CONTENTS

Cover. Image of a nanopatterned polymer brush obtained from computer simulation, showing flexible polymers (red) grafted onto a narrow stripe (gray) of a planar surface. The osmotic pressure expands the brush laterally, reducing the brush height unless the pattern is wider than a few times the polymer contour length. In the image, the stripe is much narrower than this limit (M. Patra and P. Linse).

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

ORGANIZING MOLECULAR MATTER

A most significant event for the Division of Physical Chemistry 1 during the last year was that we, together with groups at the Divisions of Theoretical Chemistry and Biophysical Chemistry of the Chemical Center, were awarded a Linné grant. The Swedish Research Council (VR) launched a call for collaborative research efforts with an obligation for a long-term support. Together with a matching grant from the university the support for the team amounts to 8.5 million SEK per annum with a projected duration of ten years. This provides a stable base financial base for the planning of research activities for the years to come.

The research program is focused on intermolecular interactions and their manifestations in a liquid environment. Four different types of problems will be addressed. The theoretical basis for the description of intermolecular interactions and their consequences are treated using both quantum chemical calculations and statistical mechanical simulations. On the next level carefully selected model systems are studied experimentally. The interplay between theory and experiment is an essential feature of the program. An important part of the experimental studies is an ongoing improvement of methods. It is very useful to have well characterized systems for which one can test the validity and usefulness of the methods. A final part of the program is to apply the understanding obtained in the basic studies for solving application problems. Here we see almost infinite possibilities and we can only select a small number of these. We find applications both in the biophysical/molecular biology field and in the industrial area.

Altogether there are nineteen senior researchers associated to the program. These range from young associate professors to senior full professors. This hopefully ensures that will be able to combine continuity with renewal in the research. The program also encourages a concentration of the efforts on a few difficult problems. It is particularly a most attractive challenge to combine strong theoretical and experimental efforts to obtain an understanding of some fundamental issues that could hardly be achieved by separate efforts.

Håkan Wennerström

RESEARCH PROJECTS

Within the broad arena of modern colloid and surface chemistry, research is largely concentrated into four loosely-bound areas: (1) Molecular assembly; (2) Adsorption and interfaces; (3) Colloidal biology; (4) Theory and modelling.

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

Molecular assembly

Phase diagram and Thermodynamics of Surfactants at low Water Contents. 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. By combining the sorption calorimetric measurements with accurate DCS measurements, a phase diagram for the dimethylamine oxide water systems has been determined. (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. In another project, the self-assembly of log chain fatty alcohol/surfactant mixtures are studied when cooled below the chain melting temperature. (P. Saveyn (Univ. of Gent), P. van der Meeren (Univ. of Gent), G. Olofsson, T. Drakenberg, T Awad, U. Olsson).

Asymmetric catanionic surfactants. Catanionic surfactants are complex salts of surfactant cations and surfactant anions (e.g. dodecyl tetra methyl ammonium dodecyl sulphonate) in the absence of additional simple salts (e.g. NaCl). Symmetric (equal alky chain lengths) catanionics form essentially stable water insoluble crystals at room temperature. In asymmetric catanionics the surfactant film may carry a net charge in mixtures with water because of a mismatch in the aqueous solubility of the two surfactant ions. The chain length mismatch also reduces the Krafft temperature significantly resulting in that these materials are water soluble already at room temperature. If the solubility difference is not too large, these surfactants form a lamellar phase in water which can swell to very high water contents due to the net bilayer charge. However a very interesting aspect is the presence of an unusual miscibility gap within the lamellar phase, which has previously been observed only in a few particular systems. (B. Silva (Porto), E. Marques (Porto), U. Olsson).

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 may be followed 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. The diffusion of surfactant molecules is restricted to the self-assembly aggregates which may form a random coil or be an infinite connected network. Both super and sub diffusion may be observed which can be described within the same formalism in terms of a generalized diffusion equation with fractional derivatives. (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. (S. Bulut, M. Zackrisson, U. Olsson, H. Wennerström; M. Gotter (Köln), R. Strey (Köln)).

Interaction between cyclodextrin and surfactants. Cyclodextrin forms inclusions complexes with surfactants. In this project we examine the stoichiometry, strength and structure of such complexes formed between α, β and γ-cyclodextrin and cationic gemini and bola surfactants. The main methods used are NMR diffusometry and NMR multi-dimensional techniques (mainly ROESY). Also conductivity measurements are used. (M. Nilsson, O. Söderman, A. Valente (Coimbra)).

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. (M. Vaccaro, O. Söderman, C. v Corswandt (Astra-Zeneca, Mölndal)).

Shear-induced formation of multi-lamellar vesicles. The equilibrium structure and phase equilibria of the lamellar phase are sometimes complicated as noted in already 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), M. Imai (Tokyo), Y. Suganuma (Tokyo).

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, M. Zackrisson, 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)).

