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Contents

Cover. Cryo-TEM micrographs of different artificially colored nonlamellar liquid crystalline nanoparticles formed by lipid self-assembly. (Justas Barauskas)
Front: glycerol monooleate/ Pluronic F127/ water reversed bicontinuous Im3m cubic phase nanoparticles viewed along the [001] direction.
Back: diglycerol monooleate/ glycerol dioleate/ Polysorbate 80/ water "coin-like" reversed hexagonal monocrystalline nanoparticles projected along [01] direction.

Paula Leckius, Media-Tryck is gratefully acknowledged for the cover design.

CHEMISTRY TODAY AND TOMORROW?

During the last decades there has been a clear trend that successful science transverse the traditional boundaries of academic disciplines. There is a certain tension between the teaching activities that are largely confined within a disciplinary division and the more eclectic research practice. There are good reasons to believe that this trend will become even more developed during the coming years. It seems necessary to find ways for academic research that are adapted to the new conditions. There are particular challenges for the chemistry subject since it is placed in the central area of science. Large fractions of the physics community is today involved in areas denoted as "biological physics", "soft condensed matter", "material science" and "nanoscience/ nanotechnology". Chemistry is an important component in all these areas of research. The "white" biology is becoming increasingly more molecularly oriented and it gradually bridges over to biochemistry. Also in medicine chemistry plays an essential role. This applies both to finding the molecular cause of deceases, finding and producing chemically well characterized compounds that cure as well as in the construction of medical devices. Chemical questions also take a central role in environmental science. That chemistry is an integral part of chemical technology is obvious, but chemistry enters also in many other branches of technology. A paradoxical consequence of the increased importance of chemistry is that there is a tendency that the subject loses its identity. Chemical research and the teaching about chemical processes is today occurring in activities that are not explicitly identified as chemistry. There is a clear challenge for the chemistry community to make itself more visible and demonstrating the usefulness of a molecular description.

Science resides in a field of tension between curiosity motivated basic research and more applied activities emanating from a need to solve problems recognized by the society. The society allocates substantial resources to academic research in science and technology. The main motive for this is a hope that one builds a base for economic growth and increased quality of life. One route to this end goes through well educated scientists/engineers. Another route goes through a commercialization or other direct applications of the results of the research. Thus we shouldn't be surprised when one in the political process tends to take specific societal needs as a basis for funding research. This trend is evident in Swedish research funding, but even more pronounced within the EU system. It is neither possible nor desirable that all research groups in a field give in to this type of external pressure. If one, on the other hand, takes a more collective perspective it is a vitalizing element if some groups have activities that to a certain degree are geared towards solving problems of obvious relevance to the society at large. In this respect, chemistry is at an advantage since there is often a short distance between the fundamental scientific questions and the problems in technology, in medicine and of environmental issues.

Making research policies involves to some extent steering science towards fields that are projected as particularly fruitful. Such an ambition should always be accompanied by the insight that such projections are uncertain on the five to ten year time-scale. Progress in science is driven both by external influences from the society and by an internal dynamics. These two factors are typically out of pace. It is a hallmark of the good academic institution to have a pluralistic attitude in responding to external and internal influences. For the individual research group it is, on the other hand, often necessary to give the research agenda a more clear focus. Which are then the external factors that will influence the chemical research in the coming decade?

A most important factor is the clear realization, also in political circles, that the amount of fossil fuel is limited. It is of particular relevance that oil is getting a bit scarce relative to the demand. This has resulted in noticeable increases in the price and this trend will probably continue. This has already stimulated a search for alternative or complementary liquid fuels. Another consequence is that there will be an increased incentive to replace mineral oil products as starting chemicals in industrial synthetic processes. Another development of outmost importance is the work on determining the genes of humans and other organisms. One hope, among several others, is that establishing the information on genes will result in new possibilities for medical therapies. Implementing such therapies will involve chemical considerations in an important and crucial way. Today computers are available to all scientists and the capacity for computations is steadily increasing. Simulations and other numerical methods are applied in a steadily increasing way in chemistry. Theory is becoming a more and more important tool for focusing experimental investigations. Environmental issues are becoming increasingly relevant in a world of globalization. The carbon dioxide emission issue represents just a tip of an iceberg. The society will, in the future, ask for more and more detailed knowledge about chemical processes in the air, in the water and in the soil.

In the future chemistry will continue to develop in its position between fundamental and applied science. There are many scientific challenges ahead. There are also some threats to the subject. Without a continued decline in the enrollment of chemistry students the basis for recruiting scientists, in academia and industry, will erode. The fact that other disciplines find chemical questions increasingly interesting and relevant is properly handled a strength of the subject, but it requires an active approach based on mutual respect. Science is difficult and there is a need for many types of skills and knowledge.

Håkan Wennerström

RESEARCH PROJECTS

Within the broad arena of modern colloid and surface chemistry, research is largely concentrated into seven loosely-bound areas: (1) Surfactant self-assembly; (2) Polymers, solutions, gels, and phase behavior; (3) Polymer-surfactant systems; (4) Protein and protein-amphiphile systems; (5) Adsorption and surface forces; (6) Experimental methodology in colloidal science and (7) Theory and 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 Surfactants. The uptake of water in 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. Both non-ionic (ethylene oxide based and sugar surfactants) and ionic surfactants are investigated. By combining the sorption calorimetric measurements with accurate DCS measurements, glass transitions in two alkyl maltosides have been identified. (V. Kocherbitov (Malmö University), O. Söderman).

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

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

Living polymers and living networks. Some surfactants form giant micelles in solution that can be longer than several micrometers. These solutions have properties similar to polymer solutions, however with some significant differences. The size distribution is not fixed but varies with concentration and temperature. Moreover,

micelles may break and reform which influences the dynamics. For these reasons the are often referred to as "living polymers". Furthermore, there are also systems where the micelles form connected (branched) network, similar to a bicontinuous microemulsion. Here the morphology resembles that of polymer gels and one may refer to a "living network". In this project we compare phase behavior of living polymer and living network systems and we have studied the effect of shear flow on the liquid structure and in particular the shear induced formation of a nematic phase of wormlike micelles. The structural transformation is followed either by small angle neutron scattering (rheo-SANS) or by NMR measurements (rheo-NMR). The growth of "living polymers" with increasing concentration is an unresolved problem. Simple mean field models predict that the number averaged contour lengths varies approximately as the square root concentration while one in the analysis of recent experiments have found a much higher exponent. An important complication in the analysis of experimental data is the interactions and how they influence e.g. the osmotic compressibility. Here we are combining static and dynamic light scattering, and NMR self-diffusion experiments, to investigate the growth law in dilute solutions. (S. Bulut, K. Bryskhe, J. Hamit, U. Olsson, T. Kato (Tokyo), R. Angelico, L. Ambrosone and A. Ceglie (Campobasso), G. Palazzo (Bari), K. Mortensen (Risø, Denmark).

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

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

Physico-chemical characterisation of micellar properties of PEG 12-acyloxy-stearates. Recent work with PEG 12-acyloxy-stearates (PEG-12-AS) has revealed remarkable properties of these amphiphilic compounds with regard to cell damage effects. For PEG1500 12-acyloxy-stearates with acyloxy groups of 14 to 18 carbon atoms no effects on red blood cells or intestinal cells were observed. The same

behaviour was found for methyl-PEG2000 12-acyloxy-stearates. The mechanism behind these very unusual properties is still unknown. To understand the underlying mechanism, systematic studies of bulk properties of PEG-12-AS are carried out. Phase diagrams, micellar structure as well as the nature of lyotropic liquid crystals found are determined. The surfactant dynamics is investigated by means of NMR diffusometry. (C. McNamee, O. Söderman, C. v Corswant (Astra-Zeneca, Mölndal))

Shear-induced formation of multi-lamellar vesicles. The equilibrium structure and phase equilibria of the lamellar phase are sometimes complicated as noted in early studies by Ekwall and Fontell. This complication appears to be due to the formation of multi-lamellar vesicles ("onions") under shear, which can originate simply by shaking the sample. A systematic study is performed on nonionic surfactant- water systems where the structure of the lamellar phase under shear is investigated using small angle neutron and light scattering. Depending on the temperature, that governs the monolayer spontaneous curvature, we can identify two distinct regions corresponding to "onions" (lower temperature) and planar bilayers (classical lamellar phase, higher temperature). The equilibrium structure at zero shear, however, appears to be the classical lamellar structure. The onion size varies with the applied shear rate or shear stress. In systematic experiments, it was found that the onion states obtained at large strain values are reversible and correspond to true steady states. (U. Olsson, B. Medronho (Coimbra), M. Miguel (Coimbra), W. Richtering (Aachen), C. Schmidt (Paderborn).

