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Cover:

Picture (front): Formation of giant vesicles composed of phospholipid and a fluorescent lipid analogue. (By Emma Sparr.)

Picture (back): CSI image of a dissolving tablet, containing Pemulen TR2 (polymer) and 2wt% Griseofulvin (drug) after ~ 6h dissolving in water. The top part of the picture represents the solution and the bottom part the dry tablet. The peaks represent, from right to left, drug, polymer, polymer, drug and water. (By Patrik Knöös.)

INTRODUCTION

Physical Chemistry on the move

The year of 2010 has been a year when many changes at the Division of Physical Chemistry either happened or began. The move to a new location that had been announced for some time finally began with a first step in August. The second and final step of the move is actually taking place as this is written. The end result is that we will all have moved from building IV to newly renovated offices and similarly fresh laboratories at levels +1 and +2 of building III of the Chemical Center. The move has progressed smoothly and we now have adequate space for all the equipment that has recently been acquired - you will find many new items in the list on p. 28-35.

However significant the physical move and the acquisition of new equipment may be, the greatest news of the year is undoubtedly that we have been able to recruit Peter Schurtenberger, Anna Stradner and Malin Zachrisson-Oskolkova as coworkers. This is a big boost for the science at the Division of Physical Chemistry. We are convinced that these recruitments will lead to a rejuvenation of our research with the establishment of several new research directions. Peter's research in the area of soft matter can reach new dimensions by combining scattering methods with the theoretical and experimental techniques already established here. Both Anna and Malin will mainly concentrate on the study of the physical chemistry of proteins. This involves applying the methods and concepts of colloid science to problems of association and aggregation. Again, their relocation offers large opportunities through the possibility of combining scattering methods with other techniques already well established at the division. A sign of immediate international recognition of the new Physical Chemistry team is that the Division has already been selected as a partner, with responsibilities in light scattering and nuclear magnetic resonance, in the EU-sponsored infrastructure in soft matter (see p. 29 for details).

The year of 2010 was also a year of change of Division leadership. It was my last as head of the Division and I have also left all other missions of an administrative character. It is time to move on and let younger people take the lead. The new head of the Division is Lennart Piculell with Viveka Alfredsson as deputy. There is also a new Division steering group that, in addition to Lennart and Viveka, consists of Peter and Olle Söderman. Olle is also the new person academically responsible for the subject of "Physical Chemistry". Ulf Olsson takes a position in the steering group of the Department of Chemistry.

For me personally 2010 has been a year where I have been closing down some of my scientific activities. I have kept the involvement in a major research program in material science funded by the Foundation for Strategic Research (SSF) and my engagement as a member and internal advisor of the Linneaus Programme "Organizing Molecular Matter". The majority of my time for research, which is rather extensive, is now devoted to penetrating some more fundamental scientific issues. Previously neither the time nor the urge for obtaining research funding allowed for such activities. Some of the results will be published as regular papers, but some will appear only on my departmental homepage.

This is the last time I contribute in a leading position to the Annual Report of the Division of Physical Chemistry. The first in the series of such reports appeared 21 years ago covering the activities of 1989. Below I quote the introduction I then wrote:

Why an annual report?

“During the last few years we have had a marked increase in the range and scope of the research activities at our department. This is partly due to the fact that several new senior research positions, mainly financed by the Swedish Natural Science Research Council (NFR), have been allocated to the department.

We are now in the position where there are several groups within the department that operate relatively independently. This creates a need for exchange of information and coordination, both with respect to activities within the department, but also, and more significantly, with respect to external national and international contacts. The present report has been compiled to partially fulfill these needs.

For anyone planning to join the department for a longer or shorter period, the report should serve as an overview of the research activities, their extent and the number of scientist involved in a particular field. If, as we hope, the report is produced during a number of years, it provides a very good opportunity to see how the research programs are developing. For us it can also serve as an instrument to judge the successes and failures of individual projects over a more long-term basis.”

Looking back at the 21 issues that have appeared, and comparing the present one with the first 1989 issue, I can only conclude that the motivation for an Annual Report expressed in 1990 is equally valid in 2011. It has clearly been the case that the Annual Report has been the very useful communication link that was anticipated in 1990.

Håkan Wennerström

RESEARCH PROJECTS

Theoretical work - Statistical mechanics

Structural properties of polar liquids (Contact person: Per Linse)

The long-range structural properties of liquids composed of molecular dipoles are 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. The theoretical analysis is based on electrostatic fluctuation formulas obtained using dielectric continuum theory. These describe the magnitude of the fluctuating electric multipole moments within spherical volumes inside a polar liquid, as a function of the radius of the volume and the dielectric constant of the fluid. The predictions from these formulae are compared with the results of computer (Monte Carlo and molecular dynamics) simulations of strongly polar liquids. The project is aimed at i) elucidating how accurately the structure and energetics of these liquids are described by dielectric continuum theory, and ii) investigating the accuracy of different schemes used to handle the long-range electrostatic interactions in computer simulations.

The research during 2010 was divided into the following sub-projects:

1. *The development of dielectric fluctuation formulas for polar liquids under spherical confinement, and comparison with simulation results obtained from a droplet of dipolar particles.* The agreement between theory and simulation is very good, and both investigations show that the fluctuations are greatly reduced as the cavity surface is approached. Furthermore, the fluctuations perpendicular to the surface are more strongly reduced than those parallel to the surface.

2. *Calculation of the van der Waals (vdW) interaction free energy between spherical bodies of classical dipolar fluid.* The analytic approach uses the dielectric fluctuation formulas developed within the project, and the results show excellent agreement with those obtained using the classical limit of Lifshitz theory. However, our relatively straightforward formalism goes beyond the linear response approximation inherent in Lifshitz theory, and thus provides the first truly exact calculation of the classical vdW interaction between fluid bodies. The analytical dielectric continuum results are compared to results for a molecular model fluid obtained using a combined simulation and perturbation theory approach. The agreement between the models is shown to be surprisingly good, down to separations between the bodies of molecular dimensions.

3. *A unified approach to calculating solvation free energies of different dipolar species using electric fluctuations.* The straightforward approach uses probability distributions of dipoles and electric fields to describe the solvation process in a very general way. In addition to recovering a number of classical results, we derive an expression for the solvation free energy of a spherical dielectric subvolume inside an infinite dielectric medium. The solvation free energy is also analyzed in detail by decomposing it into its energetic and entropic constituents. (Joakim Stenhammar, Per Linse, Gunnar Karlström (Theoretical Chemistry), and Martin Trulsson (Theoretical Chemistry))

The dielectric approximation (Contact person: Håkan Wennerström)

In the theoretical description of surface forces an aqueous medium is typically described as a dielectric continuum. This often leads to quantitatively accurate descriptions. However, the continuum description of the solvent breaks down at short separations and one must turn to a molecular picture. Through computer simulations we study the relation between the continuum and the fully molecular description of charged surfaces interacting at short range in a dipolar solvent. (Luis Pegado, Bo Jönsson (Theoretical Chemistry), Gunnar Karlström (Theoretical Chemistry) and Håkan Wennerström). Project completed 2010.

Dielectric and retardation behavior of dipolar liquids (Contact person: Per Linse)

A long-standing challenging property of dipolar liquids is their attenuation of Coulomb interaction between ions and how that depends on the orientational structure of the fluid. Extensive Monte Carlo simulations have been performed to address two central questions: (i) development of a novel approach to extract the dielectric property of a molecular polar fluid and (ii) the effect of the retardation on the orientational structure, which is coupled to the dielectric response of the dipolar fluid.

General expressions for two-center electrostatic potential fluctuations and its use to determine (i) the effective interaction between simple ions in a dipolar solvent and (ii) the dielectric permittivity of the solvent are proposed. Such two-center potential fluctuations were determined from Monte Carlo simulations of spherically confined dipolar particles embedded in a dielectric medium described by using an image charge approximation. The deduced dielectric permittivities increased with increasing dipolar moment, and at large dipole moments the effective interaction displayed an attractive first minimum.

A strongly coupled dipolar fluid confined in a sphere has been examined by Monte Carlo simulations using a modified distance-dependent pair interaction to emulate retardation effects. The effective dipole-dipole interaction and a property closely related to Kirkwood's g -factor have been analyzed for potentials with different distances at which the retardation effects became effective. The retardation effects were found to brake the otherwise long-range orientational ordering occurring in strongly coupled dipolar fluids. (Per Linse, Gunnar Karlström, (Theoretical Chemistry) and Clifford Woodward (University College University of NSW Australian Defense Force Academy, Australia))

Dynamics of polymer adsorption (Contact person: Per Linse)

The dynamics of the adsorption of uncharged homopolymers in good solvent appearing in systems composed of a polymer solution placed near attractive, but initially polymer-free, surfaces have been 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 and nematic order of adsorbed polymers.

After a diffusion of the polymer to the vicinity of the surface, four succeeding phases were identified: distortion, attachment, spreading, and final contraction 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. In the extended spreading phase,

the polymer continues to spread on the surface. Finally at long times, for flexible 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, whereas for stiff polymers a nematic ordering of adsorbed polymers was obtained. This final process is connected to the slow relaxation of the number of adsorbed polymers.

In the first sub-project, polymers with different flexibility and attractive segment-surface interaction were considered. Large differences in equilibrium structure and adsorption structure and dynamics were found. In the second sub-project, adsorption from solution comprising two different types of polymers was investigated. Polymers with different chain length and/or flexibility were considered. Generally, an initial adsorption layer dominated by short chains that later was replaced by longer chains was observed (Niklas Källrot, Per Linse). Project completed 2010.

Polyelectrolyte complexes (Contact person: Per Linse)

Structural properties and the topology of polyelectrolyte complexes formed by a long polyion and shorter and oppositely charged polyions of varying length in solution have been investigated under different conditions by Monte Carlo simulations using a coarse-grained model. The extension of individual polyions has been characterized by their radius of gyration, whereas the composition and the internal topological structure of the complexes by their net charge and a novel analysis describing how the shorter polycations link to monomers of the longer polyanion, respectively. Conditions have been found at which the polyanion and a given number of polycations form distinguishable complexes differing in (i) the polyanion conformation and (ii) the fraction of polycations being in extended and collapsed states. Thus, at equilibrium these polyelectrolyte complexes display a stepwise variation of the degree of intracomplex disproportionation of the polycations (also referred to as a intrachain segregation), the appearing of an intracomplex disproportionation in agreement with previous theoretical predictions. The coexistence of different polyelectrolyte complex structures appeared at charge equivalence for PA with 30 monomers and beyond charge equivalence for a longer polyanion. A broad polyanion size distribution and a bimodal polycation size distribution appeared as a consequence of the coexistence of different polyelectrolyte complex structures. (Per Linse, Rita Dias and Alberto Pais (University of Coimbra, Portugal)).

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

Through the web-portal www.fkem1.lu.se/sm, launched 2003, softwares for solving general problems in mainly statistical mechanics are accessible. The softwares were primarily developed as research tools, but have frequently been used in advanced undergraduate classes and in national PhD courses.

From the web-portal, further information about each software (except one) can be obtained, reference manuals and sample input files can be retrieved, and the softwares can be executed for test purposes and minor production runs. The softwares are: . DIELEC Calculation of the electrostatics in the presence of spherical dielectric discontinuities.

FIDS ¹ Calculation of the fluctuation interaction between two dielectric spheres. MOLSIM ² 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.

Parallel version employing MPI since 1997. Used in about 150 publications.
NR Analysis and simulation of neutron reflectivity data.
OZ Solution of the Ornstein-Zernike equation with a closure (MSA, PY, HNC, RY, ZH, and RHNC) for particles with central forces.
PB Solution of the one-dimensional Poisson-Boltzmann equation for different boundary conditions and symmetries.

