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Cover: BAM images of a DODAB monolayer at the air-water interface. The bright and dark regions in the image are liquid condensed and liquid expanded domains respectively. If DNA is injected below the film into the subphase, the DODAB condensed aggregates are destabilized by the electrostatic coupling of the DNA macromolecule. Instead, a less denser film is formed. (Marité Cardénas)

## COLLOIDAL BIOLOGY. AN EMERGING RESEARCH AREA.

One of the old roots of colloid science is found in biology. A well known example is the observation by the botanist Robert Brown that pollen particles move constantly in an aqueous dispersion. Around 1900 there were large activities in the colloid area and even Einstein in the year of 1905 also published the classical theoretical analysis of brownian motion at equilibrium and those who made the first advances in biochemistry at this time often identified themselves as colloid scientists. However with the rapid advances in biochemistry/molecular biology the colloid aspect of the field was largely forgotten and colloid science was for a long period primarily a discipline for technical applications. In recent years we have seen a revival of the science aspects of the area driven by advances in the understanding of intermolecular interactions, cooperative phenomena and condensed phases. One can now describe and understand the properties of increasingly complex systems. It is clear that colloid science has reached such a level that it can contribute with much larger consequences to the understanding of a range of processes in biological systems, than was possible during the first half of the previous century.

In the description of specific projects you find later in this booklet there is a substantial number that address different biology inspired problems. A comparison with previous issues reveal that the fraction of biologically oriented projects is increasing and we foresee that this trend will be sustained for some time. Basic concepts of colloid science like the surface force issue has wide applications in biochemistry and molecular biology. In order to arrive at fruitful applications of these concepts from a colloid science point of view, one has to focus on problem areas combining generality and relevance. In our present view, these areas are found for systems where several types of macromolecules (proteins, polysaccharides or polyelectrolytes) and/or amphiphiles interact to form a functional or destructive unit. Systems that previously were considered too complex for a molecular characterization now successively become available to fundamental studies.

The specific projects in the area that are currently pursued at the department can be classified into four general themes: i) Colloidal stability and cooperative association. ii) Adsorption and adhesion at interfaces. iii) Molecular transport in complex systems. iv) Composite particles in vivo and in vitro. It is clear that amyloid fibril formation is an example of colloidal instability although the phenomenon is typically not discussed in such terms. The formation of lipid rafts and cavioli in biological membranes provides examples of cooperative association of lipids presumably assisted by the presence of cholesterol acting as a lineactant in the two-dimensional system of the membrane. Living systems are full of interfaces and they have adopted to regulate adsorption/desorption processes. When such systems are perturbed by implants, surgery or other physical damages there is a stress on the system that can lead to undesired responses triggered by adsorption processes. The living system is not in equilibrium and there occurs continuous molecular transport. In addition to all intracellular trafficking there are also important transport processes on a somewhat larger scale occurring over stacks of cells. This is central both in the lung and across the skin and it is also a central issue for uptake of drugs in the intestine. In the living cell many central functions are performed in organelles which from a colloid perspective can be identified as composite particles. There is a challenge not only to unravel the molecular interactions leading to the formation of these complex structures, but in a wider perspective it should be possible to utilize the basic principles for in vitro functions. A first simple goal for such

in vitro applications is to find methods for packing/unpacking of biologically active macromolecules like DNA.

It seems clear to us that modern colloid science has much to offer in the development of an understanding of biology from a fundamental perspective. The primary challenge is to strike a balance between the general and the specific. The most useful understanding is obtained if both these aspects are properly considered. The only practical long term way to achieve such a combination is to operate in a cooperative way where scientists with different knowledge combine their efforts.

Håkan Wennerström Björn Lindman

## 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) Polymer solutions and gels; (3) Polymer-surfactant systems; (4) Protein-amphiphile interactions; (5) Adsorption and surface forces; (6) New experimental methodologies and instrumentation development; 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. (Jan Cocquyt (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 several systems for the understanding of this phenomenon. (A. Khan, E. Marques (Porto), H. Edlund (Sundsvall), C. La Mesa (Rome)).

**Ternary phase behavior of cationic/nonionic mixed surfactants in water.** The complete phase diagram of didodecyldimethylammonium bromide (DDAB) mixed with the nonionic octa-ethyleneglycol mono n-dodecyl ether (C12E8) in water was made at 25 °C. It was observed that all the single phases of the binary surfactant/water systems are extended when the other surfactant is added and some of the phases are strongly temperature-dependent. The phases were identified by crossed polaroids, SAXS, 2H-NMR and optical microscopy. (E. Feitosa, A. Khan, B. Lindman).

**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). (U. Olsson, R. Angelico, L. Ambrosone and A. Ceglie (Campobasso, Italy), G. Palazzo (Bari, Italy), C. Schmidt and D. Burgemeister (Paderborn/Freiburg, Germany) and 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. (M. Gotter (Köln), U. Olsson, H. Wennerström; R. Strey (Köln)

**Divalent surfactants.** Used as stabilizers for asphalt emulsions and for disinfection, these surfactants provide a good test case for theories of micellar aggregation. Basic properties of divalent surfactants with monovalent counterions have been studied for some time. Electrostatic theories account well for bulk properties. Work is now centered on studies of the adsorption of divalent surfactants, with special emphasis on Gemini surfactants, from solution onto silica surfaces. Adsorption isotherms are determined by means of ellipsometry, and the properties (aggregation numbers, etc.) of the adsorbed micelles are probed with fluorescence quenching methods. Poisson-Boltzmann level theories are used to rationalise the experimental findings. (O. Söderman, P. Hansson).

**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)).

**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 transition to onions from planar bilayers involves an intermediate structure with cylindrical symmetry. (U. Olsson, Florian Nettekheim (Kiel) and Walter Richtering (Aachen), Peter Lindner (ILL Grenoble), K. Mortensen (Risø)).

**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. S. 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 in dilute aqueous solution.** The project involves the investigation of block copolymer vesicles 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 are formed by either extrusion from dilute solutions of dispersed lamellar phase of the block copolymer. 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 experimental techniques employed are cryo-TEM, dynamic and static light scattering and self-diffusion measurements by NMR. (K. Bryskhe, J. Jansson, D. Topgaard, K. Schillén, U. Olsson).

**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 and hydrophobically modified polymers.** 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. Different surfactants differ markedly in their ability to compete with the amylose-HMHEC complexation. Cyclodextrins also compete efficiently with the complexation. (M. Egermayer, M. Karlberg, 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 (Department of Surgery) 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).

**Capillary-induced forces between particles/surfaces 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 excluded. 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 (latex or silica) have an affinity to 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. The CIPS gives rise to a long-range attractive force, operating over distances far exceeding the dimensions of a polymer coil. The effects of the polymer length, the length asymmetry (for ternary polymer solutions), the solution composition, and the range and magnitude of the attractive force have been analysed. 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. (M. Olsson, L. Piculell, P. Linse, F. Joabsson (Camurus AB), H. Wennerström).

**Interactions between hydrophobically modified polymers and cyclodextrins.** Rheology in mixed systems of HM-PEG and cyclodextrins, CD, or HM-EHEC and CD is investigated. For HM-EHEC the viscosity as a function of CD-concentration first decreased strongly, and at excess CD the viscosity became virtually the same as in a solution of the unmodified parent polymer. The ability to form a complex depends both on the structure of the hydrophobic group and on the size of the cavity of the CD molecule. The complex constant,  $K$ , has been determined for several combinations of different CD:s and different hydrophobic groups. For HM-PEG the viscosity reduction was even more dramatic, and terminating a small fraction (10% or below) of the total amount of polymer hydrophobic tails reduced the viscosity to a level almost corresponding to that of the unmodified parent polymer. (L. Karlson, K. Thuresson, B. Lindman).

**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. Initial studies focus on the rate of ultimate release of polymer into the surrounding bath, particularly for polydisperse polymer samples. The release rate has been recorded systematically for 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. (A. Körner, L. Piculell, A. Larsson (Chalmers), B. Wittgren (AstraZeneca Mölndal)).

