The BSc and MSc projects offered by the Soft and Complex Matter Lab for 2023/24 are given in the following pages, and they can also be found here:

https://www.ntnu.no/machform/report.php?key=176077xc31903f2c1

Pickering emulsions for food applications



Enormous food waste worldwide has huge environmental and cost efficiency impact. Chemical deterioration caused by e.g. oxidation of lipids, vitamins and other food constituents are causes of waste. Many foods are emulsions stabilized by surfactants. Apart from providing physical stability to the emulsions, the emulsifier type and the physical structure of the emulsions can affect chemical stability.

Conventional surfactants have dominated emulsion science due to their ease of use, relatively low cost and control. However, their future industrial use is under threat, because of formulation foaming problems and the need to reduce volatile organic compounds and carbon footprints. The use of socalled Pickering particles for production of physically stable emulsions may be a solution to these problems and may also improve the oxidative stability of the emulsions.

This project explores ways to use edible solid particles such as starch or proteins to stabilize Pickering emulsions for food applications. The ideas include (i) forming so called Pickering emulsion film where emulsion is sprayed or printed on the food grade substrates, (ii) optical interrogation of individual Pickering droplets and (iii) measuring and modelling X-ray and neutron data probing the emulsion interface. The project is connected to the ITN Project http://www.pickfood.eu The project assumes close collaboration with associated PhD students. Travels to other laboratories within the network might be included.

The exact details will be refined with the MSc candidate.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Supervisors: Jon Otto Fossum <u>fossum@ntnu.no</u>, Matti Knaapila, <u>matti.knaapila@ntnu.no</u>; Paul Dommersnes <u>paul.dommersnes@ntnu.no</u>, Kenneth Knudsen <u>kenneth.knudsen@ife.no</u> and PhD students working on the project

Competitive CO2 capture using clay minerals: From science to innovation.

Motivation: Continuous and increasing release of greenhouse gases, in particular CO2, to the atmosphere has a detrimental impact on our environment. In addition to emission reduction, it is imperative to establish effective ways of capturing these gases. The Soft and Complex Matter Lab previously proved that certain clay minerals (Fig.1) are competitive to other relevant porous materials for CO2 capture¹, and



Fig. 1: Smectite clay mineral

recently, our group reported^{2,3} a <u>hitherto overlooked mechanism</u> for CO2 capture by clay (Fig. 2). In that recent work, we combined experimental results from (synchrotron and home-lab) powder X-ray diffraction (PXRD)⁴, Raman spectroscopy, and inelastic neutron scattering (INS) supported by density functional theory calculations (DFT). In experiments synthetic clays were studied to investigate CO2 sorption mechanisms in a pure defect free system.

Role of student in project:

We want to continue the investigations of synthetic clay since there are several aspects of the new CO2 capturing mechanism that are not understood yet. We also want to investigate natural clays in the context of the new mechanism with the purpose of establishing the base for industrial applications. Experiments



Fig. 2: Model for nano-scale crystalline swelling in clay in response to CO2 exposure. The CO2 interacts <u>only</u> with, and causes swelling only of, chlorite-like layers.

that need to be performed are the same ones as those mentioned above, in particular using abundant and environmentally friendly iron rather that less friendly and less abundant nickel as hitherto.

Requirements: Enthusiasm and curiosity about nanoscale methods, materials science condensed matter physics and physical chemistry. Background in condensed matter physics, nanotechnology or materials science is beneficial.

