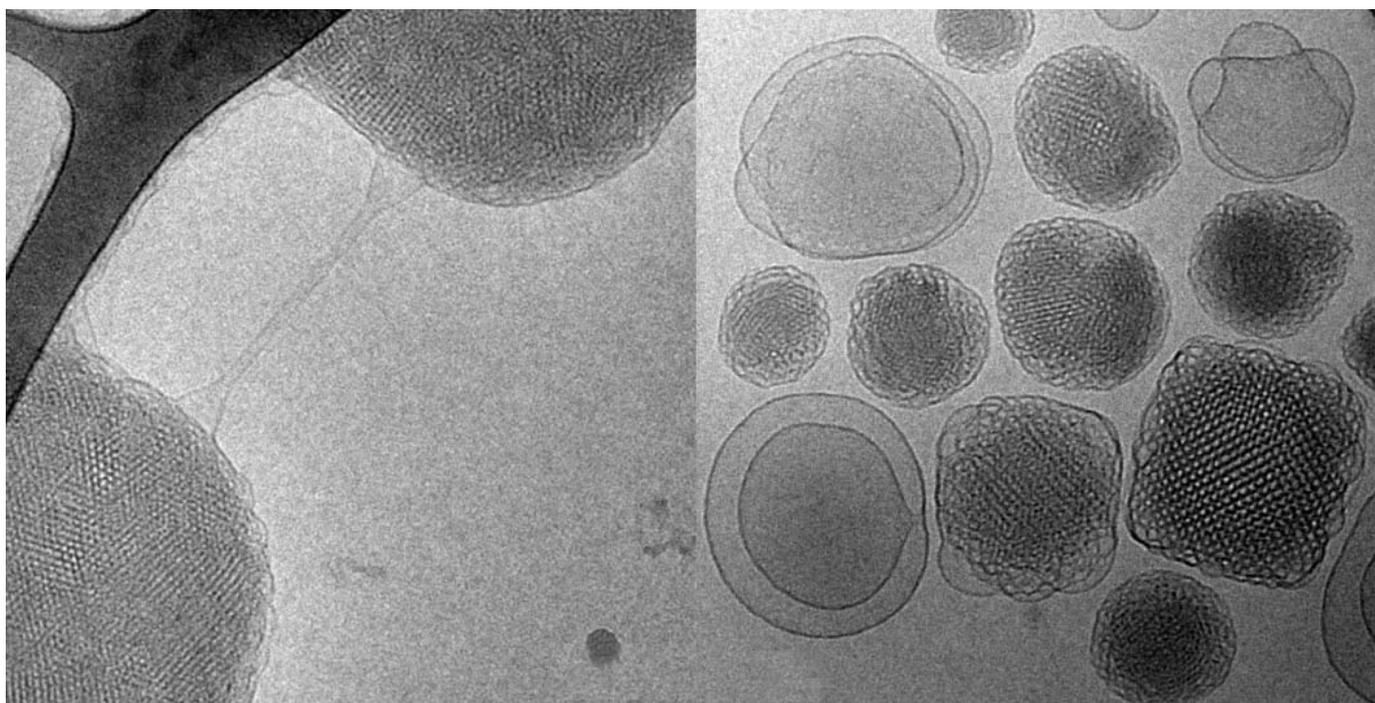


# PHYSICAL CHEMISTRY 1

CHEMICAL CENTRE, SCIENCE FACULTY



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Cover: Formation of different microstructures such as cubosomes, hexosomes, vesicles by lipolysis of cubic liquid crystal dispersions of monoolein as images by cryo-TEM. (image recorded by J. Borné)

This report is produced by Ali Khan and the layout is designed by Johan Reimer



Ali Khan



Johan Reimer

## 2001: A PHD ODYSSEY

My generation grew up with an image of 2001 created by the famous Stanley Kubrick movie from '68. As we all know, reality was to become completely different. From our spot on the globe we can report that the most futuristic scenes seen around here – some orders of magnitude less spectacular than those painted by Kubrick – were a couple of outrageous apartments at the Malmö housing fair, “Bo01”. Unlike Kubrick’s movie, the housing fair was a disastrous commercial failure, so may be the future doesn’t sell too well anymore.

Be that as it may, but one of our own most memorable arrangements in 2001 had – superficially, at least – more to do with the past than with the future. For some time, the idea had been growing among us that it would be interesting and useful to get some systematic feedback from our “old” PhDs, who got their degree at our department. We were wondering: What do they think now, in retrospect, about their PhD education? What turned out to be most useful or valuable? What were the bad parts? And, do they have some good advice for those of us who are now struggling to finish their theses?

So, we sent out a very ambitious questionnaire to those 24 PhDs who got their degrees from Phys Chem 1 during 1996-2000. We were very pleased to receive similarly ambitious answers from no less than 17 of them, and I had a somewhat demanding, but very interesting, task during late summer to summarize all the (anonymous) answers. The summary was then distributed to the former and present PhD students, and to all active PhD advisors at the department.

Most importantly, we followed up the questionnaire with a reunion in October. At the reunion, 17 old PhDs, 22 present PhDs, and 9 current thesis advisors from the department spent half a day together, devoted to the theme “Before and after D-day”. We started with an afternoon of lively group discussions, and then we threw a party. It was wonderful that so many of our former PhD students found it worthwhile to visit and give feedback to their old department. The “before D-day” crowd found it very valuable to discuss with those that were now safely past the thesis submission. Conversely – and interestingly – a few of the old PhDs are now active advisors to PhD students, and they found a day devoted to PhD education quite valuable professionally.

We were pleased to find that the overwhelming majority of the old PhDs were quite satisfied with the contents of their PhD education, and with the atmosphere at the department. This does not mean that there was no criticism, but it was not systematic. In fact, the opinions about what was most valuable also varied within wide ranges. The differences in views on the “dos and don’ts” of PhD education reflect not only differences in personalities, but also differences in current job situations. One of the difficulties in optimizing PhD education is, obviously, that we don’t know what a given PhD student will be doing in his/her life after D-day.

I daresay that all of us who participated came out with a better appreciation of the spectrum of opinions about, and the general complexity of, PhD education. Hopefully, this will help us all to better understand and handle problems that we may encounter in the future. Since we found the exercise quite rewarding, both intellectually and socially, we are thinking of doing something similar soon again. I believe the sequel to “2001: A Space Odyssey” was called “2010”. Maybe we will act sooner.

Lennart Piculell



## 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).

**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); Aerosol OT-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).

**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. 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) 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.

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, H. Wennerström; P. Uhrmeister and R. Strey (Köln)).

**Divalent surfactants.** Used as stabilizers for asphalt emulsions and for disinfection, these surfactants provide a good test case for theories of micellar aggregation. Basic properties of divalent surfactants with monovalent counterions

have been studied for some time. Electrostatic theories account well for bulk properties. Work is now centered on studies of the adsorption of divalent surfactants, with special emphasis on Gemini surfactants, from solution onto silica surfaces. Adsorption isotherms are determined by means of ellipsometry, and the properties (aggregation numbers, etc.) of the adsorbed micelles are probed with fluorescence quenching methods. Poisson-Boltzmann level theories are used to rationalise the experimental findings. (O. Söderman, B. Jönsson, 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)).

**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. (A. Khan, U. Olsson, J. Reimer, O. Söderman, C. Whiddon, I. Johansson (Akzo Nobel)).

**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. (T. Le, U. Olsson, K. Mortensen (Risø), Walter Richtering, (Kiel), Florian Nettekheim (Kiel), Cesare Oliviero (Cosenza), Johannes Zipfel (ILL Grenoble), Peter Lindner (ILL Grenoble)).

**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. Melander, D. Topgaard, M. Nydén (Chalmers), P. Linse, 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 draw-backs, most importantly a low long-term chemical stability in aqueous solution. Within the present project, novel non-ionic surfactants synthesised from renewable resources 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).

### **Polymers, Solutions, Gels and Phase Behavior**

**Effect of glycols on the microstructure of lyotropic liquid crystals formed by poly(ethylene oxide)-poly(propylene oxide) block copolymers.** Isothermal phase diagrams have been studied for ternary systems consisting of a poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) triblock copolymer (Pluronic F127, Pluronic P105, or Pluronic L44), water, and a cosolvent (glycerol, propylene glycol, ethanol, glucose, polyethylene glycol, or PEG400). Our systematic data allow us to address the following aspects: (i) effect of glycols on the phase behavior of Pluronics in water, (ii) effect of temperature on the Pluronic-water-glycol phase behavior, (iii) effect of Pluronic PEO content on the Pluronic-water-glycol phase behavior, and (iv) effect of Pluronic molecular weight on the Pluronic-water-glycol phase behavior. The trends observed in the phase behavior are confirmed and reinforced by microstructural information on the role of glycols on the block copolymer obtained from small-angle X-ray scattering. (R. Ivanova, P. Alexandridis, B. Lindman).

