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Front cover. Left: representative snapshot of an adsorbed flexible polyion on a net neutral cationic surface with mobile surface charges. Right: Contour plot of the average net charge of $20 \times 20 \text{ \AA}^2$ squares, obtained from Monte Carlo simulations with a fixed polyion conformation. The color code for a selected number of contour intervals is given. (Rita Dias)

Back cover. Schematic picture of a hexagonal phase with anionic DNA and rodlike cationic CTA micelles which are distorted to reduce the electrostatic free energy. (Daniel Topgaard)

WHAT IS A CENTER OF SCIENTIFIC EXCELLENCE?

During the last year there has in Sweden been a focus on scientific centers of excellence. All major research-funding agencies have geared substantial parts of their funds towards supporting activities under this concept. The signs are that this trend will continue for some time. This naturally raises the question of what constitutes a center of scientific excellence. There are reasonably well-established criteria for evaluating excellence of specific research achievements and also for judging the excellence among individual researchers. When it comes to centers of excellence the issue is much more tricky. Should the whole be judged simply as the sum of the parts? What are reasonable criteria for being a part of the whole? What is the time frame over which a center of excellence should operate before one can evaluate the performance? How scientifically focused should the activities be? What is the relevant output; scientific results, PhDs, industrial collaborations, courses/education, conferences, books, activities towards the public, ...?

When it comes to funding specific proposals, it must be the funding agency itself that has the privilege of interpretation. However, it is useful for us, as scientists belonging to a common research group, to reflect over these issues and provide answers that can guide us in our own planning. In our scientific activity at the Division of Physical Chemistry 1 we find it essential to establish long-term goals and policies that are based on an unbiased analysis of the specific situation, rather than an uncritical following of the current trends.

We have produced this Annual Report since 1989. The collection of these reports provides details of the scientific activities over fifteen years, presented in the contexts of a number of themes that has characterized the work at the division. It is, in fact, our contention that such a detailed and coherent documentation of the activities of a scientific group is unique for Sweden. Whether or not the quality of these scientific activities corresponds to those of a scientific center of excellence can only be answered by others. However, we here wish to take the opportunity to discuss some of the softer issues related to coordinated scientific activities.

At the division there are at present six professors, two lecturers and three assistant professors (forskarassistenten). Additionally, there are postdoctoral students, graduate students, visiting scientists, adjunct scientists and technical staff. What is this, more than a mere collection of people with a common administration and some common responsibilities with respect to teaching? It is and has been our policy that it should be a lot more.

Cooperation should be present in as many respects as possible. We share a scientific focus on Colloid Science with an inclusive interpretation of what this area encompasses. This provides a basis for a coordinated PhD education with an unusually rich program, by Swedish standards, of actively taught courses, typically in cooperation with colleagues at other Swedish universities. The doctoral students have direct access to expertise knowledge from a group of seniors often resulting in co-publication among seniors and/or graduate students. Through an active dialogue among seniors, postdocs and graduate students we share knowledge but also achieve mutual stimulation. By using equipment in different types of projects instruments can be adequately maintained and efficiently used. By sharing common tasks among several individuals each person can, to a larger degree than would otherwise have been possible, focus on tasks where her/his strengths are used.

In addition to their core scientific activities, seniors are often involved in collaborative projects of a broader character. These can be in the form of national programs, EU-financed activities or direct cooperation with industries. Typical for all these cases is that two or more seniors are engaged. For foreign short- or long-term guests the focus on colloid science in general, and the effort to keep an open attitude, provides a basis for a scientifically fruitful exchange. Furthermore, by recruiting permanent and visiting graduate students on a broad international basis we ensure a truly international atmosphere within the group. On an everyday basis there are typically ten or more nationalities represented during coffee time. Additional international stimulation is obtained by organizing meetings and symposia on a regular basis.

We have above described the context in which we perform our scientific investigations. A survey of previous annual reports reveals that these activities have resulted in a consistently high publication rate with around 40 published papers 1989 rising to 78 this year with many contributions of high international visibility. Annually on average four students have received their doctor's degree, with an all time high of nine in 2004. The challenge to keep up with the rapid scientific development was eased by the fact that we have the privilege to see two assistant professors (forskarassistenter) financed by the Research Council joining the division.

It is along these lines that we develop our vision of a Center of Scientific Excellence.

Björn Lindman

Per Linse

Lennart Piculell

Ulf Olsson

Olle Söderman

Håkan Wennerström

RESEARCH PROJECTS

Within the broad arena of modern colloid and surface chemistry, research is largely concentrated into seven loosely-bound areas: (1) Surfactant self-assembly; (2) Polymers, solutions, gels, and phase behavior; (3) Polymer-surfactant systems; (4) Protein and protein-amphiphile systems; (5) Adsorption and surface forces; (6) Experimental methodology in colloidal science and (7) Theoretical modelling.

Many projects involve two or more of these subjects and some projects have aspects that fall outside all seven of these themes.

Surfactant Self-assembly

Phase diagram and Thermodynamics of Alkylglucoside surfactants. The uptake of water in alkylglucoside surfactants is investigated by means of a sorption calorimeter. The device simultaneously measures the water activity as a function of water content and the partial molar enthalpy of mixing water with the surfactant. From the data, accurate water/surfactant compositions vs. temperature phase diagrams are obtained. In addition, using the thermodynamic properties of the phases and phase transitions, phase boundaries are constructed on the basis of thermodynamic modeling. By combining the sorption calorimetric measurements with accurate DCS measurements, glass transitions in two alkyl maltosides have been identified. (V. Kocherbitov (Malmö University), O. Söderman).

Long chain surfactants. Double chain cationic surfactants may form vesicles above the chain melting temperature, T_c . In a vortexed dispersion all chains freeze when the dispersion is cooled below T_c . However, in a sonicated dispersion it was found from NMR experiments that approximately 50 % of the chains remain in a fluid state even far (20-30 °C) below T_c . The reason for the stability of this supercooled state, and how frozen and fluid domains are distributed is still unclear. Work is extended to other lipid surfactants and lipids where similar observations have been made. In a more detailed DSC study of the chain melting/freezing process two separate steps involving similar enthalpy changes were observed. One of the processes showed slow kinetics in the freezing direction, and has therefore not always been recognized. (J. Cocquyt (Univ. of Gent), P. van der Meer (Univ. of Gent), G. Olofsson, U. Olsson).

Catanionic surfactant mixtures. Mixtures of oppositely charged surfactants (catanionic mixtures) exhibit novel solution and interfacial properties. The interplay between electrostatic effects and surfactant molecular geometry allows a rich diversity of phase behavior. The phase behavior and microstructure of several catanionic mixtures have been explored. Recently, it has been observed that the catanionic mixtures consisting of almost identical cationic and anionic surfactant pair exhibit different phase behaviour between the anionic-rich and the cationic-rich area at high water concentration. We are investing, by following the phase behaviour and phase structure for several systems for the understanding of this phenomenon. (A. Khan, E. Marques (Porto), H. Edlund (Sundsvall), C. La Mesa (Rome)).

Living polymers and living networks. Some surfactants form giant micelles in solution that can be longer than several micrometers. These solutions have properties similar to polymer solutions, however with some significant differences. The size distribution is not fixed but varies with concentration and temperature. Moreover, micelles may break and reform which influences the dynamics. For these reasons 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 is followed either by small angle neutron scattering (rheo-SANS) or by NMR measurements (rheo-NMR). The growth of “living polymers” with increasing concentration is an unresolved problem. Simple mean field models predict that the number averaged contour lengths varies with the concentration as $\langle L \rangle \sim \phi^{0.5}$ while one in the analysis of recent experiments have found the exponent 1.1-1.2. An important complication in the analysis of experimental data is the interactions and how they influence e.g. the osmotic compressibility. Here we are combining static and dynamic light scattering, and NMR self-diffusion experiments, to investigate the growth law in dilute solutions. (S. Bulut, K. Bryskhe, J. Hamit, U. Olsson, T. Kato (Tokyo, Japan), R. Angelico, L. Ambrosone and A. Ceglie (Campobasso, Italy), G. Palazzo (Bari, Italy), C. Schmidt and D. Burgemeister (Paderborn), K. Mortensen (Risø, Denmark).

Bilayer membrane kinetics. The phase lamellar-to-”sponge” phase transition involves a topological transformation of a bilayer membrane. In the lamellar phase the bilayer has a planar topology while it is multiply connected in the so-called “sponge” or L3 phase. Topology transformations are believed to involve the fusion or fission of membranes. With nonionic surfactants the phase transformation can occur by a minor change in temperature. Using deuterium as “phase-detection” the transition has been investigated in both directions. The sponge-to-lamellar transition appears to occur via a nucleation and growth process while the opposite transition rather involves a random fusion of adjacent bilayer membranes. To investigate the bilayer structure in more detail, The transitions are also studied by small angle neutron scattering experiments. A Sponge-to-lamellar transition can also be induced by shear flow and this was studied by rheo-birefringence. (U. Olsson, H. Wennerström; M. Gotter (Köln), R. Strey (Köln), F. Nettekheim (Kiel), C. B. Müller (Kiel), W. Richtering (Aachen)).

Alternative surfactants. Industrial interest continues in novel, especially biodegradable, surfactants like alkyl polyglucosides synthesised from renewable sources. Little research has been devoted to these systems. Phase diagrams, aggregate structure and microemulsion formation with model, and industrial compounds are investigated. Special interest is focussed on the liquid-liquid phase separation in binary and pseudo-binary alkylglucosides/water systems. The aim is to identify molecular factors that govern the phase behavior and so facilitating design of applications. Studies of polyglucoside/polymer interactions have been initiated. Solution properties of an acyl-N- methylglucamide and an ethoxylated fatty acid amide are also under exploration. Also an amino acid based surfactant, with applications as mild soap, is investigated in terms of the aqueous phase behavior, in particular the formation of a micellar cubic phase. (A. Khan, M. Nilsson, U. Olsson, J. Reimer, O. Söderman, C. Whiddon, I. Johansson (Akzo Nobel), D. Kaneko and K. Sakamoto (Ajinomoto Co. Japan))

Physico-chemical characterisation of micellar properties of PEG 12-acyloxy-stearates. Recent work with PEG 12-acyloxy-stearates (PEG-12-AS) has revealed remarkable properties of these amphiphilic compounds with regard to cell damage effects. For PEG1500 12-acyloxy-stearates with acyloxy groups of 14 to 18 carbon atoms no effects on red blood cells or intestinal cells were observed. The same behaviour was found for methyl-PEG2000 12-acyloxy-stearates. The mechanism behind these very unusual properties is still unknown. To understand the underlying mechanism, systematic studies of bulk properties of PEG-12-AS are carried out. Phase

diagrams, micellar structure as well as the nature of lyotropic liquid crystals found are determined. The surfactant dynamics is investigated by means of NMR diffusometry. (C. McNamee, O. Söderman, C. v Corswandt (Astra-Zeneca, Mölndal))

Shear-induced formation of multi-lamellar vesicles. The equilibrium structure and phase equilibria of the lamellar phase are sometimes complicated as noted in 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. (U. Olsson, B. Medronho (Coimbra), M. Miguel (Coimbra), F. Nettesheim (Kiel), W. Richtering (Aachen), P. Lindner (ILL Grenoble), K. Mortensen (Risø), C. Schmidt (Paderborn), D. Burgemeister (Paderborn)).

Thermodynamics of microemulsions. The common behavior of many microemulsion system with, e.g. the so-called Winsor I, II and III equilibria and the formation of lamellar phases at higher surfactant concentrations is qualitatively rather well understood. Here, the interfacial description, based on the curvature elasticity of the surfactant film, is a useful approach to understand the thermodynamics (structure and phase equilibria) of microemulsions and related phases. The key ingredients in this description are the spontaneous curvature of the surfactant film and two elastic moduli, the bending rigidity, which is a stiffness parameter and the saddle splay modulus which tells about the preferred topology of the surfactant film. Many efforts have been made to measure these quantities but it is difficult and different approaches or methods often give significantly different results. Particularly difficult it is to measure the saddle splay modulus. In this project we investigate a number of microemulsion systems with nonionic surfactants, varying the chain length of the oil. Depending on the oil chain length, and hence the degree of “oil penetration” (short oils penetrate or solvate the surfactant alkyl chains better) the microemulsion phase behavior is quantitatively and well as in some parts qualitatively different. It appears that oil penetration affects not only the spontaneous curvature but also the elastic moduli. (J. Balogh, H. Kaper, U. Olsson, J. Skov Pedersen (Aarhus, Denmark))

Stability of bilayer vesicles. The stability of bilayer vesicles is an intriguing problem. While an essentially unlimited stability or lifetime is often observed experimentally a vesicle dispersion may still be a trapped metastable state. One reason for a very slow equilibration is that Ostwald ripening in these systems can be a very slow process that does not even lead to a coarsening. Fusion of vesicles could be an effective coarsening mechanism, but for many systems it appears to be a rare event. In this project we aim to study fusion rates and how this is influenced by the curvature elastic properties of the bilayer film. (S. Bulut, U. Olsson, H. Wennerström)

Emulsions. NMR techniques are used to study oil- in- water and water- in- oil type emulsions with varying volume fractions. Self-diffusion data show that molecules of the dispersed phase undergo restricted self- diffusion whereas unbounded diffusion is the rule for the dispersion medium. The self- diffusion data can be used to determine

emulsion characteristics such as droplet size, size distribution and interdroplet interactions. In a related project new methods that allow the study of high internal phase ratio emulsions (concentrated emulsions) by means of the NMR self-diffusion approach have been developed. Here we focus on methods to investigate short- and long-time diffusion of the dispersed phase. In addition, the diffusional transport of active substances solubilized in the emulsions is investigated. Concentrated emulsions are also being used as model systems in developing methods to study porous media by means of pulsed field gradient NMR. In particular the new method of modulated field gradients is being used in the study of such emulsions. (C. Malmberg, D. Topgaard, O. Söderman).

Non-ionic surfactants as solubility enhancers in pharmaceutical formulations.

Aqueous formulations of hydrophobic drugs often require the use of solubility enhancers that increase the concentration of the active substance to therapeutically acceptable levels. Traditionally, PEG based surfactants have been used for this purpose. These surfactants have, however, certain pronounced drawbacks, most importantly a low long-term chemical stability in aqueous solution. Within the present project, novel non-ionic surfactants synthesised from renewable resources, primarily alkylglycosides, are studied as potential alternatives to PEG based surfactants in pharmaceuticals. The investigations include characterisation of non-ionic micellar systems by spectroscopic and light scattering techniques, as well as studies of novel preparative methods for incorporation of hydrophobic molecules in non-ionic micelles. The project is a co-operation between Physical Chemistry 1 and AstraZeneca R&D Lund. (C. Ericsson, S. Ulvenlund, O. Söderman).