Mixed solutions of amino-acid-based surfactants. Mixed solutions of surfactants based on arginine and glutamate, as well as their mixtures with synthetic surfactants, were examined with respect to phase behaviour and aggregate structure. Mixed solutions show vesicle formation as for several other catanionic systems. For mixed systems of an arginine and a glutamate-based surfactant a spontaneous formation of dispersions of both lamellar, reversed hexagonal (HexasomesR) and cubic phase (CubosomesR) were obtained. Specially noteworthy was the fact that for the first time Cubosomes , which do not need a stabilizer, were found. (Collaboration with Coimbra Univ., M. Miguel, M. Rosa) and Univ. Barcelona, M. R. Infantes, C. Moran). (B. Lindman, M. Rosa, M. Miguel).

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). Project completed.

Phase behaviour of aqueous "complex salts" of oppositely charged polymer and surfactant. We use a 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)).

Ionic surfactants with polymerizable counterions. The results of the preceding project include phase diagrams of mixtures of complex salts (surfactant ions with polymeric counterions) with conventional ionic surfactants (with monomeric counterions). Such phase diagrams actually predict the outcomes of polymerization processes, where the monomeric counterions of a surfactant ion are gradually polymerized into polymeric counterions. In a newly started project, we test these predictions by using ionic surfactants with polymerizable counterions. Indeed, the polymerization of acrylate counterions of alkyltrimethylammonium surfactants yields phases in accordance with the equilibrium phase diagrams determined previously. These polymerization processes are of fundamental and practical interest. For instance, they are closely analogous to processes where highly ordered mesoporous silica materials are produced by the polymerization of silicates in the presence of surfactants. (S. Santos, L. Piculell, O. Karlsson, M. Miguel (Coimbra University)).

Molecular dynamics and nanoscale organization in molecular matter. Several types of intermolecular interactions, e.g., steric, electrostatic, and hydrophobic, affect the dynamic behavior of large molecules in crowded system. NMR offers a unique possibility of resolving different molecules and molecular sites even in rather complex mixtures. For colloidal and biological systems with reduced molecular mobility and sample heterogeneity on the nano- to micrometer scale, solid-state NMR methods with magic-angle spinning are necessary in order to extract high-resolution spectroscopic information. Dynamic and site-resolved information can be correlated in multidimensional experiments. The aim of this project is to develop and apply modern multidimensional solid-state NMR techniques for the study of molecular dynamics and organization in a series of colloidal systems. (P. Choudhary, E. Sparr, V. Alfredsson, L. Piculell, D. Topgaard).

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). Project completed.

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).

Cross-linked DNA gels. DNA molecules, both single- and double-stranded, 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. An extensive comparative study of the deswelling of both ss- and ds-DNA gels on addition of several cosolutes- metal ions of different valency, proteins, polyamines and other polycations and cationic surfactants- have been performed. Both thermodynamic and kinetic aspects, as well as reversibility of volume changes, have been considered. (D. Costa, M. Miguel (Coimbra), P. Hansson (Uppsala), S. Schneider, B. Lindman).

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_iEO_j) in dilute aqueous solution are studied using dynamic and static light scattering in combination with differential scanning and isothermal titration calorimetry. Small-angle X-ray scattering and depolarized dynamic light scattering are also employed. The aim is to study the block copolymer-surfactant interaction, the mixed micelles formed as well as the retarded kinetics of the shape transition of the mixed micelles. (D. Löf, K. Schillén, G. Olofsson, A. Niemiec, W. Loh (UNICAMP, Brazil), O. Glatter (University of Graz, Austria)).

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).

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, T. Costa and M. da G. Miguel (University of Coimbra, Portugal), K. Schillén, B. Lindman).

Extensional rheology, shear rheometry and dynamic light scattering measurements on systems of cylindrical surfactant micelles and block copolymer-nonionic surfactant mixed micelles. 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 by using shear rheometry, extensional rheology and dynamic light scattering in combination. The rheological properties (and growth) of cationic cylindrical surfactant micelles in aqueous solution are studied under three different flow fields: simple shear, opposed-jets flow (which approximates uniaxial extension) and porous media flow (which includes simultaneously shear and elongational components of the flow). The retarded kinetics of the sphere-to-rod transition of mixed micelles of PEO-PPO-PEO triblock copolymer and nonionic C_iEO_j surfactants is also being investigated. By using zero-shear rheology as a function of time and temperature the time-dependence of the transition is followed and the results are in good agreement with those obtained from time-resolved static and dynamic light scattering measurements. (D. Löf, K. Schillén, M. Torres and A. J. Müller (Universidad Simón Bolívar, Venezuela)).

Supramolecular aggregates of amphiphilic gadolinium complexes as contrast agents for magnetic resonance imaging applications. Magnetic resonance imaging (MRI) is an imaging technique with cellular resolution that is widely used as a diagnostic tool in clinical practice. In this project, new potential blood pool contrast agents based on amphiphilic gadolinium complexes and amphilphiles that contain a bioactive peptide with target specificity are being developed. The structures of the self-assembled aggregates (lamellar aggregates, vesicles and micelles) in aqueous solution are characterized by means of dynamic light scattering, cryo-TEM and small-angle neutron scattering. (M. Vaccaro, L. Paduano, G. Mangiapia, G. Morelli, A. Accardo and D. Tesauro (University of Naples, Italy), E. Gianolio and S. Aime (University of Turin, Italy), D. Löf, K. Schillén, O. Söderman).