**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 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 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. Schillén, K. Bryskhe, J. Jansson, U. Olsson).

**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 a hydrophobically modified polymer (HMHEC). 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. Small amounts of added surfactant destroy the amylose-HMHEC complexation by competitive association to HMHEC and, presumably, also by complexation between the surfactant and amylose (M. Egermayer, I. Chronakis, 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 Lena Holmdahl (Östra Hospital, University of Göteborg) 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 (Björn Lindman).

**Capillary-induced forces between particles in polymer solutions near phase separation.** The stability of polymer solutions is studied when colloidal particles are added to solutions. The added particles can induce phase separation in the solution, if the polymer solution itself is close to phase separation. We have shown that the induced phase separation is due to formation of a new phase between the particles, a capillary phase. The formation of a capillary phase in the gap between the particles is driven by a lower surface energy for this phase, compared to the bulk phase. Polymer systems investigated have been of two kinds; ternary systems e.g. PEO/dextran/water and quasi-binary systems e.g. EHEC/water. In both kinds of systems, capillary induced phase separation occurs. Some parameters that affect the formation of capillary induced phase separation are molecular weight of the polymers, the affinity for the polymers to the surface, the composition of the sample and the distance between the particles in the solution. (M. Olsson, F. Joabsson, P. Linse, L. Piculell)

**Capillary-induced phase separation.** The formation of a capillary phase in segregating mixed polymer solutions confined between two planar walls has been modelled by using a lattice mean-field theory for flexible polymers in solution. A capillary-induced phase separation (CIPS) may appear in systems where the two polymer components display different preference for the wall, the preference being either of energetic or entropic origin. A long-range attractive force operating between the walls across the polymer solution is associated with the CIPS. The effects of the chain length asymmetry, the solution composition, and the interactions with the walls on the range and the magnitude of the attractive force have been analysed. For compositions near the binodal curve and far from the critical point, the range of the attractive force exceeds far the dimension of the polymer chains. (F. Joabsson and P. Linse).

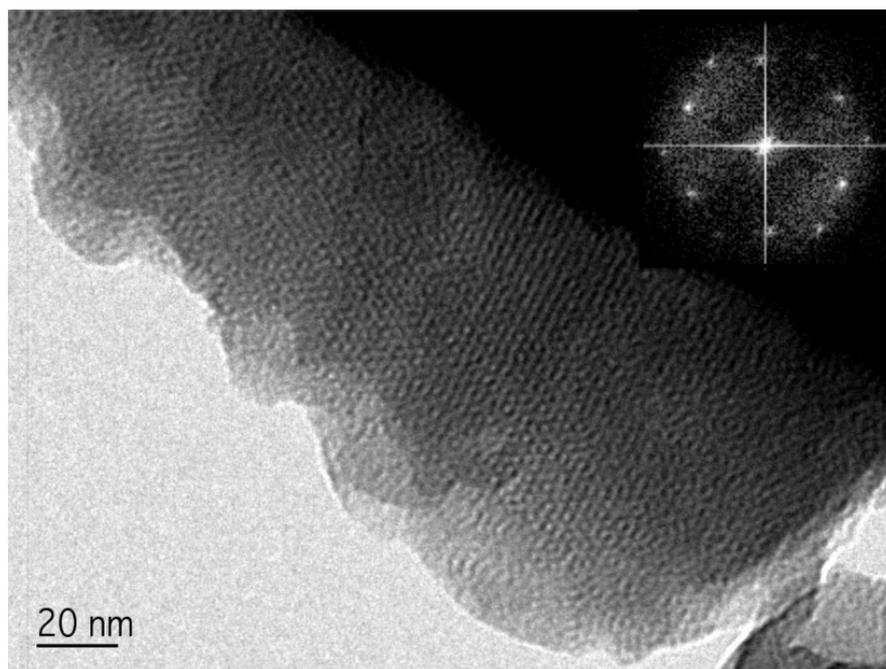
**Mixed block copolymer/graft copolymer systems.** Aqueous systems containing both a block copolymer and a hydrophobically modified water-soluble polymer are investigated with respect to self-assembly, phase behavior and rheology. The project focusses on graft copolymers derived from polysaccharides and di- and triblock copolymers, including end-capped poly (ethylene glycol). (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. 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. A remarkable decrease of the viscosity is found when small amounts of CD is added to a solution of HM-Peg. The CD seems to specifically deactivate the rheologically most important hydrophobic associations. (L. Karlson, K. Thuresson, B. Lindman).

**Correlation between structure of HM-polymers and properties of their aqueous solutions (e.g. phase behavior and rheology).** Parameters that have been varied are: the length of the polymer hydrophobic tail, the length of a spacer group between the polymer and the hydrophobic tail, and the charge density of the polymer. It was found that strongly associating groups favour network formation and phase separation, while charged groups enhances solubility. (S. Nilsson, L. Karlson, K. Thuresson, B. Lindman).

**New dissolution of dry polymers.** This new area of research has begun in 2001 as a PhD project within CAP. The aims are to closely investigate the process whereby a dry sample of a water-soluble polymer swells and finally dissolves when immersed in an aqueous solution. The concentration profile in the swollen polymer matrix, and the rate of ultimate release of polymer into the surrounding bath, are parameters that will be studied. A detailed understanding of the dissolution of dry polymer is of obvious relevance to tablet formulations of pharmaceutical drugs, but the approach is fundamental. Primary objectives are to investigate how polymer parameters such as molecular mass, polydispersity and persistence length influence the dissolution process. (A. Körner, A. Larsson (AstraZeneca Mölndal), L. Piculell).

**Mesoporous inorganic materials.** Inorganic material with pores in the meso range can be synthesised by supramolecular templating with surfactant aggregates acting as templates. 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 cubic. Characterization is primarily performed with SAX, TEM and BET. (K. Flodström and V. Alfredsson).



Transmission electron micrograph of mesoporous aluminium oxide particles formed with the anionic surfactant sodium dodecyl sulphate acting as a template.

**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)).

### Polymer-Surfactant Systems

**Vesicle formation and stability.** In recent years, there have been considerable interests in using vesicles made of long double-tailed cationic synthetic amphiphiles (e.g., dimethyldialkylammonium halides and dialkylphosphate acid esters) as vehicles for gene delivery and as membrane model systems. However, the physicochemical properties of these vesicles are still not well characterized. Size, polydispersity, thermotropic phase behavior, surface potential, permeability, and physical stability of vesicles generally depend on the preparation protocol and on the physical conditions in the bulk solution. Our objective here is to examine the effects of vesicle preparation method, concentration and counterion of the amphiphiles, temperature, and additives on vesicle formation and physical (thermodynamic and colloidal) stability. We also examine the addition of surface polymers as steric stabilizers for cationic vesicles. This study includes techniques such as differential scanning calorimetry (DSC), isothermal titration calorimetry (ITC), cryo-TEM and scattering techniques. (P. Barreireiro, G. Olofsson, E. Feitosa (Brazil)).

**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. Since the coil dimensions are (much) larger than the thickness of the water layers two phases in equilibrium form; the AOT rich phase and one phase rich in the polymer. The polymer rich phase exerts an osmotic pressure that reduces the water content in the AOT rich phase, and by compression the repeat distance is reduced. (Joint project with I. E. Pacios, A. Horta and C. S. Renamayor, Madrid; B. Lindman, K. Thuresson).

**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.** Here we take a new approach to the phase behavior of oppositely charged polymers and surfactants. Conventional studies deal with aqueous mixtures of a polyelectrolyte (e.g., sodium polyacrylate, NaPA) with a conventional surfactant (e.g., cetyltrimethylammonium bromide, CTABr or acetate, CTAAC). 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) 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 and for CTAPA/CTAAC/water. Pure CTAPA swells in water, forming first a hexagonal and then a cubic phase. The hexagonal phase can be formed with arbitrary proportions of polymeric (PA) and monomeric (Br or Ac) anions. The cubic phase is destroyed (in favour of the hexagonal phase) already at small proportions of Br anions, but it survives when Ac is used as the monomeric surfactant counterion. 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. (A. Svensson and L. Piculell; B. Cabane and P. Ilekti (Paris)).

