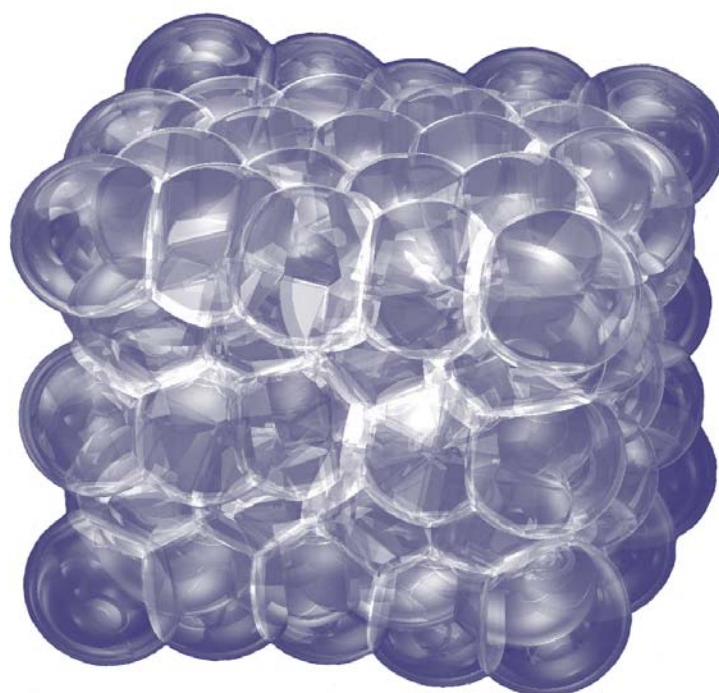


# Annual Report 2002

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Physical Chemistry 1  
Lund University  
Sweden



Cover: Schematic picture of a foam-like emulsion consisting of micrometer-size water compartments separated by a thin film of oil and surfactant.  
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This report is produced by Ali Khan and Johan Reimer.



Ali Khan



Johan Reimer

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## **SSF PROGRAMME ON COLLOID & INTERFACE TECHNOLOGY FINISHED**

In April 1997, the Board of the Swedish Foundation for Strategic Research (SSF) decided on a grant for a national programme on Colloid & Interface Technology with Lund University as host university and responsible, and with the undersigned as Programme Director.

From that time, this programme has been a very important factor for our department, with a very strong role in both our research and our Ph D training.

When the programme started, major aims were to create world-leading research programmes in areas which were new to Sweden and which are of strategic relevance for Swedish industry, to create a strong Graduate School for Ph D training and to create a national integration of both research and training.

The funding obtained amounts to a total of 64 MSEK and has been extensively used for funding Ph D projects. Other important parts were postdoc projects and a course programme.

When the programme finished, according to plans, by the end of 2002, we have inter alia seen in the programme 42 Ph D projects, 9 postdoc projects, 9 international scientific meetings of different kinds and 21 Ph D courses.

The programme has been directed by a Programme Board, the majority being leading personalities of Swedish industry. The management and administration have been made by the Programme Director, a Programme Secretary (Gerd Olofsson) and, for the course part, by a Director of Studies (Jan Christer Eriksson, Stockholm, from 2000 Krister Holmberg, Göteborg). Furthermore, there have been 6 "Area Leaders" responsible for the different research areas, and two reference groups one industrial and one international to assist in fulfilling the research strategy and securing a high quality of the research.

An extensive final report covering all types of activities, as well as comparing the results with the goals, is at present under preparation. Awaiting a thorough evaluation we can still highlight what we feel are important achievements.

Regarding the Ph D training, the programme substantially increased the number of Ph Ds in surface and colloid chemistry in Sweden and we could also see a very significant improvement of the efficiency. The study times for a Ph D were on average quite a bit lower than previously and the quality of research work high according to external evaluations.

There were Ph D projects in 7 different universities in Sweden with the main groups being in Göteborg, Lund and Stockholm. The aim was to have Ph D students work in a national context rather than in separate groups. This was achieved by "twinning" Ph D projects in different places and by having two supervisors from different universities. Very important uniting factors were the courses and the different workshops and conferences.

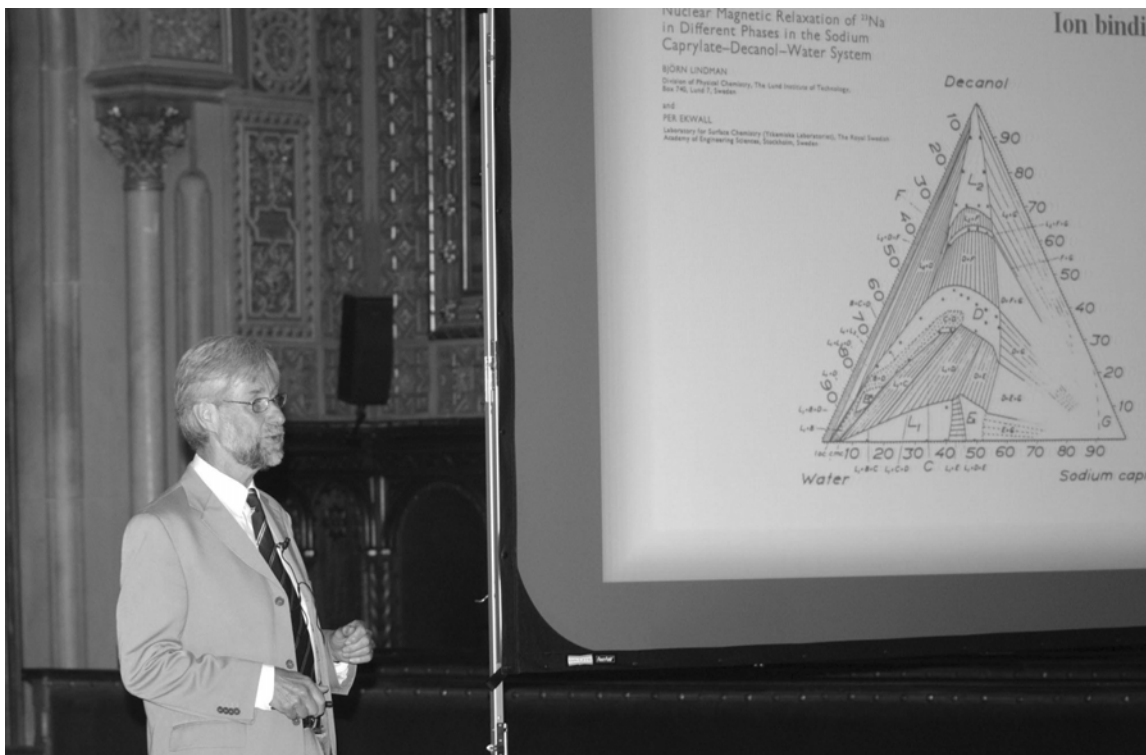
All good things come to an end and so also this programme. However, all who were involved agree that the national coordination and integration should survive and be long lasting and are prepared to work for it. Fortunately, SSF funding does not end with the programme. Thus we have obtained funding for a three-year course programme with partial funding of Ph D student salaries, as well as for two years of network activities. Regarding funding of research of senior scientists and of Ph D students, much more work needs to be done to secure a sufficiently high level of

funding, even if SSF recently awarded a joint five-year grant to Göteborg, Lund and Stockholm.

National integration and coordination have been strong parts of the programme. We expect the experience gained to be valuable on the European level in the 6<sup>th</sup> Framework Programme of the European Commission.

For the Programme Director, these 5 years have been great, full of new experiences and full of nice contacts and collaborations. Due to an efficient and experienced Board and generous help from all colleagues, his work has been much facilitated and allowed him to participate amply in both the research and the teaching parts of the programme. One person deserves to be specially mentioned, i.e. Gerd Olofsson, who acted as Programme Secretary. I wish to thank all participants in the programme for their contributions and hope you all agree to continue along the same lines during many years.

Björn Lindman



Björn Lindman giving the Kash Mittal Lecture at SIS2002 in Barcelona

## 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. Finally, the method allows for a characterization of the forces between the layers of lamellar phases. In cooperation with L. Wadsö (Building Materials). (V. Kocherbitov, O. Söderman).

**Double chain cationic surfactants.** Double chain cationic surfactants may form vesicles above the main phase transition temperature,  $T^*$ , vesicles which then may be cooled to temperatures below  $T^*$ . In one project we investigate the precipitation kinetics of catanionic structures as cationic vesicles, below  $T^*$ , are mixed with anionic surfactants. (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, including sodium dodecyl sulfate (SDS)-didodecyl dimethyl ammonium bromide (DDAB); bile salts-DDAB and dodecyltrimethylammonium chloride with hydrogenated and fluorinated sodium carboxylates of varying chain length. At high water content, stable vesicles, precipitates (catanionic solid) or two coexisting liquids may form, depending on the system. At higher surfactant concentrations, the phase behavior is dominated by the appearance of several new liquid crystalline phases. A feature of the mixed systems is that it is a trivial matter to span a range of aggregate structures, from micelles to vesicles to liquid crystals, by playing with surfactant mixing ratio and total concentration, and symmetry/asymmetry effects of alkyl chain lengths. (A. Khan, E. Marques (Porto), H. Edlund (Sundsvall), C. La Mesa (Rome)).

