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Cover pictures:
Langmuir – Blodgett monolayers of SBA-15 particles with different morphologies.
Manuscript Yana Znamenskaya Falk, Julien Schmitt and Viveka Alfredsson.

1 The work environment is important

In 2015, we made a questionnaire in the division about the psycho-social environment. To a large extent people were happy but we also encountered some aspects that were not so positive and that we have since tried to address on different levels. A work place with content co-workers and where people have an open-mind and willingness to discuss issues is worth striving for and I am here giving a personal reflection related to this issue with a special focus on equality.

I started at the division as an assistant professor in 1998; I was one of three women in the group of senior scientists. There were of course many more men. Karin Schillén had started a few months prior to me and Eva Hansson, who had been at the division for a long time, was soon to become head of the department and leave the normal division activities. Today, the number of women has increased; Emma Sparr, Malin Zackrisson-Oskolkova and Anna Stradner have joined (Eva retired several years ago). Women are stilled outnumbered by men but we are close to the desired range of 40-60%. Hence, we are on the right path! What about the younger scientists? With them, in particular with the PhD students, we have reached much further. In 2015 there were 24 PhD students, 15 of which were women. This is brilliant! So are we heading for a workplace of equal opportunities? I believe and hope so. But we still have a long way to go. The "male structures", whatever they are, still control and dominate the universities. Not strange, initially (we are talking about 800 years!) universities were institutions dedicated for men. Only in 1880 did Lund University take on its first representative of the other 50% of the population.

Knowledge and science have evolved greatly since the University of Bologna opened its doors in 1088, so why bother about equality? Isn't the major thing that we progress and develop, and does it matter who is responsible for it? My answer to that is that it matters enormously! And let´s be very fundamental. Check out this statement: *everyone has the right to education. Education shall be free, at least in the elementary and fundamental stages. Elementary education shall be compulsory. Technical and professional education shall be made generally available and higher education shall be equally accessible to all on the basis of merit.* I suppose you all recognise this as part of the declaration of human rights (article 26 to be specific). Let´s take a look at what "everybody" means. It is not just about gender; there are a number of factors such as sexuality, religion, political views etc., that defines the word "everybody". So, it does not only matter, we are obliged to strive for a workplace of gender equality and equal opportunities!

If you are a woman, should you stick around in a male dominated working place? This depends largely on the colleagues and (of course!) on the job that you do. For me, I early on, first week of my position as assistant professor, realised that my gender wasn't a big issue. I now have to use a "having kids" argument (sorry!), which by the way is not the divider for the differences in the careers for men and women, but here it serves as an example. When I started at the division I was pregnant with

my first child – it was early in the pregnancy – and I was scheduled to have a meeting with the leadership, which at the time meant Björn Lindman, Håkan Wennerström and Olle Söderman. I did not know them, had hardly met them. I felt intimidated and was anxious about how they would react to me being pregnant as when starting my career at the division. I was also very aware that this should not be considered to be a problem! We had a lunch meeting in Björn's office and started discussing and making plans. I told them of my "condition", they said, "OK, then we will just change the plans slightly". No big deal!

To conclude, we (all of us!) should continue striving to have a good work environment (by collaborating and having an open-door policy, having pub nights, coffee breaks, lunch clubs, discussions…), that accommodates "everybody". Just as with science, we will never reach the ultimate goal; we should continue talking, having an open-mind and, be aware of inequalities and fight them, and, always look out for each other!

2 Research projects

2.1 Theoretical work - Statistical mechanics

2.1.1 Portal for statistical-mechanical computation and software
(Contact person: Per Linse)

Through the web-portal www.fkem1.lu.se/sm, launched 2003, softwares for solving general problems in mainly statistical mechanics are accessible. The softwares were primarily developed as research tools, but have frequently been used in advanced undergraduate classes and in national PhD courses. From the web-portal, further information about each software can be obtained, reference manuals and sample input files can be retrieved, and the softwares can be executed for test purposes. The software's are:

DIELEC is a software for calculation of the electrostatics in the presence of spherical dielectric discontinuities. First version 2008.

MOLSIM is a software for atomistic and coarse-grain modeling of molecular, colloidal, and polymer systems, with extensive static and dynamic analyses, employing molecular dynamics, stochastic dynamics, and Monte Carlo simulation techniques. With contributions from Anna Akinchina, Fredrik Carlsson, Samuel Edgecombe, Yoshikatsu Hayashi, Pascal Hebbeker, Niklas Källrot, Björn Linse, Vladimir Lobaskin, Thomas M. Nymand, Alberto Pais, Jurij Rescic, Stefanie Schneider, Marie Skepö, Joakim Stenhammar, Anders Wallqvist, Jos van Rijssel, Erik Wernersson, and Per-Olof Åstrand. First version 1990. Parallel version employing MPI since 1997.

OZ is a software for solving the Ornstein-Zernike equation with a closure (MSA, PY, HNC, RY, ZH, and RHNC) for systems with central forces. First version 1985.

PB is a software for numerically solving the one-dimensional Poisson-Boltzmann equation for different boundary conditions and symmetries. First version 1982.

PGSE is a software for simulation of pulse gradient spin echo attenuations for spins diffusing in restricted spaces of different symmetries with permeable walls. First version 1993.

POLYMER is a software for solving lattice mean-field models containing a mixture of solvents and polymers for homogeneous (Flory-Huggins theory) and heterogeneous (Scheutjens-Fleer theory) solutions extended to polymers possessing internal degrees of freedom. First version 1991.

During 2014, MOLSIM has undergone a large structural reorganization simplifying its use, been extended to handle concave particles of arbitrary shape, and got an enhanced capacity of dynamic analyses. The ideas behind the software MOLSIM have been developed and presented in a research publication. (Jurij Rescic (University of Ljubljana) and Per Linse.)

2.1.2 Spherical dielectric boundaries

(Contact person: Per Linse)

Rapidly Rapidly convergent expressions for the Green's function of the Poisson equation for spherically symmetric systems, where the dielectric constant varies discontinuously in the radial direction, were derived. These expressions were used in Monte Carlo simulations of various electrolyte systems, and their efficiency was assessed. The simulations were performed on six types of systems having either (i) a uniform surface charge distribution, (ii) a uniform volume charge distribution, or (iii) mobile ions, which were neutralized by mobile counterions. With only the leading term of the expansion included, a precision of the polarization energy of $0.005kT$ or better was achieved, which is smaller than the statistical uncertainty of a typical simulation. The inclusion of the dielectric inhomogeneity lead to a 2.5-fold increase of the computational effort, which is modest for this type of model. The ion density distributions were investigated for different dielectric conditions. These spatial distributions were discussed in terms of the importance of (i) the direct mean-field Coulomb interaction, (ii) the surface charge polarization at the dielectric discontinuity, and/or (iii) the change in the attractive Coulomb correlations. Moreover, the accuracy of a splitting theory, based on dividing the electrostatic interaction into long and short wavelength contributions and applying different approximations on the two contributions, has been assessed against simulation results. The splitting theory works best for the case where the dielectric constant of the confining sphere is equal to or less than that of the surrounding medium. (Leo Lue (University of Strathclyde), and Per Linse.)

2.1.3 Multigraft polymers in solution

(Contact person: Per Linse)

Complexes formed by one charged and branched copolymer with an oppositely charged and linear polyion have been investigated by Monte Carlo simulations. A coarse-grained description has been used, in which the main chain of the branched polyion and the linear polyion possess the same absolute charge and charge density. The spatial extension and other structural properties, such as bond-angle orientational correlation function, asphericity, and scaling analysis of formed complexes, at varying branching density and side-chain length of the branched polyion, have been explored. In particular, the balance between cohesive Coulomb attraction and side-chain repulsions resulted in two main structures of a polyion complex. These structures are (i) globular polyion core surrounded by side chains appearing at low branching density and (ii) extended polyion core with side chains still being expelled at high branching density. The globule-to-extended transition occurred at a crossover branching density being practically independent of the side chain length. Moreover, the properties of the complexes were investigated for variable electrostatic attraction between the polymers. The complexes were relatively intact for the fractional charge

½, but at smaller charges considerable structural changes appeared. (Daniel Angelescu (Romanian Academy) and Per Linse.)

2.2 Studies of model systems

2.2.1 Self-organized structures of oppositely charged PNIPAAM diblock copolymers in aqueous solution

(Contact person: Karin Schillén)

Self-organized structures are formed in water by electrostatic attraction between two oppositely charged poly(N-isopropylacrylamide) PNIPAAM diblock copolymers, which are mixed at 1:1 charge ratio. The copolymers have the same lengths of the PNIPAAM and the charged blocks. We use dynamic and static light scattering, turbidimetry, small angle X-ray scattering, 2D- or NOESY-nuclear magnetic resonance, cryo-transmission electron microscopy, electrophoretic mobility and DSC measurements to investigate the effect of temperature and total concentration on the aggregation behavior. (Solmaz Bayati, Karin Schillén, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway) and Jan Skov Pedersen and Beatrice Plazzotta (Aarhus University, Denmark).)

2.2.2 Inclusion complex formation between thermoresponsive PNIPAAM diblock copolymers and cyclodextrin at solid/liquid interfaces

(Contact person: Karin Schillén)

Pseudopolyrotaxanes or inclusion complexes are supramolecular assemblies formed by a polymer chain, which is threaded by several cyclodextrin (CD) molecules. CDs are cyclic oligosaccharides with a hollow cavity. In this project, we investigate the inclusion complex formation between γ-CD and diblock copolymers containing thermoresponsive poly(N-isopropylacrylamide) (PNIPAAM) chains at silica/liquid interfaces. Ellipsometry, neutron reflectivity and quartz crystal microbalance with dissipation techniques are employed to study the surface properties under different conditions, such as with the presence of CD, at different temperatures and with copolymers of different PNIPAAM block lengths. (Solmaz Bayati, Karin Schillén, Tommy Nylander, Aleksandra Dabkowska, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway), Giuseppe Lazzara (University of Palermo, Italy) and Richard Campbell (ILL, France).)

2.2.3 Emulsion Coarsening

(Contact person: Ulf Olsson)

Two coarsening mechanisms of emulsions are well established: droplet coalescence (fusion of two droplets) and Ostwald ripening (molecular exchange through the continuous phase). Here we demonstrate the existence of a third mechanism, contact ripening, which operates through molecular exchange upon droplets collisions. A contrast manipulated small angle neutron scattering experiment was performed to

isolate contact ripening from coalescence and Ostwald ripening. The key parameters have been identified through a kinetic analysis using dynamic light scattering and monodisperse nanoemulsions. Contact ripening is accelerated by increasing the concentration of droplets but hindered by repulsions between droplets and highly hydrated cohesive films. These parameters can be tuned to control the magnitude of this exchange/coarsening mechanism, which is essential for both emulsion formulation and delivery of hydrophobic ingredients. (Kevin Roger, Ulf Olsson, Bernard Cabane (ESPCI, Paris), Ralf Schweins (ILL, Grenoble).) (Project completed.)

2.2.4 Anisotropic patchy protein-protein interactions

(Contact person: Malin Zackrisson Oskolkova)

In this project we are investigating the effect of anisotropy or patchiness on protein-protein interactions, using detailed Metropolis Monte Carlo computer simulations in combination with static light scattering and SAXS. The Monte Carlo simulations have been combined with static light scattering (SLS) measurements of the second viral coefficient to provide insights into the mechanism of patchy, attractive protein interactions. We use lactoferrin as model protein, since it was predicted to display anisotropic attractive interactions and the calculated values of protein-protein interactions from the simulations leads to a good quantitative agreement with the experimental data, using no adjustable parameters. The molecular origin of the attraction could be explained as a combination of a highly directional electrostatic contribution, a local charged patch, and van der Waals attraction. This gives rise to two competing electrostatic effects acting over different length scales, which is seen as an anomalous dependence in the second virial coefficient as a function of electrolyte concentration (Li et al., JPhys. Chem. B, 2015). Similar salt dependence has been observed in various proteins which points to a more general mechanism. Currently the effect of the attraction anisotropy on the scattering pattern is being explored. Recombinant variant of lactoferrin are currently being expressed in collaboration with LP3, the protein production platform at Lund University. (Weimin Li, Björn Persson (Division of Theoretical Chemistry), Mikael Lund (Division of Theoretical Chemistry), Johan Bergenholtz and Malin Zackrisson Oskolkova.)

2.2.5 Polymer mediated attractive interactions of PEGylated colloids

(Contact person: Malin Zackrisson Oskolkova)

In this project we investigate how steric interactions, by surface-grafted PEG polymer on colloidal particles, translates into effective attractions and its effect on the static structure, phase behavior and dynamics. PEGylated particles differ from the commonly used non-aqueous systems for which crystallization in the polymer shell acts to trigger the attractions. This water-based system offers a more controlled approach where the solvent quality for PEG is varied and found to smoothly regulate the interactions (Zackrisson Oskolkova et al., RCS Advances, 2015). From a

quantitative analysis of small-angle neutron scattering data we can extract the effective attraction. In contrast to what is commonly assumed, the effective attraction is found to depend on particle concentration at high volume fractions and the attraction is no-longer pairwise additive. This aspect should serve as impetus for further studies of graft-mediated interactions.

Furthermore, Core-shell particles with a fluorinated core are now being synthesized and characterized using Cryo-TEM. The fluorination serves to match the index of refraction of the solvent i.e. water, cancelling or minimizing the attractive Van der Waals (VdW) forces, normally always present in common systems. Now instead, the steric contribution to the interactions is dominating. This facilitates the study of the detailed nature of steric stabilization and destabilization and the role of VdW interactions. (Jeanette Ulama (Physical Chemistry, Göteborg University), Johan Bergenholtz (Physical Chemistry, Göteborg University and Physical Chemistry, Lund University), Giuseppe Foffi (University of Paris-Syd) and Malin Zackrisson Oskolkova.)

2.2.6 Surface adsorption versus bulk aggregation of colloidal particles

(Contact person: Lennart Piculell)

We are studying model liquid dispersions of spherical colloidal particles in contact with a flat solid surface, which is made of the same material as the particles. The particle-particle and particle-surface attractions are then increased by increasing the concentration of an added polymer depletant. Recent theoretical work by Per Linse and Håkan Wennerström has shown that in such a situation, for purely geometric reasons, the particles should adsorb to the infinite flat surface before phase separation occurs in the bulk. This prediction has been verified by ellipsometry for uncharged model systems (hydrophobically modified silica particles and silica surfaces in cyclohexane) and, also, for charged silica particles and surfaces in water. QCM and AFM are also used to study the surface phenomena. (Samia Ouhajji, Gerda Kamsma, Lennart Piculell, Tommy Nylander, A. Philipse and Remco Tuinier (University of Utrecht).)

2.2.7 Micelles and their environment – wide q-range neutron diffraction studies to probe molecular interactions essential in mesoporous silica formation

(Contact person: Viveka Alfredsson)

In this project we investigate molecular interactions in systems giving rise to mesoporous silica material. The interaction between a cationic surfactant and a variety of counterions, including a silica model (a small and stable silica molecule) has been investigated with wide q-range neutron diffraction at ISIS (UK). The aim is to get an atomistic picture of the cationic micelle with its counterions, including the silica model, and water molecules. The diffraction data are interpreted through a modelling process (EPSR) that produces 3D atomistic configurations. 29SiNMR is

used for the silica speciation. (Emelie Nilsson, Karen Edler (University of Bath and guest Professor at Lund University), Daniel T. Bowron (ISIS; UK), Sven Lidin (CAS, LU), Göran Karlström (CAS), Olle Söderman and Viveka Alfredsson.)

2.2.8 How lipid membrane are protected against osmotic stress

(Contact person: Emma Sparr)

Small, water-soluble molecules with low vapor pressure can act to protect lipid membranes against osmotic stress. Such compounds, called osmolytes, occur naturally in many organisms to regulate osmotic pressure and to prevent cell damage due to freezing or drying. For example, urea, glycerol and pyrrolidone carboxylic acid (PCA) are a part of the Natural Moisturizing Factor in human skin, and are also used in skin care products. In seeds and plants, a class of protein named dehydrins are also present to protect against dehydration.

The question addressed in the project concerns the molecular mechanism(s) behind the role of the osmolytes and dehydrins in membrane systems under osmotic stress. By studying model lipid systems using a range of methods such as sorption calorimetry, sorption balance, X-ray diffraction/scattering and NMR we aim to unravel how the presence of different polar molecules and dehydrins interacts with phospholipid bilayers. We have previously studied urea and glycerol. In on-going studies, we explore the influence of dehydrins as well as other small polar molecules such as monosacharides, TMAO and PCA. (Dat Pham, Jenny Andersson, Emma Sparr, Håkan Wennerström, Pia Harrysson (Stockholm University), Daniel Topgaard, Lars Wadsö (Building Materials, LTH), Roland Netz (FU-Berlin, Germany), Emanuel Schneck (Max-Planck Institute, Pottsdam, Germany).)

2.2.9 Effect of electrostatic interactions on the casein-PEO phase diagram in the colloid limit

(Contact person: Anna Stradner)

Here we explore the possibility to create solid-like (food) gels whose structural and mechanical properties can be varied and tailored over an extremely large range in a very controlled way through an arrested spinodal decomposition process. We exploit the use of a polymer-induced depletion interaction between food colloids such as casein micelles to tune the interparticle interaction strength and range and thus play with the interplay between spinodal decomposition and gel formation. We use aqueous mixtures of casein micelles and a low molecular weight poly(ethylene oxide) for a proof of concept and investigate the possibility to create gels with well-defined structural and mechanical properties. We investigate the phase diagram of casein–PEO mixtures and the resulting equilibrium and non-equilibrium structures using diffusing wave spectroscopy and confocal laser scanning microscopy. (Najet Mahmoudi, Anna Stradner.)