**Thermodynamics of DNA-cationic lipid interactions.** DNA and cationic liposomes form complexes that are promising candidates for gene therapy. Previous studies by Rädler et al. and Lasic et al. using synchrotron x-ray scattering and cryo-TEM have elucidated the structure and morphology of these complexes. Thermodynamic properties, however, are lacking in the literature and warrant further investigations to better understand the mechanics and biological function of these complexes. We employ calorimetric and spectroscopic techniques to measure the thermodynamics of the interactions between DNA and cationic liposomes. Our results indicate that the binding enthalpy depends on membrane charge density and bending rigidity of the lipid bilayers and on the solution conditions (ionic strength and temperature). (P. Barreleiro, G. Olofsson, Björn Lindman).

**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 catanionic mixtures, DNA compaction at vesicles was documented. (R. Dias, B. Lindman, M. Miguel).

**DNA-gemini surfactants interactions.** Gemini surfactants show great promise in the context of gene delivery. Here we investigate the interaction between DNA and various Gemini surfactants. The Geminis are systematically varied with respect to valency, spacer length and size of the hydrophobe. The methods are self-consistent field calculations and fluorescence microscopy techniques. (M. Van Eijk, O. Söderman). Project completed.

**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)

**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 differential scanning calorimetry and isothermal titration calorimetry in combination with dynamic and static light scattering 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. (R. Cardoso da Silva, J. Jansson, A. Niemiec, K. Schillén, G. Olofsson, W. Loh).

**Hydration of DNA and DNA complexes.** The thermodynamics of hydration of DNA and DNA–lipid complexes is studied using sorption calorimetry giving both free energies and enthalpies. (C. Leal, B. Lindman and G. Olofsson).

**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) combined with results from static and dynamic light scattering report on the self-association of the polymers in aqueous solution and also on their interaction with surfactants, other polymers or other additives. One recent study concerned, the solution behavior of dye-labeled PAA and the effects induced by added cationic surfactants in water. Time-resolved fluorescence spectroscopy is utilized to obtain more information on the dye excimer/dimer formation in these systems. (K. Schillén, J. S. Seixas de Melo, J. Jansson, B. Lindman, M. da Graça Miguel).

**Association between a non-ionic microemulsion and hydrophobically modified PEG.** The thickening effect of a hydrophobically modified polymer 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. (Joint project with F. Antunes and M. Miguel, Coimbra; B. Lindman K. Thuresson,).

## 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-dodecylsulfatesulfate, free from simple salts, is synthesised by the precipitation technique. The phase equilibria of the ternary system complex salt-sodium dodecylsulfatesulfate-water are investigated and the resulting phase diagram is used as fundamental for theoretical discussion and modelling. 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. (A. Stenstam, G. Montalvo, A. Khan, H. Wennerström).

**Protein-lipid interactions.** Studies on the relation between the lipid phase behavior and protein-lipid interactions make use of cryo-TEM, X-ray scattering and different NMR techniques. Mixtures of  $\beta$ -lactoglobulin (the major whey protein in milk, which is known to bind lipids) and phospholipid, are mainly investigated. The studies involve liquid crystalline (lamellar) phases, vesicle suspensions and the protein-lipid interactions at interfaces, e.g. emulsions. (T. Nylander, A. Khan; R. Bauer (Denmark); J. Skov-Pedersen (Denmark); M. Paulsson (Food Engineering); B. 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  $\alpha$ -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. *De novo* synthesis of hydrophobically modified polypeptides is also conducted. 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. Gillgren, 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. Gillgren, 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. Large research has been performed to understand the factors determining DNA compaction due to interaction with cationic surfactants or polymers in bulk solution. However, almost no research has been performed on interfacial phenomena. The co-adsorption behavior may be another important factor determining the DNA-surfactant complex efficiency for its delivery to target cells. Solid-liquid interfaces are used as a model system to facilitate the understanding of interfacial properties such as lateral organization and layer composition at technologically relevant surfaces. The main technique being used is ellipsometry, which allows *in situ* measurements of interface processes with high resolution ( $\sim 0.1$  mg/m<sup>2</sup>). Tapping Mode Atomic Force Microscopy measurements is also used to visualize the interfacial structures and therefore gain some information on lateral organization of adsorbed layers. Using surface film balance measurements, understanding is gained on the interactions of DNA with surfactant head group. Furthermore, the surface film balance technique will be used in combination with ellipsometry, 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, A. Braem, and 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, and F. Tiberg (YKI, Stockholm)).

**Surface forces in semi-dilute polymer solutions.** By using the surface force apparatus (SFA) an attractive force with a long range was observed between macroscopic surfaces immersed in mixed semi-dilute solutions of dextran and poly(ethylene oxide). The range of the force (several thousands angstroms) exceeds the size of individual polymer coils by an order of magnitude. Thus, the range is much too long to be explained by classical depletion or bridging mechanisms. The formation of a capillary condensate between the two surfaces with a polymer composition different from the composition of the bulk solution was suggested to be the underlying mechanism. Despite that ethyl (hydroxyethyl) cellulose (EHEC) is a nominally single polymer system, which has been subject to extensive purification procedures, a similar force was found to operate also in semi-dilute solutions of EHEC. However, a recent separate investigation has shown that EHEC is a multi-component system that contains a range of chemically different polymer chains. The heterogeneity is believed to stem from the manufacturing process. In a similar way as in the dextran-poly(ethylene oxide) mixture, a surface induced segregation between different polymer fractions could be the origin of the long-range attractive force in the EHEC system. (H. Wennerström, K. Thuresson, T. Nylander, F. Joabsson, P. Linse, B. Lindman).

**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) and F. Tiberg (YKI, Stockholm)).

**Behavior of hydrophobically modified polymers at surfaces.** The adsorption of HMP(E)s at surfaces is investigated. Due to their amphiphilic nature HMP(E)s are potentially interesting for stabilizing or flocculating particle and fiber systems. The project deals with the adsorption of different HMP(E)s at surfaces and the relation between their interfacial behavior and their function as stabilizers/flocculants. The adsorption is studied by time-resolved ellipsometry and reflectometry. Studies of isotherms, adsorbed layer thickness, stagnant layer thickness as well as the mass transfer rate are performed. Planar silica surface and hydrophobically modified silica surface are used as model surface and end-capped poly(ethylenoxide) is used as model polymer. (J. Carlén and F. Tiberg).

**Interfacial properties of cellulose derivatives.** Adsorption of EHEC or HM-EHEC on solid surfaces is investigated, and the effect of surfactant on the adsorbed layer is followed. The interfacial polymer-surfactant interaction was found to be correlated to the bulk-behavior of the same systems. Knowledge about the adsorbed layer is used to interpret stability investigations in the EHEC-particle system. (F. Joabsson, K. Thuresson, B. Lindman, E. Blomberg (Stockholm), A.-L. Kjöniksen (Oslo), B. Nyström (Oslo)).

**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)).

## Experimental Methodology in Colloid Science

**NMR self-diffusion experiment in porous systems.** 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. Moreover, the effect of cross-relaxation on the self-diffusion experiment is investigated and quantified. (D. Topgaard, O. Söderman).

**Diffusion in polymer systems.** The overall aim of this project is to extract information about structure and dynamics in self-associating polymer systems. The experimental technique used is the NMR PFG experiment. Ethyl(hydroxyethyl) cellulose and its hydrophobically modified version have been investigated. The interpretation of the NMR echo-decays from such systems are complicated by a number of effects such as polymer polydispersity, scaling behavior with respect to molecular weight and concentration etc. These effects are addressed and relevant information pertaining to the polymer association and gel network is extracted. (B. Håkansson, O. Söderman, M. Nydén (Chalmers)). Project completed.

**Macroscopic background gradients in PGSE NMR diffusion measurements.** Background gradients caused by susceptibility differences at the sample interfaces may seriously effect 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, 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)).

#### **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. (B. Jönsson, M. Nydén (Chalmers), H. Hagslätt (Chalmers), O. Söderman).

**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).

### **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, J. Dacic (YKI)).

**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 by a calorimetric technique and we find a pronounced break in the permeability when the relative humidity reaches the value of the liquid crystal to gel transition of the lipid. (E. Sparr, N. Markova, L. Hallin, H. Wennerström).