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

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

Emulsions. NMR techniques are used to study oil- in- water and water- in- oil type emulsions with varying volume fractions. Self-diffusion data show that molecules of the dispersed phase undergo restricted self- diffusion whereas unbounded diffusion

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

Drug nanoparticles. A significant proportion of drugs on the market are poorly soluble in water and it is expected that this will be even more pronounced in the future. Formulations of poorly water-soluble compounds offers a challenge to the formulation scientist, from the early discovery phase through the development to the launch of the pharmaceutical product. A potentially interesting way of formulating such compounds is as aqueous nanosuspensions with typical particle sizes of the order of 100 nm. The particles may be amorphous or crystalline, and in the development of such formulations one comes across a number of classical colloid and surface science problems such as nucleation and growth, Ostwald ripening and particle characterization. (U. Olsson, Lennart Lindfors (AstraZeneca))

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

Hydration of extracted skin lipids and model lipids. We aim at the characterization of the lipid component of the stratum corneum (the upper layer of the skin) at different degrees of hydration, using NMR and sorption calorimetry. This involves understanding how molecular organization as well as molecular diffusive transport occurs through the skin and thus how it can be affected. Hydration of model lipid membranes is also investigated, focusing on how small water-soluble solutes, like urea, can protect the membrane system against osmotic stress. Here, we put a special emphasis on applications of urea in skin care products. (F. Costa-Balogh, C. Silva, D. Topgaard, V. Kocherbitov (Malmö University), A. A. C. C. Pais (Coimbra University), J.J. Sousa (Coimbra University), H. Wennerström, E. Sparr)

Polymers, Solutions, Gels and Phase Behaviour

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

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

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

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

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

Dissolution of dry polymers. We closely investigate the process whereby a dry sample of a water-soluble polymer swells and finally dissolves when immersed in an aqueous solution. A detailed understanding of the dissolution of dry polymer is of obvious relevance to tablet formulations of pharmaceutical drugs, but the approach is fundamental. The release rate has been recorded systematically for dry tablets based on mixtures of a short and a long fraction of PEO. For each tablet composition, both PEO fractions are released at the same rate, but this release rate increases with an increasing proportion of the short PEO fraction. Similar results are obtained for tablets of hydroxypropylmethylcellulose or dextran. The "gel layers" surrounding the dry cores of dissolving PEO tablets have been probed during the dissolution. Tablets of short polymers soon develop a thin steady state gel layer of constant thickness, whereas tablets of long polymers yield gel layers that grow monotonically with time until the entire dry tablet core has finally disappeared. Despite differences in release rate or gel layer swelling, the shape of the release profile (the accumulation of released polymer with time) is remarkably similar for all cases: A slow initial phase is followed by an extended linear phase and, finally, a slowing down. Moreover, tablets of polydisperse polymer mixtures behave in all respects remarkably similar to tablets of nearly monodisperse polymers, as long as the tablets have the same release rates. The

dissolution of hydrophobically modified surfactant-binding polymers in surfactant solutions is currently investigated. (A. Körner and L. Piculell; A. Larsson and F. Currie (Chalmers); B. Wittgren (AstraZeneca Mölndal)).

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

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

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

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

The Ejection of Genome from Viruses. In this work light scattering was used as the main technique in order to study the ejection process of natural DNA from λ-bacteriophage. Measurements were carried out under different physical conditions and the ejection process was also studied with different DNA binding proteins added into the investigated solutions. (D. Löf, K. Schillén, A. Evilevitch (Biochemistry, Lund University)).

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

Patterned polymer brushes. Patterned polymer brushes constitute one approach to fabricate functionalized surfaces. In a newly started project, our aim is to in more depth characterized such brushes manufactured at Purdue University by, in particular, QCM, ellipsometry, and scattering methods as well as with simulation methods. (S. Zauscher (Duke University), A. Rennie (Uppsala University), F. Höök (Solid State Physics), T. Nylander, M. Patra, and P. Linse)

Polymer-Surfactant Systems

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

oppositely charged hydrophobically modified cellulose derivatives are investigated with specific focus on the charge and hydrophobe stoichiometries. Varying the electrostatic and hydrophobic associations, there are dramatic changes in rheology. (F. Antunes, B. Medronho, M. Miguel, Coimbra University, B. Lindman K. Thuresson).

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

Concentrated mixtures of oppositely charged polymer and surfactant. We use a new, simplified approach to study structures and water uptake of oppositely charged polymers and surfactants. The essence is to use the minimum number of components to map out the generic features, and to make contact between polymer/surfactant systems and conventional surfactant systems. To this end, we first synthesize the pure "complex salt" (polyion + surfactant ion) and use it as our point of departure. Binary mixtures of complex salt and water are studied, and also truly ternary mixtures involving one of the following additional components: The conventional surfactant (surfactant ion + simple monovalent counterion), the conventional polyelectrolyte (polyion + simple counterion), the corresponding polyacid (protonated polyion), or a non-polar "oil". Most experiments so far refer to alkyltrimethylammonium ($CnTA^+$) surfactant ions with polyacrylate (PA^-) counterions. Small additions of a long-chain alcohol to a complex salt rapidly change the aggregate curvature and, hence, the phase structure from cubic or hexagonal to lamellar. Less polar oils such as p-xylene or cyclohexane swell the surfactant aggregates, but have less of an effect on the aggregate curvature. If the charge density of the polyion is decreased, either by mixing in polyacrylic acid or making copolymers of sodium polyacrylate with a neutral comonomer, the curvature of the aggregates increases. This results first in a destabilization of the hexagonal phase relative to the micellar cubic phase. Moreover, the micellar aggregation number decreases, even for spherical micelles. The miscibility of the complex salt with water increases with an increasing fraction of neutral comonomers in the polyion; however, an opposing effect is found if the hydrophobicity of the neutral comonomer is increased. (J. Norrman, L. Piculell and I. Lynch; W. Loh and J. Bernardes (UNICAMP, Brazil)).

Mixtures of an associating polymer and a degradable surfactant. The addition of surfactant to a solution of an "associating" hydrophobically modified polymer generally gives rise to a dramatic change in viscosity, but the sign and magnitude of the change depends on the amount of surfactant added. The result is the development of a viscosity maximum as a function of added surfactant, where the maximum viscosity may be orders of magnitude higher than that of the surfactant-free polymer solution. We are using this sensitivity to surfactant concentration to create and study HMHEC-surfactant mixtures with a time dependent rheology, using alkali-sensitive, degradable betaine esters as surfactants. Depending on the initial amount of surfactant, the viscosity may either decrease or go through a maximum with time, as the surfactant degrades.

The rate of degradation, and thus the rate of variation of the surfactant concentration, may be controlled within wide ranges by controlling the pH of the mixture (M. Karlberg and L. Piculell, M. Stjerndahl and D. Lundberg (Chalmers)). Project completed.

The effect of poly(N,N-dimetylacrylamide) on the lamellar phase of Aerosol OT-water. The effect of a water soluble uncharged polymer (polyacrylamid) on the stability of the lamellar phase of the AOT (Aerosol OT, sodium di(ethylhexyl) sulfosuccinate)/water system is studied. Polymers with large coil dimensions, with respect to the thickness of the water layers, induces formation of two phases in equilibrium; the AOT rich phase and one phase rich in the polymer. In the case of polymers with smaller coil dimensions a nanometric sieving of polymer coils by the lamellar liquid crystal is obtained. Only the fraction of polymer chains with dimensions smaller than the thickness of water layers are able to penetrate the lamellar phase, while the fraction consisting of larger polymer chains forms an isotropic phase. When the size of polymer is small enough all can be located in the water layer. In situ polymerisation within AOT bilayers lead to phase separation. This is partly because aqueous solubility of studied polyacrylamides is temperature sensitive. At the temperature used for synthesis the polymer chains attain a globule conformation. First results could indicate that structure (tacticity) of the polymer chains varies depending on whether the polymer chains are synthesised in the lamellar phase or in solution. (Joint project with I. E. Pacios, A. Horta and C. S. Renamayor, Madrid; B. Lindman, K. Thuresson). Project completed.

Hydration of DNA surfactant complexes. The thermodynamics of hydration of DNA–cationic surfatant(lipid) complexes is studied using a sorption calorimeter that provides both the partial free energy (chemical potential) and the partial enthalpy of hydration. This provides a complete thermodynamic description of the system at the given temperature and pressure. The system is also studied using a range of advanced NMR methods for both liquids and solids. By combining the thermodynamic , spectroscopic and scattering information we obtained a detailed description of how the complex responds to changes in water activity. (C. Leal, E. Moniri, D. Topgaard, H. Wennerström, G. Olofsson).

Solid-state NMR studies of DNA-amphiphile complexes. The local molecular mobility of DNA-amphiphile complexes is investigated with ^{1}H-^{13}C magic angle spinning NMR. The two dimensional WIdeline SEparation (WISE) and Separated Local Field (SLF) experiments yield the 1H linewidth (WISE) or the residual ^{1}H-^{13}C dipolar coupling (SLF) for each resonance line in the high-resolution ^{13}C spectrum. The dynamic state of the DNA, the lipid headgroup, and hydrocarbon tail is monitored as a function of hydration level and lipid composition. (C. Leal, D. Sandström (Stockholm University), D. Topgaard)

Phase separation, adsorption behavior and delivery capacity of polyelectrolytes and oppositely charged surfactants at hydrophilic surfaces. The concentrated phase formed in dilute mixtures of polyelectrolytes and oppositely charged surfactants can be a precipitate (solid) or a coacervate (liquid) depending on parameters such as the molecular weight and charge density of the polymer, the self-assembly of the surfactant and the charge ratio of polymer vs. surfactant in the mixtures. The phase separation is of practical use in products where it is desired to obtain a deposition on a surface. The polymer-surfactant complexation can also be used as a delivery tool for an additional substance to the surface. The aim of the present project is to link the adsorption behavior of a polyelectrolyte-surfactant mixture with the characteristics of the phase separation in the bulk solution. Based on these results, an investigation regarding the delivery of an oil-in-water emulsion to a hydrophilic surface is made. A combination of

different techniques is used: in-situ ellipsometry to investigate the adsorption behavior, phase studies and turbidity measurements to look into the bulk properties, dynamic light scattering to determine the size of soluble aggregates and gel swelling experiments to investigate the polymer-surfactant binding. (A. Svensson, T. Nylander, L. Piculell, B. Lindman in collaboration with E. Johnson and R. Panandiker, Procter & Gamble, Cincinnati and R. Fabicon, Procter & Gamble, Beijing).