**Mixed block and graft copolymers.** Aqueous mixtures of two types of hydrophobically modified polymers, end modified and graft modified, are investigated with respect to their phase behaviour and viscosity. Mixtures of nonionic hydrophobically modified polysaccharides (HM-EHEC and HM-HEC) and end-modified PEO (HM-PEO) show clear evidence of mixed hydrophobic aggregation, although the effects of added HM-PEO on the modified polysaccharides are smaller than the effects of added ionic surfactants. HM-PEO with hydrophobes at both ends has stronger effects than HM-PEO modified at only one end. (M. Karlberg, K. Thuresson, B. Lindman, L. Piculell). Project completed.

**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  $^1\text{H}$  NMR and TEM. (K. Flodström, V. Alfredsson and H. Wennerström).

**Mesoporous alumina materials.** Mesostructured aluminum oxide material is synthesized using as template micellar solution of ionic surfactant. The inorganic precursors are water-soluble cation,  $\text{Al}^{3+}$  and oligocations  $[\text{Al}_{13}\text{O}_4(\text{OH})_{24}(\text{H}_2\text{O})_{12}]^{7+}$ . The aim is centered on a systematic investigation of synthesis conditions for optimizing the structure of as-synthesized mesoparticles in a wide range of concentration. Characterization is carried out by SAXS, TEM and optical microscopy (D. Angelescu, A. Khan, V. Alfredsson in collaboration with H. Caldararu, A. Carageorghieopol (Romania)). (project completed)

**Monoolein – HM-EHEC mixtures.** We are studying the interactions between the lipid monoolein 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).

**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  $\mu\text{m}$ ). 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. For example, the solution behavior of dye-labeled PAA and the effects induced by added cationic surfactants and block copolymers in water are studied. Time-resolved fluorescence spectroscopy is utilized to obtain more information on the dye excimer/dimer formation in these systems. (J. S. Seixas de Melo and T. Costa and M. da G. Miguel (University of Coimbra, Portugal), K. Schillén, B. Lindman).

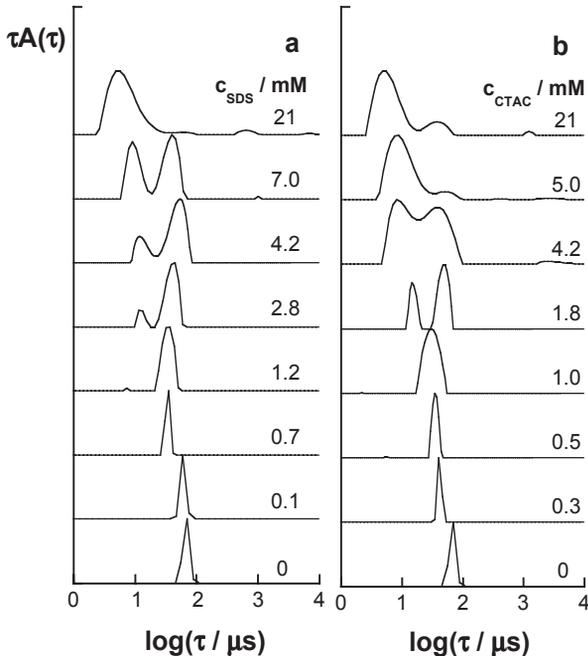
## Polymer-Surfactant Systems

**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 and addition of a second amphiphile. 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. For cationic mixtures, DNA compaction at vesicles was documented. The results are compared with those of Monte Carlo simulations. (R. Dias, A. Pais, M. Rosa, B. Lindman, M. Miguel).

**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<sub>6</sub>E) 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. (J. Jansson, D. Löf, K. Schillén, G. Ölofsson, O. Glatter (University of Graz, Austria), R. C. da Silva and A. Niemiec and W. Loh (UNICAMP, Brazil)).

**Association between hydrophobically modified polymers and surfactant self-assemblies.** The thickening effect of hydrophobically modified poly(ethylene

glycols) in a O/W microemulsion is investigated. The hydrophobically modified polymer is a triblock copolymer, alkyl end-capped poly(ethylene glycol) and the microemulsion is based on a nonionic surfactant, pentaethylene oxide dodecyl ether (C12E5) and decane. The rheological properties, such as viscosity and cross-link lifetime, vary strongly with microemulsion droplet volume fraction, with temperature and with end-caps of the polymer. The variations can be understood on the basis of interdroplet distances and interactions. Studies also include an analogous system where the surfactant self-assemblies are thermodynamically stable catanionic vesicles bearing a negative net-charge. 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 with different intensity. The vesicles are changed from spherical ones into faceted vesicles. This effect is attributed to a start 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

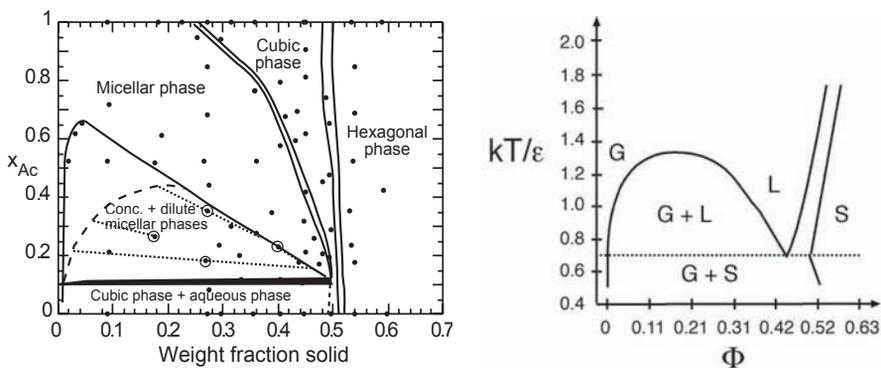


Selected relaxation time distributions obtained from DLS for a 1.0 wt % F127 solution with varying surfactant concentrations at 40 °C: (a) SDS and (b) CTAC.

considerable vesicle disruption may lead to planar bilayer, disc-like, aggregates.

Further studies include the association between hydrophobically modified carboxymethyl cellulose on one hand and either cationic vesicles or cationic polymers on the other. (F. Antunes, M. Miguel, Coimbra University, B. Lindman K. Thuresson).

**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. The experimental results (phase diagrams, SAXS data) are compared with computer simulations. 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. The  $C_{16}TAPA/C_{16}TAAc$ /water phase diagram illustrates the phase behavior of charged colloidal spheres (the micelles) with mixed monomeric/polymeric counterions. An increased fraction of polymeric counterions gives an increasing attraction, resulting in, first, a "gas-liquid" phase separation (coexistence of a dilute and a concentrated micellar phase) and, ultimately, a "gas-solid" phase separation (coexistence of essentially pure water and a cubic phase. Monte-Carlo simulations reproduce qualitatively the shift from repulsion to attraction, and show



Analogies between the  $C_{16}TAPA/C_{16}TAAc$ /water phase diagram (left) and the Temperature-Density diagram for Lennard-Jones particles (right, redrawn from Vliegenthart et. al. *Physica A* 1999, 263, 378)

that the attraction between micelles with polymeric counterions is due to polyion bridging. Small additions of a long-chain alcohol gives rise to a concentrated lamellar phase in mixtures of complex salt and water. (A. Svensson, J. Norrman, L. Piculell, W. Loh (Campinas), B. Jönsson (Theoretical Chemistry, Lund), B. Cabane (Paris)).

**Hydration of DNA and DNA complexes.** The thermodynamics of hydration of DNA and DNA–lipid complexes is studied using sorption calorimetry giving both free energy and enthalpy changes. The molecular properties of the complex is also investigated using proton NMR. (C. Leal, H. Wennerström, D. Topgaard, G. Olofsson).