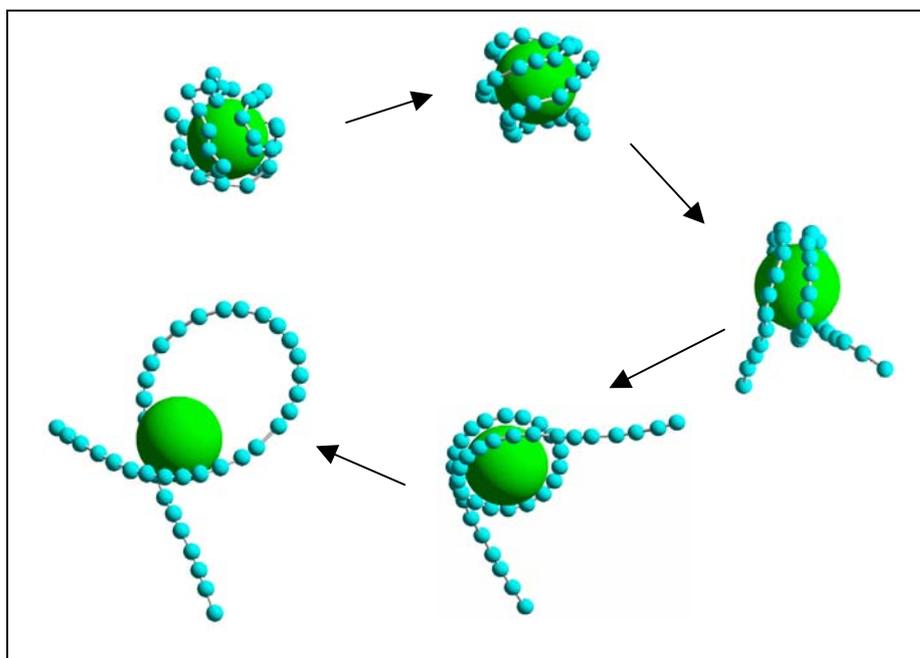
**Phospholipid–cholesterol interactions.** The hydration thermodynamics of a series of phospholipid – cholesterol mixtures have been studied using the sorption calorimeter giving both free energies and enthalpies. The system is additionally studied by the NMR quadrupolar splitting technique. From the 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).

**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 solubilised fatty acid probes, designed to exert a minimum of perturbation on the micelle. The dissociation constant is obtained from pH- titrations 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. (O. Söderman, Bo Jönsson (Theoretical 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 was 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 final results of the structure determination show two possible states differing in their degree of bending, which fits with previous indications that the sequence is inherently flexible and with reports that similar sequences are also bent. (C. H. Y. Lau (Canberra), M. Ullner).

**Solutions of charged colloids.** Model systems of charged spherical macroions and point counterions interacting solely through hard-sphere and Coulomb interaction were investigated by means of extensive Monte Carlo simulations. The parameter space investigated includes nearly all experimental colloidal solutions (in

the salt-free limit) in which the colloids are carrying up 80 (monovalent counterions) or 160 (divalent counterions) elementary charges. At a high electrostatic coupling, these systems display a thermodynamic instability and separates into two phases of widely differing electrolyte concentration. Parts of the binodal surface were determined and critical points were estimated. By employing a temperature and density scaling Monte Carlo simulation method, the determination of the critical point was much improved. Moreover, effective macroion-macroion potentials were extracted from reverse Monte Carlo simulations and at higher electrostatic coupling these potentials displayed attractive regions. The nature of the effective macroion-macroion potential has also been revisited by employing the Debye-Hückel theory. Finally, the effects replacing simple counterions with flexible ones with same or different total valence on the stability of colloidal solutions were examined by Monte Carlo simulations. (P. Linse, V. Lobaskin, J. Rescic, A. Lyubartsev (Stockholm University), D. Chan (University of Melbourne), and S. Petris (University of Melbourne)).



Configurations from simulations of a charged macroion and an oppositely charged polyion with same absolute charges at increasing bare persistence length of the polyion.

**Polyelectrolyte-macroion complex formation.** The complex formation between one charged polyelectrolyte and oppositely charged micelles has been investigated by Monte Carlo simulation. We have gained information on the structure and the complex strength at different conditions. In particular, at increasing micelle concentration the polyelectrolyte becomes saturated with micelles and the degree of overcharging increases with the chain stiffness. Moreover, the chain flexibility plays a decisive role in determining the structure of the polyelectrolyte-macroion complex and a rich spectrum of structures appear. We are currently examining in more detail the effect addition of salt on the structure of a polyelectrolyte-micelle complex as well as on the phase behavior. (M. Jonsson, 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. However, different definitions have been used and these represent different properties. This has caused apparent contradictions in the literature. To remedy the semantic confusion, four main groups of definitions have been identified and given separate names. Monte Carlo simulations illustrate the differences between different types of persistence length and also show a universal behavior for one of the definitions, the projection length. Furthermore, simulations of long chains with truncated interactions suppress end effects and reveal the influence of excluded volume effects. The aim is a better understanding of the interplay between electrostatic interactions and the conformational behavior. (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. (A. A. C. C. Pais (University of Coimbra), M. G. Miguel (University of Coimbra), B. Lindman, and P. Linse)

**Statistical-mechanical programs.** Also during 2001 the statistical mechanical computer program MOLSIM for Monte Carlo and molecular dynamics simulation has substantially been updated and extended. In particular, features facilitating simulation of polyelectrolyte solutions and cross-linked gels have been extended. The software POLYMER for lattice mean-field calculations have been ported to PC's and 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 second year (P. Linse).

**Structures of charged block copolymers.** A novel polymer system containing charged diblock polymers grafted onto a planar 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 is found that the structure of the polymer brush is decisively dependent of the relative charge of the blocks. For certain conditions, bimodal profiles appear which demonstrate the simultaneous presence of two types of chain conformations, one coiled and one stretched. (N. Shusharina; 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 examined by Monte Carlo simulations using two different models. 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. (Y. Hayashi, M. Ullner, and P. Linse).

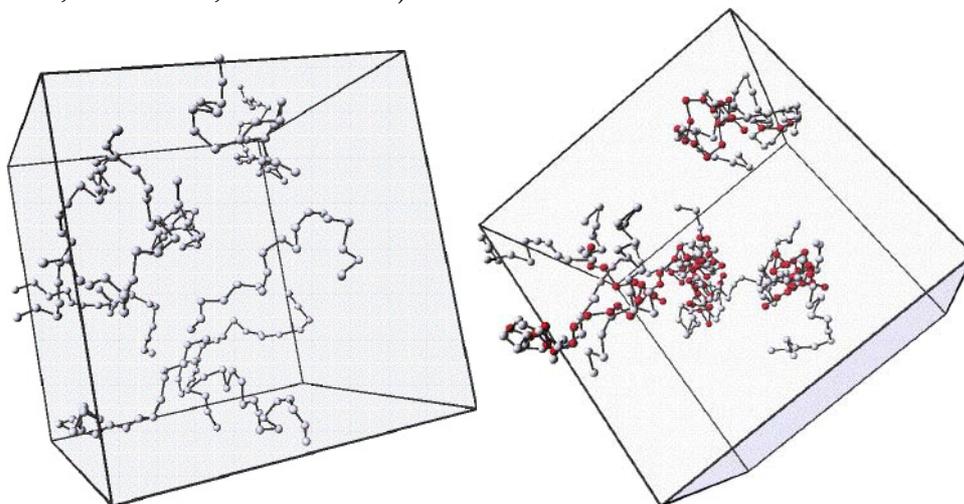


Illustration of a homogeneous polyelectrolyte solution containing 10 negatively charged chains (left) and heterogeneous solution containing 10 negatively plus 5 positively charged chains (right).

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**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. Currently, we are investigating the effect of the chain linear charged density, chain flexibility, and valence of the counterions on the swelling behavior and the structure of the gel (S. Schneider and P. Linse).

**Polyelectrolyte-protein complexation.** A simple model of lysozyme has been established, and the complexation between one polyelectrolyte and the protein model has been examined by employing Monte Carlo simulations. Beside the electrostatic interactions, a short-range attractive interaction between the polyelectrolyte and the protein accounting for hydrophobic interactions was included. The complexation as a function of pH and the electrolyte concentration has been investigated. Moreover, the oligomerization of lysozyme in aqueous solution was investigated by Monte Carlo simulations as a function of protein concentration, pH, and electrolyte screening. In particular, structure factors and equilibrium constants obtained were compared to those obtained experimentally and were found to capture the experimentally obtained effects of pH and ionic strength. (F. Carlsson (YKI), M. Malmsten (YKI), and P. Linse).