PGSE Simulation of pulse gradient spin echo attenuations for spins diffusing in restricted spaces of different symmetries with permeable walls.
POLYMER Solution of lattice mean-field models comprising a mixture of solvents and polymers for (i) homogeneous (Flory-Huggins theory) and (ii) heterogeneous (Scheutjens-Fleer theory) systems extended to polymers possessing internal degrees of freedom. Used in about 90 publications. 1) With Joakim Stenhammar. 2) With contributions from Anna Akinchina, Fredrik Carlsson, Samuel Edgecombe, Yoshikatsu Hayashi, Niklas Källrot, Vladimir Lobaskin, Thomas M. Nyman, Alberto Pais, Jurij Rescic, Stefanie Schneider, Marie Skepö, Joakim Stenhammar, Anders Wallqvist, and Per-Olof Åstrand

Studies of model systems

Physico-chemical behavior of aqueous systems containing DNA, proteins and amphiphiles. (Contact persons: Dan Lundberg and Björn Lindman)

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. 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, Karin Schillén, Viveka Alfredsson, Daniel Topgaard, Björn Lindman, Maria da Graça Miguel (University of Coimbra), Henrique Faneca (University of Coimbra), Maria C. Pedroso de Lima (University of Coimbra), Lars Nordenskiöld (Nanyang Technological University), Nikolay Korolev (Nanyang Technological), Nikolay Berezhnoy (Nanyang Technological))

Asymmetric Catanionic Surfactants (Contact person: Ulf Olsson)

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 longrange droplet-droplet interactions which depend on the concentration dependent effective droplet charge. (Bruno Silva (Porto University), Per Linse, Ulf Olsson, Eduardo Marques (Porto University))

Diffusive transport in responding membranes (Contact person: Emma Sparr)

A responding membrane is defined as a membrane that cannot be described by a simple permeability constant, but which barrier properties varies in response to changes in its environment. The permeability of such a membrane depends on the gradient of the diffusing substance, and on variations in other membrane gradients in variables such as osmotic pressure, salt concentration, pH or temperature.

The barrier properties of a responding membrane can be understood from the coupling between equilibrium phase and permeability. It is typical for the rich phase behavior of lipids that small changes in the external conditions can trigger large structural changes between lyotropic phases with distinctly different diffusion characteristics. In experimental and theoretical studies, we previously demonstrated that an external osmotic gradient can introduce heterogeneous swelling and phase transformation within the membrane, and thereby alter the membrane barrier properties. 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 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 can regulate the membrane barrier. 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 (Figure). 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 molecularly ordered films that can form spontaneously at the interface between air and solutions of micellar solutions of mixed surfactant and polyelectrolytes. (Emma Sparr, Tahereh Mokthari, Håkan Wennerström, Karen Edler (University of Bath), Christoffer Åberg (University College Dublin), Peter Nilsson, Fátima Costa-Balogh (Coimbra university, Portugal))

How small polar molecules protect membrane systems against osmotic stress

(Contact person: Emma Sparr)

Urea, under the name of carbamide, and glycerol are standard major components of skin lotions. They are claimed to act as “moisturizers” with seems to imply that have the effect of binding water in excess to what would be the case without the presence of these compounds. Compounds such as urea, glycerol and similar polar substances

occur naturally in many organisms to regulate osmotic pressure and to prevent cell damage due to freezing or drying. The question addressed in the project concerns the molecular mechanism(s) behind the role of urea and glycerol in these contexts.

By studying lipid - mixed solvent systems using a range of methods such as sorption calorimetry, sorption balance, X-ray diffraction/scattering and nuclear magnetic resonance it is possible to unravel how the presence of urea and glycerol interacts with phospholipid bilayers. The major conclusions are: i) urea and glycerol shows a near ideal mixing with water in the lipid lamellar systems. ii) The presence of urea or glycerol has only a minor effect on the gel to liquid crystal transition temperature in the presence of excess solvent. iii) Under conditions of fixed lipid to urea (or glycerol) ratio the transition to a gel state occurs at lower relative humidities than for pure aqueous systems. The “moisturizing” effect of urea and glycerol is, based on these investigations, due to a suppression of a liquid crystal to gel/solid transformation that otherwise would occur under dry conditions. (Agnieszka Nowacka, Emma Sparr, Håkan Wennerström, Daniel Topgaard, Fátima Costa-Balogh (Coimbra university, Portugal), Lars Wadsö (Building Materials, LTH))

Interaction between RNA and lipid membranes (Contact person: Emma Sparr)

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 use small single-stranded and doublestranded oligonucleotides (RNA), tRNA and long DNA. Model lipid membrane systems are zwitterionic, anionic, as well as cationic lipids. The system are studied with several techniques, including calorimetry, ellipsometry, quartz crystal microbalance (QCM-D), neutron reflectometri, fluorescence microscopy and monolayer techniques. (Agnes Michanek, Emma Sparr, Tommy Nylander, Luc Jaeger (University of California, Santa Barbara, USA), Fredrik Höök (Chalmers))

Polymerization in structured media (Contact person: Ola Karlsson)

The long-term goal of this project is to study 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. The project is run in co-operation with MIP Technologies AB, Lund. (Johanna Bailey, Ola Karlsson, Lennart Piculell)

Soluble complex salts of surfactant ions and polymeric counterions: Composite macromolecular self-assembly (Contact person: Karin Schillén)

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 (a polyion). The complex salts studied in this work consist of polyacrylate (PA_y^-) and cationic $C_{16}TA^+$ surfactant ions aggregated into micelles. They are denoted $C_{16}TAPA_y$, where y is the degree of polymerization ($y=25$ or 6000). Both are insoluble in water. To make these complex salts soluble, PEO-containing nonionic surfactants of the type $C_{12}E_j$ are added and $C_{16}TA^+/C_{12}E_j$ mixed micelles surrounded by PA_y chains are formed. Phase studies on systems containing $C_{16}TAPA_y$ complex salts in water mixed with either $C_{12}E_5$ or $C_{12}E_8$ have been carried out by visual inspection of the samples and by using synchrotron SAXS at MAX-lab. The results revealed that decreasing polyion length and increasing the PEO-chain length of the nonionic surfactant were important factors for increasing the solubility of the complex salt. We are currently investigating the composite self-assembled structures found in the L_1 -regime (i.e. the complex salt fully dissolved by $C_{12}E_8$ and $C_{12}E_{25}$) by means of DLS, isothermal titration calorimetry, cryo-transmission electron microscopy, SAXS and NMR. In a related project the copolymers poly(methacrylic acid-co-ethoxylated methacrylate) $P(MA-MAEO_{24})_{x:y}$ have been synthesized by a free-radical copolymerization and titrated with hexadecyltrimethylammonium surfactant, $C_{16}TAOH$, to produce $C_{16}TAP(MA-MAEO_{24})_{69:31}$. This copolymer displays a micellar one-phase up to 50 wt% in water. DLS and NMR are employed to study the effect of changing the concentration and temperature. (John Janiak, Karin Schillén, Lennart Piculell, Gerd Olofsson, Matija Tomšič (University of Ljubljana, Slovenia), Otto Glatter (University of Graz, Austria), Watson Loh and Ana Maria Percebom (Campinas University, Brazil).

Associative Polymer-Polymer and Polymer-Surfactant Systems: Phase Behaviour and the Influence of Chemical Reactions (Contact person: Lennart Piculell)

Polymer-surfactant pairs that associate strongly and separate out as a concentrated phase from an aqueous solution are extensively used to create water-insoluble materials, or surface coatings, with controllable properties. Two properties that are interesting to control are the water content and the packing of the surfactant aggregates in the concentrated phase. The control parameters are the detailed chemistry of the components, as well as their concentrations and proportions in the mixture. This project follows two lines of activity. One is concerned with systematic studies of the phase behavior of mixtures of associating pairs in water, using the minimum number of components to simplify the interpretation. We investigate nonionic pairs of polyacrylic acid and PEO-PPO-PEO triblock copolymers, as well as conventional cationic surfactants mixed with "complex salts" of cationic surfactant ions having acrylate-based copolymers as counterions. We study the effect of polymer length and polyion charge density for the structures formed in the concentrated phase, as well as the possibility to "redissolve" the concentrated phase by additions of excess surfactant. We also compare with simple model calculations in an attempt to extract the main physical mechanisms. The other line of research concerns using chemical reactions to modify the phase behavior. For this purpose we use surfactants containing either degradable cationic betaine esters as surfactant ions, or polymerizable acrylate ions as counterions. In both cases, we compare the outcome of the degradation or polymerization reactions

with predictions from the appropriate equilibrium phase studies, where the effects of replacing one (reactant) component with another (product) component is readily apparent. (Salomé dos Santos, Charlotte Gustavsson, Lennart Piculell, Ola Karlsson, Per Linse, Maria da Graça Miguel (University of Coimbra), Dan Lundberg (University of Coimbra)).

Porous surface layers through deposition of structured polymer-surfactant particles (Contact person: Lennart Piculell)

A porous surface layer can function as a semi-permeable barrier, as a depot for material to be released from the pores, or as a size-selective adsorbent for substances in a surrounding fluid phase. For all these functions, it is of importance to control the size of the pores, their geometry, and their orientation (for non-spherical pores) relative to the surface. As one part of the larger SSF program “Porous surface layers through polymer-assisted deposition”, this project investigates the making of porous polymer-surfactant particles from associating polymer-surfactant pairs, which are then deposited at a surface through a destabilizing mechanism. The deposition strategy is closely related to that commonly used in laundry and personal care applications to deposit particulate matter through “coacervating” polymer-surfactant formulations. The particles are made either by direct mixing or by polymerizing surfactant counterions (with or without cross-linkers) in solution, and are later studied by DLS, SAXS and cryo-TEM. The correct conditions for surface deposition of the particles (in a controlled fashion) will be studied by ellipsometry and AFM. (Charlotte Gustavsson, Lennart Piculell, Ola Karlsson, Viveka Alfredsson)

Microphase separation of diblock copolymers with strongly asymmetric repeating units (Contact person: Lennart Piculell)

For a diblock copolymer (polyA-*b*-polyB), the thermodynamic incompatibility between polyA and polyB blocks drives a microphase separation in the melt state where alternating A-rich and B-rich microdomains appear in order to minimize the contact between dissimilar polyA and polyB blocks. The segregated regions of polyA and polyB typically form structures with liquid crystalline ordering. The classical block copolymers (BCs) are conformationally symmetric, meaning that the polyA and polyB blocks have the same persistence length l_p and that the interaction between the A and B repeating units can be described by a single interaction parameter.

This project seeks to develop experimental model systems of BCs containing strongly asymmetric repeating units. For an asymmetry in l_p , we use the poly(ethylene propylene)-*b*-poly(benzyl glutamate) system (the PEP-*b*-PBLG “coil-*b*-rod” BC), with an order-of-magnitude difference in l_p of the two blocks. For a BC containing amphiphilic repeating units, we use poly(styrene)-*b*-poly(methacrylic acid), PS-*b*-PMAA, where the repeating units of the PMAA block have an amphiphilic nature. This amphiphilicity can be enhanced by replacing the carboxylic acid protons with cationic surfactant ions. Anionic polymerization is used for synthesis of these BCs and small-angle-X ray scattering is utilized for structural analysis. (Mehran Asad Ayoubi, Lennart Piculell, Ulf Olsson, Alexei Khokhlov (Moscow State University/Russian Academy of Science), Bo Nyström and Kaizheng Zhu (University of Oslo) and Kristoffer Almdal (Micro- and Nanotechnology, DTU))

Water-soluble polymers containing amphiphilic repeating units and their interactions with ionic surfactant micelles (Contact person: Lennart Piculell)

The repeating units of water-soluble polymers are usually divided into two classes: hydrophobic versus hydrophilic units. However, it is evident that typical repeating units are actually amphiphilic, since they contain functionalities of both types. Simulations by Khokhlov et al. have shown that conformational properties of polymers containing amphiphilic units are significantly different from those predicted by a model based on uniformly hydrophobic, or hydrophilic, repeating units. The main reason is that amphiphilic units possess a significant surface activity. Both the interfacial activity and the partitioning between water and hydrocarbon solvents are key parameters for a two-dimensional classification of amphiphilic repeating units. In this project we are using the two-dimensional description to classify certain acrylamide 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 repeating units should also be taken into account. (Irina Nasimova, Lennart Piculell, Alexei Khokhlov (Moscow State University/Russian Academy of Science))

Living polymers and living networks (Contact person: Ulf Olsson)