**Ionic-zwitterionic surfactant mixtures.** We are investigating the phase equilibria of lecithin mixed with cationic didodecyl dimethyl ammonium bromide (DDAB), anionic aerosol OT (AOT) in water. The binary phase behavior of DDAB, lecithin and AOT is dominated by lamellar liquid crystalline phases, On mixing lecithin with either of the ionic surfactants shows a strong tendency of forming one

extensive lamellar phase. These systems also form cubic phases in the water-poor part of the triangular phase diagrams. We are also studying the aggregate microstructure of the phases. (A. Khan, M. Fernandes, G. Montalvo, M. Miguel). (Project completed).

**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 ( $C_{12}E_8$ ) 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. The phases were identified by crossed polaroids, SAXS,  $^2H$ -NMR and optical microscopy. (E. Feitosa, A. Khan, B. Lindman).

**Wormlike micelles.** Some surfactants form giant wormlike micelles in solution that can be longer than several micrometers. These solutions have properties similar to polymer solutions, however with some significant differences. The contour length is not fixed but varies with concentration and temperature. Moreover, micelles may break and reform which may influence the dynamics. Furthermore, there are also systems where the micelles form connected (branched) network, similar to a bicontinuous microemulsion. In this project we study 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). A large difference in the dynamics and kinetics is found between systems where branching and/or fast breaking occurs and systems where breaking is slow and branching is absent. The former case may have relaxation times in the millisecond regime while in the latter case relaxation may be many orders of magnitude longer (even hours). Another interesting aspect of the wormlike micellar system is the very complex diffusion behavior observed for the surfactants, in particular in dilute and semidilute conditions. (U. Olsson (Lund), R. Angelico, L. Ambrosone and A. Ceglie (Campobasso, Italy), G. Palazzo (Bari, Italy), C. Schmidt and D. Burgemeister (Paderborn, Germany) and K. Mortensen (Risø, Denmark).

**Kinetics of fluid interfaces.** An oil in water droplet microemulsion can be brought to a non-equilibrium state by a rapid temperature quench. The approach to equilibrium involves nucleation of a bulk oil phase, and the rate for this process depends dramatically on the depth of the quench. The phase separation process involves splitting a uni-modal size distribution into a bimodal one where the larger drops at long times evolve through Ostwald ripening. The evolution of the bimodal size distribution, which at longer times is composed of two narrow peaks, can be followed by small angle neutron scattering. The reverse (solubilization) process, where the bimodal size distribution evolves into a unimodal one, can also be investigated by letting a sample return to the microemulsion phase, by temperature jump, after spending a given time in the two phase region at a lower temperature. The solubilization process depends on the initial distance from the final equilibrium. For shorter distances solubilization is a (slow) ripening process, while for large distances it involves coalescence into an intermediate bicontinuous structure and the solubilization is fast. The effect of droplet concentrations and interactions on the solubilization kinetics has also been studied by computer simulations. Here the droplets undergo Brownian motion while they also are allowed to exchange

molecules. Treating oil monomers in the continuous solvent as discrete particles allows one to follow local fluctuations in droplet size. In order to capture the full solubilization process, however, one can only follow the net flow of molecules. The simulations, involving hard sphere interactions only, are in good agreement with experiments on a nonionic system. In the continuation of the project we will investigate effects of attractive and repulsive droplet interactions on processes like solubilization and separation.

Vesicles are another example of non-equilibrium self-assembly colloids. Here, however, the ripening process appears to be far from straight forward. While the curved bilayer structures carry bending energy it turns out that that the common Helfrich bending energy does not drive a ripening process, because within this approximation the bending energy is independent of the vesicle size. When taking higher order terms into account, the vesicle curvature energy becomes radius dependent. However this radius dependence is such that it drives a ripening process where small vesicles grow and large vesicles shrink until the system eventually get trapped in a metastable size distribution. This might explain while many vesicle dispersions appear to have long time (months) stability although the global equilibrium is a lamellar phase.

In another series of experiments, relaxation processes in sponge phases were studied by temperature-jump technique. In these experiments, we found that the relaxation rate (of the light scattering intensity) increases dramatically with increasing concentration. (A. Evilevitch, J. Rescic (Ljubljana), J. Balogh, T. Le, U. Olsson, B. Jönsson (Biophysical Chemistry, Lund), H. Wennerström; P. Uhrmeister and R. Strey (Köln), Jan Skov Pedersen (Aarhus)).

**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).

**Ionic surfactants with divalent counterions.** Phase diagrams of ionic surfactants with multivalent counterions show strong counterion dependence. Specific ion effects on the phase behavior and microstructure in binary and ternary systems with dialkyl surfactants are explored. Both cationic and anionic surfactants are investigated. (A. Khan, O. Söderman; M. Nydén (Chalmers), M. Monduzzi and F. Caboi (Cagliari)). Project completed.

**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. 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, U. Olsson, J. Reimer, O. Söderman, C. Whiddon, I. Johansson (Akzo Nobel), D. Kaneko and K. Sakamoto (Ajinomoto Co. Japan)).

**Structure of lamellar phases.** 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 related to the formation of liposomes (onions) under shear, which can originate simply by shaking the sample. A systematic rheology study is performed on nonionic surfactant- water systems where the structure of the lamellar phase under shear (Couette flow) 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. (Florian Nettesheim and Walter Richtering (Kiel), Cesare Oliviero and Luigi Coppola (Cosenza), Peter Lindner (ILL Grenoble), K. Mortensen (Risø)).

**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 a 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. These block copolymer vesicles may be stabilized, electrostatically or sterically, by the addition of single- or double-chained surfactants or polymers. The break-up mechanism of the copolymer vesicles will be further explored. In the unextruded block copolymer system, under very dilute conditions, large polydisperse unilamellar vesicles are formed when raising the temperature approaching and passing the phase boundary to the two-phase region. 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 is a newly initiated research project which 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. (K. Schillén, D. Pebalk and E. B. Barmatov (Moscow State University, Russia), K. Mortensen (the Danish Polymer Centre, Risoe National Laboratory, Denmark)).

**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 HM-HEC 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. (M. Egermayer, M. Karlberg, J. Norrman, 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. (M. Olsson, P. Linse, L. Piculell, F. Joabsson, H. Wennerström).

**Mixed block copolymer/graft copolymer systems.** Aqueous systems containing both a block copolymer and a hydrophobically modified water-soluble polymer are investigated with respect to self-assembly, phase behavior and rheology. The project focuses on graft copolymers derived from polysaccharides and di- and triblock copolymers, including end-capped poly (ethylene glycol). All results indicate mixed hydrophobic associations between the different types of polymers. (M. Karlberg, B. Lindman, L. Piculell, K. Thuresson).

#### **Interactions between hydrophobically modified polymers and cyclodextrins.**

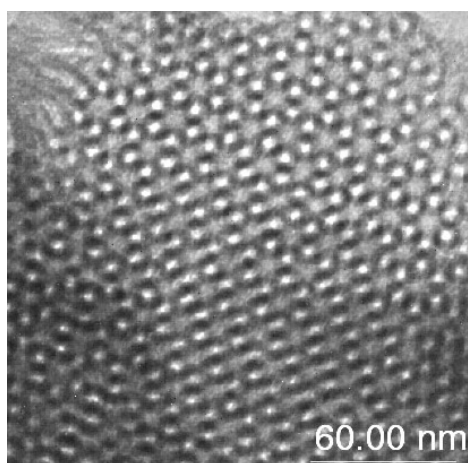
Rheology in mixed systems of HM-PEG and cyclodextrins, CD, or HM-EHEC and CD is investigated. For HM-EHEC the viscosity as a function of CD-concentration first decreased strongly, and at excess CD the viscosity became virtually the same as in a solution of the unmodified parent polymer. The ability to 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, A. Larsson (AstraZeneca Mölndal), L. Piculell).

**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, L. Piculell, K. Thuresson, B. Lindman).

**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 SAX, TEM, NMR and nitrogen adsorption measurements. (K. Flodström, V. Alfredsson and H. Wennerström).



Transmission electron micrograph of mesoporous silica with a bicontinuous cubic (Ia3d) structure. (K. Flodström).

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**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. Caragheorghopol (Romania)).

**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 the vesicles that form spontaneously at very high water content and several liquid crystalline phases at different compositions. (J. Bornè, A. Khan, T. Landh (Camurus), B. Lindman).

