Annual Report 2008

Physical Chemistry

Lund University
Sweden

CONTENTS

Cover. Two-dimensional NMR spectrum correlating ^{2}H resonance frequency (horizontal axis) with position along a sample tube (vertical axis) for a solution of a non-ionic surfactant in ^2H_2O. Equilibration in a strong centrifugal field results in an increasingly concentrated lamellar phase towards the top and pure ^2H_2O in the bottom. The ^{2}H quadrupole splittings yield the surfactant concentration profile from which the interbilayer force can be estimated. (Bulut, Åslund, Topgaard, Wennerström, Olsson)

Paula Leckius, Media-Tryck is gratefully acknowledged for the cover design.

INDUSTRY AND ACADEMIA

As has been stated so many times before, surface and colloidal chemistry represents a scientific discipline in which the distance between fundamental science and technical application is unusually short. From a practical point of view, this statement is directly reflected in the fact that Physical Chemistry maintains strong and continuous links with researchers from Industry. Furthermore, these collaborative research efforts span the widest possible range in terms of company size, from small-size high-tech companies, over mid-size companies with a strong local base, to large, multinational enterprises. The authors of this preface actually represent companies that cover the entire spectrum. Ola Karlsson represent MIP Technologies with 20 employees all based in Lund, whereas Stefan Ulvenlund represent the big pharma company AstraZeneca with thousands of staff world-wide. Nevertheless, the two of us both hold adjunct positions at the department, and actively engage in the research carried out there. This makes for an interesting reflection on the different driving forces behind academic-industrial collaboration.

Ola Karlsson – MIP Technologies

MIP Technologies develops and produces molecularly imprinted polymers (MIPs) and other 'smart' polymer materials for use in trace analysis or in advanced separations applications. The materials we make are niche polymers with tailor-made sites that facilitate selective molecular interactions. Such materials have often been described as 'artificial antibodies'. The MIPs are produced by various polymerization methods but in all cases specific interactions, molecular partitioning and polymer structure are key properties that we focus on.

Working in a rather small high-tech early stage company is of course (to use the buzz words you would expect) challenging, exciting and fun. But from time to time it can also be frustrating because of lack of critical mass in non-core but technically interesting areas.

The collaborations we have with Physical Chemistry are in a number of aspects very rewarding. For example, among the crew of Physical Chemistry one finds the 'open minded', 'knowledgeable' and not least 'creative' scientists that a small company can sometimes lack. In a more general way we can discuss and get new ideas on how to go forward with our own developments. We also have a direct collaboration on a common PhD project where we are looking at completely new polymerization techniques. In this project the core skills of MIP Technologies and Physical Chemistry in polymer design and studies of the colloidal domain have significant overlap and complementarity. This is then a good example of the classical theory of cross-fertilization at work. In this project, the PhD student (Johanna Bailey) and I both spend time at the department at the university as well as at MIP Technologies, allowing ideas to move back and forth between the department and the company.

It is too early to say if the project will lead to a commercial product or not but even if it does not we will gain knowledge in new areas as we move forward. In addition, we will have regular interactions with the permanent staff at Physical Chemistry and will get to meet students in their final studies thereby enlarging our network and creating possibilities for future recruitment. All these factors are essential for a small company to evolve. Hopefully we also bring something to the university by stimulating Physical Chemistry to search for a deeper understanding of new areas.

Stefan Ulvenlund – AstraZeneca

AstraZeneca is a multinational pharmaceutical company that maintains a strong presence in Sweden, where three of its major R&D sites are located: Södertälje (the cradle of one of the mother companies, Astra), Mölndal, and Lund. The reason that the Lund site was established in the first place was actually the proximity to the University, and the possibilities to benefit from academic-industrial cross-fertilization. Since the modest start in the mid-50's, the Lund site has grown to a major pharmaceutical R&D facility that employs about 1200 staff. Furthermore, the communication tools available to scientists have certainly evolved and multiplied dramatically over this time! Nevertheless, the proximity to the University remains a major advantage, since it is difficult to replace old-fashioned face-to-face discussions with teleconferences and electronic communication aids (no matter how elaborate). Personally, I consider it a major advantage to have my academic colleagues within walking distance from my lab at AstraZeneca. That these colleagues also happen to represent world-leading scientific expertise in a field of central important for pharmaceutics certainly doesn't hurt!

In one way or the other, I have worked together with scientists at Physical Chemistry for a decade. The collaborative projects have mostly been focused on fundamental science of relevance for pharmaceutical applications, rather than on the applications themselves. This direction is partly a matter of personal taste on my behalf, partly a result my research profile and the characteristics of my employer, AstraZeneca. In my own field of expertise (physical chemistry as applied to pharmaceutical formulation technology), a company of AstraZeneca's size has all the resources and know-how required to conduct scientific studies that are "wide", in the sense that massive data sets are collected and analyzed by primarily statistical means in a limited time frame. However, studies that are (for lack of better words) "deep" are another thing altogether. The "deep" studies I have in mind are those that are motivated primarily by scientific curiosity, yet delivers detailed understanding of the principles that underlie and determine complex phenomena. In somewhat simplistic terms, they deliver not only an answer to the question how, but also to why. Building this type of "deep" understanding is a direct investment for the future, since it has high predictive power and is applicable to many, seemingly disparate systems. I would claim that the most efficient way to achieve sufficient scientific understanding ("depth") is close collaboration between Academia and Industry - quite regardless of company size! Why? Well, as a scientist in a company culture, you are obviously assigned the role as an expert in your own scientific niche. Depending on company size, your place in the hierarchy and other factors, this niche may be small or big, but it is still a niche in which you often reign supreme within the confines of the company. However, intellectual challenges are necessary to keep you on your toes, keep you motivated, drive personal development and, ultimately, make it possible for you to deliver the high-quality science the company requires. Personally, my contacts with Physical Chemistry is what keeps me on my toes – in a way that the environment in a company, no matter how big, could achieve.

RESEARCH PROJECTS

Theoretical work - statistical mechanics

Dielectric discontinuities. A united description of the electrostatics of an arbitrary number of electrostatic multipoles, each localized in a spherical dielectric cavity, in a dielectric medium has been derived. The permanent charges as well as the polarization surface charges are described by multipole expansions in standard format. Expressions of the polarization surface charge density, the electrostatic potential energy, and the electrostatic interaction including the contribution from the polarization surface charge densities are given. Interacting electrostatic multipoles in dielectric spheres immersed in a medium with a higher (lower) relative dielectric permittivity experience a repulsive (attractive) potential term that increases in magnitude at reduced multipole separation, originating from the polarization surface charges appearing at the dielectric interfaces. Simplified expressions applied to monopoles and to two dielectric cavities are provided. Numerical examples involving monopoles and dipoles quantifying the effect of the surface polarization are also included.

The potential of mean force between two spherical and like-charged macroions in a salt-free aqueous solution has been determined using an extended primitive model and canonical Monte Carlo simulations. The systems considered covered the range from a purely repulsive to a purely attractive potential of mean force as the electrostatic coupling was increased. The macroions were modeled as spherical dielectric cavities, and the polarization surface charge densities occurring at the dielectric discontinuities were expanded in spherical harmonics. The surface polarization gave rise to (i) an attenuation of the counterion accumulation at the macroion surfaces at all cases considered, (ii) an enhanced repulsive potential of mean force in the weak to intermediate electrostatic coupling regime, and (iii) a less attractive at short separation and an enhanced attractive potential of mean force at longer macroion-macroion separation in the strong electrostatic coupling regime. (Per Linse and Jurij Rescic (University of Ljubljana, Slovenia))

Dynamics of polymer adsorption. The dynamics of adsorption and desorption of uncharged homopolymers have been investigated using a coarse-grained model comprised of a bead-spring chain and a planar surface. Brownian dynamics simulation has been used to examine the adsorption process for polymers released near the surface and with bulk properties as well as Monte Carlo simulations to explore equilibrium adsorption structures of the polymer. Systems with varying polymer contour length, polymer stiffness, and polymer-surface interaction potential have been considered. Investigations have been made on polymer extensions perpendicular and parallel to the surface and also characterized the adsorbed state in terms of loops, tails, and trains. After a diffusion of the polymer to the vicinity of the surface, three succeeding phases were identified: distortion, attachment, and relaxation phase. In the distortion phase, the polymer starts to experience the potential of the surface and becomes elongated perpendicular to the surface. In the attachment phase, the polymer makes direct contact with the surface and becomes contracted perpendicular to the surface and starts to spread on the surface. Finally, in the extended relaxation phase, the polymer continues to spread on the surface.

Furthermore, the dynamics of the adsorption process appearing in systems composed of a polymer solution placed near attractive, but initially polymer-free, surfaces were determined by Brownian dynamic simulations, and equilibrium properties of corresponding systems by Monte Carlo simulations. The properties of the systems have been analyzed by monitoring the number of adsorbed polymers, bead density profiles, time and frequency of polymer attachments, spatial extension of polymers perpendicular and parallel to the surface, and configurational characteristics. In addition to the phases described above, at long times, and connected to the slow relaxation of the number of adsorbed polymers, the extension of the polymer coils parallel to the surface was reduced, and the perpendicular extension was increased, with associated changes of the number of beads residing in tails, loop, and trains. The adsorption process was fastest for shorter polymer at higher density. (Per Linse and Niklas Källrot)

Microemulsions. Structural equilibrium properties of transient networks formed by microemulsion droplets and ABA-triblock copolymers in solution have been studied by Monte Carlo simulation. The droplets were represented by soft spheres, and the polymers were represented by junctions connected by harmonic bonds with an angular potential regulating the intrinsic chain stiffness. The interaction parameters were selected such that the end A-blocks were localized inside the droplets and the middle B-block in the continuous phase.

The influence of (i) the polymer concentration, (ii) the polymer stiffness, and (iii) the contour length of the middle B-block on the formation and the structure of the microemulsion-polymer network were investigated. An increase of the polymer-droplet number ratio had a strong impact on the network formation. Under typical conditions and at an intermediate polymer-droplet number ratio, (i) the fraction of polymers forming bridges between droplets increased from essentially zero to unity and (ii) the fraction of polymers that were forming loops decreased as the ratio of the polymer end-to-end separation and the surface-to-surface separation between neighboring droplets for a hypothetical homogeneous droplet distribution was increased from 0.5 to 2. For long and flexible polymers, a mesoscopic segregation triggered by a depletion attraction between droplets appeared, and, furthermore, for sufficiently stiff chains, only bridge conformations occurred. The percolation probability could be represented as a function of the average droplet cluster size only, across all systems.

Furthermore, the effect of (i) the droplet volume fraction, (ii) the droplet radius, and (iii) the contour length of the middle B-block on the formation and the structure of the microemulsion-polymer network at three-fold excess of the polymers were also investigated. A universal behavior of the properties investigated was found when examining the results versus the length ratio of the polymer end-to-end separation and the surface-to-surface separation between neighboring droplets for a hypothetical homogeneous droplet distribution. At a length ratio of 0.5, few polymer bridges between droplets were established and only clusters with a small number of droplets were found. However, at a length ratio of ca. 1.5 a connected network was formed and most of the polymers formed bridges between two droplets. (Per Linse and Jorge Sarragua and Alberto A. C. C. Pais (University of Coimbra, Portugal))

Polyelectrolyte gels. The swelling and mechanical properties of various interpenetrating polymer networks (IPN) have been studied by computer simulation. Six networks made from permuations of a moderately crosslinked polyelectrolyte network (ref), a moderately crosslinked neutral polymer network (net1), and a highly crosslined polyelectrolyte network (net2) were swollen in water. The swelling of the composite IPNs was discussed in terms of a balance between the osmotic pressure due to mobile counterions and the restoring force of the network chains, which act in parallel to counteract the osmotic swelling. For the ref-net2 system, the strong stretching of net2 chains increases the network restoring force and the further swelling due to the counterions is suppressed. The swollen network was then uniaxially stretched and equilibrium stress-strain plots obtained up to high extension ratios. (Samuel Edgecombe and Per Linse)

Structural properties of polar liquids. The long-range structural properties of liquids composed of molecular dipoles is a question of long-standing interest within many fields of chemistry and physics. The long range of the dipole-dipole interaction makes the structure of dipolar systems notoriously difficult to probe using computer simulations, although many techniques have been proposed to overcome these problems.

Within the present project, we combine the use of dielectric continuum theory with computer simulations to try to elucidate some fundamental properties of polar liquids. In particular, we have developed an analysis method based on the distance dependent Kirkwood factor Gk(R) to study the formation of so-called ferroelectric domains, i.e. regions exhibiting a large alignment of the dipoles. These analyses have proven successful in probing the build-up of ferroelectric structuring as the liquids become more strongly coupled. In parallel, we are using dielectric continuum theory to describe the fluctuations of electrical moments in dielectric media. The derived formulas have shown excellent agreement with results obtained from computer simulations for weakly coupled polar liquids. Hopefully, the study of how the size of these fluctuations change as the liquids become more strongly coupled can yield valuable information about the different structural properties of the systems. (Joakim Stenhammar, Gunnar Karlström and Per Linse)

Portal for statistical-mechanical computation and software. 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 package of four integrated and general programs for molecular dynamics, stochastic dynamics, and Monte Carlo simulation for molecular, colloidal, and polymer systems, including polarizable potentials, with extensive static and dynamic analyses. With contributions from Anna Akinchina, Fredrik Carlsson, Samuel Edgecombe, Yoshikatsu Hayashi, Niklas Källrot, Vladimir Lobaskin, Thomas M. Nymand, Alberto Pais, Jurij Rescic, Stefanie Schneider, Marie Skepö, Joakim Stenhammar, Anders Wallqvist, and Per-Olof Åstrand. First version 1990. Parallel version employing MPI since 1997.

NR is a software for simulation and analysis of neutron reflectivity data. First version 2007.

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.

(Per Linse)

Studies of model systems

Association behavior of block copolymers under the influence of nonionic surfactants and hydrophobically-modified polyelectrolytes. A specific group of water-soluble block copolymers that has attracted great interest in the literature is the triblock copolymers of (PEO) and poly(propylene oxide) (PPO), PEO-PPO-PEO. The more hydrophilic copolymers associate into micelles, composed of a hydrophobic PPO core and a PEO corona, established by light, X-ray (SAXS) and neutron scattering investigations. It is well-known that some of these copolymer micelles may undergo a sphere-to-rod transition at elevated temperatures. The underlying principle for this growth is the decrease of the polar PEO headgroup area at higher temperatures because of a transition to the high-energy forms of (non-polar) conformations, which is have a small or no dipole moments. In this project, mixed micelles of PEO-PPO-PEO block copolymers (e.g. P123) and C_iEO_j surfactants are studied, with a special focus on their temperature-induced sphere-to-rod transition at low surfactant content. The change in the shape transition temperature with increasing $C_{12}EO_6$ content follows the liquid-liquid phase separation temperature of the mixed system (first a decrease, then an increase) was determined using differential scanning calorimetry and visual inspection. This observation is explained by internal structural model of the mixed micelle where the added surfactant molecules lead to a change in the effective PEO head group area in the micellar corona. The retarded kinetics of the shape transition of mixed micelles of P123 and $C_{12}EO_6$ is analyzed from simultaneous time-resolved DLS and SLS measurements as well as from time-resolved titration calorimetry and time-resolved rheology and the rodlength may be obtained from depolarized DLS. The internal structure of the mixed micelles has been analyzed by SAXS, confirming that the $C_{12}EO_6$ reside in the core/corona region of the P123 micelles. The solution behavior of the mixed system consisting of pyrene-labeled poly(acrylic acid) (PAAMePy) and one PEO-PPO-PEO copolymer is investigated by using DLS, steady-state and time-resolved fluorescence spectroscopy. The DLS measurements provide information of the complex formation between PAA and copolymer micelles and the complex structure as a function of pH. (Karin Schillén, David Löf, Gerd Olofsson, Telma Costa (Coimbra Unv), W. Loh (University of Campinas, Brazil), A. J. Müller (Simon Bolivar University, Venezuela), O. Glatter (University of Graz, Austria), J. Seixas de Melo, B. Lindman and M. da G. Miguel (University of Coimbra, Portugal))

Catalysis of surface-active substrates at interfaces in dispersed media: oil in water emulsions. It is known that one efficient way to increase the rate of a catalytic reaction is to accumulate the reagents in a set of micro-reactors, distributed uniformly in the system. We propose another route to concentrate reagents in limited volume, namely, to use the interfacial adsorption of surface-active amphiphilic molecules at the boundaries of immiscible phases in, for example, oil-in-water emulsions. If the adsorbing molecules can react with each other, the interfacial layer becomes a reactor of nano-scale thickness (a "surface nano-reactor"). Computer modeling and theoretical considerations from Khokhlov's group have pointed to a possibility to control the rate of catalytic reactions carried out in emulsions. At a certain size of the emulsion droplets (several hundreds of nanometers) the reaction rate was predicted to exhibit a maximum. This could be simply explained as follows. For small droplet radii, the available surface area is too large and the concentrating effect at the interface is low. On the other hand, for large radii the surface area is too low, thus reducing the probability that the catalyst and the substrate will meet at the interface. The experimental investigation of this possibility is of special interest. Therefore, this project focuses on experiments on catalysis of surface-active substrates in oil-in-water emulsions. (Irina Nasimova, Ulf Olsson, Alexei Khokhlov (Moscow State University/Russian Academy of Science))

Diffusive transport in responding membranes. In a simplified description of membrane transport, one considers a concentration gradient across a static barrier. In a more dynamic approach, the barrier is allowed to respond by changes in lipid phase behavior along the concentration gradient, which motivates the name "responding membrane". In the presence of more than one gradient, this can lead to dramatic effects. It is typical for the rich phase behavior of lipids that small changes in the external conditions can trigger large structural changes with distinctly different diffusion characteristics. It is clear that the abruptness of phase changes can act as a kind of switch for diffusive transport, and thereby introduce non-linear elements to the transport process In this way, structure and transport are intimately coupled. This mechanism is highly relevant to biological systems where transport often occurs between regions of profoundly different properties.

