MSc Project: Molecular-dynamics (MD) simulations on polymeric vesicle architecture

(Joint MSc project between Group Theory of Polymers and Soft Matter, Applied Physics and BioOrganic Chemistry Group, Chemical Engineering and Chemistry)

Requirements: Master student
Interest in fundamental research on the formation of polymeric vesicles
No MD simulation experience required

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Introduction:

Polymersomes are an interesting group of polymeric (micro/nano) vesicles. These vesicles are formed due to the self-assembly of amphiphilic block copolymers into a well-defined nano/micro structure (100- 500 nm). Due to their ability to encapsulate cargo, e.g. antigen/peptides, it is possible to use polymersomes for drug delivery systems. By altering the composition of the block copolymer it is possible to control the polymersome size, membrane thickness and shape. For biological systems (uptake, cell response, etc.) the morphology (size, shape, membrane thickness) of these polymersomes is highly important and, consequently, we are interested in controlling these parameters. Traditionally, the morphology of assemblies of low molecular weight amphiphiles is predicted by using the packaging parameter $p = \frac{v}{a_0 l_c}$ where v = volume of the hydrophobic chain, a_0 = area of the hydrophilic head and l_c = length of the hydrophobic chain. Generally vesicles are formed when $1/2 \leq p \leq 1$.

However, in case of polymeric amphiphiles the packaging parameter is too limited. Besides interactions of the copolymer with itself, neighboring copolymers and its environment, i.e. solvent and non-solvent, the folding of the polymer is an extremely important factor and is difficult to predict without modeling.

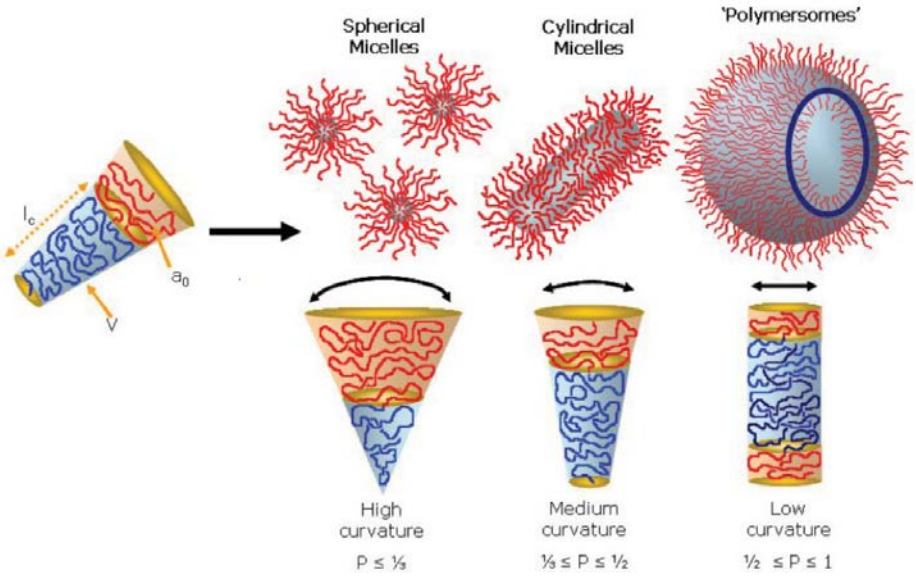

Figure 1 - Blanazs, A., Armes, S. P., & Ryan, A. J. (2009). Self-assembled block copolymer aggregates: From micelles to vesicles and their biological applications. Macromolecular Rapid Communications, 30(4–5), 267–277. https://doi.org/10.1002/marc.200800713

The **goal** of this master project is to use **computer simulations** to calculate the folding of the used block copolymers and its interactions, to **correlate its composition to the morphology**. Also, some of the formed polymersomes have semi-permeable membranes. By simulating membrane density this behavior

can be explained and predicted. Another feature closely related to this permeability is the ability of the polymersome to change its shape by changing the environment (e.g. dialysis against salt). By altering the environment of an already assembled polymersome the change in morphology can be simulated (thanks to the change of interactions of the copolymers with the environment, pressure inside and/or change in membrane density changing the permeability). As we have experimentally access to a wide range of block copolymers, we can effectively validate the model with actual polymer assemblies.

Objectives of the Master student project:

As a Master student you will be given the task to execute MD simulation answering several important research questions. These MD simulations are conducted at an atomistic level giving detailed insight in the interactions of the system. Using these simulations it is possible to explain the behavior of the polymeric vesicles our group fabricates. After simulating these interactions at the atomistic level larger scale coarse grained simulations (DPD) can be done in a more detailed fashion.