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 they 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). In a living polymer system made of reverse, slightly water swollen, lecithin micelles in cyclohexane, the stress relaxation time is around an hour. Hence, the zero shear viscosity is unusually high. The long relaxation times also allow for studying the entangled system's response to fast deformations. Here, the stress strain relationship is similar to that of rubbers. Above a certain critical strain the entangled micellar network fractures, and the micelles align in the flow direction. (Ulf Olsson, R. Angelico, L. Ambrosone and A. Ceglie (Campobasso), G. Palazzo (Bari), L. Gentile, C. Olivieri (Cosenza), K. Mortensen (Riso, Denmark))

Bilayer membrane kinetics, including vesicle fusion (Contact person: Ulf Olsson)

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 spongeto-

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 when the monolayer spontaneous curvature is negative, i.e. when the monolayer prefers to bend towards water. In this project, vesicle fusion kinetics is studied using time-resolved static and dynamic light scattering and small angle neutron scattering. In terms of the monolayer spontaneous curvature, H_0 , it was found that vesicles. (Malin Zackrisson, Ulf Olsson, Håkan Wennerström, Sandra Bulut, M. Gotter, M. Baciu Gotter and R. Strey (Köln))

Lamellar phase rheology and shear-induced formation of multi-lamellar vesicles (Contact Person: Ulf Olsson)

The equilibrium structure and phase equilibria of the lamellar phase are sometimes complicated as noted in already early studies by Ekwall and Fontell. This complication appears to be due to the formation of multi-lamellar vesicles (“onions”) under shear, which can originate simply by shaking the sample. A systematic study is performed on nonionic surfactant- water systems where the structure of the lamellar phase under shear is investigated using small angle neutron and light scattering. Depending on the temperature, that governs the monolayer spontaneous curvature, we can identify two distinct regions corresponding to “onions” (lower temperature) and planar bilayers (classical lamellar phase, higher temperature). The equilibrium structure at zero shear, however, appears to be the classical lamellar structure. The onion size varies with the applied shear rate or shear stress. In systematic experiments, it was found that the onion states obtained at large strain values are reversible and correspond to true steady states. Oriented (“single crystal”) lamellar phases still contain equilibrium defects that give them a relatively high shear viscosity and in addition make them viscoelastic. In a Couette cell, magnetic resonance chemical shift imaging has shown that the lamellarto-onion transition takes place homogeneously throughout the sample, while in the onion-to-lamellar transition, the lamellar phase first forms at the inner rotor and the growth of that phase propagates through the gap. (Ulf Olsson, B. Medronho (Coimbra), M. Miguel (Coimbra), C. Schmidt (Paderborn), M. Imai (Tokyo), Y. Suganuma (Tokyo), P. Galvosas and P. Callaghan (University of Wellington), L. Gentile and C. Oliviero Rossi (Univ. of Calabria))

PIT and PIC emulsification (Contact Person: Ulf Olsson)

In this project we re-examine the phase inversion temperature (PIT) emulsification process using model ternary nonionic surfactant/water/oil systems. This is a low-energy method that uses a physicochemical drive to produce very fine oil/water emulsions in the absence of high shear flows. We find that successful emulsification depends on two conditions. First, the mixture must be stirred at low speed throughout the whole process: this makes it possible to produce emulsions at surfactant concentrations that are too low to form an equilibrium microemulsion. Second, the stirred mixtures must be heated above a threshold called the clearing boundary (CB) and then quenched to lower temperatures. The clearing boundary is determined experimentally by a minimum in the turbidity of the stirred mixture, which results from solubilization of all the oil into swollen micelles. This matches the emulsification failure boundary corresponding to the condition $R^*C_0=1$, where R^* is the spherical radius that results from the oil/surfactant composition for monodisperse spheres and C_0 is the spontaneous spherical

curvature of the surfactant monolayer. Thus, we show that such cycles do not need to cross the PIT. In fact, sub-PIT cycles and cross-PIT cycles give exactly the same result. These conditions lead to emulsions that have a narrow size distribution and a mean diameter controlled by the oil/surfactant ratio. The typical range of those diameters is 20-100 nm. Moreover, these emulsions have an excellent metastability, in contrast with emulsions made with shorter oil and surfactant molecules. In the phase inversion composition (PIC) method, typically an oil-surfactant mixture is suddenly mixed with a large amount of water to produce an O/W emulsion. A key molecular event here is surfactant hydration. Also in this process a clearing boundary can be identified. However, the PIC mechanism, and its corresponding sequence of events, is significantly different from the PIT mechanism. The PIC mechanism involves as a fundamental step the formation of a separate oil phase. As a consequence of this separation a unimodal size distribution of the final emulsion is not possible, as it is in PIT emulsification. (Ulf Olsson, K. Roger and B. Cabane (ESPCI, Paris))

Pickering Emulsions (Contact Person: Ulf Olsson)

Pickering, or particle stabilized, emulsions have a number of interesting properties. When the particles are properly chosen, they are essentially irreversibly adsorbed at the oil-water interface, which, as a consequence, inhibits Ostwald ripening. In this project we investigate the properties of silica coated particles and their potential for stabilizing W/O emulsions. Furthermore, we want to develop a method to measure the strength of particle adsorption at the oil-water interface. (Ulf Olsson, Y. Sakazaki (Pola Chemical Industries INC, Yokohama))

Cellulose dissolution (Contact person: Björn Lindman)

The dissolution of cellulose is important for a number of industrial processes and several solvents and mixtures have been tested. On the basis of an examination of the intermolecular interactions in cellulose novel approaches to cellulose dissolution are attempted. (Björn Lindman, B. Medronho (Coimbra), L. Stigsson (KIRAM), G. Karlström and A. Holt (Theoretical Chemistry, Lund Univ.))

Investigation on effect of added drug on a model drug delivery system

(Contact person: Joakim Balogh)

Here a model drug delivery system is studied and the effect of emulsions of an added drug (lidocaine) on this system. The temperature and concentration dependence have been followed using NMR self-diffusion, light scattering and synchrotron SAXS at MAX-Lab. It was shown that not only macroscopical but also microscopical changes occur in the phase diagram. The plan is to study the specific interaction the active compound has with the surfactant film to better understand the process and to be able to predict what the effect will be in more applied systems. (Joakim Balogh, Daniel Topgaard, Karin Schillén, Antonio Lopes (ITQB, Oeiras, Portugal), Maria da Graça Miguel (University of Coimbra, Portugal) and Jan. Skov Pedersen (University of Aarhus, Denmark)) (project completed 2010)

Controlling the phase behavior of polyion-surfactant ion complex salts by cyclodextrins (Contact person: Björn Lindman)

We have previously shown that cyclodextrins can be used to decompact single DNA molecules that were compacted by cationic surfactants. Additionally, macroscopically

phase separated DNA-surfactant complexes were shown to be dissociated at sufficient cyclodextrin concentrations. In this study we look at the phase behavior of concentrated ternary systems of polyion-surfactant ion complex salt and cyclodextrins to deepen our knowledge on these interactions. Various parameters, such as polyion hydrophobicity and length, surfactant chain length, as well as salt dependence and type of cyclodextrin is addressed. Preliminary results from a system containing DNA-DTA:2-HP- β -CD:water shows a rich and very interesting phase behavior. These studies are both of biological and biotechnological interest and may also be interesting for other industrial applications. (Ulf Olsson, Azat Bilalov, Jonas Carlstedt, R. S. Dias (University of Coimbra, Portugal))

Coulomb fission (Contact person: Per Linse)

Delayed asymmetric Coulomb fission in size-selected molecular dication clusters has been recorded for the first time. Observations on $(\text{NH}_3)_n^{2+}$ clusters show that fragmentation accompanied by charge separation can occur on a microsecond time scale, exhibits considerable asymmetry, and involves a kinetic energy release of ~ 0.9 eV. The fission process has been modeled by representing the fragments as charged dielectric spheres and the calculated maximum in the electrostatic interaction energy between the fragments gives a good account of the measured kinetic energy release. A simple kinetic model shows that instrumental factors may contribute to the observation of asymmetric fragmentation. (Per Linse and Guohua Wu, Xiaojing Chen, and Anthony J. Stace (University of Nottingham, England))

Understanding ultra-dense microgel suspensions

(Contact person: Peter Schurtenberger)

Cross-linked microgels are a particular interesting class of colloids with tunable size and softness that creates particle properties situated between classical hard spheres and soft-polymeric systems. Due to their soft-repulsive nature, microgels can be packed to an effective volume fraction f_{eff} much above closed packing f_{cp} , with enormous consequences for the resulting structural and dynamic properties. In our project we aim at: 1) Understanding the particle size and structure as a function of the effective volume fraction far into the ultra-dense region $f_{\text{eff}} \gg f_{\text{cp}}$, using mainly small angle neutron scattering combined with advanced contrast variation schemes. 2) Understanding structural ordering and dynamics of microgel dispersions at high volume fractions using confocal laser scanning microscopy and scattering techniques. Here we also use the charge density as an additional and tuneable parameter to combine long-range electrostatic interaction with the intrinsic short-range soft repulsion from the cross-linked polymer network in order to probe complex equilibrium crystalline structure as predicted the theory of ionic microgels. (Priti Mohanty, Divya Paloli, Jérôme Crassous (University of Fribourg, Switzerland), Urs Gasser (PSI, Switzerland), Peter Schurtenberger)

Flexibility and conformation of giant dendronised polymers

(Contact person: Peter Schurtenberger)

In recent years an interesting new class of polymers and polyelectrolytes has been developed, the so-called dendronized polymers. The unusual structure of these polymers with their tight and highly branched layer around the backbone has raised fundamental questions in polymer science, which all have their origin in the influence

of the layer on the conformation and rigidity of the backbone. We investigate the effect of the dendrons on the chain stiffness, and look at the influence of charge and solvent on the cross-sectional conformation, the flexibility, and on the interchain correlation at higher densities using SANS, SAXS and light scattering. (Peter Schurtenberger, Dieter Schlüter (ETH Zurich, Switzerland), Reinhard Siegel (University of Fribourg, Switzerland, Sebastian Lages)

Phase behavior, structure and dynamics of anisotropic model colloids

(Contact person: Peter Schurtenberger)

Colloids are convenient model systems to study classical condensed matter problems such phase transitions, dynamical arrest, or nucleation and crystallization phenomena.

Here we aim at a fundamental understanding of the phase behavior, structure and dynamics of concentrated suspensions of anisotropic particles. We focus both on structural anisotropy in ellipsoidal particles, as well as on the effects of an additional anisotropic component in the interaction potential between particles that can be generated using magnetic particles or particles with a magnetic core. (Ilya Martchenko, Jérôme J. Crassous (University of Fribourg, Switzerland), Hervé Dietsch (University of Fribourg, Switzerland), Peter Schurtenberger)

The nature of the glass transition in microgel suspensions

(Contact person: Peter Schurtenberger)

The main aim of this project is to study the phase behaviour of concentrated suspensions of Poly(N-isopropylacrylamide) (PNIPAM) microgel particles. PNIPAM particles are very interesting as they show a thermoresponsive size, where the particle swells at low and collapses at high temperatures. The size and thus the effective volume fraction of the particles can therefore be changed through a variation of the temperature. Here we use PNIPAM microgels as convenient model systems to investigate the glass transition that occurs at volume fractions $\gg 0.6$. We also look at the influence of the intrinsic softness of these particles on dynamical arrest, and investigate the nature of the dense phases that exist at high densities. We use confocal laser scanning microscopy that allows us to track the particles in real time and determine quantities such the pair correlation function or the mean square displacement of the particles as a function of effective volume fraction. (Divya Paloli, Jérôme Crassous (University of Fribourg, Switzerland), Priti Mohanty, Urs Gasser (PSI, Switzerland), Emanuela Zaccarelli (University La Sapienza Rome, Italy), Peter Schurtenberger)

Temperature-responsive supramolecular structures based on γ -cyclodextrin and polymers containing PNIPAAm chains (Contact person: Karin Schillén)

Pseudopolyrotaxanes or inclusion complexes are supramolecular assemblies formed by a linear molecule (e.g. a polymer chain) and several ring shaped molecules such as cyclodextrin (CD). Pseudopolyrotaxanes are widely studied because the structure of the assembly can readily be tuned by means of the solution conditions as well as the molecular architecture. A precise control of such supramolecular structures by using external stimuli and the understanding of the involved mechanism is a challenge in the field for designing smart nanomaterials. CDs are cyclic oligosaccharides formed by glucopyranose units. They have a truncated cone shape with a hollow cavity, which may incorporate more or less hydrophobic solutes such as surfactants or polymer chains. Several CDs rings can thread a polymer chain assuming either a compact or

loose structure depending on the nature of the CD. In this project, we investigate the inclusion complex formation between γ -CD and polymers containing the thermoresponsive poly(N-isopropylacrylamide) (PNIPAAm) chains in solid state, in solution and at solid/liquid interfaces. Both PNIPAAm-diblock copolymers and PNIPAAm homopolymers have been studied so far. When temperature approaches the lower critical solution temperature of PNIPAAm, the CD molecules dethread. The experimental techniques employed are $^1\text{H-NMR}$, Fourier transform infrared spectroscopy, synchrotron radiation powder X-ray diffraction, steady-state fluorescence spectroscopy, differential scanning calorimetry, SLS, DLS and cryo-transmission electron microscopy. The surface properties of the PNIPAAm-diblock copolymer system are investigated using ellipsometry, neutron reflectivity and quartz crystal microbalance. Furthermore, in a related project, the formation of coacervate core micelles of cationic and anionic PNIPAAm copolymers and their interaction with CDs are studied using DLS, SAXS and isothermal titration calorimetry. (Giuseppe Lazzara, Karin Schillén, Gerd Olofsson, Viveka Alfredsson, Tommy Nylander, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway) and Matija Tomšič (University of Ljubljana, Slovenia)).