In this project we use a combined experimental and theoretical approach to explore the mechanisms for diffusive transport in responding membranes, and how external gradients that induce phase transformations and domain formation can regulate the membrane barrier (Figure 1). The experimental work involves transport studies in model lipid membranes using recently devolved system of so-called double-porous membranes where lipid lyotropic phases are confined inside the pores of a synthetic polymer membrane.

Beside the basic scientific interest in the mechanisms for steady-state transport in responding membranes, several applications in biology and technology can be seen in, for example, the barrier properties of stratum corneum (the upper layer of the skin) and the formation of plastic polymer-surfactant films. (Christoffer Åberg, Peter Nilsson, Emma Sparr, Håkan Wennerström, Daniel Topgaard, Fátima Costa-Balogh (Coimbra university, Portugal), Karen Edler (University of Bath))

Interaction between RNA and lipid membranes. In the living system, RNA (ribonucleic acid) is present in an environment that contains many substances, which can influence its structure and function. RNA occurs more often than DNA in the single-stranded form, where the apolar parts of the bases are obvious targets for interaction with hydrophobic species in the environment, e.g. lipids in the cell membrane and in the cell nucleus. We aim at revealing the basic features of RNA–lipid interactions. We study the adsorption of nucleic acids to lipid bilayers and monolayers with varying properties, and we study how interaction affect the phase behavior, which in turn provide information of how and where the interaction takes place. For this purpose, we investigated a set of model membrane systems with varying charge density and with fluid or solid acyl-chains together with RNA or DNA of different size and degree of base pairing. We study small single-stranded RNA, tRNA and long double stranded DNA, and the model lipid membrane systems are mainly chosen to mimic cell membranes and the lipids within cell nuclei (zwitterionic and anionic lipids), as well as cationic lipids. The system are studied with several techniques, including calorimetry, ellipsometry, quartz crystal microbalance (QCM-D) and monolayer techniques. (Agnes Zettergren, Emma Sparr, Tommy Nylander, Luc Jaeger (University of California, Santa Barbara, USA))

Physicochemical Behavior of Aqueous Systems Containing DNA, Proteins and Amphiphiles. The behavior of systems where DNA coexists with both proteins and amphiphiles is of great biological importance. Most notably, there are indications that interactions between the lipid portions of the cell nucleus with chromatin, which is a DNA-protein complex, are involved in organization of the chromatin and regulation of gene expression. Another example is the finding that the inclusion of proteins in DNA-lipid complexes for gene therapy can greatly enhance the transfection efficiency. Despite the biological relevance, investigations performed to study well-defined aqueous systems of DNA, protein and amphipihiles are few. The aim of this project is to gain an improved understanding of the physicochemical behavior of such systems. Of particular interest is the structure and composition of aggregates and complexes formed by the components and a multitude of techniques are applied for characterization of these. The work is focused on three classes of systems: 1) model systems of well-characterized proteins, DNA and different types of amphiphiles, 2) systems containing nucleosome core particles (NCPs), i.e. the basic unit of chromatin, which consist of DNA wrapped around a core of eight histone proteins, and different types of amphiphiles, and 3) complexes comprising plasmid DNA, amphiphiles and certain proteins that have been evaluated with regards to their efficiency in transfection experiments. (Dan Lundberg, Anna Carnerup, John Janiak, Karin Schillén, Viveka Alfredsson, Daniel Topgaard, Björn Lindman, Maria da Graça Miguel, Henrique Faneca and Maria C. Pedroso de Lima at University of Coimbra, Coimbra, Portugal; Lars Nordenskiöld and Nikolay Korolev, Nanyang Technological University, Singapore.)

Polymerization in structured media. The long-term goal of this project is to create polymers that resemble biomacromolecules in their structure and function. To that end, we study polycondensation reactions in dispersed aqueous systems at ambient or slightly elevated temperatures. The incorporation of active chemical functionalities through polymerization in structured dispersed media will produce new types of polymer. The polymerization reactions that result in such materials include multifunctional monomers, which are often amphiphilic by nature. In order to facilitate the formation of specific molecular sequences, a detailed control of the polymerization loci is a necessity, and the partitioning of the reaction components in the various phases during reaction is crucial. Initially, we study the solubility of the active components and the complex formation between them. We also study how the reaction kinetics are affected by the distribution of the reaction species and by the particle size of the dispersed phase. (Johanna Bailey, Ola Karlsson, Lennart Piculell)

Polymerization of polymerizable surfactant counterions. Polymerization in surfactant systems, typically with the objective of “freezing” or “templating” (making a polymer replica of) the surfactant structure is a very active research field. However, there are notorious problems associated with using “soft” surfactant aggregates to template “soft” polymeric materials, mainly because the polymerization reaction generally strongly affects – and often destroys – the surfactant structure. Two aspects make our approach to this problem unique: 1) We build on our a priori knowledge of the phase behavior of surfactant ions with polymeric counterions in water. 2) We perform the syntheses under conditions where the surfactant aggregates are the sole counterions to the growing chains of the polyion. This represents a quite strong constraint for the outcome of the polymerization. We introduce comonomers and/or crosslinkers in the system, with the overall aim to achieve non-random polymeric materials, whose primary structures are affected by the presence of the surfactant aggregates. For example, we synthesize, in cationic surfactant systems, linear copolymers of polyacrylate with neutral comonomers, and also cross-linked gels. Two questions will be addressed in this research: 1) To what extent can we make a soft template that still retains its structure even after the surfactant is removed? 2) Can we make a gel or a polymer that recognizes objects, for instance, such surfactant aggregates as was used for templating? (Salomé dos Santos, Lennart Piculell, Ola Karlsson (MIP Technologies) Maria Miguel (Coimbra University))

Soluble complex salts of surfactant ions and polymeric counterions: Composite macromolecular self-assembly. The aim of this project is to understand the physical chemistry of soluble complex salts in aqueous solution and the intermolecular interactions involved. A complex salt is defined as the neutral salt of surfactant ions (aggregated into highly charged micelles) that interact with a polyelectrolyte chain, which in turn acts as a large counterion (denoted “polyion”). In this project, the complex salts consist of polyacrylate (PA^-_y) and cationic $C_{16}TA^+$ surfactant ions and are denoted $C_{16}TAPA_y$, where y is the number of monomer units (or degree of polymerization). Without nonionic surfactants, at high water contents, the investigated complex salts exhibit miscibility gaps that consist of co-existing phases: a concentrated phase (either cubic or hexagonal internal structure) and a less concentrated phase. In order to make the complex salts soluble, nonionic surfactants of the type C_iEO_j (where EO stands for poly(ethylene oxide), PEO) are added. The project has two parts: a) initial phase studies of ternary mixtures of $C_{16}TAPA_y$, C_iEO_j surfactants and water, b) investigation of the composite macromolecular self-assembly in dilute solution (main part). The solution properties of these new composite self-assembled macromolecular structures at different temperatures are investigated by varying the polyion length (y = 25 or 6000) and the PEO length of the nonionic surfactant ($C_{12}EO_5$, $C_{12}EO_8$, $C_{12}EO_{23}$). The size and internal structure of the aggregates formed are investigated by using dynamic and static light scattering (DLS, SLS), small-angle X-ray scattering (SAXS). It has been found that the size is highly influenced by the temperature. Cryo-transmission electron microscopy will also be used for structural characterization. For further insight in the intermolecular interactions between $C_{16}TAPA_y$ and C_iEO_j, isothermal titration calorimetry will be employed for measurements of interaction enthalpy changes at different temperatures. Finally, the solution properties of the complex salt in organic solvents, such as tetrahydrofuran, will studied in order to create a new purification procedure of $C_{16}TAPA_y$. (John Janiak, Karin Schillén, L. Piculell, G. Olofsson, V. Alfredsson, P. Stepanek (Institute of Macromolecular Chemistry, Czech Republic), W. Loh (Campinas University, Brazil))

Condensing DNA with cationic dendrimers: means of controlling aggregate morphology. 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. (M.-L. Ainalem, A. M. Carnerup, J. Janiak, V. Alfredsson, T. Nylander and K. Schillén)

Solubilization of conjugated anionic copolymers by nonionic surfactants in aqueous solution. Interaction between the conjugated polyelectrolyte, anionic poly{1,4-phenylene-[9,9-bis(4-phenoxy- butylsulfonate)]fluorene-2,7-diyl} (PBS-PFP), and the non-ionic alkyloxyethylene surfactant n-dodecylpentaoxyethylene glycol ether (C12E5) in water is investigated. Using UV/visible and fluorescence spectroscopy, dynamic light scattering (DLS), small-angle X-ray scattering (SAXS), cryo-transmission electron microscopy (cryo-TEM) and electrical conductivity, a coherent model for this polymer-surfactant interaction is formulated, which is based on the of break-up of the PBS-PFP clusters through polymer-surfactant association and formation of cylindrical micelles containing isolated polymer chains. This process involves a careful balance between electrostatic, hydrophilic and hydrophobic interactions. Strong support for this comes from molecular dynamics simulations, which indicate stable polymer-surfactant structures and also provide support for the tendency of C12E5 to break up polymer clusters to form these mixed polumer-surfactant aggregates. Radial electron electron density profiles of the cylindrical cross-section obtained from SAXS results reveal the internal structure of such inhomogeneous species. DLS and cryo-TEM results show that at higher surfactant concentrations the micelles start to grow, possibly partially due to formation of long, thread-like species. (K. Schillén, V. Alfredsson and A. M. Carnerup, H. D. Burrows, S. M. Fonseca, C. L. Silva, A. A.C.C. Pais and A. J.M. Valente (University of Coimbra, Portugal), M. José Tapia (Univeridad de Brugos, Spain), S. Pradhan and U. Scherf (Bergische Universität Wuppertal, Germany), M. Tomšic and A. Jamnik (University of Ljubljana))

Extensional rheology, shear rheometry and dynamic light scattering measurements on systems of cylindrical surfactant micelles and block copolymer-nonionic surfactant mixed micelles. In the elongational flow technique the extensional viscosity is measured by using an uniaxial elongational flow field. An increase in the extensional viscosity, i. e. elongational thickening, may be observed in systems that are shear thinning. An example where this can occur is in systems of linear polymers, where thickening may be exhibited due to uncoiling of the polymer chain to an aligned and extended conformation, cylindrical micelles of amphiphiles, et.c. In this project we explore a variety of different systems by using shear rheometry, extensional rheology and dynamic light scattering in combination. The rheological properties (and growth) of cationic cylindrical surfactant micelles in aqueous solution are studied under three different flow fields: simple shear, opposed-jets flow (which approximates uniaxial extension) and porous media flow (which includes simultaneously shear and elongational components of the flow). The retarded kinetics of the sphere-to-rod transition of mixed micelles of PEO-PPO-PEO triblock copolymer and nonionic CiEOj surfactants is also being investigated. By using zero-shear rheology as a function of time and temperature the time-dependence of the transition is followed and the results are in good agreement with those obtained from time-resolved static and dynamic light scattering measurements. Project completed. (D. Löf, K. Schillén, M.

Torres and A. J. Müller (Universidad Simón Bolívar, Venezuela)

Supramolecular aggregates of amphiphilic gadolinium complexes as contrast agents for magnetic resonance imaging applications. Magnetic resonance imaging (MRI) is an imaging technique with cellular resolution that is widely used as a diagnostic tool in clinical practice. In this project, new potential blood pool contrast agents based on amphiphilic gadolinium complexes and amphilphiles that contain a bioactive peptide with target specificity are being developed. The structures of the self-assembled aggregates (lamellar aggregates, vesicles and micelles) in aqueous solution are characterized by means of dynamic light scattering, cryo-TEM and small-angle neutron scattering. (D. Löf, K. Schillén and O. Söderman, M. Vaccaro, L. Paduano, G. Mangiapia, G. Morelli, A. Accardo and D. Tesauro (University of Naples, Italy), E. Gianolio and S. Aime (University of Turin, Italy))

Structures formed by block copolymers containing amphiphilic repeating units. Block copolymers are composed of two or more chemically distinct and typically immiscible polymer blocks. For a diblock copolymer (poly-A + poly-B) the immiscibility between A and B blocks drives a microphase separation in the melt, with alternating A-rich and B-rich microdomains. The melt phase behavior of linear diblock copolymers with random coil blocks is determined by the overall degree of polymerization N, the volume fraction of the A component f_A, and the A-B segment-segment interaction χ. With increasing f_A from 0 to 0.5, at a fixed high value of χN, one experimentally and theoretically obtains i) A-spheres arranged in a body-centered cubic lattice, ii) A-cylinders arranged in a hexagonal lattice, iii) a region of gyroid phase and iv) alternating A and B lamellae. Very recently Khokhlov et al. reported computer simulation results for diblock copolymers where one of the blocks contains amphiphilic repeating units: One part of each amphiphilic unit interacts athermally (zero χ) with the other block, whereas the other part has a strongly repulsive interaction (strongly positive χ). The amphiphilic block is predicted to give a new morphological variation in the block copolymer phase separation, featuring thin channels and slits of amphiphilic units penetrating through the matrix of a major nonpolar components. The project seeks first to test these new predictions by experimental structural studies of block copolymers containing one hydrophobic and one strongly amphiphilic block. In order to vary the volumes of the hydrophobic and amphiphilic microdomains, a hydrocarbon solvent and/or water will be added to the system. Experimental methods include SAXS and NMR. (Mehran Asad Ayobi, Lennart Piculell, Ulf Olsson, Alexei Khokhlov (Moscow State University/Russian Academy of Science))

Water-soluble polymers containing amphiphilic repeating units and their interactions with ionic surfactant micelles. The description of water-soluble polymers is one of the main research tasks of polymer chemistry and physics. The monomer units of such polymers are usually divided into two classes: hydrophobic (H) versus polar (P) or hydrophilic (P) units (HP classification). However, from the chemical structures of typical monomer units it is evident that in most cases these are neither purely hydrophilic nor purely hydrophobic, but rather amphiphilic, since they contain functionalities of both types. Based on these considerations, a new dumbbell model (HA-model) for amphiphilic (co)polymers was introduced in the group of Khokhlov. It was shown that conformational properties of polymers containing amphiphilic units are significantly different from those predicted by the HP model. The main reason is that for amphiphilic dumbbells a location at an interface is most probable, i.e. these units possess a significant surface activity. Both the interfacial activity and the partitioning between water and hydrocarbon solvents could be key parameters for the classification of monomers and, based on these considerations, a two-dimensional classification diagram has been proposed by I.M. Okhapkin et al. The positions of monomer units of various synthetic water-soluble polymers in such a diagram was determined based on interfacial tension and partition coefficient measurements. In this project we are using the two-dimensional description to classify certain alkylacrylamide monomers with the aim to rationalize the varying tendencies of the corresponding polymers to bind to surfactant aggregates in water. Usually, the tendency of a nonionic polymer to bind ionic surfactant micelles is explained in terms of the polymer hydrophobicity. However, since a large fraction of the micellar surface contains hydrocarbon in direct contact with water, the interfacial activity of the monomer units should also be taken into account. (Irina Nasimova, Lennart Piculell, Alexei Khokhlov (Moscow State University/Russian Academy of Science))

Asymmetric catanionic surfactants. Catanionic surfactants are complex salts of surfactant cations and surfactant anions (e.g. dodecyl tetra methyl ammonium dodecyl sulphonate) in the absence of additional simple salts (e.g. NaCl). Symmetric (equal alky chain lengths) catanionics form essentially stable water insoluble crystals at room temperature. In asymmetric catanionics the surfactant film may carry a net charge in mixtures with water because of a mismatch in the aqueous solubility of the two surfactant ions. The chain length mismatch also reduces the Krafft temperature significantly resulting in that these materials are water soluble already at room temperature. If the solubility difference is not too large, these surfactants form a lamellar phase in water which can swell to very high water contents due to the net bilayer charge. However a very interesting aspect is the presence of an unusual miscibility gap within the lamellar phase, which has previously been observed only in a few particular systems. With the addition of an alkane, the lamellar phase is transformed into a water-in-oil droplet microemulsion with spherical, weakly charged droplets of low polydispersity. Using small angle neutron scattering we study the long range droplet-droplet interactions which depend on the concentration dependent effective droplet charge (B. Silva (Porto), E. Marques (Porto), Per Linse, Kell Mortensen (Copenhagen), U. Olsson).