Polymers, Solutions, Gels and Phase Behavior

Block copolymer vesicles and particles with internal structure in dilute aqueous solution. The project involves the investigation of block copolymer vesicles and particles and their stability in aqueous solution. The block copolymer used is a triblock copolymer of poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO) (PEO-PPO-PEO). Unilamellar vesicles may be formed by extrusion from dilute solutions of dispersed lamellar phase of the block copolymer. However, in the unextruded block copolymer system, under very dilute conditions, large polydisperse unilamellar vesicles are formed when a solution of unimers is heated into a two phase region where, at equilibrium, a concentrated lamellar phase coexists with a dilute solution of unimers. The internal structure, size and time stability of PEO-PPO-PEO particles are also investigated. These are formed at temperatures where the reversed hexagonal phase is in equilibrium with a unimer solution. The experimental techniques employed in the different projects are cryo-TEM, dynamic and static light scattering, self-diffusion measurements by NMR and small-angle X-ray scattering. (K. Bryskhe, K. Schillén, U. Olsson and A. Yagmur and O. Glatter (University of Graz, Austria)).

The influence of multivalent metal ions on the chain conformation of ionomers in solution. This research project concerns the investigation of the solution properties of ionomers in nonpolar organic solvents by using dynamic and static light scattering as main methods of investigation in combination with gel permeation chromatography. The synthesized ionomers are random copolymers with different multivalent counter ions of transition and rare earth metals. The purpose is to investigate the effect of the chemical nature and the concentration of multivalent ions and solvent quality on the polymer chain conformation. (D. Pebalk (Moscow State University, Russia), K. Schillén, J. Jansson, H. Sjögren).

Interactions between starch, hydrophobically modified polymers and surfactants. Amylose can form inclusion complexes where the hydrophobic tails of surfactants and lipids are included in the amylose helix. We have found a similar complexation between amylose and hydrophobically modified polymers, such as HMHEC and HMEHEC. Even small amounts of added amylose give rise to a marked viscosity increase for semidilute solutions of HMHEC, but not for non-modified HEC. The viscoelastic “gels” formed in the mixed solutions are thermoreversible and thixotropic. The gels are clear when prepared by mixing a hot solution of completely dissolved amylose with a HMHEC solution. Cold mixing results in some viscosity enhancement. Small amounts of added surfactant, even when mixed into the cold gel, destroy the amylose-HMHEC complexation by competitive association to HMHEC and, presumably, also by complexation between the surfactant and amylose. In dilute mixtures, ionic surfactants may prevent the precipitation of amylose. Different surfactants differ markedly in their ability to compete with the amylose-HMHEC complexation. Cyclodextrins also compete efficiently with the complexation. (M. Karlberg, M. Egermayer, L. Piculell).

Effects of polymers on adhesion formation in surgery. Adhesion formation is a well-known complication of abdominal and pelvic surgery. Together with Stig Bengmark and Kåre Larsson (Ideon Research Center) and Roland Andersson and coworkers (Department of Surgery, Lund University) we investigate the effect of water-soluble polymers and find very significant effects with certain hydrophobically modified polymers as well as synergistic behavior between oppositely charged polyelectrolytes (B. Lindman).

Particle-induced phase separation in polymer solutions. Added particles can induce a phase separation in a polymer solution that is close to phase separation, even under conditions when both bridging and depletion mechanisms can be ruled out. Experimentally investigated polymer solutions have been of two kinds; ternary systems (e.g. PEO/dextran/water) and quasi-binary systems (e.g. EHEC/water). The added particles (polystyrene latex or silica) have an affinity to at least one of the polymers (PEO or EHEC). The extent of the particle-induced effect for a given polymer system depends on the identity of the particle, the particle concentration, the molecular weight(s) of the polymer(s), and the polymer polydispersity. Model calculations, using a lattice mean-field theory for polymer solutions, as well as comparisons with surface force measurements, show that the effect may be explained by the formation of a new phase between the particles, a capillary phase. The capillary induced phase separation (CIPS) in the gap between the particles is driven by a lower surface energy for the capillary phase, compared to the reservoir phase, in contact with the particle surface. A Flory-Huggins model treating the particle as a very long polymer, which is attracted to the polymer component, also captures the qualitative features of attractive polymer-particle mixtures in solution. In experiments, small additions of PEO have been found to dramatically destabilise aqueous silica/dextran/water mixtures. This effect is not attributed to capillary-induced phase separation, but to a repulsion between PEO-dressed particles and dextran. Added surfactant, that adsorbs to the particle surface, may also change the particle-polymer interactions from attractive to repulsive, with consequences for the polymer-particle phase behaviour. (M. Olsson, L. Piculell, P. Linse, Leif Karlson (Akzo Nobel Surface Chemistry), F. Joabsson (Camurus AB), H. Wennerström).

Dissolution of dry polymers. We closely investigate the process whereby a dry sample of a water-soluble polymer swells and finally dissolves when immersed in an

aqueous solution. A detailed understanding of the dissolution of dry polymer is of obvious relevance to tablet formulations of pharmaceutical drugs, but the approach is fundamental. The release rate has been recorded systematically for dry tablets based on mixtures of a short and a long fraction of PEO. For each tablet composition, both PEO fractions are released at the same rate, but this release rate increases with an increasing proportion of the short PEO fraction. Similar results are obtained for tablets of hydroxypropylmethylcellulose or dextran. The “gel layers” surrounding the dry cores of dissolving PEO tablets have been probed during the dissolution. Tablets of short polymers soon develop a thin steady state gel layer of constant thickness, whereas tablets of long polymers yield gel layers that grow monotonically with time until the entire dry tablet core has finally disappeared. Despite differences in release rate or gel layer swelling, the shape of the release profile (the accumulation of released polymer with time) is remarkably similar for all cases: A slow initial phase is followed by an extended linear phase and, finally, a slowing down. Moreover, tablets of polydisperse polymer mixtures behave in all respects remarkably similar to tablets of nearly monodisperse polymers, as long as the tablets have the same release rates. The dissolution of surfactant-binding polymers in surfactant solutions is currently investigated. (A. Körner, L. Piculell, A. Larsson and F. Currie (Chalmers), B. Wittgren (AstraZeneca Mölndal)).

Interaction between functionalised soft polymer particles and inorganic surfaces. 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. With this technique we may measure the interactions between the polymer particles and inorganic substances through direct force measurements, or study the morphology of the film surface at the nanometer scale. Also, we may analyse the adhesion of individual polymer particles onto inorganic surfaces, such as titanium dioxide, silica, and mica (J.K. Dreyer, T. Nylander, L. Piculell)

Mesoporous inorganic materials. Inorganic material with pores in the meso range can be synthesised with surfactant aggregates acting as structure directing agents. We are studying the behavior of such systems. Our attention is mainly focused on silica systems formed with non-ionic block copolymers, in particular Pluronics. The structures formed are highly dependent on the length of the polymer blocks as well as on the temperature of the synthesis, and range from lamellar via hexagonal to micellar cubic. Also, addition of inorganic salts has a strong influence on the outcome of the synthesis. Characterization is performed with SAXS, TEM and nitrogen adsorption measurements. Time resolved mechanistic studies are done with in-situ SAXS (synchrotron light), in-situ ^1H NMR and TEM. (P. Linton, K. Flodström, V. Alfredsson and H. Wennerström).

Monolein – HM-EHEC mixtures. We are studying the interactions between the lipid monolein and hydrophobically modified polymer ethyl hydroxyethyl cellulose (HM EHEC) by following the phase behaviour of the aqueous system over a wide concentration range. The system exhibits a large variety of aggregate structures including vesicles that form spontaneously and several liquid crystalline phases at different compositions. (J. Bornè, A. Khan, B. Lindman). Project completed.

Development and characterization of thin polymer films for control of cell growth and gene expression. A series of Poly(N-isopropylacrylamide)-co-poly(N-tert-butylacrylamide) PNIPAM-co-PBAM polymers have been prepared and used to prepare thin films (5 μm). Cells grown on these films were found to consistently express 19 genes differently from cells grown on control surfaces. Further work is being conducted using this series of polymers of increasing surface hydrophobicity. Further work includes investigation of surfaces with increasing roughness, surfaces with different charge distributions, and eventually, surfaces made from various polymerizable lipids, which are currently being synthesized. Films are characterized using ellipsometry, contact angle measurements and AFM. This project is a collaboration between the departments of Chemistry and Pharmacology, University College Dublin and Physical Chemistry 1, Lund University. (I. Lynch, T. Nylander and B. Lindman).

Polymers labeled with fluorescent chromophores. Water-soluble polymers covalently labeled with fluorescent hydrophobic dyes have been synthesized and their solution properties are now investigated. The polymer is a polyelectrolyte, poly(acrylic acid) (PAA), and the chromophores are either pyrene or naphthalene, which are randomly attached onto the polymer. The aim is to achieve molecular understanding of the association processes in hydrophobically-modified polymer systems by using dye-labeled polymers. Fluorescence measurements (steady-state and time-resolved) report on the self-association of the polymers in aqueous solution and also on their interaction with surfactants, other polymers or other additives. The time-resolved fluorescence investigations provide detailed information on the dye excimer/dimer formation in these systems. The solution behavior of dye-labeled PAA and the effects induced by added cationic surfactants and block copolymers in water are also studied using dynamic light scattering. (J. S. Seixas de Melo and T. Costa and M. da G. Miguel (University of Coimbra, Portugal), K. Schillén, B. Lindman).

Elongational flow, rheometrical and dynamic light scattering measurements on oppositely charged polymers, cylindrical surfactant micelles and block copolymer-nonionic surfactant complexes. In the elongational flow technique the extensional viscosity is measured by using an uniaxial elongational flow field. An increase in the extensional viscosity, i. e. elongational thickening, may be observed in systems that are shear thinning. An example where this can occur is in systems of linear polymers, where thickening may be exhibited due to uncoiling of the polymer chain to an aligned and extended conformation, cylindrical micelles of amphiphiles, et.c. In this project we explore a variety of different systems using the elongational flow technique in combination with rheometry and dynamic light scattering. First, an oppositely charged polymer system of poly(sodium acrylate) and a cationic hydroxyethylcellulose derivative is studied. The purpose is to investigate the effect of total polymer concentration, added salt concentration as well as the salt valency on the extensional viscosity and the rheological and hydrodynamic properties. This will provide information of the interpolymer interaction strength. The growth of cationic cylindrical surfactant micelles (induced by salt) and the growth of PEO-PPO-PEO triblock copolymer-nonionic C₁₂E₃ surfactant complexes are other topics that currently are under investigation using these three experimental techniques. (D. Löff, K. Schillén, M. Torres and A. Müller (Universidad Simón Bolívar, Venezuela), B. Lindman, K. Thuresson, G. Olofsson).

Patterned polymer brushes. Patterned polymer brushes constitute one approach to fabricate functionalized surfaces. In a newly started project, our aim is to in more depth characterized such brushes manufactured at Purdue University by, in particular,

QCM, ellipsometry, and scattering methods as well as with simulation methods. (S. Zauscher (Duke University), A. Rennie (Uppsala University), F. Höök (Solid State Physics), T. Nylander, M. Patra, and P. Linse)

Polymer-Surfactant Systems

Association between hydrophobically modified polymers and surfactant self-assemblies or a second hydrophobically modified polymer. Studies include a system where the surfactant self-assemblies are thermodynamically stable catanionic vesicles bearing a negative net-charge and the polymers are cationic. The vesicles are composed of sodium dodecyl sulfate (SDS) and didodecyldimethyl ammonium bromide (DDAB), and the polyelectrolytes were two cationic cellulose derivatives with different charge densities. In addition, one of the polymers was hydrophobically modified. For both polymer systems, polymer-vesicle association leads to major increases in viscosity and to a gel-like behaviour. It was found that the more highly charged polymer without hydrophobic groups gives rise to more long-lived cross-links but the number of cross-links is higher with the hydrophobically modified polymer. According to microstructure studies by cryogenic transmission electron microscopy, the two polymers also affect the vesicle stability but quite differently. The vesicles are changed from spherical ones into faceted vesicles. This effect is attributed to an onset of crystallization of the surfactant films in the vesicles. Depending on the polymer architecture there may be opening of the bilayers and formation of holey vesicles. Ultimately considerable vesicle disruption may lead to planar bilayer, disc-like, aggregates. Further studies include the association between nonionic hydrophobically modified polymers and cationic vesicles. Furthermore, the rheological properties and microstructures of mixed solutions of two oppositely charged hydrophobically modified cellulose derivatives are investigated with specific focus on the charge and hydrophobe stoichiometries. Varying the electrostatic and hydrophobic associations, there are dramatic changes in rheology. (F. Antunes, B. Medronho, M. Miguel, Coimbra University, B. Lindman K. Thuresson).

Interactions between DNA and surfactant mixtures. Mixed aqueous systems of DNA and a cationic surfactant show a very strong associative phase separation. The phase behavior of these systems is investigated as a function of surfactant chain length, electrolyte addition, addition of a second amphiphile and the conformation of DNA. By fluorescence microscopy, DNA compaction is monitored on the single molecular level for simple surfactants, and surfactant mixtures, in particular mixtures between cationic and anionic surfactant. DNA conformational changes are strongly cooperative, involving a coexistence of extended and globular DNA molecules. Also it is observed that shorter chained surfactants associate preferentially with single-stranded DNA molecules, decreasing the DNA's melting temperature close to the system's phase separation. The results are compared with those of Monte Carlo simulations. (R. Dias, A. Pais, M. Rosa, B. Lindman, M. Miguel).