**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).

**The effect of poly(N,N-dimethylacrylamide) on the lamellar phase of Aerosol OT-water.** The effect of a water soluble uncharged polymer (polyacrylamid) on the stability of the lamellar phase of the AOT (Aerosol OT, sodium di(ethylhexyl) sulfosuccinate)/water system is studied. 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. Polymers with small coil dimensions are expected to have access to the water domains within the lamellar phase. The same polymer is synthesized with different coil dimensions. The variation in the ternary system with AOT, water and polymer induced by the change of the polymer size is investigated.

*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. Renamayor, Madrid; B. Lindman, K. Thuresson).

**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. (A. Bilalov, C. Leal, A. Khan, 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).

**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.

Transfection studies *in vitro* and *in vivo* are to be performed during this project. (M. Rosa, M. R. Infantes (Barcelona), M. Miguel, R. Dias, B. Lindman).

**Gel electrophoresis studies of the DNA compaction and decompaction by the addition of oppositely charged surfactants.** The mobility of DNA molecules is followed in terms of conformation and charge neutralization. (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).

**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  $\beta$ -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, A. Khan; R. Bauer (Denmark); J. Skov-Pedersen (Denmark); M. Paulsson (Food Engineering); B. Bergenstahl and R. Waninge (Food Technology)).

**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, A. Khan, J. Barauskas, F. Tibergh, 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. (T. Nylander, F. Tiberg, H. Wennerström, and P. Vandoolaeghe)

**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  $\alpha$ -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, phase equilibrium in binary surfactant-polypeptide monolayers at the air-water interface are investigated. Properties of the binary monolayers are studied in 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  $\beta$ -casein.** The interfacial properties and the structure of the adsorbed layers of a natural block copolymer,  $\beta$ -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.  $\beta$ -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)).

**Depletion interactions in DNA solutions.** In this project we use colloidal probe atomic force microscopy (AFM) to study the interaction forces between a hard colloidal sphere and a flat surface when DNA is present in solution. It is generally known that polyelectrolytes can induce strong depletion forces, either predominately attractive interactions in dilute solutions or oscillatory interactions (both attractive and repulsive, depending on separation distance) in more concentrated solutions. These forces can control the stability and processing characteristics of colloidal suspensions, so they have implications on the formulation of gene delivery systems. Additionally, the shape of the interaction force versus distance curve can give insight into the structure of DNA in solution. In particular we will study the role of the type of DNA (single or double stranded), the length of DNA relative to the persistence length (or rigidity of the DNA), and the ionic strength. (A. Braem, B. Lindman).

**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).

**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 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).

**Interfacial structure of coadsorbed DNA/surfactant layers.** The interfacial behavior of DNA solutions and mixtures of DNA and surfactants can be an important factor in the design and function of gene delivery systems. This project focuses on imaging the lateral structure of adsorbed layers of DNA and mixtures of DNA and the cationic surfactant cetyltrimethylammoniumbromide (CTAB) using atomic force microscopy (AFM). Adsorption to model cationic, anionic, and hydrophobic systems is studied for various solution compositions. We give special attention to the differences in interfacial behavior between single and double stranded DNA, as well as differently sized DNA. By varying the length of DNA studied relative to the persistence length, we can study the importance of chain flexibility in determining the interactions between DNA and CTAB at an interface. (A. Braem, M. Cárdenas, B. Lindman)

**Interaction forces between DNA and DNA-cationic surfactant complexes.**

Complexes between DNA and cationic surfactants, the so-called lipoplexes, are thought to be useful as potential vectors for gene transfection. In vivo, the complexes will encounter different types of interfaces in the blood stream (walls of protein vessels, blood cells, proteins, etc.) before being thoroughly delivered. Interactions with such interfaces are likely to occur and therefore influence the uptake behavior of the lipoplexes. Hence, in this project we use the interferometric surface force apparatus (SFA) to study the interaction between DNA and DNA-cationic surfactant complexes films adsorbed on two model surfaces i.e. hydrophilic (mica) and hydrophobic (mica-octadecyltriethoxy silane) surfaces. (J. Campos Terán, M. Cárdenas, T. Nylander, 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 in situ follow the adsorption of the different components on two solid surfaces, i. e. silica (SiO<sub>2</sub>) and titanium oxide (TiO<sub>2</sub>). 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).

**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)

**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/m<sup>2</sup>). 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. The effect of the DNA conformation in

terms of molecular weight (above and below 400bp) and single/double stranded chains is studied due to the different surfactant-induced compaction behaviour in the bulk. In order to study the effect of the surfactant chain length and counterion on the adsorption behaviour, cationic surfactants such as cetyltrimethylammoniumbromide (CTAB), cetyltrimethylammoniumchloride (CTAC), cetyltrimethylammoniumfluoride (CTAF), and dodecyltrimethylammoniumbromide (DTAB) and a gemini surfactant ( $C_{12}-C_6-C_{12}(TAB)_2$ ) are studied. (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 with a decrease in the hydrodynamic radius as a result, as well as the disappearance the fast second relaxation mode related to intramolecular motions of the macromolecule. Such compaction is also observed on the DNA coated polystyrene particles in the presence of surfactant. The time-dependence is also being investigated. The effect of the particle charge is also investigated. SANS is used to get an insight in the structure of the complexes formed. (M. Cardenas, 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).

**(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, K. Flodström, J. Borné, K. Bryskhe, A. Khan, K. Schillén, A. Stenstam).

**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. Thureson, B. Jönsson (Biophysical Chemistry, Lund)).

## Theory and Modelling

**Diffusive transport in responsive media.** We are studying molecular transport over a lamellar phase in the presence of a water gradient. 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 transport through samples of different lipid liquid crystalline phases is also studied experimentally. (Fatima Costa, E. Sparr, H. Wennerström).

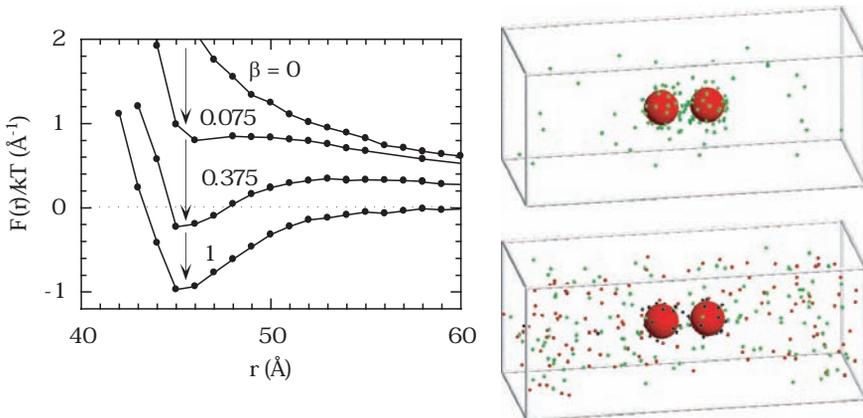
**Determination of surface potential of micelles.** The understanding and control of colloidal stability requires an understanding of the surface potential of colloidal particles. In this project we investigate the surface potential of ionic micelles by means of measuring the dissociation constant of 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)).

**Polyelectrolyte-macroion complex formation.** The complex formation between charged polyelectrolytes and oppositely charged micelles has been studied by Monte Carlo simulation. We have gained information on the structure and the complex strength at different conditions. The chain flexibility plays a decisive role in determining the structure of the polyelectrolyte-macroion complex and a rich spectrum of structures appear. The effect of addition of salt on the structure of the polyelectrolyte-micelle complex has also been examined. Finally, the phase behavior,

including the phase separation at equimolar amount of the charged macromolecules and a subsequent dedissolution, has been investigated at different conditions. (M. Škepö, A. Akinchina, and P. Linse).