**Solution behavior of reverse amphiphilic polymers (hydrophilically modified polystyrenes) in oil-continuous microemulsions.** The solution behavior of hydrophilically modified polystyrenes will be investigated. Polystyrene (PS) undergoes a coil-globule transition temperature in the region of 34 degrees C and the solution viscosity changes dramatically as the polymer conformation changes from expanded coil to collapsed globule. Introducing a responsive polymer as the backbone polymer is expected to have a dramatic influence on the polymer-droplet behavior. For example, contraction of the backbone will force the water-soluble side chains closer to each other and may, for example, cause aggregation of the polymer-connected droplet networks. Thus, the possibility of introducing a thermal responsiveness into the microemulsion will be investigated. Next, the effect of changing the interaction between the side-chains and the surfactant-stabilised water droplets will be investigated. The first side chain (PEO) interacts associatively with the surfactant stabilised water droplets. Changing the side-chain to PNIPAM will introduce a temperature dependence to the interaction, as the side-chain will become unstable in the droplet at high temperatures. And finally, a repulsive interaction between the side chains and the surfactant stabilised droplets will be investigated using the (PNIPAM-co-Ac) grafted copolymer. (I. Lynch, L. Piculell).

## **Polymer-Surfactant Systems**

**Chemical polymer gels mixed with surfactants.** The gels studied in this project are based on polymers that bind ionic surfactants. This includes slightly hydrophobic polymers (EHEC, HEC), hydrophobically modified polymers (HMHEC, cat-HMHEC), and polymers carrying charges (cat-HEC, polyacrylate, co-polymers of acrylate and nonionic monomers). The gels are immersed in “bath” solutions containing ionic surfactants, mixed ionic/nonionic surfactants, hydrophobically modified polymers, and/or salt. Binding isotherms and the equilibrium swelling/shrinking of the polymer gels are studied. Dynamic and kinetic effects are also studied, such as the surfactant self-diffusion inside the gel, and the time dependence of the volume response of the gel following changes in the composition of the swelling medium. A nice correlation is generally found between the phase behavior of the linear polymer plus surfactant, and the collapse/swelling behavior of the corresponding gel. The gel swelling experiment is found to be a useful tool in the study of polymer-surfactant interactions, since both critical association phenomena and subtle differences between different types of polymer and/or surfactant are clearly revealed. Copolymer gels containing charged and uncharged monomers may first

collapse and then reswell again on successive addition of oppositely charged surfactant to the bath solution. Reswelling occurs if the uncharged monomer by itself is hydrophobic enough to bind surfactant. Systems can be designed where the swelling response with time is non-monotonic, i.e., a rapid shrinking is followed by a slow reswelling. (J. Sjöström, I. Lynch, L. Piculell).

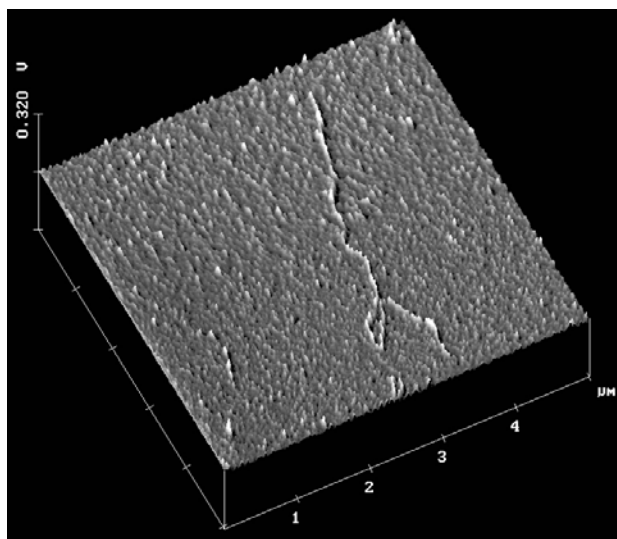
**Concentrated mixtures of oppositely charged polymer and surfactant.** We use a new approach to the study of oppositely charged polymers and surfactants. Conventional studies use aqueous mixtures of a polyelectrolyte (e.g., sodium polyacrylate, NaPA) with a conventional surfactant (e.g., cetyltrimethylammonium bromide, CTABr). Thermodynamically, such mixtures, containing 4 different ions and water, are four-component systems. By contrast, we use the "complex salt" (polyion + surfactant ion) as our point of departure. We prepare the pure complex salt (e.g., CTAPA) and study its aqueous mixtures with either the corresponding conventional surfactant (CTABr or CTAAc; Ac = acetate) or the polyelectrolyte (NaPA). Thus, we obtain truly ternary mixtures (3 different ions + water), which simplifies the interpretation immensely. Complete ternary phase diagrams have been established for CTAPA/CTABr/water, CTAPA/CTAAc/water, and NaPA/CTAPA/water. Pure CTAPA swells in water, forming first a hexagonal and then a cubic phase. The hexagonal phase exists with arbitrary proportions of polymeric (PA) and monomeric (Br or Ac) counterions. The cubic phase is destroyed (in favour of the hexagonal phase) already at small proportions of Br anions, but it survives with Ac counterions. The CTAPA/CTAAc/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 that the attraction between micelles with polymeric counterions is due to polyion bridging. (A. Svensson, J. Norrman, L. Piculell and B. Jönsson (Theoretical Chemistry, Lund), B. Cabane and P. Ilekli (Paris)).

**Mechanism of the interaction of DNA with cationic vesicles.** The scope of this project is to obtain mechanistic information in membrane systems where an oppositely-charged "guest" component is added. An example is the addition of DNA to a bilayer membrane composed of a mixture of a cationic and a neutral lipid. We are studying the kinetics of the following processes: (i) DNA condensation, (ii) formation and (iii) dissociation of the DNA-cationic vesicle complex using stopped-flow techniques (fluorescence spectroscopy, light and neutron scattering). (P. Barreleiro, Roland P. May, Björn Lindman).

**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, amino-acid 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).

**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)



3D AFM picture of a double-stranded DNA chain on mica. (A. Braem).

**Block copolymer-surfactant interactions.** Interaction between triblock copolymers of poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO), (PEO-PPO-PEO), and both ionic and nonionic surfactants in dilute aqueous solution are studied using dynamic and static light scattering in combination with differential scanning calorimetry, isothermal titration calorimetry and small-angle X-ray scattering. Polymers studied at the present have the same hydrophobic PPO block length but varying length of the hydrophilic PEO block. (J. Jansson, K. Schillén, G. Olofsson, O. Glatter (University of Graz, Austria), R. Cardoso da Silva and A. Niemiec and W. Loh (UNICAMP, Brazil)).

**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. (C. Leal, H. Wennerström, 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).

**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 in water has been 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 Graça Miguel (University of Coimbra, Portugal), K. Schillén, B. Lindman).

**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 ( $C_{12}E_5$ ) and decane. The rheological properties vary strongly with microemulsion droplet volume fraction, with temperature and with end-caps of the polymer. Particularly interesting are a maximum in viscosity as a function of droplet volume fraction, a decrease in cross-link life-time and very strong temperature dependencies. These can be understood on the basis of interdroplet distances and interactions. Recently studies have started for an analogous system where the surfactant self-assemblies are thermodynamically stable catanionic vesicles. (F. Antunes, M. Miguel, B. Lindman K. Thuresson).

**The effect of poly(N,N-dimethylacrylamide) on the lamellar phase of Aerosol OT-water.** The effect of a water soluble uncharged polymer 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.



(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. Different regions of liquid crystalline and isotropic solutions are identified. (A. Bilalov, C. Leal, A. Khan, B. Lindman).

### **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-dodecylsulfate, 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. (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, M. Cárdenas, A. Khan; R. Bauer (Denmark); J. Skov-Pedersen (Denmark); M. Paulsson (Food Engineering); B. Bergenståhl 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. (J. Borné, T. Nylander, A. Khan).

**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, H. Ljusberg-Wahren (Camurus AB, Lund); F. Caboi, M. Monduzzi (Italy)).

**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 (Clinical Physiology), 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).

## Adsorption and Surface Forces

**Interfacial behavior of DNA-cationic surfactant systems.** DNA-cationic surfactant systems are potential candidates for gene delivery. The co-adsorption behavior is an 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 ( $\sim 0.1$  mg/m<sup>2</sup>). Using surface film balance measurements, understanding is gained on the interactions of DNA with surfactant head group. Furthermore, the surface film balance technique is used in combination with ellipsometry, both to determinate the adsorbed amount and for imaging, mimicking processes at model cell

membranes. High and low molecular weight (above and below 400bp), single and double stranded DNA samples are used due to the different surfactant-induced compaction behavior in the bulk. In order to study the effect of the surfactant chain length on the adsorption behavior, cationic surfactants such as cetyltrimethylammonium- bromide (CTAB), tetradecyltrimethylammoniumbromide (TTAB) and dodecyltrimethylammonium bromide (DTAB) are studied. (M. Cárdenas, T. Nylander, B. Lindman).

**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).

**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).

**Interfacial properties of wheat proteins.** Various surface chemical techniques, like ellipsometry, surface film balance, and the surface force apparatus is used to study the interfacial interactions between pure fractions of the different wheat proteins. The interfacial properties and the interfacial interactions of the proteins are vital importance for the quality of wheats for use in food industry. (A.- C. Eliasson, J. Örnebro (Food Technology), T. Nylander).

**Interacting forces between biological macromolecules.** The interactions between salivary films adsorbed on mica surfaces are investigated using the interferometric surface force technique (SFA). Human whole saliva and purified fractions of saliva are used. These studies are of key importance for the understanding of intraoral events such as adhesion, friction and wear. Complementary neutron reflectivity measurements on the structure of the adsorbed layers have also been started. (T. Nylander, T. Arnebrant, P.-O. Glantz (Prosthetic Dentistry, Lund University), F. Tiberg).