Concentrated mixtures of oppositely charged polymer and surfactant. We use a new, simplified approach to study structures and water uptake of oppositely charged polymers and surfactants. The essence is to use the minimum number of components to map out the generic features, and to make contact between polymer/surfactant systems and conventional surfactant systems. To this end, we first synthesise the pure "complex salt" (polyion + surfactant ion) and use it as our point of departure. Binary mixtures of complex salt and water are studied, and also truly ternary mixtures involving one of the following additional components: The conventional surfactant (surfactant ion + simple monovalent counterion), the conventional polyelectrolyte (polyion +

simple counterion), the corresponding polyacid (protonated polyion), or a nonionic cosurfactant. The two first additions yield either surfactant aggregates with mixed simple/polymeric counterions, or polyions with mixed simple/surfactant counterions. By the two latter additions we regulate the charge density of either the polyion or the surfactant aggregate. Most experiments refer to alkyltrimethylammonium (C_nTA^+) surfactant ions with polyacrylate (PA^-) counterions. The aqueous complex salts form the same cubic and hexagonal structures as the conventional C_nTA surfactants with simple counterions. Additions of either polyelectrolyte or conventional surfactant to the complex salt increases its miscibility with water, owing to the entropy of mixing of the simple counterions. Small additions of a long-chain alcohol to a complex salt rapidly change the aggregate structure from cubic or hexagonal to lamellar. The infinite lamellar aggregates, neutralised by polyions, swell very little with water. These systems are thus quite similar to lamellar C_nTA /alcohol mixtures with divalent counterions (J. Norrman, L. Piculell, W. Loh (UNICAMP, Brazil)).

Block copolymer-surfactant interactions. Interaction between triblock copolymers of poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO) (PEO-PPO-PEO) and cationic, anionic and nonionic surfactants (of the type C_nE_j) in dilute aqueous solution are studied using dynamic and static light scattering and small angle X-ray scattering in combination with differential scanning and isothermal titration calorimetry. The copolymers studied at the present have the same hydrophobic PPO block length but varying length of the hydrophilic PEO block. The aim is to investigate the solution properties of block copolymers and how their self-organization is altered by the addition of surfactants. (D. Löf, J. Jansson, K. Schillén, G. Olofsson, O. Glatter (University of Graz, Austria), R. C. da Silva, A. Niemiec, W. Loh (UNICAMP, Brazil)).

Mixtures of an associating polymer and a degradable surfactant. The addition of surfactant to a solution of an "associating" hydrophobically modified polymer generally gives rise to a dramatic change in viscosity, but the sign and magnitude of the change depends on the amount of surfactant added. The result is the development of a viscosity maximum as a function of added surfactant, where the maximum viscosity may be orders of magnitude higher than that of the surfactant-free polymer solution. We are using this sensitivity to surfactant concentration to create and study HMHEC-surfactant mixtures with a time dependent rheology, using alkali-sensitive, degradable betaine esters as surfactants. Depending on the initial amount of surfactant, the viscosity may either decrease or go through a maximum with time, as the surfactant degrades. The rate of degradation, and thus the rate of variation of the surfactant concentration, may be controlled within wide ranges by controlling the pH of the mixture (M. Karlberg and L. Piculell, M. Stjern Dahl and D. Lundberg (Chalmers)).

The effect of poly(N,N-dimethylacrylamide) on the lamellar phase of Aerosol OT-water. The effect of a water soluble uncharged polymer (polyacrylamide) on the stability of the lamellar phase of the AOT (Aerosol OT, sodium di(ethylhexyl) sulfosuccinate)/water system is studied. Polymers with large coil dimensions, with respect to the thickness of the water layers, induces formation of two phases in equilibrium; the AOT rich phase and one phase rich in the polymer. In the case of polymers with smaller coil dimensions a nanometric sieving of polymer coils by the lamellar liquid crystal is obtained. Only the fraction of polymer chains with dimensions smaller than the thickness of water layers are able to penetrate the lamellar phase, while the fraction consisting of larger polymer chains forms an isotropic phase. When the size of polymer is small enough all can be located in the water layer. *In situ* polymerisation

within AOT bilayers lead to phase separation. This is partly because aqueous solubility of studied polyacrylamides is temperature sensitive. At the temperature used for synthesis the polymer chains attain a globule conformation. First results could indicate that structure (tacticity) of the polymer chains varies depending on whether the polymer chains are synthesised in the lamellar phase or in solution. (Joint project with I. E. Pacios, A. Horta and C. S. Renamayo, Madrid; B. Lindman, K. Thuresson).

Hydration of DNA surfactant complexes. The thermodynamics of hydration of DNA-cationic surfactant(lipid) complexes is studied using a sorption calorimeter that provides both the partial free energy (chemical potential) and the partial enthalpy of hydration. This provides a complete thermodynamic description of the system at the given temperature and pressure. (C. Leal, H. Wennerström, G. Olofsson).

Solid-state NMR studies of DNA-amphiphile complexes. Local molecular mobility of DNA-amphiphile complexes is investigated with 1H - ^{13}C magic angle spinning NMR. The two dimensional WIdeline SEparation (WISE) experiment yields the 1H linewidth for each resonance line in the high-resolution ^{13}C spectrum. The dynamic state of the DNA, the lipid headgroup and hydrocarbon tail is monitored as a function of hydration level and lipid composition. (D. Topgaard, C. Leal, H. Wennerström, R. W. Martin (UC Berkeley), D. Sandström (Stockholm University))

Phase separation and adsorption behavior in aqueous mixtures of polyelectrolytes and oppositely charged surfactants. 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 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. To this end, 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 and gel swelling experiments to investigate the polymer-surfactant binding. (A. Svensson, T. Nylander, L. Piculell, B. Lindman in collaboration with E. Johnson, Procter & Gamble, Cincinnati and R. Watson, R. Fabicon, Procter & Gamble, Beijing)

Light scattering studies of DNA compaction, decompaction and aggregation. By dynamic light scattering, the transitions between different states of DNA induced by surfactants and surfactant mixtures can be followed. Coexistence between coils and globules as well as a "double" cooperativity in cations surfactant binding are monitored. (O. Glatter (Graz), R. Dias, B. Lindman, M. Miguel).

Influence of hydrophobic modification of the polymer and of the charge density of the surfactant aggregates on phase behaviour, transport properties, and rheological properties in polymer surfactant systems of opposite charge. Systems composed of mixtures of surfactants and a polymer are frequently employed for rheological control and, in particular, is gel-like appearance important in many applications. If a surfactant is added to a polymer solution, dramatic changes in viscosity are found if the polymer is of the associating type, in particular if it is a hydrophobically modified water-soluble polymer. Association and complex formation between polyelectrolytes and oppositely charged surfactants frequently leads to precipitation. These complexes, being in equilibrium with an excess aqueous phase, are sometimes characterized by a long-range order (lamellar, hexagonal, or cubic).

The behavior is dependent on parameters such as charge density of the polyelectrolyte chain and the ionic strength in the medium, but also on the charge density of the surfactant aggregates. In this project we study the effect of a non ionic surfactant on the complex formation in between carboxymethyl cellulose, or a hydrophobically modified analogue, and an oppositely charged surfactant. (Joint project with I. E. Pacios, A. Horta and C. S. Renamayor, Madrid; B. Lindman, K. Thuresson).

Transport properties of colloidal sized aggregates in complex polymer systems – stability, retention, and deposition. In this project we study the fate of hydrophilic drug carriers in contact with the mucus layer in the gastrointestinal tract. The mucus layer is a complex mixture, containing among other things mucin (a negatively charged polyelectrolyte contributing to the gel like properties of the mucus layer) and lipid depots. We have chosen to investigate mixtures of mucin and a model drug carrier – a mixed micelle of a non-ionic and a cationic surfactant, the latter providing functionality and retentive properties towards the mucin matrix. Depending on composition phase separation and precipitation can take place. The structural properties of the precipitate are studied by means of SAXS and the water rich phases are investigated by a combination of different optical and analytical methods, such as PGSE-NMR, HPLC, and Cryo-TEM. (G. Lafitte, K. Thuresson (Camurus AB, Lund), O. Söderman)

DNA-surfactant complexes in water-oil mixtures. The phase behaviour and phase microstructure in ternary systems of DNA with cationic surfactant as counterion and oil and water is investigated. Complex phase diagrams with different regions of lamellar and reversed hexagonal liquid crystalline phases and isotropic solutions are identified with decanol as oil. With other water-immiscible solvents further phases occur. (A. Bilalov, C. Leal, A. Khan, B. Lindman).

DNA / Amino acid-based surfactants interaction. Gene therapy is a rapidly developing technology for the treatment of a variety of diseases and mixed systems of surfactants/lipids are already being used as packaging agents of nucleic acids. These non-viral vectors attract a great deal of interest due to their advantageous safety profile when compared to viral ones. Nevertheless, some of the used surfactants are still toxic. Amino acid-based surfactants are biodegradable, milder and less irritant than conventional ones. Studies of compaction and decompaction of DNA by amino acid-based surfactants are performed by fluorescence microscopy. The interaction between DNA and positively charged amino acid-based cationic vesicles is investigated through the study of the relation between structure and DNA/surfactant net charge ratio. The main techniques in use are Cryo-TEM and SAXS. The mechanism of interaction is being followed through ¹H NMR and NMR Self-Diffusion techniques. (M. Rosa, M. R. Infantes (Barcelona), M. Miguel, B. Lindman).

Amino Acid-Based Surfactants as DNA Condensing Agents – A Transfection Study. The aim of using amino acid-base cationic surfactants in drug and gene delivery formulations is to reduce toxic side effects. When designing cationic surfactants for gene therapy, their ability to mediate transfection can be attributed to several physical aspects: including DNA condensation due to electrostatics; and an intrinsic ability of the cationic lipids to destabilize the plasma membrane or the endosomal compartment (dependent on the mode of uptake). ALA, an arginine-based single chained cationic surfactant, is being used as a DNA pre-condensing agent. The liposome systems in study are: DOTAP:Chol (7% ethanol); CatpH (7% ethanol); and CatpH-det (7% ethanol). ALA pre-condensed DNA is added to the different liposomes formulations and transfection studies are performed. Transfection efficiency is explored as a function

of the ALA/DNA charge ratio and cationic lipid/DNA charge ratio. A thorough physical-chemical characterization of each system will be made which will clarify the main factors responsible for transfection efficiency. (M. Rosa, N. Penacho, S. Simões, C. Pedroso de Lima, M. Miguel, B. Lindman)

Cross-linked DNA gels. DNA molecules 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. (D. Costa, M. Miguel (Coimbra), P. Hansson (Uppsala), S. Schneider, B. Lindman).

Gel electrophoresis studies of the DNA compaction and decompaction by the addition of oppositely charged surfactants. The mobility of DNA molecules in the presence of surfactants is followed in terms of conformation and charge neutralization. Also the decompaction and release of the DNA from the DNA-surfactant complexes is obtained by addition of anionic surfactants. (B. Åkerman (Gothenburg), R. Dias, B. Lindman, M. Miguel).

Protein and Protein-Amphiphile Systems

Protein-surfactant interactions in solution. The aim of the project is to investigate the protein-surfactant interactions in solution. The complex salt, lysozyme-dodecyl sulfate, free from simple salts, is synthesized by the precipitation technique. The phase equilibria of the ternary system complex salt-sodium dodecylsulfate-water are investigated and the resulting phase diagram is used as fundamental for theoretical discussion and modeling. Three types of protein-surfactant aggregates are identified and they are insoluble complex, soluble complex and a gel-like aggregate. These aggregates are also formed for the system lysozyme-sodium dodecylsulfate-water. The physico-chemical properties of these aggregates are under study by a combination of different techniques, e.g. NMR diffusometry, rheology and SANS. Furthermore the redissolution of the complex by cationic surfactants is studied revealing the competition between the cationic protein versus surfactant for the interaction with the dodecyl sulfate (A. Stenstam, G. Montalvo, A. Khan, H. Wennerström). Project completed.

Protein-lipid interactions. Studies on the relation between the lipid phase behavior and protein-lipid interactions make use of cryo-TEM, X-ray scattering and different NMR techniques. Mixtures of β -lactoglobulin (the major whey protein in milk, which is known to bind lipids) and phospholipid, are mainly investigated. The studies involve liquid crystalline (lamellar) phases, vesicle suspensions and the protein-lipid interactions at interfaces, e.g. emulsions. (T. Nylander; B. Bergenstahl and R. Wånge (Food Technology); M. Paulsson (Food Engineering)).

Lipid-lipase structure function relationship. The aim is to better understand the small-scale structure of lipid aggregates, which are of important substrates for lipolytic enzymes. The aggregate structure and composition have a determining influence on the activity of the lipase. Furthermore, the aggregate structures are largely influenced by the formed catalytic products. Therefore a large part of the project is devoted to study the phase behavior and phase structure of selected mixtures of triglyceride, diglyceride, monoglyceride, fatty acids, soap, glycerol and aqueous solution, using NMR, small angle x-ray scattering and microscopy techniques. (T. Nylander, J. Barauskas, F. Tiberg, A. Svendsen (Novozymes)).

Lipid nanostructures as matrices for biologically active molecules. The use of cubic-lipid phases (e.g. in the monoolein- aqueous system) as matrices to study

immobilize enzymes and redoxactive molecules, both natural (e.g. ubiquinone, vitamin K1) is studied. Of particular interest is to study how and why the structure of the lipid aggregate changes when lipophilic compounds (e.g. membrane bound cofactors for enzymes) solubilised in the lipid matrix. The project involves both studies of the phase behavior of the lipid-lipophilic compound and/or enzyme-aqueous system as well as the activity of the enzymes and redox active compounds. (T. Nylander, V. Razumas (Lithuania); K. Larsson, F. Tiberg, H. Ljusberg-Wahren (Camurus AB, Lund); F. Caboi, M. Monduzzi (Italy).

Lipid-peptide interactions. The potential of using self-associated nano-structured lipid aqueous based as carrier for peptide drugs are exploited. This involves fundamental investigations of peptide-lipid interactions as well as effects of enzymatic degradation and permeation of biomembranes. The aim is to increase the understanding of the physicochemical factors that control the uptake of the peptides from the gastro-intestinal tract. The project involves biophysical and surface chemical studies of interactions in model systems. (T. Nylander, F. Tiberg, H. Wennerström, and P. Vandoolaeghe).

Amyloid formation and protein-lipid co-aggregation. Many human disorders belong to a family of amyloid diseases, characterized by abnormal folding of proteins into aggregates with a fibrillar structure. We have recently shown on the formation of protein-lipid aggregates when the protein aggregation is taking place in the presence of lipid membranes. The aim the project is to investigate the basic principles for such protein-lipid co-aggregation. We study the interactions between the A β protein, involved in Alzheimer's disease, and mutants of the superoxide dismutase protein, involved in amyotrophic lateral sclerosis (ALS) with model lipid membranes of different composition. The protein-lipid interactions are under study by a combination of different techniques, e.g. confocal fluorescence microscopy on giant unilamellar vesicles, combined Brewster angle microscopy and surface pressure studies of lipid monolayers, and quartz crystal microbalance (QCM-D) studies on deposited lipid bilayers. (E. Sparr, H. Wennerström, F. Höök (Solid State Physics, Lund University), M. Oliveberg (Umeå University)).