**Solutions of charged colloids.** Model systems of charged spherical macroions and counterions interacting solely through hard-sphere and Coulomb interaction were investigated by means of Monte Carlo simulations. At high electrostatic coupling, an attractive force between pairs of like-charged macroions appears. That has been investigated in more detail using a cylindrical cell model and connection with fluid simulations have been made. The influence of added multivalent salt and the role of dielectric discontinuities are currently under investigation. A simple boot-strapped Poisson-Boltzman theory has been developed and compared with simulation data for monodisperse and bidisperse solution of colloids (P. Linse, D. Angelescu (Romanian Academy), J. Rescic (University of Ljubljana), D. Chan (University of Melbourne), and S. Petris (University of Melbourne)).

**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



Left: Mean force acting between two macroions vs their separation for macroions with 60 elementary charges with monovalent counterions at increasing amount of salt containing trivalent counterions. At stoichiometric amount of trivalent counterions ( $\beta = 1$ ), the force becomes purely attractive beyond 43  $\text{\AA}$ . Right: Illustration of the small ion distribution at  $\beta = 0$  (top) and 1 (bottom) (D. Angelescu and P. Linse).

theories, representing two limiting cases. The task at hand is to improve the description based on the gained insight. (M. Ullner).

**Polyelectrolytes in confined geometries.** The distribution of polymers and polyions with counterions between spherical cavities of different sizes joined with narrow cylinders are examined by Monte Carlo simulations. A simple model system with focus on chain connectivity and Coulomb interactions is used. For equal sized cavities, the entropic barrier of the narrow cylinder forces the uncharged polymer to be localized in one of the cavities, whereas the charged polymer occupies both cavities simultaneously. As the cavity sizes are made different, the distribution of the uncharged and charged polymers displays another qualitative difference. The polymer is completely distributed to the larger cavity, even for small size differences, whereas the polyion to both cavities, unless the size differences of the cavities are made large. (A. Sousa (University of Coimbra) A. A. C. C. Pais (University of Coimbra), and P. Linse).

**Structures of charged block copolymers.** A novel polymer system containing charged diblock polymers grafted onto a surface, simple salt, and solvent has been considered in the framework of a mean-field lattice theory. On the basis of predicted volume fraction profiles of polymer segments, free ends, block junctions, and small ions, a detailed picture of the system has emerged. It was found that the structure of the polymer brush is decisively dependent of the relative charge of the blocks. For certain conditions, bimodal profiles appeared which demonstrated the simultaneous presence of two types of chain conformations, one coiled and one stretched. Currently, Monte Carlo simulations are performed to deepen the description of these systems. (N. Shusharina (University of North Carolina at Chapel Hill), A. Akinchina, 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. Currently, theories describing the complexation in polyelectrolyte solutions are being developed. (Y. Hayashi, M. Ullner, and P. Linse).

**Polyelectrolyte-protein complexation and protein adsorption.** A simple model of lysozyme has been established. Aqueous solutions of proteins and oppositely charged polyelectrolytes were studied by Monte Carlo simulations at different polyelectrolyte chain length, ionic strength, and protein-protein interaction potential as a function of the polyelectrolyte concentration. One of the protein models used represented lysozyme in aqueous environment. At strong electrostatic protein-polyelectrolyte interaction, large clusters were formed near or at equivalent amount of net protein charge and polyelectrolyte charge, whereas in excess of polyelectrolyte a redissolution appeared. The adsorption of lysozyme to a charged surface was studied also by Monte Carlo simulations at different protein concentration, protein net charge, ionic strength, and surface charge density. The protein adsorption was found to be favored by high protein concentration, high protein net charge, low ionic strength, and high surface charge density. The protein displayed a strong preferential orientation near the charged

surface. (F. Carlsson (YKI), E. Hyltner (YKI), T. Arnebrant (Malmö University), M. Malmsten (Uppsala University), 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. Pressure-density relations for polyelectrolyte gel at different crosslinking density, chain linear charged density, chain flexibility, and valence of the counterions have been determined. The polyelectrolyte gel displayed a very large swelling capacity, in agreement with experiments. Moreover, discontinuous transitions were found at attractive bead-bead interactions and/or low dielectric constant. In addition, the reduced swelling upon addition of salt and the Donnan equilibrium are currently under investigation, and a comparison with current theories on gel swelling is in progress. (S. Schneider, S. Edgecombe, and P. Linse).

**Protein-polymer interaction.** The effect of the spatial distribution of hydrophobic surface residues on the adsorption of a weakly hydrophobic polymer to proteins has been examined using a coarse-grain model solved by Monte Carlo simulations. In particular, as the strength of the hydrophobic interaction was increased, the onset of the polymer adsorption to the protein appeared first for proteins with a more heterogeneous site distribution. The degree of heterogeneity of the site distributions was quantified using the variance of the number of sites located within randomly positioned circles placed on the protein surface. Currently, the effect of finite polymer concentration and complex free energies are under investigation. (M. Jönsson, M. Skepö, P. Linse, and F. Tjernelid (Biochemistry)).

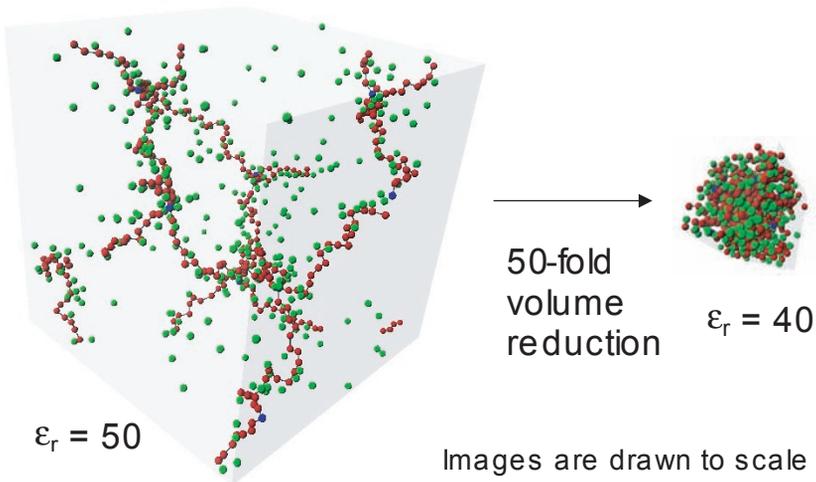
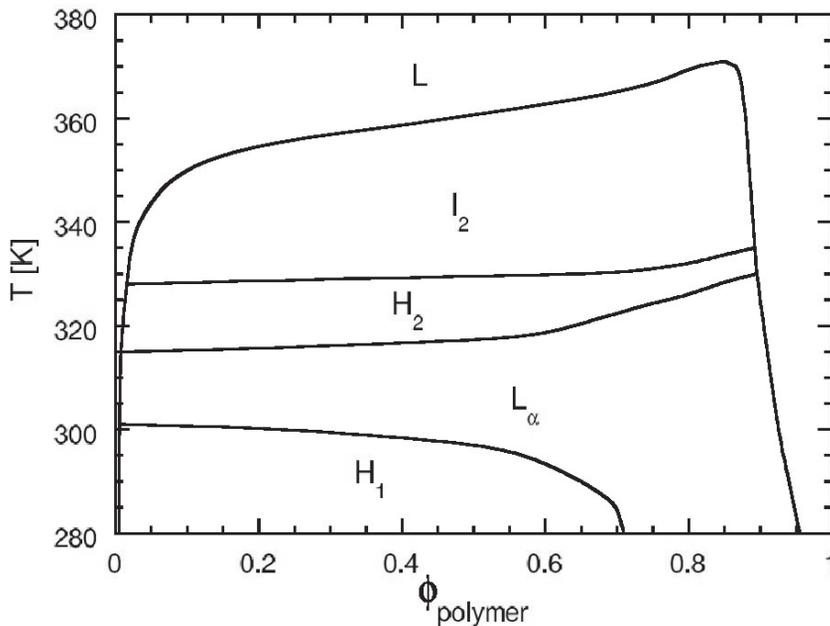


Illustration of a discontinuous collapse appearing for a charged cross-linked gel appearing at reduced permittivity of the solution (S. Schneider and P. Linse).