**Adsorption of polyelectrolytes.** An efficient and successful use of polyelectrolytes in various technological processes such as ore processing, water

treatment, papermaking and in the manufacture of different commercial products (cosmetics, paints, foodstuff, etc.) requires a deep understanding of the complex phenomenon of polyelectrolyte adsorption at solid surfaces. The objective is to establish the relation between the structure of adsorbed layer and charged density and density of hydrophobic groups on the polyelectrolyte. The research project addresses the kinetics as well as equilibrium aspects of polyelectrolyte adsorption under different solution conditions (pH, salt concentration  $c_s$ , polymer concentration  $c_p$ ). The experimental technique mainly involves ellipsometry, to study the adsorption process, atomic force microscopy (AFM), to study the structure of the formed layers, and surface force measurements, to study the interaction between the formed layers. (Y. Samoshina, T. Nylander, B. Lindman, P. Linse and P. Claesson (KTH, Stockholm) and A., Diaz (PDVSA, Intevep, Caracas, Venezuela)).

**Adsorption behavior of cationic polymer - anionic surfactant system.** Mixed cationic polymer-anionic surfactant system is extensively used in personal care products and deep understanding about adsorption of polymer-surfactant complex is required. This project deals with desorption of complex as well as adsorption under different conditions (salt concentration, polymer concentration, surfactant concentration). The main technique being used is ellipsometry. (E. Terada (Kao Corporation), B. Lindman, Y. Samoshina, T. Nylander).

### 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. Presently we are applying the method to 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).

**Macroscopic background gradients in PGSE NMR diffusion measurements.** Background gradients caused by susceptibility differences at the sample interfaces may seriously affect the accuracy of NMR self-diffusion measurements, especially at high fields. The problem is quantified and various means of overcoming improving the situation are investigated. We have also modeled the magnetic field in a standard NMR tube using the finite element method to solve the relevant differential equations. (W. Price, P. Stilbs (Stockholm), B. Jönsson (Biophysical Chemistry, Lund), O. Söderman). Project completed.

**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).

**Solution microstructure from NMR relaxation and self-diffusion measurements.** NMR relaxation time and self-diffusion measurements, as applied to the study of microstructure in surfactant systems, have a long tradition in our department. A continuous development of theoretical models over the years has turned these experimental techniques into standard tools for investigating surfactant aggregate. Recently we have used this approach to investigate the solution microstructure in some oil-water-didodecyldimethylammonium surfactants with different counterions as well as to study the microstructure in surfactants forming bicontinuous micellar aggregates in a L1 phase. Self-diffusion experiments are used to investigate a viscoelastic microemulsion formed in the L2 phase of the lecithin-water-cyclohexane system. The structure is made up of giant reverse wormlike micellar aggregates. Combined measurements of water and lecithin self-diffusion behavior gives information on structure and dynamics. For very long micelles we seem to observe the curvilinear lecithin diffusion along the micellar contour. By monitoring the time dependence of the mean square dependence we are able to obtain information on the micellar persistence length. Moreover, the methods have been used to characterize vesicle systems found in mixtures of cationic and anionic surfactants. Here, the method yields important information with regard to the presence of vesicles, their sizes and also to the dynamics of the surfactants. (U. Olsson, O. Söderman, A. Khan, E. Marques; M. Monduzzi (Cagliari), A. Ceglie (Bari), R. Angelico (Bari), G. Palazzo (Bari)).

**Ellipsometry at liquid-liquid interfaces.** Ellipsometry is developed to enable multi-angle of incidence, MAI, measurements at liquid-liquid interfaces. This involves development of instrumentation as well as in analysis of data. Our focus is studies of adsorption from the oil phase of lipids and surfactants as well as from the aqueous phase of proteins, surfactants and polymers. The studies aim at a deeper understanding of phenomena at the oil-aqueous interface of relevance to emulsion

stability and phase behavior of corresponding three-component systems. (J.-W. Benjamins, T. Nylander, K. Thuresson, B. Jönsson (Biophysical Chemistry, Lund)).

### Theory and Modelling

**Temperature dependent dispersion forces.** We are investigating the consequences for the dispersion forces of having a thermally excited radiation field. A number of conceptually important results follow. i) The asymptotic form of an atom-atom (or molecule-molecule) dispersion interaction is a potential varying as the inverse sixth power of the separation and not the inverse seventh power retarded interaction that is the present textbook result. ii) We find that generally the asymptotic form of the dispersion interaction is, on the free energy level, identical to the corresponding classical case, which amounts to a novel correspondence principle. iii) The mechanistic explanation of the so-called retardation effects in terms of delays in a signal transmission seems misleading. (H. Wennerström, B. Ninham (Florence), J. Dacic (YKI)). Project completed.

**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 a stack of lipid bilayers is also studied experimentally. (E. Sparr, H. Wennerström).

**Phospholipid–cholesterol interactions.** The hydration thermodynamics of a series of phospholipid – cholesterol mixtures have been studied using the sorption calorimeter giving both free energies and enthalpies. The system is additionally studied by the NMR quadrupolar splitting technique. From the data we construct a  $P(\text{osm}) - X(\text{cholesterol})$  phase diagram, which shows clear analogies with the corresponding  $T - X(\text{cholesterol})$  diagram. The calorimetric data also show that for cholesterol contents of  $X > 0.3$  the enthalpy of the sorption induced chain melting is virtually zero. (L. Hallin, E. Sparr, N. Markova and H. Wennerström). Project completed.

**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. Special emphasis is focused on counter-ion effects. The results are interpreted by means of state of the art Monte Carlo simulations, including effects due to the presence of a dielectric discontinuity. Further developments include accurate electrostatic calculations based on finite element methods. (C. Whiddon, O. Söderman, B. Jönsson (Theoretical Chemistry, Lund), B. Jönsson (Biophysical Chemistry, Lund)).

**Structure determination of DNA from NMR data.** The solution structure of the DNA dodecamer  $d(\text{CAATCCGGATTG})_2$  has been determined by restrained molecular dynamics simulation. The effects of the molecular dynamics force field were also investigated. Contrary to the general assumption, we could show that the non-bonded interactions of the force field can have a strong influence on the structure. In particular, with commonly used parameter values, the electrostatic interactions were too strong and governed the final result to a large degree. With reduced electrostatic interactions or none at all, the Lennard-Jones attraction could dominate and produce specific features. A purely repulsive potential for non-bonded interactions minimizes the bias, but does have a tendency for somewhat elongated structures. The study of this particular sequence was partly motivated by the fact that G/C rich regions have displayed interesting features. In particular, oligonucleotides containing the tetrad GGCC have been reported to be highly bent. Although the present structure, which contains the reverse tetrad CCGG, has indications of some ability to bend, it is best described as straight. (C. H. Y. Lau (Canberra), M. Ullner).

**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 bootstrapped Poisson-Boltzmann 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)).

**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. Skepö, A. Akinchina, and P. Linse).

**Conformational properties of polyelectrolytes.** Electrostatic persistence length has often been used as a measure of the conformational response to the intramolecular, electrostatic interactions of linear polyelectrolytes. The behaviour, given the Debye-Hückel approximation, has been an area of controversy. However, a more unified picture is emerging from a combination of Monte Carlo simulations and an analysis of the analytical approaches in the literature. First, it is important to recognise that four different types of definitions have been used and that they all represent different properties. Second, the behaviour can be divided into three regimes, depending on the relation between the screening length and chain size. Third, the description of the chain behaviour requires at least two parameters, while

most theories rely on only one, even if the initial approach would appear to be more general. Furthermore, the majority can be said to be variations to one or the other of two original one-parameter theories, representing two limiting cases. The task at hand is to improve the description based on the gained insight. (M. Ullner).

**Polyelectrolytes in confined geometries.** The effects of confining a polyion and its counterions in spherical cavities of different sizes have been investigated by Monte Carlo simulations. A simple model system with focus on chain connectivity and Coulomb interactions was used. Structure, energy, and free energy properties at different chain linear charge densities and counterion valences were determined. The results are relevant for experimental studies of polyions confined into, e.g., viruses, vesicles, and zeolyte cavities. Extension to non-spherical cavities is in progress. (A. A. C. C. Pais (University of Coimbra), M. G. Miguel (University of Coimbra), B. Lindman, 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 Buffalo), A. Akinchina, and P. Linse).