Other Aspects: The project includes travels for experiments at international synchrotron x-ray and neutron facilities. The activity is a collaboration between the Soft and Complex matter Lab at NTNU, NORCE Stavanger, Univ, Bayreuth Germany, Univ. Copenhagen Denmark and Univ. Sao Paulo Brazil.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Contact persons: Postdoc Paulo Michels Brito (<u>paulo.h.m.brito@ntnu.no</u>), Researcher Barbara Pacakova (<u>barbara.pacakova@ntnu.no</u>), Professor Jon Otto Fossum (<u>jon.fossum@ntnu.no</u>)

¹ A nano-silicate material with exceptional capacity for CO2 capture and storage at room temperature, L.P. Cavalcanti, G.N. Kalantzopoulos, J. Eckert, K.D. Knudsen & J.O. Fossum, Scientific Reports 8, 11827 (2018)

² CO2 Capture by Nickel Hydroxide Interstratified in the Nanolayered Space of a Synthetic Clay Mineral, K.W.B. Hunvik, P. Loch, L.P. Cavalcanti, K.K. Seljelid, P.M. Røren, S. Rudic, D. Wallacher, A. Kirch, K.D. Knudsen, C.R. Miranda, J. Breu, H.N. Bordallo & J.O. Fossum, Journal of Physical Chemistry C 124, 26222–26231 (2020)

³ CO2 Adsorption Enhanced by Tuning the Layer Charge in a Clay Mineral, K. W. Bø Hunvik, P. Loch, D. Wallacher, A. Kirch, L. P. Cavalcanti, M. Rieß, M. Daab, V. Josvanger, S. Grätz, F. Yokaichiya, K. Dahl Knudsen, C. Miranda, J. Breu, J. O. Fossum, Langmuir 37, 14491 (2021)

⁴ Controlled Sample Environment for Studying Solid-Gas Interactions by in situ Powder X-ray Diffraction, P.M. Røren, K.W.B. Hunvik, V. Josvanger, O.T. Buset & J.O. Fossum, Journal of Applied Crystallography 54, 1-5 (2021)

Mechanical control of 2D nanosheets.

Motivation: Graphene is a very well-known 2D material, and many different things can be done with it, among them encapsulation or wrapping of particles. Similar to graphene, clays are also 2D materials and our group are experts on clays. We can fabricate clay sheets that are 1nm thick and hundreds of micrometers wide, which would be like a very thin paper sheet. From these clay nanosheets we can make geometrical 2D cuts (similar to cuts on the first row of in the figure) using Focused Ion Beam (FIB) in the NTNU Nanolab, and by depositing drops we can achieve capillary origami (fig 1), which means that using capillary forces we achieve nano scale design/architecture with this self-assembly. This is a way of turning a 2D nano scale object into a 3D nano scale object. Similar things have been done before at the micronscale and now we want to downscale this, moving from macro scale to micron/nano scale

by using use clay nanosheets. for more information, see these references $^{1,2} \ensuremath{\mathsf{2}}$

Role of student in project: The student will carry out experiments either using microfluidic devices wrapping microdroplets or in open cells to wrap single droplets. This will be initially monitored using optical microscopy. Further characterization can be carried out using Atomic Force Microscopy (AFM) and mechanical strength or magnetic manipulation experiments. The student will work together with and be instructed by a PhD candidate and professors. To work will take place in the Soft and Complex Matter Lab. The project is a collaboration locally with the Thermal Two-Phase Flow Laboratory at the Department of Energy and Process Technology at NTNU, and internationally

with partners at École supérieure de physique et de chimie industrielles (ESPCI) (Paris), Pontifical Catholic University of Rio de Janeiro (PUC-Rio) (Brazil). The project can include training/research missions to a collaborator.

Requirements: Enthusiasm, curiosity and will to learn about soft materials science at the nanoscale. Background in physics, nanotechnology or material science is beneficial.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Contact person(s): For further details, please contact PhD candidate Yue Yu (<u>yue.yu@ntnu.no</u>) or Professor Jon Otto Fossum (<u>jon.fossum@ntnu.no</u>).



Capillary wrapping of macrodroplets (copied from https://doi.org/10.1063/1.2775288)



Inverted microscope with syringe pumps used previously by a master student on his experiments.



Sketch of a microfluidic device used for droplet creation.