**Phase behavior and structure of an ABC triblock copolymer dissolved in selective solvent.** A mean-field lattice theory has been applied to predict the self-assembly into ordered structures of an ABC triblock copolymer in selective solvent. The composition-temperature phase diagram of the C(14)PO(12)EO(17)/water system has been determined. The model predicts thermotropic phase transitions between the ordered hexagonal, lamellar, reverse hexagonal, and reverse cubic phases, as well as the disordered phase. The lyotropic effect on the formation of different structures was found to be weak (N. Shusharina (University of Buffalo), P. Alexandridis (University of Buffalo), S. Balijepalli (The Dow Chemical Co.), H. J. M. Gruenbauer (The Dow Chemical Co.), and P. Linse).

**Polarization in electric fields.** Polarization deficiency and excess ion hydration free energy at an electric field of hydrated calcium, sodium, and chloride ions have been determined by Monte Carlo simulations of a spherical cell containing either one ion and molecular water or only molecular water, subjected to an external electrical field. The permittivity of pure water decreases as the electric field is increased in quantitative agreement with previous simulation studies and the Booth theory. The excess hydration free energy depends initially quadratically on the electric field, whereas it becomes linear in the field at higher field due to dielectric saturation. The excess ion hydration free energies are in quantitative agreement with measured dependencies of the permittivity of electrolyte solution upon the ion concentration. (S. Gavryushov and P. Linse).



Composition-temperature phase diagram of the binary  $C_{14}(PO)_{12}(EO)_{17}$ /water system as predicted from lattice mean-field theory. Notation:  $H_1$ : hexagonal,  $L$ : lamellar,  $H_2$ : reverse hexagonal,  $I_2$ : reverse cubic, and  $L$ : disordered phase (N. Shusharina et al.).

**Statistical-mechanical programs.** During 2004, a web-based interface for running five different statistical mechanical computer programs (MOLSIM, OZ, PB, PGESE, and POLYMER) was launched and thereafter used in an advanced course in physical chemistry (undergraduate course) and a national course on "Polymers in solution" (graduate course). In addition, 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  $12^\circ$  to  $155^\circ$ , 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  $>10^5$  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  $-12^\circ\text{C}$  to  $+140^\circ\text{C}$ . 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  $1/\text{\AA}$ ) 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  $\psi$  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 these were installed during 2003. The new microscopes have 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 (Thermometric AB, Järfälla, Sweden).

**Rheometers.** (contact person: Krister Thuresson). A Carri-med controlled stress rheometer CSL 100 temperature controlled by 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. Since the beginning, the participating companies have been Akzo Nobel Surface Chemistry, AstraZeneca R&D Mölndal, EKA Chemicals, Lyckeby Stärkelsen, SCA Research, and Tetra Pak. The Board of CAP has an industrial majority.

CAP activities concern fundamental behaviour and applications of amphiphilic polymers, and the use of biopolymers for their preparation. The CAP research activities are 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 2003, four PhDs completed their theses financed by CAP, including Monica Egermayer and Stefanie Schneider from our department. Monica has stayed with CAP, but now at Food Technology, where she works on a post-doc project on uses of starch in oral drug delivery.

In January 2004, CAP entered stage 4 of its existence. Prior to that, CAP and its sister Competence Centres were thoroughly evaluated during 2003. We are proud to say that the international evaluators were extremely satisfied, both with the research within CAP, and with the CAP way of working together. With the transition to stage 4 there have also been some changes in the management of the centre. Thus Lennart Piculell is the new director of CAP since November 2003, following the retirement of Bengt Wesslén, and Per Linse is a new board member from 2004, replacing Lennart Piculell.

### 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 2003 the following courses were given:

- Surface Chemistry – surfactants and polymers in aqueous solutions (5 p), Degeberga with 32 participants.
- NMR – basic physics and applications (4p), Marstrand with 23 participants.
- Lipids – from solid state behaviour to membrane protein crystallization (3p), Hindås with 26 participants.
- Polymers in Solution (3p), Örenäs with 32 participants
- The Colloidal Domain (10p), Lund, Göteborg and Stockholm with 26 participants (continues during 2004).

Members of the board of the Research Programme and Research School are: Jan Svärd (Chairman; Eka Chemicals), Krister Holmberg (Chalmers University of Technology, Director of studies of the Graduate School), Björn Lindman (Lund University), and Martin Malmsten up to 15 September and after that date 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 will be achieved through courses, symposia and conferences arranged by the students themselves. The International Symposium on Surface and Colloid Chemistry for the Life Sciences was organized 6–7 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 was held 6–7 November starting with a joint session with the preceding SNSS-9, Swedish Neutron Scattering Society Meeting. This year the symposium was organized in cooperation with the Division of Surface Chemistry of the Swedish Chemical Society, The Swedish Academy of Pharmaceutical Sciences and the SSF funded COLINTECH programme, see below.

## **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 Ölofsson, chairman). It will organize in cooperation with YKOLL the annual Symposium in Surface and Colloid Science. The third 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, , Ö. 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/>). 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 take 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. (M. Paulsson, O. Santos and C. Trägårdh (Food Engineering) and T. Nylander).

## **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.lu.se](http://www.BIOSCOPE.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, 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 2002 took place in Lund. All the groups presented their results on the systems that were identified during the meeting in 2001 at Coimbra.

### **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 ongoing project “A 48-channel microcalorimeter for analysis of living cells” (in cooperation with Dr D. Hallén, Biovitrum, Stockholm) may also be 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**

#### 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 invited lectures at the Spanish Royal Society of Chemistry and Physics meeting in Madrid, and at a conference on Polymer-surfactant Interactions in Wrexham and also gave talks at YKI Member Days in Stockholm and at a COST Polymer-surfactant workshop in Rome. Furthermore he participated in a symposium on Science and Education in Coimbra, Portugal, in the European Colloid and Interface Society meeting in Florence, Italy, Simposio Iberico de Fotoquímica, Santiago de Compostela, and in the Marcus Wallenberg Prize Symposium in Stockholm. During the year Björn Lindman visited a number of universities and other research centers and in most cases he presented a lecture. The institutions visited included: University of Graz, Austria; Akzo Nobel, Stenungsund; Eka Chemicals, Karlstad University, Mid-Sweden University, Åbo Akademi University, Institute for Surface Chemistry, Royal Institute of Technology, Stockholm, Uppsala University, Procter&Gamble Research Centers in Cincinnati and Newcastle, University of Wales, Swansea, University Santiago de Compostela, and University College, Dublin. Björn Lindman was visiting professor at Department of Chemistry, Coimbra University, Portugal and was also invited by Nanjing University of Science and Technology for a stay and thereby also visited Soochow University and Zhejiang University of Science and Technology in Hangzhou.

Håkan Wennerström delivered invited talks at; the workshop "Attractive Interactions in Colloidal Systems" Bad Gastein, Austria; at the workshop "Charges in solution" Möckelnäs, Sweden; and at "Jülich Soft Matter Days" Kerkrade, The Netherlands. Håkan Wennerström visited Puchino, Russia for meeting within an INTAS project

Olle Söderman took part in a workshop on Attractive Interaction in Colloidal Systems in Bad Gastein, Austria. He was one of the organizers of the EUCHEM conference "Structure and Molecular Mobility in Heterogeneous Systems", August 27-29, in Fiskebäckskil. He also visited the University of Bayreuth, where he gave a seminar. Olle gave a invited lecture at XVII Conference of the European Colloid and Interface Society, Florence, September 21-26.