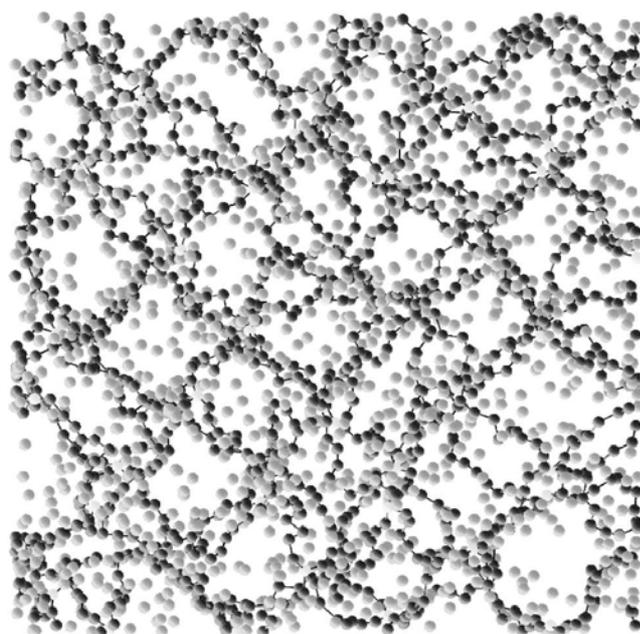


Illustration of a typical configuration of a charged crosslinked gel with charged segments (dark spheres) and counterions (light spheres). S. Schneider, unpublished data

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**Protein-polymer interaction.** Theoretical investigations of the interaction between globular water-soluble proteins and moderately hydrophobic water-soluble polymers have been initiated. The aim is to examine how the strength of the interaction depends on the spatial location of the hydrophobic patches on the protein surface and the consequences on the partitioning of the protein in aqueous two-phase polymer systems (M. Jönsson, M. Jonsson, P. Linse, and F. Tjernelid (Biochemistry)).

### **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° to 155°, a cell housing with an index matching quartz vat, a fiber optical near-monomodal detection system, a detection unit comprised of 2 matched photomultipliers in a pseudo-cross correlation arrangement. For the DLS measurements using photon correlation spectroscopy, two multiple tau digital correlators (with a total of 320 exponentially spaced channels) are utilized to obtain an initial real time sampling time of 12.5 ns. The lag time range extends from 12.5 ns up to  $>10^5$  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°C to +140°C. In addition, a differential refractometer from ALV for the determination of refractive index increments necessary for the SLS experiments is incorporated in the overall set-up with an optical fiber. (Sponsored by 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 can be used together with Optrel Multiskop. 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  $1/\text{Å}$ ) scattering reports on short-range correlations and is helpful for example in discriminating between fluid and frozen surfactant chains. (Sponsored by FRN).

**Ellipsometry.** (contact person: Tommy Nylander). The development of a high precision ellipsometer for time-resolved studies of thin adsorbed films has been successful and of great importance to several specific projects. The instrument allows precise and rapid measurements of the ellipsometric angles  $\psi$  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 Å, 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  $\mu$ l) of the sample onto a holey-carbon grid, which is subsequently immersed in liquid ethane (-183 °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.(Contact person: Vitaly Kocherbitov). 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) (contact person: Gerd Olofsson).

**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**

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 involve 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 2001 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 a research group from the Mid Sweden University in Sundsvall also participates. In addition, important research activities take place at the member companies. The Board of CAP, which includes Lennart Piculell from our department, has an industrial majority.

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.

During 2001, Fredrik Joabsson from our department, Sara Richardson from the department of Analytical Chemistry, and Magnus Norgren from Mid Sweden University, completed their theses financed by CAP. No less than six new PhD projects were launched by CAP in 2001. Two of these deal with film formation from polymer dispersions – a new area of CAP research - and are carried out at the department of Polymer Science and Technology. Another two projects, run at the departments of Biochemistry and Analytical Chemistry, concern the use of cellulases for analysis of substitution patterns in cellulose derivatives. The remaining two new CAP projects are conducted at our department. Maria Karlberg works with interactions in solution between mixed amphiphilic polymers of different architectures, and Anna Körner studies the process of dissolution of a dry polymer sample immersed in aqueous solution.

Activities during 2001 include the Research Symposium in April (where all projects were presented), and two one-day workshops, one in October on “Oppositely Charged Polymer-Colloid Mixtures” and one in November on “Association Behavior of DNA. Physico-Chemical and Biological Aspects”.

### **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 programs 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 program and an adjoining graduate school in surface and colloid technology. The funding for the 5-year period 1998-2002 amounts to 64 MSEK with 18 MSEK for 2001.

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

- ♦ create a strong fundamental national research program
- ♦ 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 program consists of a nationally coordinated research program 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 Research), 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 Program is Lund University; Program Director is Björn Lindman and Program Secretary Gerd Olofsson. Krister Holmberg (Chalmers University of Technology) is the Director of Studies of the Graduate School.

The research program is divided into 5 areas:

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

At present 41 students are enrolled in the program carrying out projects in Lund, Stockholm, Göteborg, Uppsala, Karlstad, Luleå and Sundsvall. The recruitment of students has stopped and instead postdoc:s are recruited during the final years of the program and there are now four postdocs.

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

- ♦ Surface and colloid chemistry- molecular basis and technological applications, Degeberga (25 participants)
- ♦ The Colloidal Domain, Lund, Göteborg and Stockholm (39 participants)
- ♦ Scattering methods applied to complex fluids, Ystad (29 participants)
- ♦ Microscopy- Basic principles and applications to surfactant phase science, Lund (12 participants)
- ♦ Surface characterization and analysis, Stockholm (61 participants)

The Board of 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 Stockholm and one in Lund. The 4<sup>th</sup> General Program Workshop was arranged in Lund in November with participation of the Board, senior scientists, Ph D students and members the Industrial and International Reference Groups, in all 71 participants. The program consisted of plenary lectures and presentations of Ph D student projects in a poster session in the afternoon of the first day and in two sessions of 15 min presentations the second day. During 2001 the Program has been involved as co organizer of the following events:

In January in Göteborg a conference on Nanostructured materials made from self-assembled molecules and particles with 70 participants from 18 countries.

In October in Lund a workshop on Current Applications in Thermochemistry with 70 participants from 10 countries.

Further information on the program (including the complete Program Plan) can be found at the website of the program [www.colintech.lu.se](http://www.colintech.lu.se). The e-mail address is [colintech@lu.se](mailto:colintech@lu.se)

### **The Surface and Colloid Science Center, YKOLL**

YKOLL is an interdisciplinary center on surface and colloid science at Lund University. The center 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 11–12 October, was this year organized in cooperation with the Division of Surface Chemistry of The Swedish Chemical Society, see below. As usual, the program contained an appealing blend of lectures. More than 50 posters (26 of which with authors from our department) illustrated the range of current projects within the area of surface and colloid science. There were this year 135 registered participants.

In conjunction with the Symposium there was this year a one-day seminar on "Oppositely charged polymer-colloid mixtures". The seminar, which had 53 registered participants, was organized by Per Linse and Lennart Piculell, as an activity of the Centre for Amphiphilic Polymers from Renewable Resources. Except for the keynote speaker, Paul Dubin from Indiana/Purdue Universities, the speakers at the conference were Swedish researchers, including Lennart Piculell from our department. The lectures were aimed at an audience of non-specialists, and covered fundamental as well as applied aspects of oppositely charged polymer-colloid mixtures.

**The Division of Surface Chemistry of the Swedish Chemical Society.** This new 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 first symposium in the series was held in Lund in October.

### **The Competence Center for Surfactants based on natural products**

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, 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.

### **ENGEMS – the European Network for Gemini Surfactants**

The department is a member of a European Network, which investigates Gemini surfactants with the ultimate goal to use them in gene therapy. Our contribution to the network is physical chemical investigations of Gemini's synthesized within the network. Participants from Lund are M. van Eijk and I. Söderman. The network was discontinued by the end of 2001.

### **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 Piera) and Coimbra (Maria de Graca Martins Miguel, Hugh Douglas Burrows, Eduardo Marques, Maria Luisa Leito, Maria Ermelinda da Silva Eusebio) Within the scheme, the senior scientists and post-graduate students have the possibility to visit each other's lab. Moreover, there are two workshops per year. Collaborative research activities are focused on the following areas: (a) Formation, structure and dynamics of polymer-surfactant systems, (b) Physico-chemical properties of polymer containing microemulsions and (c) Characterization of new polymer-surfactant adducts. The first network meeting took place in Coimbra (with Ali Khan and Björn Lindman representing Lund). The discussions have been lively and interactive and resulted in identifying several systems that the different groups showed interest to work with these projects.

### **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: XXX Reuniao Annual Sociedade Brasileira de Bioquímica, Caxambu, Minas Gerais; Biofunctional Polymers and Polymers at Interfaces, München, Germany; Gordon Research Conference on Chemistry of Supramolecules and Assemblies, New London, Connecticut; Gordon Research Conference on Chemistry of Polysaccharides, Mount Holyoke, Massachusetts. Björn Lindman also gave a talk at the COST Workshop on Polymer-Surfactant Systems, Coimbra, Portugal and also attended The Nobel Jubilee Symposium on Frontiers in Molecular Sciences, Örsundsbro, Sweden; Workshop on Current Applications in Thermochemistry, Lund; the Conference of the Portuguese Photochemical Society in Costa de Capariga;

The Marcus Wallenberg Prize Symposium, Stockholm; and the 14<sup>th</sup> conference of the European Colloid and Interface Society, Coimbra, Portugal. Björn Lindman was together with Lennart Piculell Conference Chair of the Conference on Amphiphilic Polymers and Gels organized by the United Engineering Foundation in Sintra, Portugal. Björn Lindman also organized together with others at the department a well-attended workshop in Lund (sponsored by the Center of Amphiphilic Polymers) on Association Behavior of DNA, Physico-chemical and biological aspects.