Living polymers and living networks. Some surfactants form giant micelles in solution that can be longer than several micrometers. These solutions have properties similar to polymer solutions, however with some significant differences. The size distribution is not fixed but varies with concentration and temperature. Moreover, micelles may break and reform which influences the dynamics. For these reasons the are often referred to as “living polymers”. Furthermore, there are also systems where the micelles form connected (branched) network, similar to a bicontinuous microemulsion. Here the morphology resembles that of polymer gels and one may refer to a “living network”. In this project we compare phase behavior of living polymer and living network systems and we have studied the effect of shear flow on the liquid structure and in particular the shear induced formation of a nematic phase of wormlike micelles. The structural transformation may be followed by small angle neutron scattering (rheo-SANS) or by NMR measurements (rheo-NMR). The growth of “living polymers” with increasing concentration is an unresolved problem. Simple mean field models predict that the number averaged contour lengths varies approximately as the square root concentration while one in the analysis of recent experiments have found a much higher exponent. An important complication in the analysis of experimental data is the interactions and how they influence e.g. the osmotic compressibility. Here we are combining static and dynamic light scattering, and NMR self-diffusion experiments, to investigate the growth law in dilute solutions. The diffusion of surfactant molecules is restricted to the self-assembly aggregates which may form a random coil or be an infinite connected network. Both super and sub diffusion may be observed which can be described within the same formalism in terms of a generalized diffusion equation with fractional derivatives. (S. Bulut, J. Hamit, U. Olsson, T. Kato (Tokyo), R. Angelico, L. Ambrosone and A. Ceglie (Campobasso), G. Palazzo (Bari), K. Mortensen (Copenhagen, Denmark), Samiul Amin (Malvern, UK))

Bilayer membrane kinetics, including vesicle fusion. The phase lamellar-to-”sponge” phase transition involves a topological transformation of a bilayer membrane. In the lamellar phase the bilayer has a planar topology while it is multiply connected in the so-called “sponge” or L3 phase. Topology transformations are believed to involve the fusion or fission of membranes. With nonionic surfactants the phase transformation can occur by a minor change in temperature. Using deuterium as “phase-detection” the transition has been investigated in both directions. The sponge-to-lamellar transition appears to occur via a nucleation and growth process while the opposite transition rather involves a random fusion of adjacent bilayer membranes. To investigate the bilayer structure in more detail, The transitions are also studied by small angle neutron scattering experiments. Nonionic vesicles spontaneously fuse at elevated temperatures. Here, vesicle fusion kinetics is tudied using time-resolved static and dynamic light scattering and small angle neutron scattering. (S. Bulut, M. Zackrisson, U. Olsson, H. Wennerström; M. Gotter (Köln), M. Baciu (Köln), I. Savic (Köln) R. Strey (Köln)).

Lamellar phase rheology and shear-induced formation of multi-lamellar vesicles. 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. (U. Olsson, B. Medronho (Coimbra), M. Miguel (Coimbra), C. Schmidt (Paderborn), M. Imai (Tokyo), Y. Suganuma (Tokyo), Cesare Oliviera (Cosenza))

Experimental methodologies

Diffusive transport of multivalent ions in cartilage. Articulate cartilage is a complex material, composed of collagenous fibers, and cells called chondrocytes, all of which are embedded in a firm gel-like ground substance. 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 n 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 will be performed on model system of cartilage made from gel-forming polymers as well as on actual in-vitro samples of cartilage will be undertaken.

Theoretical studies on diffusion of large negative divalent ions in models of healthy and damaged cartilage will be carried out. These include Brownian Dynamics simulations, which possibly will be complemented by Dynamic Density Functional Theory calculations. (Daniel Topgaard, Olle Söderman, Jan Forsman, Jonas Svensson (Department of Radiation Physics and the Joint and Soft Tissue Unit at UMAS, Malmö))

Neutron reflectometri. Neutron reflectivity (NR) measurements have been performed on stimulus-responsive polymer brushes containing N-isopropylacrylamide at different temperatures and contrasts using two different brush samples of roughly the same grafting density and layer thickness. The NR data were analyzed using a novel method employing polymer density profiles predicted from lattice mean-field theory augmented with a polymer model to describe polymer solubility that decreases with increasing temperature. The predicted density profiles at the different temperatures were self-consistent with the experimentally observed profiles; hence the experimental data lend credibility to the theory. We found that the brush thickness decreased from 220 to 160 nm and the polymer volume fraction increased from 55 to 75% when increasing temperature from 293 to 328 K. The new evaluation approach involved significantly fewer independent fitting parameters than methods involving layers of uniform densities. Furthermore, the approach can straightforwardly be extended to analyze neutron reflectivity data of grafted, weakly charged polymers that display pH-sensitive behaviour and also to block copolymers and to surfaces with adsorbed polymers. We propose that such accurate model calculations provide a tool to interpret results from NR experiments more effectively and design neutron reflectivity experiments for optimal outcome. (Tommy Nylander, Richard Campbell, Per Linse)

Polymer-surfactant interaction at liquid interface. There is considerable industrial interest in understanding the nature of surface and bulk interactions between polymers and surfactants because such mixtures are used extensively in commercial products such as shampoos and fabric conditioners.

Considerable effort over the last two decades has been devoted to gaining an understanding of the nature of the interaction between polyelectrolytes and oppositely charged surfactants in the bulk phase. Most of the work has been carried out on linear polyelectrolyte systems. These investigations showed that usually a one-phase transparent system forms in the presence of a small amount of surfactant. By increasing the bulk surfactant concentration, the solution becomes turbid, and an associative phase separation occurs (i.e., a concentrated phase enriched in both polymer and surfactant separates from a dilute aqueous phase containing mostly small ions). With further increases in the bulk surfactant concentration, the turbidity may decrease, and redissolution of the polyelectrolyte/surfactant complexes can occur. The surfactant binding in the bulk phase is usually interpreted in terms of a two-part equilibrium process.

Poly(ethylene imine) [PEI] has captured a lot of attention from the academic and industrial research communities in recent years. Factors that in particular make PEI an interesting class of polymer both from a fundamental and practical perspective:

1. The polymer size as well as molecular architecture can be readily varied from linear to hyperbranched, which affects its morphology in bulk solution and at interfaces.
2. The polyelectrolyte charge can be set by modifying the solution pH: effectively, PEI has a high positive charge density at low pH but a diminished charge density at high pH.
3. The physicochemical properties are affected by the ionic strength because the addition of electrolyte increases the surface activity of polymer/surfactant complexes.

A useful optical technique for the characterization of polymer/surfactant adsorption layers at the air/liquid interface is ellipsometry, where the reflection of elliptically polarized light depends on the dielectric (refractive index) profile normal to the interface. The phase change of light upon reflection at the surface of a polymer/surfactant solution, relative to that of a clean interface, is determined by the structure and amount of adsorbed material. We exploit ellipsometry in the present project by analyzing fluctations in the optical signal, features that would most likely not be detected in the relatively slow and macroscopic measurements made using for instance neutron reflectometry (NR). Furthermore, the comparison of ellipsometry measurements, both with changing bulk composition and evolving time, allows us to track the relative amount of adsorbed material.

We have exploited the spatial and kinetic resolution of ellipsometry to monitor the lateral movement of inhomogeneous patches of material in mixed adsorption layers of poly(ethylene imine) and sodium dodecyl sulfate at the air/liquid interface. We show that the choice of sample preparation methods can have a profound effect on the state of the interface for chemically equivalent samples. The extent of aggregation in the bulk solution on relevant time scales is affected by specific details of the polymer/surfactant mixing process, which produces varying numbers of aggregates that can become trapped in the interfacial layer, resulting in an enhanced and fluctuating ellipsometry signal. It can be beneficial to apply the surface-cleaning method of aspiration prior to physical measurements to remove trapped aggregates through the creation of a fresh interface. At low pH, the ellipsometry signal of samples with surface cleaning is remarkably constant over a factor of >500 in the bulk composition below charge equivalence, which is discussed in terms of possible adsorption mechanisms. At high pH, through observing temporal fluctuations in the ellipsometry signal of samples with surface cleaning, we reveal two important processes: there is the spontaneous adsorption of aggregates >0.2 μm in diameter into the interfacial layer, and with time there is the fusion of smaller aggregates to generate new large surface aggregates. We attribute the favorability of the adsorption and fusion processes at high pH to reduced electrostatic barriers resulting from the low surface charge density of the aggregates. It is inappropriate in this case to consider the interface to comprise a homogeneous adsorption layer that is in dynamic equilibrium with the bulk solution. Our work shows that it can be helpful to consider whether there are macroscopic particles embedded in molecular layers at the air/liquid interface for systems where there is prior knowledge of aggregation in the bulk phase. (Richard Campbell, Katrin Tonigold, Marianna Yanez, Tommy Nylander, Lennart Piculell, Imre Varga and Róbert Mészáros at Eötvös Loránd University, Budapest; Hungary; LSS Group, Institut Laue-Langevin, Grenoble, France (present affiliation of Richard Campbell))

Solid-state NMR methods for amphiphile systems. 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 necessary in order to extract 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 cationic surfactants with mono-, oligo-, and polymeric counterions, nonionic surfactants with poly(ethylene oxide) or glucoside headgroups, DNA-lipid assemblies, and synthetic analogs of the lipid mixtures in the stratum corneum. (Daniel Topgaard, Emma Sparr, Gunnar Karlström, Per Linse, Agnieszka Nowacka, Tiago Ferreira, Dan Lundberg, Azat Bilalov, Johan Reimer, Nils Bongartz, Jens Norrman, Rachel W Martin, UC Irvine)

Diffusion NMR methods for biological tissues. Molecular transport by diffusion is a crucial process for the function of biological tissues. Diffusion NMR is a powerful method to non-invasively study 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. Most of the present day diffusion NMR studies use the same basic experiment as in the pioneering works from the 60's. Here we design new protocols for estimating parameters such as the diffusion coefficient of the intracellular medium, the cell membrane permeability, and the length scale at which an inhomogeneous medium, such as brain tissue, start to appear homogeneous. 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 and gels. 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. (Daniel Topgaard, Olle Söderman, Ingrid Åslund, Samo Lasic, Freddy Ståhlberg, Medical Radiation Physics, Stina Oredsson, Cell- and Organism Biology, Karin Bryskhe and Anna Stenstam, Colloidal Resource)

Cryo-Fracture TEM. Conventional Cryo-TEM experiments requires very thin samples in order to have sufficient transmission. This is difficult to achieve with viscous samples. In this project we have developed a slightly modified specimen preparation protocol, where a (too) thick vitrified specimen is punched with a sharp object in a number of different spots. In the resulting fractures one frequently find edges that are thin enough image in transmission. Lamellar phases, including a lamellar mesh phase, hexagonal and cubic phases have been successfully imaged using this protocol. (A Gonzalez-Péréz, S. Bulut, U. Olsson)

A 12-channel microcalorimeter for use as a monitor of biological systems. The instrument is primarily intended for investigations of microbial activity in soil, of animal (human) cells and tissues and for small animals. The calorimeter is a further development of the earlier 48-channel instrument (cf. AR 2007), which mainly was intended for use in the pharmaceutical industry, at temperatures around 37 °C. The new instrument is designed for use in a wider temperature range, down to 0 °C and has larger vessels. Both instruments should be considered as analytical tools (process monitors), which are sensitive (about 10 nW) and stable (days on the µW level), but are not suitable as accurate and versatile thermodynamic tools. (Ingemar Wadsö)

A 10-channel microcalorimetric system for use in analytical and thermodynamic measurements. The new instrument has a different mechanical design and is intended as a “platform” for different reaction vessels, useful as process monitors or in accurate thermodynamic measurements. As for instrument (1) the goal is to reach highest possible sensitivity and stability, but the useful temperature range will be wider (0-150 °C). Most mechanical parts for the “platform” have been manufactured. Tests will initially be conducted by use of simple static vessels, which are suitable for some biological systems and for stability measurements of technical materials. Later more advanced vessels (of types we earlier have designed for conventional microcalorimeters) will be tested/adapted: vessels with stirring and injection devices (g, l, s), flow vessels and vessels equipped with analytical sensors such as electrodes for pH and O2 used simultaneously with the calorimetric measurements. (Ingemar Wadsö)

Colloidal biology

Amyloid formation in the presence of lipid membranes. Disease-causing amyloid fibril formation can be modulated by many factors including interactions with biological lipid membranes. An increasing amount of evidence suggests that the process of fibril formation in vivo and the mechanism of toxicity both involve membrane interactions, as reviewed in [1]. Alzheimers is probably the most well-known amyloid disease and the Alzheimer's beta peptide is originally cleaved off from the amyloid precursor protein (APP), which is a membrane incorporated protein. The cleaving site is such that the resulting Alzheimer's beta peptide, in its C-terminal part, contains 11 to 14 amino acids originally incorporated into the membrane. This gives the cleaved peptide a significant amphiphilicity, but also electrostatics are believed to be important in the membrane-peptide interaction.

We use recombinant Abeta peptide produced in Escherichia coli, which allows us to perform large scale amyloid formation assays with good statistics where the aggregation process is followed in means of thioflavin T fluorescence. The lipid membranes are introduced in the system as large unilamellar vesicles. As a model system, we have used vesicles composed of zwitterionic DOPC and mixtures of DOPC and anionic DOPS , Cholesterol and Sphingomyelin. The aggregation process itself is highly salt dependent but we can also take advantage of this salt dependence to study the electrostatics in the membrane-peptide interactions. The presence of cholesterol causes an increase in the acyl-chain ordering of the lipids, which may be important when it comes to the incorporation of the peptide into the membrane. We also study the effect of domain formation in the lipid membrane. Sphingomyelin and cholesterol are major component in the micro domains usually referred to as lipid rafts in biologic membranes.

To further study interactions of interest that we detect in the Thioflavin T assays we have different biophysical techniques available such as monolayers, giant vesicles in combination with confocal microscopy, isothermal calorimetry, NMR, SPR and Electron Microscopy. (Erik Hellstrand, Sara Linse, Emma Sparr, Dominic Walsh, University College Dublin, Patrik Brundin, BMC Neurocentrum, LU.)

Cyclodextrins in DNA decompaction. Important cellular processes involving DNA, such as transcription and replication, can be strongly affected by the extent of condensation of the chromatin fiber. The degree of condensation affects the access of regulatory factors. In synthetic gene delivery systems, the use of cationic lipids can protect and compact the large and highly biodegradable DNA molecule. Once the DNA:compacting agent complex reaches the target inside the cell, the DNA should be decompacted to be accessible to the cell machinery responsible for translating the enclosed information. Obviously, it is desirable to achieve a reversible DNA condensation process in order to be able to control the transfection efficiency. Many chemical agents have been successfully used in vitro in order to compact DNA, thus mimicking the natural process occurring in the cell. In the last years, the fundamental understanding of the compaction process using different chemical agents has improved. Various strategies have also been used in order to decompact the condensed DNA, such as the introduction of non-ionic and anionic surfactants.

It was recently reported that β-cyclodextrin (β-CD) can be used to decompact DNA:CTA complexes. Cyclodextrins are cyclic oligomers of glucose shaped like truncated cones that are resistant to degradation of human enzymes and not producing an immune response in mammals. They are therefore of interest in therapeutical applications. In general, cyclodextrins are used to encapsulate and solubilize various hydrophobic molecules (or parts of thereof) in aqueous solution by forming host-guest complexes by association of the hydrophobic parts into the hydrophobic cavity of the cyclodextrin. The inclusion complexes formed by β-CD and the cationic surfactant cetyltrimethylammonium bromide (CTAB) were investigated by Cabaleiro-Lago and coworkers, and a strong association constant was found. Both 1:1 and 2:1 β-CD:CTAB complexes were found.

In the present study, the efficiency of α-CD and β-CD (differing in size by one glucose unit and subsequently also in the effective size of the hydrophobic cavity) as well as 2-hydroxypropyl-β-CD (the 2-HP substitution increases the water solubility substantially) of various degree of substitution in the DNA decompaction process of DNA previously compacted by CTAB is investigated. The decompaction process is studied by fluorescence microscopy and fluorescence spectroscopy as well as by density and sound velocity measurements. Furthermore, the possibility of direct interactions between DNA and CD is studied by thermal melting and circular dichroism. Additionally, macroscopic phase separation studies are also being performed.

This novel approach in DNA decompaction makes it possible to control the conformation of DNA without introducing new surfactant structures into the solution and we believe it could be of interest from a gene therapy perspective. (Björn Lindman, Jonas Carlstedt, Rita Dias (University of Coimbra, Portugal), Alfredo González-Pérez (MEMPHYS, SDU, Denmark))

DNA gel nanoparticles. DNA phase separates associatively with many oppositely charged cosolutes, including surfactants, polyelectrolytes and proteins. By local arrest of the phase separation well-defined particles of long-term stability can be formed in a size range from millimetres to 100 nanometers. DNA gel particles have been produced inter alia with cetyltrimethylammonium bromide, lysozyme and chitosan. The entrapment of DNA can exceed 99 % and both single-stranded and double-stranded DNA can be used, with a preserved conformation in the particles. The particles are characterized with respect to size and size distribution as well as internal structure. The time-dependent release of DNA is investigated as well as the possibility of utilizing the particles for gene transfection. (Björn Lindman, Carmen Morán & Maria Miguel (Coimbra University))

Structure and Self-Assembly of Viruses. The project comprises studies of the packaging of DNA inside viral capsids using a density functional theory and constitutes an extension of previous computer simulations of polymers in confined geometries at the Division of Physical Chemistry. Of special interest is to investigate the liquid-crystalline transition in the spherical capsid and elucidate possible conformation transitions of DNA in confined geometry.