Morphologies and structures of aqueous dispersions of brain lipids. The self-assembly of lipids, with high degree of unsaturation, from e.g. brain and other tissues is not yet fully understood. The morphologies and structure formed by different type of brain lipids in aqueous dispersion and how the formed structures dependent on cholesterol content, buffer composition and temperature are investigated by cryo-TEM, SAXD and WAXD. (V. Alfredsson, T. Nylander; K. Larsson (Camurus Lipid Research); P. Lo Nostro and B. Ninham (University of Florence).

Lung surfactants. The alveolar surface is lined by film of submicron thickness between the epithelial cells and the alveolar lumen with the main function to lower the surface tension. The aqueous bulk structure of this layer consists of lipid bilayers forming lamellar bodies (LB:s) and tubular myelin (TM), and two hydrophilic proteins in the outside water ; SP-A and SP-D. We are studying the structure of and phase transitions in this layer with cryo-TEM and SAXD. (M. Larsson (Lund University Hospital), K. Larsson, T. Nylander).

Interactions between surfactants and polypeptides. The project is centered on a systematic investigation of the interactions between surfactants and relatively simple polypeptides, namely synthetic homo- and *co*-polymers of α -L-amino acids. The peptide-surfactant interactions in these systems are studied with respect to, on the one hand, the size, charge, hydrophobicity and conformation of the peptide and, on

the other hand, properties of the surfactant, *e.g.* charge, head group, length of the alkyl chain and micellar size. The systems are investigated by means of circular dichroism (CD), Raman/IR and NMR spectroscopy, as well as by static and dynamic light scattering techniques. Non-ionic surfactants of pharmaceutical relevance, especially alkylglucosides and sucrose esters, play a key role in the project. In addition to the studies of peptide-surfactant systems in aqueous solution, the properties of polypeptide monolayers at the air-water interface are investigated by means of surface balance experiments, as well as by AFM, ATR-IR and CD spectroscopic characterization of Langmuir-Blodgett films. The project is a co-operation between Physical Chemistry 1 and AstraZeneca R&D Lund. (H. Sjögren, S. Ulvenlund, T. Nylander).

Polypeptide and protein characterization by vibrational spectroscopy. Raman and IR spectroscopy are powerful tools in studies of polypeptide and protein conformation. In the present project, vibrational spectroscopy is used primarily to study the effects of surfactants and lipids on protein/polypeptide conformation. The studies include both aqueous systems and Langmuir-Blodgett films. In the latter case, attenuated total reflection (ATR) IR spectroscopy is utilized. (H. Sjögren, A. Stenstam, S. Ulvenlund, A. Khan).

Calorimetry of water sorption on proteins. The project deals with studies of protein - water interactions. The initial hydration of dry lysozyme is studied by means of sorption calorimetry and differential scanning calorimetry. Questions addressed include the state of the dry protein and changes in such properties as mobility and aggregation of protein molecules as water is introduced. In the current stage of the project, studies of water sorption on lysozyme are performed using sorption calorimetric technique. (V. Kocherbitov and T. Arnebrant (Malmö University), T. Nylander, G. Olofsson, and O. Söderman).

Adsorption and Surface Forces

Interfacial properties of β -casein. The interfacial properties and the structure of the adsorbed layers of a natural block copolymer, β -casein, are extensively studied by ellipsometry, surface force measurements, and neutron reflectivity measurements as well as by applying a specific proteolytic enzyme, endoproteinase Asp-N. β -Casein is a highly surface active protein from milk, which forms brush like structures at interfaces depending on the surface properties and the ionic strength and salt composition. The protein is extensively used as emulsifier and to stabilize colloidal suspensions. (T. Nylander, F. Tiberg, R. K. Thomas (University of Oxford)).

Polycation adsorption on solid-liquid interface – the response of the adsorbed layer structure to changes in bulk solution. Polyelectrolyte adsorption processes are in many cases of practical relevance kinetically controlled with the polymer molecules arrested in a “non-equilibrium” adsorption state. However, these dynamic aspects of polymer adsorption are not yet fully understood. Further assessment of the kinetic barriers for achieving equilibrium adsorption of polyelectrolytes at charged surfaces from solution can be obtained by determining how the adsorbed layer structure responds to changes in bulk solution. In many applications, these dynamic phenomena can be utilized to achieve a certain layer structure at the interface. The objective is to determine how the adsorbed layer is affected by the way we approach a certain solution condition, *i.e.* cycling and step-wise changes of pH and electrolyte concentration and step-wise increase in polyelectrolyte concentration. Cationic polyacrylamides with different linear charge density at silica surface under different solution conditions (pH, salt concentration c_s , polymer concentration c_p) were subject of this investigation.

Important characteristics of the adsorption process - adsorbed amount and effective layer thickness - were accessed by in-situ null ellipsometry. Since the silica surface charge is variable, the experiments were conducted under thoroughly controlled conditions. Data on adsorbed amount and adsorbed layer thickness were supplemented with surface charge density measurements of bare silica surface and in the presence of a polyelectrolyte adsorbed layer. Cycling of bulk solution parameters allowed us to estimate the degree of reversibility of the polyelectrolyte adsorption. (Y. Samoshina, T. Nylander, R. Bauer (Danmark)).

Adsorption of Cationic Cellulose derivatives/Anionic Surfactant Complexes onto Solid Surfaces. Knowledge of the mechanisms by which oppositely charged polymer/ surfactant complexes adsorb and interact at interfaces is prerequisite for a range of applications. There is also a fundamental interest for a deeper understanding of these phenomena. A comparative study of adsorption of cationic celluloses/SDS complexes on hydrophobic and hydrophilic surfaces has been carried out by null ellipsometry. The effect of SDS on polymer adsorption was studied under two different conditions: adsorption of polymer/SDS complexes from premixed solutions and addition of SDS to preadsorbed polymer layers. A wide range of SDS concentrations was covered in this work. The effect of the rinsing process on the adsorbed layer characteristics was also studied. The strength of the present study is that we are able to link the adsorption process to the bulk behaviour of the system. (E. Terada (Japan, Kao Corporation), Y. Samoshina, T. Nylander, B. Lindman).

Adsorption and aggregation of highly charged hydrophobically modified cationic polyelectrolytes and their complexes with oppositely charged surfactant. Hydrophobically modified polyelectrolytes are one of the polymer subclasses that are of prime importance for modification of surface properties. The adsorption behavior of these types of polymers can be adjusted both chemically and by manipulating the ionic strength or the pH of the solution, which makes them powerful tools for many industrial applications. The adsorption onto the hydrophilic silica – aqueous solution interface of hydrophobically modified polyelectrolytes with different contents of hydrophobic groups at different ionic strengths has been studied by ellipsometry and tapping mode atomic force microscopy (AFM). The kinetics of aggregate formation at the interface was followed. Path-dependence of adsorption with respect to ionic strength and also of coadsorption with SDS has been studied. Polymer layers are found to be trapped in non-equilibrium states. The composition and structure of co-adsorbed layers are also hysteretic. Furthermore, polymer/surfactant complexation can be used to guide polymer layers into different trapped states. Coadsorption from premixed solutions has been compared also with addition of surfactant to the adsorbed polymer layers. (Y. Samoshina, T. Nylander, P. Claesson, B. Lindman).

Adsorption competition between dispersants and rheological modifiers. The aim of this project is to provide a thorough understanding of the adsorption behavior and interactions between the constituents of typical water-borne paint formulations, i.e., pigments, dispersants, rheological modifiers and emulsifiers on surfaces. Null-ellipsometry is used to in situ follow the adsorption of the different components on two solid surfaces, i. e. silica (SiO₂) and titanium oxide (TiO₂). The method gives the adsorbed amount as well as the thickness of the adsorbed layer. In particular we will study the adsorption competition between the constituents, the spatial configuration of the adsorbed layers and the effect of divalent salts. This project is a collaboration with CIP (Centro de Investigación en Polímeros) COMEX, México. (J. Campos Terán, T. Nylander, B. Lindman).

Cold water cleaning techniques. It is important to develop cold water cleaning techniques both concerning energy savings and fabric care. The removal of different model soils, deposited on substrates, with a number of different surfactants is here investigated. The focus is to follow the cleaning mechanism *in situ* at different temperatures. The main technique for this project is ellipsometry. (K. Flodström, T. Nylander, B. Lindman in corporation with J. Dupont, J. Seeley, J. Zerhusen, Procter & Gamble, Cincinnati)

DNA-cationic surfactant complexes at solid interfaces. DNA-cationic surfactant systems are potential candidates for gene delivery. Extensive research has been performed to understand the factors determining DNA compaction due to interaction with cationic surfactants or polymers in bulk solution. However, almost no research has been performed on interfacial phenomena. The co-adsorption behaviour may be another important factor determining the DNA-surfactant complex efficiency for its delivery to target cells. Solid-liquid interfaces are used as a model system to facilitate the understanding of interfacial properties such as lateral organization and layer composition at technologically relevant surfaces. The main technique being used is ellipsometry, which allows *in situ* measurements of interface processes with high resolution (~ 0.1 mg/m²). Both adsorption phenomena on hydrophilic and hydrophobic surfaces are investigated. The adsorbed layer structure is further determined by means of Neutron Reflectivity. The surface force apparatus is also utilized to better understand the structure of the mixed adsorbed layers. (M. Cárdenas, J. Campos, T. Nylander, R. Thomas (Oxford University), B. Lindman).

Lipoplexes at air-water interface. Lipoplexes are complexes formed between DNA and different lipids. Using surface film balance measurements, understanding is gained on the interactions of DNA with different lipid head groups. This technique in combination with the Brewster Angle Microscopy gives an insight into the type of structures formed between DNA and different lipids. (M. Cárdenas, T. Nylander, B. Lindman).

DNA Compaction in Solution and at Polystyrene Particle Solution Interfaces. The effect of cationic surfactant (cetyltrimethylammonium bromide) on the compaction of DNA both in aqueous solution and on polystyrene particles (uncharged and charged) are studied by dynamic light scattering as the main experimental technique. The DNA macromolecule undergoes a transition from a semiflexible coil to a more compact globule in solution as a consequence of cationic surfactant binding. DNA compaction is also observed on different types of polystyrene particles in the presence of surfactant. Here dynamic light scattering and SANS is used to get an insight in the structure of the complexes formed. (M. Cardenas, C. Dreiss, D. Pebalk (Moscow State University, Russia), J. Jansson, K. Schillén, T. Cosgrove (Bristol University), T. Nylander, B. Lindman).

Experimental Methodology in Colloid Science

NMR self-diffusion experiments. In this project we study fluid motion in porous systems. The experimental method used is the pulsed gradient spin echo (PGSE) NMR technique, which is sensitive to molecular motion. With the method we can estimate molecular displacements over a wide range of time scales (from ms to several seconds). Such data convey information about structure such as pore morphology and dynamic features related to the long-range fluid diffusivity as well as to the local molecular self-diffusion. The method has been applied paper, and the water fluid motion is studied as function of water content. Other studied systems include water-containing biomaterials

such as starch and protein. Moreover, the effect of cross-relaxation on the self-diffusion experiment is investigated and quantified. (D. Topgaard, O. Söderman).

Calculations of pulsed field gradient echo decays in restrictive geometries.

The presence of barriers in the investigated systems (such as membranes) gives rise to characteristic features in the echo decays observed in the pulsed field gradient NMR experiment. In this project we use finite element calculations to predict echo decays in various different restrictive geometries. First the relevant propagator describing the random motion of the spins is calculated and then the echo decays are computed. Examples include diffusion in cylindrical geometry and in systems where the spatial distribution of the diffusing compound varies over the system. Extensions include investigations of the effects of susceptibility effects and the development of effective Brownian dynamic simulations to calculate echo decays. (B. Jönsson (Biophysical Chemistry, Lund), M. Nydén (Chalmers), H. Hagslätt (Chalmers), O. Söderman).

Chemical shift imaging of drug release from polymer gels. Release dynamics of model drugs from polymer gels is studied by means of magnetic resonance imaging. The experiment yields chemical shift-resolved NMR spectra as a function of position in one dimension. From these spectra the concentrations of species with distinct chemical shifts can be quantified with one minute time-resolution. Simple gels, composite gels containing microgel particles acting as a drug reservoir, and responsive gels where the release is triggered by the presence of a second species is studied. (D. Topgaard, I. Lynch, O. Söderman).

Diffusion NMR studies of human brain microstructure. Diffusion-weighted magnetic resonance imaging is a diagnostic tool for ischemic stroke, demyelination, and tumor detection. In this project excised brain tissue is studied by means of state-of-the-art spectroscopic diffusion NMR equipment in order to elucidate the relation between brain microstructure, water diffusion, and signal response in the clinical imaging system. (D. Topgaard, C. Malmberg, O. Söderman, J. Lätt (Radiation Physics), S. Brockstedt (Radiation Physics), F. Ståhlberg (Radiation Physics), M. Sjöbeck (Pathology))

(Cryo-)Transmission Electron Microscopy. TEM enables the direct imaging of both solid-state systems, such as mesoporous silica, but also of liquid samples. The liquid samples are frozen and transported to the microscope and subsequently studied in the microscope under cryogenic conditions. Cryo-TEM is used for direct imaging of labile systems containing biological and synthetic amphiphiles, naturally occurring polymers (polysaccharides, proteins, etc.) or synthetic polymers, liquid crystals and gels. This technique allows for direct imaging and detection of different entities found in, for example, very dilute amphiphilic systems. It is consequently possible to identify *e.g.* vesicles, micelles and cubosomes. The energy filtering-option on this microscope (Philips CM 120 bio-twin) can be used to improve the contrast, permit the observation of thicker specimens and also allow for elemental analysis. (V. Alfredsson, J. Barauskas, C. Leal, P. Linton, M. Rosa, P. Vandoolaeghe, K. Flodström, K. Bryskhe,).

Ellipsometry at liquid-liquid interfaces. Ellipsometry is developed to enable multi-angle of incidence, MAI, measurements at liquid-liquid interfaces. This involves development of instrumentation as well as in analysis of data. Our focus is studies of adsorption from the oil phase of lipids and surfactants as well as from the aqueous phase of proteins, surfactants and polymers. The studies aim at a deeper understanding of phenomena at the oil-aqueous interface of relevance to emulsion stability and phase behavior of corresponding three-component systems. (J.-W. Benjamins, T. Nylander, K. Thuresson, B. Jönsson (Biophysical Chemistry, Lund)).