2.2.10 Interactions and phase behavior of aqueous colloid – polymer mixtures and the influence of charges

(Contact person: Anna Stradner)

We investigate the use of depletion interactions to tune the interaction potential between colloids and the resulting phase behavior and the microstructure of the states that form. We use a combination of a well-defined colloid with tunable charge density and an added water-soluble polymer. We synthesize appropriate model core shell colloids consisting of a polystyrene core and an added shell that provides electrosteric stabilization. Small-angle neutron scattering combined with contrast variation techniques is used to obtain detailed information about the particle structure and the interparticle interactions. We add water-soluble polymers to create a mixed potential that we tune through appropriate variations of the ionic strength and polymer concentration. We investigate the resulting plethora of equilibrium and non-equilibrium states as a function of the strength and range of the two dominating contributions to the mixed potential, the depletion induced attraction and the soft screened Coulomb repulsion. We compare the experimentally determined phase diagrams with theoretical predictions and characterize the resulting microstructures and their dynamics through a combination of spin-echo small-angle neutron scattering (SESANS), small-angle neutron (SANS) and x-ray (SAXS) scattering and diffusing wave spectroscopy over a large range of length and time scales. (Kitty van Gruijthuijsen (University of Fribourg, Switzerland), Wim Bouwman (University of Delft, The Netherlands), Marc Obiols-Rabasa, Fei Xie, Jan Forsman, Anna Stradner.)

2.2.11 On the ripening of solids

(Contact person: Ulf Olsson)

Growth of nanoparticles is investigated by use of dynamic light scattering and transmission electron microscopy. Crystalline and amorphous nanoparticles are prepared from the drug compounds felodipine, bicalutamide and linaprazan. The crystalline nanoparticles are found to be in the nanometer range and polydisperse. However, neither of the crystalline systems display any change over time and no Ostwald ripening is observed over 10 weeks. Contrary, the amorphous nanoparticles prepared from felodipine show rapid growth, in correspondence with Ostwald ripening, in a matter of minutes after preparation, under the same stabilizing conditions as the crystalline nanoparticles. The amorphous system is also found to be polydisperse, though the polydispersity decrease with time. (Manja Annette Behrens, Ulf Olsson, Urban Skantze and Lennart Lindfors (AstraZeneca R&D Mölndal).)

2.2.12 Drying interfaces

(Contact person: Emma Sparr)

At the interface between two regions, for example the air–liquid interface of a lipid solution, there can arise non-equilibrium situations. In most cases, the condensed phase is not in equilibrium with the vapor phase, and as a consequence there will be

evaporation of water and possible also other volatile components. There might also be dissolution of compounds from the gas phase into the solution. This non-equilibrium situation implies several simultaneous transport processes across the interfacial layer separating the condensed and the gas phases, which in turn can have consequences on the molecular organization in the interfacial layer. In system containing of self-assembling amphiphilic molecules or colloidal suspensions, there is then a possibility of transport-generated interfacial phase separation. This is an apparent possibility in laboratory experimental studies of amphiphilic and colloidal systems. Similar conditions also exist in living system, with obvious examples found in the lipid tear film formed on our eyes, which prevent evaporation and dry eyes, and the membrane system in the alveoli of the lung. In this study, we explore the underlying mechanisms of transport-generated interfacial phase separation using a combination of surface together with theoretical modelling solving diffusion equations. (Emma Sparr, Håkan Wennerström, Karen Edler (University of Bath), Kevin Roger (Univ Toulouse, France).)

2.2.13 Cellulose dissolution

(Contact person: Ulf Olsson)

The dissolution of cellulose is important for a number of industrial processes and several solvents and mixtures have been tested. On the basis of an examination of the intermolecular interactions in cellulose novel approaches to cellulose dissolution are attempted. It is found that for aqueous systems the presence of amphiphilic compounds can facilitate dissolution as well as prevent re-association. It is also found that kinetic parameters are important in control cellulose systems and that anomalous temperature effects are encountered, similar to the case of several other nonionic polymers. Scattering techniques and NMR are used to characterize the state of cellulose in solution and in spun fibers. (Björn Lindman, Ulf Olsson, Manja Behrens, Joel Hagman, Marta Gubitosi, Luigi Gentile, Stefan Kuczera, Pegah Nosrati, Mona Kader Hamid, Daniel Topgaard, B. Medronho (U. Algarve), Tobias Köhnke (Swerea), Carina Olsson (Swerea), Alexander Idström (Swerea), L. Alves & M. Miguel (Coimbra).)

2.2.14 Colloids with complex interactions: from model atoms to colloidal recognition and bio-inspired self-assembly

(Contact person: Peter Schurtenberger)

In this ERC Advanced Grant Project we follow nature's strategies and make a concerted experimental and theoretical effort to study, understand and control self-assembly for a new generation of responsive colloidal building blocks. We investigate the influence of anisotropy in shape and interactions on phase behavior and self-assembly in colloidal suspensions and mixtures. Using responsive particles we implement colloidal lock-and-key mechanisms and then assemble a library of "colloidal molecules" with well-defined and externally tunable binding sites using

microfluidics-based and externally controlled fabrication and sorting principles. We use them to explore the equilibrium phase behavior of particle systems interacting through a finite number of binding sites, and subject recently developed theoretical models and computer simulations to a critical test. In parallel, we will exploit them and investigate colloid self-assembly into well-defined nanostructures. We combine molecule-like colloidal building blocks that possess directional interactions and externally triggerable specific recognition sites with directed self-assembly where external fields not only facilitate assembly, but also allow fabricating novel structures. (Maxime Bergman, Jérôme J. Crassous, Thiago Ito, Adriana Mihut, Linda Månsson, Antara Pal, Feifei Peng, Per Linse, Joakim Stenhammar, Jonas Tegenfeld (Physics, Lund University), Emanuela Zaccarelly (University La Sapienza Rome, Italy), Peter Schurtenberger.)

2.2.15 Structured surface layers of hydrated polymer-surfactant assemblies (Contact person: Lennart Piculell)

A surface layer that contains both hydrophobic and hydrophilic domains can function as a semi-permeable barrier, as a depot for material to be released from the different domains, or as an absorbent of substances in a surrounding fluid phase. For all these functions, it is of importance to control the size of the domains, their geometry, and their orientation (for non-spherical pores) relative to the surface. As one part of the larger SSF program “Porous surface layers through polymer-assisted deposition”, this project investigates the making of hydrated liquid-crystalline polymer-surfactant layers from associating oppositely charged polymer-surfactant pairs. Direct application of ethanol solutions of polyion-surfactant ion “complex salts” on a surface, followed by evaporation of the ethanol, has proven to be an easy method to coat hydrophobic as well as hydrophilic surfaces with complex salt assemblies. The surface layers swell, but do not dissolve, in water, and the structures of the layers can be controlled by choice of polyion, surfactant ion and added co-surfactant, and they also respond to the humidity of surrounding air, and to solutes such as salts, acids, surfactants and polymers in a surrounding aqueous solution. Detailed SAXS studies of the liquid crystalline structures give both kinetic and equilibrium information, and confirm that the structures largely correspond to those found in studies of bulk systems of the same compositions. Detailed kinetic and equilibrium studies of the sorption/desorption of water from/to surrounding “air” give additional insights and suggest a general strategy to study the kinetics of water vapor exchange processes for thin hydrated films. (Charlotte Gustavsson, Lennart Piculell, Joaquim Li, Marc Obiols-Rabasa, Karen Edler.)

2.2.16 Phase behavior, dynamics and directed self-assembly of anisotropic model colloids

(Contact person: Peter Schurtenberger)

Here we aim at a fundamental understanding of the phase behavior, structure and dynamics of concentrated suspensions of anisotropic particles. We focus both on structural anisotropy in ellipsoidal particles, as well as on the effects of an additional anisotropic component in the interaction potential between particles that can be generated using magnetic particles or particles with a magnetic core, or with an external alternating electrical field.

We investigate the structural and dynamic properties of magnetic ellipsoidal particles in the presence of an external magnetic field using a combination of small-angle x-ray scattering, differential dynamic microscopy and magnetometry. We compare the experimental results with those obtained by computer simulations.

We also study the effect of particle anisotropy and external polarizing electrical fields with soft ellipsoidal core-shell microgel particles using a combination of confocal laser scanning microscopy and computer simulations. (Jérôme J. Crassous, Thiago Ito, Adriana Mihut, Antara Pal, Per Linse, Joakim Stenhammar, Erik Wernersson, Ann Hirt (ETH Zurich, Switzerland), Vincent Martinez and Wilson Poon (University of Edinburgh, UK), Jan Vermant (ETH Zurich, Switzerland), Peter Schurtenberger.)

2.2.17 Depletion interactions in soft particle suspensions

(Contact person: Peter Schurtenberger)

Microgels are responsive cross-linked colloidal particles with a polymeric network structure, which undergo solvation changes in response to the application of an external stimulus such as temperature, pH or electrolyte concentration. In this project, depletion interactions induced by the presence of a fraction of small microgel particles in a suspension of large microgels (PNIPAM cross-linked with MBA) are studied. Microgels are used as a versatile model system where the effective volume fraction and the strength and shape of the interaction potential can conveniently be changed via a change in temperature. In order to perform these studies, a combination of techniques such as 3D cross-correlation light scattering, ultra-small angle light scattering, small-angle x-ray and neutron scattering, confocal laser scanning microscopy and rheology is used. We characterize the effective interaction potential USS(r), ULL(r), and USL(r) between the particles, where the subscripts S and L stand for small and large particles, respectively, from measurements of the pair correlation functions g(r) combined with computer simulations. We then investigate the phase diagram and determine the structural and dynamic properties of the system as a function of temperature, mixing ratio and volume fractions of small and large particles. (Maxime Bergman, Marc Obiols Rabasa, Emanuela Zaccarelly (University La Sapienza Rome, Italy), Peter Schurtenberger.)

2.2.18 Magnetic particles

(Contact person: Per Linse)

Structure of quasi-2d solutions of dipolar superballs in the fluid state has been determined by Metropolis Monte Carlos simulations without and with the presence of an external field. Here, the superballs resemble cubes but possess rounded edges. Examination has been made for three different dipole directions with respect to the superball principal axes and at several magnitudes of the dipole moment. At a small dipole moment, the superballs are translationally and orientationally disordered, and the dipoles become partially orientationally ordered in the presence of the field parallel to the plane of the superballs. At a large dipole moment, chains of superballs are formed, and the chains become parallel in the presence of the field. The chains remain separated for the dipole in the 001-direction and form bundles for the 011- and 111-directions. The different structures obtained for the different dipole directions are interpreted in terms of how compatible the dipole-dipole interaction is with the cube-cube interaction at short separation for the different directions of the dipole moment. Hence, the structural richness appears from an interplay of the different symmetries of a cube and of the field of a dipole. (Albert P. Philipse (Utrecht University) and Per Linse.)

2.2.19 Understanding and exploiting soft and anisotropic interactions in colloidal suspensions

(Contact person: Peter Schurtenberger)

We investigate structural and dynamic properties of colloidal particles with a soft repulsive interaction potential, and study self-assembly without and with externally applied fields. The project follows the well-established tradition of using colloids as model systems in condensed matter research to unravel basic phenomena such as phase transitions, crystallization and glass formation. Here we extend this approach to responsive soft particles such as Poly(*N*-isopropylacrylamide) microgels with tunable and directional interactions. We address the following key points:

(1) We use responsive neutral microgels to re-investigate recently developed approaches to disentangle glass and jamming transitions in soft particle systems.

(2) We use binary mixtures of microgels with different sizes, charge state and transition temperature to explore the rich phase diagram in binary systems of soft particles, investigate various ordered and amorphous phases and study solid-solid phase transitions.

(3) We extend the previous work to ionic microgels and develop a quantitative description of the interaction potential of ionic microgel particles with and without an applied electric field.

(4) We use them as a convenient model system for an investigation of crystallization, melting and domain growth processes and develop analogies to classical materials such as alloys. (Maxime Bergman, Jerôme Crassous, Peter Holmqvist, Jasper Immink, Sofi Nöjd, Divya Paloli, Per Linse, Joakim Stenhammar,

Priti Mohanty (KIIT University, India), Anand Yethiray (Memorial University, St. John's, Canada), Emanuela Zaccarelli (University La Sapienza Rome, Italy), Christos Likos (University of Vienna, Austria), Jan Dhont (Forschungszentrum Jülich, Germany), Peter Schurtenberger.)

2.2.20 Inclusion complex formation between thermoresponsive PNIPAAM diblock copolymers and cyclodextrin at solid/liquid interfaces

(Contact person: Karin Schillén)

Pseudopolyrotaxanes or inclusion complexes are supramolecular assemblies formed by a polymer chain, which is threaded by several cyclodextrin (CD) molecules. CDs are cyclic oligosaccharides with a hollow cavity. In this project, we investigate the inclusion complex formation between γ-CD and diblock copolymers containing poly(N-isopropylacrylamide) (PNIPAAM) chains at silica/liquid interfaces. Ellipsometry, neutron reflectivity and quartz crystal microbalance with dissipation techniques are employed to study the surface properties under different conditions, such as with the presence of CD, at different temperatures and with copolymers of different PNIPAAM block lengths. (Solmaz Bayati, Karin Schillén, Tommy Nylander, Aleksandra Dabkowska, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway), Giuseppe Lazzara (University of Palermo, Italy) and Richard Campbell (ILL, France).)

2.2.21 Lamellar phase rheology and shear-induced formation of multi-lamellar vesicles

(Contact person: Ulf Olsson)

The equilibrium structure and phase equilibria of the lamellar phase are sometimes complicated as noted in already early studies by Ekwall and Fontell. This complication appears to be due to the formation of multi-lamellar vesicles ("onions") under shear, which can originate simply by shaking the sample. A systematic study is performed on nonionic surfactant- water systems where the structure of the lamellar phase under shear is investigated using small angle neutron and light scattering. Depending on the temperature, that governs the monolayer spontaneous curvature, we can identify two distinct regions corresponding to "onions" (lower temperature) and planar bilayers (classical lamellar phase, higher temperature). The equilibrium structure at zero shear, however, appears to be the classical lamellar structure. The onion size varies with the applied shear rate or shear stress. In systematic experiments, it was found that the onion states obtained at large strain values are reversible and correspond to true steady states. Oriented ("single crystal") lamellar phases still contain equilibrium defects that give them a relatively high shear viscosity and in addition make them viscoelastic. In a Couette cell, magnetic resonance chemical shift imaging has shown that the lamellarto- onion transition takes place homogeneously throughout the sample, while in the onion-to-lamellar transition, the

lamellar phase first forms at the inner rotor and the growth of that phase propagates through the gap. (Ulf Olsson, B. Medronho (Coimbra), M. Miguel (Coimbra), C. Schmidt (Paderborn), M. Imai (Tokyo), Y. Suganuma (Tokyo), P. Galvosas and P. Callaghan (University of Wellington), L. Gentile and C. Oliviero Rossi (Univ. of Calabria).)

2.2.22 Brush polymers at solid surfaces

(Contact person: Per Linse)

Thermo-responsive polymer layers on silica surfaces have been obtained by utilizing electrostatically driven adsorption of a cationic-nonionic diblock copolymer. The cationic block provides strong anchoring to the surface for the nonionic block of poly(2-isopropyl-2-oxazoline), referred to as PIPOZ. The PIPOZ chain interacts favorably with water at low temperatures, but above 46 °C aqueous solutions of PIPOZ phase separate as water becomes a poor solvent for the polymer. We explore how a change in solvent condition affects interactions between such adsorbed layers, and report temperature effects on both normal forces and friction forces. To gain further insight, we utilize self-consistent lattice mean-field theory to follow how changes in temperature affect the polymer segment density distributions and to calculate surface force curves. We find that with worsening of the solvent condition an attraction develops between the adsorbed PIPOZ layers, and this observation is in good agreement with predictions of the mean-field theory. The modeling also demonstrates that the segment density profile and the degree of chain interpenetration under a given load between two PIPOZ-coated surfaces rise significantly with increasing temperature. (Junxue An, Xiaoyan Liu, Andra Dedinaite and Per M. Claesson (KTH), Francoise M. Winnik (University of Montreal) Per Linse.)

2.2.23 Self-organized structures of oppositely charged PNIPAAM diblock copolymers in aqueous solution

(Contact person: Karin Schillén)

Self-organized structures are formed in water by electrostatic attraction between two oppositely charged poly(N-isopropylacrylamide) PNIPAAM diblock copolymers, which are mixed at 1:1 charge ratio. The copolymers have the same lengths of the PNIPAAM and the charged blocks. We use dynamic and static light scattering, turbidimetry, small angle X-ray scattering, 2D- or NOESY-nuclear magnetic resonance, cryo-transmission electron microscopy, electrophoretic mobility and DSC measurements to investigate the effect of temperature and total concentration on the aggregation behavior. (Solmaz Bayati, Karin Schillén, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway) and Jan Skov Pedersen and Beatrice Plazzotta (Aarhus University, Denmark).)