¹ Capillary Origami: Spontaneous Wrapping of a Droplet with an Elastic Sheet, Charlotte Py, Paul Reverdy, Lionel Doppler, Jose Bico, Benoit Roman and Charles N. Baroud, Phys. Rev. Lett. 98, 156103 (2007)

² Clay nanolayer encapsulation, evolving from origins of life to future technologies, Jon Otto Fossum, European Physical Journal Special Topics 229, 2863–2879 (2020)

Touching the nanoscale – Atomic Force Microscopy of 2D nanosheets

Motivation: Two dimensional (2D) structures belong to the new class of materials exhibiting completely new and exciting physical properties. With this class of materials, we have the experimental access to phenomena that were either just predicted theoretically or their existence was even not postulated before. Inspired by the variety of studied 2D (semi)-conductors and insulators, we work on 2D systems based on natural and synthetic layered silicates and graphene, studying their fundamental properties with the focus on their potential use in electronics¹.



Left: 3D AFM image of the single layer Na-fluorohectorite. Middle: UV LED-array for illumination of graphene oxide. **Right:** Sketch of the C-AFM experiment on heterostructure of clay (gray layers)-intercalated layers (black layers).

Role of the student in the project: The bachelor student will study different types of 2D materials and 2D heterostructures based on graphene and natural and synthetic layered silicates. The student will work on its own specific project in the home NTNU lab and Nanolab and in case of interest, participate on experimental work performed on synchrotron facilities and laboratories of collaborating partners. Master student work is related to the project Graphene-Clay systems. The Master project additionally involves sample preparation with focus on selected characterizations. The actual work will depend on the student's interest and preferences. Possible projects involve preparation and characterization of mechanically exfoliated single sheets of natural or synthetic clays; development of various methods for conversion of graphene oxide to graphene and/or investigation of its structure and electrical transport properties (UV influence); preparation and selected characterizations of multi-layered structures of graphene and clay; development of methods for preparation of macroscopic layers with desired functionality, combining clay and graphene and others. Master student will work on its own specific project in the home NTNU lab and Nanolab (AFM, SEM) and in case of interest, participate on synchrotron experiment on thin films made from 2D sheets. Master work is related to the project Graphene-Clay systems. Samples under interest include mechanically exfoliated single sheets of natural or synthetic clays, chemically exfoliated sheets of natural or synthetic clays, combination of both with graphene oxide and graphene.

Requirements: Interest in science and experimental work. Background in the condensed matter physics or nanotechnology is of high advantage. Ability to work independently under the supervision and in the larger experimental group.

Other aspects: There are several ongoing projects in the lab. Students can participate in the experiments carried at the synchrotron/neutron facilities and experiments in external collaboratiion with Indiana University-Purdue University Indianapolis USA and Univ. Bayreuth, Germany, as well as labs in Czeck Republic (Pragues) and UK.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Contact: Researcher Barbara Pacakova (<u>barbara.pacakova@ntnu.no</u>) or Professor Jon Otto Fossum (jon.fossum@ntnu.no).

¹ Large bandgap insulating superior clay nanosheets, Barbara Pacakova, Per Erik Vullum, Alexsandro Kirch, Josef Breu, Caetano Rodrigues Miranda & Jon Otto Fossum, MRS Bulletin 47, December 2022. DOI: 10.1557/s43577-022-00349-8 (2022)

Individual and collective bacterial motility in clay suspensions: Experiments and/or simulations

Motivation: Understanding the motion of bacteria in clay suspensions is critical to unlocking key biological processes in nature. The Soft and Complex Matter Lab have previously studied the locomotion of E.Coli bacteria in Laponite suspensions and have observed that the swimming velocity of the bacteria is impacted by the presence of clay mineral particles in the suspensions as depicted in Figure 1. The goal is to study the motility of different bacteria in different types of clay suspensions.



Fig 1: Schematic representation of bacteria swimming through a fluid containing clay particles.



Fig 2: Experimental setup for tacking bacteria motion in a fluid.

Role of the student: The student will study the trajectories of different bacteria in different clay suspensions using the 3D Lagrangian tracking system shown in Figure 2. The work will be done in collaboration with Professor Eric Clement at Ecole Superieure de Chimie et Physique Industrielles - ESPCI Paris. Furthermore, he/she will also perform mathematical simulations of the hydrodynamics of the bacteria motion.