Theory and Modelling

Diffusive transport in responsive media. We are studying molecular transport over a lamellar as well as cubic phases in the presence of a gradient in water chemical potential. Calculations are based on the interbilayer forces that induce swelling and phase transitions in response to the variation in boundary conditions. Our model implies non-linear transport behaviors, due to the co-operative structural transformations along the water gradient. Water and solute transport through samples of different lipid liquid crystalline phases is also studied experimentally. (F. Costa, E. Sparr, H. Wennerström).

Cohesion in cement. The hardening of cement is due to the precipitation of calcium silicate hydrate nanoparticles. In the highly basic medium these particles are strongly negatively charged but the cohesion is supposed to arise from the aggregation of these particles. We are modelling this effect as due to the attractive ion correlation effect found by us twenty years ago. This is done through Monte Carlo simulations and simple analytical approximations. (B. Jönsson (Theoretical Chemistry Lund), A. Nonat (Université de Bourgogne), B. Cabane (ESPCI, Paris), H. Wennerström).

Fundamental issues concerning surface forces. We study a number of problems concerning basic questions in the area of surface forces. This includes the molecular interpretation of the van der Waals interaction as expressed in the Lifshitz theory and its consequences for dynamic systems, the role of dissolved gas in the hydrophobic interaction, capillary induced phase separation as a mechanism for long range attractive interactions, the validity of the Derjaguin approximation and ion binding to interfaces. (H. Wennerström).

Determination of surface potential of micelles. The understanding and control of colloidal stability requires an understanding of the surface potential of colloidal particles. In this project we investigate the surface potential of ionic micelles by means of measuring the dissociation constant of solubilized fatty acid probes, designed to exert a minimum of perturbation on the micelle. The dissociation constant is obtained from pH- titrations, NMR experiments as well as from calorimetric methods. Further developments include accurate electrostatic calculations based on finite element methods. (C. Whiddon, O. Söderman, B. Jönsson (Biophysical Chemistry, Lund)).

Polymer-stabilized magnetic fluids. A class of water-based magnetic fluids has been characterized by small-angle neutron scattering (SANS) and mean-field lattice modeling. These magnetic fluids, which are specifically tailored to extract soluble organic compounds from water, consist of a suspension of ~7 nm magnetite (Fe_3O_4) nanoparticles coated with a bifunctional polymer layer comprised of an outer hydrophilic polyethylene oxide (PEO) region for colloidal stability, and an inner hydrophobic polypropylene oxide (PPO) region for solubilization of organic compounds. SANS analysis showed that the polymer shell has an inner region that is increasingly depleted of water as the fraction of PPO side chains increases. The incorporation of PPO side chains also leads to a small increase in interparticle attraction. The lattice model predicted a similar result for the hydration of the polymer shell around the nanoparticles and suggested that the shell is similar in structure to that of a PEO-PPO-PEO triblock copolymer (Pluronic) micelle. (G. D. Moeser (MIT), W. H. Green (MIT), P. E. Laibinis (Rice University), P. Linse, and T. A. Hatton (MIT))

Protein adsorption. Lysozyme adsorption to charged surfaces was studied by Monte Carlo simulations at different protein concentrations, protein net charges, ionic strengths, and surface charge densities. The lysozyme was represented by a

hard sphere with embedded positive and negative surface charges parametrically dependent on the solution pH. A short-range attractive protein-protein potential was included to represent attractive non-Coulomb forces. The charged surface was described by a hard wall with embedded charges representing a mica surface. The protein adsorption was favored by high protein concentration, high protein net charge, low ionic strength, and high surface charge density. Nevertheless, adsorption appeared also for a weakly negatively charged protein to the negatively charged surface as a result of an electrostatically favorable protein orientation at the surface. While a multipole expansion including monopole and dipole moments only was insufficient to explain preferential orientation, an expansion including also quadrupole moments provided a satisfactory picture. The adsorbed amounts obtained compared favorably with experimental results. (F. Carlsson (YKI), E. Hylltner (YKI), T. Arnebrant (Malmö University), M. Malmsten (Uppsala University), and P. Linse).

Protein-polymer interaction. Protein-polymer association in solution driven by a short-range attraction has been investigated using a simple coarse-grain model solved by Monte Carlo simulations. The effect of the spatial distribution of hydrophobic surface residues of the protein on the adsorption of weakly hydrophobic polymers at variable polymer concentration, polymer length, and polymer stiffness has been considered. Structural data of the adsorbed polymer layer and thermodynamic properties, such as the free energy, energy, and entropy, related to the protein-polymer interaction were calculated. It was found that a more heterogeneous distribution of the surface residues promotes adsorption and that this also applies for different polymer concentrations, polymer chain lengths, and polymer flexibilities. Furthermore, the polymer adsorption onto proteins with more homogeneous surface distributions displayed larger sensitivity to polymer properties like chain length and flexibility. Finally, a simple relation between the adsorption probability and the change in the free energy was found. (M. Jönsson, and P. Linse).

Polyelectrolytes in confined geometries. The distribution of neutral and charged polymers with different flexibilities between two spheres of different volumes connected by a short and narrow cylinder has been investigated by Monte Carlo simulations. The uncharged chain displayed mostly single-sphere occupancy due to high conformational entropy penalty of being in the cylindrical domain, whereas double-sphere occupancy was obtained, except for very different spherical volumes, for the charged polymer. The origin of this different occupancy stems from the counterion entropy. At increasing stiffness, a stronger preference of double-sphere occupancy was detected. (A. Sousa (University of Coimbra) A. A. C. C. Pais (University of Coimbra), and P. Linse).

Systems containing oppositely charged polyelectrolytes. Solutions of oppositely charged polyelectrolytes have been simulated using Monte Carlo simulations. Polyion complexes containing the oppositely charged polyions were formed as the number of negatively charged polyions was increased at fixed amount of positively charged polyions. With a small excess of positively charged polyions, large charged clusters were observed together with small neutral ones, while at charge equivalence only neutral clusters were formed. Simple rules to rationalize the complexation have been proposed. The effect of polydispersity in chain length and charge as well as of the role of added salt has also been addressed. Theories describing the complexation in polyelectrolyte solutions have also been developed. (Y. Hayashi, M. Ullner, and P. Linse).

Polyelectrolyte gels. A model of a cross-linked polyelectrolyte gel has been examined using Monte Carlo simulations. The simple model contained a charged defect-free network represented by linked charged beads and explicit counterions.

The polyelectrolyte gel displayed a very large swelling capacity, in agreement with experiments. Discontinuous volume transitions appeared at critical values of the depth of a short-range potential at fixed permittivity, and at critical values of the permittivity at fixed short-range potential. In particular, we observed such a transition also without the short-range potential. The volumes of the collapsed states were one to two orders of magnitude smaller than those of the swollen states. Also the deswelling upon addition of salt was investigated for gels with different charge density, crosslinking density, chain flexibility, and counterion valence. All polyelectrolyte gels underwent a deswelling upon addition of salt. The salt content in the gel was larger as compared to that predicted by an ideal Donnan equilibrium due to a more negative excess chemical potential of the salt in the gel as compared to that in the salt reservoir. The predictions of the Flory-Rehner-Donnan theory were qualitatively in agreement with our results, but displayed significant quantitative disagreement. (S. Schneider, S. Edgcombe, and P. Linse)

Conformational properties of polyelectrolytes. Electrostatic persistence length has often been used as a measure of the conformational response to the intramolecular, electrostatic interactions of linear polyelectrolytes. The behaviour, given the Debye-Hückel approximation, has been an area of controversy. However, a more unified picture is emerging from a combination of Monte Carlo simulations and an analysis of the analytical approaches in the literature. First, it is important to recognise that four different types of definitions have been used and that they all represent different properties. Second, the behaviour can be divided into three regimes, depending on the relation between the screening length and chain size. Third, the description of the chain behaviour requires at least two parameters, while most theories rely on only one, even if the initial approach would appear to be more general. Furthermore, the majority can be said to be variations to one or the other of two original one-parameter theories, representing two limiting cases. The task at hand is to improve the description based on the gained insight. (M. Ullner).

Structures of charged block copolymers. Spherical brushes composed of diblock polyampholytes (diblock copolymers with oppositely charged blocks) grafted onto solid spherical particles in aqueous solution are investigated by using the primitive model solved with Monte Carlo simulations and by lattice mean-field theory. Polyampholyte chains of compositions AB are considered. The B -block is end-grafted onto the surface and its charge is varied, whereas the charge of the A -block is fixed. Single-chain properties, radial and lateral spatial distributions of different types, and structure factors are analyzed. The brush structure strongly depends on the charge of the B -block. In the limit of an uncharged B -block, the chains are stretched and form an extended polyelectrolyte brush. In the other limit with the charges of the blocks exactly compensating each other, the chains are collapsed and form a polyelectrolyte complex surrounding the particles. At intermediate charge conditions, a polyelectrolyte brush and a polyelectrolyte complex coexist and constitute two substructures of the spherical brush. Finally, a comparison of the predictions of the two theoretical approaches is made. (N. Shusharina (University of North Carolina at Chapel Hill), A. Akinchina, and P. Linse).

Solutions of oppositely charged macroions. The structure and phase-behavior of oppositely charged macroions in solution has been studied with Monte Carlo simulations using the primitive model where the macroions and small ions are described as charged hard spheres. Size and charge symmetric, size asymmetric, and charge asymmetric macroions at different electrostatic coupling strengths are considered and the properties of the solutions have been examined using cluster

size distribution functions, structure factors, and radial distribution functions. At increasing electrostatic coupling, the macroions form clusters and eventually the system displays a phase instability, in analogy to that of simple electrolyte systems. The relation to the similar cluster formation and phase instability occurring in solutions containing oppositely charged polymers is also discussed. (J. Rydén, M. Ullner, and P. Linse)

Macroions with discrete surface charges. Monte Carlo simulations are applied to examine the role of discrete surface charges and the mobility of surface charges on the counterion distribution near a charged macroion, the mean force between two like-charged macroions, and the structure of macroion solutions. With monovalent counterions, the effects were small. However, with divalent and trivalent counterions, where the correlation effects are larger, the deviation from the conventional description of a homogeneous surface charged density becomes noticeable. (K. Qamheih (Al-Quds University) and P. Linse)

Dynamics of polymer adsorption. Brownian dynamics simulation is applied to examine the adsorption of polymers to a solid interface. The extension and shape of the chains are investigated during the adsorption process at different chain length, chain stiffness, and adsorption energy. A novel longitudinal extension of the chain before the attachment was found before the conventional transversal stretching. Our next step will be to examine the adsorption of polyelectrolytes onto charged surfaces. (N. Källrot and P. Linse)

Genome in viral capsids. A coarse-grain model has been adopted to examine the structure and free energy of genome in viral capsids by Monte Carlo simulations. Of special interest is the spatial organization of the genome inside the capsid and the stability of the complex at different genome length and flexibility. (D. Angelescu, R. Bruinsma (University of California Los Angeles), and P. Linse)

Statistical-mechanical programs. During 2004, a web-based interface for running five different statistical mechanical computer programs (MOLSIM, OZ, PB, PGESE, and POLYMER) was used in advanced undergraduate courses in physical chemistry. In addition, the program MOLSIM for Monte Carlo and molecular dynamics simulation has substantially been updated and extended (P. Linse).

INSTRUMENTS AVAILABLE AT THE DEPARTMENT

NMR. (contact person: Olle Söderman). The department has a Bruker DMX200 NMR spectrometer, delivered towards the end of 1994. The spectrometer is well equipped and allows performance of a variety of modern NMR experiments, such as solid-state experiments, advanced relaxation measurements and diffusion experiments. In addition, the department has at its disposal a Bruker DMX100 spectrometer and a Bruker MSL 100 spectrometer interfaced to a variable field electromagnet. (Sponsored by FRN and Kjell and Märta Beijers Stiftelse).

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

Dynamic and Static Light Scattering. (contact person: Karin Schillén).

A) A laser light scattering goniometer system from ALV GmbH, Langen, Germany, for simultaneous angular dependent determination of dynamic light scattering (DLS) and static light scattering (SLS). The goniometer system is suitable for DLS experiments, such as determination of diffusion coefficients and size distributions in polymer solutions and surfactant micellar solutions, studies on polymer gels and glasses. In addition, depolarized DLS measurements for studies on optical asymmetric systems and determination of rotation diffusion coefficients can be performed. The system is also utilized for SLS experiments, i.e. determination of molecular weight, radius of gyration, and second virial coefficients in macromolecular solutions. The system includes a diode-pumped solid-state laser from Coherent (532 nm, 400mW), laser beam focusing optics including a laser beam attenuator, a goniometer with a rotary table of an angular range of 12° to 155°, a cell housing with an index matching quartz vat, a fiber optical near-monomodal detection system, a detection unit comprised of 2 matched photomultipliers in a pseudo-cross correlation arrangement. For the DLS measurements using photon correlation spectroscopy, two multiple tau digital correlators (with a total of 320 exponentially spaced channels) are utilized to obtain an initial real time sampling time of 12.5 ns. The lag time range extends from 12.5 ns up to >105 s, which makes it possible to detect particle sizes from 1 nm up to 5000 nm in radius. The temperature range of the DLS/SLS goniometer system is -12°C to +140°C. In addition, a differential refractometer from ALV for the determination of refractive index increments necessary for the SLS experiments is incorporated in the overall set-up with an optical fiber. (Sponsored by the former Swedish Natural Science Research Council (NFR).)

B) For the characterization of molecular weight and studies of conformation changes or association processes in macromolecular systems, a multi-angle desktop 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 (633 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 organic solvents but batch analysis may also be performed. (Sponsored by FRN.)

Surface film balance. (contact person: Tommy Nylander). A Nima technology 611 Langmuir trough with a surface film balance (Wilhelmy plate) was acquired during 1997. The instrument is equipped with a dipper to prepare Langmuir-Blodgett films. It can also be used for dynamic contact angle measurements, while simultaneously recording the surface film pressure. In addition a KSV minitrough was acquired 2000 and used together with the Optrel Multiskop ellipsometer. Both surface film balances are equipped to measure the surface potential (Sponsored by Crafoord Foundation).