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: Université Pierre et Marie Curie, Paris; Université Paris-Sud, Orsay; ESPCI, Paris; PDVSA-Intevep, Los Teques, Caracas, Venezuela; Universidad de Los Andes, Mérida, Venezuela; Universidad Simon Bolivar, Caracas, Venezuela; Rome University, Rome; Procter&Gamble Research Center, Rome; Rutgers University, Piscataway, New Jersey; Chalmers University of Technology, Göteborg; University of Göteborg; MidSweden University, Sundsvall; SCA Research, Sundsvall; The Swedish Pulp and Paper Research Institute, Stockholm; Universidade Nova de Lisboa, Costa de Capariga, Portugal; Department of Chemistry, University of Coimbra, Portugal; Department of Physical Chemistry, Uppsala University; Institute for Surface Chemistry, Stockholm; Royal Institute of Technology, Stockholm. Björn Lindman was visiting professor at Department of Chemistry, Coimbra University and Université Pierre et Marie Curie, Paris.

Håkan Wennerström delivered the invited talks at Particles 2001, in Orlando Fl.; at Physics Meets Biology, in Helsinki, with an additional contribution at the affiliated summer school and the Workshop on Current Applications in Thermochemistry, Lund. Olle Söderman organized one session and presented a talk at the 15th Annual Meeting of the European Colloid and Interface Society (ECIS) in Coimbra, Portugal. He also took part in several network meetings in connection with his participation in ENGEMS (European Network for Gemini Surfactants) and SNAP (the competence center for Surfactants based on Natural Products). Together with Ingemar Wadsö, he organized a one-day symposium on Current Applications in Thermochemistry, Lund, on the occasion of the retirement of Gerd Olofsson.

Per Linse delivered invited seminars/talks at Henrich-Heine Universität Düsseldorf; Forschungszentrum Jülich, Germany; at the conference, Particles 2001, Orlando; at the annual research seminar of the Center for Amphiphilic Polymers (CAP), Bäckaskog Castle; at the minisymposium, Forces between charged macroions, Lund University; at the miniconference on Charged systems, Göteborg University. Per also presented a Poster at the SIMU conference on Bridging the time-scale gap, at Konstanz, Germany. Vladimir Lobaskin, and Stefanie Schneider also attended the SIMU conference and presented posters. Stefanie presented a poster at the CAP research seminar. Per Linse and Shusharina Nadezhda presented both oral and posters at the EuroConference on the Physics of Surfactants and Polymers at Interfaces, Evora, Portugal. Per Linse, Magnus Ullner, Marie Jonsson, Stefanie Schneider, J. Rescic, Y. Hayashi and Anna Akinshina, gave oral presentation at the ECIS conference at Coimbra. Linse, Ullner, Jonsson, Schneider, Akinshina, Hayashi and Nadezhda gave oral presentation at YKOLL symposium, Lund. Per, Stefanie, Yoshikatsu and Magnus exhibited posters and also gave oral presentation at the SSF Colloid and Interface Technology workshop, Lund. Linse presented Poster at the conference on the Interface of Biology, Chemistry and Physics Il Cioccio, Italy. Nadezhda and Linse gave oral presentation at the Euro Conference on the Interfaces

and Thin Films of Polymers and Colloidal Systems, Acquafredda di Maratea, Italy. Marie and Stefanie gave invited seminar at the Physical Chemistry, Uppsala University.

Gerd Olofsson organized and actively participated three symposiums/workshops - Surface and Colloid Science (YKOLL), Current Applications in Thermochemistry, and Association Behavior of DNA, Physico-chemical and Biological Aspects. Lennart Piculell organized, chaired and gave a talk at the international conference on Amphiphilic Polymers and Gels in Sintra, Portugal. Other contributions from the department were an invited talk by Ulf Olsson, and posters by Rodrigo Cardoso da Silva, Rita Dias, Helen Gillgren, Karin Schillén, and Anna Svensson. Lennart organized, together with Per, a one-day seminar for CAP on oppositely charged polymer-colloid mixtures; gave invited seminar/talk at the Van't Hoff Laboratory for Physical and Colloid Chemistry at the University of Utrecht; at SCA Hygiene Products, Mölndal; at the Danish Polymer Centre at Risø, Denmark; and at SIK, Gothenburg. Ulf Olsson Viveka Alfredsson, Katarina Flodström and Joakim Balogh, visited Aarhus University where Ulf gave a seminar. Ulf also presented a seminar at the Köln University. Karin Schillén presented the research activities within the Foundation of Strategic Research program Colloid and Interface Technology at a symposium for all programs of the Foundation of Strategic Research, at Stockholm and also presented poster at the SSF Program Colloid and Interface Technology. Karin attended the workshop on Association Behavior of DNA at Lund. Karin Schillén, Karin Bryskhe & Jörgen Jansson presented posters at XV ECIS conference, Coimbra and YKOLL workshop, Lund. Viveka and Katarina attended the conference on nanostructured materials made from self-assembled molecules and particles, at Hindås, Sweden, and presented poster. Katarina also presented posters at the 13<sup>th</sup> International zeolite conference, Montpellier and YKOLL workshop, Lund. Gemma Montalvo presented a poster at YKOLL, Lund; and attended the workshops on oppositely charged polymer-colloid system and Current applications in thermochemistry, Lund.

Rita Dias gave two oral presentations, one at the ECIS Conference, Coimbra and the other, at the workshop in Coimbra on Polymer-Surfactant Interactions. Rita and Paula Barreleiro presented posters at the Conference on Assembly and Self-Assembly at the Interface of Biology, Chemistry and Physics, Il Ciocco, Italy and at the workshop on Association Behavior of DNA, Lund. Ali Khan was a guest scientist for one month at Camillo La Mesa's Lab by the invitation of the Faculty of science, University of Rome, "La Sapienza", gave several seminars in the faculty of science. He also gave invited seminar at the chemistry department, University of Palermo.

## 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 is 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 member of the Research Council of The Swedish Pulp and Paper Research Institute. He is a member of The Royal Swedish Academy of Engineering Sciences, of The Royal Swedish Academy of Sciences and of

The Royal Physiographic Society in Lund. He is Program Director for the national program on Colloid & Interface Technology sponsored by the Swedish Foundation for Strategic Research. 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 attended the 41st IUPAC General Assembly in Brisbane, Australia as secretary of the IUPAC Physical Chemistry Division Committee. Gerd is chairman of the newly founded Division of Surface Chemistry of the Swedish Chemical Society and was responsible for the organization of the Symposium on Surface and Colloid Science in October in Lund. Gerd is a member of the Advisory Board for *Thermochimica Acta*. Olle Söderman served on the PhD Thesis committee for Alex Evilevitch, Physical Chemistry, Lund University. Lennart Piculell served on PhD Thesis committees for Charlotte Wiberg, Cell and Molecular Biology, Lund University, Niklas Lorén, Chalmers Institute of Technology and Fredrik Tufvesson, Food Technology, Lund University. Lennart was a member of the committee for PhD education at the Chemical Center, a member of a special committee evaluating the basic chemistry courses at the faculty of science, LU. Both Lennart and Per Linse were members of the program committee of the Center for Amphiphilic Polymers. Lennart also served as a member of the editorial boards of the *Food Hydrocolloids* and *Carbohydrate Polymers*. He acted as an external reviewer for NSF research proposal, the chair in Biotechnology/Biopolymer chemistry NTNU, Norway, the "lektorat" at Uppsala University and the "docentur" at Uppsala University. Ulf Olsson served as a member of the PhD thesis committee for Markus Johnsson at Uppsala University. Tommy Nylander served as an external examiner for the thesis of Nobou Maeda at the Department of Applied Mathematics, Australian National University, Canberra. Karin Schillén was a member of the board of the Foundation of Strategic Research program "Colloid and Interface Technology".

## 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, Eva Hansson and Olle Söderman taught parts of the course. Johan Reimer and Marie Jonsson were in charge of the laboratory exercises. Bengt Jönsson and Ulf Olsson gave lectures during the second chemistry course, and Eva Hansson, Lennart Piculell, Olle Söderman and Magnus Ullner 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 shares the teaching with Bengt Jönsson.