Requirements: Enthusiasm and interest in Soft Matter cooperative dynamics and Flow dynamics. Background in soft matter and physical chemistry.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Contact persons: Postdoc Andrew Akanno (<u>andrew.akanno@ntnu.no</u>) or Professor Jon Otto Fossum (jon.fossum@ntnu.no).

Flow and structural behavior of clay suspensions: Experiments or simulations

Motivation: Understanding the individual or collective behavior of clay particles in different environments is the focus of what we do at Soft and Complex Matter Laboratory. We have previously studied the suspension behavior of the clay minerals Sodium Fluorohectorite and Laponite as a function of particle concentration and ionic strength, and one of our central goals is to understand the evolution of the suspension flow and how this is connected to underlying micro- and nanostructures under different conditions. This will provide insight into the complex nature particle suspensions and help to explain the phenomena of complex fluids.







Viscosity behavior of a suspension of clay platelet shaped particles

Role of the student: The student will prepare different suspensions of clay particles in different solvent conditions. He/she will study the flow and deformation behavior of the clay suspensions using a Rheometer. Structural characterization will be done using Small Angle X-ray Scattering (SAXS at NTNU and at international synchrotron facilities), Small Angle Neutron Scattering (SANS at international neutron facilities) and Small Angle Light Scattering (SALS). The student will setup and implement Small Angle Light Scattering (SALS) System with our Rheometer for simultaneous structural and flow information under shear stress. Optical microscopy is also important for this project. The experiments will be based at the Soft and Complex Matter Lab (softcomlab.com). Some special microscopies will be done in the Thermal Two-Phase Flow Laboratory at the Department of Energy and Process Technology at NTNU, and internationally with partners and the Mechanical Engineering department, NTNU. This is a collaboration with the Institute for Complex Systems, Sapienza University, Rome, Italy, and in the latter case we are also looking for a student interested in simulations. The work will be carried under the instruction and supervision of Postdoc researchers and Professors.

Requirements: Enthusiasm and curiosity about Soft Matter and Rheology. Background in condensed matter physics, materials science and/or physical chemistry.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Contact persons: Postdoc Andrew Akanno (<u>andrew.akanno@ntnu.no</u>) or Professor Jon Otto Fossum (jon.fossum@ntnu.no).

Self-assembly of new 2D hybrid nanomaterials

Motivation: Smectite clay and graphene nanolayers are examples of 2D materials¹. This class of materials have been employed to develop new type of composites with extraordinary proprieties, such as mechanical magnetic and electric. The motivation of the current project is to self-assemble 2D materials together with magnetic nanoparticles, branched polymers, etc. to produce new hybrid materials with designed proprieties.



Figure1 : Clay nanosheet decorated with magnetic nanoparticle. Images obtained in Scanning Transmission Electron Microscopy (STEM) at NTNU Nanolab. The bright dots in each image are the magnetic nanoparticles on top of clay nanosheets.

Role of the student in the project: The student will focus on nano-functionalization protocols for clay nanosheets and/or graphene oxide and the self-assembly process together with different materials, like magnetic nanoparticles and branched polymers. The hybrid materials will be characterized by X-ray Scattering techniques (mainly SAXS), Electron Microscopy (SEM and STEM), Atomic Force Microscopy (AFM), Spectrometry, UV-Vis, Zeta potential, and other relevant techniques. The Master students will work and under guidance in the Soft and Complex Matter Lab. NTNU NANOLAB also will be use in the project. Some experiments will be done in international synchrotron X-ray or neutron facilities. This project is in collaboration with Univ. Bayreuth, Germany and University of São Paulo, Brazil

Preferred selection criteria: Interest in science and experimental work. Background in condensed matter physics, materials science or nanotechnology will be advantageous. Ability to work independently under the supervision and in the larger experimental group.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Contact persons: Postdoc Paulo Michels Brito (<u>paulo.h.m.brito@ntnu.no</u>), Researcher Barbara Pacakova (<u>barbara.pacakova@ntnu.no</u>), Professor Jon Otto Fossum (<u>jon.fossum@ntnu.no</u>)