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

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 γ and D , thus, allowing

unique studies of the evolution of both the thickness and density (refractive index) of adsorbed surfactant and polymer layers with time. The possibility of working at different wavelengths provides an additional source of information on complex systems as well as flexibility to optimize the optical contrast of the systems studied. Continued efforts are invested in upgrading this instrument to improve its potential for studies of fast interfacial processes occurring on the nanometer scale. During 1998 we acquired an additional ellipsometer, an Optrel Multiskop (Optrel, Berlin Germany). This instrument has been fitted with sample cells to measure at the solid-liquid, liquid-liquid and liquid-air interfaces. Apart from doing null-ellipsometry we can also do imaging ellipsometry, Brewster Angle Microscopy, Surface plasmons as well as operate it in waveguide mode. (Sponsored by FRN).

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

Multimode scanning probe microscope (contact person: Tommy Nylander). A Multimode Scanning Probe Microscopy (Nanoscope-III) was purchased jointly by Physical Chemistry 1 and the Department of Food Technology from Digital Instruments Inc. in April 96. The instrument can be operated as both a scanning tunneling microscope (STM) and an atomic force microscope (AFM). With its many configurations the instrument can scan and image a wide variety of samples with scan sizes from atomic level up to 125 by 125 microns. As an AFM, traditional contact mode experiments in air and liquid and TappingMode experiments in air have been available for many years. More recent equipment purchases allow users to image surfaces with TappingMode in fluid environments, perform lateral force microscopy (LFM) measurements of topography and friction, and make force measurements using a colloidal probe. In the latter mode, a spherical particle is adhered to an AFM cantilever and colloidal forces between the probe and surface in a fluid environment can be studied. Other force measurements are also possible using standard cantilevers or chemically modified cantilevers. (Sponsored by FRN).

Optical Microscopy. (contact person: Olle Söderman). The Department has a Zeiss Axioplan Universal microscope equipped with differential interference contrast and a 35 mm photo camera MC 100 as well as with a 100W mercury short-arc lamp and a system of filters to allow the fluorescence microscopy observations. The microscope is further equipped with a high-sensitivity SIT video camera and an image processor, Argus 20, (Hamamtsu Photonics, Japan) together with the Macintosh-based image analysis software. (Sponsored by FRN & Crafoord Foundation).

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

Rheometers. (contact person: Krister Thuresson). A Carri-med controlled stress

rheometer CSL 100 temperature controlled by a Peltier system. Measuring systems; cone and plate (solvent trap) in acrylic (4 cm, 1° and 6 cm, 1°) and stainless steel (4 cm, 1° and 6 cm, 1°). (Sponsored by Nils and Dorthi Troëdsson Research Foundation).

A Physica UDS 200 controlled stress rheometer. Measuring systems temperature controlled by a Peltier system; cone and plate in acrylic (2.5 cm, 1°, 5 cm, 1°, 7.5 cm, 1°), cone and plate in stainless steel (2.5 cm, 1°, 5 cm, 1°, 7.5 cm, 1°), plate and plate in stainless steel (2.5 cm and 5 cm). Measuring systems temperature controlled by a cylindrical temperature system and an external water bath; cup and bob (2.5 cm) and a double gap measuring device, both in stainless steel.

Vibrational spectroscopy. (contact person: Olle Söderman). Two Fourier transform spectrometers from BioRad are available at the department, namely the infrared spectrometer FTS6000 and the FT Raman spectrometer. Raman and IR spectroscopy are powerful tools in studies of polypeptide and protein conformation. In the present projects, vibrational spectroscopy is used primarily to study the effects of surfactants and lipids on protein and polypeptide conformation. Also, conformational studies of peptides deposited as Langmuir-Blodgett films are conducted by means of attenuated total reflection techniques (ATR-IR) in cooperation with AstraZeneca.

COLLABORATIVE RESEARCH PROGRAMS

The Centre for Amphiphilic Polymers, CAP

The Centre for Amphiphilic Polymers from Renewable Resources (CAP) at Lund University has been in existence since 1995. It is part of the national Competence Centre Programme supported by VINNOVA, the Swedish agency for innovation systems. CAP is jointly funded by Lund University, VINNOVA, and a group of industrial companies. Companies participating since the beginning are Akzo Nobel Surface Chemistry, AstraZeneca R&D Mölndal, EKA Chemicals, Lyckeby Stärkelsen, SCA Research, and Tetra Pak, and in 2004, CAP could welcome Celanese Emulsions Norden AB as a new member company. Lennart Piculell is the director of CAP since November 2003. Per Linse is a member of the Board, which has an industrial majority.

CAP activities concern fundamental behaviour and applications of amphiphilic polymers, and the use of biopolymers for their preparation. CAP research is mainly localised at Lund University, but also at the member companies. The scientific work in CAP is carried out as ca. 20 PhD or postdoc projects covering all aspects of amphiphilic polymers, including synthesis/modification, characterisation, physical-chemical behaviour, and theoretical modelling. Research activities are directed towards all four main areas of application of amphiphilic polymers: Polymer solutions, polymer gels, polymers at interfaces, and polymeric materials. Dr Charles Buchanan (Eastman, USA) and professor Terence Cosgrove (University of Bristol, UK) are the two members of the international scientific advisory board of CAP.

In January 2004, CAP entered, at full speed, the stage 4 of its existence. During 2004 a new member company joined (cf above), no less than six new projects were launched, and three PhD students financed by CAP, including Karin Bryskhe and Martin Olsson from our department, completed their theses. Activities included the CAP annual symposium, a tour for PhD students to the member companies in the Gothenburg region, and a mini-symposium on polymer-particle dispersions attended by ca. 60 delegates from academia and industry.

2005 will be CAP's 10th and final year. To mark the 10 successful years of CAP, the 5th Annual Surface and Colloid Symposium in Lund on November 16-18 this year

will have “Amphiphilic Polymers” as its theme. The topics of the symposium mirror the topics of CAP research, and the speakers will include CAP researchers as well as invited leading international scientists in the area.

Colloidal Structures from Self-association, COLINTECH and the Research School in Colloid and Interface Technology.

Colloidal Structures from Self-association, COLINTECH, is a five-year research programme funded by the Swedish Foundation for Strategic Research, SSF. It started January 1, 2003 and the total funding is 14.5 MSEK. Research groups at the Chalmers Institute of Technology, the Institute for Surface Chemistry (YKI)/ Royal Institute of Technology and Lund University, i.e. our department are active in the programme. The research topics include the preparation of hard and soft nanoparticles through dynamic self-assembly, dynamics of non-equilibrium self-assembly dispersions, and structuring complex systems at interfaces.

SSF has granted 9.5 MSEK for the period 2003–2005 for a prolongation of the Research School in Colloid and Interface Technology. The Research School organizes courses, often in the form of summer schools, on a national level and, in addition, takes care of the “course year” for a limited number of PhD students. The activities of the research programme supports the Research School and *vice versa*.

During 2004 the following courses were given:

- Surface Chemistry – surfactants and polymers in aqueous solutions (5 p), Degeberga with 25 participants.
- Surface analysis (2 p), Stockholm with 18 participants.
- Stability of dispersions (3 p), Stockholm with 30 participants.
- Mesoporous crystals and related nano-structured materials, Stockholm. Workshop organized with Professor Osamu Teresaki, Stockholm University.
- The Colloidal Domain (10p), Lund, Göteborg and Stockholm with 26 participants (2003- 2004).

Members of the board of the Research Programme and Research School are: Jan Svård (Chairman; Eka Chemicals), Krister Holmberg (Chalmers University of Technology, Director of studies of the Graduate School), Björn Lindman (Lund University), and Bruce Lyne (Institute of Surface Chemistry).

An SSF grant of 350 000 SEK for National Net-working Activities in Surface and Colloid Technology during 2003–2004 is managed by the same Board. The aim is to give PhD students opportunities to meet, learn and discuss various fields in surface and colloid science with particular relevance for the life sciences. This was achieved through courses, symposia and conferences arranged by the students themselves. The International Symposium on Surface and Colloid Chemistry Applied to Nanoscience was organized 18-19 November in Lund in cooperation with the Division of Surface Chemistry of the Swedish Chemical Society, The Swedish Academy of Pharmaceutical Sciences, and the Surface and Colloid Science Center at Lund University, see below.

Lund University is the host university of all three programmes.

The Surface and Colloid Science Center, YKOLL

YKOLL is an interdisciplinary centre on surface and colloid science at Lund University. The centre currently involves the Departments of Analytical Chemistry, Applied Microbiology, Biochemistry, Biotechnology, Food Engineering, Food Technology, Inorganic Chemistry, Medical Microbiology, Physical Chemistry 1, Polymer Technology, and Technical Analytical Chemistry, as well as individual research groups from Theoretical Chemistry and from the Department of Experimental

Research at Malmö Hospital. The annual symposium 2004, titled International Symposium on Surface and Colloid Chemistry Applied to Nanoscience, was held 18–19 November. It was preceded by a half-day symposium on Cell–Protein–Surface Interactions. The symposia were organized in cooperation with the Division of Surface Chemistry of the Swedish Chemical Society, Malmö University and the SSF funded COLINTECH programme, see above.

The Division of Surface Chemistry of the Swedish Chemical Society.

This Division of the Swedish Chemical Society was founded 2001 to promote contacts between chemists interested in surface and colloid chemistry (Gerd Olofsson, chairman). It will organize in cooperation with YKOLL the annual Symposium in Surface and Colloid Science. The fourth symposium in the series was held in Lund in November.

The Competence Center for Surfactants based on natural products, SNAP

The department is a member of a competence center in which the aim is to utilize raw materials from various natural resources as the basis for the production of surfactants. The center is administrated by the Royal Institute of Technology in Stockholm, and its structure is similar to the CAP described above, involving universities, research institutes and companies. Participants from Lund are C. Ericsson, M. Nilsson, J. Reimer, C. Whiddon, O. Söderman and S. Ulvenlund.

NorFA Network

A three-year nordic-baltic network, sponsored by NorFA (Nordic Academy for Advanced Study), on Quality and Health Aspects of Milk Components, co-coordinated by Dr. Jeanette Otte at KVL (The Royal Veterinary and Agricultural University) in Copenhagen, Denmark was started 2002 (<http://www.mli.kvl.dk/dairy/NORFA/>). A one year prolongation of the project was granted in the end of 2004. The participating institutions are Food Technology, Food Engineering, Physical Chemistry 1 at Lund University; Food Science, Swedish University of Agricultural Sciences; Food Science, Agricultural University of Norway; Dairy and Food Science, The Royal Veterinary and Agricultural University, Denmark; Department of Molecular and Structural Biology, University of Aarhus, Denmark, Unit for Nutrition Research at University of Iceland and Landspítali-University Hospital, Reykjavik, Iceland, Food Technology, Food Research Institute, Finland; Institute of Food Processing, Tallin Technical University, Estonia; Food Technology, Kaunas University of Technology, Lithuania.

New strategies for oral delivery of drug peptides and peptidomimetics

A 3 year collaborative project involving Camurus AB and Physical Chemistry 1 was granted 2003 by VINNOVA (Swedish Agency for Innovation Systems) and SSF (Swedish Foundation for Strategic Research) within the so-called VINST program dedicated to support SME. The aim of the project is to develop more effective peptide carriers and during this process also increase the understanding of the physicochemical and biological problems involved in oral bioavailability of peptides and proteins. Oral administration of peptide and protein drugs has so far been hampered by low bioavailability, due to the presence of effective permeation barriers and lack of peptide stability in the gastro-intestinal tract. The project involves extensive interdisciplinary

activities and cross-fertilization of projects. The basic approach will be to use self-associated nano-structured lipid carrier and exploit special properties, which can provide protection against enzymatic degradation and enhanced permeation of biomembranes. Scientifically the project will span biophysical studies of lipids and peptides to in vivo studies of uptake mechanism for peptides and proteins. (T. Nylander, H. Wennerström; F. Tiberg and K. Larsson Camurus AB)

EU-shared cost project- MODSTEEL

The department took part in a 4 year EU-shared cost project entitled "The Improvement of construction materials used in the food industry to lengthening processing time" (Acronym MODSTEEL and Contract no. G5RD-1999-00066) and co-coordinated by Prof. Marie Paulsson Food Technology, LU and includes partners from Sweden, Greece, Portugal, France and Germany. Fouling of processing equipment upon heating is one of the major problems in the dairy industry as deposit formation limits the desired heat transfer required for the microbiological safety of the product, reduces the flow and leads to pressure build up, whereas bacterial adhesion in the cooling section can lead to post-pasteurization microbial contamination. Cleaning at regular intervals is essential to overcome these problems. However, this requires interruption of processing, use of cleaning agents and large amounts of rinsing water, all attributing negatively to the cost of a process and leading to environmental problems. The aim of the project is to minimize fouling and to reduce cleaning by altering the surface properties of the heating surface, i.e. steel, to make it less attractive for the fouling components. The Lund team mainly contributes with ellipsometry studies of protein adsorption on different modified stainless steel surface as a function of temperature and flow rate as well as characterization of surface properties and modeling. The project formally ended in May 2004. (M. Paulsson, O. Santos and C. Trägårdh (Food Engineering) and T. Nylander).

EU-STREP FP6 project- NEONUCLEI

The department was granted a 4 year EU-FP6 STREP in the NEST PATHFINDER project within Synthetic Biology, entitled "Self-assembly of synthetic nuclei: key modules for semibiotic chemosynthetic systems" (Acronyme NEONUCLEI and Contract no.12967) and coordinated by Prof. George Attard, University of Southampton, UK. NEONUCLEI will develop transcription-competent synthetic analogues of cell nuclei. These particles, termed neonuclei, will be obtained through self-assembly/organisation in mixtures of DNA, macromolecules (or nanoparticles), and lipids. The composition of the neonuclei will be chosen to produce particles with internal nano-architectures capable of sustaining gene transcription upon the addition of transcription factors. The DNA of the neonuclei will contain a gene cluster (or tandem repeats of the same gene). The genes will be separated by sequences designed to induce DNA compaction in response to specific chemical or physical stimuli. This will be exploited to establish non-biological control over the transcription of parts, or all, of the DNA. These control sequences offer the opportunity for multiple transcription control strategies and provide the capability of implementing temporally co-ordinated synthesis of multiple gene products. Neonuclei represent a key enabling step in the realisation of semi-biotic systems: these are systems and devices that combine synthetic non-natural functional systems with systems of biological origin. The neonuclei will be integrated with biological systems, or with isolated components, to produce novel semi-biotic devices capable of the controlled in situ synthesis of complex bio-molecules on demand. Physical chemistry 1 mainly contributes in providing understanding

formation, morphology and structure of relevant self-assembly structures, DNA-surfactant/particle interaction, DNA compaction, morphology and structure of formed entities (T. Nylander, V. Alfredsson, B. Lindman, U. Olsson, H. Wennerström).