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 quite 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)).

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 1H NMR and TEM. (P. Linton, V. Alfredsson and H. Wennerström).

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, I. Åslund, G. Rata, O. Söderman).

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, I. Åslund, 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).

Adsorption and Interfaces

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).

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. Mixed polymer systems, both nonionic and ionic, have been extensively tested in animal experiments in the Department of Surgery, Lund University. Major reductions in adhesion formation have been obtained, much above products used in clinics. Studies based on the systems we have designed have formed the basis of two doctoral thesis in surgery. (B. Lindman).

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).

Stimulus-responsive polymer brushes on surfaces. Patterned polymer brushes constitute one approach to fabricate functionalized surfaces. Our aim is to in more depth characterized such brushes manufactured at Purdue University by, in particular, QCM, ellipsometry, and neutron reflectivity as well as with simulation methods. (S. Zauscher (Duke University), A. Rennie (Uppsala University), F. Höök (Solid State Physics), R. Campbell, T. Nylander, M. Patra, and P. Linse).

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, O. Santos, T. Nylander, L. Piculell, B. Lindman in collaboration with E. Johnson and R. Panandiker, Procter & Gamble, Cincinnati).

DNA compaction in solution and at particle solution interfaces. 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. DNA adsorption has also large implications for the fabrication of nano-structures using e.g. 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. The contribution of nonspecific interactions to the overall interactions of thiol-ssDNA and dsDNA macromolecules with gold nanoparticles is here very important. Dynamic light scattering, cryogenic transmission electron microscopy 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, J. Barauskas, J. L. Brennan and M. Brust (University of Liverpool, UK), T. Cosgrove (Bristol University), T. Nylander, B. Lindman).

Colloidal Biology

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 (Camurus AB, Lund), M. Monduzzi (Italy)).

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).

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

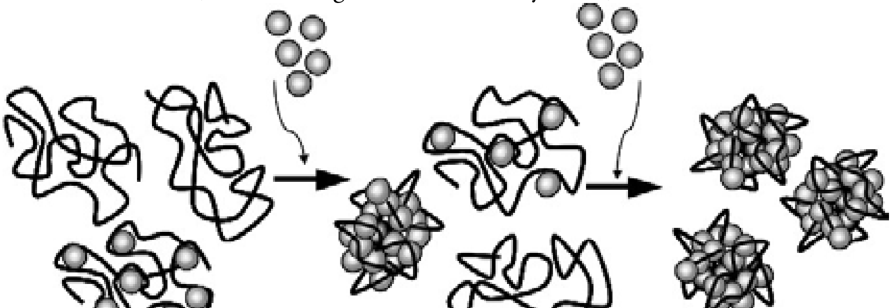
Amyloid formation and protein-lipid co-aggregation. Many human disorders belong to a family of amyloid diseases, characterized by abnormal folding of proteins into aggregates with a fibrillar structure. We have recently shown on the formation of protein-lipid aggregates when the protein aggregation is taking place in the presence of lipid membranes. The aim the project is to investigate the basic principles for such protein-lipid co-aggregation. We study the interactions between the A protein, involved in Alzheimer's disease with model lipid membranes of different composition. (E, Sparr, S. Linse (Biophysical Chemistry, Lund University) H. Wennerström).

Interaction 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), NMR, monolayer techniques, fluorescence microscopy and fluorescence spectroscopy. (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).

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).

Interactions between DNA and cationic dendrimers. Dynamic light scattering and steady-state fluorescence spectroscopy are utilized to investigate the interaction between poly(amido amine) (PAMAM) dendrimers and double stranded (ds) DNA. The aim is to study the formation process of dsDNA-dendrimer aggregates and their internal structure. (M.-L. Örberg, K. Schillén, T. Nylander).



Proposed binding model for discrete aggregates formed between DNA and PAMAM dendrimers of generation 4. A coexistence of coils and globules are shown for low ratios of dendrimers/DNA (rmolar <30) and only compacted globules are displayed for higher amount of dendrimers in dilute solutions below charge neutrality.

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, A. Gonzáles Pérez, B. Lindman, M. Miguel).

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. The co-adsorption behaviour may be another important factor determining the DNA-surfactant complex efficiency for its delivery to target cells. Solid-liquid interfaces are used as a model system to facilitate the understanding of interfacial properties such as lateral organization and layer composition at technologically relevant surfaces. The main technique being used is ellipsometry, which allows in situ measurements of interface processes with high resolution (~0.1 mg/m2). Both adsorption phenomena on hydrophilic and hydrophobic surfaces are investigated. The adsorbed layer structure is further determined by means of Neutron Reflectivity. The surface force apparatus is also utilized to better understand the structure of the mixed adsorbed layers. (M. Cárdenas (Malmö University), J. Campos, T. Nylander, R. Thomas (Oxford University), B. Lindman).

