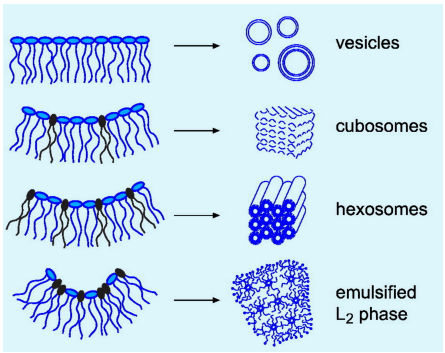
Automated phase recognition of liquid crystalline phases in soft matter (M.Sc./speciale)

The formation of liquid crystalline phases is common in many soft matter systems from lipids to block copolymers and the go-to method to study this is Small-angle X-ray Scattering (SAXS) where a particular phase displays a signature scattering signal. In many cases there are phase transitions between different morphologies, for example due to temperature or pressure changes (see figure below) but also in biological systems as during fat digestion [1]. There have been several softwares developed but none that really convincingly handles dynamic data and also without any automated phase recognition strategy. This is the topic of this project where you will design and write a new piece of software to do exactly that. Depending on progress this might involve extending to include Machine Learning for automation and to handle samples with co-existing phases.

Figure: (right) Time-resolved SAXS on a model lipid system showing a pressure induced phase transition. (below) Illustration of lipids forming liquid crystal phases.



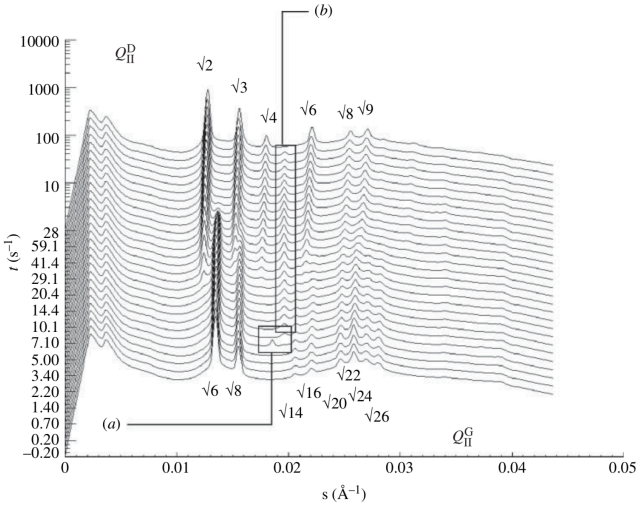


Figure 9. Time-resolved X-ray diffraction plots of the G–D transition induced at T=59.5°C by a pressure-jump from 600 to 240 bar (Squires *et al.* 2005). The intensities are plotted logarithmically

Prerequisites:

✓ Preferably coding experience in Python

As a student you will learn about:

✓ self-assembly and geometry and topology of liquid crystal phases in soft matter
✓ code development and small-angle scattering
✓ be a part of the Structural Food Physics and Soft Matter Self-Assembly research group

Supervisor(s):
Martin Cramer Pedersen (mcpe@nbi.ku.dk) and Jacob Kirkensgaard (jjkk@nbi.ku.dk)

[1] Meiland, Kirkensgaard, Boyd et al., Comparing the lipid self-assembly behaviour and fatty acid composition of plant-based drinks to bovine milk during digestion , Food Chemistry - in review

ABC star block copolymer self-assembly under hyperbolic confinement (M.Sc./speciale)

Numerical simulations reveal a family of hierarchical and chiral multicontinuous network structures self-assembled from a melt blend of Y-shaped ABC and ABD three-miktoarm star terpolymers [1]. These mesostructures are among the most topologically complex morphologies identified to date and represent an example of hierarchical ordering within a hyperbolic pattern, a unique mode of soft-matter self-assembly. In this project the idea is to use a new simulation setup to investigate the self-assembly of model block copolymers under different hyperbolic constraints, i.e. where the polymer are forced to assemble within a thin curved film. The project will involve coding up a range of new analysis routines to understand topological transitions and relate to mappings into the hyperbolic plane, see figure below [2].