Influence of hydrophobic modification of the polymer and of the charge density of the surfactant aggregates on phase behaviour, transport properties, and rheological properties in polymer surfactant systems of opposite charge. Systems composed of mixtures of surfactants and a polymer are frequently employed for rheological control and, in particular, is gel-like appearance important in many applications. If a surfactant is added to a polymer solution, dramatic changes in viscosity are found if the polymer is of the associating type, in particular if it is a hydrophobically modified water-soluble polymer. Association and complex formation between polyelectrolytes and oppositely charged surfactants frequently leads to precipitation. These complexes, being in equilibrium with an excess aqueous phase, are sometimes characterized by a long-range order (lamellar, hexagonal, or cubic). The behavior is dependent on parameters such as charge density of the polyelectrolyte chain and the ionic strength in the medium, but also on the charge density of the surfactant aggregates. In this project we study the effect of a non ionic surfactant on the complex formation in between carboxymethyl cellulose, or a hydrophobically modified analogue, and an oppositely charged surfactant. (Joint project with I. E. Pacios, A. Horta and C. S. Renamayor, Madrid; B. Lindman, K. Thuresson).

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

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

DNA / Amino acid-based surfactants interaction. Gene therapy is a rapidly developing technology for the treatment of a variety of diseases and mixed systems of surfactants/lipids are already being used as packaging agents of nucleic acids. These non-viral vectors attract a great deal of interest due to their advantageous safety profile when compared to viral ones. Nevertheless, some of the used surfactants are still toxic. Amino acid-based surfactants are biodegradable, milder and less irritant than conventional ones. Studies of compaction and decompaction of DNA by amino acid-based surfactants are performed by fluorescence microscopy.

The interaction between DNA and positively charged amino acid-based catanionic vesicles is investigated through the study of the relation between structure and DNA/surfactant net charge ratio. The main techniques in use are Cryo-TEM and SAXS. The mechanism of interaction is being followed through 1H NMR and NMR Self-Diffusion techniques. (M. Rosa, M. R. Infantes (Barcelona), M. Miguel, B. Lindman).

Amino Acid-Based Surfactants as DNA Condensing Agents – A Transfection Study. The aim of using amino acid-base cationic surfactants in drug and gene delivery formulations is to reduce toxic side effects. When designing cationic surfactants for gene therapy, their ability to mediate transfection can be attributed to several physical aspects: including DNA condensation due to electrostatics; and an intrinsic ability of the cationic lipids to destabilize the plasma membrane or the endosomal compartment (dependent on the mode of uptake). ALA, an arginine-based single chained cationic surfactant, is being used as a DNA pre-condensing agent. The liposome systems in study are: DOTAP:Chol (7% ethanol); CatpH (7% ethanol); and CatpH-det (7% ethanol). ALA pre-condensed DNA is added to the different liposomes formulations and transfection studies are performed. Transfection efficiency is explored as a function of the ALA/DNA charge ratio and cationic lipid/DNA charge ratio. A thorough physical-chemical characterization of each system will be made which will clarify the main factors responsible for transfection efficiency. (M. Rosa, N. Penacho, S. Simões, C. Pedroso de Lima, M. Miguel, B. Lindman).

Cross-linked DNA gels. DNA molecules have been covalently cross-linked to form chemical gels. Addition of electrolytes causes a deswelling of the gels. From the volume changes the association of oppositely charged cosolutes with DNA can be monitored. For cationic surfactants a dramatic compaction is noted as well as the formation of different ordered microstructures. (D. Costa, M. Miguel (Coimbra), P. Hansson (Uppsala), S. Schneider, B. Lindman).

Electrostatics and deformations during DNA-amphiphile swelling. The swelling behavior with respect to maximal water content and characteristic distances of the unit cell dimension of a stoichiometric DNA:amphiphile complex is studied under the influence of added salt. The aim is to obtain qualitative and quantitative information on the contribution of attractive electrostatic forces and repulsive deformation forces upon DNA:amphiphile swelling. (C. Leal, E. Mori, L. Pegado and H. Wennerström)

Block copolymer-surfactant interactions. Interaction between triblock copolymers of poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO) (PEO-PPO-PEO) and nonionic surfactants (of the type C_iE_j) in dilute aqueous solution are studied using dynamic and static light scattering in combination with differential scanning and isothermal titration calorimetry and cryo-TEM. The aim is to study the block copolymer-surfactant interaction, the mixed complexes formed by the block copolymers in aqueous solution as well as the kinetics of the complex growth. (D. Löf, K. Schillén, G. Olofsson, A. Niemiec, W. Loh (UNICAMP, Brazil), H. T. Davis (University of Minnesota, U.S.A.)).

Protein and Protein-Amphiphile Systems

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

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

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

A**myloid formation and protein-lipid co-aggregation.** Many human disorders belong to a family of amyloid diseases, characterized by abnormal folding of proteins into aggregates with a fibrillar structure. We have recently shown on the formation of protein-lipid aggregates when the protein aggregation is taking place in the presence of lipid membranes. The aim the project is to investigate the basic principles for such protein-lipid co-aggregation. We study the interactions between the Aβ protein, involved in Alzheimer's disease, and mutants of the superoxide dismutase protein, involved in amyotrophic lateral sclerosis (ALS) with model lipid membranes of different composition. (E, Sparr, H. Wennerström, M. Oliveberg (Stockholm University)).

I**nteraction between poly nucleic acids and phospholipids.** In the living system, DNA and RNA are present in an environment that contains many other substances, e.g. lipids in cell membranes and in the cell nuclei, which may influence its structure and function. RNA occurs more often than DNA in the single-stranded form, where the apolar parts of the bases are obvious targets for hydrophobic interaction with other species. We aim at revealing the basic features of DNA-phospholipid and RNA–phospholipid interactions. We study double stranded DNA, single stranded DNA and RNA, and the model lipid membrane systems are chosen to mimic cell membranes and the lipids within cell nuclei, in order to better understand the functions of intra nuclear lipids. These systems are studied with several techniques, including dynamic light scattering, cryo-TEM, differential scanning calorimetry, isothermal titration calorimetry, ellipsometry, quartz crystal microbalance (QCM-D) and fluorescence spectroscopy. We detect interaction in almost all systems investigated, showing the

strongest effects for RNA and single-stranded DNA. It is also observed that RNA and DNA can induce domain formation in mixed model membranes. (M-L. Örberg, A. Zettergren, T. Nylander, E. Sparr, V. Alfredsson, F. Höök (Solid State Physics, Lund University), B. Lindman).

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

Lung surfactants. The alveolar surface is lined by film of submicron thickness between the epithelial cells and the alveolar lumen with the main function to lower the surface tension. The aqueous bulk structure of this layer consists of lipid bilayers forming lamellar bodies (LB:s) and tubular myelin (TM), and two hydrophilic proteins in the outside water ; SP-A and SP-D. We are studying the structure of and phase transitions in this layer with cryo-TEM and SAXD. Another aspect of the project is the diffusion in through the interfacial lipid membrane with complex structure that implies a diffusional permeability that is different for hydrophilic and hydrophobic substances. The transport processes is theoretically analyzed considering the dynamic conditions. (M. Larsson (Lund University Hospital), T. Nylander, K. Larsson, C. Åberg, E. Sparr, H. Wennerström)

Interactions between surfactants and polypeptides. The project is centered on a systematic investigation of the interactions between surfactants and relatively simple polypeptides, namely synthetic homo- and co-polymers of α-L-amino acids. The peptide-surfactant interactions in these systems are studied with respect to, on the one hand, the size, charge, hydrophobicity and conformation of the peptide and, on the other hand, properties of the surfactant, e.g. charge, head group, length of the alkyl chain and micellar size. The systems are investigated by means of circular dichroism (CD), Raman/IR and NMR spectroscopy, as well as by static and dynamic light scattering techniques. Non-ionic surfactants of pharmaceutical relevance, especially alkylglucosides and sucrose esters, play a key role in the project. In addition to the studies of peptide-surfactant systems in aqueous solution, the properties of polypeptide monolayers at the air-water interface are investigated by means of surface balance experiments, as well as by AFM, ATR-IR and CD spectroscopic characterization of Langmuir-Blodgett films. The project is a co-operation between Physical Chemistry 1 and AstraZeneca R&D Lund. (H. Sjögren, S. Ulvenlund, T. Nylander).

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

Adsorption and Surface Forces

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

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

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

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

Adsorption competition between dispersants and rheological modifiers. The aim of this project is to provide a thorough understanding of the adsorption behavior and interactions between the constituents of typical water-borne paint formulations,

i.e., pigments, dispersants, rheological modifiers and emulsifiers on surfaces. Null-ellipsometry is used to in situ follow the adsorption of the different components on two solid surfaces, i. e. silica (SiO_2) and titanium oxide (TiO_2). The method gives the adsorbed amount as well as the thickness of the adsorbed layer. In particular we will study the adsorption competition between the constituents, the spatial configuration of the adsorbed layers and the effect of divalent salts. This project is a collaboration with CIP (Centro de Investigación en Polímeros) COMEX, México. (J. Campos Terán, T. Nylander, B. Lindman).

DNA-cationic surfactant complexes at solid interfaces. Extensive research has been performed to understand the factors determining DNA compaction due to interaction with cationic surfactants or polymers in bulk solution. However, almost no research has been performed on interfacial phenomena. The co-adsorption behaviour may be another important factor determining the DNA-surfactant complex efficiency for its delivery to target cells. Solid-liquid interfaces are used as a model system to facilitate the understanding of interfacial properties such as lateral organization and layer composition at technologically relevant surfaces. The main technique being used is ellipsometry, which allows in situ measurements of interface processes with high resolution (~0.1 mg/m^2). Both adsorption phenomena on hydrophilic and hydrophobic surfaces are investigated. The adsorbed layer structure is further determined by means of Neutron Reflectivity. The surface force apparatus is also utilized to better understand the structure of the mixed adsorbed layers. (M. Cárdenas (Malmö University), J. Campos, T. Nylander, R. Thomas (Oxford University), B. Lindman).