Per Linse delivered invited talks; at the workshop on "Attractive Interaction in Colloidal Systems", Graz, Austria at 9th Dresden Polymer Discussion on the topic of "Polyelectrolytes", Meissen, Germany; and at the ESP and EMLG conference "Molecular liquids: routes from local order to large-scale co-operativity", Il Cioccio, Italy. Per Linse also gave oral presentations at the annual meeting of the American Institute of Chemical Engineers, San Francisco, USA and invited seminars at Dow Chemicals, Midland, USA and at the Department of Chemical Engineering, University of Berkeley, USA

Ulf Olsson took part in a workshop on Attractive Interaction in Colloidal Systems in Bad Gastein, Austria He gave invited lectures at AstraZeneca, Charnwood, England, on a work shop on high dose inhalation drug delivery and at the 2<sup>nd</sup> PSI Summer School on "Structure and Dynamics of Soft Condensed Matter", Zuoz, Switzerland. He also visited the Physics Department of University of Fribourg, Switzerland where he gave a lecture.

Lennart Piculell gave an invited lecture at Polymer-Surfactant Interactions, Wrexham, UK.

Tommy Nylander attended a planning meeting in Paris, France to setup a EU-

network of Excellense (SENSE). He also attended a NORFA conference on “Milk Proteins – Quality and Health Aspects” in Wadahl, Norway where he gave an oral presentation on the structure of adsorbed milk proteins. Tommy Nylander also attended the yearly project meeting of the EU-RTD project MODSTEEL, where he gave an introductory lecture on Surface and Colloid Chemistry and project meeting with Friesland Coberco in Deventer, The Netherlands. He also attended the Biocomplexity conference at University of Southampton, UK, ECIS 2003 in Florence, Italy, and the Bioscience Program meeting at Chalmers University of Technology, Gothenburg, Sweden. Tommy Nylander gave an invited lecture at Utrecht University, The Netherlands on Lipase and lipid structure. He also organized the NorFa network (Quality and Health Aspects of Milk Components) meeting in Lund 13-14 of September. As a coordinator EU-STREP FP6 project BIOSCOPE he went for negotiations in Brussels, Belgium. He also did Neutron reflectivity measurements at ISIS, Didcot, UK.

Karin Schillén gave a talk at the department of Chemistry, Karlstad University, and presented a poster at International Summer School and Workshop “Hairy Interfaces and Stringy Molecules”, Odense, Denmark.

Ingemar Wadsö gave an invited lecture at 39th Japanese Conference on Calorimetry and Thermal Analysis, Hiroshima, Japan an also gave talks at 15. Ulm-Freiberger Kalorimetritage, Freiberg, Germany; at Medicta 2003, Porto, Portugal; at CCTA 9, Zakopane, Poland; and at XIIIth International Society for Biological Calorimetry, Würzburg, Germany

Gerd Olofsson visited the Instituto de Chimica, University of Campinas, Campinas, Brazil, where she gave a couple of seminars.

Magnus Ullner gave invited lectures at Forschungszentrum, Jülich, Germany and at the 2<sup>nd</sup> PSI Summer School on “Structure and Dynamics of Soft Condensed Matter”, Zuoz, Switzerland, and presented a poster at “New Approaches and Perspectives in Polymer Physics”, Bad Honnef, Germany. He also held a JSPS fellowship in Japan for two months, mainly staying at the Department of Physics, Kyoto University, but also visiting the Department of Physics, Tohoku University, Sendai, and the Department of Polymer Chemistry, Kyoto University, presenting 1-2 seminars at each location.

Fredrik Tiberg gave invited lectures at EuroConference on Complex Fluid Interfaces, San Felieu de Guixols, Spain; at Drug Delivery Partnerships, Cologne, Germany; and at Drug Delivery: Latest Technology and Strategic Partnerships, Munich, Germany.

Fredrik Tiberg, Cecilia Leal, Katarina Flodström, Martin Olsson, Marité Cárdenas, Anna Akinchina, Johanna Borné and Rita Dias gave oral presentations and Karin Schillén, Justas Baruskas, Magali Deleu, Iseult Lynch, Anna Stenstam, Vitaly Kocherbitov, Anna Svensson, Monica Rosa, Carin Malmborg and Viveka Alfredsson presented posters at 17th Conference of the European Colloid & Interface Science Society, Florence, Italy.

Viveka Alfredsson presented a poster at the Biocomplexity conference at University of Southampton, UK.

Jörgen Jansson gave a seminar at the Institute of Physical Chemistry, University of Graz, Graz, Austria

Stefanie Schneider delivered an oral presentation at the annual meeting of the Center for Amphiphilic Polymers (CAP), Hemmeslöv, Sweden and gave invited

seminars at BASE, Ludwigshafen, Germany and at the institute of solid state research, Research Center Jülich, Germany

Anna Akinchina gave oral presentations at the workshop “Charges in Solution”, Möckelnäs, Sweden and presented posters at 298 WE-Heraeus-Seminar “New Approaches and Perspectives in Polymer Physics”, Bad Honnef, Germany, and at the summer school “Hairy Interfaces and Stringy Molecules”, Odense, Denmark.

Samuel Edgecomb gave an invited seminar at Uppsala University, Sweden.

The department organized the yearly meeting of the Surface and Colloid section of the Swedish Chemical Society, entitled “International Symposium on Surface and Colloid Chemistry for the Life Sciences”. The meeting attracted 150 participants from many different countries and was organized jointly with the 9th Swedish Neutron Scattering Society Meeting (SNSS-9) 5-7 of November. 7 internationally well-renowned lecturers gave invited lectures and a majority of the department members presented posters at the meeting. The meeting 2004 will also be held in Lund 18-19 of November and dedicated to “Surface and Colloid Chemistry Applied to Nanoscience” (<http://www.ykoll.fkem1.lu.se/>).

## EXTERNAL PROFESSIONAL ACTIVITIES

Björn Lindman is 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. Björn Lindman was an evaluator of the Fibre Science and Communication Network at Mid-Sweden University in Sundsvall and a member of the chemistry panel of the Academy of Finalnd. He was an external examiner for Jan Gustafsson's Ph D thesis at Åbo Akademi, Finland of Gerd Persson's Ph D thesis at Mid-Sweden University in Sundsvall and of Jennifer McManus' Ph D thesis, National University of Ireland; he was in the evaluation committee for a chair in Chemistry at Aalborg University, Denmark

Håkan Wennerström was a member of the Nobel committee for chemistry; Chairman for the board of graduate studies of the Faculty of Science, Lund University and Chairman of the committee for physical and theoretical chemistry of the national research council

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

Lennart Piculell was member of the board and deputy director of the Center for Amphiphilic Polymers, CAP (jan-oct), since November 2003 he is Director of CAP. Lennart served on PhD thesis committees for Lina Karlsson, Stefanie Schneider and Anna Stenstam. Lennart also served as a member of the editorial boards of the Food Hydrocolloids and Carbohydrate Polymers. Lennart was a member of the granting committee for Physical and Theoretical Chemistry, Swedish Research Council, and member of the international advisory committee for the IUPAC Macro 2004 conference, Paris France

Olle Söderman is the chairman of the Graduate Studies board at the Natural Science Faculty. He also serves on the Lund University advisory board for Graduate Studies. He was also active in a mentor program initiated by the Natural Science faculty aimed at supporting female researchers in the beginning of their academic career. Finally, he was a member of the Election Committee that elects members of the Lund University board.

Per Linse was an external examiner for Johan Mathias Lundgren's PhD Thesis, School of Chemistry, University of Bristol, UK. Per was a member of the program committee of the Center for Amphiphilic Polymers, CAP.

Tommy Nylander was mentor for the Food Industry program Meny. He was also a member of the Scientific Committee of ECIS2003 in Florence. He also acted as an evaluator of research proposals to the Italian Ministry for Education University and Research (MIUR), Food Characterization/Process/Product Research Program of US department of Agriculture National Research Initiative, Australian Research Council and Chalmers University of Technology's Bioscience Program. Tommy Nylander served in the thesis committee of Linda Karlsson, Linköping University as well as Maria von Bahr and Cecilia Hahn-Berg at Lund University.

Ulf Olsson was external examiner for Mari Kadi's Ph.D. thesis at Uppsala University

Ingemar Wadsö was a member of the Advisory Committees at the meetings of International Society for Biological Calorimetry in Würzburg 2003 and the IUPAC Conference of Chemical Thermodynamics in Beijing 2004.