Experimental methodologies

Diffusive transport of multivalent ions in cartilage (Contact person: Olle Söderman)

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 proteoglycans 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 $(\text{Gd-DTPA})^{2-}$ as a contrast in MRI to monitor the concentration of proteoglycans and therefore the state of the cartilage. In healthy cartilage the concentration of $(\text{Gd-DTPA})^{2-}$ will be low, while in damaged cartilage it would be high leading to T_1 -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 T_1 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. (Jenny Algotsson, Daniel Topgaard, Olle Söderman, Jan Forsman (Division of Theoretical Chemistry, LU) and Jonas Svensson and Leif Dahlberg (Department of Radiation Physics and the Joint and Soft Tissue Unit at UMAS, Malmö))

Polymer-surfactant interaction at liquid interface

(Contact person: Tommy Nylander)

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 as well as at interfaces because such mixtures are used extensively in commercial products such as shampoos and fabric conditioners. 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. In practise these system are used under non-equilibrium conditions. In this project we focus on the implications of the nonequilibrium complex formation and aggregation on the structure and properties of the interfacial layer, mainly on liquid interfaces. We exploit ellipsometry in the present project by analyzing fluctuations 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). Ellipsometry, surface tension and neutron reflectometry measurements, both with changing bulk composition and evolving time, we can track the relative amount of adsorbed material as well as composition of the formed layer (neutron reflectometry). 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 polyelectrolytes and oppositely charge surfactants 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 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. (Marianna Yanez, Tommy Nylander, Lennart Piculell, Richard Campbell (ILL, France), Katrin Tonigold (Ulm University), Imre Varga and Róbert Mészáros (Eötvös Loránd University, Budapest; Hungary))

Solid-state NMR methods for amphiphile systems

(Contact person: Daniel Topgaard)

Several types of intermolecular interactions, e.g., steric, electrostatic, and hydrophobic, affect the dynamic behavior of large molecules in a crowded system. NMR offers a unique possibility of resolving different molecules and molecular sites even in rather complex mixtures. For colloidal systems with reduced molecular mobility and sample heterogeneity on the nano- to micrometer scale, solid-state NMR methods with magic-angle spinning are 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. (Agnieszka Nowacka, Tiago Ferreira, Daniel Topgaard, Emma Sparr, Per Linse, Dan Lundberg, Azat Bilalov, Johan Reimer, Olle Söderman, Stefan Ulvenlund, Christina Wende, Rachel W Martin (UC Irvine) Gunnar Karlström (Theoretical Chemistry), Jens Norrman, Nils Bongartz)

Diffusion NMR methods for biological tissues (Contact person: Daniel Topgaard)

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, Freddy Ståhlberg (Medical Radiation Physics) Stina Oredsson (Cell- and Organism Biology), Samo Lasic, Karin Bryskhe and Anna Stenstam (Colloidal Resource AB))

A 12-channel microcalorimeter for use as a monitor of biological systems

(Contact person: Ingemar Wadsö)

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. The instrument should be considered as analytical tools (process monitors), which are sensitive (about 10 nW) and stable (days on the μ W 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 (Contact person: Ingemar Wadsö)

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 the 12-channel instrument 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

(Contact person: Emma Sparr)

The starting point of this project is the recent realization that lipid membranes seem to play pivotal roles in the pathogenesis of the protein misfolding disorders, e.g., Alzheimer and Parkinson diseases. An increasing amount of evidence suggests that the process of fibril formation in vivo and the mechanism of toxicity involve membrane interactions. The objective of the project is to explore the basic principles of how aggregating amyloid protein influence the lipid membrane barrier and the underlying interactions between the aggregating protein and the lipid membrane. We use recombinant A β and α -synuclein peptides 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 unilamellar vesicles. One important goal of the present project is to further understand how the aggregating amyloid protein can influence the membrane barrier properties and thus affect the transport of the protein itself as well as other substances. We also investigate whether transport amyloid can occur over a pure model membrane in the absence of the membrane proteins and uptake systems inherent to cells, and if the aggregating peptide affect the membrane integrity to diffusional transport of small molecules. Finally, we study lipid-peptide association using different biophysical techniques, including monolayers technique, confocal microscopy on giant unilamellar vesicles, NMR, ellipsometry, QCM-D, neutron reflectivity and electron microscopy. (Erik Hellstrand (Division of Biophysical Chemistry, LU), Marie Grey, Emma Sparr, Agnieszka Nowacka, Daniel Topgaard, Sara Linse and Martin Lundqvist (Division of Biochemistry and Structural Biology, LU), , Patrik Brundin (Wallenberg Neurocenter, LU), Ronald Melki (Laboratoire d'Enzymologie et Biochimie Structurales, CNRS, Gif-sur-Yvette, France), Marie-Louise Ainalem (ESS AB), Tommy Nylander)

Condensing DNA with cationic dendrimers: means of controlling aggregate morphology (Contact persons: Karin Schillén, Tommy Nylander)

Dynamic light scattering, cryogenic TEM and steady-state fluorescence spectroscopy are utilized to investigate the interaction between cationic poly(amido amine) (PAMAM) dendrimers and double stranded DNA. This systematic study reveals how the size, composition and morphology of aggregates formed between DNA and PAMAM dendrimers are affected by dendrimer size and charge. (Marie-Louise Ainalem, Anna Carnerup, John Janiak, Viveka Alfredsson, Tommy Nylander, Karin Schillén)

DNA gel particles and cross-linked DNA gels (Contact person: Björn Lindman)

Through an interfacial diffusion mechanism DNA particles were prepared and studied with respect to internal structure and DNA release. A large difference in internal structure between different DNA conformations for surfactant systems point to the

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

Structure and self-assembly of viruses (Contact person: Per Linse)

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 [1] 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 the spatial distribution or biaxial nematic order of polymers of arbitrary length and rigidity inside a spherical cavity is proposed. The local order of different chain segments is considered as an alignment to a spatially varying director field of cylindrical symmetry. The steric interactions are taken into account in the second virial approximation. Polymer density and orientational order distributions inside the spherically cavity are the principal results. It was found that short and flexible polymers are located at the center of the sphere and are orientationally disordered. Upon increasing polymer length and/or polymer rigidity, the location of the polymer is continuously shifted towards the surface of the spherical cavity and the polymer segments become gradually more aligned. Parameters have been selected to model the behavior of genomes in spherical viral capsids. (Nikolay N. Oskolkov, Per Linse, Alexei R. Khokhlov (Moscow State University, Russia))

The skin as a barrier to molecular diffusion (Contact person: Emma Sparr)

At normal conditions there is a substantial water gradient over the skin as it separates the water-rich inside of the body from the dry outside. This leads to a variation in the degree of hydration along the skin and changes in this gradient may affect the structure and function of skin. Similarly, the skin is exposed to other gradients in, e.g., metabolic gases, temperature, pH, applied drugs etc. In this study we raise the questions: How do changes in these gradients across skin affect its permeability? In a recent study, we have shown that the permeability of the skin barrier increases abruptly at low water gradients, corresponding to high degrees of skin hydration, and that this effect is reversible. The results are explained on basis that the skin is a responding membrane, for which small changes in the environment can lead to major changes in membrane structure, which in turn affect its transport properties. This phenomenon is highly relevant to drug delivery applications due to its potential of temporarily opening

the skin barrier for transdermal delivery of drugs and subsequently closing the barrier after treatment.

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 intact stratum corneum under varying conditions, using NMR and sorption calorimetry. This is combined with transport studies of different drugs across intact stratum corneum in the presence several gradients. (Sebastian Björklund, Emma Sparr, Agnieszka Nowacka, Daniel Topgaard, Johan Engblom (Biofilms; Malmö university), Krister Thuresson (Hemocue), Lars Wadsö (Building materials, LTH), Joke Bouwstra (Leiden university), Vitaly Kocherbitov (Malmö University), Véronique Burnier (L'ORÉAL, Paris), Bernard Cabane (ESPCI, Paris))

Peptide self-assembly (Contact person: Ulf Olsson)

The development of modern peptide chemistry has opened for the possibility of custom peptide synthesis that allows for systematically investigating the relationship between a specific oligopeptide molecular structure and the macroscopic phases and structures formed in such systems. Understanding the assembly behavior of peptides is important in not only designing nanomaterials for a desired functionality but also for combating neurodegenerative diseases such as Alzheimer and Parkinson's disease which are strongly associated with an accumulation of amyloid forming peptides in the brain. In this newly started project we focus initially on the self-assembly behavior of short simple and synthetic peptides, AnK, where n is varied in the range 4-10 (A=alanine, L=lysine). These peptides allows for a systematic investigation of e.g. the hydrophobicity and peptide length on the self-assembly behavior.

A6K in water forms very long hollow nanotubes with a (monodisperse) diameter of 52 nm, for concentrations above a critical aggregation concentration, $c_{ac} \approx 11$ %. Because of the large aspect ratio, the nanotubes form a nematic phase or a hexagonal phase. Work is now proceeding to investigate the self-assembly behavior of the analogue peptides A4K, A8K, and A10K. (Celen Çenker, Ulf Olsson, Malin Zackrisson, Mikael Lund (Division of Theoretical Chemistry), S. Bucak (Istanbul), I. Hamley (Reading), V. Castelletto (Reading))

DNA-lipid complexes (Contact person: Ulf Olsson)

Systems containing DNA, cationic cosolutes and phospholipids have a broad biological and biotechnological significance. For example, in the cell nucleus of eukaryotic cells, there is an intricate interplay between DNA, cationic proteins and lipids self-assembling into complex structures. This self-organisation is still far from being understood and in particular concerning the role of the lipids present. Important transfection agents are based on a mixture of cationic amphiphiles (surfactants of lipids) and neutral zwitterionic lipids. Understanding the interaction between the zwitterionic lipids and DNA would give a better basis for designing lipoplex formulations for transfections. In view of this significance we investigate the aqueous phase behavior of the “complex salt” DNA-amphiphilic cation (e.g. dodecyl trimethyl ammonium (DTA)) when mixed with various lipids. The ternary DNA-DTA/water/lecithin system shows a rich phase diagram with several liquid crystalline phases. Of particular interest is the first

observation of a DNA containing bicontinuous cubic phase. (Björn Lindman, Ulf Olsson, A. Bilalov (Kazan State Technological University))

Understanding concentrated protein solutions (Contact person: Anna Stradner)

The main objective of this project is to measure and understand intermolecular interactions in concentrated protein solutions and mixtures. We use a combination of different scattering methods (SANS, SAXS, static and dynamic light scattering), and compare the results with the predictions from numerical simulations. (Anna Stradner, Peter Schurtenberger, Mikael Lund, Giuseppe Foffi (EPFL, Switzerland), George Thurston (Rochester Institute of Technology, USA))