Prerequisites:

- ✓ **Preferably coding experience - not so important in what language**

As a student you will:

- ✓ **get an understanding of the fundamentals of DPD and MD**
- ✓ **learn about polymer physics/chemistry**
- ✓ **learn about complex self-assembly and hyperbolic geometry**

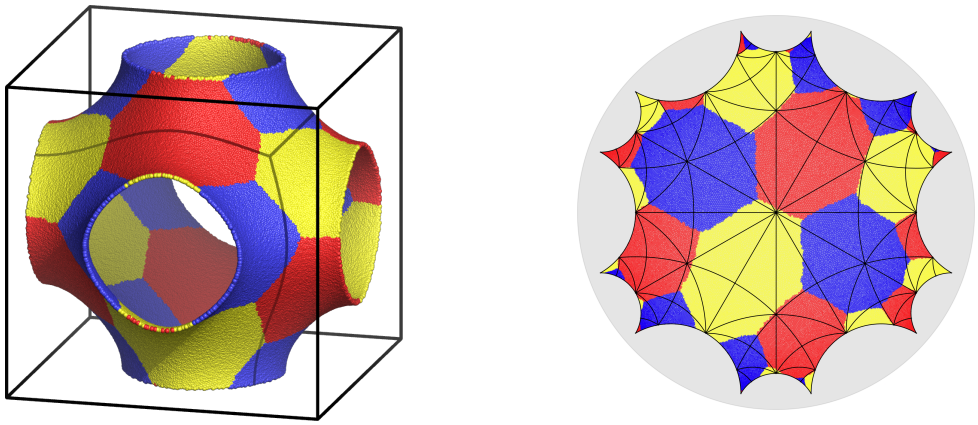


Figure: (left) ABC stars forming a tiling pattern on the P-surface. (right) Back-mapping into the hyperbolic plane allows to unfold the pattern for detailed analysis.

Supervisors:
Martin Cramer Pedersen (mcpe@nbi.ku.dk) and Jacob Kirkensgaard (jjkk@nbi.ku.dk)

References:

[1] Kirkensgaard JJK, Evans, de Campo and Hyde, PNAS, 111, 4, 1271-1276 (2014)
[2] Pedersen MC, Hyde ST, Ramsden S and Kirkensgaard JJK, Mapping hyperbolic order in curved materials, Soft Matter, 2023, 19, 1586

Computational modeling of photosynthetic membranes (M.Sc./speciale)

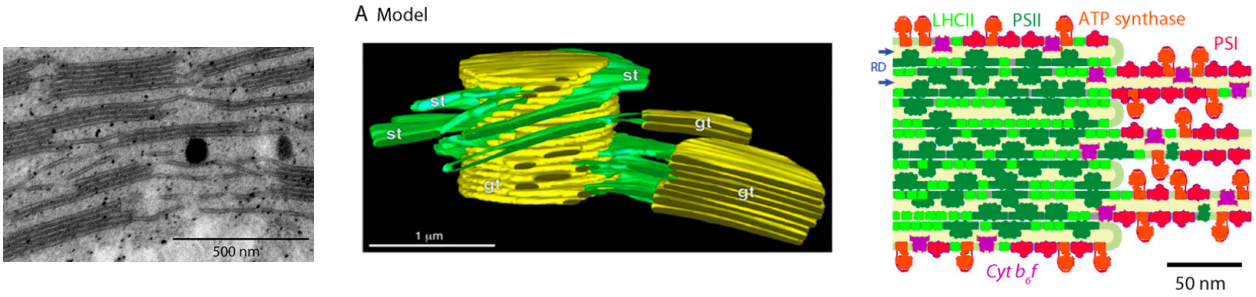
The main photosynthetic machinery in plants and cyanobacteria are embedded in biomembranes called *thylakoids* [2]. The thylakoids host an array of membrane bound proteins that harvest light and convert light to chemical energy. We have access to new experimental data suggesting a better understanding of how this membrane system behaves dynamically as photosynthesis takes place during illumination. In this project the idea is to try and understand this behavior using computational modeling. The main methodology to be employed are dynamic triangulated surface simulations combined with coarse-grained molecular dynamics [1]. You will setup a model system trying to describe the so-called grana stacks (see Figure below) and how the stack behaves dynamically upon illumination.

<u>Prerequisites:</u>

- ✓ **Preferably coding experience - not so important in what language**

<u>As a student you will:</u>

- ✓ **get an understanding of the fundamentals of coarse-grained molecular dynamics and triangulated surface simulations**
- ✓ **learn about photosynthetic membranes and soft matter physics and self-assembly**



<u>Figure:</u> (left) Grana stacks inside chloroplast in plants (middle) 3D tomography data of grana stack (right) Model of the membrane arrangement in the stack.