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

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

Nanoparticle-protein and nanoparticle-cell interactions. Immediately upon contact with physiological solutions, e.g. serum or plasma, a layer of proteins is deposited onto the surface of a nanoparticle. This has consequences for the nanoparticle stability and aggregation, the proteins stability and aggregation, the protein functioning, and it is this adsorbed protein layer that is actually in contact with the cells. In this project we are interested to understand the nature and composition of the adsorbed protein layer, as a function of the nanoparticle characteristics (size, shape, composition), and to investigate the consequences of protein adsorption for cellular response to nanoparticles. (I. Lynch S. Linse (Biophysical Chemistry)).

Interactions between DNA and Gold Nanoparticles. Gold nanoparticles modified by thiol-derivatized singlestranded (ss)DNA (thiol-ssDNA) are promising building blocks for nanoscale materials and are used in various applications in bioanalysis. In this project, the contribution of nonspecific interactions to the overall interactions of thiol-ssDNA and dsDNA macromolecules with gold nanoparticles is investigated. Dynamic light scattering and cryogenic transmission electron microscopy are utilized to directly measure and visualize the changes in particle size and appearance during functionalization of gold nanoparticles with thiol-ssDNA and nonthiolated dsDNA.(M. Cárdenas (Malmö University), J. Barauskas, K. Schillén, T. Nylander, J. L. Brennan and M. Brust (University of Liverpool, UK))

Experimental Methodologies in Colloid Science

NMR self-diffusion experiments. In this project we study fundamental aspects of the pulsed gradient spin echo (PGSE) NMR technique applied to fluid motion in porous systems. 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. (D. Topgaard, C. Malmborg, O. Söderman).

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

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

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

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

Theory and Modelling

Diffusive transport in responding membranes. A combined theoretical and experimental approach is applied to gain insight into the mechanisms for diffusive transport in responding lipid membranes in the presence of several gradients. We study how an external gradient that induce structural transformations and domain formation in the membrane can be used as a regulating mechanism to control the barrier properties and introduce non-linear transport behavior. Beside the basic scientific interest in these mechanisms, several applications in biology and technology can be seen in, for example, the barrier properties of stratum corneum (the upper layer of the skin) and controlled release systems for drug delivery. (C. Åberg, F. Costa-Balogh, J Engblom (Zelmic AB), H. Wennerström, E. Sparr).

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

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

The dielectric approximation. In the theoretical description of surface forces an aqueous medium is typically described as a dielectric continuum. This often leads to quantitatively accurate descriptions. However, the continuum description of the solvent breaks down at short separations and one must turn to a molecular picture. Through computer simulations we study the relation between the continuum and the fully molecular description of charged surfaces interacting at short range in a dipolar solvent. (L. Pegado, B. Jönsson, G. Karlström, H. Wennerström).

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

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

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

Polyelectrolyte gels. The volume and structural changes upon the addition of oppositely charged macroions to crosslinked polyelectrolyte gels have been investigated by Monte Carlo simulations using a coarse-grained model. Initially the gel undergoes a deswelling, but after approximately equivalent amount of macroions the gel starts to swell again. The deswelling is greatest for small and highly charged macroions. The role of the network properties on the deswelling has also been examined. The initial deswelling is understood in terms of a replacement of confined counterions with macroions, thereby reducing the osmotic pressure originating from the counterions. At these conditions macroions are located near network nodes with various degree of network chains wrapping them. At charge equivalence, a profound change of the network structure has appeared. At these conditions the cohesive electrostatic interaction and the excluded volume effect of the macroions strongly influence the equilibrium volume. Our model system reproduces many characteristic experimental observations of polyelectrolyte gels containing oppositely charged surfactants. (S. Edgecombe and P. Linse)

Structures of charged block copolymers. The structure of spherical brushes formed by symmetric diblock polyampholytes end-grafted onto small spherical particles in salt-free aqueous solution is examined within the framework of the primitive model using Monte Carlo simulations. Three different chain flexibilities, corresponding to flexible, semiflexible, and stiff blocks, are considered at various polyampholyte linear charge densities and grafting densities. The link between the two blocks is flexible at all conditions, and the grafted segments are laterally mobile. Radial and lateral spatial distribution functions of different types and single-chain properties are analyzed. The brush structure strongly depends on the chain flexibility. With flexible chains, a disordered polyelectrolyte complex is formed at the surface of the particle, the complex becoming more compact at increasing linear charge density. With stiff blocks, the inner blocks are radially oriented. At low linear charged density, the outer blocks are orientationally disordered, whereas at increasing electrostatic interaction the two blocks of a polyampholyte are parallel and close to each other, leading to an ordered structure referred to as a polyampholyte star. As the grafting density is increased, the brush layer becomes denser but single-chain properties are only marginally affected. (A. Akinchina and P. Linse)

Nanopatterned polymer brushes. Structural properties of polymer brushes on nanopatterned surfaces in good solvent have been determined by computer simulations. Scaling relations for the brush height and brush width are proposed. The properties of the central part of the patterned brush remain constant as long as the pattern is wider than a few times the brush height. The results agree qualitatively with recent AFM experiments, but some quantitative differences call for a reassessment of experimental procedures. In addition, the interaction between a nanopatterned polymer brush and a rigid pyramidal body representing an AFM tip has been investigated using molecular dynamics (MD) simulation. The computed forces for varying position and penetration depth are systematically contrasted with the density and pressure tensor profiles of the unperturbed brush. For weak penetration of the AFM tip in the brush, we find that the force can quantitatively be computed from the properties of the unperturbed brush after folding with the geometry of the AFM tip. This steric effect leads to a force profile that is significantly wider than the physical brush. The structure of the perturbed brush has also been examined, and we show that for deep penetration of the AFM tip more than half of the force originates from the reorganization of the brush. (M. Patra and P. Linse)

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

Solutions of oppositely charged macroions. The structure and phase-behavior of oppositely charged macroions in solution has been studied with Monte Carlo simulations using the primitive model where the macroions and small ions are described as charged hard spheres. Size and charge symmetric, size asymmetric, and charge asymmetric macroions at different electrostatic coupling strengths are considered and the properties of the solutions have been examined using cluster size distribution functions, structure factors, and radial distribution functions. At increasing electrostatic coupling, the macroions form clusters and eventually the system displays a phase instability, in analogy to that of simple electrolyte systems. The relation to the similar cluster formation and phase instability occurring in solutions containing oppositely charged polymers is also discussed. (J. Rydén, M. Ullner, and P. Linse)

Modeling of prolin rich protein 1. Structural properties of the acidic proline rich protein PRP-1 of salivary origin in bulk solution and adsorbed onto a negatively charged surface have been studied by Monte Carlo simulations. A simple model system with focus on electrostatic interactions and short-ranged attractions among the uncharged amino acids has been used. In addition to PRP-1, some mutants were considered to assess the role of the interactions in the systems. Contrary to polyelectrolytes, the protein has a compact structure in salt-free bulk solutions, whereas at high salt concentration the protein becomes more extended. The protein adsorbs to a negatively charged surface, although its net charge is negative. The adsorbed protein displays an extended structure, which becomes more compact upon addition of salt. Hence, the conformational response upon salt addition in the adsorbed state is the opposite as compared to that in bulk solution. The conformational behaviour of PRP-1 in bulk solution and at charged surfaces as well as its propensity to adsorb to surfaces

with the same net charge are rationalized by the block polyampholytic character of the protein. The presence of a triad of positively charged amino acids in the C-terminal was found important for the adsorption of the protein. (M. Skepö (Malmö University), T. Arnebrandt (Malmö University), and P. Linse)

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

Genome in viral capsids. Structural features of polyelectrolytes as single-stranded RNA or double-stranded DNA confined inside viral capsids and the thermodynamics of the encapsidation of the polyelectrolyte into the viral capsid have been examined for various polyelectrolyte length by using coarse-grained model solved by Monte Carlo simulations. The capsid was modeled as a spherical shell with embedded charges and the genome as a linear jointed chain of oppositely charged beads, and their sizes corresponded to those of a scaled-down T=3 virus. Counterions were explicitly included, but no salt was added. The encapisdated chain was found to be predominantly located at the inner capsid surface, in a disordered manner for flexible chains and in a spool-like structure for stiff chains. The distribution of the small ions was strongly dependent on the polyelectrolyte-capsid charge ratio. The encapsidation enthalpy was negative and its magnitude decreased with polyelectrolyte length, whereas the encapsidation entropy displayed a maximum when the capsid and polyelectrolyte had equal absolute charge. The encapsidation process remained thermodynamically favorable for genome charges ca. 3.5 times the capsid charge. The chain stiffness had only a relatively weak effect on the thermodynamics of the encapsidation. (D. Angelescu, R. Bruinsma (University of California Los Angeles), and P. Linse)

Hydrophobic effect in aqueous electrolyte solutions. The hydrophobic interaction between two methane molecules in salt-free and high salt-containing aqueous solutions and the structure in such solutions have been investigated using an atomistic model solved by Monte Carlo simulations. Monovalent salt representing NaCl and divalent salt with the same nonelectrostatic properties as the monovalent salt have been used to examine the influence of the valence of the salt species. In salt-free solution the effective interaction between the two methane molecules displayed a global minimum at close contact of the two methane molecules and a solvent-separated secondary minimum. In 3 and 5 M monovalent salt solution, the potential of mean force became slightly more attractive and in a 3 M divalent salt solution the attraction became considerably stronger. The structure of the aqueous solutions was determined by radial distribution functions and angular probability functions. The distortion of the native water structure was increased with ion valence. The increase of the hydrophobic attraction was associated with (i) a breakdown of the tetrahedral

structure formed by neighboring water molecules and of the hydrogen bonds between them and (i) the concomitant increase of the solution density. (M. Jönsson, M. Skepö (Malmö University), and P. Linse)