On the submicellar structure of casein micelles and their aggregation behaviour (Contact person: Tommy Nylander)

This work aims to relate the nano- and microscopic structures formed in milk based products to macroscopic effects such as gel strength and syneresis. The substructure of the casein micelle will be revealed by using model systems systematically built up by the different components, by mainly using light scattering, and small angle neutron scattering (SANS) with contrast matching using perdeuterated proteins. In order to reveal the aggregation process of casein micelles we are using SESANS (Spin-Echo-Small-Angle-Neutron-Scattering), which allows following the formation of structure at a wide length scales from 10nm-20 μ m. The objective of the study is to reveal the substructure and aggregation process of casein micelles and the relation between the two. (Sofie Botegård (ESS AB), Tommy Nylander, Marie Paulsson (Food Technology), Carl Holt (University of Glasgow), Wim Bouwman (University of Delft))

Molecular matter for specific functions

Mesoporous silica – formation and functional materials

(Contact person: Viveka Alfredsson)

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 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 mesostructured 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))

Foam films (Contact person: Per Linse)

The influence of counterions and coins on the stability and thickness of foam films stabilized by anionic dodecyl sulfate (DS-) has been studied in a thin film pressure balance. Particularly, the effect on the properties of foam films of (i) the counterions Li^+ , Na^+ , and Cs^+ of DS- and (ii) monovalent inorganic salts added to sodium dodecyl sulfate (SDS) solutions is considered. The interactions within the foam films were correlated to the adsorption behavior of the ions at the film surfaces. An increasing ionic size lead to an increased adsorption, which in the case of anions gave a thicker and more stable films and in the case of cations to the opposite effect. A strong anion effect was observed although the film surfaces were already negatively pre-charged by the anionic DS- leading to the conclusion that the impact of ions on the foam films was dominated by ion specific rather than electrostatic interactions. A maximum in the film thickness as a function of salt concentration appeared for a salt concentration below the surfactant concentration. This was interpreted as arising from two counteracting effects: (i) a charging of the film surfaces leading to a dominating increased film-film repulsion occurring below the maximum and (ii) a screening of the electrostatic film-film repulsion dominating above the maximum. (Per Linse and Natascha Schelero, Gabi Hedicke, and Regine v. Klitzing (Berlin Institute of Technology, Germany))

Modeling of the adsorption of bottle-brush polymers onto surfaces

(Contact person: Per Linse)

A new class of polymers composed of the monomers monomers poly(ethylene oxide) methyl ethyl methacrylate (PEO₄₅MEMA) and methacryloxyethyl trimethylammonium chlorid (METAC) have recently been synthesized by Vareikis and coworkers. Depending on the monomer ratio, polymers continuously ranging from uncharged bottle-brush polymer ($X = 0$) to highly charged polyelectrolyte ($X = 100$) are available. Solution and as well as adsorption properties of this class of polymers are currently of large experimental interest.

To further understand the adsorption mechanism of this class of polymer onto various solid surfaces, we have performed model calculations using a lattice mean field theory. The bottle-brush polymers were modeled as being composed of two types of main-chain segments: charged segments and uncharged segments with an attached side chain. We have been able to capture the major experimental findings for adsorption on mica and on silica oxide, made predictions that we currently are testing experimentally, and provided further insight into the adsorption.

In our first sub-project, model calculations were made for various main-chain compositions (various value of X) for adsorption on mica-like and silica-like surfaces. The mica-like surface possesses a constant negative surface charge density and no special affinity, whereas the silica-like surface has a constant negative surface potential and a positive affinity for the side chains of the bottle-brush polymers. The model was able to reproduce a number of salient experimental features characterizing the adsorption of the bottle-brush polymers for the full range of the composition variable X on the two surfaces, and thereby quantifying the different nature of the two surfaces with respect to electrostatic properties and nonelectrostatic affinity for the polymer. In our second sub-project, model calculations were extended to cover bottle-brush polymers with different length of side chains. With the mica-like surface, at low X the surface excess became smaller and at $X \geq 25$ it became larger with increasing side-chain length. Hence, the value of X at which the surface excess displays a maximum increased with

the side-chain length. However, with the silica-like surface the surface excess increased with increasing side-chain length at all $X < 100$, and the maximum of the surface excess appeared at $X \approx 10$ independent of the side-chain length. (Per Linse and Per Claesson (KTH, Stockholm))

Low interfacial tension microemulsions for practical applications

(Contact person: Ulf Olsson)

The high solubilization capacity and the ultra low interfacial tension exhibited by microemulsions make them desirable for a broad range of applications including enhanced oil recovery, soil and aquifer remediation, consumer and pharmaceutical formulation, chemical reaction media and nanoparticle preparations. In this project we investigate various microemulsion formulations, targeted for practical applications, combining phase diagram and interfacial tension studies. Systems studied include ionic surfactant in combination with oppositely charged hydrotropes with the aim to optimize the overall surfactant efficiency. (Ulf Olsson, I. Kayali and K. Qamhie (Al-Quds University, Jerusalem), L. Bemhart and R. Strey (University of Köln))

Hydrophobically modified polymers in pharmaceutical tablet formulations

(Contact person: Lennart Piculell)

Hydrophobically modified polymers are water-soluble polymers that contain a small proportion of strongly hydrophobic functionalities attached to the polymer backbone. Such polymers are not traditionally used as excipients in pharmaceutical drug tablets. In this project, we study how the hydrophobic modification as such, and the possible presence of other amphiphilic molecules such as surfactants, affect the drug release properties of tablets made from hydrophobically modified poly(acrylic acid). (Patrik Knöös, Lennart Piculell, Marie Wåhlgrén (Food Technology) and Stefan Ulvenlund)

Interaction between functionalised soft polymer particles and inorganic surfaces

(Contact person: Lennart Piculell)

When water evaporates from a dispersion of polymer particles, the particles are forced together developing a coherent film. Therefore soft polymer particles are widely used as binders in a range of applications, including water based paints, glue, and paper coatings. It is generally found that chemically modified particles have superior properties in films that include inorganic pigment particles, resulting in improved mechanical properties and water resistance of the film. In this project, the effect of the functionalisation of the polymer particles on their film formation and interactions with inorganic surfaces is studied, primarily by atomic force microscopy (Project completed 2010). (Tommy Nylander, Lennart Piculell, Ola Karlsson, J.K. Dreyer)

Phase separation, adsorption behavior and delivery capacity of polyelectrolytes and oppositely charged surfactants at surfaces (Contact person: Lennart Piculell)

The concentrated phase formed in dilute mixtures of polyelectrolytes and oppositely charged surfactants can be a precipitate (solid) or a coacervate (liquid) depending on parameters such as the molecular weight and charge density of the polymer, the self-assembly of the surfactant and the charge ratio of polymer vs. surfactant in the mixtures. The phase separation is of practical use in products where it is desired to obtain a deposition on a surface. The polymer-surfactant complexation can also be

used to deliver an additional substance to the surface. The aim of the present project is to link the adsorption behavior of a polyelectrolyte-surfactant mixture with the characteristics of the phase separation in the bulk solution. Based on these results, the delivery of an oil-in-water emulsion to a hydrophilic and hydrophobic surfaces are studied. A combination of different techniques is used: in-situ ellipsometry to investigate the adsorption behavior, phase studies and turbidity measurements to look into the bulk properties, dynamic light scattering to determine the size of soluble aggregates and gel swelling experiments to investigate the polymer-surfactant binding. (Asger Bjørn Petersen, Wei Wang, Tommy Nylander, Lennart Piculell, E. Johnson, R. Panandiker and M. Sivik (Procter & Gamble, Cincinnati))

Associative effects of polyacrylates in surfactant systems

(Contact person: Björn Lindman)

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

Alginate particles as vehicles for gene therapy (Contact person: Ulf Olsson)

Major efforts to obtain efficient means of gene therapy have lead to important improvements but there are still problems with low efficiency and toxicity. The objective of this project is to use a novel approach to produce a biocompatible gene therapy formulation based on particles of alginate gel containing the DNA to be delivered. The particles will be characterized using a range of techniques with regards to physicochemical character and biological activity. (Alexandra Machado, Dan Lundberg, Ulf Olsson, Björn Lindman, Maria da Graça Miguel (University of Coimbra), António J. Ribeiro (University of Coimbra), Francisco J. Veiga (University of Coimbra))

Cleaning technology in high temperature food processing - from fundamental understanding to sustainable and safe food processing

(Contact person: Tommy Nylander)

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

is cleaned as environmental friendly as possible and simultaneously guaranteeing that it is always totally cleaned, reducing the risk of food safety or quality hazards due to improperly cleaned equipment. (Tommy Nylander, Fredrik Innings (Tetrapak AB), Christian Trägårdh and Marie Paulsson (Food Technology), Niklas Lorén (SIK AB, The Swedish Institute for Food and Biotechnology Structure and Material Design))

Understanding the dissociation of pharmaceutical salts

(Contact person: Daniel Topgaard)

Active pharmaceutical ingredients (API) are active chemicals used in the manufacture of drugs. APIs poor solubility in water leads to many problems in the pharmaceutical industry, one of the biggest being the poor uptake in vivo. Many of the APIs that are manufactured today are formulated as salts with a suitable counter-ion instead of in its free form. Such salts are often found to have a higher transient solubility in biologically relevant fluids, with enhanced uptake in the body. The problem is that these API salts are very sensitive to water, and at a certain water activity a given salt will dissociate to its free form. The central questions of the project are when and how the pharmaceutical salt dissociates in the presence of moisture, and how this process influences the physical and chemical stability of solid dosage forms. The dissociation is studied with newly developed solid-state nuclear magnetic resonance spectroscopy methods giving information on molecular mobility and phase behavior at the relevant moisture contents. (Sanna Gustavsson, Daniel Topgaard, Stefan Ulvenlund and Johan Reimer)

SCIENTIFIC INSTRUMENTATION

Surface techniques

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 and 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).

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

Quartz crystal microbalance with dissipation monitoring (QCM-D)

(Contact person: Tommy Nylander)

The instrument is from Q-Sense fitted with E4 and E1 module and is able to collect, both the dissipation and the resonance frequency of a quartz crystal. These data can be used to follow the formation of thin films (nm) such as proteins, polymers and cells onto surfaces, in liquid by using a flow system at controlled temperature. The advantage with measurements at several frequencies and the dissipation is that we can determine the adsorbed film is rigid or water-rich (soft). The instrument is equipped with a Q-Sense Ellipsometry Module (for the Q-Sense E1 system), which enables simultaneous QCM-D and ellipsometric measurements on the same substrate. Thus we can determine both the adsorbed amount and the water content in adsorbed layer. (New instrument, sponsored by The Knut and Alice Wallenberg Foundation.)

Multimode scanning probe microscope (Contact person: Emma Sparr)

A XE-100 AFM system from ST Instruments (Park systems) was installed in 2011. The instrument can be operated to image topography and friction on small and medium size

samples both in air and in liquid (up to 70°C). The instrument consists of completely decoupled XY & Z scanners by using flexure guided scan system for all three axes, closed/open-loop scan, XY flexure scanner with zero background curvature, motorized Z stage, motorized focus stage, precision motorized XY sample stage and direct on-axis optics. The system also includes high resolution digital CCD camera with digital zoom. (New instrument, sponsored by The Knut and Alice Wallenberg Foundation.)

Surface force apparatus (SFA) (Contact person: Tommy Nylander)

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

Surface film balance (Contact persons: Tommy Nylander and Emma Sparr)

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

Surface tension, surface rheology and contact angle

(Contact person: Tommy Nylander)

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

Scattering techniques

Dynamic and static light scattering (DLS and SLS) (Contact person: Karin Schillén)

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 $-12\text{ }^{\circ}\text{C}$ to $+140\text{ }^{\circ}\text{C}$ (if the refractive index matched liquid changed) and is controlled to $\pm 0.01\text{ }^{\circ}\text{C}$ 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.)