¹ Clay nanolayer encapsulation, evolving from origins of life to future technologies, Jon Otto Fossum, Eur. Phys. J. Special Topics 229, 2863–2879 (2020)

Colors from nanostructures

Motivation: There are two type of colors, chemical (pigments and dyes) and physical colors (scattering of light). The rainbow or the color of soap bubbles are examples of physical colors, also called structural colors. In nature, for example butterfly wings have bright colors due to scattering of light from nanostructures (Fig 1 left). Currently, there is a large scientific effort to recreate biological structural colors using sustainable artificial systems. In our lab, we achieved such structural colors by using nanosheets derived from clay minerals (Fig 1 right)^{1,2,3}. Clay minerals are widely used materials in industry. one of the most abundant natural materials on earth and they are environmentally friendly and non-toxic. Clay nanosheets can be suspended in water and they can self-organize into structures that make structural colors.





Figure 1 (left): Nature structural colors and their nanostructures. (right): Structural colors from nano-functionalized clay nanosheets suspensions achieved in our lab.

Role of the student in the project: The student will focus on nano-functionalization protocols for clay nanosheets, preparation of clay suspension for production of structural colors. Beyond this, the project will develop protocols for fixation of suspension nanostructures in hydrogels and polymer films. The structural colors/films will be characterized by X-ray Scattering techniques (mainly SAXS), Electron Microscopy (SEM and STEM), Atomic Force Microscopy (AFM), Spectrometry, UV-Vis, Zeta potential, and other relevant techniques. The student will work under guidance in the Soft and Complex Matter Lab. NTNU Nanolab will also be used in the project. Some experiments will be done in international synchrotron X-ray or neutron facilities. This project is in collaboration with Univ. Bayreuth, Germany.

Requirements: Interest in science and experimental work. Background in the condensed matter physics, material science or nanotechnology will be advantageous. Ability to work independently under the supervision and in a larger experimental group.

Other aspects: Students can participate in the experiments carried at the synchrotron/neutron facilities and experiments in external collaboratiion with Univ. Bayreuth or Max Plamck Institute Dresden, Germany.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Contact: Postdoc Paulo Michels Brito (<u>paulo.h.m.brito@ntnu.no</u>), or Professor Jon Otto Fossum (<u>jon.fossum@ntnu.no</u>)

¹ Bright, noniridescent structural coloration from clay mineral nanosheet suspensions, P. H. Michels-Brito, V. Dudko, D. Wagner, P. Markus, G. Papastavrou, L. Michels, J. Breu, J. O. Fossum, Science Advances 8, DOI: 10.1126/sciadv.abl8147 (2022)

² Norwegian SciTech News, - Published Feb 3, 2022

https://norwegianscitechnews.com/2022/02/natures-colours-can-replace-toxic-pigments/

³ physicsworld: optics and photonics - Published Feb 20, 2022

https://physicsworld.com/a/clay-nanosheets-produce-bright-structural-colours/

Physics of swarming: simulation and theory

Master/project thesis in theoretical physics. Contact person: Paul Dommersnes, Professor Email: <u>paul.dommersnes@ntnu.no</u>



Swarming:

Animals often come together and form large groups moving collectively in a coordinated fashion, which is called swarming or flocking. The collective behavior can be anything from simple (e.g. all moving in the same direction) to extremely chaotic. It has long been thought that swarming can be understood by simple interaction rules between the animals and that swarming should exhibit universal characteristics. The development of imaging techniques has revealed that swarming of cells is common inside our body, the cells sometimes form coordinated motion (e.g. in wound healing) or in chaotic turbulent like motion. There is also currently much experimental effort into emulating swarming matter both at microscopic ("artificial cells") and macroscopic scales (robots, drones), which is known as "synthetic" or artificial active matter. Swarming models are therefore not just interesting from a theoretical perspective; they have real applications in fields like cell biology, robotics and modern materials science.