A density functional theory of packaging of double stranded DNA inside a viral capsid is developed. The main idea of the work is to apply the mathematical apparatus elaborated in the theories on nematic ordering [1, 2] to describe the arrangement principles of a long persistent polymeric chain under the conditions of confined geometry. In this case the local self-assembly of different segments of the chain can be considered as a liquid-crystalline phase with non-constant (distorted) director. To take into account the energy of nematic distortion, the elastic continuum theory has been used. The director of the ordered nematic phase was specified for the particular case of bend distortion, which models the well-known spool-like [3] conformation of DNA inside a spherical viral capsid. The elastic constant of the bend distortion was calculated in accordance with Grosberg's method [4].

The developed density functional theory accounts for excluded volume interactions in Onsager's second virial approximation [1, 2]. The inhomogeneous free-energy functional was minimized with respect to polymer density and order parameter of DNA segments. As a result, the polymer density and orientational order distribution profiles throughout the volume of capsid were obtained.

At the present moment the predictions of the theory are being explored and comparison with experimental data is in progress. (Nikolay N. Oskolkov, Per Linse, Alexei R. Khokhlov (Moscow university))

The skin as a barrier to molecular diffusion. The upper part of the human skin, stratum corneum, is one important example of a responding barrier membrane in biology. The skin can be exposed to rather extreme gradients in water, temperature and in other species, and these gradients may affect the molecular structure in the barrier membrane. One example of this is that the water flux through skin shows nonlinear response to variations in water activity with a distinct decrease in permeability at water activities below 0.85-0.9. This non-linearity indicates a structural change in the skin that also alter the transport properties in a profound way.

The main goal of this project is to couple stratum corneum barrier properties to stratum corneum lipid structure, and to explore how this is affected by, e.g. hydration, "moisturizers". These studies aim to understand how molecular diffusive transport occurs through the SC and thus how it can be affected.

We aim at the characterization of the lipid component of the stratum corneum and in model lipid membranes under varying conditions, using NMR and sorption calorimetry. This is combined with transport studies of different drugs across intact stratum corneum under the same conditions. (Sebastian Björklund, Emma Sparr, Agnieszka Nowacka, Daniel Topgaard, Johan Engblom (Malmö university), Krister Thuresson (Camurus AB), Lars Wadsö (Building materials, LTH), Joke Bouwstra (Leiden university), Vitaly Kocherbitov (Malmö University))

DNA-lipid complexes. DNA-lipid interactions play a significant biological and biotechnological role but remain poorly understood. In investigations of mixed lipid-DNA systems a novel bicontinuous cubic phase, composed of lecithin, water and dodecyltrimethylammonium with DNA as counterion (DNA-DTA), was identified. In the same system also, a lamellar phase and normal and reverse hexagonal phases are formed. Model calculations indicate that the cubic phase is normal, i.e. being composed of DNA chains and water incorporated in polar group bilayers separating two hydrophobic domains containing hydrocarbon tails of lipids. Work is extended to other DNA-lipid systems. (Azat Bilalov, Ulf Olsson, Björn Lindman)

Lipid chain freezing in dilute vesicle dispersions. In this project we investigate the thermal behavior of lipids in dilute dispersions of uni-lamellar vesicles. Main focus is on charged lipids. As the main model system, we have chosen the long chain synthetic lipid octadecyl dimethyl ammonium bromide, DODAB. However, also other lipids have been investigated. Lipid bilayers may often undergo several transitions as a function of the temperature. Cooled below the so called main transition, Tm, the alkyl chains stretch and form a viscous glass-like, still disordered, state. Decreasing the temperature further there may be one or several additional sub-gel transitions where the chains pack in a more ordered lattice. The DODAB system show a main transition at ca. 40 °C and sub-gel transition at ca. 36 °C. The formation of the gel phase is very rapid, and behave essentially as barrier free. In the formation of the subgel phase, on the other hand, a significant barrier is involved, and the gel phase can be super cooled more than 20 °C before the sub-gel formation can be observed.

The thermal behavior of charged lipids is also dependent on the vesicle size. A most striking observation is that for small (≈50 nm) vesicles there is an incomplete chain freezing when the vesicles are cooled below Tm. In large vesicles, the gel phase may easily nucleate and grow from several spots along the bilayer, and such vesicles are often found to be facetted or polyhedral shaped, resembling a poly-crystalline material, when imaged by cryo-TEM from lower temperatures.

In small vesicles, the number of nucleation events are few, perhaps only one or two. When a flat solid domain grows in a small vesicle, this results in an additional bending deformation the super-cooled remaining fluid part. If the bilayer bending rigidity is large, as it is for charged lipids, this additional curvature stress may be large enough to terminate the growth of the solid domain, leaving a gel-fluid coexistence in a single vesicle. The relative fractions of gel and fluid depends on the vesicle size and on the degree of super cooling. (Pieter Saveyn (Gent University), Ulf Olsson, Malin Zackrisson, Paul van der Meeren (Gent University), Teyencheri Narayanan (ESRF, Grenoble))

Peptide self-assembly. 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 not only for 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.

Here we study the self-assembly of small peptides into nanotubes, ribbons, fibres etc. The solvent is mainly water of varying pH and salinity, but also less polar solvents are used. A preliminary study performed on the short synthetic oligopeptide A6K in water, showed the formation of nano-tubes of a well defined diameter above a critical concentration. (see figure above) Because of the large aspect ratio, the tubes further assemble into a liquid crystalline phase, presumably of nematic ordering. (Celen Cenker, Ulf Olsson, Irem Nasir (Yeditpe University Istanbul), Seyda Bucak (Yeditpe University Istanbul), Ian Hamley (Univ. of Reading), Valeria Castalletto (Univ. of Reading) Mikael Lund, (Theoretical Chemistry), Malin Zackrisson))

Organizing molecular matter for specific functions

Adsorption of macromolecules to responsive surfaces. The adsorption of colloids of varying sizes and charges onto a surface that carries both negative and positive charges, representing a membrane, has been investigated using a simple model employing Monte Carlo simulations. The membrane was made of positive and negative charges (headgroups) that were allowed to move along the membrane, simulating the translational diffusion of the lipids, and were also allowed to protrude into the solution, giving rise to a fluid and soft membrane. When an uncharged colloid was placed in the vicinity of the membrane, a short-range repulsion between the colloid and the membrane was observed and the membrane deflected to avoid coming into contact with the colloid. When the colloid was charged, the membrane response was twofold: the headgroups of the membrane moved toward the colloid, as if to partly embrace it, and the positive headgroups of the membrane approached the oppositely charged colloid, inducing the demixing of the membrane lipids (polarization). The presence of protrusions enhanced the polarization of the membrane. Potential of mean force calculations showed that protrusions gave rise to a more long-range attractive colloid-membrane potential that had a smaller magnitude at short separations. (Per Linse, Rita Dias and Alberto A. C. C. Pais (University of Coimbra, Portugal))

Cryogenic transmission electron microscopy – imaging lyotropic liquid crystals. Cryogenic transmission electron microscopy is a powerful tool for investigating structures/particles in liquid samples. One major drawback is the sample preparation where specimens of viscous liquids are difficult or, in some cases, even impossible to prepare with the normal cryogenic plunge methodology. In this project the aim is to develop methodologies to prepare specimens of viscous samples, in particular of lyotropic liquid crystals. Lyotropic liquid crystals have structures (see inserted micrograph) equivalent to those formed by mesostructured silica materials (c. f. the OMM project Mesoporous silica – formation and functional materials). Electron micrographs offer unique information regarding the structure of materials as direct information is obtained (Both amplitude and phase are obtained as compared to diffraction which do not provide the phase information). The structures of mesoporous materials have been solved with electron microscopy using a methodology developed by Professor Osamu Terasaki and coworkers at Stockholm University (SU). In collaboration with the group at SU we will use this methodology for the study of structures formed by lyotropic liquid crystals. Other interesting aspects of liquid crystals that can be investigated are for instance domain sizes, intergrowths and defects. (Juanfang Ruan, Anna Carnerup, Viveka Alfredsson, Yasuhiro Sakamoto and Osamu Terasaki (Stockholm University), Matthias Mörgelin (Medicin, LU))

Mesoporous silica – formation and functional materials. In this project we are i) seeking an understanding of the mechanisms that control and make possible the formation of mesoscopically ordered silica materials and ii) functionalizing the silica surface to obtain a temperature sensitive material which can controllably uptake/release biomolecules by a "temperature switch".

i) The formation proceeds via a cooperative assembly process in water where amphiphilic molecules in the presence of an inorganic source self assemble into a material that is highly ordered on the mesoscopic scale yet atomically amorphous. Previous studies, mainly done with with in-situ SAXS, TEM and in-situ NMR, has taught us that the crystallisation follow a non-classical route, including a step where smaller particles organize in an oriented manner into larger silica flakes. This mechanism is now used to produce films of mesostructred materials.

ii) Once the structure directing amphiphile is removed a porous silica material remains. We are functionalizing the inner silica surface with a polymer whose hydrophilicity can be controlled by temperature. This composite material will be used as carrier for biomolecules. (Peter Linton, Nina Reichhardt, Viveka Alfredsson, Tommy Nylander, Håkan Wennerström, Vitaly Kocherbitov, (MaH), Beate Klösgen (SDU, Denmark))

Modeling of the adsorption of bottle-brush polymers onto surfaces. A new class of polymers composed of the monomers monomers poly(ethylene oxide) methyl ethyl methacrylate (PEO45MEMA) and methacryloxyethlyl trimethylammonimum chlorid (METAC) have recently been synthesized by Vareikis and coworkers. Depending on the momoner ratio, polymers continuously ranging from a highly charged polyelectrolyte to an uncharged bottle-brush polymer are available. Solution and as well as adsorption properties have this class of polymer are currently of large experimental interest.

To further understand the adsorption mechanism of this class of polymer onto various solid surfaces, we are currently performing model calculations using a lattice-mean field theory. We are able to capture the major experimental findings for adsorption on mica and on silica oxide and to provide further insight into the adsorption. (Per Linse and Per Claesson (KTH, Stockholm))

Scaling behavior of nanopatterned polymer brushes. Previously, we have investigated that the height of polymeric and biopolymeric nanostructures, fabricated by surface-initiated polymerization, depends dramatically on the feature foot-print size of the initiator pattern. More recently, we have analyzed experimental brush heights obtained for different foot-print sizes, polymer molecular weights, and surface grafting densities using recent scaling relations obtained from a coarse-grained model. We found good agreement between the experimental data and the theoretical predictions. Our results thus indicate that the scaling predictions provide a useful tool for the design and fabrication with polymeric and biomacromolecular nanostructures on surfaces. (Per Linse, Woo-Kyung Lee and Stefan Zauscher (Duke University, USA))

INSTRUMENTS AVAILABLE AT THE DEPARTMENT

NMR. (contact person: Daniel Topgaard). The department has Bruker AV-200 and AV-500 NMR spectrometers, both being equipped for high-performance diffusion studies. The AV-500 in addition has microimaging as well as solid-state and high-resolution magic-angle spinning capabilities. (Sponsored by VR/KFI).

Dynamic and static light scattering. (contact person: Karin Schillén).

Light scattering equipments

1) 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 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 20° to 150°, a cell housing with an cylindrical quartz vat (filled with a refractive-index matching liquid, toluene), 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, the latest ALV-7004 multiple tau digital correlator is utilized to produce the time pseudo-cross correlation function of the scattered intensity. It has an initial real sampling time of 25 ns and a lag time range that extends from 25 ns to up to 54975.6 s, which makes it possible to detect 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 differential refractometer with one He-Ne laser from ALV for the determination of refractive index increments necessary for the SLS experiments. (Sponsored by the former Swedish Natural Science Research Council, NFR, and by Knut and Alice Wallenbergs Stiftelse, KAW.)

2) For convenient DLS and SLS measurements and determination of eletrophoretic mobility (or zetapotential), a Zetasizer Nano ZS from Malvern Instruments Ltd, Worshestershire, UK, is available. The instruments measures DLS and SLS at a set angle of 173° using the NIBS technology. The zetapotential (or electrophoretic mobility) measurements using M3-PALS technology are performed at 17°. The laser used is a 4 mW He-Ne laser (632.8 nm) and the detection unit comprises an avalanche photodiode. The temperature range of the instrument is 2-90 °C. (Sponsored by Crafoordska Stiftelsen.)

3) 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.)

Surface force apparatus. (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).

Surface film balance. (contact person: Tommy Nylander). 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. In addition 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 (Sponsored by Crafoord Foundation).

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 angles y and D, thus, 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).

Transmission electron microscopy with cryo facilities. (contact person: Viveka Alfredsson). At the national Centre for High Resolution Electron Microscopy (nCHREM) three electron microscopes are available. Two of the microscopes are operated at an accelerating voltage of 300kV and use a field emission gun as electron source: the JEOL3000F has many analytical possibilities, such as EDAX and EELS and the JEOL3000SFF is dedicated for protein crystallography and is equipped with a He-cooled stage. The third microscope is a Philips CM 120 bio-twin, dedicated for cryo-imaging. There are a number of different sample preparation equipments available at nCHREM. For more information, check out http://www.materialkemi.lth.se/nchrem/. (Sponsored by NFR, Crafoord Foundation and Knut and Alice Wallenberg foundation).

Multimode scanning probe microscope. (contact person: Tommy Nylander). A Multimode Scanning Probe Microscopy (Nanoscope-III) was purchased jointly by Physical Chemistry and the Department of Food Technology from Digital Instruments Inc. in April 96. The instrument can be operated as both a scanning tunneling microscope (STM) and an atomic force microscope (AFM). With its many configurations the instrument can scan and image a wide variety of samples with scan sizes from atomic level up to 125 by 125 microns. As an AFM, traditional contact mode experiments in air and liquid and TappingMode experiments in air have been available for many years. More recent equipment purchases allow users to image surfaces with TappingMode in fluid environments, perform lateral force microscopy (LFM) measurements of topography and friction, and make force measurements using a colloidal probe. In the latter mode, a spherical particle is adhered to an AFM cantilever and colloidal forces between the probe and surface in a fluid environment can be studied. Other force measurements are also possible using standard cantilevers or chemically modified cantilevers. (Sponsored by FRN).

SAXS. (contact person: Ulf Olsson). The instrument is a Kratky compact camera equipped with a linear position sensitive detector (MBraun, Graz), and a Seifert ID 3000 (3.5 kW) generator. Equipped with two separate detectors, the instrument may record, simultaneously, the scattered intensity at both 'low' and 'wide' angles. The wide-angle (q-range 1.3--1.8 1/Å) scattering reports on short-range correlations and is helpful for example in discriminating between fluid and frozen surfactant chains. (Sponsored by FRN).

Optical microscopy. (contact person: Ulf Olsson). The Department has a Zeiss Axioplan Universal microscope equipped with differential interference contrast and a 35 mm photo camera MC 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, Argus 20, (Hamamtsu Photonics, Japan) together with the Macintosh-based image analysis software. (Sponsored by FRN & Crafoord Foundation).

Calorimeters. (contact person: Gerd Olofsson). A double twin isothermal microcalorimeter for the simultaneous determination of sorption isotherms and differential sorption enthalpies of vapors on solids. Isothermal titration microcalorimeter 2277 TAM Thermal Activity Monitor System.

Rheometers. (contact person: Ulf Olsson). A Carri-med controlled stress rheometer CSL 100 temperature controlled by a Peltier system. Measuring systems; cone and plate (solvent trap) in acrylic (4 cm, 1° and 6 cm, 1°) and stainless steel (4 cm, 1° and 6 cm, 1°). (Sponsored by Nils and Dorthi Troëdsson Research Foundation). A Physica UDS 200 controlled stress rheometer. Measuring systems temperature controlled by a Peltier system; cone and plate in acrylic (2.5 cm, 1°, 5 cm, 1°, 7.5 cm, 1°), cone and plate in stainless steel (2.5 cm, 1°, 5 cm, 1°, 7.5 cm, 1°), plate and plate in stainless steel (2.5 cm and 5 cm). Measuring systems temperature controlled by a cylindrical temperature system and an external water bath; cup and bob (2.5 cm) and a double gap measuring device, both in stainless steel.

SAXS at MAX. The Physical Chemistry department, in particular through Malin Zackrisson and Ulf Olsson continue to work with Yngve Cerenius concerning the devlopment of the beam line I711 at Max-lab and the possbilities there for small angle scattering experiments (SAXS). The beamline is now fully operational on SAXS but e.g. sample environment is continuously upgraded, with the aim to develop it into a first class SAXS instrument. For further details on the SAXS instrument see the I711 home page at http://maxsun5.maxlab.lu.se/beamlines/bli711/ .