Karin Schillén served as chairman on PhD Thesis committees for Monica Egermayer, Physical Chemistry 1, Lund University. She was also an external examiner for Gunilla Carlsson's licentiate thesis at Karlstad University.

Krister Thuresson was an external examiner for Anna Imberg's Ph. D. thesis at the Faculty of Pharmacy, Uppsala University and of Cecilia Groth's licentiate thesis at Chalmers University of Technology.

## **COURSES AND TEACHING**

The department is strongly involved in the undergraduate education of physical chemistry and colloid and surface science. Viveca Alfredsson and Karin Schillén gave lectures and exercises during the first semester courses where also Magnus Ullner was involved in the exercises. During the second semester there is 10 credit course dedicated to classical physical chemistry where Olle Söderman is the course responsible and also gave a major part of the lectures and exercises. This course is based on the well known text book of Atkins. A basic course on colloids, based on the book "Introduction to Soft Matter" was taught by Ulf Olsson and Magnus Ullner, with some additional lectures by Håkan Wennerström on colloidal biology. During this course, the students also receive 4h lectures on drug formulations, as an example of applied colloid science, kindly given by Jan-Erik Löfroth of AstraZeneca, Mölndal.. The advanced colloid course was given by Håkan Wennerström and Lennart Piculell. This course is based on the text book "The Colloidal Domain" by Fennell Evans and Håkan Wennerström. A second advanced physical chemistry course, devoted to methods to study colloidal systems was given by Olle Söderman, Per Linse and Ulf Olsson. The methods discussed during this course are NMR, scattering and statistical mechanical simulations. Håkan Wennerström on behalf of the department, delivered a total of 15 hrs lectures on environmental chemistry. Finally, a number of our graduate students serve as teaching

assistants on all courses given by the department.

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 2003, the course was held, for the 12<sup>th</sup> 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 2003, the department had a turnover of ca 36.5 million SEK. From the University we obtained 15.6 million of which 1.3 million is to cover undergraduate teaching; 3.6 million, for graduate students; and 10.7 million to cover 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 5.4 million SEK, The Swedish Agency for Innovation Systems (VINNOVA) which finances more applied projects, supports us with 4.9 million, mainly via the 2 Competence Center CAP and SNAP, during the fiscal year. We also received 1.9 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. 2.1 million. Finally, we received 1.3 million SEK from The European Commission.

## ALI KHAN RETIRED

Ali Khan retired in September 2003. Ali did his undergraduate studies in former east-Pakistan (now Bangladesh) and received a PhD from the University of Manchester, UK, in 1967. After his doctoral studies, he worked for several years in Africa. Ali came to the Physical Chemistry II department at the Technical Faculty, Lund University in 1978. After a few years, he moved to Physical Chemistry 1, where he has been active ever since. Ali has contributed scientifically mainly within the field of surfactant phase science. Among his achievements are important work in 'catanionic surfactants' (Ali coined this now generally accepted term for these surfactants) as well as work centered on surfactants with divalent counter ions. He has also been instrumental in editing the department's Annual Report, and has played an important social role in making the stays of our many guests easier, both by helping with practical matters and by opening his house to them (Ali is an excellent chef!). After his retirement, Ali still maintains ties with the department by taking part in a number of ongoing research projects. During the COST meeting on Polymer-Surfactant systems arranged at the University of Calabria in January 2004, one session was dedicated to Ali Khan's work.

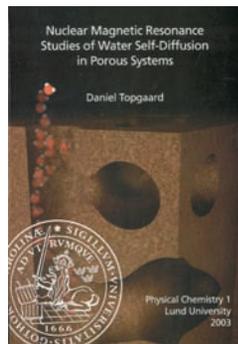
## DOCTORAL THESIS

February 28, 2003

**Daniel Topgaard**

Nuclear Magnetic Resonance Studies of  
*Water Self-Diffusion in Porous Systems*

Opponent: Prof. Dr. Rainer Kimmich,  
Sektion Kernresonanzspektroskopie,  
Ulm University, Germany

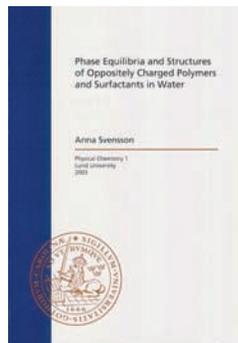


April 25, 2003

**Anna Svensson**

*Phase Equilibria and Structures of Oppositely Charged Polymers and Surfactants in Water*

Opponent: Prof. Per Stenius,  
Laboratory of Forest Products Chemistry,  
Helsinki University of Technology, Finland



May 17, 2003

**Monica Egermayer**

*Complexation between hydrophobically modified polymers and amylose.*

*Gelation and competition by surfactants*

Opponent: Dr. Taco Nicolai,  
Université du Maine, France

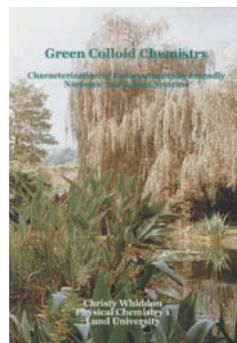


May 23, 2003

**Christy Whiddon**

*Green Colloid Chemistry:  
Characterization of Environmentally  
Friendly Nonionic Surfactant Systems*

Opponent: Prof. Larry Romsted  
Rutgers, The State University of New Jersey,  
USA

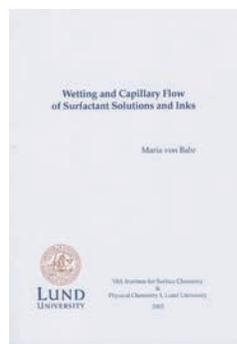


June 4, 2003

**Maria von Bahr**

*Wetting and Capillary Flow of Surfactant  
Solutions and Inks*

Opponent: Dr Colin Bain,  
University of Oxford, UK

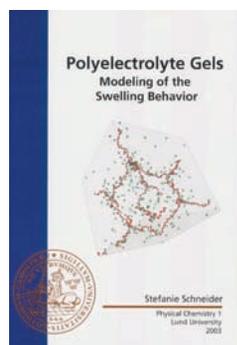


September 19, 2003

**Stefanie Schneider**

*Polymer Gels: Modeling the Swelling Behavior*

Opponent: Prof. Dr. Kurt Kremer,  
Max-Planck Institute for  
Polymer Research, Mainz, Germany

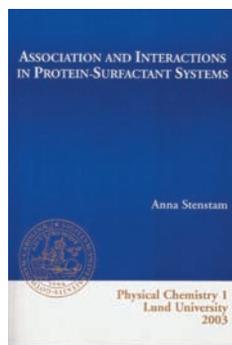


October 24, 2003

**Anna Stenstam**

*Association and Interactions in  
Protein-Surfactant Systems*

Opponent: Prof. Göran Lindblom,  
Department of Chemistry,  
Biophysical Chemistry, Umeå University

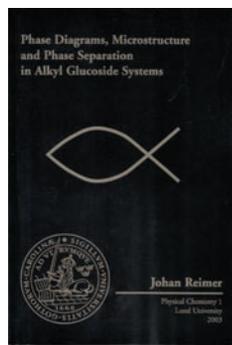


November 28, 2003

**Johan Reimer**

*Phase Diagrams, Microstructure and  
Phase Separation in Alkyl Glucoside Systems*

Opponent: Prof. Bengt Kronberg, Institute for  
Surface Chemistry, Stockholm



## MEMBERS OF THE DEPARTMENT Scientists/Teachers

Viveka Alfredsson, assistant professor  
Justas Barauskas, postdoc  
Azat Bilalov, postdoc  
Alan Braem, postdoc  
José Campos, postdoc  
Magali Deleu, postdoc  
Sergei Gavryushov, postdoc  
Eva Hansson, associate professor, dean  
Markus Johnsson, postdoc  
Alexey Kabalnov, visiting professor  
Lina Karlsson, postdoc  
Ali Khan, associate professor  
Björn Lindman, professor  
Per Linse, professor  
Iseult Lynch, postdoc  
Vitaly Kocherbitov, postdoc