Adsorption of macromolecules to responsive surfaces. It has been observed, by fluorescence microscopy, that DNA adsorbs onto catanionic vesicles and cationic liposomes, in a compacted conformation, whereas it presents an extended conformation when adsorbed at cationic lipid bilayers deposited on a glass substrate. These experimental results have prompted a Monte Carlo study where we analyse the interaction of a negatively charged polyion with a surface consisting of sets of negative and positive charges, which are allowed to move in the xy plane, simulating the lateral diffusion of lipids in membranes, and also to protrude individually into the "solution". It is shown that the adsorption behaviour is determined by the length and stiffness of the polyelectrolyte, overall charge of the membrane, and mobility of charges in a non-trivial manner. When the membrane retains some positive charge, the discrimination based on the stiffness is low, but less flexible polyelectrolytes show a higher degree of adsorption if the charges are frozen, compatible with a smaller loss in internal entropy, while in the case of mobile charges adsorption is still almost complete, irrespective of the intrinsic stiffness. When the membrane becomes neutral or slightly negative the general view is that flexible polyions adsorb better for both mobile and frozen charges than stiffer ones. These findings go beyond the conventional adsorption behaviour of a polyion at homogeneously charged surfaces. When individual protrusions are considered the adsorption of the polyelectrolyte is further enhanced. The surface response to the adsorbing macromolecule is two-fold: (i) the displacement of the surface particles out of the surface plane and towards the macromolecule and (ii) the polarization of the surface with the concentration of positive charges near the oppositely charged molecule. (R. Dias, A. A. C. C. Pais, (University of Coimbra), and P. Linse).

Statistical-mechanical programs. During 2005, a web-based interface for running five different statistical mechanical computer programs (MOLSIM, OZ, PB, PGESE, and POLYMER) was used in advanced undergraduate courses in physical chemistry. (P. Linse)

INSTRUMENTS AVAILABLE AT THE DEPARTMENT

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

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

Dynamic and static light scattering. (contact person: Karin Schillén).

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

B) For the characterization of molecular weight and studies of conformation changes or association processes in macromolecular systems, a multi-angle desktop instrument for SLS measurements is available. The instrument is a Dawn DSP-F MALLS photometer (Wyatt Technology Corp., Santa Barbara, California) equipped with a 5 mW He-Ne laser (633 nm). The intensity of the scattered light is measured using photodiodes at 18 different angles simultaneously. The instrument is connected to a gel permeation chromatography system for on-line molecular weight determinations in organic solvents but batch analysis may also be performed. (Sponsored by FRN.)

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

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

Ellipsometry. (contact person: Tommy Nylander). The development of a high precision ellipsometer for time-resolved studies of thin adsorbed films has been successful and of great importance to several specific projects. The instrument allows precise and rapid measurements of the ellipsometric angles y and D, thus, allowing unique studies of the evolution of both the thickness and density (refractive index) of adsorbed surfactant and polymer layers with time. The possibility of working at different wavelengths provides an additional source of information on complex systems as well as flexibility to optimize the optical contrast of the systems studied. Continued efforts are invested in upgrading this instrument to improve its potential for studies of fast interfacial processes occurring on the nanometer scale. During 1998 we acquired an additional ellipsometer, an Optrel Multiskop (Optrel, Berlin Germany). This instrument has been fitted with sample cells to measure at the solid-liquid, liquid-liquid and liquid-air interfaces. Apart from doing null-ellipsometry we can also do imaging ellipsometry, Brewster Angle Microscopy, Surface plasmons as well as operate it in waveguide mode. (Sponsored by FRN).

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

Multimode scanning probe microscope. (contact person: Tommy Nylander). A Multimode Scanning Probe Microscopy (Nanoscope-III) was purchased jointly by Physical Chemistry 1 and the Department of Food Technology from Digital Instruments Inc. in April 96. The instrument can be operated as both a scanning tunneling microscope (STM) and an atomic force microscope (AFM). With its many configurations the instrument can scan and image a wide variety of samples with scan sizes from atomic level up to 125 by 125 microns. As an AFM, traditional contact mode experiments in air and liquid and TappingMode experiments in air have been

available for many years. More recent equipment purchases allow users to image surfaces with TappingMode in fluid environments, perform lateral force microscopy (LFM) measurements of topography and friction, and make force measurements using a colloidal probe. In the latter mode, a spherical particle is adhered to an AFM cantilever and colloidal forces between the probe and surface in a fluid environment can be studied. Other force measurements are also possible using standard cantilevers or chemically modified cantilevers. (Sponsored by FRN).

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

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

Rheometers. (contact person: Krister Thuresson). A Carri-med controlled stress rheometer CSL 100 temperature controlled by a Peltier system. Measuring systems; cone and plate (solvent trap) in acrylic (4 cm, 1° and 6 cm, 1°) and stainless steel (4 cm, 1° and 6 cm, 1°). (Sponsored by Nils and Dorthi Troëdsson Research Foundation).

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

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

Collaborative Research Programs

The Centre for Amphiphilic Polymers, CAP

The Centre for Amphiphilic Polymers from Renewable Resources (CAP) at Lund University has been in existence since 1995. It is part of the national Competence Centre Programme supported by VINNOVA, the Swedish agency for innovation systems. CAP is jointly funded by Lund University, VINNOVA, and a group of member companies currently including Akzo Nobel Functional Chemicals, AstraZeneca R&D Mölndal, Celanese Emulsions Norden AB, Eka Chemicals, Lyckeby Stärkelsen, SCA Research, and Tetra Pak. Lennart Piculell is the director of CAP and Per Linse is a member of the Board, which has an industrial majority.

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

The year 2005 was originally meant to be the last year of CAPs existence, but owing to a sizeable number of ongoing projects (18 projects at the beginning of 2005), the duration of CAP was extended to June 2006. In 2005, the CAP graduate students Dane Momcilovic from Technical Analytical Chemistry and Maria Karlberg from our department successfully defended their PhD theses. The traditional two-day CAP annual meeting was held in May at Klitterbyn with 45 participants from industry and academia. The program was dominated by exciting lectures from 12 young CAP researchers who were close to finishing their respective projects.

To mark the 10 successful years of CAP, the 5th Annual Surface and Colloid Symposium in Lund on November 16-18 had "Amphiphilic Polymers" as its theme. Per Linse was the chair of the organizing committee. The topics of the symposium mirrored the topics of CAP research and the speakers included CAP researchers, reviewing the accumulated progress made during CAPs existence, as well as invited leading international scientists in the area. The 120 participants included international as well as Scandinavian researchers, with a strong representation from industry. In connection with the Symposium, CAP organized a half-day Open Forum on the Competence Centre as an Instrument for Collaborative Research, where representatives from Lund University, CAP academic researchers, CAP member industries, and VINNOVA presented their views and experiences.

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

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

self-assembly, dynamics of non-equilibrium self-assembly dispersions, and structuring complex systems at interfaces.

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

During the final year 2005 the following courses were given:

- Surface Chemistry - surfactants and polymers in aqueous solutions (5 p), Degeberga with 18 participants.
- DCS - basic principles and applications to phase science (3 p), Örenäs Slott, with 26 participants.
- Phase Behavior of Soft Matter, (3 p) Örenäs Slott, 32 participants

In addition, the graduate students organized a three days workshop. This workshop was organized by and open only for graduate students apart from three invited distinguished foreign scientists: Roland May, Robert Tilton and Brian Vincent.

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

The Division of Surface Chemistry of the Swedish Chemical Society.

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

The Competence Center for Surfactants based on natural products, SNAP

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

NorFA Network

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

Research Institute, Finland; Institute of Food Processing, Tallin Technical University, Estonia; Food Technology, Kaunas University of Technology, Lithuania.

New strategies for oral delivery of drug peptides and peptidomimetics

A 3 year collaborative project involving Camurus AB and Physical Chemistry 1 was granted 2003 by VINNOVA (Swedish Agency for Innovation Systems) and SSF (Swedish Foundation for Strategic Research) within the so-called VINST program dedicated to support SME. The aim of the project is to develop more effective peptide carriers and during this process also increase the understanding of the physicochemical and biological problems involved in oral bioavailability of peptides and proteins. Oral administration of peptide and protein drugs has so far been hampered by low bioavailability, due to the presence of effective permeation barriers and lack of peptide stability in the gastro-intestinal tract. The project involves extensive interdisciplinary activities and cross-fertilization of projects. The basic approach will be to use self-associated nano-structured lipid carrier and exploit special properties, which can provide protection against enzymatic degradation and enhanced permeation of biomembranes. Scientifically the project will span biophysical studies of lipids and peptides to in vivo studies of uptake mechanism for peptides and proteins. (T. Nylander, H. Wennerström; F. Tiberg and K. Larsson Camurus AB)

EU-STREP FP6 project- NEONUCLEI

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

EU-STREP FP6 project- BIOSCOPE

The department was granted a 3 year EU-FP6 STREP in the Nanoscience and technology area entitled "Self-reporting biological nanosystems to study and control

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

CIPSNAC

EU research training network "CIPSNAC: Colloidal and interfacial properties of synthetic nucleic acid complexes-assembly of nanostructured DNA particles and surfaces (EU-MRTN-CT-2003-504932). The Research Training Network (RTN), started in 2002, focus upon DNA nanoparticles and surfaces. In this specific field, a relationship between the structure, thermodynamic stability, enzymatic accessibility and gene transfer or detection efficiency has not been established so far. To date, physico-chemical characterization has only been carried out sporadically on isolated gene transfer systems. The establishment of phase diagrams as well as gene transfer efficiencies as a function of a large range of variables is time consuming. Therefore, this RTN project will bring about a concerted action of expert groups to address these problems. The fascinating frontier is to study the assembly of DNA surfactant complexes at the molecular level. The RTN will define model systems and key parameters such that a systematic theoretical approach becomes feasible. The partners are from Lund, Coimbra, Munich, Dublin and Paris. (B. Lindman, responsible for Lund group)

EU Project "Mercury"

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

As part of the project the essential parts of two titration calorimeters will be donated to our colleagues in Argentina and Peru. One of the instruments has been sent to Argentina. The other is nearly ready.