COLLABORATIVE RESEARCH PROGRAMS

POLYSURF

This is a Transfer of Knowledge (TOK) Development Scheme (DEV) funded within the Marie Curie Program of the European Union. The overall objective of the project is to increase the knowledge and research level of the host organisation, Institute of Textiles at the University of Maribor, on the creation of tailored and/or smart fibre forming polymers and materials that would be able to control the release of various active compounds or to create new tailored fibre surface properties for different end-applications in the area of technical textiles, such as medical, therapeutic, hygienic and protective textiles. The project will transfer knowledge of innovative fibre surface modification technologies based on (WP2) colloidal micro-hydro-gelation, (WP3) nano-micro-(en)capsulation and (WP4) polymer surface coating. Additionally, (WP1) innovative biotechnological, green-chemistry, chemical and physical catalysis tools, or their combination will be applied to activate and/or modify polymer surfaces and/or colloidal particles/layers created using ecologically and toxicologically suitable processes. According to the diversity of the knowledge and expertise that shall be transferred, the project will build a highly multidisciplinary scientific group, cutting across different established research areas, i.e. textile chemists, physical chemists, biological catalysts and colloidal engineers, that will be able to prepare colloidal particles, coatings and multi-layers, and subsequently apply them to different suitably eco-pre-activated and/or modified natural and synthetic polymer surfaces. The new fibre materials with upgraded properties can be exploited either to enhance the bulk properties of existing products for better performance, or to create new value-added products with smart and/or tailored surface characteristics based on the multi-functionality. The project objective will be realised through training, module-based courses and several research activities by outgoing seconded and incoming recruited more experienced (MER) and experienced (ER) researchers that will be able to provide the necessary inputs in these areas. (B. Lindman)

Biopolymers based surfactants - stabilization and functionalization of particles and surfaces

The COST-project "Biopolymers based surfactants - Stabilization and functionalization of particles and surfaces" aims at increasing the knowledge of processes at surfaces and interfaces and factors tuning them at the molecular scale. An interdisciplinary effort to study the interaction of surfactants, derived from high and low molecular biological sources, with different kinds of substrates, as soft and hard particles and structured polymer surfaces, is envisioned. This activity will focus on the stabilization of the systems and the functionalisation of different surfaces. This has extended social and industrial interest as these results will provide advanced hygienic and technical materials as well as new insight into critical medical field, as for example the biocompatibility of implants. This requires a multidisciplinary approach i.e. synthesis and activation of materials, characterization and understanding of surface properties and processes at the molecular and supramolecular level. A theoretical description of these systems will allow to predict the properties of final products based on their chemical composition and the structure of the surface active compounds and substrates. Modification of these surfactants as well as the dispersed and macroscopic substrates will change their interaction abilities and functionalities. The results will enable us to understand, and ultimately control, the structure-property relationship and create new materials with excellent surface specificity. (B. Lindman)

The division of surface chemistry of the swedish chemical society.

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. The main activity of the Division is to organize the Annual Surface and Colloid Symposium in Lund. The aim of the 8th Symposium was to highlight the role of surface and colloid science for the synthesis and processing of advanced polymeric and inorganic materials. Four main topics were covered, namely, polymers and organic coatings, materials from renewable resources, porous materials and nanoparticles.

NEONUCLEI

The department was granted a 4 year EU-FP6 STREP in the NEST PATHFINDER project within Synhetic Biology, entitled "Self-assembly of synthetic nuclei: key modules for semibiotic chemosynthetic systems" (Acronyme NEONUCLEI and Contract no.12967) and coordinated by Prof. George Attard, University of Southampton, UK. NEONUCLEI will develop transcription-competent synthetic analogues of cell nuclei. These particles, termed neonuclei, will be obtained through self-assembly/organisation in mixtures of DNA, macromolecules (or nanoparticles), and lipids. The composition of the neonuclei will be chosen to produce particles with internal nano-architectures capable of sustaining gene transcription upon the addition of transcription factors. The DNA of the neonuclei will contain a gene cluster (or tandem repeats of the same gene). The genes will be separated by sequences designed to induce DNA compaction in response to specific chemical or physical stimuli. This will be exploited to establish non-biological control over the transcription of parts, or all, of the DNA. These control sequences offer the opportunity for multiple transcription control strategies and provide the capability of implementing temporally co-ordinated synthesis of multiple gene products. Neonuclei represent a key enabling step in the realisation of semi-biotic systems: these are systems and devices that combine synthetic non-natural functional systems with systems of biological origin. The neonuclei will be integrated with biological systems, or with isolated components, to produce novel semi-biotic devices capable of the controlled in situ synthesis of complex bio-molecules on demand. Physical Chemistry mainly contributes in providing understanding formation, morphology and structure of relevant self-assembly structures, DNA-surfactant/particle interaction, DNA compaction, morphology and structure of formed entities (T. Nylander, V. Alfredsson, B. Lindman, U. Olsson, H. Wennerström).

BIOCONTROL

EU Marie Curie research training network "BIOCONTROL" aims at controlling biological functions at, respectively on, bio-interfaces. It is based on the recent recognition of the importance of structure and properties of bio-interfaces, e.g. biological membranes, for a multitude of life processes. We now know that the evolution of atherosclerosis, cancer, immunity and viral infections, neurodegenerative disorders (Alzheimer, Prion diseases, etc.) and aging depend on perturbations of such interfaces. However, we need to improve our knowledge of the underlying molecular mechanisms in order to design efficient drugs and to meet the challenges in regenerative medicine and tissue engineering. This requires a deeper understanding of processes and interactions at bio-interfaces in terms of biology, biochemistry, biophysics and structure. The two major scientific objectives of BIOCONTROL are to: Provide fundamental knowledge of the forces and molecular mechanisms that regulate the interactions and biological processes taking place in and around biological membranes. Construct bio-mimetic surfaces and self-assembled structures that enable external control of biological and biotechnological processes, such as, cell adhesion and cell cycle regulation. Real progress in the field can only be achieved by breaking traditional academic borders. This requires the education of new researchers that are trained in cross-disciplinary and collaborative work. Therefore the major educational objective of BIOCONTROL is to train of a new category of 'life science' experts who can work across disciplines. This will be achieved by an unprecedented interdisciplinary training programme comprising (bio)physicists, biologists, (bio)chemists, surface chemists and computational biologists. (T. Nylander, V. Alfredsson). (http://biocontrol.tau.ac.il/)

SOCON

EU Marie Curie research training network "SOCON" focus on aqueous films, which are either confined between two solid surfaces or by air (foam film) or oil (emulsion film), respectively. SOCON put emphasis on complex self-organising systems of environmentally friendly components, such as sugar-based surfactants and polymeric carbohydrate derivatives, but we will also use traditional surfactants and polymers. The interest in the former class of surfactants and polymers is motivated by the fact that they can be made from renewable materials and that they have favourable properties with respect to applications in various fields. Most applications explore surfactant mixtures as well as surfactant-polymer mixtures. Hence, to advance the increased use of more environmentally friendly components synergistic and antagonistic effects in multicomponent systems have to be understood. In fact, this is one essential element of the joint network research. The wide range of systems which will be examined have in common self-assembly and strong surface activity. The four main objectives of the network are to: determine the relation between self-assembled structures in bulk solution, at one interface, and confined between two interfaces. SOCON will advance the understanding of the relations between changes in self-organised structures due to confinement and surface forces. This includes how the nature of the interface influences self-assembled surface structures and thus surface interactions. The emphasis will be on multicomponent systems. understand, predict, and control trapped non-equilibrium structures at interfaces and the corresponding surface forces. establish the correlation between properties of single films and complex colloidal systems. This includes macroscopic foams, emulsions and dispersions. promote the use of new environmentally friendly compounds in products and processes based on complex colloidal systems. For this purpose novel composite polymers and surfactants will be synthesized from natural building blocks. (P. Linse, T. Nylander). (http://www.mcrtn-socon.org/)

NANOGROWTH

This EPSRC (UK) founded project studies the fundamental aspects of crystal growth in nanoporous materials. It involves the application of a powerful set of complementary techniques to the study of crystal growth of open-framework materials comprising: atomic force microscopy, high resolution transmission and scanning electron microscopies, in-situ NMR with enhanced data processing, X-ray diffraction and mass spectrometry. A substantially better understanding of the synthesis process is likely to yield important economic benefits, for example, better process control, increased efficiency in reagent usage, improved reproducibility and the capacity to modify or tailor products for specific applications. (V. Alfredsson) (http://www.ucl.ac.uk/nanogrowth/index.htm)

Conferences, Travels and Seminars

Björn Lindman gave plenary lectures at the Polyelectrolytes 2008 conference, Coimbra, Portugal, the Austrian-Slovenian Polymer Meeting, Graz, 7th Liquid Matter Conference, Lund, Sweden, and 22th Conference of the European Colloid and Interface Society (ECIS2008), Cracow Poland, and keynote or invited lectures at CESIO 2008 – 7th World Surfactants Congress, Paris, the International Conference on Physical Organic Chemistry, ICPOC-19, Santiago de Compostella, Spain, the17th International Symposium on Surfactants in Solution (SIS), Berlin (2 lectures), and the Dynamical Arrest Conference, Taormina, Sicily. He also gave talks at the COST workshops on “Biopolymer based surfactants – stabilisation and functionalisation of particles and surfaces” at Schloss Seggau, Austria and Rome, Italy. He also attended the Semi - Biotic Systems Conference in Malta. During the year Björn Lindman visited a number of universities and other research centers and in most cases he presented a lecture. The institutions visited included: University of Maribor, Slovenia; University of Florence, Italy; BASF Research Center, Ludwigshafen, Germany; Procter & Gamble Research Centers, Cincinnati; Novo Nordisk, Copenhagen; Ecole des Mines de Paris, Sophia Antipolis, France; Karl-Franzens-Universität Graz, Austria; University of Santiago de Compostela, Spain; Åbo Akademi University, Turku, Finland; Beiersdorf Research Center, Hamburg, Germany; Cognis Research Center, Düsseldorf, Germany; Greenwich University, U.K.; University of Palermo, Italy; Università La Sapienza, Rome, Italy; Akzo Nobel Surface Chemistry, Stenungsund, Sweden; GlaxoSmithKline Research Center, Weybridge, UK; Björn Lindman also visited national research councils in conjunction with reviewing research proposals. Björn Lindman was visiting professor at the Department of Chemistry, Coimbra University, Portugal.

Håkan Wennerström gave invited presentations at AKZO_Nobel, Sassenheim, The Netherlands, Metting of the Swedish Theoretical Chemistry Society, Vålådalen and Dynamical Arrest conference in Taormina, Sicily.

Ulf Olsson gave invited talks at the Nanotech Europe 2008 conference in Copenhagen and at the Procter and Gamble Minisymposium on concentrated dispersions in Bruxells. He was also invited to the brainstorming meeting UPBL9 on the ESRF Upgrading Beamlines dedicated to time-resolved scattering/diffraction experiments. He also participated in the following meetings: the 5th Nordic Workshop on Scattering from Soft Matter in Trondheim, the annual meeting of the Swedish Neutron Scattering Society in Stockholm, the deGennes Days in Paris, ECIS 2008 in Krakow, the annual MAX-lab User Meeting in Lund and the 8th Annual Surface and Colloid Symposium in Lund.

Per Linse gave a invited oral presentation at the 8th Annual Surface and Colloid Symposium, Lund, Sweden.

Lennart Piculell gave two lectures at the 10th course on “Glycosciences”, an international summer course organized by the graduate school VLAG in Wageningen, the Netherlands and two lectures at “Polyelectrolytes - assembly interfacial and solution properties”, a national course organized by the Chalmers Soft Matter Graduate School. Lennart also gave a plenary lecture at the international conference “Polyelectrolytes 2008” in Coimbra, Portugal and plenary and keynote lectures at the Joint Polymer and Colloid and Surface Science Global Community of Practice Symposium in at Procter & Gamble, Cincinnati, USA.

Olle Söderman gave an invited talk at the European Detergents Conference

(EDC) held in Würzburg. He presented a seminar during a visit with Reinhard Strey, Physical Chemistry, Cologne university.

Tommy Nylander gave invited talks at Polymer and Colloid & Surface Science COP, Procter & Gamble, Cincinnati, USA 21-24 April 2008; ILL symposium on "Surface and Interfaces in Soft Matter and Biology: The Impact and Future of Neutron Reflectivity, Institute Laue Langevin, Grenoble France, 21-23 of May 2008; Keynote lecture at Surfactant in Solution Conference, Berlin, Germany, 18-22 August 2008; Institute Laue Langevin, Grenoble France, 11 September 2008; SPARK workshop, Unilever, Port Sunlight, UK 16-17 September; Meeting to celebrate the Barry Ninham Chair of Natural Science, Australian National University, Canberra, Australia, 8 December 2008; Materials and Complexity VI, ANU, Kioloa, Australia 9-12 December 2008.

Karin Schillén presented two posters at at each of the following three conferences: 7th Liquid Matter Conference, Lund, Sweden; ECIS2008, Cracow, Poland and at 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for Advanced Materials", Lund, Sweden.

Viveka Alfredsson gave an invited seminar in the Department of Materials Science and Metallurgy, University of Cambridge, UK.

Emma Sparr gave an invited lectures at the conference "Controlling drug delivery" organized by Läkemedelsverket, Lund, Sweden, and on "Biomembranes" at Nano2Life Research School (European Network of Excellence in nanobiotechnology), Lund, Sweden.

Daniel Topgaard gave oral presentations at Second workshop on soft matter, Coimbra, Portugal and at American Chemical Society 236th National Meeting, Philadelphia, USA

Ola Karlsson presented posters at 48th Microsymposium Polymer Colloids: From Design to Biomedical and Industrial Applications, Prauge, Czech Republic and at 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for Advanced Materials", Lund, Sweden.

Bruno Silva presented posters at Fifth Nordic workshop on scattering from Soft Matter, Trondheim, Norway and at ECIS2008.

Nikolay Oskolkov presented posters at the 7th International Symposium on Polyelectrolytes (Polyelectrolytes 2008), Coimbra, Portugal; 7th Liquid Matter Conference, Lund, Sweden and 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for Advanced Materials", Lund, Sweden

Marie-Louise Ainalem (neé Örberg) gave oral presentations at the Nordic Soft-Matter Scattering meeting, Trondheim, Norway, at the 12th Swedish Neutron Scattering Society meeting, Stockholm, Sweden, as well as at "Surfaces and interfaces in soft matter and biology", in honor of Robert K. Thomas, ILL, France. Oral seminars were in addition presented at the 7th NEONUCLEI meeting, Krapperup, Sweden as well as at the 8th NEONUCLEI meeting on Malta.

Jonas Carlstedt visited University of Coimbra, Portugal were he gave a talk. He also gave an oral presentation at the Neonuclei meeting, Krapperup. Sweden and presented posters at Polyelectrolytes 2008, Coimbra, Portugal; Liquid matter conference, Lund, Sweden; Semi-biotics conference, Malta and 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for Advanced Materials", Lund, Sweden

John Janiak presented posters at 7th Liquid Matter Conference, Lund, Sweden and at 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for

Advanced Materials", Lund, Sweden.

Niklas Källrot presented posters at the 6th International Symposium of Molecular Order and Mobility in Polymer Systems, St Petersburg, Russia and at Polyelectrolytes 2008, Coimbra, Portugal.

Luis Pegado gave an oral presentation at the "7th Liquid Matter Conference" in Lund, Sweden and presented a poster at the workshop "Electrostatic effects in soft matter" in Barcelona, Spain.

Salome Santos gave an oral presentation at Polyelectrolytes 2008, Coimbra, Portugal and presented a poster at the "7th Liquid Matter Conference" in Lund, Sweden.

Joakim Stenhammar presented posters at the ESF workshop Electrostatic Effects in Soft Matter, Barcelona, Spain; 7th Liquid Matter Conference, Lund, Sweden and 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for Advanced Materials", Lund, Sweden.

Christoffer Åberg presented posters at 7th Liquid Matter Conference, Lund, Sweden and at 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for Advanced Materials", Lund, Sweden.

Ingrid Åslund delivered an oral presentation at 9th Magnetic Resonance in Porous media, Cambridge, MA, USA and presented a poster at 8th Annual Surface and Colloid Symposium "Surface and Colloid Science for Advanced Materials", Lund, Sweden

External professional activities

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, The open Physical Chemistry Journal, 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 Royal Physiographic Society in Lund, and honorary corresponding member of Romaniae Scientiarium Societas. He is cofounder and honorary member of the European Colloid & Interface Society (ECIS). For the period 2006-2009 Björn Lindman is President of the International Association of Colloid and Interface Scientists (IACIS). He was also evaluator of research and training networks and research programs for the European Commission as well as evaluator of research programs for the Norwegian Research Council. He was external examiner for the Ph D thesis defences of Jorge Sarraguca, Coimbra University, Portugal and Rodrigo Brito, University of Porto, Portugal.

Håkan Wennerström is member of The Royal Swedish Academy of Sciences and The Royal Swedish Academy of Engineering Sciences; member of the Nobel Committee for Chemistry; member of NT-rådet; the board for science and technology within the Swedish Research Council and member of the boards for research development within Lund University.