2.2.24 The interaction between amphiphilic block copolymers and and bile salts

(Contact person: Karin Schillén)

The long-term aim of this project is to investigate the possibility of using amphiphilic block copolymers instead of ion exchange resins in the therapy of bile acid diarrhea and hypercholesterolemia. The polymers investigated are nonionic triblock copolymers of poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO) or cationic poly(N-isopropylacrylamide) (PNIPAAM) or PEO diblock copolymers. Bile salts are biological surfactants with a rigid four-ring system, not completely hydrophobic because of the presence of some hydroxyl groups, joined to a carboxylic head by an alkyl chain. In this project, physiochemical studies of the interaction between the anionic bile salts, typically sodium glycodioxycholate (NaGDC), and PEO-PPO-PEO copolymers of various block lengths are carried out by means of dynamic and static light scattering (DLS, SLS), small angle X-ray scattering (SAXS) and small angle neutron scattering in combination with differential scanning calorimetry. The experiments reveal that the bile salt interacts with the copolymers forming, at low bile salt concentrations, a large copolymer-rich complex by association of NaGDC monomers to the block copolymer micelle. The micelle disintegrates upon increasing the concentration of bile salt passing different aggregation states. The association aggregates between bile salt and cationic PNIPAAM copolymers are currently being investigated by SAXS, DLS and SLS. (Solmaz Bayati, Karin Schillén, Luciano Galantini (University of Rome “La Sapienza”, Italy), Kenneth D. Knudsen (Institute for Energy Technology, Kjeller, Norway), Bo Nyström and Kaizheng Zhu (University of Oslo, Norway).

2.3 Experimental methodologies

2.3.1 Diffusive transport of multivalent ions in cartilage

(Contact person: Olle Söderman)

Articulate cartilage is a firm gel-like complex material, composed of collagenous fibers and cells called chondrocytes. The chondrocyte cells produce proteoglycans which bind to hyaluronic acid, forming large highly hydrophilic aggregates. These aggregates are entangled with each other and with the collagen fibrils forming what can best be described as a hydrogel that sits within the collagen network. In the general accepted model of the morphology of cartilage, the collagen fibrils associate into columnar structures that extend outward from the bone. The protoeglycans are highly charged due to the presence of sulfate and carboxylic groups. The break-down of cartilage results in a lowering of the concentration of the proteoglycans. It has been suggested to use (Gd-DTPA)2- as a contrast in MRI to monitor the concentration of proteoglycans and therefore the state of the cartilage. In healthy cartilage, the concentration of (Gd-DTPA)2- will be low, while in damaged cartilage it would be high leading to T1-contrast in MRI.

There are some fundamental questions in this context. What is the dynamics of the Gd-complex in cartilage? How does one quantify the T1 contrast in terms of the state of the cartilage? On the experimental side, NMR diffusometry and micro imaging techniques are applied on model system of cartilage made from gel-forming polymers as well as on actual in-vitro samples of cartilage.

In addition, computer simulations on a model system of cartilage with the aim of going beyond the use of an ideal Donnan equilibrium approach in the analysis of experimental data pertaining to distribution of (Gd-DTPA)2 from MRI-data are performed.

Finally, a theoretical framework for the transport and concentration of ions in cartilage starting from a non-equilibrium situation is developed. This forms the basis for numerical calculations based on the finite element method. (Jenny Algotsson, Daniel Topgaard, Olle Söderman, Peter Jönsson, Jan Forsman (Division of Theoretical Chemistry, LU), Jonas Svensson and Leif Dahlberg (Department of Radiation Physics and the Joint and Soft Tissue Unit at UMAS, Malmö).)

2.3.2 Polymer-surfactant interaction at liquid interface

(Contact person: Tommy Nylander)

The project aims to understanding of the nature of the interaction between polyelectrolytes and oppositely charged surfactants at interfaces in relation to the bulk phase, with particular attention to non-equilibrium effects. We study polyelectrolyte systems of relevance for commercial products such as shampoos and fabric conditioners, but also model systems such at cationic dendrimers and anionic surfactants. We have demonstrated that the choice of sample preparation methods can have a profound effect on the state of the interface for chemically equivalent samples. This is particularly apparent in the phase separation region, where the extent of aggregation in the bulk solution on relevant time scales is affected by the polymer/surfactant mixing process, which in turn the structure and composition of the interfacial layer. The studies include experimental studies using ellipsometry, QCM-D, neutron reflectometry and light scattering as well as theoretical modeling. (Marianna Yanez, Tommy Nylander, Lennart Piculell, Per Linse, Richard Campbell (ILL, France), Katrin Tonigold (Ulm University), Imre Varga and Róbert Mészáros (Eötvös Loránd University, Budapest; Hungary).)

2.3.3 Solid-state NMR methods for soft matter

(Contact person: Daniel Topgaard)

Several types of intermolecular interactions, e.g., steric, electrostatic, and hydrophobic, affect the dynamic behavior of large molecules in a crowded system. NMR offers a unique possibility of resolving different molecules and molecular sites even in rather complex mixtures. For colloidal systems with reduced molecular mobility and sample heterogeneity on the nano- to micrometer scale, solid-state NMR methods with magic-angle spinning are required for extracting high-resolution

spectroscopic information. Dynamic and site-resolved information can be correlated in multidimensional experiments. The experimentally determined parameters have simple geometrical definitions and can be estimated using theoretical approaches such as molecular dynamics simulations. The NMR methods are applied to a series of colloidal systems including nonionic surfactants with poly(ethylene oxide) or glucoside headgroups, lipid/cholesterol membranes, synthetic analogs of the lipid mixtures in the stratum corneum, and lung surfactant extracts. (Daniel Topgaard, Sanna Gustavsson, Dat Pham, Jenny Andersson, Emma Sparr, Tiago Ferreira, Olle Söderman, Samuli Ollila, Johan Reimer, Stefan Ulvenlund (CR Competence).)

2.3.4 Diffusion MRI methods development

(Contact person: Daniel Topgaard)

Molecular transport by diffusion is a crucial process for the function of biological tissues. Diffusion NMR and MRI are powerful methods for non-invasively studying molecular motion on the micrometer length scale and millisecond time scale. By following the self-diffusion of molecules in a cellular system, information about structure and dynamics on the cellular scale can be obtained. Within this project we design new experimental protocols for estimating parameters such as cell shape, orientation, and membrane permeability. The structure of biological materials, or the transport behavior of molecules within these materials, can often be mimicked by carefully designed colloidal model systems such as emulsions, gels, and liquid crystals. The new methods are first tested by simulations, subsequently applied to colloidal model systems, simple cellular systems and excised tissue, and finally implemented in the context of medical MRI. (Stefanie Eriksson, Daniel Topgaard, Olle Söderman, Markus Nilsson and Freddy Ståhlberg (Lund BioImaging Center), Samo Lasic and Karin Bryskhe (CR Development), Carl-Fredrik Westin (Harvard Medical School), Hans Knutsson (Linköping University).)

2.3.5 Development of multi-channel isothermal microcalorimeters for monitoring of living organisms

(Contact person: Ingemar Wadsö)

Isothermal microcalorimeters are used in thermodynamic work, but can also be designed for use as general monitors of e.g. the “activity” of biological systems. It has for many years been predicted that such techniques will become of practical importance in different areas of applied biology. However, due to their low sample throughput those prospects have not been realized. Our calorimetric development work is focused on that problem, using “multi-channel” techniques, i.e. instruments where many samples can be measured simultaneously and thus increasing the sample throughput.

Several years ago we finished the development of a 48-channel instrument, which primarily was designed for measurements of the activity of microorganisms, mammalian cells and biopsies in the pharmaceutical industry and in clinical

laboratories. A commercial version of the instrument has now been developed by SymCel, Stockholm. It is expected that their regular marketing of the instrument will start in early 2016.

A first version of a 9-channel instrument has been built. It is primarily intended for measurements of activities of living cells, tissues and small animals. The measurement principle is the same as for the 48-channel instrument, but the sample vessels are larger. The new instrument design will allow the use of a flow-through technique for the sample assemblies, which will facilitate automatization of the measurements.

2.4 Colloidal biology

2.4.1 Oligomeric alkylglycosides - sustainable production of a novel class of biodegradable surfactants with added and controllable functionality, from renewable resources.

(Contact person: Tommy Nylander)

Non-ionic surfactants constitute a group of chemicals with enormous, yet under-appreciated, impact on our daily lives and our environment. These surfactants are key functionality-bearing constituents in products as diverse as household detergents, laundry powder, pharmaceutics, cosmetics, personal care products and agrochemicals. In applications that involve direct interaction or physical contact with living organisms, non-ionic surfactants are preferred over ionic ones, due their lower toxicity and irritancy. However, the most common non-ionic surfactants, which are based on polyethyleneglycol (PEG), are derived from ethyleneoxide, a hazardous chemical of petrochemical origin. The aim for this project is to give scientific proof of concept for a new sustainable surfactant that could replace and even outperform existing non-ionic petrochemical based surfactants. Our innovative technology is based on enzymatic methods for surfactant synthesis and uses renewable materials, such as cyclodextrins and starch, to produce alkylglycosides comprising oligomeric head-groups with up to fourteen hexose units. The aim with this project is to obtain detailed understanding of the structure-function relationships on the molecular level to be able to rationally design OMAGs and further develop of the manufacturing process. This will allow successful transfer of this novel sustainable technology platform to application. This framework project is funded by Formas and is a collaboration between Food Technology (Marie Wahlgren and Stefan Ulvenlund), Biotechnology (Patrick Adlercreutz) and Enza Biotech (Stefan Ulvenlund and Patrick Adlercreutz).

2.4.2 Viscoelastic properties of concentrated protein solutions and mixtures assessed via tracer microrheology

(Contact person: Anna Stradner)

The viscosity of protein solutions often experiences a sudden increase when the concentration reaches a threshold value. For the vast majority of proteins it is currently hard to predict the exact location of this liquid-solid transition from the solution properties at low concentration only. In view of the high cost/low availability of highly interesting proteins such as antibodies, where a viscosity increase can inhibit the injection of effective doses, or eye-lens proteins, where the physiological concentration is naturally very high to achieve the refractive properties needed, it is commonly not viable to investigate this type of systems using macroscopic methods such as classical rheology due to the large sample volumes needed. Instead we use Dynamic Light Scattering (DLS) based microrheology where we can extract information about the viscoelastic behaviour of the various protein solutions by measuring the motion of inert tracer particles embedded in a small sample volume. We also work on the synthesis of tracer particles that meet all requirements for a systematic investigation of the viscoelastic properties of different protein solutions and mixtures as a function of concentration and solvent conditions. (Tommy Garting, Nicholas Skar-Gislinge, Anna Stradner.)

2.4.3 Calbindin D_{9k} as a protein component for a model cytosol

(Contact person: Anna Stradner)

The knowledge of interactions between proteins in crowded mixtures, as they exist in the interior of living cells, is essential since they ultimately determine their stability, phase behavior, solution structure and dynamics. As a first step on our way to establish a well-defined model cytosol with a complete experimental description of the effective interactions and the resulting solution structure and thermodynamic stability, we need to identify individual proteins that differ in size and charge and are suitable components for our generic cell cytosol.

One potential candidate is calbindin D_{9k}, a monomeric calcium-binding protein of the S100 family of the calmodulin-related proteins, involved in Ca^{2+} buffering and in trans-cellular transport of Ca^{2+} ions. We investigate the solution structure of calbindin D_{9k} using SAXS and quantify the protein-protein interactions through second virial coefficients as a function of the calcium binding state (holo and apo) and the screening conditions, both experimentally and via Monte Carlo computer simulations. In a next step we study the interactions/aggregation behaviour of calbindin with the oppositely charged lysozyme. (Najet Mahmoudi, Coralie Pasquier, Mikael Lund, Sara Linse, Jeppe Lyngsø and Jan Skov Pedersen (Aarhus University), Anna Stradner.)

2.4.4 Responsive colloids interacting with lipid bilayers (Contact person: Emma Sparr)

We investigate interactions between thermoresponsive microgel particles and lipid model membranes. We have previously shown that spherical PNIPAM microgel particles adsorb to fluid lipid bilayers in monolayers with crystalline packing. Here we will focus on soft responsive isotropic and anisotropic microgel particles as well as lipogel composite particles. As model membranes, we use supported bilayers as well small and giant vesicles where we systematically very lipid composition.

We investigate dynamics of the microgel particles and their assembly near or within the membrane and the rate by which they are adsorbed. The study also concerns how particle-membrane interactions are affected by the nature of the lipid bilayer, e.g. fluidity, curvature, charge and domain formation. As an example, for lipid systems with segregated fluid and solid domains, the soft microgel particles preferentially adsorb to fluid domains into highly ordered 2D hexagonal arrays, rather than to solid domains, where almost no adsorbed particles were observed. (Adriana Mihut, Meina Wang, Aleksandra Dabkowska, Jerome Crassous, Ellen Rieloff, Tommy Nylander, Peter Schurtenberger, Emma Sparr.)

2.4.5 Model membranes on novel sensing support (Contact person: Tommy Nylander)

As nanowires (NWs) gain momentum in biological applications, it is becoming increasingly important to understand the molecular interactions at these sophisticated interfaces. Membrane-mediated processes play a key role in many biological functions and supported lipid bilayers are excellent model systems for the study of membranes and membrane-integrated proteins. Furthermore, for many cell organelles, membranes are curved. With this in view, we recently developed a hybrid system consisting of membrane-like phospholipid bilayers supported by NW forests, which allows the formation of bilayers with controllable curvature as a matrix for biomolecular interaction. We seek to use the hybrid system to monitor membrane processes, including mechanical properties of the membrane and interactions with biomolecules. This work is funded by the nmC@LU together with the Organizing Molecular Matter (OMM) Linné Centre of Excellence as well as Carl Tryggers Stiftelse. (Tommy Nylander, Aleksandra Dabkowska, Christelle Prinz (Solid State Physics, LU), Heiner Linke (Solid State Physics, LU), Hanna Wacklin (ESS AB), Emma Sparr.)

2.4.6 Protein structure and interactions involved in antigen presentation (Contact person: Malin Zackrisson Oskolkova)

In the responsive immune system major histocompatibility complex class I (MHC I) proteins plays a key role in the recognition of intracellular pathogens (virus and cancer). The main task of the MHC-I proteins is to present antigens, which may impose a hazard to the cell. The antigen processing and loading onto MHC-I

molecules takes place in the intracellular environment, when the antigen-MHC-I complex is transferred to the cell surface for detection by circulating CD8 + T cells. The mechanism of this antigen presentation involves the formation of a so-called MHC-I peptide-loading complex (PLC) where several proteins are involved. One of these proteins, which help to stabilize, facilitate and edit the peptide-loading complex, is Tapasin, a chaperone transmembrane protein. We are interested in investigating the solution structure and behavior of Tapasin in a first step to understand the connection between that and its biological function. The project is done in collaboration with Kajsa M. Paulsson, head of the Antigen Presentation group at the Faculty of Medicine. (Weimin Li, Kajsa M. Paulsson (Experimental Medical Science, Faculty of Medicin), Malin Zackrisson Oskolkova.)

2.4.7 Cataract formation and eye lens transparency
(Contact person: Anna Stradner)

The understanding of protein solutions, their dominant interactions and their complex phase behavior is an important topic that has greatly profited from the well established experimental and theoretical toolbox of colloid physics. Initially, these developments were primarily driven by attempts to better understand and improve protein crystallization. However, issues of interparticle interactions, aggregation, cluster formation and dynamical arrest in protein solutions have to be seen in a broader context. Understanding interparticle interactions in protein solutions is for example of central importance to gain insight into the origin of protein condensation diseases such as Creutzfeldt Jakob, Alzheimer, Parkinson or cataract. In this project we study the structural and dynamic properties of concentrated eye lens protein solutions and mixtures with the long-term goal of shedding light on the molecular origins of cataract formation, still the major cause of blindness worldwide. We primarily use scattering experiments (light, neutron and x-ray scattering) as well as phase diagram determination and rheological measurements together with course grained computer simulations based on colloidal models to achieve a quantitative understanding of protein interactions in the eye lens. (Saskia Bucciarelli, Tommy Garting, Najet Mahmoudi, Bela Farago (ILL Grenoble, France), Cristiano de Michele (La Sapienza, Rome), Francesco Sciortino (La Sapienza, Rome), George Thurston (Rochester Institute of Technology, USA), Mikael Lund, Peter Schurtenberger, Anna Stradner.)

2.4.8 Scanning SAXS study of bone
(Contact person: Ulf Olsson)

Bone is a complex material with a hierarchical structure, where the main building blocks are the protein type I collagen and a crystalline mineral phase usually referred to as carbonated hydroxyapatite. These two very different components are closely associated in fibrils that form an interconnected network, which detailed arrangement depends on species and type of tissue. With collagen being tough but soft and

hydroxyapatite being rigid but brittle, together they form a nanocomposite that provides bone with its unique mechanical properties of strength and toughness.

In this project we collaborate with the group of Hanna Isaksson division of Biomedical Engineering, Faculty of Engineering on the characterization of bone structure in e.g. fracture healing using scanning SAXS. Scattering studies are often combined with e.g. FTIR microscopy, that reports on the spatial distribution of bone composition. (Hanna Isaksson (Biomedical Engineering), Jörn Dövling Kaspersen, Ulf Olsson, Martin Bech (Medical Radiation Physics), Magnus Tägil (Department of Orthopaedics), Mikael Turunen and Jukka Jurvelin (Kuopio, Finland), Ana Labrador & Sebastian Lages (MAX IV laboratory), Jan Skov Pedersen (Aarhus).)