EU-STREP FP6 project- BIOSCOPE

The department was granted a 3 year EU-FP6 STREP in the Nanoscience and technology area entitled "Self-reporting biological nanosystems to study and control bio-molecular mechanisms on the single molecule level" (Acronyme BIOSCOPE and Contract no. NMP4-CT-2003-505211, www.BIOSCOPE.fkem1.lu.se) and coordinated by Tommy Nylander at the department. BIOSCOPE will develop new nano-scale tools allowing unprecedented insight into bio-molecular mechanisms at biological interfaces on the scale of single molecules. The key element in the BIOSCOPE strategy is to involve the bimolecular system itself as part of the nanoscopic instrument which in various ways reports to the out-side world about its current local state. The objectives of BIOSCOPE are 1.) To develop instrumentation and methods for manipulation of enzymes and enzyme activity at the nano-scale providing insight into the bimolecular mechanisms on a single molecule level. 2.) To develop novel forms of integration, at the nano-level, of enzymes and non-biological systems such as nanoparticles, artificial membranes, electrical field or force field traps. 3.) To confine several enzymes to surfaces of nanoparticles or membranes on a less than 10 nm scale in order to achieve a self-organized assembly with concerted as well as controllable bioaction superior to the simple sum of the same individual enzymes. Apart from co-ordinating the project, Physical chemistry 1 mainly contributes in providing understanding formation, morphology and structure of self-assembly structures on the nanoscopic scale (T. Nylander, V. Alfredsson, J. Barauskas H. Wennerström).

COST Project

The network "Polymer-surfactant interactions: From modelling to applications" sponsored by the management committee for the European Concerted Action, COST, D 15 is formed by the following groups: Lund (Ali Khan, Björn Lindman, Olle Söderman, Ulf Olsson), Rome (Camillo La Mesa, Bianca Sesta, Giacomo Gente, Paolo Gasbarrone, Livio Persi), Calabria (Giuseppe Antonio Ranieri, Mario Terenzi, Luigi Coppola, Cesare Oliviero), Barcelona (Maria Rosa Infante, Pere Clapes, Aurora Pinazo, Eulalia Piera) and Coimbra (Maria de Graca Martins Miguel, Hugh Douglas Burrows, Eduardo Marques, Maria Luisa Leito, Maria Ermelinda da Silva Eusebio) Within the scheme, the senior scientists and post-graduate students have the possibility to visit each other's lab. Moreover, there are two workshops per year. Collaborative research activities are focused on the following areas: (a) Formation, structure and dynamics of polymer-surfactant systems, (b) Physico-chemical properties of polymer containing microemulsions and (c) Characterization of new polymer-surfactant adducts. The network meeting for the year 2004 took place in Calabria. There was also a meeting for all groups active within COST in Nice during the fall of 2004.

CIPSNAC

A new 4 year EU research training network "CIPSNAC: Colloidal and interfacial properties of synthetic nucleic acid complexes-assembly of nanostructured DNA particles and surfaces (EU-MRTN-CT-2003-504932) was set-up during 2004. The Research Training Network (RTN) will focus upon DNA nanoparticles and surfaces. In this specific field, a relationship between the structure, thermodynamic stability, enzymatic accessibility and gene transfer or detection efficiency has not been

established so far. To date, physico-chemical characterization has only been carried out sporadically on isolated gene transfer systems. The establishment of phase diagrams as well as gene transfer efficiencies as a function of a large range of variables is time consuming. Therefore, this RTN project will bring about a *concerted action* of expert groups to address these problems. The fascinating frontier is to study the assembly of DNA surfactant complexes at the molecular level. The RTN will define model systems and key parameters such that a systematic theoretical approach becomes feasible. The partners are from Lund, Coimbra, Munich, Dublin and Paris. (*B. Lindman, responsible for Lund group*)

EU Project “Mercury”

The project deals with problems related to mercury pollution in Latin America, e.g. the recovery of mercury (ionic, organic) and the effect of mercury in living plant materials. Participating laboratories are in Europe and in Latin America. The role of the Lund group is primarily to design and test a new titration micro-calorimeter that is equipped with electrodes (pH, Hg). It will be used for thermodynamic characterisation of Hg complexes. Our long term project “A 48-channel microcalorimeter for analysis of living cells” is also included in the EU project. (*I. Wadsö*).

EU Marie Curie Training Site on Surface and colloid technology-self-assembled structures of biological and technological relevance (Contract No HPMT-CT-2000-00150)

Research Areas and Facilities

Doctoral fellowships are offered for 3 to 12 months in the following research areas of surface and colloid science:

- 1) Fundamental work in surface and colloid science of direct relevance for industry. The focus will be on lipids, protein, surfactants and polymers of biological origin and relevance. Research can be a short distance from commercialization.
- 2) Polar lipid/aqueous systems used as model matrices to mimic biological processes. This includes the phase behavior of lipids, which effects the binding of proteins/polypeptides and processes.
- 3) Liquid crystalline phases as well as other self-assembled aggregates like micelles and vesicles formed by polar lipids, surfactants and polymers in aqueous media, used to encapsulate drugs, enzymes, vitamins or any other active molecules.

Fellows will be given access to “state of the art” facilities and training. The research studies will be part of their requested training and there will be close liaisons between Lund and their home universities.

For further information contact

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CONFERENCES, TRAVELS AND SEMINARS

Björn Lindman gave plenary lectures at the 10th National Symposium on Colloids and Interface Chemistry, Xi'an, China, and the European Colloid and Interface Society (ECIS) conference in Almeria, Spain and invited lectures at the 15th Surfactants in Solution (SIS) conference, Fortaleza, Brazil, at the Akzo Nobel Innovation Day honoring Prof. Martin Hellsten, Stenungsund. He also talked at COST Polymer-surfactant workshops in Arcavata di Rende and Barcelona. He was President of the Scientific Committee of the meeting of the Portuguese Chemical Society in Coimbra. Björn Lindman was invited to Taiwan (host Prof. Ya-wun Yang) by the National Science Council on its "Honorable Visitor Program" and gave several lectures including the National Taiwan University Medical Center and the Chemistry Department, the National Tsinghua University and the National Taiwan University Nano-Center. 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: Univ. of Calabria, Italy, Univ. Paris-Sud, Orsay, Ludwig-Maximilian University, München, Swedish Forest Research Institute, STFIPackforsk, Stockholm, Nestlé Research Center, Lasusanne, Jotun Research Center, Sandefjord, Norway, Åbo Akademi University, Trondheim University, Shaanxi Normal University, Xi'an, China, Peking University, Chinese Academy of Sciences, Beijing, Uppsala University, Akzo Nobel, Stenungsund, Eka Chemicals, Institute for Surface Chemistry, Royal Institute of Technology, Stockholm. Björn Lindman was visiting professor at Department of Chemistry, Coimbra University, Portugal.

Håkan Wennerström delivered invited talks at: "Short Range Interactions in Soft Condensed Matter" Regensburg, Germany; at "Membrane Domains and Fluctuations" Graz, Austria; and at "Faraday Discussions: The Dynamics and Structure of the Liquid-Liquid Interface" Cambridge, UK

Olle Söderman lectured at two EU-sponsored COST meetings during 2004. He also presented a talk at the workshop on Short Range Interactions in Soft Condensed Matter in Regensburg in February and gave a seminar at the Jozef Stefan institute in Ljubljana during a visit in June.

Per Linse delivered a invited talk at the workshop on "Electrostatic interactions and biophysics", Minneapolis, USA. He also gave oral presentation at the "Algorithms for Macromolecular Modelling IV" meeting Leicester, UK and a invited seminar at Princeton University, USA.

Lennart Piculell visited USA where he gave two lectures at Procter & Gamble, Cincinnati, an invited lecture at the conference "Polyelectrolytes 2004" in Amherst, and a lecture at the 78th ACS Colloids symposium at Yale. He stayed two weeks at UNICAMP, Campinas, Brazil, as part of a research collaboration. In Brazil he gave two lectures at UNICAMP and one lecture at the Riberai Preto campus of University of São Paulo. He organized a one-day minisymposium on polymer-particle dispersions for CAP.

Ulf Olsson delivered invited seminars at the meeting of the Belgian Particle, Colloid & Interface Society at Gembloux Agricultural University, at Procter and Gamble, Bruxells, and at the annual meetings of the Danish and the Swedish Neutron Scattering Societies. Ulf also participated at the workshop on "Our Future Light Source" organized by Max-lab in Lund. He also made short visits to Ghent University and Köln University. Ulf Olsson also participates in a popular science seminar series open to the public and organized annually by the City Library of Malmö in collaboration with

Lund University. This year, he gave a lecture on electrostatic forces, using examples ranging from DNA compaction to the mechanism of thunderstorms.

Ingemar Wadsö gave talks at the Calorimetry Conference in Santa Fe, New Mexico, USA and in Barcelona, Spain. He also visited University of Surrey, Guilford, UK for discussions in connection with the EU project.

Tommy Nylander gave invited talks at University of Leuven, Leuven, Belgium, University of Southern Denmark, Odense, Denmark, Novozymes, Bagsvaerd, Denmark, and Duke University, Durham, North Carolina, USA. He also organized the Kick-off meeting and 1st meeting of the EU-funded project, BIOSCOPE, in Lund and Copenhagen, respectively as well as the "International Symposium on Surface and Colloid Chemistry Applied to Nanoscience" at Lund University in November. He also gave a talk at the Workshop on "Short range interactions in soft condensed matter –from solutions to materials and biological systems" at University of Regensburg, Germany and at NorFA meeting on "Quality and Health Aspects of Milk Components" at Kaunas University of Technology, Tallinn, Estonia. He also attended the CIPSNAC (EU Marie Curie Research Training Net-work) project meeting in Munich in July as well as the Swedish Neutron Scattering Society meeting in Studsvik. He also made traveled to ILL, Grenoble, France, ISIS at Rutherford-Appleton Laboratory, Didcot, UK and Jülich, Germany for Neutron scattering and reflectivity measurements.

Gerd Olofsson gave an invited lecture at 18th IUPAC International Conference on Chemical Thermodynamics in Beijing, China.

Magnus Ullner gave an oral presentation at Polyelectrolytes 2004, Amherst, Massachusetts, USA

Karin Schillén presented a poster at XVIII European Colloid and Interface Society Conference, Almeria, Spain and gave an invited talk at the annual CAP meeting at Järavallen, Sweden

Stefan Ulvenlund gave an oral presentation at "Drug Delivery – New Routes to Innovative Formulations", Medeon, Malmö, Sweden He also presented posters at the "Workshop in Controlled Drug Delivery – Current Swedish Research", Gothenburg, Sweden

Emma Sparr gave oral presentations at the 5th International Conference on Biological Physics, Göteborg, Sweden, and at a symposium on delivery systems and membranes, Coimbra, Portugal. She also gave an invited seminar at the department of Biochemistry and Biophysics, Stockholm University, and presented a poster at the Xth International Symposium on Amyloidosis, Tours, France.

Markus Johnsson gave a seminar at the two day symposium "Beyond aqueous borders" in the honour of Prof. Jan B. F. N. Engberts at the University of Groningen, The Netherlands. He also presented a poster at the BioTech Forum Science Conference in Copenhagen, Denmark

Katarina Flodström visited Procter & Gamble, Cincinnati, USA and Duke University, Durham, USA where she gave a seminar. She also delivered an oral presentation at the workshop on Small Angle Scattering from Soft Matter, Lund, Sweden and presented a poster at MCRM 2004 (Mesoporous Crystals and Related nano-structured Materials), Stockholm, Sweden

Joakim Balogh, Justas Barauskas, Karin Bryskhe, Marité Cárdenas, Rita Dias, Caroline Ericsson, Jörgen Jansson, Cecilia Leal, Jens Norrman and Johan Reimer gave oral presentations and Fatima Costa presented a poster at the 15th Surfactants in Solution (SIS) conference, Fortaleza, Brazil

Rita Dias delivered an oral presentations at the CIPSNAC meeting in Munich, Germany, and at the COST D15 “Interfacial Chemistry and catalysis” meeting in La Colle sur Loup, France.

Cecilia Leal gave oral presentations at “XIX Encontro da Sociedade Portuguesa de Química”, Coimbra, Portugal and at “DNA and Chromosomes: Physical and Biological Approaches”, Cargese.

Jörgen Jansson gave an oral presentation at the workshop on Small Angle Scattering from Soft Matter, Lund, Sweden.

Sam Edgcombe gave a invited seminar at BioMedical Center, Uppsala University, Sweden and presented a poster at the “18th Conference of the European Colloid and Interface Society”, Almería, Spain

Marité Cárdenas gave an oral presentation at the CIPSNAC Workshop in Munich, Germany and at the Swedish Neutron Scattering Society SNSS-10 in Studsvik, Sweden.

Fatima Costa presented posters at LogP2004 – the 3rd Lipophilicity Symposium in Zurich, Switzerland and at American Society of Pharmaceutical Scientist Annual Conference in Baltimore, USA

In January the department organized the first Scandinavian workshop on scattering from soft matter. The meeting attracted about 40 participants from the Nordic countries, and focused mainly on small angle scattering X-ray and neutron scattering. The meeting was very appreciated by the participants and it was agreed upon that this meeting should be organized annually with the next meeting (2005) to be held in Copenhagen. With these meetings, it is also the objective to create a platform where young Scandinavian scientists can find scientific support when performing scattering studies for example neutron scattering at large-scale facilities.

The department organized the yearly meeting of the Surface and Colloid section of the Swedish Chemical Society, entitled “Surface and Colloid Chemistry Applied to Nanoscience”. The meeting attracted 150 participants from many different countries and was organized with a satellite symposium on Cell-Protein-Surface Interactions 17-19 of November. 14 internationally well-renowned lecturers gave invited lectures and a majority of the department members presented posters at the meeting. The meeting 2005 will also be held in Lund 16-18 of November and dedicated to “Amphiphilic Polymers” (<http://www.ykoll.fkem1.lu.se/>).