Lennart Piculell is a section editor for the Polyelectrolytes section of Current Opinion in Colloid and Interface Science, a member of the editorial board of Carbohydrate Polymers, and a member of the international organizing committee of the biannual International Polyelectrolyte Symposia. He is a member of the board of the Department of Chemistry at Lund University and the Chairman of the Division of Surface Chemistry of the Swedish Chemical Society. He was also on the program committee and the local organizing committee of the annual three-day 8th annual surface and colloid science symposium, organized by Division of Surface Chemistry and Physical Chemistry, that took place in November in Lund, with 116 registered participants. He is a member of the program committee for Formula VI, an international conference to be held in Stockholm 2010. He is the director of the Linnaeus center OMM. He served in 2008 as a faculty opponent at the PhD defense of Rikard Lingström at KTH in Stockholm, and as a member of the grading committee at the thesis defense of Martin Turesson, Theoretical Chemistry, Lund University.

Tommy Nylander was external examiner for the PhD thesis of Pedro Reis, Chalmers University of Technology, Gothenburg 5 May 2008 and Csaba Kotsmár, Physical Chemistry, University of Potsdam, Germany, December 2007. Tommy Nylander was a chairman of the expert panel for Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning 2008 and he is also a member of Subcommittee 9 of the Scientific Council at Institute Laue Langevin, Grenoble France. Tommy Nylander was member of Scientific Advisory Group as well as the Stake Holder Advisory Group for ESS- Scandinavia

Karin Schillén was external examinator for the PhD thesis of Lone Weilby, Department of Science, Systems and Models, Roskilde University, Denmark and Atoosa Maleki, Department of Chemistry, University of Oslo, Norway. Karin also served on PhD thesis committee for Sanja Bulut, Lund University and was deputy member of the board of the Department of Chemistry.

Viveka Alfredsson was external examinator for the PhD thesis of Steven Hant, University of Southampton, UK. Viveka also served on PhD thesis committee for Keiich Miyasaka, Stockholm University, Markus Nilsson, Lund University and Juanfang Ruan, Stockholm University.

Emma Sparr served on PhD thesis committee for Pauline Vandoolaeghe, Lund University and Andreas Dahlin, Chalmers. Emma was member of a review panel in the committee for physical and theoretical chemistry of the national research council. Emma held popular science seminars at the Science Faculty day and at the KILU department day.

Daniel Topgaard served on the PhD thesis committee for Ulrika Brath, Biophysical Chemistry, Lund University.

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 on all courses given by the division. Johan Reimer has the main part of his position within the undergraduate education, where he among other things administrates the first-year chemistry courses.

The first year of chemistry studies at the Chemical Center 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 chemistry course during the spring semester, Viveka Alfredsson, Emma Sparr, Johan Reimer and Per Linse were involved in lectures and leading exercises and question hours, whereas Viveka Alfredsson, Daniel Topgaard and Johan Reimer gave the course during the fall semester. The topic of the first-year physical chemistry course is thermodynamics and quantum mechanics. 2008 was the first year this course was given in its new re-organized form and it is based on the book of P.W. Atkins

"Physical Chemistry". Karin Schillén is the head teacher for this course and she gave the lectures in thermodynamics and the exercise sessions in thermodynamics were given by Christoffer Åberg.

As regards higher courses, the division gives one basic and one advanced course in surface and colloid chemistry and two advanced physical chemistry courses. The introductory colloid and surface chemistry course is headed by Ulf Olsson and was taught by Ulf and Lennart Piculell. The advanced surface and colloid chemistry course, given during the fall semester, was taught by Lennart Piculell (main teacher) along with Tommy Nylander, Emma Sparr, Christoffer Åberg and Håkan Wennerström. This course is based on the text book "The Colloidal Domain" by Fennell Evans and Håkan Wennerström. Two advanced physical chemistry Master courses were given during the spring semester by Daniel Toopgaard (nuclear magnetic resonance, NMR, techniques) and Ulf Olsson (scattering techniques). Christoffer Åberg gave also the exercise sessions at the Master course "Chemist's Modelling Tools".

Finally, Björn Lindman was one of the teachers at the annual course on surfactants and polymers in aqueous solution, this year given in Lisbon and he also taught courses at Coimbra University, Portugal and at a national course at Åbo Academi University, Finland. Lennart Piculell delivered three popular lectures at "Naturvetenskap- och teknikdagar för gymnasister" in March, a series of lectures in science and engineering aimed at Swedish high school students. Per Linse and Lennart Piculell organized a one-week international PhD course "Polymer in Solutions" at Örenäs Castle. Håkan Wennerström contributed to the graduate course: How to write research application at the Science faculty.

7TH LIQUID MATTER CONFERENCE

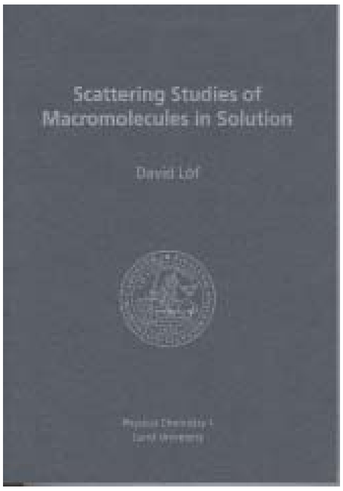
Under the auspices of the European Physical Society a Liquid Matter Conference is held every third year. Lund had been selected as the venue for the 2008 meeting. The conference was held June 27th to July 1st and the presentations were given at the Student union house, the University aula and at Palestra all localized at the heart of the town close to the cathedral. The conference attracted close to 600 active participants. The scientific program was divided into eleven themes: Simple liquids: ionic and quantum liquids and liquid metals; Water and aqueous solutions; Liquid crystals; Polymers, polyelectrolytes and biopolymers; Colloids; Films, foams and surfactants; Confined liquids and interfacial phenomena, Supercooled liquids, glasses and gels; Phase transitions and nucleation; Non-equilibrium systems and rheology; Biological and biomimetic fluids. There were ten plenary lectures, 22 invited lectures and additionally more than 40 contributed talks. Additionally there were more than 450 posters presented in the student union building. The Liquids group of the European Physical Society also awarded Henk Lekkerkerker and Peter Pusey with the Liquids Prize and they both presented prize Lectures at the meeting.

The local organization was lead by Håkan Wennerström with strong support by Johan Reimer, Magnus Ullner, Jan Forsman, Johan Bergenholtz (Gothenburg) with invaluable assistance by post-doctoral and graduate students. The social highlight of the conference was the Conference Dinner held at the Chemical Center. A big thank goes to all who made the practical arrangements go so smoothly.

Håkan Wennerström

DOCTORAL THESIS

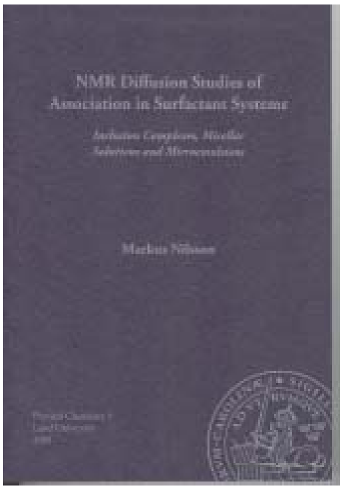
March 14, 2008
David Löf
Scattering Studies of Macromolecules in Solution.
Opponent: Prof. Stefan Egelhaaf,
Institut für Physik der kondensierten Materie,
Heinrich-Heine-Universität, Düsseldorf,
Germany



Scattering Studies of
Macromolecules in Solution

David Löf

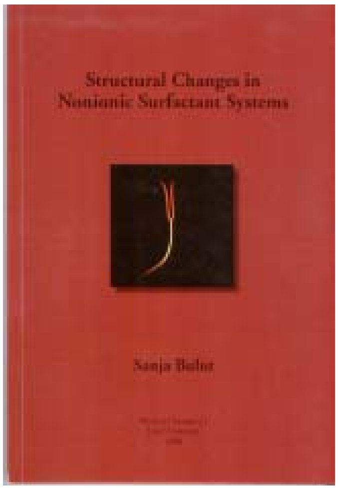
March 28, 2008
Markus Nilsson
NMR Diffusion Studies of Association in Surfactant Systems - Inclusion Complexes, Micellar Solutions and Microemulsions.
Opponent: Prof. Claudia Schmidt
Department Chemie, Universität Paderborn,
Germany



NMR Diffusion Studies of
Association in Surfactant Systems

Markus Nilsson

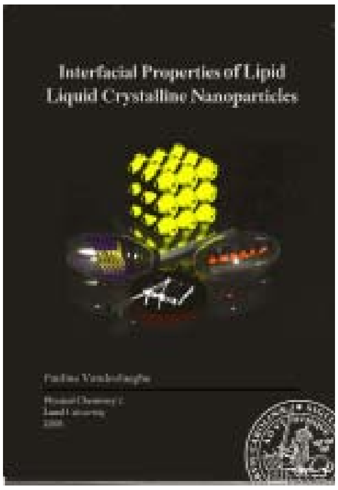
April 18, 2008
Sanja Bulut
Structural Changes in Nonionic Surfactant Systems.
Opponent: Assoc. Prof. Lise Arleth,
Department of Basic Sciences and Environment/
Biophysics, University of Copenhagen,
Denmark



Structural Changes in
Nonionic Surfactant Systems

Sanja Bulut

September 18, 2008
Pauline Vandoolaeghe
Interfacial Properties of Lipid Liquid Crystalline Nanoparticles.
Opponent: Prof. Ka Yee Lee,
Chemistry Department, University of Chicago,
USA



AWARDS

Björn Lindman received the Overbeek Gold Medal of the European Colloid & Interface Society.

Håkan Wennerström has been awarded the Celsius medal in gold, the Highest Award of The Royal Society of Sciences at Uppsala University.

The Board of the Division of Detergent Chemistry of the German Chemical Society honored Olle Söderman with the Award of the Division of the Detergent Chemistry.

Emma Sparr recieved an individual grant (SEK 8.5 million) for “Future Research Leaders” from The Swedish Foundation for Strategic Research (SSF). The grant is intended for innovative research and given young scientists who have the potential to and are prepared to become future leaders of academicand industrial research in Sweden

Daniel Topgaard received Innovation Prize by Öhrlings PricewaterhouseCoopers and LUAB (with Karin Bryskhe and Anna Stenstam, Colloidal Resource) and first price in Venture Cup South (with Karin Bryskhe and Anna Stenstam, Colloidal Resource) for the invention of OncoPulse.

MEMBERS OF THE DEPARTMENT

Scientists/Teachers

Viveka Alfredsson, associate prof.
Daniel Angelescu, postdoc
Azat Bilalov, postdoc
Anna Carnerup, postdoc
Alfredo Gonzáles Pérez, postdoc
Ola Karlsson, adjunct prof.
Ali Khan, associate prof. em.
Samo Lasic, postdoc
Björn Lindman, prof.
Per Linse, prof.
Dan Lundberg, postdoc
Maria G. Miguel, visiting prof.
Peter Nilsson, postdoc
Tommy Nylander, prof.
Gerd Olofsson, associate prof.
Ulf Olsson, prof.
Nikolay Oskolkov, postdoc
Lennart Piculell, prof.
Gabriel Rata, postdoc
Johan Reimer, lecturer
Juangfang Ruan, postdoc
Karin Schillén, prof.
Emma Sparr, assistant prof.
Olle Söderman, prof.
Fredrik Tiberg, adjunct prof.
Daniel Topgaard, assistant prof.
Stefan Ulvenlund, assistant prof.
Ingemar Wadsö, prof. em.
Hoa Wang, postdoc
Wei Wang, postdoc
Håkan Wennerström, prof.

Technical-Administrative Personnel

Barbro Hansson, administrator
Majlis Larsson, administrator
Ingegerd Lind, MSc, engineer
Lennart Nilsson, MSc, electrical engineer
Gull-Britt Odeskog, administrator

Graduate students working on a Ph. D. Thesis

Marie-Louise Ainalem
Mehran Asad Ayoubi
Johanna Bailey
Sebastian Björklund
Sanja Bulut
Jonas Carlstedt
John Janiak
Niklas Källrot
Peter Linton
David Löf
Markus Nilsson
Agnieszka Nowacka
Luis Pegado
Nina Reichhardt
Salomé Santos
Joakim Stenhammar
Pauline Vandoolaeghe
Agnes Zettergren
Christoffer Åberg
Ingrid Åslund

GUESTS

Ar, Gönül, Universität zu Köln, Germany (L)
Arleth, Lise, University of Copenhagen, Denmark
Attard, Phil, University of Sydney, Australia (L)
Baciu, Magdalena, Universität zu Köln, Germany (S)
Bilalov, Azat, Kazan State Technological University, Russia (L)
Black, Camilla, University of Southampton, UK (L)
Bode, Marieke, University of Utrecht, The Netherlands (L)
Bongartz, Nils, Universität zu Köln, Germany (L)
Bucak, Seyda, Yeditepe University Istanbul, Turkey (L)
Catanoiu, Gabriela, Universität zu Köln, Germany (S)
Cenker, Celen, Yeditepe University Istanbul, Turkey (L)
Clemens, Anna, RWTH Aachen, Germay (L)
Douezan, Stephane, ESPCI Paris, France (L)
Edwards, Mark, Glaxo Smith Kline, UK (S)
Eeman, Marc, Gembloux Agricultural University, Belgium (L)
Egelhaaf, Stefan, Heinrich-Heine-Universität, Düsseldorf, Germany (S)
Eryilmaz, Onur, , Turkey (L)
Ferreira, Tiago, University of Coimbra, Portugal (L)
Fras, Lidija, University of Maribor, Slovenia (L)
Gilliams, Richard, University of Southampton, UK (L)
Gracia, Louise, Glaxo Smith Kline, UK (S)
Gröber, Gerhard, Umeå University, Sweden (S)
Johansson, Christian, Uppsala University, Sweden (S)
Kabalnov, Alexey, Hewlett Packard, USA (S)
Kayali, Ibrahim, Al-Quds University, Jerusalem, Palestine (L)
Kayali, Khawla, Al-Quds University, Jerusalem, Palestine (L)
Khokhlov, Alexei, Moscow State University, Russia (S)
Krivtsova, Elena, Kazan State Technological University, Russia (L)
Küster, Simon, RWTH Achen, Germany (S)
Lee, Ka Yee, University of Chicago, USA (S)
Loh, Watson, University of Campinas, Brazil (S)
Lundberg, Dan, University of Coimbra, Portugal (L)
Machado, Alexandra, University of Coimbra, Portugal (L)
Majcen, Natasha, Glaxo Smith Kline, UK (S)
Max, Eva, University of Bayreuth, Germany (L)
Medronho, Bruno, University of Coimbra, Portugal (L)
Melnikov, Sergey, Unilever R&D Vlaardingen, The Netherlands (S)
Monduzzi, Maura, University of Cagliari, Italy (S)
Nasimova, Irina, Moscow State University, Russia (L)
Nasir, Irem, Yeditepe University, Turkey (L)
Nordenskiöld, Lars, Nanyang Technological University, Singapore (S)
Norrman, Jens, University of Coimbra, Portugal (S)

Persson, Rasmus, Astra Zeneca R&D Mölndal, Sweden (S)
Saveyn, Pieter, Ghent University, Belgium (S)
Savic, Ivana, Universität zu Köln, Germany (L)
Schelero, Natascha, TU Berlin Institut für Chemie, Germany (S)
Schmidt, Claudia, Paderborn University, Germany (L)
Silva, Bruno, University of Porto, Portugal (L)
Snowden, Martin, Glaxo Smith Kline, UK (S)
Štepánek, Petr, Inst. of Macromolecular Science, Czech Republic (S)
Stepisnik, Janez, Jozef Stefan Institute, Slovenia (S)
Suganuma, Yukiko, Ochanomizu University, Japan (L)
Tkavc, Tina, University of Maribor, Slovenia (L)
Tonigold, Katrin, Ulm University, Germany (L)
Valente, Artur, University of Coimbra, Portugal (S)
Yanez, Marianna, Universidad Simón Bolívar, Venezuela (L)
Zackrisson, Malin, Zürich, Switzerland (S)

(L)= Long-term (S)= Short-term

WELCOME TO VISITORS

Dear Visitor,

We receive many guests, who stay with us from a few hours or a day of discussions, seminar etc., to one or more years for postdocs and foreign students. Visitors are very important for us and help us to improve our level of research and education. Careful planning can significantly improve these visits. The Annual Report partly serves the purpose of introducing a person to our department prior to a call.

We hope to continue to have many visitors and here we give some information, which may be helpful for you if you plan to visit us.

To arrange a visit, you may contact an appropriate member of our department. Depending on the nature of the visit different arrangements may be made. Help with accommodation can be provided by Majlis Larsson. In many cases we have found that smaller, less formal seminars, lead to better information exchange.

The Chemical Center and Lund can be reached in many ways. Below we give some useful hints:

We recommend the visitors to fly to Kastrup Airport, Copenhagen. Then, take a train (frequency every 20 min.) from Kastrup Airport over the Öresund bridge to Malmö (30 min). At Malmö railway station, change to a local train (Pågatåg) to Lund railway station (15-20 min). You may take a taxi from Malmö to Lund (about 20 km). Also, there are few direct train connections between Copenhagen airport and Lund railway station.