2.4.9 Amyloid interaction with lipid membranes

(Contact person: Emma Sparr)

Amyloid protein aggregation is associated with over 30 known diseases in humans. In amyloid plaques associated with several amyloidogenic diseases, tightly associated lipids have been identified. For several of the amyloid disorders, protein aggregation has also been associated with membrane disruption in cells and in model lipid systems. In this project, we investigate interactions between aggregating amyloid proteins and lipid membranes, and we explore the basic principles of the amyloid-lipid coaggregation

The proteins -synuclein is found in the protein aggregates characteristic for Parkinson disease. In this project, we study interactions between -synuclein and lipid membranes. We use model membranes with varying lipid compositions, and biological membranes in isolated exosomes. We study protein-lipid co-aggregation, membrane assoication and the consequences of protein-lipid interaction on aggregation kinetics and membrane intergrety. In this project we explore different biophysical techniques, including PT ssNMR, confocal microscopy on giant unilamellar vesicles, fluorescence correlation spectroscopy, fluorescence spectroscopy, QCM-D, neutron reflectivity and cryo-TEM. (Ricardo Gaspar, Ilaria Idini, Aleksandra Dabkowska, Veronica Lattanzi, Sara Linse (Division of Biochemistry and Structural Biology, LU), Tommy Nylander, Ulf Olsson, Daniel Topgaard, Celine Galvagnion (Cambridge University, UK).)

2.4.10 Condensing DNA with cationic dendrimers: means of controlling aggregate morphology and membrane penetration

(Contact person: Tommy Nylander)

Dynamic light scattering, cryogenic TEM and steady-state fluorescence spectroscopy are utilized to investigate the interaction between cationic poly(amido amine) (PAMAM) dendrimers and double stranded DNA. This systematic study reveals how the size, composition and morphology of aggregates formed between DNA and PAMAM dendrimers are affected by dendrimer size and charge. In gene therapy one often utilizes vehicles with the ability to condense DNA and thereby

protect DNA against degradation, transport DNA across membranes as well as regulate gene expression. One such compacting agent is dendrimers. We have found that the compacting agent not only condenses the DNA chain, but can also on its one be transported across a model membrane. This might help the complex to be transported across the membrane. We are investigating the conditions, such as membrane and dendrimer properties, under which this occurs using ellipsometry, QCM-D, neutron reflectometry and different fluorescence techniques. (Marianna Yanez, Marie-Louise Ainalem (ESS AB), Syma Khaled (University of Southampton), Anna Carnerup, John Janiak, Viveka Alfredsson, Tommy Nylander, Dan Lundberg, Karin Schillén.)

2.4.11 DNA gel particles and cross-linked DNA gels

(Contact person: Björn Lindman)

Through an interfacial diffusion mechanism DNA particles were prepared and studied with respect to internal structure and DNA release. A large difference in internal structure between different DNA conformations for surfactant systems point to the role of hydrophobic interactions. Release properties of the gel particles, which can be manufactured in the size range from 100 nm to mm, are investigated. DNA gel particles are made from mixtures of DNA with cationic surfactants, proteins and polymers and also for other polymers. DNA molecules, both single- and double-stranded, have been covalently cross-linked to form chemical gels. Addition of electrolytes causes a deswelling of the gels. From the volume changes the association of oppositely charged cosolutes with DNA can be monitored. For cationic surfactants a dramatic compaction is noted as well as the formation of different ordered microstructures. An extensive comparative study of the deswelling of both ss- and ds-DNA gels on addition of several cosolutes – metal ions of different valency, proteins, polyamines and other polycations and cationic surfactants - have been performed. Both thermodynamic and kinetic aspects, as well as reversibility of volume changes, have been considered. The release of DNA and incorporated proteins are investigated, in particular related to triggering release. (Björn Lindman, Carmen Morán (Univ. Barcelona), Diana Costa (Univ. Beira Interior) and Maria Miguel (Coimbra University).)

2.4.12 Structure and self-assembly of viruses

(Contact person: Per Linse)

The role of the genome in the assembly of icosahedral viral capsids has been investigated by molecular dynamics simulation of a coarse-grained model, in which the capsomers carry explicit charges and the polynucleic acid is represented by a bead-spring chain. The co-assembly process was contrasted with the self-assembly of uncharged capsomers. In the co-assembly, the capsomers first associated to the polyion and then rearrange into a capsid, whereas the self-assembly proceeded through a spontaneous nucleation and growth of partial capsids. The polyion

backbone stiffness was found to have a significant effect on the co-assembly process; polyions of intermediate flexibility gave the fastest and most faithful assembly process. Addition of a small amount of monovalent salt also improved both speed and fidelity of the co-assembly process. Moreover, the capsid assembly process in terms of cluster size development and encapsulation efficiency was investigated by employing different polyion topologies from linear to dendritic ones. With increased branching degrees of the polyion, the encapsulation process is significantly steered to the formation of icosahedral T1 capsids. The dendritic polyions were entirely encapsulated in an ordered capsid structure for all the designed polyion/capsid charge ratios considered. (Ran Zhang, Erik Wernersson, and Per Linse.) (Project completed.)

2.4.13 The skin as a barrier to molecular diffusion

(Contact person: Emma Sparr)

The human skin is a large (ca. 2 m2) membrane that separate regions with profoundly different properties. This implies that several simultaneous transport processes occur across a non-equilibrium system. The skin is a vital organ, and its outer layer, stratum corneum (SC) forms the barrier that prevents from desiccation and protects against the uptake of hazardous chemicals. SC also highly attractive as a target for directed and controlled delivery of drugs.

We aim at a characterization of the material properties of the SC by coupling macroscopic SC barrier properties to its molecular structure and dynamics. Diffusional transport across SC can be regulated by changes in the skin environments. One example is the abrupt increase in SC permeability at high degrees of SC hydration, called occlusion effect. Through a complementary experimental and theoretical approach, we have provided a molecular explanation to this effect.

We investigate how different classes of solvents and small molecules used as penetration enhancers or moisturizers influence the molecular properties of SC components and the macroscopic barrier properties of the skin. We also study the differences between healthy and diseased SC, focusing on psoriasis skin. We characterize the lipid and protein components in intact stratum corneum using natural abundance PT ssNMR, scattering and sorption techniques. (Dat Pham, Enamul Mujumdar, Sebastian Björklund, Emma Sparr, Daniel Topgaard, Johan Engblom (Biofilms; Malmö University), Joke Bouwstra (Leiden University), Bernard Cabane (ESPCI, Paris), Andreas Sonesson (Dermatology, Lund University), Ola Bergendorff (Dermatology, Lund University).)

2.4.14 Molecular crowding: towards a better understanding of concentrated protein solutions and mixtures

(Contact person: Anna Stradner)

There is an increasing awareness that a quantitative understanding of the cellular machinery requires considerable advancement of our current understanding of concentrated (or crowded) protein mixtures present in the cytosol. The main objective

of this project is thus to measure and understand intermolecular interactions in concentrated protein solutions and mixtures as well as their dynamics. We use a combination of different scattering methods (SANS, SAXS, Static and Dynamic Light Scattering, Neutron Spin Echo (NSE) experiments), and compare the results with the predictions from numerical simulations. We in particular focus on the influence of interactions and their anisotropy on the diffusion of proteins. We can show that incorporating patchiness and thus interaction anisotropy has a dramatic effect on the dynamics and shifts the simulation results significantly towards matching our experimental results on the local short time dynamics of concentrated solutions of one of the lens proteins obtained from NSE.

In order to reach quantitative agreement with experiments at all volume fractions, we optimize our model by incorporating information based on the molecular structure of the protein. We use this refined anisotropic interaction potential as a starting point for simulating binary protein mixtures and comparing with data from NSE experiments and structural investigations. (Saskia Bucciarelli, Tommy Garting, Marc Obiols-Rabasa, Johan Bergenholtz, Bela Farago (ILL Grenoble, France), Olaf Holderer (Jülich Centre for Neutron Science (JCNS), Germany), Jin Suk Myung (FZ Juelich, Germany), Gerrit Vliegenthart (FZ Jülich), Roland Winkler (FZ Jülich), Gerhard Gompper (FZ Jülich), Jan Dhont (FZ Jülich), George Thurston (Rochester Institute of Technology, USA), Mikael Lund, Sara Linse, Peter Schurtenberger, Anna Stradner.)

2.4.15 Supramolecular structures of bile salt derivates in aqueous solutions (Contact person: Karin Schillén)

Surfactants prepared by chemical modification of bile salts, e.g. sodium cholate derivatives, show a rich self-assembly in aqueous solution. The supramolecular structures formed range from small micelles, networks of thin threads (homogenous fibers), tubules, long (on the “μm” -mm length scale) rod-like objects (“poles”) to twisted ribbon-like structures. The formation of these assemblies depends on the kind of modification, pH and temperature. The temperature response is particularly interesting since it is fast and reversible. Cryo-TEM, circular dichroism, SAXS at MAX IV laboratory and light scattering techniques are employed to explore these various morphologies and the driving force of their formation. The formation of tubules occurs around body temperature and the tubules are further investigated using water-diffusion NMR. (Karin Schillén, L. Galantini and V. Pavel (University of Rome “La Sapienza”, Italy), Ulf Olsson, Daniel Topgaard.)

2.4.16 Studies of osteopontin and casein self-assembly in the context of biomineralisation: applications in food, health and biomaterials (Contact person: Tommy Nylander)

Many biofluids are super saturated with respect to hydroxyapatite (HA) by forming complexes between phosphopolypeptides/phosphoproteins and amorphous calcium

phosphate (ACP). The purpose is to maintain the integrity of bones and teeth without mineralising the surrounding soft tissues. Our long-term goal is to provide a unified model of the structure and mechanism of the formation of the complex between ACP and different phosphorylated proteins/peptides, based on the hypothesis that the process is controlled by protein self-assembly. The structures of composite materials comprising phosphopolypeptides and calcium phosphate with very different neutron scattering length densities are well suited to being studied by neutron scattering and diffraction methods. We will use NMR techniques to study the formation of these composites as well as interfacial techniques to study their interfacial behavior of relevance for biomineralization. In combination with recombinant phosphoprotein expression and isotope labelling, novel nano-, micro- and macro-structures will be fabricated and their size and medium resolution substructures determined. (Susana Teixeira, Sam Lenton and Giuseppe Zaccai (ILL), Carl Holt (University of Glasgow), Tommy Nylander, Daniel Topgaard.)

2.4.17 Peptide self-assembly

(Contact person: Ulf Olsson)

The development of modern peptide chemistry has opened for the possibility of custom peptide synthesis that allows for systematically investigating the relationship between a specific oligopeptide molecular structure and the macroscopic phases and structures formed in such systems. Understanding the assembly behavior of peptides is important in not only designing nanomaterials for a desired functionality but also for combating neurodegenerative diseases such as Alzheimer and Parkinson's disease which are strongly associated with an accumulation of amyloid forming peptides in the brain. In this newly started project we focus initially on the self-assembly behavior of short simple and synthetic petides, AnK, where n is varied in the range 4-10 (A=alanine, L=lysine). These peptides allows for a systematic investigation of e.g. the hydrophobicity and peptide length on the self-assembly behavior. A6K in water forms very long hollow nanotubes with a (monodiperse) diameter of 52 nm. Because of the large aspect ratio, the nanotubes form a nematic phase or a hexagonal phase. The nanotube walls are crystalline and the tube formation involves crystal growth processes including oriented fragment attachments. Increasing the peptide concentration, close packing is obtained and there is a first order phase transition to a lamellar phase with the peptide now forming planar bilayers. Increasing the number of hydrophobic alanines to A8K and A10K, aggregation begins at lower peptide concentrations. Also, they do not aggregate into tubes. Instead they form fibrils, a few 100 nm long, with a rectangular cross section of ca. 8 nm x 4 nm. (Axel Rüter, Celen Cenker, Ulf Olsson, Mikael Lund (Division of Theoretical Chemistry), Karl-Erik Bergqvist (Centre for Analysis and Synthesis), S. Bucak (Istanbul), Paul Bomans, Heiner Friedrich and Nico Sommerdijk (Eindhoven), Theyencheri Narayanan (ESRF, Grenoble).)

2.4.18 Lung surfactants

(Contact person: Emma Sparr)

The alveolar surface is lined by film of submicron thickness between the epithelial cells and the alveolar lumen with the main function to lower the surface tension. The aqueous bulk structure of this layer consists of lipid bilayers forming lamellar bodies (LB:s) and tubular myelin (TM), and two hydrophilic proteins in the outside water ; SP-A and SP-D. We are studying the interfacial and bulk structure of and phase transitions in this lung surfactant extracts and model systems using ssNMR, SAXS/WAXS, ellipsometry, monolayer techniques and cryo-TEM. Another aspect of the project is the diffusion in through the interfacial lipid membrane with complex structure that implies a diffusional permeability that is different for hydrophilic and hydrophobic substances. (Jenny Andersson, Tommy Nylander, Marcus Larsson (Lund University Hospital), Tiago Ferreira (Martin Luther universität Halle-Wittenberg, Germany), Emma Sparr.)

2.5 Molecular matter for specific functions

2.5.1 Nanoparticle-protein interactions – towards understanding cellular response to nanoparticles

(Contact person: Peter Schurtenberger)

In this project we investigate and model interactions between nanoparticles and proteins in serum and cellular environments. We characterize their properties (size, polydispersity, surface charge density etc.) and the resulting interaction potential and particle stability as a function of solvent conditions (pH, ionic strength).

We study the interactions of these particles with a set of model proteins covering a representative array of protein sizes and charges. We investigate the fate of the particles in a crowded mixture of proteins, thus mimicking the interaction of nanoparticles with the cell cytoplasm. Experimentally, we combine several scattering techniques (Static and dynamic light scattering, depolarized light scattering, small-angle x-ray and neutron scattering, confocal and electron microscopy), various labeling schemes that allow for the detection of complex formation, and numerical simulations. (Marc Obiols Rabasa, Sandor Balog and Alke Fink (University of Fribourg), Peter Schurtenberger.) (Project completed.)

2.5.2 Phase separation, adsorption behavior and delivery capacity of polyelectrolytes and oppositely charged surfactants at surfaces

(Contact persons: Tommy Nylander and Lennart Piculell)

An enhanced surface adsorption is typically obtained from dilute mixtures of a polyelectrolyte and an oppositely charged surfactant under conditions when there is a bulk associative phase separation in the mixture. This phenomenon is used in everyday products (e.g., shampoos, laundry detergents) that are specifically designed

to produce deposited surface layers. Often the phase-separation and enhanced deposition can be obtained by a simple dilution process. The same process can also be used to deliver some additional substance to the surface together with the polyion-surfactant ion complexes. As an example, the co-deposition of emulgated silicone oil droplets onto hydrophilic and hydrophobic surfaces has been studied for formulations containing anionic surfactant and cationic polymers of varying hydrophobicity. The aim of the present project is to provide fundamental understanding of the kinetics of this process by combining models of kinetics with experimental data by obtained by using surface techniques such as neutron reflectometry and ellipsometry as well as scattering techniques to reveal the changes in composition at the interface versus time. (James Holdaway, Tommy Nylander, Lennart Piculell; E. Johnson, P. Ellingson, B. Schubert (Procter & Gamble, Cincinnati).)

2.5.3 Cleaning technology in high temperature food processing – from fundamental understanding to sustainable and safe food processing
(Contact person: Tommy Nylander)

Food products are heat treated in order to assure the food safety and to increase the shelf life of the product. An unwanted consequence of the thermal treatment is the formation of a deposit, fouling, onto exposed surface of the processing equipment. The challenge is to remove these deposits within minimal time and without using excessive amount of energy, water and chemicals. The key question that this work aims to answer is which mechanisms dominate and limit the efficiency during cleaning of deposits in process equipment for dairy or dairy based products. Focus will be to answer the question in relation to different: process parameters, detergent properties and deposit compositions and structures. The final vision is to establish a classification map that enables tailor made and optimized cleaning routines based on deposit composition, deposit structure, detergents and cleaning mechanisms. This scientific PhD project, granted within the Cross-disciplinary food research Programme by FORMAS and VINNOVA, will be followed by applied projects at Tetra Pak Processing Systems where the results will be verified in full scale for further implementation into new processing solutions. (Tommy Nylander, Fredrik Innings (Tetrapak AB), Christian Trägårdh and Marie Paulsson (Food Technology), Niklas Lorén (SIK AB, The Swedish Institute for Food and Biotechnology Structure and Material Design).)

2.5.4 Model membranes on nanostructured sensing supports
(Contact person: Tommy Nylander)

This project aims to study the mechanism of formation and structure of complex lipid bilayers, a lipid composition that mimics biological membranes (i.e. composed of several lipid types) on a variety of substrates including structured surfaces consisting of nanowire forests. This will allow membranes with tailored properties to be developed for applications in key membrane processes, such as antimicrobial

peptide activity, protein interactions, and DNA transfection. We will investigate the use of nano-wire "forests" developed by Lars Samuelson's group at Solid State Physics, Lund University as a support for free standing lipid bilayers and means to sense membrane mechanical properties, such as lateral stress, as well as biomolecular interactions and activity with and in the membrane. Financed by OMM and nmC@Lund. (Tommy Nylander, Aleksandra Dabkowska, Emma Sparr, Heiner Linke and Christelle Prinz (Solid State Physics), Hanna Wacklin (ESS AB).)