Multangle laser light scattering (MALLS) (Contact person: Karin Schillén)

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

3D Light scattering instrument (Contact person: Peter Schurtenberger)

The instrument from LS Instruments is used for simultaneous dynamic and static light scattering with transparent and turbid samples. It is equipped with a HeNe laser light source, wavelength $\lambda_0 = 632.8\text{ nm}$ and a maximum power of 35 mW. The sample is filled into cylindrical glass cells of a diameter of 3, 5 or 10 mm or 10 mm square cells and placed in the temperature controlled index-matching bath. The scattered light is detected within an angular range of 15 to 140° by two efficient Avalanche Photo Diodes and processed by a Flex correlator in a 3D cross-correlation configuration. In aqueous samples we have access to scattering vectors $0.0034 \leq q \leq 0.025\text{ nm}^{-1}$. The apparatus is equipped with a sample goniometer to characterize non-ergodic samples.

Multi-angle 3D-goniometer system (Contact person: Peter Schurtenberger)

The instrument allows time-resolved measurements of dynamic and static light scattering in transparent and turbid samples using the technique of 3D cross-correlation at four angles simultaneously. The apparatus is equipped with a diode-pumped solid-state laser (wavelength $\lambda_0 = 532\text{ nm}$) with a maximum power of 200 mW. The sample is filled into cylindrical glass cells of a diameter of 3, 5 or 10 mm or square cells with diameter 10 mm and placed in the temperature controlled index-matching bath. The scattered light is detected within an angular range of 10 to 150° by two photomultiplier tubes at each angle and processed by a Flex correlator in a 3D cross-correlation configuration. Thus four intensity correlation functions are obtained simultaneously, one for each scattering angle measured. In aqueous samples we have access to scattering vectors $0.0027 \leq q \leq 0.031\text{ nm}^{-1}$.

Ultra small angle light scattering (USALS) (Contact person: Peter Schurtenberger)

The instrument is used for simultaneous dynamic and static light scattering at ultra-small angles using a CCD camera. The scattered light is detected from 0.3° to 6° , corresponding to length scales from a few hundred nanometers to a fraction of a millimetre. Time resolved static measurements with a time resolution of approx. 100 msec. Multispeckle correlation functions are processed in real-time, thereby allowing measurements of a set of intensity autocorrelation functions at different q -values using measurement times that are comparable to the longest correlation time. A multitau correlation scheme is adopted (delay time space quasi-logarithmically), requiring thereby less data storage and processing time. This allows one to calculate time- and pixel-averaged correlation functions in real time. Multiple exposure times are used in order to optimize the mean intensity level for all scattering vectors. The instrument is equipped with a HeNe laser light source with a wavelength of 632.8nm and a maximum power of 35 mW. The sample is filled into squared glass cells with path lengths ranging from 10 μm to 1 mm and placed in a temperature-controlled sample environment. The instrument is designed to study both ergodic and non-ergodic samples

Diffusive wave spectrometer (DWS) (Contact person: Peter Schurtenberge)

The instrument is used for characterization of extremely turbid samples and is equipped with diode-pumped solid-state laser (wavelength of 660 nm) with a maximum power of 70 mW. The apparatus is implemented with a "Two-Cell Echo Technique" which allows reducing measurement times down to only a few minutes even for slowly relaxing and solid-like materials. The sample is filled into squared glass cells of 1 – 10 mm and placed in a temperature controlled sample environment (15-70 $^\circ\text{C}$). The scattered light is detected with two efficient Avalanche Photo Diodes in transmission and processed by a multi-tau/linear correlator using pseudo-crosscorrelation as well as echo measurements. Also possible are experiments using backscattering geometry as well as CCD camera-based multispeckle measurements. The equipment runs with a powerful software solution (LS-Instruments, Fribourg, Switzerland) for data acquisition and analysis (combined correlation-echo measurements, single-, multi-speckle analysis, user defined multi-run scripts, online microrheology analysis and full data access).

Electrophoretic light scattering

(Contact persons: Karin Schillén and Peter Schurtenberger)

Two Zetasizer Nano ZS instruments from Malvern Instruments Ltd, Worshestershire, UK, are available for convenient DLS and SLS measurements as well as for determination of eletrophoretic mobility (or zetapotential) in both aqueous and non-aqueous dispersions. The required particle diameter ranges from 3.8 nm to 10 μm with concentrations up to 40 % (w/v) depending on sample. A conductivity range from 0 to 200 mS cm^{-1} is required. The instrument measures DLS and SLS at a set angle of 173° using the NIBS technology. The zetapotential (or electrophoretic mobility) measurements by means of M3-PALS technology are performed at 17° . The instrument is equipped with a 4 mW He-Ne laser (wavelength of 632.8 nm) with an automatic laser attenuator that allows for measurements at sample transmissions ranging from 100 % to 0.0003 %. The detection unit comprises an avalanche photodiode. The temperature range of the instrument is 2-90 $^\circ\text{C}$. (Sponsored by Crafoordska Stiftelsen)

Small/wide angle X-ray spectrometer (SAXS and WAXS).

(Contact person: Peter Schurtenberger)

This instrument combines a X-ray focusing optics with a block collimator which produces an intense, monochromatic primary beam. The primary beam is focused through the sample allowing fast measurements of the scattering pattern, even from samples with low contrast. The scattering signal is detected by a CCD camera for SAXS and a 2D imaging plate detection system for WAXS. The apparatus is implemented with a SAXSess camera using a X-ray generator (PANalytical, PW 3830) with a sealed copper tube. The X-ray generator offers a maximum power of 4.0 kW and an operating range of 20-60 kV and 10-100 mA. A Göbel mirror and a Kratky block collimation system (line-shaped beam) is used to convert the divergent polychromatic X-ray beam into a focused line shaped beam of Cu-K $_{\alpha}$ radiation. Holders for liquid and solids are available. The instrument design makes it possible to investigate particles length scales from 0.25 nm (thanks to the wide angle extension system) up to 40 nm. Thus, q values range from $\leq 0.077 \text{ nm}^{-1}$ (corresponding to a Bragg value $\geq 82 \text{ nm}$) up to $\approx 8 \text{ nm}^{-1}$ (SAXS) and $\approx 29 \text{ nm}^{-1}$ (SWAXS).

Nuclear magnetic resonance (NMR)

(Contact person: Daniel Topgaard)

Two Bruker Avance II spectrometers are available at Physical Chemistry: one 500 MHz system from 2007 and one 200 MHz system originally installed in 1994 and upgraded in 2006. Both spectrometers are equipped for high-performance diffusion studies. The 500 MHz has accessories for microimaging, solid-state, and high-resolution magic-angle spinning experiments. (Sponsored by VR/KFI.)

- Bruker Avance II 500

Magnet: 11.7 T / 500 MHz, 54 mm UltraShield

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

- Bruker Avance II 200

Magnet: 4.7 T / 200 MHz, 89 mm

Probes: BBO 10mm ($^{31}\text{P}/^{15}\text{N}/^1\text{H}$), DIF-25 5mm (^1H)

Microscopy

Optical microscopy (Contact person: Emma Sparr)

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

Confocal scanning laser microscope (Contact person: Peter Schurtenberger)

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

Transmission electron microscopy with cryo facilities

(Contact person: Viveka Alfredsson)

The national Centre for High Resolution Electron Microscopy (nCHREM) at the Department of Chemistry has two transmission electron microscopes. The Philips CM120 BioTWIN Cryo is a microscope dedicated for cryo-imaging. It is operated at 120 kV. The BioTWIN objective lens gives high contrast and the resolution is 0,34 nm. The microscope is equipped with an energy filter imaging system (Gatan GIF 100) and digital multiscan CCD cameras (Gatan 791). There is an Oxford CT 3500 Cryoholder and transfer system. The JEOL3000F is an analytical high-resolution transmission electron microscope with a field-emission electron source and an operating accelerating voltage of 300kV. The microscope is equipped with video-rate camera, and a 2 x 2 k CCD camera for HR image recording. The structural resolution is 0.17 nm in conventional mode, and 0.13 nm in STEM mode with high-angle annular detector. The microscope has an Oxford XEDS system and a Gatan Imaging Filter (2 x 2 k) for analysis of chemical composition with a spatial precision below 1 nm. Specialised holders for specimen transfer at liquid nitrogen temperature, insitu heating, scanning tunneling microscopy with simultaneous TEM viewing etc are available. More information about nCHREM can be found at <http://www.materialkemi.lth.se/nchrem/index.html>. (Sponsored by NFR, Crafoord Foundation and Knut and Alice Wallenberg foundation.)

Calorimetry**Differential scanning calorimeter (DSC)** (Contact person: Emma Sparr)

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

Isothermal titration calorimeters (ITC)

(Contact persons: Emma Sparr & Gerd Olofsson)

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

* Isothermal titration microcalorimeter 2277 TAM Thermal Activity Monitor System.

Reaction calorimeter (Contact person: Ola Karlsson)

The energy released as heat by a process is directly proportional to the rate of reaction and by monitoring the reaction in a calorimeter detailed kinetics can be revealed.

In 2011 we will get a Chemical Process Analyser CPA202 from Chemisens. It is a high precision factory pre-calibrated calorimeter made in Hastelloy C276 with a useful volume of 10 – 180 ml, which can be continuously varied during experiments. The temperature range for experiments is -50 °C to + 200 °C and it is possible to operate in a pressure range from vacuum up to 20 bars. The temperature resolution for an experiment is 0.001 °C and the power resolution is 0.001 Watt in the standard reactor and in the so called HighSens Reactor, which will be used for e.g. adsorption kinetics, crystallization, dissolution of tablets and micellization it will be possible to perform studies with a power resolution of 0.1mW at a volume of 10 -180 ml. (New instrument, sponsored by The Knut and Alice Wallenberg Foundation.)

Sorption calorimeter (Contact person: Gerd Olofsson)

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

Rheology**Rheometers** (Contact person: Ulf Olsson)

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.

A rheo-small angle light scattering (SALS)/microscopy instrument based on the MCR301 rheometer from Anton Paar has recently been installed (New instrument, sponsored by the Knut and Alice Wallenberg Foundation). The rheometer works with both Couette and cone-and-plate geometries. For simultaneous rheology and SALS or microscopy experiments a transparent plate-plate or cone-and-plate geometry is used with the optical axis in the gradient direction.

Advanced rheometric expansion system (ARES)

(Contact person: Peter Schurtenberger)

The Advanced Rheometric Expansion System (ARES) is a true strain-controlled instrument, where the application of strain and the measurement of stress are separated. The sample is subjected to either a dynamic (sinusoidal) or steady shear strain deformation, and then the resultant torque expended by the sample in response to this shear strain is measured. The motor applies shear strain; the transducer measures torque. Strain amplitude and frequency are set by the operator, with the actual sample deformation determined by the measured motor, and transducer, displacement. The instrument is implemented with the transducer 1 K FRT (torque range 0.004 – 20.0 g•cm and normal force range 2.0 – 2000.0 gmf). The operational temperature range is between -30°C and 150°C with temperature stability at thermal equilibrium of ± 0.1 °C, which is controlled with a Peltier system. The actual available geometries are: cone and plate (50 mm, 0.04 rad, 25 mm, 0.04 rad), plate and plate in (50 mm) and couette (16.5 mm bob, 17 mm cup and 32 mm bob and 34 mm cup).

Spectrophotometers

UV-Vis spectrophotometer (Contact person: Ingegerd Lind)

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

Fluorescence spectrophotometer (Contact person: Emma Sparr)

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

COLLABORATIVE RESEARCH PROGRAMS

Organizing Molecular Matter (Contact person: Lennart Piculell)

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

SSF–“Porous surface layers through polymer-assisted deposition” (Contact person: Håkan Wennerström)

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

SoftComp (Contact person: Peter Schurtenberger)

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

European Soft Matter Infrastructure (ESMI)

(Contact person: Peter Schurtenberger)

Free access to soft matter infrastructure, synthesis facilities, first-class instrumentation and a fast supercomputer will be offered by the new EU project ESMI, planned to start in January 2011. ESMI consists of three main parts:

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

- Networking: A dissemination and educational plan will be implemented to foster a culture of cooperation between research infrastructures and scientific communities

- Joint Research Activities - A number of research projects are funded to improve the existing infrastructure.