PUBLICATIONS

(1) Angelescu, D.; Linse, P.
Modelling of icosahedral viruses.
Curr. Opin. Colloid Interface Sci. 2008, 13, 389-394.

(2) Angelescu, D.; Linse, P.; Nguyen, T. T.; Bruinsma, R. F.
Structural transitions of encapsidated polyelectrolytes.
Eur. Phys. J. 2008, 25, 323-334.

(3) Angelescu, D. G.; Linse, P.
Viruses as supramolecular self-assemblies: modelling of capsid formation and genome packaging.
Soft Matter 2008, 4, 1981-1990.

(4) Barauskas, J.; Cervin, C.; Tiberg, F.; Johnsson, M.
Structure of lyotropic self-assembled lipid nonlamellar liquid crystals and their nanoparticles in mixtures of phosphatidyl choline and alpha-tocopherol (vitamin E).
Phys. Chem. Chem. Phys. 2008, 10, 6483-6485.

(5) Barauskas, J.; Nylander. t.
"Microstructure of Lyotropic Lipid Liquid Crystals and Delivery Vehicles for Food Ingredients" (Ed. Garti, N.), In "Controlled release technologies for targeted nutrition" Woodhead Publishing Limited, Cambridge, UK (2008) pp. 107-131.

(6) Bulut, S.; Gonzalez Perez, A.; Olsson, U.
Cryo-fracture TEM: direct imaging of a random mesh phase.
Langmuir 2008, 24, 22-25.

(7) Bulut, S.; Hamit, J.; Olsson, U.; Kato, T.
On the concentration-induced growth of nonionic wormlike micelles.
Eur. Phys. J. 2008, 27, 261-273.

(8) Cardenás, M.; Nylander, T.
"Adsorption of DNA and DNA-surfactant complexes at solid surfaces" In Interaction of DNA with Surfactants and Polymers (Eds. Lindman, B. and Dias, R.) (2008), Blackwell Publishing, 291-315

(9) Cárdenas, M.; Schillén, K.; Alfredsson, V.; Duan, R.-D.; Nyberg, L.; Arnebrant, T.
Solubilization of sphingomyelin vesicles by addition of a bile salt.
Chem. Phys. Lipids 2008, 151, 10-17.

(10) Cifra, P.; Linse, P.; Nies, E.
Energy-driven asymmetric partitioning of a semiflexible polymer between interconnected cavities.
J. Phys. Chem. B 2008, 112, 8923-8927.

(11) Corkery, R. W.; Fogden, A.
On the formation and structure of nanometric polyhedral foams: Toward the dry limit.
Langmuir 2008, 24, 10443-10452.

(12) Costa, M. C.; Moran, M. C.; Miguel, M. G.; Lindman, B.
"Cross-linked DNA Gels and Gel Particles." In DNA Interactions with polymers and surfactants, edited by Rita Dias and Björn Lindman: Wiley, 2008. 353-365.

(13) Costa-Balogh, F. O.; Sparr, E.; Sousa, J. J. S.; Pais, A.
Drug Release and Skin Permeation from Lipid Liquid Crystalline Phases.
Prog. Colloid Polym. Sci. 2008, 135, 119-129.

(14) De Vico, L.; Pegado, L.; Heimdal, J.; Söderhjelm, P.; Roos, B.
The ozone ring closure as a test for multi-state multi-configurational second order perturbation theory (MS-CASPT2).
Chem. Phys. Lett. 2008, 461, 136-141.

(15) Deleu, M.; Paquot, M.; Nylander, T.
Effect of fengycin, a lipopeptide produced by Bacillus subtilis, on model biomembranes.
Biophysical Journal 2008, 94, 2667-2679.

(16) Dias, R.; Linse, P.
Colloid Adsorption onto Responsive Membranes.
Biophysical journal 2008, 94, 3760-3768.

(17) Dias, R.; Magno, L.; Valente, A.; Das, D.; Das, P.; Maiti, S.; Miguel, M.; Lindman, B.
Interaction between DNA and Cationic Surfactants: Effect of DNA Conformation and Surfactant Headgroup.
J. Phys. Chem. B 2008, 112, 14446-14452.

(18) Dias, R.; Miguel, M. G.; Lindman, B.
"DNA as an amphiphilic polymer." In DNA Interactions with polymers and surfactants, edited by Rita Dias and Björn Lindman: Wiley, 2008. 367-378.

(19) dos Santos, T.; Medronho, B.; Antunes, F. E.; Lindman, B.; Miguel, M.
How does a non-ionic hydrophobically modified telechelic polymer interact with a non-ionic vesicle? Rheological aspects.
Colloids Surf., A 2008, 319, 173-179.

(20) Edgecombe, S.; Linse, P.
Monte Carlo simulation of two interpenetrating polymer networks: Structure, swelling, and mechanical properties.
Polymer 2008, 49, 1981-1992.

(21) Erkselius, S.; Wadsö, L.; Karlsson, O.
Drying rate variations of latex dispersions due to salt induced skin formation.
J. Colloid Interface Sci. 2008, 317, 83-95.

(22) Ferreira, T.; Medronho, B.; Martin, R. W.; Topgaard, D.
Segmental order parameters in a nonionic surfactant lamellar phase studied with 1H-13C solid-state NMR.
Phys. Chem. Chem. Phys. 2008, 10, 6033-6038.

(23) Gaweda, S.; Moran, M. C.; Pais, A. A. C. C.; Dias, R.; Schillén, K.; Lindman, B.; Miguel, M. G.
Cationic agents for DNA compaction.
J. Colloid Interface Sci. 2008, 323, 75-83.

(24) Gonzalez Perez, A.; Dias, R.; Nylander, T.; Lindman, B.
Cyclodextrin-surfactant complex: A new route in DNA decompaction.
Biomacromolecules 2008, 9, 772-775.

(25) Gonzalez Perez, A.; Olsson, U.
Cryo-fracture TEM: direct imaging of viscous samples.
Soft Matter 2008, 4, 1625-1629.

(26) Greene, G. W.; Zappone, B.; Zhao, B.; Söderman, O.; Topgaard, D.; Rata, G.; Israelachvili, J. N.
Changes in pore morphology and fluid transport in compressed articular cartilage and the implications for joint lubrication.
Biomaterials 2008, 29, 4455-4462.

(27) Jadhav, V.; Maiti, S.; Dasgupta, A.; Das, P. K.; Dias, R.; Miguel, M.; Lindman, B.
Effect of the head-group geometry of amino acid-based cationic surfactants on interaction with plasmid DNA.
Biomacromolecules 2008, 9, 1852-1859.

(28) Jausovec, D.; Angelescu, D.; Voncina, B.; Nylander, T.; Lindman, B.
The antimicrobial reagent role on the degradation of model cellulose film.
J. Colloid Interface Sci. 2008, 327, 75-83.

(29) Karlson, L.; Olsson, M.; Boström, G.; Piculell, L.
Influence of added surfactant on particle flocculation in waterborne polymer-particle systems.
J. Coat. Technol. Res. 2008, 5, 447-454.

(30) Karlström, G.; Stenhammar, J.; Linse, P.
Effects of different boundary conditions on the long-range structure of polar liquids.
J. Phys.: Condens. Matter 2008, 20, 494204- 1--9.

(31) Kirsebom, H.; Rata, G.; Topgaard, D.; Mattiasson, B.; Galaev, I.
In situ H-1 NMR studies of free radical cryopolymerization.
Polymer 2008, 49, 3855-3858.

(32) Kocherbitov, V.; Ulvenlund, S.; Kober, M.; Jarring, K.; Arnebrant, T.
Hydration of microcrystalline cellulose and milled cellulose studied by sorption calorimetry.
J. Phys. Chem. B 2008, 112, 3728-3734.

(33) Leal, C.; Rognvaldsson, S.; Fossheim, S.; Nilssen, E. A.; Topgaard, D.
Dynamic and structural aspects of PEGylated liposomes monitored by NMR.
J. Colloid Interface Sci. 2008, 325, 485-493.

(34) Leal, C.; Sandström, D.; Nevsten, P.; Topgaard, D.
Local and translational dynamics in DNA-lipid assemblies monitored by solid-state and diffusion NMR.
Biochim. Biophys. Acta, Biomembr. 2008, 1778, 214-228.

(35) Leal, C.; Wennerström, H.
"Hydration of DNA-amphiphile complexes" in DNA interactions with plymers and surfactants, edited by R. Dias and B. Lindman: Wiley, USA 2008, 239-251

(36) Lindfors, L.; Forssen, S.; Westergren, J.; Olsson, U.
Nucleation and crystal growth in supersaturated solutions of a model drug.
J. Colloid Interface Sci. 2008, 325, 404-413.

(37) Lindman, B.; Dias, R.; Miguel, M. G.; Moran, M. C.; Costa, D.
"Manipulation of DNA by Surfactants " In Highlights in Colloid Science, edited by E. Platikanov and D. Exerowa, Weinheim: Wiley-VCH, 2008. 179-202.

(38) Linse, P.
Electrostatics in the presence of spherical dielectric discontinuities.
J. Chem. Phys. 2008, 128.

(39) Linton, P.; Alfredsson, V.
Growth and morphology of mesoporous SBA-15 particles.
Chem. Mater. 2008, 20, 2878-2880.

(40) Maleki, A.; Lafitte, G.; Kjoniksen, A.-L.; Thuresson, K.; Nyström, B.
Effect of pH on the association behavior in aqueous solutions of pig gastric mucin.
Carbohydr. Res. 2008, 343, 328-340.

(41) Marques, E.; de Oliveira Brito, R.; Silva, S.; Rodriguez-Borges, J.; Vale, M.; Gomes, P.; Araujo, M.; Söderman, O.
Spontaneous Vesicle Formation in Catanionic Mixtures of Amino Acid-Based Surfactants: Chain Length Symmetry Effects.
Langmuir 2008, 24, 11009-110017.

(42) Misiunas, A.; Talaikyte, Z.; Niaura, G.; Razumas, V.; Nylander, T.
Thermomyces lanuginosus lipase in the liquid-crystalline phases of aqueous phytantriol: X-ray diffraction and vibrational spectroscopic studies.
Biophys. Chem. 2008, 134, 144-156.

(43) Nilsson, L.; Löf, D.; Bergenståhl, B.
Phenolic Acid Nanoparticle Formation in Iron-Containing Aqueous Solutions.
J. Agric. Food Chem. 2008, 56, 11453-11457.

(44) Nilsson, M.; Valente, A. J. M.; Olofsson, G.; Söderman, O.; Bonini, M.
Thermodynamic and kinetic characterization of host-guest association between bolaform surfactants and alpha- and beta-cyclodextrins.
J. Phys. Chem. B 2008, 112, 11310-11316.

(45) Nylander, T.; Arnebrant, T.; Bos, M. A.; Wilde, P. "Protein-emulsifier interactions" In "Food emulsifiers and their applications", 2nd ed (eds. Hasenhuettl, G. L. and Hartel, R. W.) Chapman and Hall, New York (2008) 89-171.

(46) Nylander, T.; Campbell, R. A.; Vandoolaeghe, P.; Cardenas, M.; Linse, P.; Rennie, A. R.
Neutron reflectometry to investigate the delivery of lipids and DNA to interfaces.
Biointerphases 2008, 3, FB64-FB82.

(47) Pacios, I. E.; Lindman, B.; Thuresson, K.
Polyelectrolyte–surfactant complexes with long range order.
J. Colloid Interface Sci. 2008, 319, 330-337.

(48) Papancea, A.; Valente, A. J. M.; Patachia, S.; Miguel, M.; Lindman, B.
IPVA-DNA cryogel membranes: Characterization, swelling, and transport studies.
Langmuir 2008, 24, 273-279.

(49) Pegado, L.; Jönsson, B.; Wennerström, H.
Ion-ion correlation attraction in a molecular solvent.
J. Chem. Phys. 2008, 129, 184503.

(50) Pegado, L.; Jönsson, B.; Wennerström, H.
Like-charge attraction in a slit system: pressure components for the primitive model and molecular solvent simulations.
J. Phys.: Condens. Matter 2008, 20, 494235.

(51) Peron, N.; Campbell, R.; Nylander, T.; Vareikis, A.; Makuska, R.; Gilanyi, T.; Meszaros, R.
Competitive Adsorption of Neutral Comb Polymers and Sodium Dodecyl Sulfate at the Air/Water Interface.
J. Phys. Chem. B 2008, 112, 7410-7419.

(52) Piculell, L.; Norrman, J.; Svensson, A.; Lynch, I.; Bernardes, J. S.; Loh, W.
Ionic surfactants with polymeric counterions.
Adv. Colloid Interface Sci. 2008, 147-48 228-236.

(53) Ramos, S.; Campos-Terán, J.; Mas-Oliva, J.; Nylander, T.; Castillo, R.
Forces between Hydrophilic Surfaces Adsorbed with Apolipoprotein AII Alpha Helices.
Langmuir 2008, 24, 8568-8575.

(54) Rescic, J.; Linse, P.
Potential of mean force between charged colloids: Effect of dielectric discontinuities.
J. Chem. Phys. 2008, 129, 114505-1--9.

(55) Rosa, M.; Penacho, N.; Simoes, S.; Lima, M. C. P.; Lindman, B.; Miguel, M. G.
DNA pre-condensation with an amino acid-based cationic amphiphile. A viable approach for liposome-based gene delivery.
Mol. Membr. Biol. 2008, 25, 23-34.

(56) Sarraguca, J. M. G.; Pais, A. A. C. C.; Linse, P.
Structure of microemulsion - ABA triblock copolymer networks.
Langmuir 2008, 24, 11153-11163.

(57) Saveyn, P.; Cocquyt, E.; Sinnaeve, D.; Martins, J.; Topgaard, D.; Meeren, P.
NMR Study of the Sorption Behavior of Benzyl Alcohol Derivatives into Sonicated and Extruded Dioctadecyldimethylammonium Chloride (DODAC) Dispersions: The Relevance of Membrane Fluidity.
Langmuir 2008, 24, 3082-3089.

(58) Schillén, K.; Jansson, J.; Löf, D.; Costa, T.
Mixed Micelles of a PEO-PPO-PEO Triblock Copolymer (P123) and a Nonionic Surfactant ($C_{12}EO_6$) in Water. A Dynamic and Static Light Scattering Study.
J. Phys. Chem. B 2008, 5551-5562.

(59) Silva, B.; Marques, E.; Olsson, U.
Unusual Vesicle-Micelle Transitions in a Salt-Free Catanionic Surfactant: Temperature and Concentration Effects.
Langmuir 2008, 24, 10746-10754.

(60) Sparr, E.
“Osynlig rörelse.” In interdisciplinary antholgy “TEMPO”, edited by H. Sandberg and M. Cronqvist: Makadam förlag, 2008.

(61) Stengel, G.; Simonsson, L.; Campbell, R.; Höök, F.
Determinants for Membrane Fusion Induced by Cholesterol-Modified DNA Zippers.
J. Phys. Chem. B 2008, 112, 8264-8274.

(62) Stubenrauch, C.; Tessendorf, R.; Salvati, A.; Topgaard, D.; Sottmann, T.; Strey, R.; Lynch, I. Gelled polymerizable microemulsions. 2. Microstructure.
Langmuir 2008, 24, 8473-8482.

(63) Tauraite, D.; Razumas, V.; Nylander, T.; Butkus, E.
Interfacial behavior of ferrocene- and 1,4-naphthoquinone-based compounds, and their mixtures with monoolein at the air/water interface.
Z. Naturforsch., B: Chem. Sci. 2008, 63, 1093-1100.

(64) Terama, E.; Ollila, O.; Salonen, E.; Rowat, A.; Trandum, C.; Westh, P.; Patra, M.; Karttunen, M.; Vattulainen, I.
Influence of Ethanol on Lipid Membranes: From Lateral Pressure Profiles to Dynamics and Partitioning.
J. Phys. Chem. B 2008, 112, 4131-4139.

(65) Wadsö, L.; Anderberg, A.; Åslund, I.; Söderman, O.
An improved method to validate the relative humidity generation in sorption balances.
Eur. J. Pharm. Biopharm. 2008, 72, 99-104.

(66) Vandoolaeghe, P.; Rennie, A. R.; Campbell, R.; Thomas, R. K.; Höök, F.; Fragneto, G.; Tiberg, F.; Nylander, T.
Adsorption of cubic liquid crystalline nanoparticles on model membranes.
Soft Matter 2008, 4, 2267 – 2277

(67) Vandoolaeghe, P.; Rennie, A. R.; Campbell, R.; Nylander, T.
Neutron Reflectivity Studies of the Interaction of Cubic-Phase Nanoparticles with Phospholipid Bilayers of Different Coverage (dagger).
Langmuir 2008, 25, 4009–4020

(68) Zhang, J.; Nylander, T.; Campbell, R.; Rennie, A. R.; Zauscher, S.; Linse, P.
Novel evaluation method of neutron reflectivity data applied to stimulus-responsive polymer brushes.
Soft Matter 2008, 4, 500-509.