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).

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).

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).

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. With shorter alcohols particularly complex phase diagrams were observed. (A. Bilalov, C. Leal, A. Khan, B. Lindman). Project completed.

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). Project completed.

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 has been 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). Project completed.

The ejection of genome from viruses. In this work light scattering is used as the main technique in order to study the ejection process of natural DNA from λ-bacteriophage. Measurements are carried out under different physical conditions and the ejection process is also studied with different DNA binding proteins added to the investigated solutions. (D. Löf, K. Schillén, A. Evilevitch (Biochemistry, Lund University), B. Jönsson (Biophysical Chemistry, Lund University).

Theory of Colloids

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. The experimental work involves transport studies in skin and in model lipid membranes. For these studies we recently devolved a system of so-called double-porous membranes where the lipid lyotropic phases are confined and aligned inside the pores of a synthetic polymer membrane. 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). (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. (C. Whiddon, O. Söderman, B. Jönsson (Biophysical Chemistry, Lund).

Dynamics of polymer adsorption. The dynamics of adsorption and desorption of uncharged homopolymers have been investigated using a coarse-grained model comprised of a bead-spring chain and a planar surface. Brownian dynamics simulation has been used to examine the adsorption process for polymers released near the surface and with bulk properties, and Monte Carlo simulations to explore equilibrium adsorption structures of the polymer. Systems with varying polymer contour length, polymer stiffness, and polymer-surface interaction potential, have been considered. Investigations have been made on polymer extensions perpendicular and parallel to the surface and also characterized the adsorbed state in terms of loops, tails, and trains. After the diffusion of the polymer to the vicinity of the surface, three succeeding phases were identified: distortion, attachment, and relaxation phase. In the distortion phase, the polymer starts to experience the potential of the surface and becomes elongated perpendicular to the surface. In the attachment phase, the polymer makes direct contact with the surface and becomes contracted perpendicular to the surface. Finally, in the extended relaxation phase, the chain polymer spreads on the surface. (N. Källrot and P. Linse).

Polyelectrolyte gels. Volumes and other structural properties of polyelectrolyte gels in equilibrium with pure water have been determined by Monte Carlo simulations. The role of chain length polydispersity and topological network defects of four different networks with varying crosslinking density, monomer charge, and chain stiffness have been investigated. Generally, a chain length polydispersity reduced the gel volume, whereas the presence of chains with one end detached from the crosslinker (severed chains) led to an increased gel volume. Polyelectrolyte networks displayed the largest and uncharged polymer the smallest dependence on chain length polydispersity. The effect of severed chains was strongest for flexible polyelectrolyte gels and weakest for uncharged networks and stiff polyelectrolyte gels. Mechanical properties of uncharged and charged polymer gels were also investigated through uniaxially stretching and compared with theory. Furthermore, the volume and structural changes upon the addition of oppositely charged macroions to crosslinked polyelectrolyte gels have also been investigated. 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 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 aqueous solution is examined within the framework of the so-called primitive model using Monte Carlo simulations. The properties of the two blocks are identical except for the sign of their charges. 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 thickness responded differently for flexible and nonflexible chains, depending on a different balance between electrostatic interactions and excluded volume effects. In addition, the interaction between such composite colloidal particles composed of a spherical core and grafted AB-diblock polyampholytes are investigated. The B-block is end-grafted onto the core of the colloid and its linear charge density is varied, whereas the linear charge density of the A-block is fixed. Brush structure of a single colloid, the mean force between two colloids, and the structure of solutions of such colloids have been determined for different linear charge densities of the B-blocks and block lengths. Many features of the present system are controlled by the charge of the B-blocks. In the limit of uncharged B-blocks, (i) the grafted chains are stretched and form an extended polyelectrolyte brush, (ii) a strong repulsive force is operating between two colloids, (iii) and the solution is thermodynamic stable and displays strong spatial correlation among the colloids. In the limit where the charges of the two types of blocks exactly compensate each other, (i) the chains are collapsed and form a polyelectrolyte complex surrounding the cores, (ii) an attractive force appears between two colloids, and (iii) strong colloid clustering appears in the solution. These features become more pronounced as the length of the polymer blocks is increased, and a phase instability occurs at sufficiently long chains. A comparison with properties for other related colloidal particles is also provided. (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. Furthermore, we have analysed experimental brush heights obtained for different foot-print sizes, polymer molecular weights and surface grafting densities using the scaling relations obtained from simulations. We found good agreement between the experimental data and the theoretical predictions. Our results thus indicate that the scaling predictions provide a useful tool for the design and fabrication with polymeric and biomacromolecular nanostructures on surfaces. Finally, the interaction between a nanopatterned polymer brush and a rigid pyramidal body representing an AFM tip has been investigated using molecular dynamics 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, W.-K. Lee (Duke University), S. Zauscher (Duke University), 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).