The extensive design work on the 48-channel instrument has successfully been completed. The project, which has been conducted in cooperation with Dr Dan Hallén, Stockholm, has also received support from non-EU sources. As a direct result the work in Lund, Hallén has formed a new instrument company, "SymCel" (initially in some

contact with KTH). The industrial version of the instrument is primarily built for the characterization of cell-drug interactions in the pharmaceutical industry. SymCel has applied for a patent of the instrument.

I intend to design slightly different versions for use in ecology and clinical analysis. A third instrument, an analytical device for sublimation and characterization of crystals, has been designed and tested in cooperation with Lars-Erik Briggner, Astra-Zeneca, Lund. That instrument is now used in routine work at Astra-Zeneca (in Lund and at a subsidiary in England).

Publication of the three instruments is presently being prepared. (I. Wadsö)

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

Research Areas and Facilities

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

- 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.
- 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.
- 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.

The contract was concluded in april 2005.

CONFERENCES, TRAVELS AND SEMINARS

Björn Lindman gave plenary lectures at the 11th International Conference on Organized Molecular Films, Sapporo, Japan and the 1st Iberian Symposium on Colloids and Interfaces, Salamanca, Spain, and invited lectures at the symposia on Surface Chemistry, Self-Assembly and Cell Biology, and Cosmetic Nanotechnology, at the American Chemical Meeting, Washington, D. C., at the Science and Engineering of Advanced Materials Strategic Workshop, Dublin, Ireland, at the Materials Sciences 2005 Conference, Göteborg, at the workshop On the shoulders of Fourier and Stokes: Stilbs and NMR, Stockholm, at the 5th Annual Surface and Colloid Symposium, Amphiphilic Polymers, Lund. He also attended the 19th Conference of the European Colloid and Interface Society, Geilo, Norway, the Nobel Symposium on Controlled Nanoscale Motion in Biological and Artificial Systems, Bäckaskog Slott, Sweden, the Marcus Wallenberg Prize Symposium, Stockholm, the 2nd Workshop on Colloidal and Interfacial Properties of Synthetic Nucleic Acid Complexes, Penacova, Portugal, the Nobel Workshop on Fundamentals of Biomolecular Function: Nucleic Acids, Proteins and Membranes, Coimbra, Portugal and the 8th Portuguese Meeting on Photochemistry, Coimbra, Portugal. 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: Universidad de Granada, Procter & Gamble Research Center, Cincinnati, Karlstad University, Institute of Genomics and Integrative Biology, Delhi, Indian Association for the Cultivation of Science, Kolkata, Jadavpur Univversity, Kolkata, University College Dublin, P&G Kobe Research Center, Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Kao Research Center, Wakayama, Yokohama National University, BASF Research Center, Ludwigshafen, Germany, Pola Research Center, Yokohama, Universidad Salamanca, Chalmers University of Technology, Göteborg, Akzo Nobel Surface Chemistry, Stenungsund, University of Ljubljana, Slovenia, University of Maribor, Slovenia, GlaxoSmithKline Research Center, Weybridge, UK, Columbia University, New York, Swedish Forest Research Institute, Stockholm, Uppsala University, Eka Chemicals, Göteborg, Institute for Surface Chemistry, Stockholm, Royal Institute of Technology, Stockholm. Björn Lindman also visited national research councils in conjunction with reviewing research proposals. Björn Lindman was visiting professor at the Department of Chemistry, Coimbra University, Portugal.

Håkan Wennerström delivered invited talks at: "First International Symposium on Delivery of Functionality in Complex Food Systems", Lausanne, Switzerland; at the CIPSNAC meeting in Penacova, Portugal and on a seminar at Department of Physical Chemistry , Oxford University, UK.

Lennart Piculell gave an invited lecture at the "European Polymer Congress 2005" in Moscow. Maria Karlberg gave an oral contribution at the same conference.

Lennart delivered an invited lecture at the SOCON annual meeting in Aarhus, Denmark. He was also a member of the organizing committee and chairman of the program committee of the 5th Annual Surface and Colloid Symposium, Amphiphilic Polymers in Lund

Per Linse delivered invited plenary lecture at European Polymer Congress, Moscow, Russia and invited oral presentations at the workshop on "Macroion complexation: Fundamentals and applications", Wageningen, The Netherlands and "5th International Discussion Meeting on Relaxation in Complex Systems", Lille France. He also gave invited seminars at Utrecht University, The Netherlands and KTH, Sweden.

Ulf Olsson gave invited a plenary lecture at 19th Conference of the European Colloid and Interface Society, Geilo, Norway, invited talk at 5th Annual Surface and Colloid Symposium, Amphiphilic Polymers in Lund and a seminar at Procter and Gamble, Bruxells. He also attended SSF workshop on material science in Göteborg, the annual meeting of the Swedish Neutron Scattering Society, Göteborg. Ulf visited Bari University, Italy and Coimbra University, Portugal and performed neutron scattering at: ILL Grenoble, France and Paul Scherrer Institute, Villigen, Switzerland.

Karin Schillén presented two posters at a workshop on Scattering from Soft Matter, Kgs. Lyngby, Denmark,

Anna Svensson visited Procter & Gamble, Cincinnati, USA where she gave a seminar and held a 1-day workshop called Hands-on experience of liquid crystalline phases and phase diagrams.

Emma Sparr presented a poster at the Nobel Symposium "Fundamentals of Biomolecular Functions: Nucleic Acids, Proteins and Membranes" in Coimbra, Portugal

Justas Barauskas gave an oral presentation at The Annual European Conference on Micro & Nanoscale Technologies for the Biosciences (Nanotech), Montreux, Switzerland.

Rita Dias, Justas Barauskas and Geraldine Lafitte gave oral presentations at 19th Conference of the European Colloid and interface Society (ECIS) in Geilo, Norway

Justas Barauskas and Geraldine Lafitte also gave an oral presentation at "First International Symposium on Delivery of Functionality in Complex Food Systems", Lausanne, Switzerland.

Rita Dias and Monica Rosa gave oral presentations at the CIPSNAC meeting in Penacova, Portugal, and presented posters at the Nobel Workshop "Fundamentals of Biomolecular Function: Nucleic Acids, Proteins and Membranes" Coimbra, Portugal

Rita Dias also gave an oral presentation at the Final Evaluation meeting of COST D15 "Interfacial Chemistry and catalysis" meeting in Maribor, Slovenia, and presented a poster at and at the NEONUCLEI meeting in Southampton, UK.

Monica Rosa also presented a poster at the "13th Annual Congress of ESGT", Prague, Czech Republic.

Ola Karlsson gave invited lectures at 5th Annual Surface and Colloid Symposium. Amphiphilic Polymers, Lund, Sweden and at YKI Member Days, Stockholm, Sweden

Samuel Edgecombe gave oral presentations at 44th Macromolecular Symposium, in Prague, Czech Republic and at the Student Conference in Fiskebäckskil, Sweden

David Löf spent 10 weeks with the "Grupo de Polimeros" in University Simon Bolivar, Venezuela, and gave an oral presentation at "XI Coloquio Venezolano de Polímeros Conference", Caracas, Venezuela David was one of the directors and chairman for the student conference at Gullmarsstrand in Fiskebäckskil, Sweden where he also contributed with an oral presentation.

Markus Nilsson stayed two weeks at University of Vigo, Spain, as part of a research collaboration.

Marie-Louise Örberg delivered an oral presentation at the 2nd Neonuclei meeting in Southampton, UK.

Cecilia Leal presented a poster at "The 4th Alpine conference on solid-state NMR", Chamonix, France.

The department organized the yearly meeting of the Surface and Colloid section of the Swedish Chemical Society, entitled "5th Surface and Colloid Symposium.

Amphiphilic Polymers". The meeting attracted 120 participants included international as well as Scandinavian researchers, with a strong representation from industry. A majority of the department members presented posters at the meeting. In connection with the Symposium CAP organized a open forum on "The Competence Centre as an Instrument for Collaborative Research"

The meeting 2006 will also be held in Lund 15-17 of November and dedicated to "Lipid-Peptide Interactions and Biological Function"

(http://www.chemsoc.se/sidor/KK/ytkemi/surfaceandcolloid.htm /)

EXTERNAL PROFESSIONAL ACTIVITIES

Björn Lindman was on the Advisory or Editorial Boards of Cellulose, Advances in Colloid and Interface Science, Current Opinion in Colloid & Interface Science and Journal of Dispersion Science and Technology. Björn Lindman is also member of the Research Council of The Swedish Pulp and Paper Research Institute. He is a member of The Royal Swedish Academy of Engineering Sciences, of The Royal Swedish Academy of Sciences and of The Royal Physiographic Society in Lund. He is Director for a national program on Colloid & Interface Technology sponsored by the Swedish Foundation for Strategic Research and also a member of the Collegium of this foundation. Björn Lindman was external examiner (opponent) for Dan Lundberg's thesis defense, Chalmers University of Technology, Göteborg.