(68) Åberg, C.; Pairin, C.; Costa, F.; Sparr, E.
Responding double-porous lipid membrane: Lyotropic phases in a polymer scaffold.
Biochim. Biophys. Acta, Biomembr. 2008, 1778, 549-558.

(66) Åberg, C.; Wennerström, H.; Sparr, E.
Transport Processes in Responding Lipid Membranes: A Possible Mechanism for the pH Gradient in the Stratum Corneum.
Langmuir 2008, 24, 8061-8070.

(67) Åslund, I.; Cabaleiro-Lago, C.; Söderman, O.; Topgaard, D.
Diffusion NMR for Determining the Homogeneous Length-Scale in Lamellar Phases.
J. Phys. Chem. B 2008, 112, 2782-2794.

SEMINARS

Study of translational dynamics in water, confined fluids, and fluidized granular systems by novel NMR technique.
Janez Stepisnik, University of Ljubljana, Slovenia

NMR investigations of nematic liquid crystals in shear flow.
Claudia Schmidt, Department of Chemistry, University of Paderborn., Germany

A long and twisted journey of Cubic Membranes: from structure to function.
Yuru Deng, Dept. of Physiology, Yong Loo Lin School of Medicine National University of Singapore, Singapore

Interaction between Crosslinked Polyelectrolyte Gels and Oppositely Charged Surfactants.
Peter Nilsson, Dept. Pharmacy, Uppsala

Scattering Studies of Macromolecules in Solution.
David Löf, Physical Chemistry, Lund University, Sweden

Pathways and Kinetics of Surfactant Phase Transitions.
Stefan Egelhaaf, Institut für Experimentalphysik Heinrich-Heine-Universität Düsseldorf, Germany

Removal of fatty soils from hard surfaces by polymer - surfactant mixed solutions.
Daniel Angelescu, Physical Chemistry, Lund University, Sweden

NMR Diffusion Studies of Association in Surfactant Systems Inclusion Complexes, Micellar Solutions and Microemulsions.
Markus Nilsson, Physical Chemistry, Lund University, Sweden

The lateral structure of biological membranes and some lesson from model systems.
Luis A. Bagatolli, MEMPHYS - Center for Biomembrane Physics SDU, Denmark

Structural Changes in Nonionic Surfactant Systems.
Sanja Bulut, Physical Chemistry, Lund University, Sweden

Transport of DNA and latex-particles in liposome-nanotube networks.
Björn Åkerman, Chalmers University of Technology, Sweden

Small-angle scattering on bionanosystems.
Lise Arleth, Faculty of Life Sciences, University of Copenhagen, Denmark

Membrane-Protein Assemblies Involved in Diseases: A Biophysical Approach.
Gerhard Gröbner, Biophysical Chemistry, Umeå University

Self-assembled Structures Based in Hybrids Fluoro-Hydro surfactants.
Alfredo Gonzalez-Perez, Physical Chemistry, Lund University, Sweden

Luciferin chemistry: principles of chemiluminescence.
Roland Lindh, Chemical Physics, Lund University, Sweden

Diffusive Transport in Responding Lipid Membranes.
Christoffer Åberg, Physical Chemistry, Lund University, Sweden

Amorphous and crystalline drug nanoparticles.
Ulf Olsson, Physical Chemistry, Lund University, Sweden

Nanobubbles: From Little Things Big Things Grow.
Phil Attard, University of Sydney, Australia

Interfacial properties of lipid liquid crystalline nanoparticles.
Pauline Vandoolaeghe, Physical Chemistry, Lund University, Sweden

Collapse Mechanism of Lung Surfactant.
Ka Yee Lee, Institute för Biophysical dynamics, University of Chicago, USA

Applications of Colloidal Delivery Systems for Structural Design of Functional Foods.
Sergey Melnikov, Unilever Food and Health Research Institute. Vlaardingen, The Netherlands

Influence of pH on Aggregation Morphology of Multiheadgroup Surfactant and its Application in Assembling Nanostructure.
Wei Wang, Chinese Academy of Science, Beijing, China

Meso- and nanoscale analysis of the conditioning effect on human hairs
Eva Max, University of Bayreuth, germany

Electrostatic interactions in chromatin.
Lars Nordenskiöld, Nanyang Technological University, Singapore

Formation of Mesostructured Polymer-Surfactant Films at the Air-Solution Interface.
Karen Edler, University of Bath, UK

Self-association of polymers and surfactants in mixed solvents.
Petr Stepanek, Institute of Macromolecular Chemistry, Prague, Czech Republic

The liquid-crystalline ordering approach to the packaging of DNA inside viral capsids.
Nikolay Oskolkov, Physical Chemistry, Lund University, Sweden

Synthesis and Supramolecular Properties of New Inositol Surfactants
Nils Bongartz, University of Cologne

Microscopy study of porous materials
Ruan Juanfang, Division of Structural Chemistry, Stockholm University, Sweden

Thomas-Fermi One-Electron Analysis with Kohn-Sham Correction - New Insight into Atoms, Molecules and Reactivity of Metal Clusters
Sture Nordholm, University of Gothenburg, Sweden

The Dynamic Pathway of Polymer Adsorption
Niklas Källrot, Physical Chemistry, Lund University, Sweden

Gravitational Settling of Small Particles in Complex Geometries.
Alexey Kabalnov, Hewlett Packard, San Diego, USA

Control of DNA accessibility and gene expression by PAMAM dendrimers
Marie-Louise Ainalem, Physical Chemistry, Lund University, Sweden

The physical chemistry of respiration
Emma Sparr, Physical Chemistry, Lund University, Sweden

PATENT

Hallén, D. and Wadsö, I.
A device, method and vessel assembly for the measurement of heat flow at least for one sample. International publication number: WO 2007/139498 A1 (International publication date 2007-12-06).

MANUSCRIPTS

Ainalem, M.; Carnerup, A. M.; Janiak, J.; Alfredsson, V.; Nylander, T.; Schillén, K.
Condensing DNA with Poly(amido amine) Dendrimers: Means of Controlling Morphology and Size of the Formed Aggregates
Soft Matter, 2009, 5, 2310 - 2320

Antunes, F., Marques, E., Miguel, M., Lindman, B.
Polymer-vesicle association
Adv. Colloid Interface Sci., in press

Briggner, L.-E.; Céolin, R.; Giovannini, J.; Payraudeau.; Wadsö, I.
Design and testing of a small-scale sublimation apparatus.
J. Therm. Anal. Cal. In press

Costa, D.; Reischl, M.; Kuzma, B.;Brumen, M.; Zerovnik, J.; Ribitsch, V.; Miguel, M. G.; Lindman, B.
Modelling the surfactant uptake in cross-linked DNA gels
J. Disp. Sci. Techn., in press

Costa, D., Pais, A. A. C. C., Miguel, M. G., Lindman, B.
Cross-Linked DNA Gels: Degradation and Release Properties.
Submitted

Costa, T.; Miguel, M. da G; Lindman, B.; Seixas de Melo, J. S.; Schillén, K.
Complex Formation between a Fluorescently-Labeled Polyelectrolyte and a Triblock Copolymer
J. Phys. Chem. B 2009, 113, 6205-6214

Costa, T.; Schillén, K.; Miguel, M. da G; Lindman, B.; Seixas de Melo, J. S.
Association of a Hydrophobically-Modified Polyelectrolyte and a Block Copolymer Followed by Fluorescence techniques
J. Phys. Chem. B 2009, 113, 6194-6204

Costa-Balogh, F.O.; Sparr, E.; Sousa, J.J.S.; Pais, A.A.C.C
Drug release from lipid liquid crystalline phases: relation with phase behaviour
J Pharm, Submitted

Dias, R. S., Morán, M. C., Costa, D., Miguel, M. G., and Lindman, B.
DNA-surfactant systems: Particles, gels and nanostructures in Nano-science: colloidal background, V. M. Starov, Ed.,. Taylor&Frances, 2009,

Eeman, M.; Olofsson, G.; Sparr, E.; Nylander, T.; Paquot, M.; Deleu, M.
Thermodynamic changes associated with the interaction of fengycin, a biologically active lipopeptide, with stratum corneum mimicking membrane models
Biochim Biophys Acta, submitted

Eeman, M; Pegado, L ; Dufrene, YF ; Paquot M ; Deleu M
Influence of environmental conditions on the interfacial organisation of fengycin, a bioactive lipopeptide produced by Bacillus subtilis
J. Colloid Interface Sci., 2009, 329, 253-264

González-Pérez, A., Carlstedt, J., Dias, R. S., Lindman, B.
Cyclodextrins in DNA decompaction,
submitted

Jaušovec, D.; Voncina, B.; Angelescu, D.; Nylander, T.; Lindman, B.
Enzymatic degradation of model cellulose film pre-treated with antimicrobial agent
J. Disp. Sci. Techn., in press

Khamhieh K., Nylander T., Ainalem M-L.
Analytical model study of Dendrimer-DNA complexes.
Biomacromolecules, 2009, Accepted

Källrot, N.; Dahlqvist, M.; Linse, P.
Dynamics of polymer adsorption from bulk solution onto planar surfaces
Macromolecules, Accepted

Laranjeira, T., Morán, M. C., Ribeiro, A., Miguel, M. G. and.Lindman, B.
Chitosan particles for DNA delivery: Effect of chitosan molecular weight on formation and release characteristics. New development in Chitosan-DNA particles
Submitted

Leal, C.,Bilalov, A. and Lindman, B.
The effect of post-added ethylene glycol surfactants on DNA-cationic surfactant/water mesophases
Submitted

Lindman, B.
Microemulsions- a vital fundamental research area moving rapidly into applications while having its scientific basis in other surfactant self-assembly systems In "Microemulsions:Properties and Application" edited by M. Fanun, Taylor and Francis/CRC press, 2009.

Lindman, B.
Some Thoughts about Microemulsions in Microemulsions, Edited by C. Stubenrauch, Wiley, Oxford, UK, 2009, pp 15-23.

Lindman, B., Karlström, G.
Nonionic polymers and surfactants: Temperature anomalies revisited
Comptes Rendus Chimie, 2009, 12, 121-128..

Lundberg, D., Carnerup, A., Schillén, K., Miguel, M. G., and Lindman, B.
Phase Behavior and Aggregate Structure in Dilute Aqueous Mixtures of Lysozyme and Salmon Testes DNA - a Model Investigation of Protein-DNA Interactions
Submitted

Löf, D.; Tomšic, M.; Glatter, O.; Fritz-Popovski, G.; Schillén, K.
Structural Characterization of Nonionic Mixed Micelles Formed by C12EO6 Surfactant and P123 Triblock Copolymer
J. Phys. Chem. B 2009, 113, 5478-5486.

Morán, M. C., Baptista, F. R., Ramalho, A., Miguel, M. G., Lindman, B.
DNA Gel Particles: Effect of the Cationic Agent on the Particle Size
Submitted

Morán, M. C., Pais, A.A.C.C., Ramalho, A., Miguel, M. G., Lindman, B.
Mixed protein carriers for modulating DNA release
Submitted

Olofsson, G.; Loh, W.
On the use of titration calorimetry to study association of surfactants in aqueous solution.
J. Braz. Chem. Soc., In press

Sarragua, J.; Pais, A. A. C. C.; Linse, P.
Influence of droplet radius and concentration in the formation of microemulsion--ABA-triblock copolymers networks
Soft Matter, 2009, 5, 140–147

Silva, B. F. B.; Marques, E. F.; Olsson, U.; Linse, P.
Size, shape, and charge of salt-free catanionic microemulsion droplets: a small-angle neutron scattering and modeling study
J. Phys. Chem., Submitted

Sparr, E.; Åberg, C.; Nilsson, P.; Wennerström, H.
Diffusive transport in responding lipid membranes
Soft Matter, submitted

Stenhammar, J.; Linse, P.; Malmqvist, P.-Å.; Karlström, G.
Electric multipole moment fluctuations in polar liquids
J. Chem. Phys., Accepted

Tonigold, K.; Varga, I.; Nylander, T.; Campbell, R.A.
Effects of Aggregates on Mixed Adsorption Layers of Poly(ethylene imine) and Sodium Dodecyl Sulfate at the Air/Liquid Interface.
Langmuir, 2009, 25, 4036-4046

Vaccaro M.; Mangiapia G.; Radulescu A.; Schillén K.;, D'Errico G.; Morelli G.; Paduano L.
Colloidal Particles Composed of Amphiphilic Molecules Binding Gadolinium Complexes and Peptides as Tumor-Specific Contrast Agents in MRI: Physico-Chemical Characterization
Soft Matter, 2009, DOI: 10.1039/b820804b

Vandoolaeghe, P.; Barauskas, J.; Johnsson, M.; Tiberg, T.; Nylander, T.
Interaction between Lamellar (Vesicles) and Nonlamellar Lipid Liquid-Crystalline Nanoparticles as Studied by Time-Resolved Small-Angle X-ray Diffraction
Langmuir, 2009, 25, 3999-4008.

Vandoolaeghe, P.; Campbell, R. A.; Rennie,A. R.; Nylander, T.
Adsorption of Intact Cubic Liquid Crystalline Nanoparticles on Hydrophilic Surfaces: Lateral Organization, Interfacial Stability, Layer Structure, and Interaction Mechanism.
J. Phys. Chem. C, 2009, 113, 4483-4494

Vandoolaeghe, P.; Rennie, A. R.; Campbell, R. A.; Nylander, T.
Neutron Reflectivity Studies of the Interaction of Cubic-Phase Nanoparticles with Phospholipid Bilayers of Different Coverage.
Langmuir, 2009, 25, 4009-4020.

Wadsö, I.
Characterization of microbial activity in soil by use of isothermal microcalorimetry.
J. Therm. Anal. Cal., 2009, 95, 843-850

Wahlgren, M.; Löwenstein Christensen, K.; Valentin Jörgensen, E.; Svensson, A.; Ulvenlund, S.
Oral-Based Controlled-Release Formulations Using Poly(Acrylic Acid) Microgels.,
Drug Dev. Ind. Pharm accepted.

Wennerström, H.; Olsson, U.
Microemulsions as models
C.R.Chimie 12, 4-17, 2009.

Åberg, C.; Sparr, E.; Edler, K.; Wennerström, H.
Non-Equilibrium Phase Transformations at the Air-Liquid Interface
Langmuir, submitted

TELEPHONE LIST

Physical Chemistry
Centre for Chemistry and Chemical Engineering
P.O. Box 124
SE-221 00 Lund
Telephone. +46 46 2228150
Facsimile: +46 46 2224413
Web Address: www.fkem1.lu.se

Direct phone: +46 46 22+extention

Name	**Extension**	**Home phone no.**
Marie-Louise Ainalem	24504	046-152422
Manuel Alatorre Meda	28188	
Viveka Alfredsson	28155	046-152979
Mehran Asad Ayoubi	28154	
Johanna Bailey	28154	
Joakim Balogh	28188	046-142758
Azat Bilalov	23677	
Sebastian Björklund	24682	
Jonas Carlstedt	28163	046-146775
Celen Cenker	28188	
Fatima Costa	28188	
Tiago Ferreira	23247	
John Janiak	23248	
Ola Karlsson	20112	
Tomas Kjellman	29480	
Patrik Knöös	28188	040-6325823
Niklas Källrot	24682	040-6112052
Majlis Larsson	28150	046-293834
Samo Lasic	28204	
Ingegerd Lind	23489	046-292845
Björn Lindman	28160	046-141547
Per Linse	28151	046-140548
Peter Linton	23332	040-915291
Dan Lundberg	28148	
Alexandra Machado	28188	
Lennart Nilsson	28249	046-148810
Peter Nilsson	23677	
Agnieszka Nowacka	23247	
Tommy Nylander	28158	046-145492
Gerd Olofsson	28185	046-51835
Ulf Olsson	28159	046-53312
Nikolay Oskolkov	23677	
Luis Pegado	24954	
Lennart Piculell	29518	046-128912
Nina Reichhardt	23332	
Johan Reimer	28133	046-120424
Juangfang Ruan	24812	
Yukari Sakazaki	24504	

Salome Santos	28163	
Karin Schillén	21439	046-123322
Emma Sparr	21536	046-127497
Joakim Stenhammar	23248	040-6671578
Olle Söderman	28603	040-151292
Krister Thuresson	046-2865748	
Fredrik Tiberg	046-2864692	
Daniel Topgaard	28204	046-306976
Stefan Ulvenlund	046-337847	046-143531
Ingemar Wadsö	28180	046-2116228
Hoa Wang	24954	
Wei Wang	28154	
Håkan Wennerström	29767	046-142980
Marianna Yanez Arteta	23332	
Malin Zackrisson	28163	
Agnes Zettergren	24682	0707-877061
Christoffer Åberg	28148	0736-742132
Ingrid Åslund	24812	046-2718518

NMR lab	29462
Surface force lab	24147
Light-scattering lab	29185

E-mail addresses:	firstname.surname@fkem1.lu.se (å,ä,ö=a,a,o)
Example:	Hakan.Wennerstrom@fkem1.lu.se

This report is produced by Johan Reimer

LUND
UNIVERSITY

Physical Chemistry

Center for Chemistry and Chemical Engineering

P.O. Box 124, SE-221 00 Lund
Phone: +46 46 222 8150
Fax: +46 46 222 44 13