Maria da Graça Miguel, visiting professor (Coimbra University)  
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  
Olle Söderman, professor  
Krister Thuresson, assistant professor  
Fredrik Tiberg, adjunct 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  
Maria von Bahr (*jointly with Institute for Surface Chemistry, Stockholm*)  
Joakim Balogh  
Jan-Willem Benjamins  
Karin Bryskhe  
Sanja Bulut  
Marité Cárdenas  
Rita Dias  
Samuel Edgecomb  
Monica Egermayer  
Caroline Ericsson  
Katarina Flodström  
Yoshikatsu Hayashi  
Jörgen Jansson  
Malin Jönsson  
Maria Karlberg  
Anna Körner  
Géraldine Lafitte  
Cecilia Leal  
Peter Linton  
David Löf  
Carin Malmborg  
Marcus Nilsson  
Jens Norrman  
Martin Olsson  
Yulia Samoshina  
Stefanie Schneider  
Helen Sjögren  
Anna Stenstam  
Johanna Stiernstedt (*jointly with Institute for Surface Chemistry, Stockholm*)  
Anna Svensson  
Daniel Topgaard

Pauline Vandoolaeghe  
Christy Whiddon

## Technical-Administrative Personnel

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

## GUESTS

Antunes, Filipe, University of Coimbra, Portugal, (S)  
Ardeleanu, Magdalena, Imperial College of Science, UK, (L)  
Attard, George S., University of Southampton, UK, (S)  
Bain, Colin, University of Oxford, UK, (S)  
Bergenholtz, Johan, Göteborg Univ, Sweden, (S)  
Bilalov, Azat, Kazan State Technological University, Russia, (L)  
Braem, Alan, Carnegie Mellon Univ, USA, (L)  
Cabane, Bernard, ESPCI, Paris, France, (S)  
Cocquyt, Jan, University of Gent, Belgium, (L)  
Colsenet, Roxane, Université H. Poincaré Nancy 1, France, (L)  
Cornen, Sophie, Ecole Nationale Supérieure de Chimi de Paris, 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, , Belgium, (L)  
Edlund, Håkan, Mid Sweden University, Sweden, (S)  
El-Nokaly, Maga, Procter & Gamble, Cincinnati, USA, (S)  
Endou, Rihei, Tohoku University, Japan, (L)  
Feitosa, Eloi, IBILCE/UNESP, S.J, Brazil, (L)  
Franzén, Stefan, University of California, USA, (S)  
Gogłowski, Mark, Procter & Gamble, Cincinnati, USA, (S)  
Gotter, Martin, University of Cologne, Germany, (L)  
Hansson, Per, Uppsala University, Sweden, (S)  
Holmberg, Krister, Chalmers University of Technology, Sweden, (S)  
Kaper, Helena, , Germany, (L)  
Kayalaj, Ibrahim, , Palestine, (L)  
Kimmich, Rainer, University of Ulm, Germany, (S)  
Kremer, Kurt, Max-Planck-Institute for polymer research, Germany, (S)  
Kronberg, Bengt, YKI, Stockholm, Sweden, (S)  
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Loh, Watson, Universidade Estadual de Campinas, Brazil, (L)  
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Malmsten, Martin, Uppsala University, Sweden, (S)  
Marques, Eduardo, University of Porto, Portugal, (L)  
McNamee, Cathy, , Nederländerna, (S)  
Miguel, Maria, University of Coimbra, Portugal, (L)  
Misiunas, Audrius, Institute of Biochemistry, Vilnius, Lithuania, (L)  
Montalvo, Gemma, Universidad de Alcalá, Spain, (L)

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Morales, Daniel, , Spanien, (L)  
Mortensen, Kjell, Danish Polymer Centre RISØ, Denmark, (S)  
Nicolai, Taco, Université du Maine, France, (S)  
Ninham, Barry, Australian National University, Canberra, Australia, (S)  
Nordén, Bengt, Chalmers University of Technology, Sweden, (S)  
Norizoe, Yuuki, Tohoku University, Japan, (S)  
Pacios, Isabel, The Universidad Nacional de Educación a Distancia, Spain, (L)  
Pais, Alberto Canelas, University of Coimbra, Portugal, (L)  
Pebalk, Dmitri, Moscow State University, Russia, (L)  
Qamhieh, Kwawla, Al-Quds University, Jerusalem, Israel, (L)  
Regev, Oren, Ben - Gurion University of the Negev, Israel, (S)  
Richtering, Walter, University of Kiel, Germany, (S)  
Romsted, Larry, Rutgers, The State University of New Jersey, USA, (S)  
Rosa, Monica, , Portugal, (L)  
Sakamoto, Yasuhiro, , Japan, (L)  
Scheibel, Jeffrey, Procter & Gamble, Cincinnati, USA, (S)  
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Stenius, Per, Technical University, Helsinki, Finland, (S)  
Svärd, Jan, EKA Chemicals, Bohus, Sweden, (S)  
Takemasa, Makato, , Japan, (L)  
Terada, Eiji, , Japan, (L)  
Tilton, Robert D., Carnegie Mellon University, USA, (S)  
Vandoolaeghe, Pauline, , France, (L)  
Vincent, Brian, Univ Bristol, UK, (S)  
Zauscher, Stefan, Duke University, USA, (S)  
Zhu, Yong, Procter & Gamble, Cincinnati, USA, (S)  
Åkerman, Björn, Chalmers University of Technology, Sweden, (S)

(L)= Long-term

(S)= Short-term

**PUBLICATIONS**

1. Akinchina, A.; Linse, P.  
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2. Amenitsch, H.; Edlund, H.; Khan, A.; Marques, E. F.; La Mesa, C.  
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3. Andersson, M.; Alfredsson, V.; Kjellin, P.; Palmqvist, A. E. C.  
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4. Angelescu, D. G.; Linse, P.  
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Langmuir 2003, 19, 9661-9668.
5. Angelico, R.; Burgemeister, D.; Ceglie, A.; Olsson, U.; Palazzo, G.; Schmidt, C.  
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6. Antunes, F. E.; Thuresson, K.; Lindman, B.; Miguel, M. G.  
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7. Balinov, B.; Mariette, F.; Söderman, O. "NMR studies of emulsions with particular emphasis on food emulsions." In *Food Emulsions*, edited by S. Friberg. New York: Marcel Dekker, Inc., 2003.  
Barauskas, J.; Landh, T.  
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8. Barauskas, J.; Razumas, V.; Talaikyte, Z.; Bulovas, A.; Nylander, T.; Tauraitė, D.; Butkus, E.  
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9. Barreleiro, P. C. A.; Lindman, B.  
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10. Bastos, M.; Bai, G.; Qvarnström, E.; Wadsö, I.  
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11. Borné, J.; Nylander, T.; Khan, A.  
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12. Cardenas, M.; Braem, A.; Nylander, T.; Lindman, B.  
DNA compaction at hydrophobic surfaces induced by a cationic amphiphile.  
*Langmuir* 2003, 19, 7712-7718.
13. Carlsson, F.; Malmsten, M.; Linse, P.  
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*J. Am. Chem. Soc.* 2003, 125, 3140-3149.
14. de Melo, J. S.; Costa, T.; Miguel, M. D.; Lindman, B.; Schillen, K.  
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*J. Phys. Chem. B* 2003, 107, 12605-12621.
15. Dias, R. S.; Pais, A.; Miguel, M. G.; Lindman, B.  
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*J. Chem. Phys.* 2003, 119, 8150-8157.
16. Egermayer, M.; Norrman, J.; Piculell, L.  
Gels of hydrophobically modified hydroxyethyl cellulose cross-linked by amylose: Competition by added surfactants.  
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17. Egermayer, M.; Piculell, L.  
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*J. Phys. Chem. B* 2003, 107, 14147-14150.
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