<u>Supervisors:</u>
Weria Pezeshkian (weria.pezeshkian@nbi.ku.dk) and Jacob Kirkensgaard (jjkk@nbi.ku.dk)

<u>References:</u>

[1] Pezeshkian W and Ipsen J, Mesoscale simulation of biomembranes with FreeDTS, Nature Communications, 2024, 15:548
[2] Jakubauskas D, Mortensen K, Jensen PE and Kirkensgaard JJK, Small-Angle X-ray and Neutron Scattering on Photosynthetic Membranes, Frontiers of Chemistry, 2021, 9, 631370

Striping the Gyroid: numerical pattern formation on hyperbolic surfaces

In previous work we have explored pattern formation on hyperbolic surfaces using particle-based molecular simulations relevant to self-assembled structures found in soft matter systems, for example block copolymers [1]. We have also developed new tools to explore such patterns by mapping from surfaces in 3D to curved 2D space allowing exiting new possibilities for analysis and visualization [2]. In this project we wish to pursue similar questions using a more continuous field-based approach. Initially this means setting up code to solve a partial differential equation on triple-periodic minimal surfaces, for example the Swift–Hohenberg equation or similar approaches describing pattern-formation in 2-phase systems. Depending on progress we might expand this into more complex, physical models.

Prerequisites:
- ✓ Basic knowledge of partial differential equations and related numerical methods
- ✓ Interest in soft condensed matter physics, geometry, and numerical models
- ✓ Preferably Python coding experience

As a student you will:
- ✓ Implement a numerical scheme to solve PDEs on period minimal surfaces
- ✓ Learn about complex soft matter self-assembly and hyperbolic geometry
- ✓ Explore the role of curvature in material science

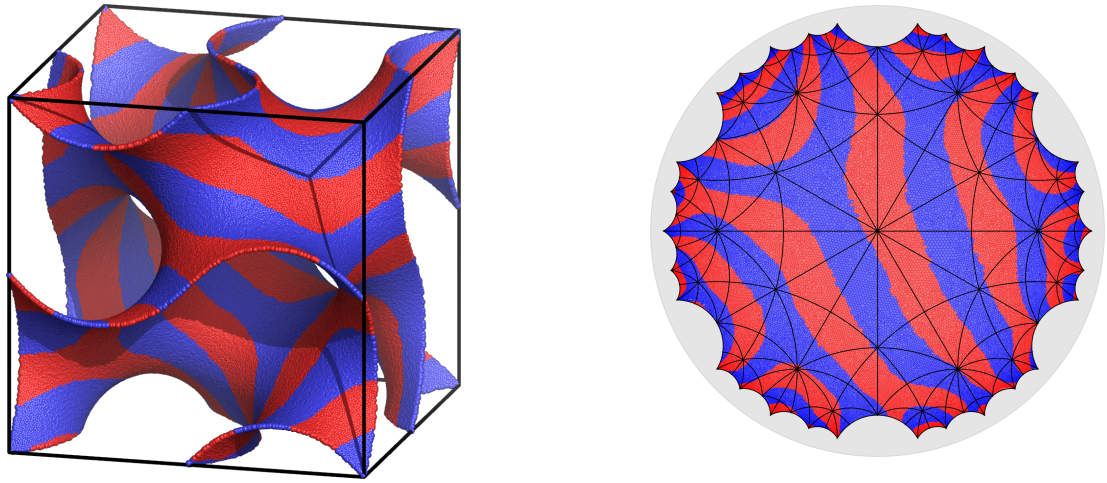


Figure: Simulated stripe pattern on the Gyroid minimal surface shown on the surface embedded in E^3 and in the universal cover of the Gyroid, hyperbolic two-space, H^2.