Biopolymers based surfactants - stabilization and functionalization of particles and surfaces

(Contact person: Björn Lindman)

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.

BIOCONTROL (Contact person: Tommy Nylander)

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 biomimetic 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 program comprising (bio)physicists, biologists, (bio)chemists, surface chemists and computational biologists. (T. Nylander, V. Alfredsson) (<http://biocontrol.tau.ac.il/>)

NANOGROWTH (Contact person: Viveka Alfredsson)

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>).

NordForsk Network (Contact person: Tommy Nylander)

Nordic Milk Science Initiatives, 2008-2011 (NordicMilk Network). Research within dairy science has a long tradition in the Nordic and Baltic countries and the level of the research has been on high international standard. Recent research has revealed in cow's milk many protective components and their derivatives displaying a range of bioactivities. The research has been focused on product and process development directly related to the traditional use of the milk raw material. This also involves health and nutritional aspects as well as linking the genetic variants of the milk components to the product quality. This project joins multidisciplinary research groups from five Nordic countries and two Baltic countries who are working on milk compounds related

to health and technological aspects. This project will join high know-how in chemical, analytical, technological, structural, in vitro studies and human clinical studies related to milk compounds. (Tommy Nylander) https://portal.mtt.fi/portal/page/portal/www_en/Projects/Nordicmilk

Division of Surface Chemistry of the Swedish Chemical Society

(Contact person: Lennart Piculell)

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 theme of the 10th Symposium in 2010 was “Molecular Processes at Solid Surfaces”, with contributions addressing fundamentals as well applications in diverse fields such as surface modification, biology and geology. A new feature in 2010 was a session dedicated to presentations from PhD students. Tommy Nylander was the chairman of the program committee, and Jonas Carlstedt, Charlotte Gustavsson, John Janiak, Tomas Kjellman, Joakim Stenhammar, Marianna Yanez and Lennart Piculell were on the local organizing committee.

Strategic Research Areas at Lund University

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

CONFERENCES, TRAVELS AND SEMINARS

Björn Lindman gave invited lectures at the Otto Glatter Workshop, Prague; the International Conference on Nanoscopic Colloid and Surface Science (NCSS 2010) Makuhari, Chiba, Japan; SEPAWA, Fulda, Germany; 18th International Symposium on Surfactants in Solution, Melbourne, Australia (2 lectures); Avant Hair Care Symposium, Wayne, New Jersey. He also gave a talk at the COST workshop on “Biopolymer based surfactants – stabilisation and functionalisation of particles and surfaces” in Barcelona, Spain. He also attended the International Soft Matter Conference in Granada, Spain, the symposium “Colloidal Dispersions in Nanoscience” in Borovets, Bulgaria and the 23th Conference of the European Colloid and Interface Society (ECIS) in Prague. Björn Lindman organized and chaired with Indian colleagues a workshop on: “Manipulation of DNA with cosolutes”, funded by Swedish International Development Cooperation Agency (SIDA), in Kumarakom, Kerala, India. He also gave a lecture at the workshop. 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: Nanyang Technological University, Singapore; Procter&Gamble Research Center, Cincinnati; GlaxoSmithKline Research Center, Weybridge, UK; Cognis Research Center, Düsseldorf, Germany; Universidade Beira Interior, Covilha, Portugal; Instituto de Química Avanzada de Catalunya CID-CSIC, Barcelona, Spain; University of Porto, Portugal; Kazakh Technical University, Almaty, Kazakhstan; Henkel Research Center, Düsseldorf; InnovNano Research Center, Aljustrel, Portugal; Beiersdorf, Research Center, Hamburg; Akzo Nobel Surface Chemistry, Stenungsund, Sweden; Pola Research Center, Yokohama, Japan; Kao Research Center, Tokyo, Japan; Procter&Gamble Research Center, Kobe, Japan; Novo Nordisk Research Center, Copenhagen. Björn Lindman was visiting professor at the Department of Chemistry, Coimbra University, Portugal and at Nanyang Technological University, Singapore.

Lennart Piculell gave invited lectures at the conferences Formula VI, Stockholm, European Detergents Conference (EDC) 2010, Fulda, Germany, and the 10th International Symposium on Polyelectrolytes in Shanghai. Together with Patrik Knöös he also attended a symposium on Drug Transport and Delivery in Göteborg in June.

Håkan Wennerström gave invited lectures at the German Biophysical Society Meeting, Gomadingen and gave a plenary lecture at FORMULA VI in Stockholm.

Per Linse presented a poster at the 20th Annual Surface and Colloid Symposium in Lund, Sweden, as well as at the Theoretical Chemistry Symposium in Lund, Sweden.

Ingemar Wadsö gave a plenary lecture at the 16th International Conference on Biological Calorimetry in Lugo, Spain.

Peter Schurtenberger gave invited plenary lectures at International Soft Matter Conference in Granada, Spain and at MAXlab Annual User Meeting in Lund, Sweden. He gave invited keynote lectures at American Chemical Society Spring National Meeting in San Francisco, USA and at ILL 2020 Vision - Future directions in neutron science in Grenoble, France. He gave invited lectures at the following international conferences, workshops and summer schools: International Workshop on Modern Light Scattering Technologies in Düsseldorf, Germany, International summer school on “The power of neutron scattering techniques in nano and bio sciences” in Jaca, Spain. He also gave invited seminars at the following Universities and Industry Research Centers: Institute of Materials Seminar, Ecole Polytechnic Fédéral de Lausanne (EPFL) in Lausanne, Switzerland; School of Physics Seminar, University of Edinburgh in Edinburgh, UK; Institute for Science and Technology Austria Seminar in Klosterneuburg, Austria;

Physics Colloquia, Università Degli Studi di Milano in Milan, Italy; School of Chemical Engineering and Analytical Science Seminar, University of Manchester; Fribourg Chemical Society in Fribourg, Switzerland; Novo Nordisk Research at Novo Nordisk Park, Måløv, Denmark.

Tommy Nylander gave an invited talk at YKI, Institute for Surface Chemistry. He gave two invited overview talks at workshops for PhD students and researchers at “Molecular Self-assembly and Interaction” and “Proteins: Expression, Folding, Structure and Function” at Center for Bioengineering and Biotechnology, China University of Petroleum. He also gave an invited talk at the Scientific workshop for inauguration of new neutron reflectometer Super-Adam at ILL, “Next generation neutron reflectometer” at the ILL, Grenoble, Biomaterials workshop, Malmö University, University of Newcastle, NSW, Australia, 4 November, Applied Maths, Australian National University, Canberra, Australia and Institute of Biochemistry, Vilnius University, Vilnius, Lithuania. He gave talks at Biophysical Society Meeting in San Francisco, USA, Food Colloids 2010, Grenada, European Colloid and Interface Society Meeting, Neutrons and Food –Ansto workshop, Sydney, Australia, Surfactant in Solution, Melbourne, Australia. Tommy Nylander co-organised Annual Swedish Neutron Scattering Society meeting and the International Workshop on Biointerfaces, Lund, Sweden

Ulf Olsson attended the Nordic workshop on “Scattering from Soft Matter” in Helsinki, and presented a plenary lecture at the World Congress on Emulsions in Lyon. He also presented a lecture at workshop organized within the NEQ-SOFT program at Ochanumizu University, Tokyo. He presented a lecture at the workshop “Beamlines at MAX IV” and, in addition, organized a workshop “The Soft Matter Beamline” at the Annual MAX-lab User Meeting in Lund. He visited and gave talks at POLA Chemicals in Yokohama, the Institute of Biophysics and Nanosystems Research of the Austrian Academy of Science in Graz, Austria and at the Kazan State Technological University, Russia.

Karin Schillén gave an invited lecture at Workshop in the honour of Otto Glatter at the XXIV (ECIS)Conference in Prague, Czech Republic. She presented a poster at the 10th Annual Surface and Colloid Symposium Molecular Processes at Solid Surfaces, Lund, Sweden. Karin Schillén visited the Department of Chemistry, University of Palermo, Palermo, Italy and held an invited seminar.

Viveka Alfredsson gave an oral presentation at the 16th International Zeolite Conference joint with the 7th International Mesosstructured Materials Symposium in Sorrento, Italy. She also gave an invited oral presentation at the 17th International Microscopy Congress in Rio de Janeiro, Brazil.

Emma Sparr gave invited lectures at the International Conference on Cosmetic Innovations (COSM’Innov), Orléans, France and at the International meeting on Biointerfaces/SNSS, Lund, Sweden. She also gave an oral presentation at Biophysical Society Annual Meeting, San Fransisco, USA and an invited seminar at Umeå University.

Daniel Topgaard gave invited lectures at the “Workshop on manipulation of DNA with cosolutes”, Kumarakom, Kerala, India and the “FG 1145 kick off meeting”, Wittenberg, Germany.

Joakim Stenhammar presented posters at the 8th Liblice Conference on the Statistical Mechanics of Liquids in Brno, Czech Republic and at the 20th Annual Surface and Colloid Symposium in Lund, Sweden. He also gave an oral presentation at

the 8th European Conference on Computational Chemistry in Lund, Sweden.

Charlotte Gustavsson presented a poster at the 10th ASCS in Lund, Sweden.

Tomas Kjellman presented a poster at 16th International Zeolite Conference (16th IZC) joint with the 7th International Mesoporous Materials Symposium (7th IMMS) in Sorrento, Italy. He also visited a group of professor Osamu Terasaki at the Korean Institute of Science and Technology (KAIST), Daejeon, South Korea for 2.5 weeks to learn about the use of low voltage High Resolution Scanning Electron Microscopy (HR-SEM) and Cross Section Polishing to extract information about the detailed structure of mesoporous silica.

Patrik Knöös attended and presented a poster at the following conferences last year: FLÅK Workshop in Brösarp; Formula VI, Stockholm; Drug Transport and Delivery, Gothenburg; 10th ASCS in Lund.

Marianna Yanez gave a College 9 seminar in the Institute Laue-Langevin in Grenoble, France. She presented a poster at the “Annual Swedish Neutron scattering society meeting and the International Workshop on Biointerfaces” in Lund and at “Molecular Processes at Solid Surfaces. 10th ASCS in Lund. She also gave an oral presentation at the “Eighth Nordic Workshop on Scattering from Soft Matter” in Kjeller, Norway.

Agnes Michanek and Marie-Louise Ainalem presented posters at the Biophysical Society Annual Meeting, San Fransisco, USA.

John Janiak gave an oral presentation at the XXIV European Colloid and Interface Society (ECIS) conference in Prague, Czech Republic. He also presented a poster at the 10th ASCS in Lund.

Giuseppe Lazzara presented a poster at the VII Nordic Workshop on Scattering from Soft Matter in Helsinki, Finland. He also gave oral presentations at the XXXII National Congress on Calorimetry, Thermal Analysis and Applied Thermodynamics in Trieste, Italy, and at the XXIV European Colloid and Interface Society (ECIS) conference in Prague, Czech Republic.

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 Scientiarum Societas*. During the year he was elected foreign member of the *Academia das Ciências de Lisboa*, the Portuguese Academy of Sciences. He is cofounder and honorary member of the European Colloid & Interface Society (ECIS). For the period 2006-2009 Björn Lindman was President of the International Association of Colloid and Interface Scientists (IACIS) and now acts as immediate-past-President. 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, Czech and Italian Research Councils, and Lundbeckfonden, Denmark. Björn Lindman is also President of the Overbeek Foundation

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 “*Soft Matter*”, 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 chairing the local organizing committee of the annual three-day “*10th Annual Surface and Colloid Science Symposium*”, organized by Division of Surface Chemistry and Physical Chemistry, that took place in Lund. He was a member of the program committee for “*Formula VI*”, an international conference held in Stockholm 2010. He is the director of the Linnaeus center OMM. He was a member of the grading committee at the thesis defense of Harald Kirsebom, Biotechnology, Lund University.