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. In addition, we have examined two extensions of the model, dodecahedral distribution of the capsid charges and addition of salt. In the former case, the radial distribution of the genome was unaffected, whereas a dodecahedral distribution appeared at an reasonable dodecahedral distribution of the capsid charges, in agreement with experiments. Upon addition of salt, the adsorption of the genome onto the inner capsid surface was reduced. (D. Angelescu, J. Stenhammar, R. Bruinsma (University of California Los Angeles), and P. Linse).

Effective interaction potentials for alkali and alkaline earth metal ions. The potential of mean force acting between two simple ions surrounded by SPC/E water have been determined by molecular dynamics simulations using a spherical cavity approach. Such effective ion–ion potentials were obtained for Me–Me, Me–Cl^-, and Cl^-–Cl^- pairs, where Me is Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, Sr^{2+}, and Ba^{2+} cation. The ionic sizes estimated from the effective potentials are not pair-wise additive, a feature in the frequently used primitive model for electrolytes. The effective potentials were used in Monte Carlo simulations with implicit water to calculate mean ion activity coefficients of LiCl, NaCl, KCl, $MgCl_2$, $CaCl_2$, $SrCl_2$, and $BaCl_2$. Predicted activities were compared with experimental ones in the electrolyte concentration range 0.1 M to 1 M. A qualitative agreement for LiCl and a satisfactory agreement for NaCl were found, whereas the predictions for KCl by two K^+ models were less coherent. In the case of alkaline earth metal ions all experimental activities were successfully reproduced at c = 0.1 M. However, at higher concentrations similar deviations occurred for all divalent cations, suggesting that the dependence of the permittivity on the salt concentration and the polarization deficiency arising from the ordering of water molecules in the ion hydration shells are important in such systems. (S. Gavryushov (Engelhardt Institute of Molecular Biology) 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).

Statistical-mechanical programs. During 2006, 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 Bruker AV-200 and AV-500 NMR spectrometers, both being equipped for high-performance diffusion studies. The AV-500 in addition has microimaging as well as solid-state and high-resolution magic-angle spinning capabilities. (Sponsored by VR/KFI).

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 both organic and aqueous 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: Ulf Olsson). 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.

SAXS at MAX

During 2006 work was begun to modify the crystallography beam line I711 at Max-lab in order to allow for small angle scattering experiments (SAXS). The idea being that this beam line in the future will serve as a shared small angle and crystallography beam line. Malin Zackrisson and Ulf Olsson are here working closely with the beam line manager Yngve Cerenius to develop it into a first class SAXS instrument. The first small angle test experiments were carried out at the end of April. During the rest of the year work continued on optimizing the optics and on the development of the sample environment. From 2007 SAXS experiments on the I711 beam line are available through the regular MAX-lab beam time application system. For further details on the SAXS instrument see the I711 home page at http://maxsun5.maxlab.lu.se/beamlines/bli711/ .

COLLABORATIVE RESEARCH PROGRAMS

The Centre for Amphiphilic Polymers, CAP

On June 30, 2006, the Centre for Amphiphilic Polymers from Renewable Resources (CAP) at Lund University was terminated. CAP had then been in existence for eleven years. It was part of the national Competence Centre Programme supported by VINNOVA, the Swedish agency for innovation systems. CAP was jointly funded by Lund University, VINNOVA, and a group of member companies, including Akzo Nobel Functional Chemicals, AstraZeneca R&D Mölndal, Celanese Emulsions Norden AB, Eka Chemicals, Lyckeby Stärkelsen, SCA Research, and Tetra Pak. Since 2004, Lennart Piculell was the director of CAP and Per Linse a member of the Board.

CAP activities concerned fundamental behaviour and applications of amphiphilic polymers, and the use of biopolymers for their preparation. CAP research was mainly localised at Lund University, but also at the member companies. The scientific work in CAP was typically carried out as PhD or postdoc projects covering all aspects of amphiphilic polymers, including synthesis/modification, characterization, physical-chemical behaviour, and theoretical modeling. Research activities were 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) were the two members of the international scientific advisory board of CAP.

The final year of CAP was a very active one. Ten projects were still running at the beginning of the year, and no less than six CAP PhD students, including Anna Körner from our department, successfully defended their theses in 2006. The final annual meeting in May in Lund attracted 65 participants. Special features of this meeting were that all persons active within CAP throughout the years were invited, and that one session was devoted to feedback from the former CAP PhD students, who are now employees of a large number of industrial companies and universities inside and outside of Sweden.

Testimonies from the participating partners as well as consistent reports from a series of international evaluations all show that CAP was an extremely successful centre. Over the years, the scientific production from a total of 55 CAP projects has resulted in ca. 240 scientific papers, 34 PhD theses, and numerous presentations at international conferences. Besides the high productivity, one of the most important achievements of CAP was to establish a multiply connected network of contacts and collaborations across the traditional boundaries between disciplines, between companies, and between industry and academia. Over the years, roughly 180 people have been actively involved in CAP. This extended network of contacts will undoubtedly continue to play a significant role in successful research collaboration for a long time after the formal termination of CAP.