Supervisor(s):
Martin Cramer Pedersen (mcpe@nbi.ku.dk) and Jacob Kirkensgaard (jjkk@nbi.dk)

References:
[1] Kirkensgaard JJK, Evans, de Campo and Hyde, Hierarchical self-assembly of a striped gyroid formed by threaded chiral mesoscale networks, PNAS, 111, 4, 1271-1276 (2014)
[2] Pedersen MC, Hyde ST, Ramsden S and Kirkensgaard JJK, Mapping hyperbolic order in curved materials, Soft Matter, 19, 1586 (2023)

Jacob Kirkensgaard

Structural Food Physics and Soft Matter Self-Assembly

X-ray and neutron scattering investigations of nanostructures in materials
Coarse-grained simulations of soft matter self-assembly

Contact:
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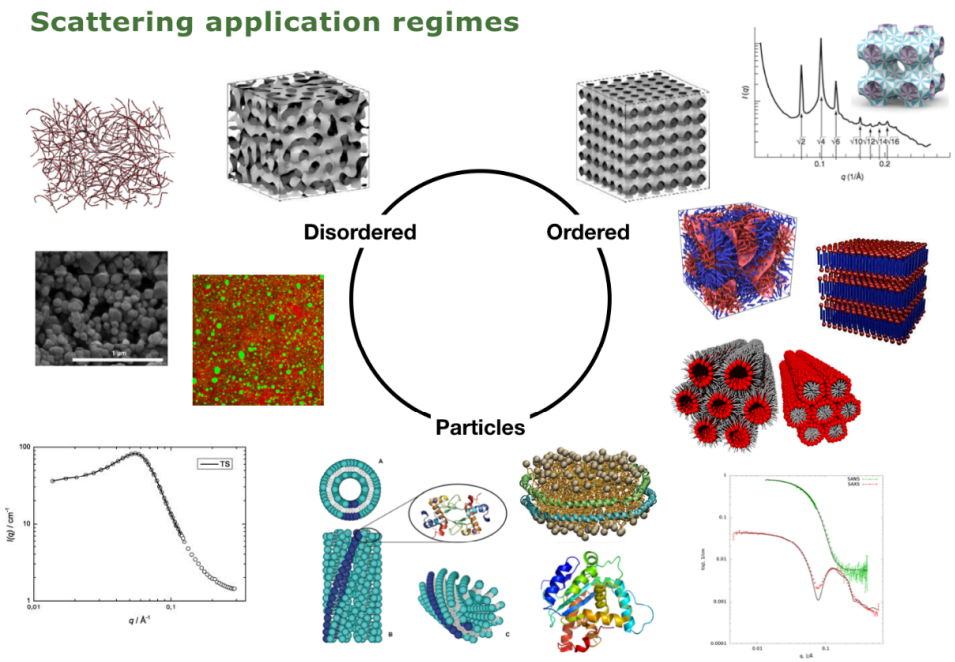

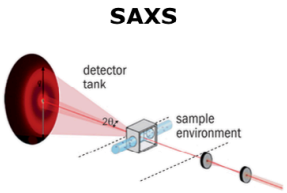

In general my research is centered around mesoscale self-assembly and particularly the formation of geometrically and topologically complex structures in soft matter systems, both synthetic systems like block copolymers and amphiphilic molecules and from various biological systems, for example photosynthetic membranes and biomacromolecules. I have combined expertise in coarse-grained molecular dynamics simulations of soft matter self-assembly and in structural investigations using small-angle x-ray and neutron scattering techniques. I have worked on a number of systems within synthetic biology, food science, electrochemistry, lipid and fatty acid polymorphism, biopolymers and complex synthetic polymers. I am heading a new hub within the Nanoscience center focused on Structural Food Physics and Soft Matter Self-Assembly and I am employed jointly at NBI and FOOD at KU. I am running two in-hhouse SAXS/WAXS instruments which make a nice platform for projects. In terms of specific projects, the following are some current ideas - but others could easily be formulated to accommodate your particular interests:

Potential project headlines:

Nanostructural effects of high pressure processing in food production (experimental)

Ethylcellulose-based oleogel structure (experimental)

Block-copolymer self-assembly in solution (experimental)

RheoSAXS studies of polymer or fibrous soft matter (experimental)

Computational topology of soft matter self-assembly (w. Martin C. Pedersen, NBI, theoretical)

Simulation of block copolymer or active matter self-assembly under hyperbolic confinement (w. MC. Pedersen, NBI, theoretical)

Examples of recent or ongoing projects:

Role of nanostructure on lipid oxidation studied with light scattering, x-ray scattering and electron spin resonance (MSc, Nano)

Nanostructural transitions during digestion of fat-based food (BSc, Nano)

Simulation of diblock copolymer self-assembly on hyperbolic surfaces (BSc, Physics)