As regards higher courses, the department gives one basic and one advanced course in surface and colloid chemistry. The basic course, which is a biannual event, is headed by Ulf Olsson and taught by Ulf, Lennart Piculell and Karin Schillén. The advanced surface and colloid chemistry course is organized and taught by Håkan Wennerström (main teacher) along with Lennart Piculell. Per Linse and Karin Schillén also took part in the teaching of the course- It is given one a year during the

fall semester, and is based on the book by Håkan Wennerström and Fennel Evans. 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.

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 2001, the course was held, for the tenth consecutive year, in Barcelona and the same course was also held for the first time in the US (Danbury, Connecticut) in both cases with Björn Lindman as one of the teachers. Björn Lindman also gave a course on surfactant and polymer solutions at Coimbra University and at PDVSA-Intevep, Los Teques, Venezuela 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 Program (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. Within the SSF program, there were two courses for the Ph. D. students. One organized by Gerd Olofsson on DSC – basic principles and applications to phase studies with Galina Chernik as the main teacher. The second course entitled Microscopy - Basic principles and applications to surfactant phase science was arranged by Ali Khan. Oren Regev (Israel). Viveka Alfredsson and Ali Khan were the teachers. Ingemar Wadsö gave short courses for Ph. D. students on Isothermal Microcalorimetry at the University of Tucuman, Tucuman, Argentina and University of Campinas, Campinas, Brazil. Olle Söderman was in charge and one of the four teachers for the Ph. D. course given on NMR basic physics and applications as a part of the Colloid and Interface Technology research school. 30 graduate students attended the course.

Lennart Piculell and Olle Söderman gave popular lectures for high school (gymnasium) students and teachers visiting Lund University. Olle talked about soaps and Lennart, on gels. Anna Svensson and Anna Stenstam presented several chemical shows for the high school students.

## **FINANCIAL SUPPORT**

For the fiscal year 2000/2001 the department had a turnover of ca 35 million SEK, which is higher compared to the fiscal year 1999/2000. From the University we obtained 15.2 million of which 2.7 million is to cover undergraduate teaching; 3.4 million, for graduate students; and 9.1 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 are: The Natural Science Research Council (NFR), the Swedish Research Council of Engineering Sciences (TFR), which provide us a support of, respectively, 2.5 million and 1.2 million SEK. The Swedish Board for Industrial and Technical Development (NUTEK/Vinnova) which finances more applied projects supports us with 3.7 million, mainly via the Competence Center, during the fiscal year. We also received 11.5 million SEK from The Swedish Foundation for Strategic Research (SSF), which is an important funding agency for supporting novel research venture in Sweden. We are grateful for support from

private industry, directly and via their foundations, amounting to ca. 0.36 million, and 0.48 million from The European Commission.

## DOCTORAL THESIS

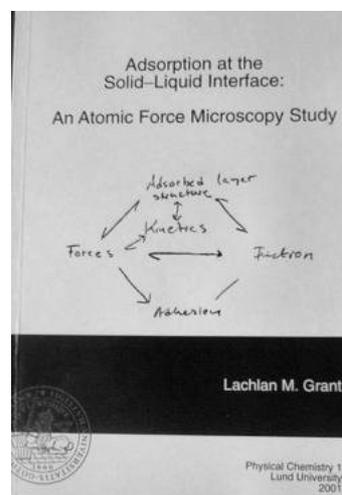
January 24, 2001

**Lachlan M. Grant**

*Adsorption at the Solid-Liquid Interface:  
An Atomic Force Microscopy Study*

Opponent: Dr. Robert K. Thomas

Physical & Theoretical Chemistry, Oxford, UK



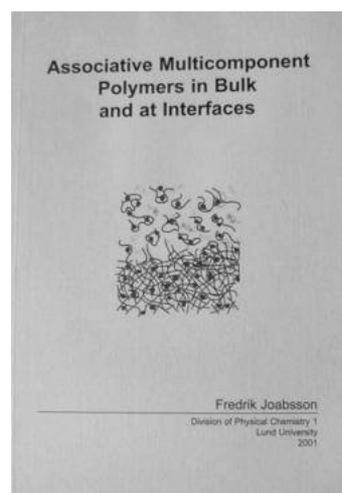
March 23, 2001

**Fredrik Joabsson**

*Associative Multicomponent  
Polymers in Bulk  
and at Interfaces*

Opponent: Prof. Per Claesson

Department of Chemistry  
and Surface Chemistry, KTH, Stockholm

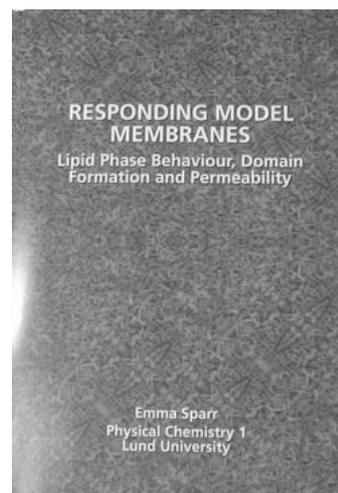


May 11, 2001

**Emma Sparr**

*Responding Model Membranes.  
Lipid Phase Behavior, Domain  
Formation and Permeability*

Opponent: Prof. Gregor Cevc  
Technical University, Munich

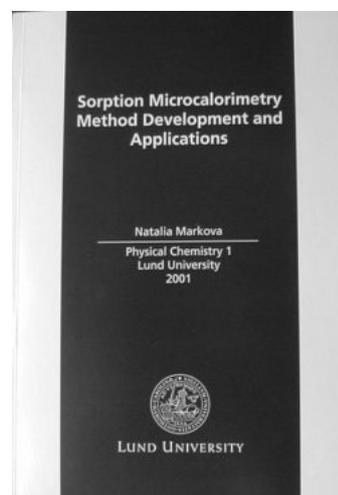


October 26, 2001

**Natalia Markova**

*Sorption Microcalorimetry:  
Method Development  
and Applications*

Opponent: Dr. Jean Rouquerol  
MADIREL, Marseille

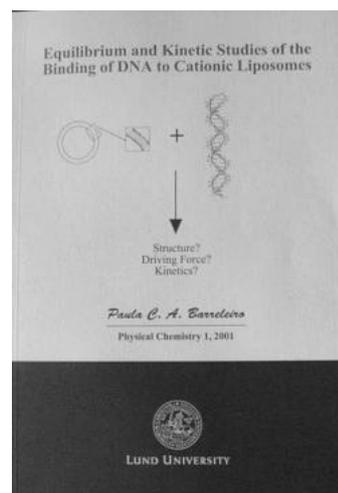


November 6, 2001

**Paula Barreleiro**

*Equilibrium and Kinetic Studies of the  
Binding of DNA to Cationic Liposomes*

Opponent: Prof. J. O. Rädler  
Sektion Physik Ludwig-Maximilians  
Universität München

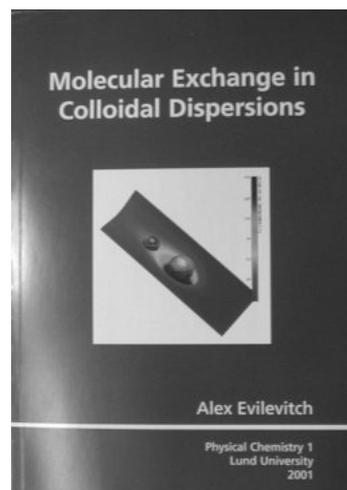


November 27, 2001

**Alex Evilevitch**

*Molecular Exchange in  
Colloidal Dispersions*

Opponent: Prof. William M. Gelbart  
Dept. of Chemistry and Biochemistry  
University of California