Colloidal Structures from Self-association, COLINTECH.

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 University of Technology, 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-equlibrium self-assembly dispersions, and structuring complex systems at interfaces.

Members of the board of the Research Programme: Jan Svärd (chairman; Eka Chemicals), Krister Holmberg (Chalmers University of Technology), Björn Lindman (Lund University) and Bruce Lyne (Institute for Surface Chemistry).

The Division of Surface Chemistry of the Swedish Chemical Society.

The Division of Surface Chemistry of the Swedish Chemical Society was founded in 2001 to promote contacts between chemists interested in surface and colloid chemistry. The current Lund representative to the board is Lennart Piculell. The main activity of the Division is to organize the Annual Surface and Colloid Symposium in Lund. The sixth symposium, held in November 2006, had as its the theme “Lipid-Peptide Interactions and Biological Functions”, with Tommy Nylander on the scientific committee. Sanja Bulut, Samuel Edgecombe, Niklas Källrot, Agnes Zettergren, Christoffer Åberg and Lennart Piculell constituted the local organizing committee.

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. The program terminated during 2006.

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)

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).

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)

BIOCONTROL

EU Marie Curie research training network "BIOCONTROL" aims at controlling biological functions at, respectively on, bio-interfaces. It is based on the recent recognition of the importance of structure and properties of bio-interfaces, e.g. biological membranes, for a multitude of life processes. We now know that the evolution of atherosclerosis, cancer, immunity and viral infections, neurodegenerative disorders (Alzheimer, Prion diseases, etc.) and aging depend on perturbations of such interfaces. However, we need to improve our knowledge of the underlying molecular mechanisms in order to design efficient drugs and to meet the challenges in regenerative medicine and tissue engineering. This requires a deeper understanding of processes and interactions at bio-interfaces in terms of biology, biochemistry, biophysics and structure.

The two major scientific objectives of BIOCONTROL are to:

- Provide fundamental knowledge of the forces and molecular mechanisms that regulate the interactions and biological processes taking place in and around biological membranes.
- Construct bio-mimetic surfaces and self-assembled structures that enable external control of biological and biotechnological processes, such as, cell adhesion and cell cycle regulation.

Real progress in the field can only be achieved by breaking traditional academic borders. This requires the education of new researchers that are trained in cross-disciplinary and collaborative work.

Therefore the major educational objective of BIOCONTROL is to train of a new category of 'life science' experts who can work across disciplines. This will be achieved by an unprecedented interdisciplinary training programme comprising (bio)physicists, biologists, (bio)chemists, surface chemists and computational biologists. (T. Nylander, V. Alfredsson). (http://biocontrol.tau.ac.il/)

SOCON

EU Marie Curie research training network "SOCON" focus on aqueous films, which are either confined between two solid surfaces or by air (foam film) or oil (emulsion film), respectively. SOCON put emphasis on complex self-organising systems of environmentally friendly components, such as sugar-based surfactants and polymeric carbohydrate derivatives, but we will also use traditional surfactants and polymers. The interest in the former class of surfactants and polymers is motivated by the fact that they can be made from renewable materials and that they have favourable properties with respect to applications in various fields. Most applications explore surfactant mixtures as well as surfactant-polymer mixtures. Hence, to advance the increased use of more environmentally friendly components synergistic and antagonistic effects in multicomponent systems have to be understood. In fact, this is one essential element of the joint network research. The wide range of systems which will be examined have in common self-assembly and strong surface activity. The four main objectives of the network are to:

- determine the relation between self-assembled structures in bulk solution, at one interface, and confined between two interfaces. SOCON will advance the understanding of the relations between changes in self-organised structures due to confinement and surface forces. This includes how the nature of the interface influences self-assembled surface structures and thus surface interactions. The emphasis will be on multicomponent systems.
- understand, predict, and control trapped non-equilibrium structures at interfaces and the corresponding surface forces.
- establish the correlation between properties of single films and complex colloidal systems. This includes macroscopic foams, emulsions and dispersions.
- promote the use of new environmentally friendly compounds in products and processes based on complex colloidal systems. For this purpose novel composite polymers and surfactants will be synthesized from natural building blocks.

(P. Linse, T. Nylander). (http://www.mcrtn-socon.org/)

NANOGROWTH

This EPSRC (UK) founded project studies the fundamental aspects of crystal growth in nanoporous materials. It involves the application of a powerful set of complementary techniques to the study of crystal growth of open-framework materials comprising: atom ic force microscopy, high resolution transmission and scanning electron microscopies, in-situ NMR with enhanced data processing, X-ray diffraction and mass spectrometry. A substantially better understanding of the synthesis process is likely to yield important economic benefits, for example, better process control, increased efficiency in reagent usage, improved reproducibility and the capacity to modify or tailor products for specific applications.