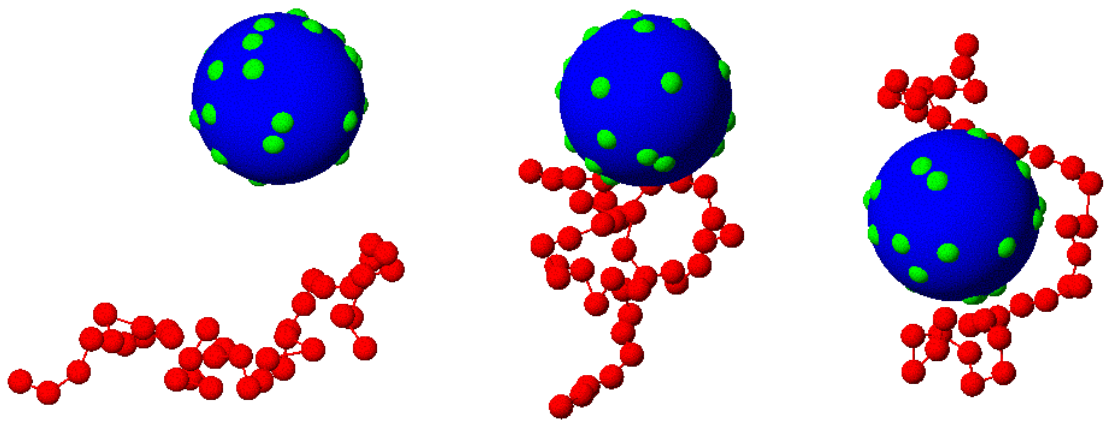
**Systems containing oppositely charged polyelectrolytes.** Solutions of oppositely charged polyelectrolytes often display a phase separation where one phase is rich in both polymer components. The conditions of such phase separations have been investigated by Monte Carlo simulations. Two different linear charge densities were considered, and structure factors, radial distribution functions, and polyion extensions were determined. A redistribution of positively charged polyions involving strong complexes formed between the oppositely charged polyions appeared as the number of negatively charged polyions was increased. The nature of the complexes was found to depend on the linear charge density of the chains. The simplified model involving the screened Coulomb potential gave qualitatively similar results as the model with explicit small ions. The role of added salt has also been addressed. (Y. Hayashi, M. Ullner, and P. Linse).

**Polyelectrolyte gels.** A model of a cross-linked polyelectrolyte gel has been examined using Monte Carlo simulations. The simple model contained a charged defect-free network represented by linked charged beads and explicit counterions. Pressure-density relations for the polyelectrolyte gel, a corresponding nonionic polymer gel, and several partly or fully degraded gels have been determined. The polyelectrolyte gel displayed a very large swelling capacity, in agreement with experiments. The swelling mechanism and chain properties have been examined and compared with current theories on gel swelling. The effect of the crosslinking density, chain linear charged density, chain flexibility, and valence of the counterions on the



swelling behavior and the structure of the gel has also been examined (S. Schneider 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. (M. Jönsson, M. Skepö, P. Linse, and F. Tjerneld (Biochemistry)).



Snapshots illustrating protein-polymer configurations at increasing hydrophobic interaction (left to right) between hydrophobic protein residues and polymer segments (Malin Jönsson et al.).

**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. Moreover, 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. (F. Carlsson (YKI), E. Hyltner (YKI), T. Arnebrant (YKI), M. Malmsten (YKI), and P. Linse).



Snapshots illustrating a solution containing positively net charged proteins: (left) without polyion, (middle) with stoichiometric amount of polyanion where strong protein-polyion complexation appears, and (right) excess amount of polyanion where the complexes are redissolved (F. Carlsson et al.).

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**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).

**Statistical-mechanical programs.** Also during 2002 the statistical mechanical computer program MOLSIM for Monte Carlo and molecular dynamics simulation has substantially been updated and extended. In particular, two-dimensional Ewald summation has been implemented for simulating charged species near surfaces. The software POLYMER for lattice mean-field calculations is regularly used in undergraduate courses. A license agreement of using the POLYMER software with a major international chemical company has been extended for a third year (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 Laser light scattering goniometer system from ALV GmbH, Langen, Germany, is a measuring system 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 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 NFR.).

B) For characterizations of molecular weight and studies of conformation changes or association processes, 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). Since October 1996 we have access to a bio-microscope dedicated for biological and cryo-samples. The microscope, a Philips CM 120 bio-twin, has a point-to-point resolution of 3.4  $\text{\AA}$ , which is suitable for biological, colloidal systems and materials. The microscope is equipped with two digital cameras (Gatan Multi-scan CCD) for rapid and high quality image recording. An energy filter (GIF100) is attached to the microscope. The filter is used for enhancing the contrast and for imaging of thicker samples by removing inelastic electron scattering, or for getting the elemental information of the sample by selecting the inelastic electron scattering. Cryo-TEM enables direct imaging of liquid specimens. The specimen is prepared by blotting a tiny drop (ca. 5  $\mu\text{l}$ ) of the sample onto a holey-carbon grid, which is subsequently immersed in liquid ethane ( $-183\text{ }^\circ\text{C}$ ). The sample then immediately vitrifies. The specimen is transported to the microscope and images are recorded, all under cryogenic conditions (liquid nitrogen temperature). Other sample preparation methods available are for example freeze-fracturing and replica techniques. For

traditional TEM, with solid-state samples, the specimen is normally prepared by crushing the sample in a volatile solvent and dispersing it on to the holey-carbon grid. For further information about the microscope see [www.materialkemi.lth.se/biomic/index.html](http://www.materialkemi.lth.se/biomic/index.html) (Sponsored by NFR, Crafoord Foundation and Knut and Alice Wallenberg foundation).

**Multimode scanning probe microscope** (contact person: Alan Braem). 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: Ali Khan). 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) and a high-sensitivity differential scanning calorimeter MicroCal MC-2 (Microcal Inc., Northampton, MA)

**Polarimeter.** (contact person: Lennart Piculell). To measure conformational changes a Jasco DIP-360 polarimeter is used. The polarimeter can be thermostated to perform temperature sweep measurements.

**Rheometer.** (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).

**Vibrational spectroscopy.** (contact person: Anna Stenstam). 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.

**UV-Vis spectrometer.** (contact person: Krister Thuresson). A Perkin Elmer lambda 14 UV/Vis is used to perform absorbance measurements (190-1100 nm). The spectrometer is PC controlled with UV Winlab Software designed by Perkin Elmer. The temperature of the sample is controlled via a connected Haake water bath.

## **COLLABORATIVE RESEARCH PROGRAMS**

### **The Centre for Amphiphilic Polymers, CAP**

The Centre for Amphiphilic Polymers from Renewable Resources (CAP) was founded in 1995 as a part of the Competence Centre Programme initiated by NUTEK (the Swedish Board for Technical and Industrial Development). CAP activities concern fundamental behavior and applications of amphiphilic polymers, and the use of biopolymers for their preparation. CAP is jointly funded by the University, VINNOVA, and a group of industrial companies. During 2002 the participating companies were Akzo Nobel Surface Chemistry, AstraZeneca R&D Mölndal, EKA Chemicals, Lyckeby Stärkelsen, SCA Research, and Tetra Pak. CAP research activities are mainly localized at Lund University, but also at the member companies. The Board of CAP, which includes Lennart Piculell from our department, has an industrial majority. A scientific advisory board was formed in 2002; its two members are Dr Charles Buchanan (Eastman, USA) and professor Terence Cosgrove (University of Bristol, UK).

The scientific work in CAP is carried out as ca. 20 PhD or postdoc projects covering all aspects of amphiphilic polymers, including synthesis/modification, characterization, physical-chemical behavior, 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.

In 2002, Jesper Sjöström from our department completed his thesis financed by CAP. Two new PhD projects were launched, one dealing with molecular mass distributions of cationic starch derivatives and one with starches in dispersions and emulsions. The two projects are carried out at Technical Analytical Chemistry and Food Technology, respectively.

Much effort was spent during 2002 on planning for the future: stage IV of CAP (2004-2005) and beyond. Among other activities, this process involved thorough interviews with all CAP members, discussing new ideas and research priorities.

### **National Research Programme in Colloid and Interface Technology.**

The Swedish Foundation for Strategic Research (Stiftelsen för Strategisk Forskning, SSF) is the most important funding agency for supporting novel research

ventures in Sweden. The Foundation supports research programmes and graduate schools in science, technology and medicine in order to strengthen Sweden's long-term competitiveness. Since colloid and interface science is an active research field in Sweden and has broad industrial relevance, the Foundation decided in 1997 to finance a national research programme and an adjoining graduate school in surface and colloid technology. The funding for the 5-year period 1998-2002 amounted to 64 MSEK with 18.56 MSEK for the last year 2002.

The main objectives of the Research Programme/Graduate School are to:

- create a strong fundamental national research programme
- further the development of the selected technologically important sub-fields, and at the same time promote more functional flows of knowledge and competence between the scientific institutions in this area in Sweden on the one hand, and the corresponding technological sectors of industry on the other.

The programme consists of a nationally coordinated research programme and a graduate school. The large majority of the research projects are conducted as PhD student projects.

The program has a Board with industrial majority composed of the following members: Jan Svärd (Chairman; Eka Chemicals), Conny Bogentoft (Karolinska Innovation), Ulf Carlson (SCA), Kåre Larsson (Camurus), Bengt Nordén (Chalmers University of Technology), Karin Schillén (Lund University) and Per Stenius (Helsinki Institute of Technology). The host university of the Programme is Lund University; Programme Director is Björn Lindman and Programme Secretary Gerd Olofsson. Krister Holmberg (Chalmers University of Technology) is the Director of Studies of the Graduate School.