Peter Schurtenberger was a member of the Swiss National Research Council, the General Secretary, European Colloid and Interface Society, the Liquids Board of the European Physical Society, the Scientific Advisory Committee of the Swiss Light Source and the Organizing Committee 10th European Summer School on “*Scattering Methods Applied to Soft Condensed Matter*”, Bombannes, France. He was also a member of the Network Governing Board and Chairman of the Experimental Platform of the European Network of Excellence SoftComp. Editorial Board, *Colloid & Polymer Science*. Peter Schurtenberger was section Editor, *Current Opinion in Colloid and Interface Science* and sat in the Advisory Board (Kuratorium), “*Physik in unserer Zeit*”.

Ulf Olsson served on the PhD thesis assessment committees for Manuel Alatorre Meda, University of Santiago de Compostela, and Jacob Judas Kain Kirkensgaard, Copenhagen University

Viveka Alfredsson was an opponent for Licentiate Thesis of Miia Klingstedt, Stockholm University and a Faculty opponent for Lu Han, Stockholm University. She was a member of the PhD thesis Committee of Andreas Sundblom, Chalmers and of the PhD thesis Committee of Salomé dos Santos, Lund University. She was also external examiner for PhD thesis of Bin Yang, University of Bath, UK. Viveka Alfredsson served as advisor (sakkunnig) for a lecturer position at Stockholm University. She was Member of Council of the International Mesostructured Materials Association and a member of the departments (KILUs) equality group. (jämställdehets- och likabehandlingsgrupp).

Tommy Nylander served as thesis examiner for the PhD thesis of Karla Webb, University of Manchester, Manchester, UK, and Marc Eeeman, Gembloux Agro-Bio-Tech, Université de Liège, Gembloux, Belgium. He was a member of Formas (The Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning) standing evaluation committee for Products and processes based on renewable and recycled resources. He was member of the evaluation panel for beam time applications NIST Centre for Neutron Research, Gaithersburg, USA and ISIS, Rutherford Appleton Laboratory, Oxfordshire, UK. In addition he was evaluator of research proposals for BBSRC – Biotechnology and Biological Sciences Research Council and MIUR – Ministero dell’Istruzione, dell’Università e della Ricerca, Italy. Tommy Nylander is a member of the Scientific Advisory Group and The Stakeholders Group of European Spallation Source – Scandinavia.

Karin Schillén is deputy Member of the grading committee of the PhD thesis defense for Ingrid Åslund, Physical Chemistry, Lund University. She was the head teacher in Physical Chemistry with the responsibility of organizing the teaching given by the members of the Division of Physical Chemistry. She was also a member of the board of the undergraduate studies in chemistry at the Department of Chemistry, Lund University.

Emma Sparr served on PhD thesis committee for Raghu Sankhar (MEMPHYS, SDU Odense, Denmark).

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 Department of Chemistry consists of four 5-week chemistry courses (which are given both during the fall and the spring semesters), one 10-week course in mathematics and one 10-week course in physical chemistry. In the first basic chemistry course during the spring semester, Emma Sparr, Viveka Alfredsson and Johan Reimer were involved in lectures and leading exercises and question hours, whereas Daniel Topgaard, Viveka Alfredsson, and Johan Reimer gave the course during the fall semester. The topic of the first-year physical chemistry course is thermodynamics and quantum mechanics and it is based on the textbook of P. W. Atkins and J. De Paula "Atkins' Physical Chemistry". Karin Schillén is the main teacher for this course and she gave the lectures in thermodynamics together with Viveka Alfredsson, who also led the corresponding exercise sessions.

As regards higher courses, the Division gives one basic course and one advanced Master course in surface and colloid chemistry and two Master courses in experimental physical chemical methods. The introductory colloid and surface chemistry course was taught by Ulf Olsson, Lennart Piculell, Håkan Wennerström and Stefan Ulvenlund. The advanced surface and colloid chemistry course, given during the fall semester, was taught by Emma Sparr along with Lennart Piculell, Håkan Wennerström, Tommy Nylander and Joakim Stenhammar. This course is based on the textbook "The Colloidal Domain" by Fennell Evans and Håkan Wennerström. The additional two Master courses were given during the spring semester by Daniel Topgaard (nuclear magnetic resonance, NMR, techniques) and by Ulf Olsson along with Tommy Nylander and Yngve Cerenius from MAX-lab (scattering techniques).

Karin Schillén continued to lead the PhD course in scattering "Advanced Scattering" in the spring semester of 2010 based on the textbook "Neutrons, X-Ray and Light Scattering: Introduction to an Investigative Tool for Colloidal and Polymeric Systems" edited by Peter Lindner and Thomas Zemb.

Two additional PhD courses were initiated during 2010. The first is a course in physical chemistry "Advanced Physical Chemistry" headed by Ulf Olsson in collaboration with the Divisions of Theoretical Chemistry and Chemical Physics at Department of Chemistry and the Department of Theoretical Physics. This course is based on the book "Physical Chemistry" by R. Stephen Berry, Stuart A. Rice and John Ross. The second PhD course is a course on ellipsometry led by Tommy Nylander together with Bengt Jönsson from the Department of Biophysical Chemistry.

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 in-house courses for industry.

Lennart Piculell gave his popular science lecture on "edible and inedible gels" on three occasions for Swedish high school students visiting Lund University.

SEMINARS 2010

Microcalorimetric techniques for chemistry and biology. Ingemar Wadsö (Physical Chemistry)

Controlling DNA compaction and the interaction with model biomembranes. Marie-Louise Ainalem (Physical Chemistry)

Understanding the physics of molecular motors. Heiner Linke (Nanometer Structure Consortium, Solid State Physics, Lund university)

Imaging and reaction dynamics in model membranes: Soft Nanoscience. Steven Boxer (Stanford University)

Peptide penetration through membrane (Curvature vs. Penetration). Kazutami Sakamoto (Tokyo University of Science)

Simple Alcohols in Microemulsion Systems of Nonionic Surfactant and their Structure in Bulk – SAXS, DLS and Monte Carlo Studies. Matija Tomsic (University of Ljubljana)

Phase diagrams of carbon nanotube-based systems. Oren Regev (Ben-Gurion University of the Negev)

Liquid crystals: Present and future materials and their applications. Per Rudquist (Microtechnology and Nanoscience, Chalmers)

Thermodynamical and structural analysis of block copolymer self-assembly in water. Effect of additives. Giuseppe Lazzara (Physical Chemistry)

Soft Matter for Energy Applications. Alexandar Matic (Condensed Matter Physics, Chalmers)

Morphological transitions of bilayer membranes triggered by external forces. Yukiko Suganuma (Department of Physics, Ochanomizu University, Japan)

DNA breathing and melting. Tobias Ambjörnsson (Computational Biology and Biological Physics, Dept Theoretical Physics, LU)

Physical chemical aspects of the greenhouse effect. Håkan Wenneström (Physical Chemistry)

Understanding Joint Lubrication: Friction Force Microscopy of Lubricin and Hyaluronic Acid. Debby Chang (Duke University)

How to have fun making a living of Physical Chemistry - From cow blood and medical devices to portable toilets. Anna Stenstam & Kajsa Bryskhe (Colloidal Resource AB)

Stiastite - A mechanism for solid solubility and a question of order. Sven Lidin (Division of Polymer & Materials Chemistry)

Protein condensation diseases seen with the eyes of a soft matter scientist. Anna Stradner (Adolphe Merkle Institute/University of Fribourg)

Morphology & Physiology by NMR Gradientology. Samo Lasic (Colloidal Resource / Physical Chemistry)

Specific examples of mechanism and structure determination of reactions and compounds in organic chemistry (with surprising results!) Asger Björn Petersen (Physical Chemistry)

The influence of discrete surface charges and surface charge clusters on the force between charged surfaces. Malek Khan (Physical chemistry, Uppsala University)

Gradient Based NMR to Measure Material Properties. Ingrid Åslund (Physical Chemistry)

Bilayers at the hydrophilic solid aqueous interface: adsorption, deposition, and removal. Robert K. Thomas (Physical & Theoretical Chemistry Laboratory, University of Oxford)

Self-assembly of three-phase "star polyphiles". Generalised foams, novel lyotropes and some ideas regarding tricontinuous patterns. Stephen Hyde (Dept Applied Mathematics, Australian National University, Canberra)

Tracer diffusion of particles in gels. Taco Nicolai (Polymères Colloïdes et Interfaces, Le Mans, France)

Mesoscale Structure and Structural Adaptability of Chloroplast Thylakoid Membranes. Dorthe Posselt (Department of Science, Roskilde University, Denmark)

Local pressure calculations from molecular dynamics simulations: applications to membrane proteins and lipid droplets. Samuli Ollila (Biological and Soft matter physics, Tampere University of Technology, Finland)

The role of molecular solvents in double layer forces. Luis Pegado (Physical Chemistry, LU)

Self-birthing of Vesicle. Yuka Sakuma (Department of Physics, Ochanomizu University, Japan)

Structural and dynamical properties of confined liquids: an experimental and numerical analysis. Alfred Delville (Université d'Orléans, France)

Phase separation dynamics in membranes: effects of bulk fluid. Shigeyuki Komura (Department of Chemistry, Tokyo Metropolitan University)

Hydration of biomimetic membranes - laser spectroscopy studies. Magnus Johansson (Surface and Corrosion Scienc, KTH)

Evolution of the Global Internal Dynamics of a Living Cell Nucleus during Interphase. Eric Freyssingéas (Université de Lyon, Laboratoire de Physique)

Self-Assembly of Bile Salt Derivatives. Luciano Galantini (Sapienza University of Rome, Italy)

Associative polymer-polymer and polymer-surfactant systems: phase behaviour and the influence of chemical reactions. Salome Santos (Physical Chemistry)

Spatial distribution of proteins and surfactant micelles in charged polymer networks Per Hansson (Pharmaceutical Physical Chemistry, Uppsala University)

AWARDS

The IFSCC Honourable Mention Award 2010 was given to Eric Johnson for his presentation, at the IFSCC conference 2010, of results from the long-standing research collaboration between Physical Chemistry and Procter & Gamble (IFSCC = the International Federation of Societies of Cosmetics Chemists). The presentation was also published as a paper in the IFSCC Magazine (E. S. Johnson, J. J. Zhang, L. Piculell, O. Santos, M. Clauzel, A. V. Svensson, T. Nylander: Polymer-Surfactant Phase and Surface Interactions Leading to New Models for Cationic Polymer Chemistries. IFSCC Magazine 3/4 (2010) 1-9).

Peter Schurtenberger was elected as an Honorary Member of the European Colloid and Interface Society

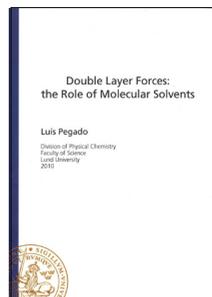
Björn Lindman became foreign member of the Academia das Ciências de Lisboa, the Portuguese Academy of Sciences.

DOCTORAL THESES

Luis Pegado

Double Layer Forces: the Role of Molecular Solvents

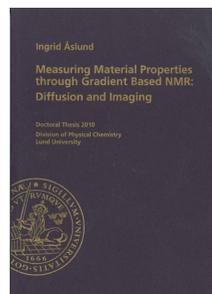
Opponent: Professor Alfred Delville, Université d'Orléans, France



Ingrid Åslund

Measuring Material Properties through Gradient Based NMR: Diffusion and Imaging

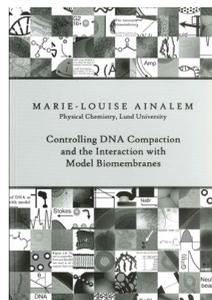
Opponent: Prof Dr. William S. Price, University of Western Sydney, Australia



Marie-Louise Ainalem

Controlling DNA compaction and the interaction with model biomembranes

Opponent: Professor Steven Boxer, Stanford University, USA



Salomé dos Santos

Associative Polymer-Polymer and Polymer-Surfactant Systems: Phase Behaviour and the Influence of Chemical Reactions

Opponent: Per Hansson, Uppsala University, Sweden



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WELCOME TO VISITORS

Dear Visitor,

We receive many guests, who stay with us from a few hours or a day of discussions, seminars 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 division 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 division. 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.

We recommend our visitors to fly to Kastrup Airport, Copenhagen. Then, take a train (frequency every 20 min.) from Kastrup Airport over the Öresund bridge directly to Lund railway station (takes approx. 45 min).

Visit the Kemicentrum website for further information:
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