^3 and its critical chain length is l_c=1.419 nm with an optimum headgroup area of a_o=0.65 nm^2

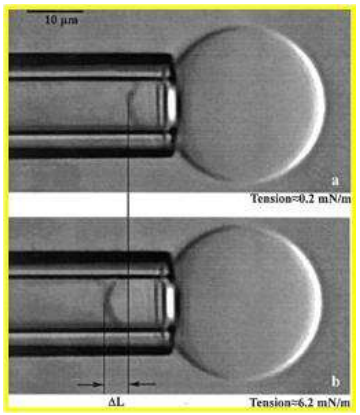
What shape micelles are formed by this amphiphile?

Vesicle formation

When bi-layers are formed in solution, there is an excess energy associated with the exposed hydrophobic tail groups at the edges of the structure







The bi-layers can offset this energy by folding around to close themselves off and form an isolated shell or vesicle

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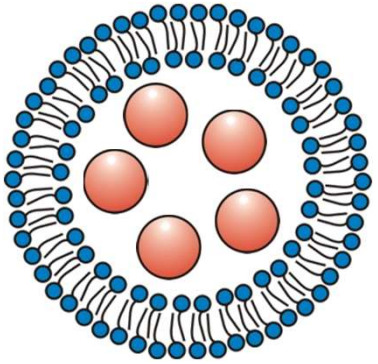
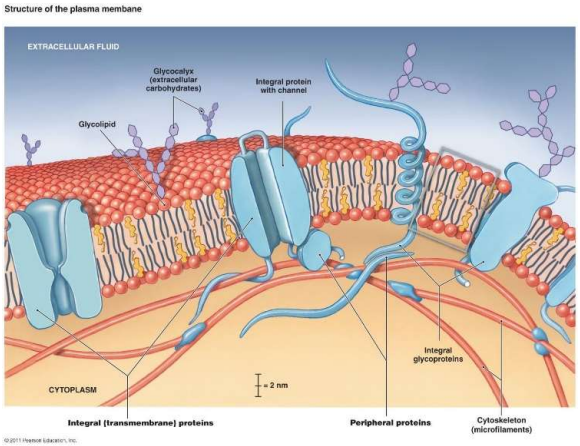
Vesicles

Vesicles are closed structures and can be used to encapsulate materials in their interior for use in drug delivery → Covid vaccine

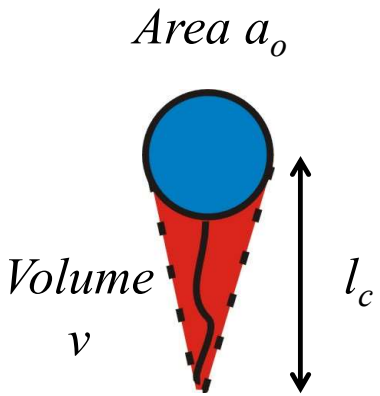
Vesicles are also an excellent model of mammal cells for use in biophysics experiments

The cell wall contains a number of other components but the majority component is amphiphilic molecules known as lipids.





Key points



Amphiphiles have a hydrophilic charged headgroup and a hydrophobic tail which enables them to drastically reduce the cost of an interface

When dispersed in water these spontaneously self-assemble into micelles of different shapes.

The shape is controlled by the value of the shape parameter:

$$\frac{v}{l_c a_0}$$