Swarming simulation models:

The most well-known (and simplest) model for swarming is due to Vicsek (1995). It is a kind of minimal "Ising model" for swarming and consist of self-propelled particles with mutual velocity alignment interactions (and some noise). The transition to collective directed motion appears as a first order phase transition[1]. There are many other simulation/theoretical models currently being developed for swarming motion, see e.g. reference [2] and [3]. The Project will consist of working with and developing simulation models such as populations of many self-propelled Brownian particles with mutual interactions, and may also include analytical continuum/fluid dynamical type modelling of large swarms. The focus will be on simple models that may find universal applications.

The project is suitable for both Master thesis and specialization Project.





References:

- [1] T. Vicsek, A. Zafeiris, Collective motion, Physics Reports, (2012) <u>https://arxiv.org/abs/1010.5017</u>
- [2] Hydrodynamics of Soft Active Matter, M. C. Marchetti et al , Reviews of Modern Physics (2013) https://arxiv.org/abs/1207.2929
- [3] Cooperative motion of active Brownian spheres in three dimensional dense suspensions Wysocki, A, R. G. Winkler, and G. Gompper, EPL (2014) <u>https://arxiv.org/pdf/1412.2692.pdf</u>
- [4] Collective Motion of Humans in Mosh and Circle Pits at Heavy Metal Concerts, Silverberg, Bierbaum, Sethna, Cohen, Physical Review Letters (2013) <u>https://arxiv.org/abs/1302.1886</u>

[5] Fluid Dynamics of Bacterial Turbulence, J. Dunkel et al, Physical Review Letters (2013) https://arxiv.org/abs/1302.5277

Talk on various forms of active matter by Julia Yeomans: <u>https://www.youtube.com/watch?v=UfY9HMUVUnY</u> Wikipedia articles: <u>https://en.wikipedia.org/wiki/Active_matter</u> <u>https://en.wikipedia.org/wiki/Swarm_behaviour</u>

Movie of swarming bacteria: <u>https://www.youtube.com/watch?v=q27Jn3h4kpE</u> Swarming/flocking birds (starlings): <u>https://www.youtube.com/watch?v=V4f_1_r80RY</u>

Predicting lifetime of ultra-strong carbon composites by combining analytics and machine learning



This project explores ways to combine two non-destructive monitoring methods to monitor long fibre reinforced composite with semi-crystalline polymer matrix. The project focuses on oriented carbon composite with single orientation direction and other materials. The idea is to use data based modelling to find out whether we can monitor crack formation and crack propagation using specific electrical characterizations (particularly impedance based) first when assisted by direct structural data from X-ray based methods and subsequently without direct structural information. The ultimate goal is to use these ideas to estimate the remaining useful lifetime in composite structures. Travels to other laboratories (University of Oslo, University of Helsinki, Deutches Elektronen-Synchrotron DESY or collaborating company laboratories) might be included. The project is connected to the research project funded by the Dutch Polymer Institute.

The exact details will be refined with the MSc candidate.

Specialization Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Supervisors: Matti Knaapila, <u>matti.knaapila@ntnu.no</u>; and Alexander Harold Sexton, <u>alexander.h.sexton@ntnu.no</u>





Effect of temperature in agglomerates and aggregates formation of silica powders.

Motivation: There exist a large variety of amorphous silica powder products for various applications in various industries, for example fumed, precipitated or colloidal silicas. They differ by their production process and have different characteristic properties. Microsilica, a by-product from Si production, is one such product. It is special as compared to other amorphous silica in that it has a low specific surface area and no aggregate structure, it consists of spherical primary particles. Because of its nature, being a by-product, its properties depend somewhat on the details of the Si production process. Considering measuring its characteristics and fundamental properties, it is a very difficult material, since it has very wide particle size distribution (PSD) and various small amounts of contaminant particles incorporated. Nevertheless, for further development of applications, a more detailed understanding of those properties is required. Some of the contaminants can be removed with a heat treatment of the product, however the changes in performance observed after heat treatment indicate that the microsilica is changed in a more fundamental way. To exactly describe and measure those changes in physical and chemical properties would be very interesting and useful for the development of new applications of microsilica.