2.5.5 Finding a protocol for adsorbing disc-like mesoporous silica particles with the pores parallel to the surface normal

(Contact person: Viveka Alfredsson)

In In this project the aim is to deposit mesoporous silica particle with controlled orientation onto a support surface. We work with a modified version of the well-known 2D hexagonal silica material denoted SBA-15. In this material primary mesopores are oriented in parallel with the surface normal. It is generally difficult to form a layered silica surface with pores in this orientation, typically the pores will orient along the underlying support surface. In our synthesis protocol disclike particles are formed in a well-characterized process and our aim is to take advantage of the shape and/or growth behavior in order to deposit the particles with the desired orientation.

We have successfully deposited a monolayer of oriented particles by two methods, drop deposition and using a Langmuir-Blodgett through. The latter permit homogenous depositions several cm2 in size. We have controlled the porous properties of such a monolayer using QCM-d.

The project is part of the SSF-program "Porous surface layers formed through polymer-assisted deposition". (Yana Znamenskaya (Post Doc), Julien Schmitt (Post Doc), Tomas Kjellman (PhD student), Prof. Viveka Alfredsson (PI), Prof. Karen Edler (University of Bath), Prof. Håkan Wennerström, Vitaly Kocherbitov (MaH), Sebastian Björklund (MaH). Project completed in 2015.

2.5.6 The role of the co-structure directing agent in the formation of mesostructured silica

(Contact person: Viveka Alfredsson)

One synthesis strategy of mesoporous silica utilizes a so-called co-structure-directing agent believed to serve as a link between the silica network and the structure-directing amphiphile. This synthesis strategy, discovered and developed by Shunai Che and her group in Shanghai, has proven to be very versatile and a large number of structures can be obtained by small variations of the synthesis parameters. In this project we are investigating the molecular interactions involved and the role of the co-structure-directing agent. (Ruiyu Lin, Karen Edler (University of Bath and guest Professor at Lund University), Shunai Che (Shanghai Jiatong University, China), Daniel Topgaard, Lennart Piculell, and Viveka Alfredsson.)

2.5.7 Controlled deposition of lipid liquid crystalline nanoparticles to obtain biofunctional surfaces

(Contact person: Tommy Nylander)

Investigation of non-lamellar nanoparticles formed by dispersion of self-assembled lipid liquid crystalline phases is stimulated by their many potential applications in science and technology; resulting from their unique solubilizing, encapsulating and space-dividing nature. Our aim is to control the interfacial behavior of lipid liquid crystalline nanoparticles (LCNPs) at surfaces to facilitate the exploitation of such systems for a number of potentially interesting uses, including preparation of functional surface coatings and uses as carriers of biologically active substances. We have shown that LCNPs can form well-defined layers at the solid-liquid interface with a structure and coverage that is determined by the interplay between self-assembly properties of the lipids and lipid surface interactions, respectively. Financed by Swedish Foundation for Strategic Research. (Tommy Nylander, Debby Chang, Fredrik Tiberg (Camurus AB), Justas Barauskas (Vilnius University).)

2.5.8 Associative effects of polyacrylates in surfactant systems

(Contact person: Björn Lindman)

Effects of surfactants on the rheology of water-soluble polymers are investigated as a function of charge density, cross-linking and hydrophobicity. The delicate balance between restoring hydrophobic interactions and osmotic swelling can be critically controlled by small concentrations of surfactants, which can change the viscosity by several orders of magnitude. (Björn Lindman, Filipe Antunes (Coimbra University), Hans-Martin Haake and Björn Klotz (Cognis/BASF, Düsseldorf).)

2.5.9 Following the nucleation and growth of a material using cryogenic transmission electron microscope

(Contact person: Viveka Alfredsson)

Cryogenic TEM is used as a tool to visualize the stages of formation of a chiral mesoporous structured material; the synthesis was designed and developed by Shunai Che. We follow the formation process from the micellar solution to the final particles, that have either tube or rod morphology dependent on synthesis temperature. We are collaborating with the group of Prof. Ishi Talmon at the Technion in Haifa in Israel. (Ruiyu Lin, Juanfang Ruan (presently at Osaka University, Japan), Ishi Talmon (Technion, Israel), Shunai Che (Shanghai Jiaotong University, China) and Viveka Alfredsson.)

2.5.10 Alternative Diesel Fuel

(Contact person: Ulf Olsson)

Alternative fuel from renewable resources has been receiving increased attention worldwide due to the expected depletion of fossil fuel and the environmental hazardous nature of emissions associated with its combustion. Diesel exhaust poses one of the major health hazards to human. The particulate matter or soot and the nitrogen oxide compounds released directly to the environment can cause serious health problems. Vegetable oils, being renewable, with similar energy content to diesel, can be a viable alternative fuel. However, due to their high viscosity, they can't be injected directly without engine modifications. Reducing viscosity can be achieved through the trans esterification process, in which the oils react with alcohol, commonly methanol, to yield the corresponding fatty methyl ester, known as biodiesel. The produced biodiesel has many attractive properties. It is compatible with diesel, renewable and it produces lower emission of greenhouse gases and pollutants like soot and polycyclic hydrocarbons. On the other hand, some technical problems associated with its usage, like the poor low temperature properties and the increased NO_x exhaust emissions still need to be solved.

Phase behavior of the three components, 1-propanol, water and oil is studied at 10, 25, and 40 C. Biodiesel, limonene and diesel are used as oil phases. NMR self-diffusion measurements are performed to investigate the microstructure of the one-phase regions. Tie lines in the two-phase regions are determined both by proton NMR analysis and compared with theoretical calculations. NMR self-diffusion results for the different components in these systems do not show any sign of confinement or obstructions, demonstrating these mixtures to be structureless solutions. A good agreement between the experimental and calculated phase behavior is obtained. The determined tie lines in the two-phase regions show higher affinity of 1-propanol to water than to oil. (Ibrahim Kayali, Khawla Qamhieh, Chemboli K. Jyothi, Ulf Olsson.)

2.5.11 Combining mesoporous silica with microgel particles

(Contact person Viveka Alfredsson)

In this project we explore different methods of combining mesoporous silica particles (SBA-15) with different morphologies with microgel in order to obtain a responsive material. We make use of several approaches: combining the particles in a layer-by-layer strategy – in order to create an assembly mimicking nacre, by synthesising the microgel (i.e. PNIPAAM) linked to the silica particles or by synthesising the PNIPAAM in the presence of silica particles. The composite particles are characterised using confocal microscopy. We explore how the anisotropy of the particles respond to an electric field. (Julien Schmitt, Jerôme Crassous, Peter Schurtenberger and Viveka Alfredsson.)

3 Scientific instrumentation

3.1 Surface techniques

3.1.1 Ellipsometry

(Contact person: Tommy Nylander)

The development of a high precision ellipsometer for time-resolved studies of thin adsorbed films has been successful and of great importance to several specific projects. The instrument allows precise and rapid measurements of the ellipsometric anglesandthus, allowing unique studies of the evolution of both the thickness and density (refractive index) of adsorbed surfactant and polymer layers with time. The possibility of working at different wavelengths provides an additional source of information on complex systems as well as flexibility to optimize the optical contrast of the systems studied. Continued efforts are invested in upgrading this instrument to improve its potential for studies of fast interfacial processes occurring on the nanometer scale.

During 1998 we acquired an additional ellipsometer, an Optrel Multiskop (Optrel, Berlin Germany). This instrument has been fitted with sample cells to measure at the solid-liquid, liquid-liquid and liquid-air interfaces. Apart from doing null-ellipsometry we can also do imaging ellipsometry, Brewster Angle Microscopy, Surface plasmons as well as operate it in waveguide mode. (Sponsored by FRN).

A spectroscopic ellipsometer, Horiba UVISEL-ER-AGAS Spectroscopic Ex-Situ Ellipsometer for the FUV-VIS-NIR Range with Automatic Goniometer and Motorised Mapping Stage that allow determination of the thin film properties within the spectral range from 190-2100 nm was purchased in 2010. The spectroscopic ellipsometer incorporates phase modulation technology to characterize polarization changes at high frequency (50 kHz), and without any mechanical movement. The Uvisel is equipped with a Multi Channel System for Parallel Spectra Acquisition for kinetic studies of thin films within the spectral range from 190 to 810 nm. The instrument is equiped with measuring cells for measurements at the solid-liquid and air-liquid interface under controlled conditions. (Sponsored by the Knut and Alice Wallenberg Foundation.)

3.1.2 Quartz crystal microbalance with dissipation monitoring (QCM-D)

(Contact person: Tommy Nylander)

The instrument is from Q-Sense fitted with E4 and E1 module and is able to collect, both the dissipation and the resonance frequency of a quartz crystal. These data can be used to follow the formation of thin films (nm) such as proteins, polymers and cells onto surfaces, in liquid by using a flow system at controlled temperature. The advantage with measurements at several frequencies and the

dissipation is that we can determine the adsorbed film is rigid or water-rich (soft). The instrument is equipped with a Q-Sense Ellipsometry Module (for the Q-Sense E1 system), which enables simultaneous QCM-D and ellipsometric measurements on the same substrate. Thus we can determine both the adsorbed amount and the water content in adsorbed layer. (Sponsored by the Knut and Alice Wallenberg Foundation.)

3.1.3 Scanning probe microscope

(Contact person: Emma Sparr)

A XE-100 AFM system from ST Instruments (Park systems) was purchased in 2011. The instrument can be operated to image topography and friction on small and medium size samples both in air and in liquid. The instrument consists of completely decoupled XY & Z scanners by using flexure guided scan system for all three axes, closed/open-loop scan, XY flexure scanner with zero background curvature, motorized Z stage, motorized focus stage, precision motorized XY sample stage and direct on-axis optics. The system also includes high resolution digital CCD camera with digital zoom. (Sponsored by the Knut and Alice Wallenberg Foundation.)

3.1.4 Surface force apparatus (SFA)

(Contact person: Tommy Nylander)

The Surface Force Apparatus allows the direct measurement of the interaction between two molecularly smooth surfaces (usually mica) in a crossed cylinders geometry. The separation between surfaces is measured interferometrically up to 0.1 nm resolution. The force is calculated from deflection of a double cantilever spring with an accuracy of ca 10-8 N. The SFA is being successfully used to identify and quantify most of the fundamental interactions occurring between surfaces, namely van der Waals, electrostatic double-layer, hydration, hydrophobic and steric forces, in different colloidal systems. (Sponsored by FRN.)

3.1.5 Surface film balance

(Contact persons: Tommy Nylander and Emma Sparr)

Three different equipments optimized for different purposes: 1) A Nima technology 611 Langmuir trough with a surface film balance (Wilhelmy plate) was acquired during 1997. The instrument is equipped with a dipper to prepare Langmuir-Blodgett films. It can also be used for dynamic contact angle measurements, while simultaneously recording the surface film pressure. 2) A KSV minitrough was acquired 2000 and used together with the Optrel Multiskop ellipsometer. Both surface film balances are equipped to measure the surface potential. 3) A 20 ml Langmuir micro-trough from Kibron. The equipment includes surface pressure sensor, a window in the bottom of the trough for microscopy, a temperature control plate, and a multiwall plate for surface pressure

measurements. (Sponsored by Crafoord Foundation and Per-Eric and Ulla Schyberg's foundation.)

3.1.6 Surface tension

(Contact person: Tommy Nylander)

The Drop and Bubble Shape Tensiometer PAT-1 from SINTERFACE, Germany, allows measuring quite a number of interfacial properties. In addition to the properties of a standard drop and bubble instruments it allows, surface and interfacial tension of liquids, static and dynamic contact angle according to the sessile drop method, surface rheological studies to measure the dilational elasticity and viscosity, fast oscillations with extra module ODBA-1, 0.1 s resolution over a period of seconds up to days and an injection system that allows adding another solution to an already formed drop. (Sponsored by the Knut and Alice Wallenberg Foundation.)

3.2 Scattering techniques

3.2.1 Dynamic and static light scattering (DLS and SLS) goniometer system

(Contact person: Karin Schillén)

The laser light scattering goniometer system from the ALV Gmbh, Langen, Germany, is a measuring system for simultaneous angular dependent determination of DLS and SLS. The ALV/DLS/SLS-5022F, CGF-8F compact based, system includes CW Helium-Neon (He-Ne) gas laser (632.8 nm with a output of 22 mW), laser beam focusing optics (including a laser beam attenuator and a Glan laser polarizer prism), a goniometer with a rotary table with the angular range of about 15° to 150°, a cell housing with an cylindrical quartz vat (filled with a refractive-index matching liquid, cis-decahydronaphtalene, decaline), a fiber optical near-monomodal detection system with a possible depolarized light detection, a detection unit comprises of two matched avalanche photodiodes that is put in a pseudo-cross correlation arrangement. For the DLS measurements using photon correlation spectroscopy, an ALV-7004 multiple tau digital correlator with an initial real sampling time of 25 ns and 4 x 312 channels covering ≈12 decades in lag time is utilized to produce the time pseudo-cross correlation function of the scattered intensity. This make it possible to measure particle sizes from 1 nm up to about 5000 nm. The temperature range of the vat is –12 °C to +140 °C (if the refractive index matched liquid changed) and is controlled to ± 0.01 °C by a F32 Julabo heating circulator. In addition, also included in the overall set-up, is a ALV/DR-1 differential refractometer with a He-Ne laser for determination of refractive index increments (dn/dc) necessary for the determination of molar masses by SLS experiments. The limited accuracy of the refractive index is ≤ 2 x

10-6 refractive index units. (Sponsored by the former Swedish Natural Science Research Council, NFR, and by Knut and Alice Wallenbergs Stiftelse, KAW.)

3.2.2 Instrument for dynamic and static light scattering and electrophoretic mobility measurements

(Contact person: Karin Schillén)

For convenient DLS and SLS measurements along with determination of electrophoretic mobility (or zeta potential) in both aqueous and non-aqueous dispersions, a Zetasizer Nano ZS from Malvern Instruments Ltd, Worshestershire, UK, is available. The instrument measures DLS and SLS at a set angle of 173° using the NIBS technology. The accessible particle-diameter range is 0.3 nm – 10 µm in concentrations up to 40 % (w/v) depending on sample and the molecular weight range is 980–2107 g/mol. The zeta potential measurements in the conductivity range of 0-200 mS/cm are performed at 17 ° using M3-PALS technology (particle diameters from 3.8 nm to 100 µm). The instrument is equipped with a 4 mW He-Ne laser (wavelength of 632.8 nm) with an automatic laser attenuator that allows for measurements at sample transmissions ranging from 100 % to 0.0003 %. The detection unit comprises an avalanche photodiode. The temperature range of the instrument is 2–90 °C. (Sponsored by the Crafoord Foundation.)

3.2.3 Multi-angle static light scattering desktop instrument

(Contact person: Karin Schillén)

For characterization of molecular weight and studies of conformation changes or association processes in macromolecular systems, a multi-angle laser light scattering instrument for SLS measurements is available. The instrument is a Dawn DSP-F MALLS photometer (Wyatt Technology Corp., Santa Barbara, California) equipped with a 5 mW He-Ne laser (632.8 nm). The intensity of the scattered light is measured using photodiodes at 18 different angles simultaneously. The instrument is connected to a gel permeation chromatography system for on-line molecular weight determinations in aqueous solvents but batch analysis may also be performed. (Sponsored by NFR.)

3.2.4 3D Light scattering instrument

(Contact person: Marc Obiols-Rabasa)

The instrument from LS Instruments is used for simultaneous dynamic and static light scattering with transparent and turbid samples. It incorporates the 3D cross-correlation technology for eliminating the contributions from multiple scattering. It is equipped with a 3D modulation unit, which implements the newest development to increase signal-to-baseline and leads to an almost four-fold improvement in the cross- correlation intercept compared to standard 3D technology. The instrument is equipped with a HeNe laser light source, wavelength $\lambda 0$= 632.8nm and a

maximum power of 35 mW. Samples can be measured in cylindrical glass cells (with a diameter of 3, 5 or 10 mm) or 10 mm square cells and placed in the temperature controlled index- matching bath. The scattered light is detected within an angular range of 15 to 140° by two efficient Avalanche Photo Diodes and processed by a Flex correlator in a 3D cross-correlation configuration. In aqueous samples we have access to scattering vectors $0.0034 \leq q \leq 0.025$nm-1. The apparatus is equipped with an upper sample goniometer to characterize non-ergodic samples.

3.2.5 Multi-angle 3D-goniometer system

(Contact person: Marc Obiols-Rabasa)

The instrument allows time-resolved measurements of dynamic and static light scattering in transparent and turbid samples using the technique of 3D cross-correlation at four angles simultaneously. The apparatus is equipped with a diode-pumped solid-state laser (wavelength $\lambda 0 = 532$ nm) with a maximum power of 200 mW. Samples can be measured in cylindrical glass cells (with a diameter of 3, 5 or 10 mm) or 10 mm square cells and placed in the temperature controlled index-matching bath. The scattered light is detected simultaneously at 4 angles within an angular range of 10 to 150° by two photomultiplier tubes at each angle, and processed in real time by a 8 channel Flex correlator in a 3D cross-correlation configuration. Thus four intensity correlation functions are obtained simultaneously, one for each scattering angle measured. In aqueous samples we have access to scattering vectors $0.0027 \leq q \leq 0.031$ nm-1.

