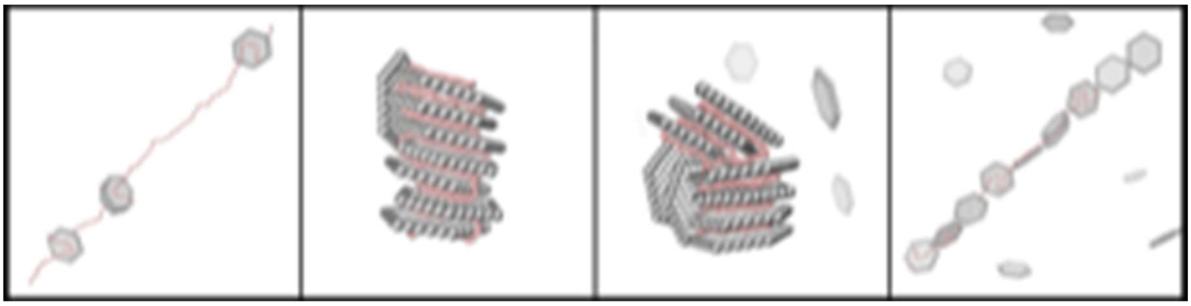

Method tags: Molecular dynamics simulations, atomistic and coarse-grained modelling, SAXS
Scientific tags: Material science, macromolecular and colloidal chemistry
Link to research group: https://www.teokem.lu.se/people/seniors/skepoe/
Contact Information:
Title of Project: Clay, an ancient material with great future
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Lab: Skepö research group

In Skepö research group we use a combination of computer simulations and experiments to understand, describe and predict complex solutions with focus on macromolecules. Unlike small molecules, a macromolecule often consists of a "chain" of several repeating units and some well-known examples are polymers, proteins and DNA. In Skepö research group, we study, for example, disordered proteins found in saliva, antimicrobial peptides that we hope can partially replace antibiotics, and polyacrylic acid, which is a commonly used polymer in industrial processes. We are interested in how these macromolecules interact with each other in solution and how they behave near different interfaces for example clay. Of particular interest is what structure they adopt and what happens when the concentration or physical conditions, such as temperature, change. Although the macromolecules we study have completely different applications, the fundamental understanding is based on the same physico-chemical principles, which form the basis for the development of our models. Our simulations are computationally intensive and can take from weeks to months to complete. Therefore, they are performed on large computer clusters such as LUNARC, Lund University's computer center for high-performance computing. Our synchrotron light and neutron measurements are made at international research facilities.

The purpose of the master thesis project is to expand the use of clays as a sustainable and environmentally friendly material. Clay is one of the oldest materials used in mankind. For example, some of the earliest pottery shards recovered are dated to around 14,000 BC, and were found in central Honshu, Japan. Besides its use in ceramics, clay has been an important material for construction since ancient times and is still used as bricks and tiles. The unique properties of clays have allowed the discovery of several more applications. Many clay minerals swell in water and yield aqueous dispersions with interesting rheological and structural properties. Clays are made of platelets with a thickness of about 1 nm and lateral dimensions varying from 25 nm in synthetic Laponite clays to 1000 nm in natural montmorillonite. These colloidal platelets are anisotropic with respect to charge, since they have a negatively charged surface, surrounded by an oppositely charged rim (pH dependent). When water is added, the clay platelets become ionized and a rising osmotic pressure in the solution causes the clay to swell. Semi-dilute dispersions with volume fractions above 0.5% can behave as gels (they have a yield stress), and upon drying, they form films with excellent barrier properties. These are often used in surface coatings, paper and polymer films, household, and personal care products. Depending on the size, the platelets can form a lamellar structure making it a seemingly perfect model system for an electrical double layer, where the swelling and stability in saline solution depend strongly on counterion valency and surface charge density. The situation is, however, from a structural point slightly less ideal. Clay is normally not a homogeneous lamellar material, it is rather better described as a disordered structure of stacks of platelets, sometimes called tactoids.

In this project focus will be on the interaction with charged (bio)polymers. The aim of the project is to achieve a molecular understanding of how the linear charge density and charge distribution affects the interaction with clay. For this purpose, a combination of computer simulations and SAXS will be used.