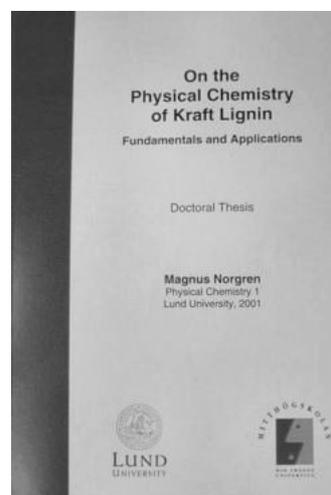


December 14, 2001

**Magnus Norgren**

*On the Physical Chemistry of Kraft Lignin.  
Fundamentals and Applications.*

Opponent: Prof. Lars Ödberg  
Assi Domän AB, Stockholm



## MEMBERS OF THE DEPARTMENT

### Scientists/Teachers

Paschalis Alexandridis, (on leave), assistant professor  
Viveka Alfredsson, assistant professor  
Alan Braem, postdoc  
Marcel van Eijk, postdoc  
Kristen Eskilsson, assistant professor  
Eva Hansson, associate professor, dean  
Bengt Jönsson, associate professor  
Ali Khan, associate professor  
Vitaly Kocherbitov, postdoc  
Tomas Landh, senior researcher, (Camurus Lipid Research Foundation)  
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	Marie Jonsson
Joakim Balogh	Malin Jönsson
Paula Barreleiro	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> )	Natalia Markova
Merité Cárdenas	Carin Melander
Joakim Carlén	Mary Molund
Fredrik Carlsson ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )	Magnus Norgren ( <i>jointly with Mid Sweden University, Sundsvall</i> )
Rita Dias	Martin Olsson
Monica Egermayer	Maria Palsander ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )
Caroline Ericsson	Johan Reimer
Jonny Eriksson ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )	Yulia Samoshina
Alex Evilevitch	Stefanie Schneider
Katarina Flodström	Jesper Sjöström
Helen Gillgren	Emma Sparr
Lachlan Grant ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )	Anna Stenstam
Yoshikatsu Hayashi	Johanna Stiernstedt ( <i>jointly with Institute for Surface Chemistry, Stockholm</i> )
Jörgen Jansson	Anna Svensson
Fredrik Joabsson	Daniel Topgaard
	Christy Whiddon

### Technical-Administrative Personnel

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

**GUESTS**

Alberius, Peter, Stockholm (S)  
Allahyarov, Elshad, University of Düsseldorf, Germany (S)  
Álvarez, Marta, Spanien, Marie Curie Student Fellowship (L)  
Angelescu, Daniel, Bucharest, Marie Curie Student Fellowship (L)  
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Cevc, Gregor, Techn. Univ. Munich (S)  
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Kapashmiri, Abha, Stockholm (S)  
Kazutami Sakamoto, Ajinomoto Co., Japan (S)  
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Mariette, Francois, France (L)  
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McLoughlin, Daragh, Univ College Dublin (L)  
Me'lnikov, Segey, Unilever, Vlaardingen, Nederland (S)  
Miguel, Maria, Univ Coimbra, (L)  
Miller, Reinhard, Max Planck Inst., Potsdam, Germany (S)  
Moreno, Ignacio, Univ Austral de Chile, Valdivia, Chile (S)  
Nettesheim, Florian (Kiel) Marie Curie Student Fellowship (L)  
Niemic, Anna, Department of Chemistry, University of Krakow, Poland (L)  
Ninham, Barry, Australian National University, Canberra (L)  
Nordén, Bengt, Chalmers University of Technology (S)  
Oliviero, Cesare, University of Cosenza, Italy (L)  
Pais, Alberto, University of Coimbra (S)  
Palazzo, Gerardo, Bari(S)  
Persson, Bertil, Univ Hospital, Lund (S)  
Premachandran, Raman, USA (S)  
Regev, Oren, Ben Gurion University, Israel (S)  
Richtering, Walter, Christian-Albrechts-Univ., Kile, Germany (S)  
Rouquerol, Jean, MADIREL, Marseille (S)  
Rädler, Joachim, Ludwig-Maximilian Univ., München (S)  
Sandström, Pär, Chalmers Univ of Technology, Göteborg (S)  
Schmidt, Claudia, Freiburg, Germany (S)  
Shigematsu, Mikiji, Japan (S)  
Stenius, Per, Technical University, Helsinki, Finland (S)  
Stilbs, Peter, KTH, Stockholm (S)  
Svingen, Roine, Chalmers Univ of Technology, Göteborg (S)  
Svärd, Jan, EKA Chemicals, Bohus (S)  
Takasuke Matsuo, Osaka Univ Japan (S)  
Takayoshi Kimura, Kinki Univ Japan (S)  
Thomas, Robert, Oxford, UK (S)  
van Stam, Jan, Karlstad univ (S).  
Vincent, Brian, Univ Bristol, UK (S)  
Vlachy, Vojko, University of Ljubljana, Slovenia (S)  
Wyn, Brown, Uppsala (S)  
Åkerman, Björn, Chalmers University of Technology (S)  
Ödberg, Lars, AssiDomän, Stockholm (S)

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

## GERD OLOFSSON RETIRED

Gerd Olofsson retired on August 1, 2001. Her scientific career started at Uppsala University in the early sixties where she passed the licentiate degree in inorganic chemistry in 1964. Afterwards she joined Stig Sunner's Thermochemistry Laboratory at Lund University resulting in her doctoral dissertation in 1968, on donor – acceptor interactions between antimony pentachloride and carbonyl compounds and a promotion to assistant professor in thermochemistry.

After her dissertation, Gerd's central research theme has been in the broad area of thermodynamic investigations of aqueous solutions with the main experimental tool being different calorimetric techniques also with many important methodological contributions. During the last 20 years her work has concentrated on surface and colloid chemical problems, which has led to a fruitful co-operation with several scientists at Physical Chemistry 1. Many doctoral students and guest scientists have benefited from Gerd's untiring engagement in their scientific problems and their theoretical and experimental training.

Gerd has built up a very extensive scientific network, partly as a result of her long-time work for the International Union of Pure and Applied Chemistry (IUPAC). During more than 10 years she was a member of the Commission on Thermodynamics. Among other missions she was involved in preparation of IUPAC Recommendations for assignments of uncertainties of thermodynamic data and for their presentation in the literature. Another extensive project involved definition of basic thermodynamic functions and concepts and recommendations for their symbols. Following her service in the Commission she was elected to the Division Committee of IUPAC's Physical Chemistry Division. During the time 1996-2001 she was secretary of the Committee, a very demanding position during a time period when the Union was reorganized.

The colloid and surface science community know Gerd not only through her research on solutions of surfactants, polymers and polymer-surfactant systems but also for her very successful conference arrangements and her role in different networks and organizations. Meetings include the Surfactants in Solution (SIS) conference in 1982, the Annual Surface and Colloid Symposia in Lund (12 so far) and many more. She was a driving force of a European Network on water-soluble polymers and of YKOLL, the Surface and Colloid Science Center at Lund University. She is the program secretary of the Colloid & Interface Technology program.

There is much more to add and much more to come since fortunately Gerd's retirement is only formal. She continues to be very active in research and supervision

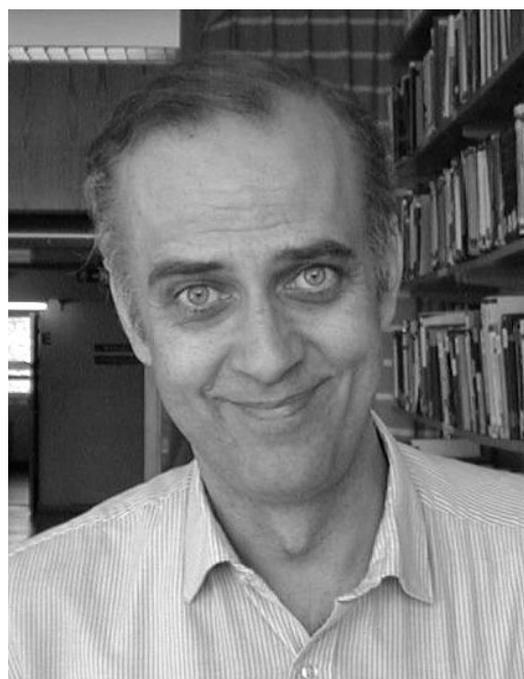


as well as in the direction of the department and remains as program secretary for the national program.

To honor Gerd an international conference “Current Applications in Thermochemistry” was held in Lund in October under the chairmanship of Ingemar Wadsö and Olle Söderman. A large number of Gerd’s colleagues, from industry and academia in Sweden as well as from many European countries, Japan and United States contributed to a very interesting scientific event and to a memorable celebration.

## BENGT JÖNSSON CHANGED DEPARTMENT

Towards the end of 2001, Bengt Jönsson left the department to take up a position at Biophysical Chemistry at the Technical Faculty, Lund University. Bengt has worked at the department since obtaining his PhD exam in 1981. His research has been multifaceted: from applied work concerned with dewatering of peat to the development of electrostatic theories. He has also been heavily involved in teaching and has consistently obtained very good evaluations from his students. Perhaps a quote from a student evaluation is appropriate here: “Bengt loves to explain, which is good. Bengt’s lectures are of high standards and his patience with our (sometimes stupid) questions is immense!”



We wish Bengt all the best in his continued academic career.

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8. Ashbaugh, H. S.; Lindman, B.  
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14. Carlsson, F.; Linse, P.; Malmsten, M.  
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15. Carlsson, F.; Malmsten, M.; Linse, P.  
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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.

It is also possible from few European countries to fly to Sturup Airport Malmö. Take the airport bus to Lund (40 min journey).

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