3.2.6 Electrophoretic light scattering

(Contact person: Marc Obiols-Rabasa)

A Zetasizer Nano Z instrument from Malvern Instruments Ltd, Worshestershire, UK, is available for eletrophoretic mobility (or zetapotential) measurements in both aqueous and non-aqueous dispersions using M3-PALS technology. The required particle diameter ranges from 3.8 nm to 10 µm. A conductivity range from 0 to 200 mS cm-1 is required. The instrument is equipped with a 4 mW He-Ne laser (wavelength of 632.8 nm) with an automatic laser attenuator that allows for measurements at sample transmissions ranging from 100 % to 0.0003 %. The detection unit comprises an avalanche photodiode. The temperature range of the instrument is 2-90 °C.

3.2.7 Ultra small angle light scattering (USALS)

(Contact person: Marc Obiols-Rabasa)

The instrument is used for simultaneous dynamic and static light scattering at ultra- small angles using a CCD camera as a position sensitive 2D-detector. The scattered light is detected from 0.3o to 6o, corresponding to length scales from a

few hundred nanometers to a fraction of a millimeter. Time resolved static measurements can be performed with a time resolution of approx. 100 msec.

Multispeckle correlation functions are processed in real-time, thereby allowing measurements of a set of intensity autocorrelation functions at different q-values using measurement times that are comparable to the longest correlation time. A multitau correlation scheme is adopted (delay time space quasi-logarithmically), requiring thereby less data storage and processing time. This allows one to calculate time- and pixel-averaged correlation functions in real time. Multiple exposure times are used in order to optimize the mean intensity level for all scattering vectors. The instrument is equipped with a HeNe laser light source with a wavelength of 632.8nm and a maximum power of 35 mW. The sample is filled into square glass cells with path lengths ranging from 10 μm to 1 mm and placed in a temperature-controlled sample environment. The instrument is designed to study both ergodic and non-ergodic samples.

3.2.8 Diffusive wave spectrometer (DWS)

(Contact person: Marc Obiols-Rabasa)

The instrument is used for the characterization of extremely turbid samples and is equipped with a diode-pumped solid-state laser (wavelength of 660 nm) with a maximum power of 70 mW. The apparatus implements a “Two-Cell Echo Technique” which allows to cover a very large range of time scales while reducing measurement times down to only a few minutes even for slowly relaxing or solid-like (non-ergodic) materials. Samples are measured in square glass cells with path lengths of 1 – 10 mm and placed in a temperature controlled sample environment (15-70 oC). The scattered light is measured in transmission with two efficient Avalanche Photo Diodes and processed by a multi-tau/linear correlator using pseudo-crosscorrelation. Also possible are experiments in backscattering geometry and CCD camera-based multispeckle measurements. The instrument is controlled and data is analyzed with a powerful commercial software solution (LS-Instruments, Fribourg, Switzerland) which allows for combined correlation-echo measurements, single-, multi-speckle analysis, user defined multi-run scripts, online microrheology analysis and full data access.

3.2.9 Small/wide angle X-ray spectrometer, SAXS (Kratky system)

(Contact person: Anna Stradner)

This instrument combines an X-ray focusing optics with a block collimator which produces an intense, monochromatic primary beam. The primary beam is focused through the sample allowing fast measurements of the scattering pattern, even from samples with low contrast. The scattering signal is detected by a CCD camera for SAXS and a 2D imaging plate detection system for WAXS. The apparatus is implemented with a SAXSess camera using an X-ray generator (PANalytical, PW 3830) with a sealed copper tube. The X-ray generator offers a

maximum power of 4.0 kW and an operating range of 20-60 kV and 10-100 mA. A Göbel mirror and a Kratky block collimation system (line-shaped beam) is used to convert the divergent polychromatic X-ray beam into a focused line shaped beam of Cu-Kα radiation. Holders for liquid and solids are available. The instrument design makes it possible to investigate particles length scales from 0.25 nm (thanks to the wide angle extension system) up to 40 nm. Thus, q values range from ≤ 0.077 nm^{-1} (corresponding to a Bragg value ≥ 82 nm) up to ≈ 8 nm^{-1} (SAXS) and ≈ 29 nm^{-1} (SWAXS).

3.2.10 Small/wide angle X-ray spectrometer, SAXS (pinhole system)

(Contact person: Anna Stradner)

This is a fully automated and remotely controllable Small Angle X-Ray Scattering instrument. The x-ray source is a high brilliance microfocus sealed tube with shaped multilayer optics, yielding a monochromatic high intensity beam at very low power. The beam shaping is initially handled by the shaped multilayer, and then further collimated by 3 sets of 4-bladed slits. The beam path is evacuated by an oil-free high speed pump allowing full pump-down to clean operating pressures in 4 minutes. The sample area comes with an XY-theta goniometer for alignment and positioning of samples for both transmission and grazing incidence work. The scattering signal is detected by a state- of-the-art pixelized solid state detector (synchrotron style), combining the best of single photon counting, dynamic range and robustness. The motion of the detector allows the user to make measurements over a very large q-range. The integrated data management (with detailed system information being carried over in date-headers interpretable by the data-reduction software) facilitates the task of monitoring, data-collection, data-reduction and data-interpretation.

Sample holders/stages available:

- Versatile ambient plate for disposable capillaries
- JSP capillary stage with temperature control
- WAXS capillary stage with temperature control
- Flow-through cell

The available q range extends from ≈ 0.003 $Å^{-1}$ up to ≈ 2.5 $Å^{-1}$.

3.2.11 Super ADAM – An Advanced Neutron Reflectometer for the Analysis of Materials (CRG Instrument located at ILL, Grenoble, France)

(Contact persons: Tommy Nylander (Physical Chemistry) and instrument responsible at ILL, Alexei Vorobiev)

Super ADAM is operated jointly by Uppsala University, Lund University and Linköping University and financed by Swedish Research Council. This reflectometer, which currently is the only operating Swedish Neutron instrument,

for the analysis of materials is an angle dispersive fixed wavelength machine with horizontal scattering geometry. The instrument has two operation modes: A high flux option (focusing monochromator made of intercalated graphite), mainly dedicated for soft matter research, and a lower flux option but with an improved Q resolution. It offers unique possibilities especially for measurements on magnetic samples due to the high resolution and the possibility of high polarisation and an accurate polarisation analysis.

3.3 NMR

3.3.1 NMR

(Contact person: Daniel Topgaard)

Bruker Avance II spectrometers operating at 200 and 500 MHz are available at Physical Chemistry. Both spectrometers are equipped for high-performance diffusion studies. The 500 MHz instrument has accessories for microimaging, solid-state, and high-resolution magic-angle spinning experiments. (Sponsored by VR/KFI.)

Bruker Avance II 500

Magnet: 11.7 T / 500 MHz, 54 mm UltraShield

Probes: TXI 5mm XYZ-Gradient (1H/13C/15N), BBO 5mm XYZ-Gradient (31P-15N/1H), multinuclear DIF-30 and MIC-5 (1H, 2H/1H, 7Li/1H, 23Na/1H, 13C/1H, 31P/1H), H/X CP-MAS 4mm (1H/31P-15N), E-free CP-MAS 4mm (13C/31P/1H), H/X CP-MAS 2.5mm (1H/31P-15N), TXI HR-MAS 4mm Z-Gradient (1H/13C/31P)

Bruker Avance II 200

Magnet: 4.7 T / 200 MHz, 89 mm

Probes: BBO 10mm (31P-15N/1H), DIF-25 5mm (1H)

3.4 Microscopy

3.4.1 Optical microscopy

(Contact person: Emma Sparr)

The division has a Zeiss Axioplan Universal microscope equipped with differential interference contrast and a High Resolution Microscopy Camera AxioCam MRm Rev. 3 FireWire, Illuminator HBO 100 as well as with a 100W mercury short-arc lamp and a system of filters to allow the fluorescence microscopy observations. The microscope is further equipped with a high-sensitivity SIT video camera and an image processor, AxioVision 4 together with the Macintosh-based image analysis software. (Sponsored by FRN and Crafoord Foundation.)

3.4.2 Confocal microscopy

(Contact person: Peter Schurtenberger)

This instrument allows recording brilliant, high-resolution images to illustrate morphological features of fixed or slowly moving samples as well as monitoring high- speed dynamic processes by fast time-course studies. The equipment is implemented with five true spectral confocal channels simultaneously with a prism spectrometer for high transmittance and tunability. Illumination regimes are switchable in microseconds for fast dynamic measurement and the beam can be split instantly for new dyes or laser lines. The apparatus mounts up to 2 channels for spectral FLIM allowing resolved fluorescence life-time imaging and 3 laser lines: a HeNe laser (543 and 633 nm), an Argon laser (458, 476, 488 and 514 nm) and an IR (800 to 1100 nm). A fast resonant scanner (50 frames/sec at 512 x 256 pixels) and a non-resonant scanner (1400 lines/sec) are also implemented. The objective is mounted on a piezo-stage for fast z-scanning (50 frames/sec at 256 x 128 pixels).

In 2012, the system was upgraded with SMD Detection package FCS (high quantum efficiency, 2 APD). The system acquires and analyzes FCS and FCCS (Fluorescence Cross-Correlation Spectroscopy) data. Both methods focus on quantitative analysis of transport and binding processes. (Sponsored by the Knut and Alice Wallenberg Foundation.)

3.4.3 (Cryo) Transmission electron microscopy

(Contact person: Viveka Alfredsson)

The Philips CM120 BioTWIN Cryo located in the national Centre for High Resolution Electron Microscopy (nCHREM) at KILU is a microscope dedicated for cryo-imaging. It is operated at 120 kV. The BioTWIN objective lens gives high contrast and the resolution is 0,34 nm. The microscope is equipped with an energy filter imaging system (Gatan GIF 100) and digital multiscan CCD cameras (Gatan 791). There is an Oxford CT 3500 Cryoholder and transfer system. We have secured means, via infrastructure grants from the Science Faculty and LTH, to replace the Philips microscope with a new instrument. In 2016 a 200 kV FEG instrument, equipped for cryoimaging and tomography, will be installed.

At nCHREM there are two other transmission electron microscopes and a scanning electron microscope. More information about nCHREM can be found at: The National Center for High Resolution Electron Microscopy (nCHREM).

3.5 Calorimetry

3.5.1 Differential scanning calorimeter (DSC)

(Contact person: Emma Sparr)

A VP-ITC Differential Scanning Microcalorimeter with a Pressure Perturbation Calorimetry accessory from MicroCal (GE Healthcare) was purchased in 2010. This is a sensitive microcalorimeter for samples in solution. The instrument has an active cell volume of ca 0.5 ml, and it operates for temperatures between –10oC to +130oC. The cells consist of non-reactive Tantalum 61TM for excellent chemical resistance, and they are fixed-in-place for reproducible ultrasensitive performance with low maintenance. The system uses a Peltier element for precise temperature control. It allows for user selectable temperature scan rates (0oC to 90oC per hour upscans), allowing studies of fast or slow transition processes. (Sponsored by the Knut and Alice Wallenberg Foundation.)

3.5.2 Isothermal titration calorimeters (ITC)

(Contact person: Emma Sparr)

* A VP-ITC Isothermal Titration Microcalorimeter from MicroCal (GE Healthcare) was purchased in 2010. This is an ultrasensitive microcalorimeter for samples in solution. The instrument has an active cell volume of ca 1.4 ml, and it operates for temperatures between 2ºC to 80ºC. The cells consist of non-reactive Hastelloy→ for excellent chemical resistance, and they are fixed-in-place for reproducible ultrasensitive performance with low maintenance. The system includes precision liquid delivery system for accurate and reproducible injections and user-selectable mixing speeds to match sample conditions. (Sponsored by the Knut and Alice Wallenberg Foundation.)

* Isothermal titration microcalorimeter 2277 TAM Thermal Activity Monitor System.

3.5.3 Reaction calorimeter

(Contact person: Ola Karlsson)

The energy released as heat by a process is directly proportional to the rate of reaction and by monitoring the reaction in a calorimeter detailed kinetics can be revealed. In 2011 we got a Chemical Process Analyser CPA202 from Chemisens. It is a high precision factory pre-calibrated calorimeter made in Hastelloy C276 with a useful volume of 10 – 180 ml, which can be continuously varied during experiments. The temperature range for experiments is -50°C to +200°C and it is possible to operate in a pressure range from vacuum up to 20 bars. The temperature resolution for an experiment is 0.001°C and the power resolution is 0.001 Watt in the standard reactor and in the so called HighSens Reactor, which will be used for e.g. adsorption kinetics, crystallization, dissolution of tablets and micellization it

will be possible to perform studies with a power resolution of 0.1mW at a volume of 10 – 180 ml. (Sponsored by the Knut and Alice Wallenberg Foundation.)

3.5.4 Sorption calorimeter

(Contact person: Emma Sparr)

A double twin isothermal microcalorimeter for the simultaneous determination of sorption isotherms and differential sorption enthalpies of vapors on solids. The instrument was developed in-house by L Wadsö and N Markova.

3.6 Rheology

3.6.1 Rheometers

(Contact person: Ulf Olsson)

A Physica UDS 200 stress controlled rheometer. Various cone and plate geometries with Peltier temperature control. A Couette geometry and a double gap measuring device, both in stainless steel, temperature controlled by circulated thermostated water. An Anton Paar MCR301 stress controlled rheometer equipped with additional transparent tools (plate-plate and cone and plate geometries) to allow for simultaneous small angle light scattering or microscopy detection.

3.6.2 Advanced rheometric expansion system (ARES)

(Contact person: Peter Schurtenberger)

The Advanced Rheometric Expansion System (ARES) is a true strain-controlled instrument, where the application of strain and the measurement of stress are separated. The sample is subjected to either a dynamic (sinusoidal) or steady shear strain deformation, and then the resultant torque expended by the sample in response to this shear strain is measured. The motor applies shear strain; the transducer measures torque. Strain amplitude and frequency are set by the operator, with the actual sample deformation determined by the measured motor, and transducer, displacement.

The instrument is implemented with the transducer 1 K FRT (torque range 0.004 – 20.0 g•cm and normal force range 2.0 – 2000.0 gmf). The operational temperature range is between -30oC and 150oC with temperature stability at thermal equilibrium of ±0.1 oC, which is controlled with a Peltier system. The actual available geometries are: cone and plate (50 mm, 0.04 rad, 25 mm, 0.04 rad), plate and plate in (50 mm) and couette (16.5 mm bob, 17 mm cup and 32 mm bob and 34 mm cup).

3.7 Spectrophotometers

3.7.1 UV-Vis spectrophotometer

(Contact person: Maria Södergren)

A Cary 300 Bio UV-Vis spectrophotometer with 4-position automatic cell holder with temperature sensor, stirrer and connected water bath was purchased in 2007.

3.7.2 Fluorescence spectrophotometer

(Contact person: Emma Sparr)

A Cary Eclipse Fluorescence spectrophotometer for fluorescence, phosphorescence or chemi/bio luminescence was purchased in 2007. The instrument includes both 4-position automatic cell holder with temperature sensor, stirrer and connected water bath as well as a microplate reader. Equipment also include the automated polarizer accessories. (Sponsored by the Crafoord foundation.)

4 Collaborative Research Programs

4.1 Organizing molecular matter

(Contact person: Emma Sparr)

In 2005, the Swedish Research Council (VR) launched a call for proposals of collaborative research efforts from strong Swedish research environments with the prospect of long-term (10 years) "Linnaeus support". A group of nineteen senior researchers from the divisions of Physical Chemistry, Theoretical Chemistry and Biophysical Chemistry at the Department of Chemistry, Lund University, responded with a proposal called Organizing Molecular Matter (OMM). The program was accepted and was operational from June 2006, with a funding of 7.5 MSEK from VR and 1 MSEK from Lund University. The OMM research program, which can be found together with accounts of ongoing research at the OMM website (http://www. omm.lu.se), focuses on intermolecular interactions and their manifestations in a liquid environment. The interplay between theory and experiment is an essential feature of the program. The theoretical basis for the description of intermolecular interactions and their consequences are treated using quantum chemical calculations and statistical mechanical simulations. Carefully selected model systems are studied experimentally, and an important part of the experimental studies is an ongoing improvement of methods. A final part of the program is to apply the understanding obtained in the basic studies for solving applied problems both in the biophysical/molecular biology field and in the industrial area. By the end of 2010, a total of 23 new PhD and postdoctoral projects had been initiated within OMM, and each of these projects typically involves two or more OMM scientists. OMM also contributes substantially to the salaries of four young senior scientists. In addition, OMM organizes a series of weekly seminars, occasional workshops, and two annual meetings.

4.2 European Soft Matter Infrastructure (ESMI)

(Contact person: Peter Schurtenberger)

Free access to soft matter infrastructure, synthesis facilities, first-class instrumentation and a fast supercomputer is offered by the new EU project ESMI. ESMI consists of three main parts:

- TransNational Access - ESMI provides (free of charge, travel and accommodation included) access to the offered infrastructure (full range of synthesis facilities, a comprehensive set of specialized experimental techniques, fast supercomputer and theoretical support for data interpretation) to researchers or research teams. An Online Proposal Submission System is available under the ESMI web portal. Experimental access will be coordinated through Physical Chemistry (Peter Schurtenberger)

- Networking: A dissemination and educational plan has been implemented to foster a culture of cooperation between research infrastructures and scientific communities
- Joint Research Activities - A number of research projects are funded to improve the existing infrastructure.