EXTERNAL PROFESSIONAL ACTIVITIES

Björn Lindman was Regional Editor of Colloid & Polymer Science and was on the Advisory or Editorial Boards of Cellulose, Advances in Colloid and Interface Science, Current Opinion in Colloid & Interface Science and Journal of Dispersion Science and Technology. Björn Lindman is also member of the Research Council of The Swedish Pulp and Paper Research Institute. He 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. He is Director for a national program on Colloid & Interface Technology sponsored by the Swedish Foundation for Strategic Research and also a member of the Collegium of this foundation.

Håkan Wennerström was chairman of the Nobel Committee for Chemistry, regular member of the board of the Science and Technology Committee of the Swedish Research Council, swedish representative in the Physical Sciences and Engineering Standing Committee (PESC) of the European Science Foundation, member of The

Royal Swedish Academy of Engineering Sciences, member of The Royal Swedish Academy of Sciences, member of The Royal Physiographic Society in Lund, member of the Scientific Group of the Chemistry Department, Lund University, member of the scientific innovation group (Iderådet), Lund University.

Lennart Piculell is the director of the Center for Amphiphilic Polymers (CAP) since November 2003. He is a member of the Board of the Faculty of Science, Lund University. He is a section editor for the Polyelectrolytes section of *Current Opinion in Colloid and Interface Science*, and a member of the editorial boards of *Food Hydrocolloids* and *Carbohydrate Polymers*. He acted as chairman, and served on the thesis committees, at the thesis defenses of Katarina Flodström and Yoshikatsu Hayashi. He was a member of the International Advisory Boards of the "European Polymer Congress – 2005" in Moscow, and the "8 International Hydrocolloids Conference" in Trondheim, 2006

Per Linse was a member of panel for Chemical Engineering, VR, member of the program committee and a member of the board of the Center for Amphiphilic Polymers, CAP. Per served on PhD thesis committee for Jörgen Jansson.

Olle Söderman served on PhD thesis committees for Jan Willem Benjamins and Karin Bryskhe in Lund and for Claire Vautrin at CEA Saclay, France

Tommy Nylander was one of the two external examiners for Torben Ishøj's PhD thesis at Copenhagen University in November and member of the evaluation committee for Johan Kostelas PhD thesis at Uppsala University in October. Tommy Nylander was also appointed member of the Advisory Committee of *Journal and Colloid and Interfaces Science*.

Gerd Olofsson is chairman of the Division of Surface Chemistry of the Swedish Chemical society.

Viveka Alfredsson was member of the organizing committee for "Mesoporous Crystals and related nanostructured Materials, a symposium and workshop that took place in Stockholm June 1-5, 2004.

Karin Schillén was a deputy member of the board of the Chemical Center and member of the research board of the chemistry division at the Chemical Center "Forskningsnämnden vid kemiska sektionen (NF)". Karin served on PhD thesis committee for Fernando E.Ortega-Ojeda, Food Technology.

AWARDS

Björn Lindman received the Molecular Science Award of the Chinese Academy of Sciences.

COURSES AND TEACHING

Members of the department are involved in a number of undergraduate courses. The first year of chemistry studies at the Chemical Center consists of three 9-week chemistry courses and a 9 week course in mathematics. These courses are given both during the fall and spring semesters. In the first two basic chemistry courses Viveka Alfredsson, Lennart Piculell, Karin Schillén and Olle Söderman were involved in lectures and leading exercises and question hours. The topic of the third first-year course is thermodynamics and introductory quantum mechanics and spectroscopy. Here, Olle Söderman is the head teacher for this course and Olle gave the lectures and exercise sessions in thermodynamics together with Karin Schillén.

As regards higher courses, the department gives one basic and one advanced

course in surface and colloid chemistry and one advanced physical chemistry course. The basic course, which is a biannual event, is headed by Ulf Olsson and was taught by Ulf, Lennart Piculell, Martin Olsson and Sam Edgecombe. The advanced surface and colloid chemistry course is organized and taught by Håkan Wennerström (main teacher) along with Lennart Piculell, Tommy Nylander and Per Linse. It is given once a year during the fall semester, and is based on the book by Håkan Wennerström and Fennel Evans. The advanced physical chemistry course is given once a year during the spring semester and is taught by Per Linse, Ulf Olsson and Olle Söderman. This course is focussed on methodology and is divided into three parts: (i) Small angle scattering and light scattering (Ulf), (ii) NMR (Olle), and (iii) statistical mechanics and computer simulations (Per). Håkan, on behalf of the department, delivered a total of 15 hrs lectures on environmental chemistry for the undergraduate students. Finally, a number of our graduate students serve as teaching assistants on all courses given by the department. We also teach colloid science at the technical faculty, where Stefan Ulvenlund and Björn Lindman teach part of a colloid course for engineering student given by the food technology department.

When teaching undergraduate courses we also emphasize industrial applications since it represents the future activities for many of the students. We visit industries, and for a number of years we also have had an invited guest from industry to lecture on pharmaceutical applications of colloid and interface science. Here we are particularly grateful to Jan-Erik Löfroth, AstraZeneca, Mölndal, who, on a regular basis, come to give 4 hours of lectures on drug delivery for the students of the basic surface and colloid course.

The Institute for Surface Chemistry, YKOLL and Chalmers University of Technology jointly organize an annual course on surfactants and polymers in aqueous solution directed towards a European audience. In 2004, the course was held, for the 13th consecutive year, in Lisbon. Björn Lindman was one of the three teachers on the course Surface and colloid chemistry - molecular basis and technical applications for undergraduate and Ph. D students arranged by the Colloid & Interface Technology Programme (SSF) in Degeberga, Sweden. Björn Lindman and Stefan Ulvenlund taught on a course on surface and colloid chemistry at the Technical Faculty of Lund University.

FINANCIAL SUPPORT

For the fiscal year 2004, the department had a turnover of ca 31.0 million SEK. From the University we obtained 14.0 million of which 1.0 million is to cover undergraduate teaching, and the rest for graduate students, salaries of professors, associate professors and assistant professor, technical and administrative personnel, and basic expenses including rents of offices and laboratories. Government research agencies that give support to the research is: The Swedish Research Council (VR), which provide us a support of 5.0 million SEK, The Swedish Agency for Innovation Systems (VINNOVA) which finances more applied projects, supports us with 5.2 million, mainly via the 2 Competence Center CAP and SNAP, during the fiscal year. We also received 2.3 million SEK from The Swedish Foundation for Strategic Research (SSF), which is an important funding agency for supporting novel research ventures in Sweden. We are grateful for support from private industry, directly and via their foundations, amounting to ca. 1.6 million. Finally, we received 2.9 million SEK from The European Commission.

DOCTORAL THESIS

February 13, 2004

Jonny Eriksson

*Interfacial behaviour of surfactants and enzymes:
studies at model surfaces*

Opponent: Prof. Thomas Arnebrandt,
Malmö Högskola

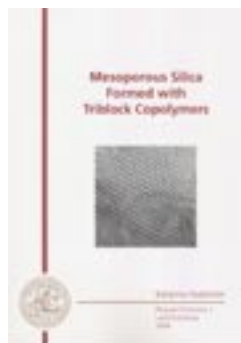


April 2, 2004

Katarina Flodström

Mesoporous silica formed with triblock copolymers

Opponent: Prof. Michael W. Anderson,
UMIST, UK



May 7, 2004

Jan-Willem Benjamins

*Ellipsometry studies of liquid interfaces.
New methodology and applications*

Opponent: Prof. Reinhard Miller,
Max-Planck-Institut für Kolloid- und
Grenzflächenforschung, Golm/Potsdam,
Germany



May 28, 2004

Yoshikatsu Hayashi

Oppositely charged polyelectrolytes in solution

Opponent: Prof. Aatto Laaksonen,
Stockholms universitet



October 8, 2004

Jörgen Jansson

The interaction between triblock copolymers and surfactants in dilute aqueous solution

Opponent: Prof. Peter Schurtenberger,
Université de Perolles, Switzerland

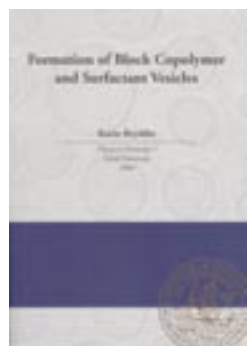


November 13, 2004

Karin Bryskhe

Formation of blockcopolymers and surfactant vesicles

Opponent: Prof. Mats Almgren,
Uppsala universitet



November 26, 2004

Yulia Samoshina

Polyelectrolytes on surfaces and their complexes with surfactants. Thermodynamics versus kinetics

Opponent: Prof. Regine V. Klitzing,
Institute für Physikalische Chemie, Christian-
Albrechts-Universität zu Kiel, Germany



December 10, 2004

Martin Olsson

Particle-induced phase separation in aqueous solutions containing colloidal particles and adsorbing polymers

Opponent: Prof. Wilson C. K. Poon,
University of Edinburgh, UK



December 17, 2004

Marité Cárdenas Gómez

DNA compaction at surfaces

Opponent: Dr. Joachim Rädler,
Ludwig-Maximilians Universität München,
Germany



MEMBERS OF THE DEPARTMENT

Scientists/Teachers

Viveka Alfredsson, associate professor
Justas Barauskas, postdoc
Azat Bilalov, postdoc
José Campos, postdoc
Magali Deleu, postdoc
Rita Dias, postdoc
Eva Hansson, associate professor, dean
Markus Johnsson, postdoc
Alexey Kabalnov, visiting professor
Lina Karlsson, postdoc
Ali Khan, associate professor em
Jakob Kisbye Dreyer, postdoc
Björn Lindman, professor
Per Linse, professor
Iseult Lynch, researcher
Maria da Graça Miguel, visiting professor
Cathy McNamee, postdoc
Tommy Nylander, associate professor
Gerd Olofsson, associate professor
Ulf Olsson, professor
Lennart Piculell, professor
Johan Reimer, lecturer
Karin Schillén, associate professor
Emma Sparr, assistant professor
Anna Svensson, researcher
Olle Söderman, professor
Krister Thuresson, assistant professor
Fredrik Tiberg, adjunct professor
Daniel Topgaard, assistant professor
Magnus Ullner, associate professor
Stefan Ulvenlund, assistant professor
Ingemar Wadsö, professor em
Håkan Wennerström, professor

Graduate students working on a Ph. D. Thesis

Anna Akinchina	Géraldine Lafitte
Joakim Balogh	Cecilia Leal
Jan-Willem Benjamins	Peter Linton
Karin Bryskhe	David Löf
Sanja Bulut	Carin Malmberg
Marité Cárdenas	Markus Nilsson
Samuel Edgecomb	Jens Norrman
Caroline Ericsson	Martin Olsson
Katarina Flodström	Yulia Samoshina
Yoshikatsu Hayashi	Helen Sjögren
Jörgen Jansson	Pauline Vandoolaeghe
Malin Jönsson	
Maria Karlberg	
Anna Körner	

Technical-Administrative Personnel

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

GUESTS

Almgren, Mats , Uppsala University, Sweden, (S)
Anderson, Michael W. , UMIST, UK, (S)
Angelescu, Daniel, Romanian Academy, Romania, (L)
Antunes, Filipe, University of Coimbra, Portugal, (S)
Arnebrandt, Thomas, Malmö University, Sweden, (S)
Attard, George S., University of Southampton, UK, (S)
Bilalov, Azat, Kazan State Technological University, Russia, (L)
Braem, Alan, Carnegie Mellon Univ, USA, (L)
Cabaleiro-Lago, Celia, Spain (L)
Cocquyt, Jan, University of Gent, Belgium, (L)
Colsenet, Roxane, Université H. Poincaré Nancy 1, France, (L)
Costa, Diana, University of Coimbra, Portugal, (L)
Costa, Fatima, University of Coimbra, Portugal, (L)
Costa, Telma, University of Coimbra, Portugal, (L)
Deleu, Magali, Gembloux Agricultural University , Belgium, (L)
Eeman, Marc, Gembloux Agricultural University, Belgium, (L)
Endou, Rihei, Tohoku University, Japan, (L)
Esteban, Isabel, Universidad a Distancia, Spain, (L)

Johnson, Eric, Procter & Gamble, Cincinnati, USA, (S)
Kaper, Helena, Christian-Albrechts-Universität zu Kiel, Germany, (L)
Klitzing, Regine V., Christian-Albrechts-Universität zu Kiel, Germany, (S)
Laaksonen, Aatto, Stockholm University, Sweden, (S)
Lam, Yee, USA, (L)
Loh, Watson, Universidade Estadual de Campinas, Brazil, (L)
Marques, Eduardo, University of Porto, Portugal, (L)
Medronho, Bruno, University of Coimbra, Portugal, (L)
McNamee, Cathy, Nederländerna, (S)
Miller, Reinhard, Max-Planck-Institut, Golm/Potsdam, Germany, (S)
Monduzzi, Maura, Cagliari University, Italy (S)
Mourad, Maurice, Utrecht University, the Netherlands, (L)
Nordén, Bengt, Chalmers University of Technology, Sweden, (S)
Pacios, Isabel, The Universidad Nacional de Educación a Distancia, Spain, (L)
Pais, Alberto Canelas, University of Coimbra, Portugal, (L)
Patra, Michael, Helsinki University of Technology, Finland, (S)
Pebalk, Dmitri, Moscow State University, Russia, (L)
Pegado, Luis, University of Coimbra, Portugal, (S)
Poon, Wilson C. K., University of Edinburgh, UK, (S)
Popescu, Georgeta, University of Bucharest, Romania, (L)
Ragout, Sylvaine, ENSCP, France (L)
Rosa, Monica, University of Coimbra, Portugal, (L)
Rädler, Joachim, Ludwig-Maximilians Universität München, Germany, (S)
Sakamoto, Yasuhiro, Stockholm University, Sweden, (L)
Schurtenberger, Peter, Université de Perolles, Switzerland, (S)
Silva Cláudia, University of Coimbra, Portugal, (L)
Speicien, Vilma, Litauen, (L)
Taixeira, Cilâne, Åbo Akademi (S)
Torres, Miguel, Universidad Simón Bolívar, Venezuela (L)
Vaccaro, Mauro, Italien (L)
Valente, Artur, University of Coimbra, Portugal, (L)
Varandras, Antonio, University of Coimbra, Portugal, (S)
Watson, Randall, Procter & Gamble, Beijing, China (S)
Zauscher, Stefan, Duke University, USA, (S)

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

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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, seminar etc., to one or more years for postdocs and foreign students. Visitors are very important for us and help us to improve our level of research and education. Careful planning can significantly improve these visits. The Annual Report partly serves the purpose of introducing a person to our department prior to a call.

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

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

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

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

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