Håkan Wennerström was chairman of the Nobel Committee for Chemistry, regular member of the board of the Science and Technology Committee of the Swedish Research Council, Swedish representative in the Physical Sciences and Engineering Standing Committee (PESC) of the European Science Foundation, member of the Scientific Group of the Chemistry Department, Lund University, member of the scientific innovation group (Idérådet), Lund University and member of the "Liquids group" of the European Physical Society.

Lennart Piculell is the director of the Center for Amphiphilic Polymers (CAP) since November 2003. He was a member of the Board of the Faculty of Science, Lund University also during 2005. He is a section editor for the Polyelectrolytes section of Current Opinion in Colloid and Interface Science, a member of the editorial boards of Food Hydrocolloids and Carbohydrate Polymers and a member of the international organizing committee of the biannual International Polyelectrolyte Symposia. He was an external examinor at the thesis defense of Isabel Couillet (Université Louis Pasteur, Strasbourg) and served on the thesis committees at the thesis defenses of Olivera Trifunovic (Food Engineering, LU) and of Helen Sjögren, where he also was the chairman. LP was the coordinator and main author of a major proposal to VINNOVA for a new so-called VINN Excellence Center entitled "High Performance Colloid and Surface Materials (HIPECS)". The proposal, backed by 10 small and large industrial companies, has reached the interview stage in 2006; a final decision will be taken in June 2006.

Per Linse was a member of the board and member of the program committee of CAP. Per served on the PhD thesis committee for Christian Persson Lund University.

Ulf Olsson was Chairman of the board of undergraduate studies, board member of the Swedish Neutron Scattering Society and member of a review panel for the Committee for Research Infrastructure of the Swedish Research Council Ulf served

on PhD thesis committees of Jan Cocquyt, Ghent University and Malin Zackrisson, Göteborg University.

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

Karin Schillén was a deputy member of the board of the Chemical Center and member of the research board of the chemistry division at the Chemical Center "Forskningsnämnden vid kemiska sektionen (NF)". Karin served on PhD thesis committees for Malin Zackrisson, Göteborg University, Gunilla Carlsson, Karlstad University and Anette Munch Elmér, Lund University.

AWARDS

Björn Lindman received the Victoria Professor Memorial Award, of the Indian Association for the Cultivation of Science and Award of Coimbra University, Portugal.

Daniel Topgaard received the Ingvar Carlsson Award from The Swedish Foundation for Strategic Research and the Fabian Gyllenbergs Award of The Royal Physiographic Society in Lund.

COURSES AND TEACHING

Members of the department are involved in a number of undergraduate courses. The first year of chemistry studies at the Chemical Center consists of three 9-week chemistry courses and a 9 week course in mathematics. These courses are given both during the fall and spring semesters. In the first two basic chemistry courses Viveka Alfredsson, Per Linse, Karin Schillén, Emma Sparr, Olle Söderman Daniel Topgaard and Christoffer Åberg were involved in lectures and leading exercises and question hours. The topic of the third first-year course is thermodynamics and introductory quantum mechanics and spectroscopy. Here, Karin Schillén is the head teacher for this course and Karin gave the lectures and exercise sessions in thermodynamics together with Olle Söderman. Johan Reimer has the main part of his position within the undergraduate education, where he among other things administrates the first year courses.

As regards higher courses, the department gives one basic and one advanced course in surface and colloid chemistry and one advanced physical chemistry course. The basic colloid course is headed by Ulf Olsson and was taught by Ulf, Lennart Piculell, and Sam Edgecombe. Half of this course was for the first time given at the same time in the Engineering School together with Björn Bergenståhl and the department of Food Technology. Also Stefan Ulvenlund was involved in the teaching of this course. The collaboration with the Engineering Faculty is interesting and we hope it can be developed further. The advanced surface and colloid chemistry course is organized and taught by Lennart Piculell (main teacher) along with Tommy Nylander, Emma Sparr Per Linse and Håkan Wennerström. It is given once a year during the fall semester, and is based on the book by Håkan Wennerström and Fennel Evans. The advanced physical chemistry course is also given once a year during the spring semester and is taught by Per Linse, Ulf Olsson and Olle Söderman. This course is focused on methodology and is divided into three parts: (i) Small angle scattering and light scattering (Ulf), (ii) NMR (Olle), and (iii) statistical mechanics and computer simulations (Per). Håkan, on behalf of the department, delivered a total of 15 hrs lectures on environmental chemistry for the undergraduate students. Finally, a number of our graduate students serve as teaching assistants on all courses given by the department.

When teaching undergraduate courses we also emphasize industrial applications since it represents the future activities for many of the students. We visit industries, and for a number of years we also have had an invited guest from industry to lecture on pharmaceutical applications of colloid and interface science. Here we are particularly grateful to Krister Thuresson at the Camurus Company for allowing visits and for taking the time to explain practical surface and colloid science to our students.

On the graduate level most senior members of the department also participate and organize various graduate courses, many of which have been given within the national research school in Colloid and Interface Technology, COLINTECH.

Björn Lindman was one of the teachers on the annual course on surfactants and polymers in aqueous solution, this year given both in Lisbon and Basking Ridge, New Jersey.

EVA HANSSON RETIRED

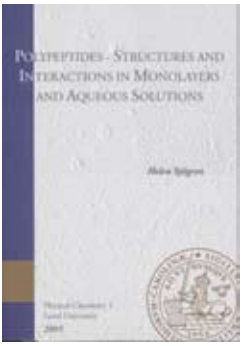
Eva Hansson retired 31/12 2005. Eva has been with our department longer than anyone else and was employed from 1962. After completing her Ph D in physical chemistry in 1973 on a thesis entitled "*On the structures of solid rare earth oxalates and malonates.*" She became a senior lecturer in our department from 1972, with tenure from 1978. Eva has during decades been a key teacher in the Chemical Center and taught a large number of courses during several years. Eva proved early also her management and administration skills and has, therefore, been trusted with many important responsibilities at the department, faculty and university levels. This has included the responsibility for the teaching in chemistry (1983-1996), vice-dean for undergraduate studies at the Faculty of Science (1993-1999), member of the Board of Lund University and during the period 2000-2005 President of the Chemical Center. It is no doubt that Eva's excellent work in these positions will give a long-lasting benefit.

Obviously, this has strongly helped also our department. However, here we wish to stress the very important role she has had in our department during all years. In particular has her talent as an enthusiastic teacher been important for generations of students. In addition she has constantly modernized the different courses. When Björn Lindman arrived to the Department of Physical Chemistry 1 as a new chair professor and head of department in 1978, he was immediately struck by Eva's wish and ability to update both her own knowledge and the chemistry curriculum. Thus she immediately had the ambition to get involved in the research in surface and colloid chemistry introduced in the department, doing research on the structure of cubic liquid crystalline phases together with late Krister Fontell, as well as to design a new course in this area. The teaching on colloids and surfaces has progressively broadened and become a cornerstone in our undergraduate program.

(Photo by Tommy Ljungdell)

DOCTORAL THESIS

June 2, 2005
Caroline Ericsson
Alkylglycoside Surfactants - Self-Assembly, Solid-State Properties and Interactions with Hydrophobic Molecules
Opponent: Dr Matthew Lynch, Procter & Gamble Company, Cincinnati, Ohio, USA



September 9, 2005
Helen Sjögren
Polypeptides - Structures and Interactions in Monolayers and Aqueous Solutions
Opponent: Prof. Paavo K. J. Kinnunen, Helsinki Biophysics and Biomembrane Group, University of Helsinki, Finland

September 16, 2005
Maria Karlberg
Synergistic Interactions Involving Amphiphilic Polymers in Solution
Opponent: Dr. Peter Griffiths, Cardiff University, UK

November 4, 2005
Anna Akinchina
Charged Polymers at Spherical Surfaces
Opponent: Dr. Helmut Schiessel, Universiteit Leiden, The Netherlands

FINANCIAL SUPPORT

For the fiscal year 2005, the department had a turnover of ca 33.2 million SEK. From the University we obtained 12.9 million of which 1.1 million is to cover undergraduate teaching, and the rest for graduate students, salaries of professors, associate professors and assistant professor, technical and administrative personnel, and basic expenses including rents of offices and laboratories. Government research agencies that give support to the research is: The Swedish Research Council (VR), which provide us a support of 5.6 million SEK, The Swedish Agency for Innovation Systems (VINNOVA) which finances more applied projects, supports us with 3.8 million, mainly via the 2 Competence Center CAP and SNAP, during the fiscal year. We also received 3.2 million SEK from The Swedish Foundation for Strategic Research (SSF), which is an important funding agency for supporting novel research ventures in Sweden. We are grateful for support from private industry, directly and via their foundations, amounting to ca. 4.2 million. Finally, we received 3.6 million SEK from The European Commission.

MEMBERS OF THE DEPARTMENT

Scientists/Teachers

Viveka Alfredsson, associate prof.
Justas Barauskas, postdoc
Rita Dias, postdoc
Katarina Flodström, researcher
Eva Hansson, dean
Markus Johnsson, postdoc
Lina Karlsson, postdoc
Ola Karlsson, adjunct prof.
Ali Khan, associate prof. em.
Jakob Kisbye Dreyer, postdoc
Björn Lindman, prof.
Per Linse, prof.
Iseult Lynch, researcher
Maria G. Miguel, visiting prof.
Tommy Nylander, associate prof.
Gerd Olofsson, associate prof.
Ulf Olsson, prof.
Lennart Piculell, prof.
Johan Reimer, lecturer
Karin Schillén, associate prof.
Emma Sparr, assistant prof.
Anna Svensson, researcher
Olle Söderman, prof.
Krister Thuresson, assistant prof.
Fredrik Tiberg, adjunct prof.
Daniel Topgaard, assistant prof.
Stefan Ulvenlund, assistant prof.
Ingemar Wadsö, prof. em.
Håkan Wennerström, prof.