(V. Alfredsson) (http://www.ucl.ac.uk/nanogrowth/index.htm)

EU Project “Mercury”

The EU project Mercury (ICA4-CT-2002-10055), dealing with problems related metal pollution in Latin America, was extended over 2006. The construction of an isothermal micro titration calorimeter has been completed and has, as part of the EU project, been donated to The Catholic University of Santa Maria, Arequipa, Peru. (I. Wadsö).

ELAPNET

The purpose of this Programme ALFA II - project is to build up collaboration between universities that are conducting teaching and research activities at undergraduate and graduate and graduate levels in areas related to synthesis and characterisation of polymeric materials by promoting exchange of undergraduate, graduate students and staff. This will help to reinforce the quality of education in those institutions and to increase the diffusion these activities in other universities. (B. Lindman)

POLYSURF

This is a Transfer of Knowledge (TOK) Development Scheme (DEV) funded within the Marie Curie Program of the European Union. The overall objective of the project is to increase the knowledge and research level of the host organisation, Institute of Textiles at the University of Maribor, on the creation of tailored and/or smart fibre forming polymers and materials that would be able to control the release of various active compounds or to create new tailored fibre surface properties for different end-applications in the area of technical textiles, such as medical, therapeutic, hygienic and protective textiles. The project will transfer knowledge of innovative fibre surface modification technologies based on (WP2) colloidal micro-hydro-gelation, (WP3) nano-micro-(en)capsulation and (WP4) polymer surface coating. Additionally, (WP1) innovative biotechnological, green-chemistry, chemical and physical catalysis tools, or their combination will be applied to activate and/or modify polymer surfaces and/or colloidal particles/layers created using ecologically and toxicologically suitable processes. According to the diversity of the knowledge and expertise that shall be transferred, the project will build a highly multidisciplinary scientific group, cutting across different established research areas, i.e. textile chemists, physical chemists, biological catalysts and colloidal engineers, that will be able to prepare colloidal particles, coatings and multi-layers, and subsequently apply them to different suitably eco-pre-activated and/or modified natural and synthetic polymer surfaces. The new fibre materials with upgraded properties can be exploited either to enhance the bulk properties of existing products for better performance, or to create new value-added products with smart and/or tailored surface characteristics based on the multi-functionality.

The project objective will be realised through training, module-based courses and several research activities by outgoing seconded and incoming recruited more experienced (MER) and experienced (ER) researchers that will be able to provide the necessary inputs in these areas. (B. Lindman)

Biopolymers based surfactants - Stabilization and functionalization of particles and surfaces

The COST-project "Biopolymers based surfactants - Stabilization and functionalization of particles and surfaces" aims at increasing the knowledge of processes at surfaces and interfaces and factors tuning them at the molecular scale. An interdisciplinary effort to study the interaction of surfactants, derived from high and low molecular biological sources, with different kinds of substrates, as soft and hard particles and structured polymer surfaces, is envisioned. This activity will focus on the stabilization of the systems and the functionalisation of different surfaces. This has extended social and industrial interest as these results will provide advanced hygienic and technical materials as well as new insight into critical medical field, as for example the biocompatibility of implants. This requires a multidisciplinary approach i.e. synthesis and activation of materials, characterization and understanding of surface properties and processes at the molecular and supramolecular level. A theoretical description of these systems will allow to predict the properties of final products based on their chemical composition and the structure of the surface active compounds and substrates. Modification of these surfactants as well as the dispersed and macroscopic substrates will change their interaction abilities and functionalities. The results will enable us to understand, and ultimately control, the structure-property relationship and create new materials with excellent surface specificity. (B. Lindman)

CONFERENCES, TRAVELS AND SEMINARS

Björn Lindman gave plenary lectures at the Polylectrolytes 2006 conference, in Dresden, and the 53. SEPAWA Congress with European Detergents Conference, Würzburg, and keynote or invited lectures at 16th International symposium on surfactants in solution (SIS), Seoul, at Symposium and Workshop on Innovative Biopolymers, Polysaccharides – from Discovery to Commercialization, Fiskebäckskil, at the symposium on Functional Chemistry honouring Prof. Krister Holmberg, Göteborg, the Jubilee Symposium of the Institute of Physcial Chemistry, Åbo Akademi, Åbo, Finland honouring Prof. J. B. Rosenholm, at the symposium on Organizing Molecular Matter , Lund, and at the 12th Conference of the International Association of Colloid and Interface Scientists (IACIS) in Beijing. He also attended the 20th Conference of the European Colloid and Interface Society (ECIS) Budapest, Neonuclei Workshops, in Penacova, Portugal, and München, Colloidal and Interfacial Properties of Synthetic Nucleic Acid Complexes (CIPSNAC) Workshops in Dublin and Paris, and COST Workshops in Rome and Barcelona. He was also invited to the meeting celebrating the 25th year jubilee of the Chemical Institute of the Chinese Academy of Sciences in Beijing. During the year Björn Lindman visited a number of universities and other research centers and in most cases he presented a lecture. The institutions visited included: Université Paul Sabatier, Toulouse, Victoria University of Wellington, New Zealand, CSIRO, Sydney, Australia, University College, Dublin, University La Sapienza Rome, IIQAB-CSIC, Barcelona, Université Paris Sud, Orsay, Astra Zeneca, Göteborg, Procter & Gamble Research Centers, Cincinnati, Schwalbach and Brussels, BASF Research Center, Ludwigshafen, Germany, Xinjiang University, Urümqi, Chalmers University of Technology, Göteborg, Akzo Nobel Surface Chemistry, Stenungsund, GlaxoSmithKline Research Center, Weybridge, UK, Uppsala University, Institute for Surface Chemistry, Stockholm, Royal Institute of Technology, Stockholm, KAIST, Korea Advanced Institute of Science and technology. Daejon. 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, Nanyang Technological University, Singapore, and Pontifica Universidad Católica, Santiago de Chile.