The research programme is divided into 5 areas:

1. Dynamic surface forces (leader, Per Claesson, S),
2. Aqueous polymer mixtures and gels (Lennart Piculell),
3. Chemical reactions in organised media (Krister Holmberg, G),
4. Interfacial aspects of cellulose (Fredrik Tiberg, S), and
5. Concentrated dispersions (Ulf Olsson and Lennart Bergström, S)

During 2002 39 students and 7 post. doc.s were enrolled in the programme carrying out projects in Lund, Stockholm, Göteborg, Uppsala, Karlstad, Luleå and Sundsvall.

Five courses (also open to students outside the programme) were given during the year.

- Surface and Colloid Chemistry – molecular basis and technological applications (5 p), Degeberga, with 14 participants.
- The Colloidal Domain – where physics, chemistry, biology, and technology meet (10 p) Lund, Göteborg and Stockholm from November 2001 to February 2002 with 38 participants.
- Microscopy- basic principles and applications to surfactant phase science (5 p), Lund, with 14 participants.
- Wetting and capillarity (3 p), Utö, September with 28 participants. This course was given in collaboration with the French Embassy.
- Graduate student conference in colloid and interface science (2 p), Fiskebäckskil with 27 participants. This course was arranged by 3

programme Ph D students and was only open for students in the programme.

The Graduate School in Colloid and Interface Technology will continue as the Foundation of Strategic Research decided on its meeting in June 2001 to provide MSEK 9.5 for a three-year prolongation of the Graduate School to cover costs of courses, direction, administration and financing of salaries of Ph D students during the course part of the Ph D training.

During the year there were two Board meetings, one in Bohus and one in Lund.

During 2002 the Programme was involved in organizing two sizeable international conferences:

June 14-18 in Lund the conference Polyelectrolytes 2002 took place, Ca. 200 participants from all over the world, and including the leading scientists in the field, attended a very successful event

The annual Programme Workshop was combined with an international conference on Colloid and Interface Technology. Fundamentals and Applications. Ca. 20 world-leading scientists gave invited talks and in addition there were talks by senior scientists from the programme and a large poster session where all programme projects were presented. The conference was held in Lund, November 6-8 with about 200 participants.

### **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, held 6 – 8 November, was this year organized in cooperation with the SSF programme on Colloid and Interface Technology and the Division of Surface Chemistry of the Swedish Chemical Society, 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 Olofsson, chairman). It will organize in cooperation with YKOLL the annual Symposium in Surface and Colloid Science. The second 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, J. Reimer, C. Whiddon, V. Kocherbitov, O. Söderman and S. Ulvenlund.



### **NorFA Network**

A three-year nordic-baltic network, sponsored by NorFA (Nordic Academy for Advanced Study), on Quality and Health Aspects of Milk Components, co-ordinated by Dr. Jeanette Otte at KVL (The Royal Veterinary and Agricultural University) in Copenhagen, Denmark was granted in the end of 2001 and will be set-up during 2002. 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.

### **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-ordinated 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).

### **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 Píera) 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.

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### **CONFERENCES, TRAVELS AND SEMINARS**

Björn Lindman gave plenary or invited lectures at a number of international conferences: Self-assembly- The Future, Massa Marittima, Tuscany; Symposium on Starch, Turku, Finland; EUROCHEM I, Toulouse; 14<sup>th</sup> Surfactants in Solution, Barcelona; Ingvar Danielsson Symposium, Turku, Finland; workshop on Cationic-anionic mixed colloids, Saclay, France. Björn Lindman also attended the 15<sup>th</sup> conference of the European Colloid and Interface Society, Paris.

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: National and Autonomous University of Mexico, Mexico City; Center of Polymer Research, CIP, Tepexpan, Mexico; Department of Applied Surface Chemistry, Chalmers University of Technology, Göteborg; Procter&Gamble Research Centers in Cincinnati, Brussels and Rome; MidSweden University, Sundsvall; Department of Physical Chemistry, Åbo Akademi University, Finland; Department of Chemistry, University of Porto; SCA Research, Sundsvall; Malmö University; The Swedish Pulp and Paper Research Institute, Stockholm; Department of Chemistry, University of Coimbra, Portugal; Department of Pharmaceutical Chemistry, Uppsala University; Institute for Surface Chemistry, Stockholm, Sweden; Royal Institute of Technology, Stockholm; Universidad Nacional de Educación a Distancia, Madrid. Björn Lindman was visiting professor at Department of Chemistry, Coimbra University, Portugal.

Håkan Wennerström delivered invited talks at; XII International Conference on Surface Forces, Zvenigorod, Russia; at 17<sup>th</sup> IUPAC Conference on Chemical Thermodynamics, Rostock, Germany; at the Annual Meeting of the Colloid and Surface Science branch of the Chemical Society of Japan, Sendai, Japan; and at International Workshop on "Renaissance of Colloid and Interface Chemistry in Nanotechnology Era", Matsushima, Japan.

Håkan Wennerström organized the International Symposium Colloid and Interface Technology: Fundamentals and Applications, Lund, Sweden. At the symposium, Lennart Piculell, Ulf Olsson and Fredrik Tiberg held invited lectures and 30 posters were presented by people from the department.

Olle Söderman presented two posters at the 6<sup>th</sup> International Conference on Magnetic Resonance in Porous Media in Ulm. He also presented a seminar at CEMAGREF, Rennes.

Per Linse gave a invited lecture at University of Kyoto, Japan, and delivered oral presentation at the symposium "Chain molecules at interfaces: SCF theory and experiment, Wageningen, The Netherlands and at the 4<sup>th</sup> International symposium on "Molecular Order and Mobility in Polymer Systems", St. Petersburg, Russia. Per Linse, Yoshikatsu Hayashi and Rita Dias presented posters at the IUPAC Polymer Conference on "The Mission and Challenges of Polymer Science and Technology", Kyoto, Japan. Marie Skepö and Fredrik Carlsson gave oral presentations at the conference "Particles 2002", Orlando, Florida, USA. Marie also gave an invited lecture at M: Ludwig-Maximilian University, München, Germany and delivered an oral presentation at the conference "Condensed Matter and Materials Physics", Brighton, UK. Anna Akinchina delivered an oral presentation at CCP5 "Summer School on Molecular Simulation", London, UK. Stefanie Schneider delivered an oral presentation at the "Europolymer Conference 2002" of the European Polymer Federation (EPF), Gargnano.

Lennart Piculell and Martin Olsson presented posters at Fundamentals and applications, Oud Poelgeest, The Netherlands. Lennart also visited Aventis Pharma, Paris, France. Martin also presented a poster at the symposium "Chain Molecules at Interfaces, SCF Theory and Experiment", Wageningen, The Netherlands.

Anna Svensson, Stefanie Schneider and Magnus Ullner gave oral presentations and Anna Stenstam, Cecilia Leal, Karin Schillén, Marite Cárdenas, Anna Akinchina, Marie Skepö, Fredrik Carlsson, and Yoshikatsu Hayashi presented posters at the conference "Polyelectrolytes 2002", Lund, Sweden

Lennart Piculell, Alan Braem and Vitaly Kocherbitov gave oral presentations and Carin Malmberg, Christy Whiddon, Iseult Lynch, Joakim Balogh, Malin Jönsson

and Rita Dias presented posters at XVIth Conference of the European Colloid and Interface Society, Paris, France

Gerd Olofsson and Karin Schillén visited the Instituto de Chimica, University of Campinas, Campinas, Brazil where lectures and seminars were held. Gerd also gave a Ph D course on "DSC – Basic principles and applications to phase changes". Karin also gave a seminar at Department of Chemistry, University of Sao Paulo, Ribeirao Preto, Brazil. Gerd visited and presented lectures at the National Central University and Chung-Yung University, Chung-Li. She also visited the Department of Chemistry and School of Pharmacy at the National Taiwan University in Taipei, Taiwan.

Ingemar Wadsö gave a lecture at 17th IUPAC Conference of Chemical Thermodynamics" in Rostock, Germany.

Viveka Alfredsson and Katarina Flodström visited Åbo Akademi, Finland where Viveka gave a seminar.

Tommy Nylander gave a three-day course at Procter & Gamble, Cincinnati USA as well as an invited lecture. He attended the mid-term meeting of the EU-RTD project MODSTEEL (Improvement of construction materials used in the food industry to lengthening processing time) in Oporto, Portugal, NorFA project (Quality and Health Aspects of Milk Components) workshop in Liseleje, Denmark as well as the REFILL2002 (Neutron reflectivity: Progress in the study of interfaces) workshop in Grenoble.

Magnus Ullner delivered seminars and oral presentations at the CERC3 Young Chemists' Workshop Water-Soluble Polymers and Their Hydrogels, Vaalbeek, Belgium; Forschungszentrum Jülich, Germany; and Kyoto University, Japan. He has also presented a poster at the IUPAC Polymer Conference on the Mission and Challenges of Polymer Science and Technology (IUPAC-PC2002).