For example, a study of the physical properties as function of heat treatment temperature could improve our understanding. Therefore, we propose SAXS measurements of microsilica heat treated up to a different temperature, or if possible, in-situ heat treatment and simultaneous SAXS measurement of microsilica.



Figure 1: A) TEM of microsilica – spheres of wide distribution, B) TEM of microsilica dispersed in PA6.6 – all primary spheres separated from each other – no aggregates/agglomerates

What the student will do: Familiarize with characteristic properties of microsilica and characterization techniques used. Receive one (or more) sample of microsilica and characterize as good as possible. Prepare heat treated powders from that sample at various heat treatment temperatures. Take SAXS measurements of the original and heat-treated samples. Analyse and interpret the resulting SAXS data, summarize results in a report.

Other Aspects: This topic is a collaboration with Elkem Silicon Products.

Supervisor: Jon Otto Fossum (NTNU); **Contact person:**, Leander Michels (NTNU/ELKEM), Andrea Freitag (ELKEM)

References:

1 The chemistry of silica, R. K. Iler, John Wiley & Sons, 1978





Norwegian University of Science and Technology

Title: H2O adsorption in meso- and nanopores of silica powders.

Motivation: There exist a large variety of amorphous silica powder products for various applications in various industries, for example fumed, precipitated or colloidal silicas. They differ by their production process and have different characteristic properties. Microsilica, a by-product from Si production, is one such product. It is special as compared to other amorphous silica in that it has a low specific surface area and no aggregate structure, it consists of spherical primary particles. Because of its nature, being a by-product, its properties depend somewhat on the details of the Si production process. Considering measuring its characteristics and fundamental properties, it is a very difficult material, since it has very wide particle size distribution (PSD) and various small amounts of contaminant particles incorporated. Nevertheless, for further development of applications, a more detailed understanding of its properties is required. One of the interesting properties is the adsorption and desorption of H2O on the silica surface, including possible internal and inter-particle pore adsorption/desorption. The details of the H2O adsorption/desorption of that material and its impact on various performance properties are not well understood. A microsilica which has never been wetted behaves fundamentally different from one, which has been wetted and subsequently dried.



Figure 1: A) TEM of microsilica – spheres of wide distribution, B) TEM of microsilica dispersed in PA6.6 – all primary spheres separated from each other – no aggregates/agglomerates

What the student will do: Familiarize with characteristic properties of microsilica and characterization techniques used. Receive one (or more) sample of microsilica and characterize it as good as possible using various analytical techniques. Take an H2O adsorption isotherm measurement (probably gravimetric, at room temperature) of microsilica using suitable instrument, or alternatively by hand over saturated salt solutions. Take SAXS measurements of that microsilica sample (from Elkem) for the sample having adsorbed various equilibrium coverages of H2O. Alternatively, try to perform SAXS measurements in-situ during isotherm measurement. For that experiment, design, construct and built a suitable sample cell, perform measurements, analyse and interpret resulting isotherm and SAXS data, summarize results in form of a report.

Other Aspects: This topic is a collaboration with Elkem Silicon Products.

Supervisor: Jon Otto Fossum (NTNU); **Contact person:**, Leander Michels (NTNU/ELKEM), Andrea Freitag (ELKEM)

References:

- 1 The chemistry of silica, R. K. Iler, John Wiley & Sons, 1978
- 2 Layer growth of methane on MgO: An adsorption isotherm study, A. Freitag, J. Z. Larese, Phys Rev. B V62/12, 2000





Norwegian University of Science and Technology

Master's project possibilities on aqueous microsilica dispersions

Motivation: Microsilica powder is a side-product of the Si production process. This amorphous silica has been characterized to consist of spherical particles with wide particle size distribution (see picture). This material is used for applications in various industries, for example the polymer, construction, oil field and refractories industries. Therefore, there is a large interest in better understanding the properties of microsilica and its dispersions. Aqueous dispersions of microsilica appear to be a complex system, with interesting properties. The various application areas also pose challenges to producers of such dispersions, one of them being long term dispersion stability. Unstable behavior of such dispersions can be categorized into various processes related to sedimentation, particle agglomeration, gelation and combinations thereof. The main factors for dispersion instability are believed to be: silica loading, presence of various contaminants, unstable pH, sensitivity to environmental temperature and wide particle size distribution.