Graduate students working on a Ph. D. Thesis

Anna Akinchina
Joakim Balogh
Sanja Bulut
Samuel Edgecombe
Caroline Ericsson
Malin Jönsson
Maria Karlberg
Niklas Källrot
Anna Körner
Géraldine Lafitte
Cecilia Leal
Peter Linton
David Löf
Carin Malmborg
Markus Nilsson
Jens Norrman
Helen Sjögren
Pauline Vandoolaeghe
Christoffer Åberg
Marie-Louise Örberg

Technical-Administrative Personnel

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

GUESTS

Almgren, Mats, Uppsala University, Uppsala, Sweden (S)
Brito, Rodrigo, University of Porto, Portugal (L)
Barreleiro, Paula, Henkel KGaA, Duesseldorf, Germany (S)
Chernik, Gerlina, St. Petersburg State University, Russia (L)
Ciunel, Katarzyna, Technical University, Berlin (L)
Das, Prasanta, Indian Association for the Cultivation of Science, India (L)
Davies, Ted, University of Minnesota, USA (S)
Deleu, Magali, Gembloux Agricultural University, Belgium (L)
de Vries, Renko, Wageningen University, The Netherlands (S)
Dreano, Marie, Ecole Nationale Supérieure de Chimie de Paris, France (L)
Eeman, Marc, Gembloux Agricultural University, Belgium (L)
Esteban, Isabel, Universidad Nacional de Educación a Distancia, Spain (L)
Glatter, Otto, University of Graz, Austria, (S)
Gotter, Martin, University of Cologne, Germany, (L)
Gradzielski, Michael, Technische Universität Berlin, Germany (S)
Griffiths Peter, Cardiff University, UK (S)
Guiot, Camille, Ecole Nationale Supérieure de Chimie de Paris, France (S)
Holmqvist, Peter, Forschungszentrum Jülich, Germany (S)
Imai, Masayuki, Japan (S)
Johannesson, Espen, Åbo akademi, Finland (S)
Johansson, Ingegärd, Akzo Nobel Surfactants, Stenungsund, Sweden (S)
Kaper, Helena, Christian-Albrechts-Universität Kiel, Germany (L)
Kinnunen, Paavo, University of Helsinki, Finland (S)
Klitzing, Regine v., Christian-Albrechts-Universität Kiel, Germany (S)
Korolev, Nikolay, Nanyang Technological University, Singapore (S)
Leaver, Marc, University of Central Lancashire, UK, (S)
Li, Junbai, Chinese Academy of Sciences, Beijing, China (S)
Liu, Yaqian, BASF, Ludwigshafen (Rhein), Germany (S)
Lynch, Matthew, Procter & Gamble Company, Cincinnati, USA (S)
Lyubartsev, Alexander, Stockholm University, Sweden (S)
Maiti, Souvik, Institute of Genomics and Integrative Biology, Delhi, India (L)
Marques, Eduardo, University of Porto, Portugal, (S)
Matsuo, Goh, Hokkaido University, Sapporo, Japan (L)
McNamee, Cathy, Nederländerna, (L)
Medronho, Bruno, University of Coimbra, Portugal (L)
Misiunas, Audrius, Institute of Biochemistry, Vilnius, Lithuania (L)
Monduzzi, Maura, Università di Cagliari, Italy (S)
Mourad, Maurice, Utrecht University, The Netherlands (L)
Müller, Alejandro, Universidad Simón Bolívar, Venezuela (S)
Nakaya, Kaor, Japan (S)
Neumann, Peter, BASF, Ludwigshafen, Germany (S)
Noolandi, Jaan, Stanford University, USA (S)
Patra, Michael, Helsinki University of Technology, Finland (S)
Pegado, Luis, University of Coimbra, Portugal, (L)
Penacho, Nuno, University of Coimbra, Portugal, (S)
Popescu, Georgeta, University of Bucharest, Romania (L)
Salvati, Anna, University of Florence, Italy (L)
Santos, Tiago University of Coimbra, Portugal, (L)

Sarraguca, Jorge University of Coimbra, Portugal, (L)
Schiessel, Helmut, Universiteit Leiden, The Netherlands (S)
Silva Cláudia, Portugal, (L)
Takemasa, Makoto, Waseda University, Tokyo, Japan (L)
Tam, Michael, Nanyang Technological University, Singapore (L)
(L)= Long-term (S)= Short-term

PUBLICATIONS

(1) Alfredsson, V.
Cryo-TEM studies of DNA and DNA-lipid structures.
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(11) Bo, A. D.; Schweitzer, B.; Felippe, A. C.; Zanette, D.; Lindman, B.
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(12) Bryskhe, K.; Bulut, S.; Olsson, U.
Vesicle formation from temperature jumps in a nonionic surfactant system.
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(13) Bryskhe, K.; Schillén, K.; Olsson, U.; Yaghmur, A.; Glatter, O.
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(14) Cabaleiro-Lago, C.; Nilsson, M.; Söderman, O.
Self-diffusion NMR studies of the host-guest interaction between beta-cyclodextrin and alkyltrimethylammonium bromide surfactants.
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(15) Cárdenas, M.; Dreiss, C. A.; Nylander, T.; Chan, C. P.; Cosgrove, T.; Lindman, B.
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Dynamics and energetics of the self-assembly of a hydrophobically modified polyelectrolyte: Naphthalene-labeled poly(acrylic acid).
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WELCOME TO VISITORS

Dear Visitor,

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

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

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

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

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

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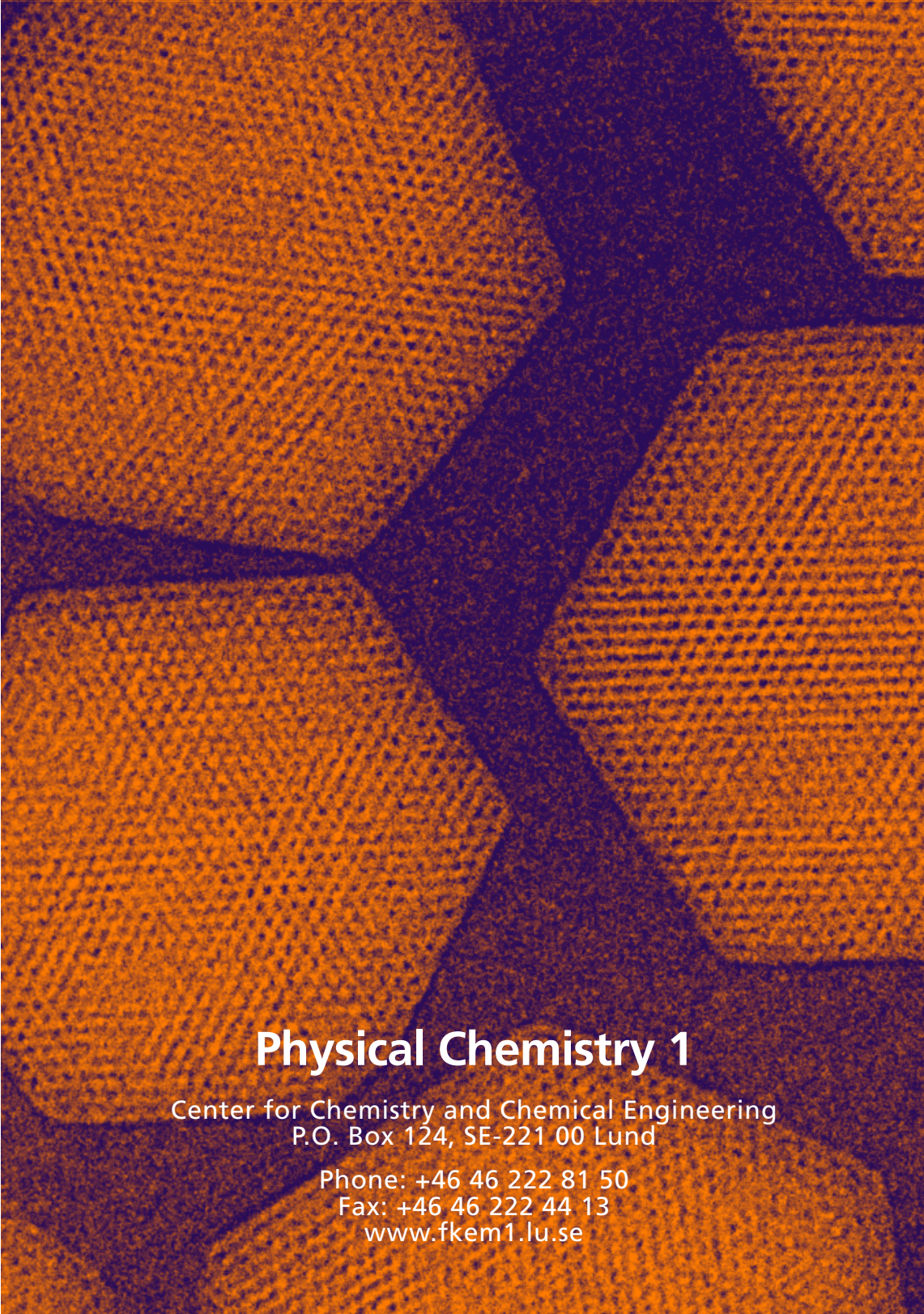

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