4.3 SSF – ”Porous surface layers through polymer-assisted deposition”

(Contact person: Håkan Wennerström)

This project started in July 2009 and is a five-year research programme financed by the Swedish Foundation for Strategic Research (SSF). The goal of the program is to develop a method for a controlled deposition of mesoporous colloidal particles on surfaces and to apply the method on three types of porous particles. The basic strategy is to gradually destabilize an initially stable colloidal dispersion to achieve surface deposition rather than bulk aggregation. For this we use a potentially phase separating polymer to achieve colloidal stability/instability. The transition stability-instability should be smooth, which allows for an ordered equilibrium deposition layer. In one project we model theoretically the process to identify useful tuning parameters. In one experimental project flat mesoporous silica particles are deposited on a surface to give micrometer thick layers with pores of well defined size and orientation. Such layers can be used for separating small solutes from larger ones through a diffusional membrane transport. Another application is in tapes with a graded porous layer to be used as precise meters for relative humidity. In a third project we deposit porous liquid crystalline particles. Such particles can be loaded with an enzyme producing an enzymatically active surface coating. The fourth project aims at synthesizing soft mesoporous gel particles through in situ polymerization. In a surface layer of the particles the porosity can respond to changes in the properties of the bulk liquid such as pH or salt content. Porous responsive surface layers have a large potential in drug formulation. (L. Piculell, P. Linse, V. Alfredsson, T. Nylander and H. Wennerström.)

4.4 Division of Surface and Materials Chemistry of the Swedish Chemical Society

(Contact person: Viveka Alfredsson)

The Division of Surface Chemistry of the Swedish Chemical Society was founded in 2001 to promote contacts between chemists interested in surface and colloid chemistry.

From 2011, the scope of the division was widened to include also materials chemistry.

The main activity of the Division is to organize an annual conference. Viveka Alfredsson is serving as member of the board.

4.5 NordForsk Network

(Contact person: Tommy Nylander)

Nordic Milk Science Initiatives, 2008-2011 (NordicMilk Network). Research within dairy science has a long tradition in the Nordic and Baltic countries and the level of the research has been on high international standard. Recent research has revealed in cow's milk many protective components and their derivatives displaying a range of bioactivities. The research has been focused on product and process development directly related to the traditional use of the milk raw material. This also involves health and nutritional aspects as well as linking the genetic variants of the milk components to the product quality. This project joins multidisciplinary research groups from five Nordic countries and two Baltic countries who are working on milk compounds related to health and technological aspects. This project will join high know-how in chemical, analytical, technological, structural, in vitro studies and human clinical studies related to milk compounds.
https://portal.mtt.fi/portal/page/portal/www_en/Projects/Nordicmilk

4.6 SoftComp

(Contact person: Peter Schurtenberger)

Softcomp is a Network of Excellence (NoE) with the aim to establish a knowledge base for an intelligent design of functional and nanoscale soft matter composites. Since December 2009 it has a durable structure organized as a Consortium, which is self- financed by the partners. It supports research visits between partner institutions, and organizes and supports a number of schools, lab courses, workshops and conferences.

4.7 Strategic Research Areas and Lund University

nmC@LU is an interdisciplinary research environment in nanoscience. One focus of the multi-disciplinary Nanometer Structure Consortium at Lund University (http:// nano.lth.se) is on materials science and synthesis. Viveka Alfredsson, Tommy Nylander, Ulf Olsson are associated with this program. Multipark is a translational program that ranges from pre-clinical research to studies on the life situation of patients with Parkinson's disease (www.med.lu.se/multipark). Emma Sparr is associated partner in this program, participating in subproject dealing with biophysical studies of protein-membrane interactions.

4.8 EU FP7-PEOPLE-2013-ITN – BIBAFOODS Network

(Contact person: Tommy Nylander)

This project was granted during autumn 2013 and started 1 February 2014. The "BIopolymer BAsed FOOd Delivery Systems" (BIBAFOODS) network will train young researchers for the advancement of food science and technology, by providing them with the complementary skills necessary to develop the future sustainable food industry and entrepreneurial skills crucial for creating biotechnological food oriented start-up companies. This collaborative training network will combine the complementary training capabilities of each individual partner institution to improve the trainees' chances for employment and promote health and welfare in the EC by providing the capability to develop novel functional foods. The scientific focus of the research training is on colloidal delivery systems to protect and deliver active components via foods, resulting in novel functional foods. The development of these systems is to be based on only food-grade ingredients and upon economical feasible processes. The hypothesis is that the materials and coatings can be made responsive to the external chemical conditions and therefore suitable for controlled releases targeted at a desired stage during food processing or at a specific point during digestion of the food, e.g. in the intestinal tract. This will involve probiotic bacteria and enzymes that are liberated and allowed to be active in a controllable way. The ultimate successful materials ensure stability of the active component during long term storage prior to food production, during food production or during digestion, but at the same time liberating the active component at the right point. The behaviour and interaction of the delivery systems will be studied by simulation of gastric and intestinal conditions and by implementation in food production and formulation into probiotic products. BIBAFOODS will train 14 young researchers distributed among 11 industrial and academic partners, among them Physical Chemistry, Lund University.

4.9 Avancell

(Contact person: Ulf Olsson)

Avancell is a research network with focus on cellulose involving scientists from Södra Skogsägarna, Swerea IVF, Lund University, Chalmers and Coimbra University. With combined efforts and research collaborations, the network focuses on the dissolution and regeneration of cellulose.

4.10 Biocatalytic functionalisation of hemicellulose from waste (BIOFUNC)

(Contact persons: Henrik Stålbrand (Biochemistry) and Tommy Nylander (Physical Chemistry))

Softwood hemicellulose (galactoglucomannan, GGM) is one of Sweden's major renewable resources that make up 25% of the wood. GGM is, however, currently discarded in industrial waste-streams and its potential is not sufficiently explored. In BIOFUNC we will develop sustainable processes to substitute GGM structure and thereby transform it to a versatile and excellent renewable resource for novel high-performance products with added value. For this purpose we will develop new biotechnical processes for GGM recovery and enzyme-aided conversion to added value products that replace existing non-renewable products, but also have entirely novel added functionality. The outcome will be novel surfactants and a new family of polymers with special functions (e.g. controlled degradability, cellulose/wood/surface adhesiveness, acrylate latex/emulsion stabilisation). Thus the enzymatic route enable production of these high-value GGM-derivatives from GGM recovered from a low-value stream. This framework project is funded by Swedish Strategic Research and coordinated by Prof. Henrik Stålbrand (Biochemistry).

4.11 Development of a multi-channel isothermal microcalorimeter for monitoring of the activity of living organisms.

(Contact person: Ingemar Wadsö)

For more than 60 years isothermal microcalorimetry has been used in measurements of the rate of heat production in living organisms. Results are often used as a measure of their "activities" and it has repeatedly been predicted that such techniques will become useful in many areas of applied biology, e.g. in the pharmaceutical industry and in clinical laboratories. However, the low sample throughput of available instruments has prevented their use in practical work. In 1999 a joint project with Dan Hallén (at the pharmaceutical company Pharmacia & Upjohn, Stockholm) was initiated. The aim was to develop a multi-channel isothermal microcalorimeter for the simultaneous measurement of many samples, thus leading to an increased sample throughput.

A 48-channel instrument was designed and built in Lund. Results of test experiments carried out in Stockholm were very satisfactory; the detectability approached 10 nW and the 24 h baseline stability was better than 50 nW. In 2004 Hallén formed a company, SymCel, for the development of a commercial version of the Lund instrument. The close contact with Lund continued until Hallén's premature death in 2011. SymCel was reconstructed and the development work continued. However, the contacts between SymCel and Lund became marginal

until the development work on the commercial instrument system was almost completed in 2014. Its 48-channel microcalorimeter was essentially the same as the Lund instrument, whereas electronics and other peripherals were much improved. The properties of the instrument system are presently investigated by scientists from Sweden (I. Wadsö, J. Suurkuusk and M. Jansson) and Switzerland (O. Braissant and T. Wenzler). The study, (coordinated by I. Wadsö) is expected to be completed in early 2016.

4.12 Anisotropic Forces in Colloid Chemistry

(Contact person: Peter Schurtenberger)

The main objective of this multi-investigator project is to explore generic phenomena caused by anisotropic colloidal interactions in dense suspensions. Such interactions are of great relevance in as disperse fields as materials science, nanotechnology and many branches of molecular biology. This objective will be accomplished by engineering, synthesizing and assembling concentrated soft matter systems of both artificial and biological origin, which will then be measured and analyzed using state of the art experimental and theoretical tools. The main emphasis is on dynamic properties, where there is a clear lack of knowledge in a rapidly expanding area of science. We focus on 3 main goals: (i) to understand how anisotropic inter-particle interactions influence the self-assembly and diffusion of complex colloidal particles in dense suspensions; (ii) to understand and exploit anisotropic interactions of particles, of synthetic or biological origin, with lipid membranes; and (iii) to use the thus generated knowledge to unravel generic features of the dynamics of macromolecules and particles of biological origin in dense solutions such as those found in the interior of living cells. The project combines several parallel research efforts connecting systems of synthetic and biological origin to highlight features of general applicability, and is also based on an extensive international collaboration involving several key research groups. We combine the toolbox of experimental and theoretical colloid chemistry with state-of-the-art characterization techniques, computer simulations and molecular biology methodologies. (co-PI's: Johan Bergenholtz, Jerôme Crassous, Per Linse, Ulf Olsson, Peter Schurtenberger, Emma Sparr, Anna Stradner, Håkan Wennerström; international collaborators: Jan Dhont (Forschungszentrum Jülich, Germany), Gerhard Gompper (Forschungszentrum Jülich, Germany), Christos Likos (University of Vienna, Austria), Albert Philipse (University of Utrecht, Netherlands), George Thurston (Rochester Institute of Technology, USA).)

4.13 MoReLife - Molecular Recognition in Life

(Contact person: Malin Zackrisson Oskolkova)

The network aims to promote development of competences and infrastructures. MoReLife participates in and arranges symposia, discussion meetings and retreats to increase dialogue contribute to establishment and development of key infrastructures. See web page: http://www.med.lu.se/morelife

5 Conferences, Travels and Seminars

Solmaz Bayati gave an invited seminar at the Department of Chemistry, University of Rome ”Sapienza” during her short-time stay. Solmaz presented a poster at Colloids and surfaces in biology and biomaterials – A symposium on surface and material chemistry in Uppsala, Sweden.

Maxime Bergman presented a poster at the International School of Physics “Enrico Fermi” Course 193 - Soft Matter Self-Assembly in Varenna, Italy, and also presented a poster at the NanoLund Annual Meeting in Lund, Sweden.

Saskia Bucciarelli presented a poster at the Workshop on recent Developments In Non-Equilibrium Physics “Luxembourg out of Equilibrium” in Luxembourg, Luxembourg. She also gave a presentation at the 29th annual conference of the European Colloid and Interface Society (ECIS) in Bordeaux, France.

Jérôme Crassous gave a talk at the IACIS 2015 47th Conference of the German Colloid Society, Mainz, Germany.

Aleksandra Dabkowska gave a plenary lecture at the Neutron and Muon Users Meeting in Leicestershire, UK and an invited seminar at the Laboratoire de Génie Chimique Université de Toulouse, France. She also gave oral presentations at the VI European Conference on Neutron Scattering in Zaragoza, Spain as well as the Materials Research Society (MRS) Spring Meeting in San Francisco, USA.

Tommy Garting gave a poster presentation at Jülich Soft Matter Day 2015 in Bad Honnef, Germany.

Peter Holmqvist gave an oral presentation at the 15th Conference of International Association of Colloid and Interface Science (IACIS) in Mainz, Germany.

Jasper Immink presented a poster at the Enrico Fermi Summer School, Soft matter Self-assembly.

Peter Jönsson gave invited lectures at the conferences: 1st Imaging for Life (Sweden, Lund), Nanoscience for Human Health (Sweden, Gothenburg), and Colloids and Surfaces in Biology and Biomaterials (Sweden, Uppsala).

Weimin Li gave an oral presentation at the European Colloid and Interface Society 2015 in Bordeaux, France, and attended as COST member.

Ruiyu Lin presented a poster at the conference of 9th International mesostructured Materials Symposium in Brisbane, Australia.

Björn Lindman was a co-chairman of the International Workshop on Polyelectrolytes in Chemistry, Biology and Technology in Singapore and also gave a lecture on this meeting. He received the triannual Life-Time Achievement Award of IACIS (International Association of Colloid and Interface Scientists) at the IACIS Conference in Mainz, where he also gave a plenary lecture. He gave a plenary lecture at the conference “Smart and green interfaces: Fundamentals and diagnostics” in Sofia, Bulgaria. He also attended the 27th Conference of the European Colloid and Interface Society (ECIS) in Bordeaux, France and gave a

lecture at Université de Lorraine, Nancy.Furthermore, Björn Lindman was Guest Professor at the Mid-Sweden University, FSCN - Fibre Science and Communication Network, and at Nanyang Technological University, Singapore.

Najet Mahmoudi gave an oral presentation entitled “Connecting structure and mechanics in arrested spinodal decomposition protein gels” at the “Arrested Gels: Dynamics, Structure & Applications Meeting” in March 2015 (Cambridge, UK).

Janne-Mieke Meijer gave an oral presentation at the 16th Conference on Small Angle Scattering (SAS 2015), in Berlin, Germany.

Adriana Mihut gave a talk at the IACIS 2015 47th Conference of the German Colloid Society, Mainz, Germany.

Linda Månsson presented posters at the conference Nanoparticle Synthesis and Assembly: Faraday Discussion 181 in Chicago, USA, at the International School of Physics “Enrico Fermi” Course 193 - Soft Matter Self-Assembly in Varenna, Italy, and at the NanoLund Annual Meeting in Lund, Sweden.

Emelie Nilsson presented a poster at the conference 9th International Mesostructured Materials Symposium in Australia, Brisbane.

Tommy Nylander gave an oral presentation at the 15th Conference of the International Association of Colloid and Interface Scientists, Mainz, Germany; European Conference on Neutron Scattering, Zaragoza, Spain and invited keynote talks at the Research Neutron Source Heinz Maier-Leibnitz (MLZ) user meeting, Munich, Germany; Super ADAM CRG inauguration meeting ILL, Grenoble, France; Conference on Green Biopolymers and Energy Conversion and Storage, Linköping University, Sweden; European Colloid and Interface Society Meeting, Bordeaux, France; International Chemical Congress of Pacific Basin Societies (Pacifichem) 2015, Honolulu, Hawaii, USA and a plenary talks at the RACIRI (Röntgen-Angström-Cluster (RAC) and the Ioffe-Röntgen-Institute (IRI)) summer school, Rügen Germany; International Symposium “Hierarchical Dynamics in Soft Materials and Biological Matter”, Kyoto, Japan. He also gave invited talks at University of Alberta, Edmonton, Canada; Novozymes, Bagsvaerd, Denmark; Tohoku University, Sendai, Japan; Federal University of Rio Grande do Sul, Porto Allegre, Brasil and a lecture at the Bibafoods course at Universidad de Alcalá, Alcalá de Henares, Spain.

Sofi Nöjd gave an oral presentation at the 5th conference of the International Association of Colloid and Interface Scientists in Mainz, Germany, and presented a poster at the 29th conference of the European Colloid and Interface Society, Bordeaux, France.

Marc Obiols-Rabasa gave an oral presentation at the VI European Conference on Neutron Scattering (ECNS) in Zaragoza, Spain, and a poster presentation at the 16th International Conference on Small-Angle Scattering (SAS) in Berlin, Germany.

Ulf Olsson was invited to present a Distinguished iNANO Lecture at Aarhus University and also gave an invited lecture at the 48th Heyrovsky Discussion:

Progress in Electrochemistry at Liquid-Liquid Interfaces and Liquid Membranes, in Trest, Czech Republic. He also attended the Nordic workshop Scattering from Soft Matter in Stockholm, and gave an invited lecture at the SoFun school "Soft Matter for Functional Materials" in Carcans, France, in connection to the ECIS conference in Bordeaux.

Antara Pal presented a poster at the NanoLund Annual Meeting 2015 in Lund, Sweden and visited Professor Wilson Poon's lab in University of Edinburgh, UK, for an ESMI granted experimental project.

Lennart Piculell gave an invited lecture at the Workshop on Polyelectrolytes in Chemistry Biology and Technology in Singapore and a keynote lecture at the 29th conference of the European Colloid and Interface Science (ECIS) in Bordeaux, France. Furthermore, Lennart Piculell made an invited 2.5 week visit at UNICAMP (the University of Campinas) in Brazil. During the visit, he gave invited lectures at UNICAMP, at PUC-Rio (Pontifícia Universidade Católica do Rio de Janeiro) and at the University of São Paulo.

Karin Schillén gave an invited seminar at Department of Fibre and Polymer Technology, The Royal Institute of Technology KTH, Stockholm, Sweden. She attended the conference Colloids and surfaces in biology and biomaterials – A symposium on surface and material chemistry in Uppsala, Sweden. Karin was at a 2-week research visit at the Department of Chemistry, University of Rome "Sapienza".

Julien Schmitt presented a poster at the IMMS9 (International Mesostructured Material Symposium 9) in Brisbane, Australia and gave an oral presentation at the SAS 2015 (16th Conference on Small Angle Scattering) in Berlin, Germany.