Rita Dias, Cecilia Leal and Johan Reimer gave oral presentations and Caroline Ericsson presented a poster at 14<sup>th</sup> Surfactants in Solution symposium (SIS-2002) in Barcelona. Rita also gave a talk at Kyoto University. Jörgen Jansson presented a talk at 6<sup>th</sup> European Summer School on "Scattering Methods Applied to Soft Condensed Matter", Bombanne, France. Jörgen also visited Institute of Physical Chemistry, University of Graz, Austria where he gave two seminars. Marite Cárdenas delivered an oral presentation at REFILL Grenoble, France and presented a poster at Particles and Polymers at Interfaces. International Workshop. Leiden, The Netherlands.

## **Polyelectrolytes 2002**

A large event during this year for our department was the arrangement of the symposium Polyelectrolytes 2002, which was the 4<sup>th</sup> in a series of International Symposia on Polyelectrolytes that began in 1995. The symposium was held June 15 to June 19 at Kårhuset in Lund. The symposia serve as a forum for polyelectrolyte researches worldwide. This year, special attention was paid to mixtures of oppositely charged polymer and colloids. A collection of papers will be published in a special issue on polyelectrolytes in the Journal of Physical Chemistry.

Nearly 200 participants, the far largest number so far in this forum, were welcomed to a sunny Lund and to listen on nearly 50 oral presentations and examine about 100 poster presentations. Although the majority of the participants were European, far-distance guests from South America, Japan, and Australia were present. The outdoor dinner at Kulturen gave the participants rich possibilities to explore new

aspects of Swedish culture and to establish new personal contacts in a relaxed environment. Surely, all participants felt satisfied when they returned back after nearly four intense days.

The arrangement was a joint effort between the division of Theoretical Chemistry and Physical Chemistry 1 with Bo Jönsson, Per Linse, Gerd Olofsson, Lennart Piculell, and Magnus Ullner in the organizing committee. There is always a lot of work to prepare and carry through such an event, and special thanks to all of you that enthusiastically assisted with the successful arrangement.

Financial support was received from The Swedish Research Council, The Foundation for Strategic Research through the Colloid & Interface Technology research program, American Scientific Publishers and the following industrial companies: Akzo Nobel, AstraZeneca, Lyckeby Stärkelsen, and SCA. This support was very helpful and is gratefully acknowledged.



### **Colloid and Interface Technology: International Symposium on Fundamentals and Applications**

During 2002 the research programme **Colloid and Interface Technology** ran for its final fifth year. It was then decided that the regular annual meeting of the participants should be extended to take the form of an international symposium, which took place in Lund 6<sup>th</sup> to 8<sup>th</sup> of November. The symposium also acted as the yearly meeting of the newly formed section in Surface and Colloid Section of the Swedish Chemical Society. Fourteen internationally renowned scientists gave plenary lectures and in addition two young Swedish recipients of the AKZO-Nobel award in surface and colloid science presented their work. Programme activities consisted in that six area leaders summarized the scientific achievements during the five years of activity. There was also a poster session where graduate students and other participants had the opportunity to present their work in more detail. The symposium attracted around 200 participants who got an overview of many of the currently dynamic areas of colloid science both from a purely scientific and from a more applied perspective.

### **The Björn Lindman Symposium.**

On November 9th, friends, colleagues, and present and former students of Björn Lindman gathered in Lund for a one-day symposium held to celebrate Björn on the occasion of his 60th birthday. The topics discussed this day by the various invited speakers shaped a chronological odyssey through Björn's scientific interests and

achievements over the past 30 years. The opening talk was given by Sture Forsén who highlighted the pioneering NMR work performed by Björn and his collaborators in the 1970's. As the only speaker from abroad, Gordon Tiddy also took the responsibility to discuss a few topics outside the area of colloid science. Towards the end of the day the topics approached Björn's more current activities, and the final talk was presented by Maria Miguel, discussing their recent DNA work. Fortunately, Maria also had time to show some slides from the Miguel/Lindman family album, confirming that Björn, indeed, has a number of other interests, besides the science.

All agreed that the symposium was a big success. The odyssey through 30 years of colloid science was interesting. There are not many occasions like this, where one gets the chance to follow the development of a particular scientific topic. Then, in the evening, we all enjoyed a magnificent dinner in the main University building. When it was time to go home we all felt that we had spent a wonderful day in Björn's companion.



(Photo by Peter Stilbs, KTH)

## EXTERNAL PROFESSIONAL ACTIVITIES

Björn Lindman is Regional Editor of Colloid & Polymer Science and was on the Advisory or Editorial Boards of Langmuir, Cellulose, Advances in Colloid and Interface Science, Current Opinion in Colloid & Interface Science and Journal of Dispersion Science and Technology. He was a member of the Board of the Camurus Lipid Research Foundation and of the Industrial Committee of the Institute for Surface Chemistry. Björn Lindman is also a 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 was the Programme Director for the national program on Colloid & Interface Technology sponsored by the Swedish Foundation for Strategic Research. Björn Lindman was external examiner for El-Ouafi Alami's Ph D thesis at Chalmers University of Technology and 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. Gerd is a member of the Advisory Board for *Thermochimica Acta*.

Olle Söderman acted as a reviewer of proposals for the National Research Council. He was a member of the board for Undergraduate Studies at Natural Science Faculty Lund University.

Per Linse served on PhD Thesis committees for Patrik Gavelin, LU. Both Per and Lennart Piculell were members of the program committee of the Center for Amphiphilic Polymers, CAP.

Lennart Piculell served on PhD thesis committees for Mats Rundlöf (Royal Institute of Technology), Leif Karlson and Marie Skepö. Lennart also served as a member of the editorial boards of the *Food Hydrocolloids* and *Carbohydrate Polymers*. Lennart was a member of the committee for PhD education at the Chemical Center, and Member of the board of CAP

Ulf Olsson acted as examiner for the thesis of Lise Arleth at the department of Mathematics and Physics, the Royal Veterinary and Agricultural University in Copenhagen, Denmark.

Tommy Nylander served in the PhD thesis committee for Kristina Lodaite and Dietlind Adlercreutz at Lund University, Liselott Lindh at Malmö University as well as Mikael Kjellin, Goran Bogdanovic, and Mark Plunkett at KTH, Stockholm.

Karin Schillén was a member of the board of the Foundation of Strategic Research program “Colloid and Interface Technology”.

Ingemar Wadsö is 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. Ingemar is also a member of the Advisory Board for *J. Chem. Thermodynamics*.

Viveka was a member of the Master thesis (lic avhandling) committee for Mats Lundberg, University of Lund.

## AWARDS

Björn Lindman received the first Kash Mittal Award for “his outstanding achievements in colloid chemistry” and was appointed “excellent researcher” by the Swedish Research Council.

Håkan Wennerström received the Lectureship Award of the Division of Colloid and Surface Chemistry of the Chemical Society of Japan.

## BARRY NINHAM HONORARY DOCTOR

In May we had the pleasure to acknowledge the long-term collaboration with the Department of Applied Mathematics in Canberra and in particular with professor Barry Ninham by awarding him an Honorary Doctorate at Lund University. Barry has made a number of both long and short visits to our department, but even more significant is that he has encouraged younger researchers at his group to spend time with us and correspondingly has he received a range of young scientists from Lund at the department in Canberra.



## COURSES AND TEACHING

Members of the department are involved in a number of undergraduate courses. The first year of chemistry studies at the Chemical Center consists of three 9-week courses. These courses are given two times a year, one, during the fall semester and the other, during the spring semester. For the introductory course, Eva Hansson was the head teacher and Viveka Alfredsson and Eva Hansson taught parts of the course. Karin Schillén gave lectures during the second chemistry course, and Lennart Piculell, Magnus Ullner and Karin Schillén were involved in leading exercises and question hours. The topic of the third first-year course is thermodynamics and introductory quantum mechanics and spectroscopy. Olle Söderman is the head teacher for this course and gives the lectures and exercise sessions in thermodynamics.

As regards higher courses, the department gives one basic and one advanced course in surface and colloid chemistry and one advanced physical chemistry course. The basic course, which is a biannual event, is headed by Ulf Olsson and taught by Ulf, Lennart Piculell, Karin Schillén and Viveka Alfredsson. The advanced surface and colloid chemistry course is organized and taught by Håkan Wennerström (main teacher) along with Lennart Piculell. Per Linse also took part in the teaching of the course. It is given once a year during the fall semester, and is based on the book by Håkan Wennerström and Fennel Evans. The advanced physical chemistry course is given once a year during the spring semester and is taught by Per Linse, Ulf Olsson and Olle Söderman. Håkan, on behalf of the department, delivered a total of 15 hrs lectures on environmental chemistry, a new course started in chemical center for the undergraduate students and Anna Stenstam also took part to assist the students in their project work. Finally, a number of our graduate students serve as teaching assistants on all courses given by the department.