Project 1: Role of silica loading in the physical-chemical behavior of silica dispersions: Project 1 will focus on the impact of the solid content on physical-chemical behavior of silica dispersions and their stability. Dispersions with various microsilica loadings will be made and characterized by using various analytical technics. The focus of the characterization will be small angle scattering (SAXS) with the objective to try to assess and compare the microstructure of the silica formed in the aqueous dispersions, agglomerate and particle network formation and similar phenomena.



Project 2: Role of pH, cation type and concentration for stability of microsilica dispersions: Project 2 will study the effect of pH, salt type and concentration on stability of aqueous silica dispersions. Microsilica dispersions with various pH and salt contents will be prepared and characterized by using various analytical technics, with focus on SAXS.

What students will do in the projects: The student will learn how to prepare aqueous dispersions of silica and to characterize them with various analytical technics. Variables to be considered are microsilica loading, pH and salt type/content. Experimental techniques being used include among others rheology for determination of physical properties, laser diffraction for evaluation of particle/agglomerate size distributions (PSD) and small angle scattering (SAXS) for investigation of the microstructure/morphology of the systems, agglomeration, and network formation processes.

Other Aspects: This topic is a collaboration with Elkem Silicon Products.

Supervisor: Professor Jon Otto Fossum (NTNU); Contact persons: Researchers Leander Michels (NTNU/ELKEM), Karina Kovalchuk (ELKEM) References:

- 1 The chemistry of silica, R. K. Iler, John Wiley & Sons, 1978
- 2 Cost reduction in Rubber Processing, *Specialty silica for Processing improvement and Reduction of Mixing Energy* Andrea Freitag, Gerd Schmaucks, pp 110-130
- 3 Lea's Chemistry of Cement and Concrete ed., Peter C. Hewlett, *Microsilica as an Addition*, Per Fidjestøl, Robert Lewis

Surface science studies of doped supported graphene layers

Motivation

The unique electronic properties and high stability of graphene layers due to strong sp2-hybridized bonds have triggered a large interest in the scientific community over the last couple of decades. Adsorption on nanostructured surfaces is of relevance for many applications in catalysis as well as for adsorption of greenhouse gases. The objective is to investigate properties of doped graphene layers on different substrates.



Figure 1 Left: LEED image of graphene supported on ruthenium. Middle: Structure of a graphene layer on a hexagonal substrate. Right: Sample holder assembly inside the ultra-high-vacuum chamber.

Role of the student in the project

Formation of graphene on metallic substrates may be obtained by heating so that carbon impurities in the bulk segregates to the surface or by exposure to carbon containing gases at elevated temperatures, or by exposure to carbon containing gases like e.g., ethylene at elevated temperatures. The graphene layer can be identified by e.g., LEED (Low Energy Electron Diffraction) as shown in Fig.1.

In this project, electronic properties, and adsorption of greenhouse gases carbon dioxide and methane will be studied in ultra-high vacuum by use of X-ray photoelectron spectroscopy (XPS), temperature programmed desorption (TPD). Atomic force microscopy (AFM) may be used to image the surfaces. Nanostructured surfaces serve as model systems for studying doped surfaces by surface analytical tools. The student will perform sample preparation, data acquisition and analysis with assistance from members of the research group.

Workload

Project (15 ECTS) or Master thesis (30 or 60 ECTS)

Requirements

Interest in experimental work. Some knowledge of condensed matter physics is an advantage, but not a necessary requirement. Ability to work independently under supervision in the laboratory.

Contact person(s)

For further details of project description, please contact steinar.raaen@ntnu.no