Peter Schurtenberger gave invited lectures at the following international conferences, workshops and summer schools: the Workshop on "Arrested Gels" – Cambridge, UK, the Faraday Discussion on "Nanoparticle Synthesis and Assembly" – Chicago, USA, the Jülich Research Alliance on Soft Matter Science (JARA-SOFT) Opening Ceremony – Jülich, Germany, the SoftComp Annual Meeting – Ancona, Italy, the Workshop on "Advanced Light Scattering Technologies" – Fribourg, Switzerland, the International School of Physics "Enrico Fermi" on "Soft Matter Self-Assembly" – Varenna, Italy, and the Jülich Center for Neutron Scattering Workshop "Neutron Scattering on Nano-Structured Soft Matter: Synthetic- and Bio-Materials" – Tutzing, Germany. Peter Schurtenberger also gave an invited seminar at the Adolphe Merkle Institute, Fribourg, Switzerland.

Emma Sparr gave invited talks at TU Berlin (Germany) and Laboratoire de Génie Chimique. Toulouse. She also presented invited lectures at the Skin days in Malmö and at the interdisciplinary PhD student course SkinResQ in Gothenborg.

Anna Stradner gave a keynote lecture at the ECNS2015 (VI European Conference on Neutron Scattering) in Zaragoza (Spain).

Daniel Topgaard gave a plenary lecture at the 13th International Conference on Magnetic Resonance Microscopy, Tächnische Universität München, Germany, and invited lectures at the 36th Danish NMR meeting, Lund, Sweden; Workshop on diffusion phenomena in NMR, Karlsruhe Institute of Technology, Germany; and Microimaging inauguration, Swedish NMR Center, Gothenburg University, Gothenburg, Sweden.

6 External professional activities

Viveka Alfredsson served as the Faculty Opponent for Arto Ojuvo at Stockholm University.

Peter Jönsson was on the advisory board for the research graduate school Advanced Microscopy Research Environment (ADMIRE) at Lund University, Sweden.

Ola Karlsson was chair of the examination committee when Annika Weiber's Ph.D. thesis, "Aromatic Polymers Functionalized with Anionic and Cationic Groups for Ion Exchange Membranes", was publicly defended at LTH, Lund, Sweden.

Björn Lindman was on the Advisory or Editorial Boards of Advances in Colloid and Interface Science, Current Opinion in Colloid & Interface Science, Fine Chemicals, Colloid&Polymer Science, and Journal of Dispersion Science and Technology. Björn Lindman is a member of The Royal Swedish Academy of Engineering Sciences, of The Royal Swedish Academy of Sciences and of the The Royal Physiographic Society in Lund as well as foreign member of science academies in Portugal and Romania. He is "docent" at Åbo Akademi, Finland. He is cofounder and honorary member of the European Colloid & Interface Society (ECIS).

Tommy Nylander served as thesis examiner (opponent) for the PhD theses of Xin Wang, Royal Institute of Technology - KTH, Stockholm; Niko Penttinen, University of Eastern Finland, Joensuu, Finland. He was member of the evaluation panel for beam time applications NIST Centre for Neutron Research, Gaithersburg, USA and chaired the panel for Biology at MLZ, Munich. Tommy Nylander was also a visiting professor at Institute of Chemistry, Chinese Academy of Sciences, Beijing, China.

Ulf Olsson was board member of the MAX IV Laboratory, and also served on the Science Advisory Committee of the Swiss spallation neutron source, SINQ. He is the spokesperson for the CoSAXS beamline project at MAX IV.

Lennart Piculell is a section editor for the Polyelectrolytes section of Current Opinion in Colloid and Interface Science and a member of the international organizing committees of the biannual International Polyelectrolyte Symposia. He is also a member of the AkzoNobel Nordic Prize Award Committee.

Karin Schillén served at two PhD thesis defenses during the year; she was the chairman and the deputy member of the PhD grading committee at the defense of Charlotte Gustavsson at the Division of Physical Chemistry and she was a member of the PhD grading committee of Christian Porsch at the Department of Fibre and Polymer Technology, The Royal Institute of Technology KTH, Stockholm, Sweden. She is the head teacher in Physical Chemistry. Karin was elected to be a

member of the Surface and Material Section at the Swedish Chemical Society at the annual meeting of the section.

Peter Schurtenberger was a member of the Chocolate Scientific Advisory Council of Mars Chocolate UK Ltd., member of the international expert committee of the PRIDE program of the Luxembourg National Research Fund, evaluator for the Excellence Initiative of the Government of Spain, chairman of the Scientific Review Board of the European Soft Matter Infrastructure ESMI, coordinator of the Experimental Infrastructure and member of the Program Executive Committee of ESMI, member of the Network Governing Board and chairman of the Experimental Platform of the European Network of Excellence SoftComp, member of the ESS SANS Scientific Advisory Panel, member of the MAX IV CoSAXS Beamline Scientific Advisory Panel, member of the International Program Committee of the European Conference on Neutron Scattering ECNS in Zaragossa, Spain, 2015, and he was on the Editorial Board of the journals Colloid & Polymer Science and Soft Matter, and Section Editor of Current Opinion in Colloid and Interface Science. He is a member of the Royal Swedish Academy of Sciences, the Royal Swedish Academy of Engineering, the Royal Physiographic Society of Lund, a fellow of the British Royal Society of Chemistry, and an honorary member of the European Colloid and Interface Society (ECIS).

Emma Sparr was in the panel for Marie Skłodowska Curie International Career Grant (INCA) evaluation at the Swedish Research Council (VR). She was a member of the election committee for the board of the Swedish Research Council and at the Swedish Chemical Society. Emma Sparr was chairing the panel for electing new members to the Young Academy of Sweden 2015. Emma Sparr served on the PhD grading committee for Boris Kharkov (KTH) and Karin Magnusson (Linköping University). At Lund university, Emma Sparr was the director of the Linnaeus center OMM.

Anna Stradner was a member of the Program Executive Committee of the European infrastructure project ESMI (European Soft Matter Infrastructure), for which she also served as the Gender Officer and as the chairperson of the ESMI Gender Review Panel. Anna Stradner organized an international one-day Symposium taking place in Lund on ”Wormlike Micelles, Equilibrium Clusters and Colloidal Molecules: 35 Years of Soft Matter and Scattering” with 12 invited speakers and more than 90 participants. Anna Stradner served as a reviewer for the US-Israel Binational Science Foundation and as a guest editor for a special issue on ”Biocolloids and Colloids in Biology” in Colloids and Surfaces B: Biointerfaces.

Daniel Topgaard served as examiner for the PhD thesis of Mikhail Zubkov, Western Sydney University, Australia.

7 Outreach activities

Emma Sparr was a teacher at a Summer research school for high school pupils "Forskarmöten" (arranged by the young academy of Sweden). Emma Sparr presented her research to L'ORÉAL and GSK scientists. She also gave popular science seminars within the seminars at the NMT days for upper secondary school pupils, and she performed experiments together with primary school pupils at Vårfruskolan.

8 Awards

Aleksandra Dabkowska was awarded the B.T.M. Willis by the joint committee of the Institute of Physics (IOP) Neutron Scattering Group and the Faraday Division of the Royal Society of Chemistry (RSC).

Björn Lindman was awarded the IACIS "Life-time achievement award" in Mainz, Germany, in May.

9 Distinctions

Peter Schurtenberger is elected as a member of the Royal Swedish Academy of Engineering and elected as a member of the Royal Physiographic Society of Lund.

10 Honorary Doctorate at Lund University

Our long-time friend and collaborator, Professor Yeshayahu (Ishi) Talmon, Wolfson Chair in Chemical Engineering at Technion in Haifa, Israel, received an Honorary Doctorate at the Faculty of Science and participated in the doctoral conferment ceremony in Lund Cathedral in May.

11 Courses and Teaching

Members of the Division of Physical Chemistry are involved in a number of undergraduate courses and a number of our graduate students serve as teaching assistants in the laboratories. Karin Schillén is the head teacher in Physical Chemistry with the responsibility of organizing the teaching given by the members of the Division of Physical Chemistry.

The first year of chemistry studies at the Department of Chemistry consists of four 5-week chemistry courses (which are given both during the fall and the spring semesters), one 10-week course in Mathematics and one 10-week course in Physical Chemistry. In the first basic course in General and Analytical Chemistry during the spring semester, Malin Zackrisson Oskolkova and Viveka Alfredsson were leading exercises and question hours, whereas Peter Jönsson did the corresponding teaching during the fall semester together with Daniel Topgaard who gave the lectures. The topic of the first-year Physical Chemistry course is thermodynamics and quantum mechanics and it is based on the textbook of P. W. Atkins and J. De Paula "Atkins' Physical Chemistry". Karin Schillén is the main teacher and course responsible for this course and she gave the lectures in thermodynamics together with Viveka, who also led the corresponding exercise sessions.

As regards higher courses, the Division gives one Bachelor course and one advanced Master course in Surface and Colloid Chemistry and two Master courses in experimental physical chemical methods. The introductory Colloid and Surface Chemistry course was taught by Ulf Olsson, Lennart Piculell and Stefan Ulvenlund. The advanced course in Surface and Colloid Chemistry, given during the fall semester, was taught by Emma Sparr (course responsible) along with Lennart, Joakim Stenhammar, Tommy Nylander, Anna Stradner Peter Schurtenberger and Per Linse. This course is based on the textbook "The Colloidal Domain" by Fennell Evans and Håkan Wennerström. The other two Master courses were given during the spring semester, one on nuclear magnetic resonance techniques taught by Daniel and one on scattering methods, which was taught by Ulf.

Viveka Alfredsson taught on the course Physical Chemistry (B09).

Björn Lindman taught on the Ph D student course in Surfaces and Colloids at Nanyang Technological University, Singapore and on a Ph D course on colloids at the BIBAFOODS meeting in Coimbra as well as the national Ph D course on Surface Chemistry in Marstrand. Björn Lindman was one of the teachers at the annual industry course on Surfactants and Polymers in Aqueous Solution, given in Lisbon.

12 Seminars

PhD Student Saskia Bucciarelli, Physical Chemistry, Lund University
A scattering study of concentrated lens protein solutions and mixtures - Towards understanding the molecular origin of presbyopia

Dr. Christoffer Åberg, University of Groningen, the Netherlands
Bio-Nano Interactions: Quantitative Insights on How Nanoparticles Interact with Cells

Dr. Bruno Silva, Iberian Nanotechnology Laboratory, Braga, Portugal
Out-of-equilibrium self-assembly pathways: From functional structures for gene delivery to microfluidic manipulation of soft materials

Dr. Enamul Mojumdar, Physical Chemistry, Lund University
Lipid model to elucidate the molecular organization in the skin barrier

PhD Student Ruiyu Lin, Physical Chemistry, Lund University
The co-structure directing agent (CSDA) approach of mesoporous silica formation – exploring the assembly characteristics

Dr. Janne-Mieke Meijer, Physical Chemistry, Lund University
Shape Induced Phase Transitions In Crystals Of Colloidal Cubes

Associate Professor Christelle Prinz, Division of Solid State Physics, Lund University
Nanowires: a promising tool for applications in Biology

Dr. Marc Obiols-Rabasa, Physical Chemistry, Lund University
New insight into the characterization of protein-nanoparticle interactions

Professor Robin Ras, Aalto University, Finland
Dynamics at superhydrophobic surfaces

Professor Istvan Furo, KTH Royal Institute of Technology
Dispersing carbon nanotubes in water: some insights, some questions

Dr. Antara Pal, Physical Chemistry, Lund University
Colloidal Crystals: Beyond Hard Spheres

Student Maxim Morin, Physical Chemistry, Lund University
Phase Diagram of PEGylated Core-Shell Particles, Caprice of The Flocculation Boundary

PhD Leonie van 't Hag, Chemical and biomolecular engineering at the University of Melbourne, Australia
The use of lipidic self-assembly materials for amphiphilic protein and peptide encapsulation

Wormlike Micelles, Equilibrium Clusters and Colloidal Molecules: 35 Years of Soft Matter and Scattering
A one-day seminar.

Stefan Egelhaaf, Düsseldorf, Germany
Speckles - Here, There and everywhere

Ulf Olsson, Lund, Sweden
The hard sphere microemulsion, and beyond

Jan Skov Pedersen, Aarhus, Denmark
SANS study of polystyrene stars with advance labeling: A small birthday present that took almost 20 years to make

George Thurston, Rochester, USA
Model for Screened, Charge-Regulated Electrostatics of an Eye Lens Protein: Bovine GammaB-Crystallin

Frank Scheffold, Fribourg, Switzerland
Colloidal photonics: from cataract formation to photonic band gap materials

Wilson Poon, Edinburgh, UK
The physics of food: simplicy in complexity?

Katharina Fromm, Fribourg, Switzerland
Silver Nanobullets against Implant and other Infections

Alke Fink, Fribourg, Switzerland
The interaction of nanoparticles with cells: what have we learnt so far?

Willem Kegel, Utrecht, the Netherlands
Spontaneous formation of virus-like shells in soft colloidal dumbbells

Matthias Ballauff, Berlin Germany
Thermosensitive Colloidal Atoms and Molecules as Model Systems for Condensed Matter

Christos Likos, Vienna, Austria
Electrostatic and elastic interactions of microgels and polymer brushes

Rudolf Klein, Konstanz, Germany
Remarks on the slow acceptance of the Copernican revolution

Dr. Suman Peel, University of Bristol, UK
Fabrication of polymer supported bilayers as cellular membrane mimics: Vesicle remodeling by hard and soft interfaces

Student Emil Gustafsson, Physical Chemistry, Lund University
Synthesis and characterization of amine-functionalized microgel particles and their subsequent assembly into colloidal molecule-like clusters by droplet-based microfluidics

Professor Erica J. Wanless, The University of Newcastle, Newcastle, Australia
Anion specific effects in weak polybasic brushes

Adjunct Senior Lecturer Hanna Wacklin, Physical Chemistry, Lund University, and European Spallation Source ESS AB
Probing membrane structure using neutron reflection - elucidating the effect of lipid composition on the mechanism of membrane binding toxins and antimicrobials

Student Mikael Novén, Physical Chemistry, Lund University
Orientation of Sticks and Spheres - Estimating Tensor Shape and Orientation Distribution using Diffusion NMR

Student Viktor Persson, Lund University
Rheology of linseed oil based paints

Student Sujata Paudel, Lund University
DLS based microrheology in concentrated protein solutions

Professor Per Persson, Department of Biology, Lund University
Reactivity of iron (oxyhydr)oxide nanoparticles and the effects on geochemical processes

Dr. Nicholas Skar-Gislinge, Physical Chemistry, Lund University
Self-Association and Viscosity of High Concentration Antibodies

Dr. Erik Wernersson, Theoretical Chemistry, Lund University
Shape Matters: Modelling Colloidal Ellipsoids

PhD Student Charlotte Gustavsson, Physical Chemistry, Lund University
Environmentally Responsive Surface Coatings of Polyion-Surfactant Ion Complex Salts

Dr. Eric Johnson and Dr. Pete Ellingson from the Procter & Gamble Company
The Ph.D. Job Search: Tips for Finding Jobs in Industry

Bachelor Student Marina Huber, University of Paderborn
Quantitative Silicon NMR Study of the Stability of Cubic Polysilsesquioxane

Bachelor Student Simon Blazy, University of Paderborn
Testing the hypothesis of Pollack water

PhD Student Dat Pham, Physical Chemistry, Lund University
The skin as a barrier to molecular diffusion

Dr. Alexander Buell, Cambridge University
Physico-chemical studies of peptide and protein self-assembly

Johan Bergenholtz, Visiting Professor at Physical Chemistry, Lund University, and Professor at Chalmers University of Technology in Gothenburg
Instrumental smearing - how to include it in modeling of SAXS data

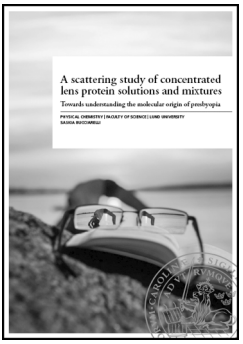
PhD Student Weimin Li, Physical Chemistry, Lund University
Understanding anisotropic attractions between proteins

13 Doctoral theses

Saskia Bucciarelli

A scattering study of concentrated lens protein solutions and mixtures - Towards understanding the molecular origin of presbyopia

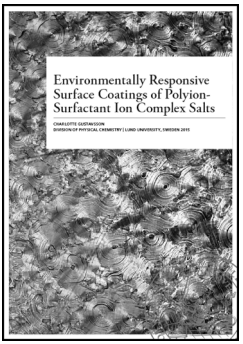
Opponent: Professor Lise Arleth,
University of Copenhagen, Denmark



Charlotte Gustavsson

Environmentally Responsive Surface Coatings of Polyion-Surfactant Ion Complex Salts

Opponent: Professor Lars Wågberg,
KTH Royal Institute of Technology, Stockholm



Divya Paloli, Department of Chemistry, University of Fribourg, Switzerland

Structure and Dynamics of Ultradense Microgels

Thesis written under the supervision of Professor Peter Schurtenberger, Physical Chemistry, Lund University

External expert: Professor Thomas Hellweg, University of Bielefeld, Germany

14 Publications

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On the role of hydrophobic interactions in cellulose dissolution and regeneration: Colloidal aggregates and molecular solutions
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16 People

16.1 Scientists/Teachers

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17 Contact Information

Welcome to visitors

We have many guests who stay with us for a few hours or a day of discussions, seminars etc., to one or more years for postdocs, foreign students and guest professors. Visitors are very important to us and help us to improve our level of research and education.

We recommend our visitors to fly to Kastrup Airport, Copenhagen. Then take a train from Kastrup Airport over the Øresund Bridge directly to Lund railway station (takes approximately 35 min.).

Visit the Kemicentrum website for further travel information: www.kc.lu.se/english/visitors/directions

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