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

The Institute for Surface Chemistry, YKOLL and Chalmers University of Technology jointly organize an annual course on surfactants and polymers in aqueous



solution directed towards a European audience. In 2002, the course was held, for the 11<sup>th</sup> consecutive year, in Lisbon and the same course was also held for the first time in Mexico at Centro de Investigación en Polímeros, Tepexpan in both cases with Björn Lindman as one of the teachers. Björn Lindman also gave courses on surfactant and polymer solutions at Coimbra University, University of Porto and at Procter & Gamble Research Centers in Cincinnati, Brussels and Rome and 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 2002, the department had a turnover of ca 34.5 million SEK. From the University we obtained 14.3 million of which 1.3 million is to cover undergraduate teaching; 2.8 million, for graduate students; and 10.2 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 3.9 million SEK, The Swedish Agency for Innovation Systems (VINNOVA) which finances more applied projects, supports us with 4.7 million, mainly via the 2 Competence Center CAP and SNAP, during the fiscal year. We also received 8.2 million SEK from The Swedish Foundation for Strategic Research (SSF), which is an important funding agency for supporting novel research ventures in Sweden. We are grateful for support from private industry, directly and via their foundations, amounting to ca. 1 million. Finally, we received 0.9 million SEK from The European Commission.

## DOCTORAL THESIS

May 3, 2002

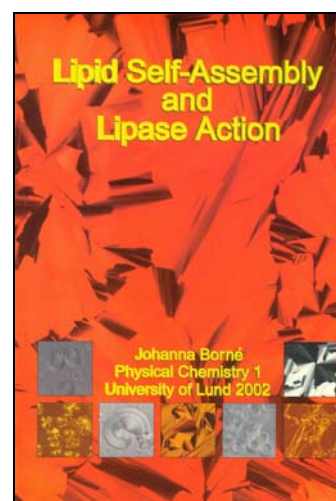
**Johanna Borné**

*Lipid Self-Assembly and Lipase Action*

Opponent: Prof. George S. Attard

Department of Chemistry

University of Southampton

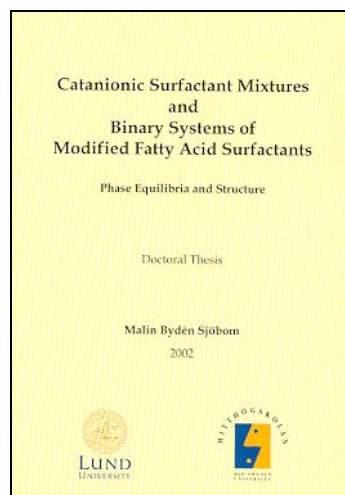


May 17, 2002

**Malin Bydén Sjöbom**

*Catanionic Surfactant Mixtures and Binary Systems of Modified Fatty Acid Surfactants – Phase Equilibria and Structure*

Opponent: Prof. Jarl B. Rosenholm  
Department of Physical chemistry  
Åbo Akademi University

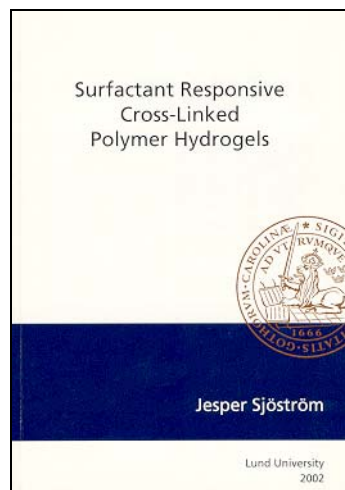


May 25, 2002

**Jesper Sjöström**

*Surfactant Responsive Cross-Linked Polymer Hydrogels*

Opponent: Docent Per Hansson  
Department of Physical Chemistry  
Uppsala University

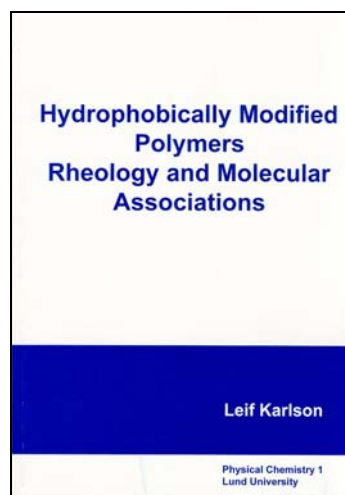


October 4, 2002

**Leif Karlson**

*Hydrophobically Modified Polymers Rheology and Molecular Associations*

Opponent: Dr. Ilias Iliopoulos  
Matiere Molle & Chimie  
E.S.P.C.I., Paris



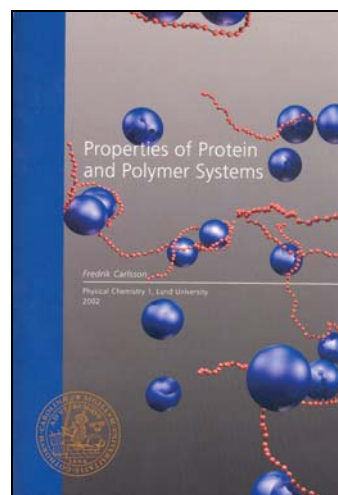
October 31, 2002

**Fredrik Carlsson**

*Properties of Protein and Polymer Systems*

Opponent: Prof. Eric Dickinson

Procter Department of Food Science,  
University of Leeds, UK



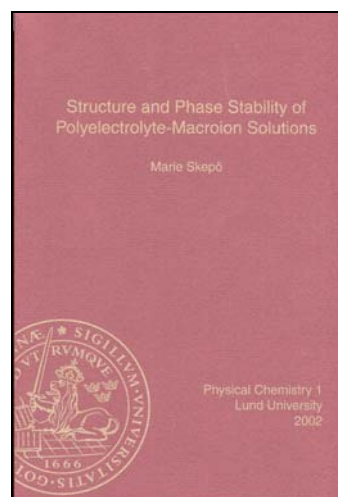
November 23, 2002

**Marie Skepö**

*Structure and Phase Stability of  
Polyelectrolyte-Macroion Solutions*

Opponent: Prof. Avinoam Ben-Shaul

Department of Physical Chemistry,  
Hebrew University, Israel



## MEMBERS OF THE DEPARTMENT

### Scientists/Teachers

Paschalis Alexandridis, (on leave), assistant professor

Viveka Alfredsson, assistant professor

Justas Barauskas, postdoc

Azat Bilalov, postdoc

Alan Braem, postdoc

José Campos, postdoc

Sergei Gavryushov, postdoc

Eva Hansson, associate professor, dean

Ali Khan, associate professor

Vitaly Kocherbitov, postdoc

Tomas Landh, senior researcher

Björn Lindman, professor

Per Linse, professor

Iseult Lynch, Postdoc

Maria de Graca Miguel, visiting professor (Coimbra University)

Gemma Montalvo, postdoc

Tommy Nylander, associate professor  
 Gerd Olofsson, associate professor  
 Ulf Olsson, professor  
 Lennart Piculell, professor  
 Karin Schillén, assistant professor  
 Olle Söderman, professor  
 Krister Thuresson, assistant professor  
 Fredrik Tiberg, adjunct professor  
 Magnus Ullner, assistant professor  
 Stefan Ulvenlund, assistant professor  
 Ingemar Wadsö, professor em  
 Håkan Wennerström, professor

### Graduate students working on a Ph. D. Thesis

Anna Akinchina	Jörgen Jansson
Maria von Bahr ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )	Malin Jönsson
Joakim Balogh	Maria Karlberg
Jan-Willem Benjamins	Leif Karlson
Johanna Borné	Anna Körner
Karin Bryskhe	Cecilia Leal
Malin Bydén-Sjöbom ( <i>jointly with Mid Sweden University, Sundsvall</i> )	Carin Malmberg
Marité Cárdenas	Mary Molund
Joakim Carlén	Jens Norrman
Fredrik Carlsson ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )	Martin Olsson
Rita Dias	Johan Reimer
Monica Egermayer	Yulia Samoshina
Caroline Ericsson	Stefanie Schneider
Jonny Eriksson ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )	Helen Sjögren
Alex Evilevitch	Jesper Sjöström
Katarina Flodström	Marie Skepö
Yoshikatsu Hayashi	Anna Stenstam
	Johanna Stiernstedt ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )
	Anna Svensson
	Daniel Topgaard
	Christy Whiddon

### Technical-Administrative Personnel

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

**GUESTS**

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Vacklin, Hanna, UK, (L)  
Vincent, Brian, Univ Bristol, UK, (S)  
von Rybinski, Wolfgang, Henkel, Düsseldorf, (S)  
Yang, Ya-Wun, National Taiwan University, Taiwan, (S)  
Zanatti, João Pedro, Ambassador, Embassy of Portugal, Stockholm, (S)  
Åkerman, Björn, Chalmers University of Technology, Göteborg, (S)  
Ödberg, Lars, AssiDomän AB, Stockholm, (S)

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

## PUBLICATIONS

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8. Borne, J.; Nylander, T.; Khan, A.  
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## WELCOME TO VISITORS

Dear Visitor,

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

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

To arrange a visit, you may contact an appropriate member of our department. Depending on the nature of the visit different arrangements may be made. Help with accommodation can be provided by Majlis Larsson. Ali Khan has the general responsibility for visitors, such as working place for long-term visitors and schedules for certain short-term visitors. In many cases we have found that smaller, less formal seminars, lead to better information exchange.

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

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

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