Håkan Wennerström delivered invited talks at “Structure and molecular properties of liquid water” in June, Stockholm and XX ECIS, Budapest, Hungary

Olle Söderman attended the XX ECIS, Budapest, Hungary and a COST workshop in Barcelona.

Ulf Olsson delivered invited lectures at XIII International Conference of Small-angle Scattering, Kyoto, Japan and the Soft Matter workshop organized by the Yukawa Institute for Theoretical Physics, at Kyoto University, Japan. Ulf visited and gave seminars at: Unilever, Port Sunlight, UK, Kao Corporation, Tokyo, Japan, Ajinomoto Co. Kawasaki, Japan, Tokyo Metropolitan University, Japan, Coimbra University, Portugal, Theoretical Physics department, Lund University and visited Ochanimizu University, Tokyo, Japan. He also attended 3rd Scandinavian workshop on Scattering from Soft Matter, Uppsala, Sweden, XX ECIS, Budapest, Hungary, and 6th Surface and Colloid Symposium, Lund, Sweden.

Per Linse delivered invited oral presentation at the 94th Bunsen Colloquium, Bayreuth, Germany and at the 6th International symposia on Polyelectrolytes, Dresden, Germany. He also gave invited seminars at Duke University, North Carolina, North Carolina State University, Raleigh, University of North Carolina, Chapel Hill, University of Amherst, Massachusetts, Stanford University, and University of Gothenburg. Per

Linse was visiting professor at Duke University, North Carolina March-April (5 weeks), University of Amherst, Massachusetts April-May (5 weeks) and Stanford University (1 week).

Lennart Piculell gave plenary lectures at 8th International Hydrocolloids Conference, Trondheim, Norway and 19 IUPAC International Conference on Chemical Thermodynamics, Boulder, USA, and invited lectures at 9th European Training Course on Carbohydrates "Summer Course Glycosciences", Wageningen, the Netherlands and European Science Foundation Exploratory Workshop Ch@ins: the limits of neutrality, Compiègne, France. Lennart also gave two invited lectures at Procter & Gamble, Cincinnati, USA. Lennart attended Polyelectrolytes 2006, Dresden, Germany where he was a member of the international advisory board.

Ingemar Wadsö gave keynote lecture at XIVth Conference of International Society for Biological Calorimetry, Sopot, Poland and oral presentations at 2nd International Symposium on Calorimetry and Chemical Thermodynamics, Campinas, Sao Paulo, Brazil and at The Calorimetry and Thermal Analysis Conference (Calcat '06) in Santiago de Compostela, Spain.

Gerd Olofsson gave an invited lecture at 2nd International Symposium on Calorimetry and Chemical Thermodynamics in Campinas, Sao Paulo, Brazil. In November, Gerd spent two weeks at UNICAMP (Universidade Estadual de Campinas), Campinas, Sao Paulo, Brazil, as part of research collaboration.

Tommy Nylander gave two invited presentations at the American Chemical Society spring meeting in Atlanta, on DNA compaction and nano-constructs as well as on polymer-surfactant interactions at interfaces. He also gave a presentation at 12th IACIS, Beijing, China.

Karin Schillén gave invited talk at Third Scandinavian Workshop on Scattering from Soft Matter, Uppsala, Sweden. She also gave oral presentations at XX ECIS, Budapest, Hungary and 12th IACIS, Beijing, China.

Viveka Alfredsson gave an invited lecture at the Max Planck Institute for Coal Research in Mülheim, Germany.

Emma Sparr presented a poster at the Biophysical Society Annual Meeting 2006 in Salt Lake City, USA.

Rita Dias delivered an oral presentation at 6th Surface and Colloid Symposium, Lund, Sweden and presented a poster at the 6th International symposia on Polyelectrolytes, Dresden, Germany.

Johan Reimer gave an oral presentation at 12th IACIS, Beijing, China.

Daniel Angelescue presented a poster at XX ECIS, Budapest, Hungary.

Joakim Balogh presented posters at Third Scandinavian Workshop on Scattering from Soft Matter, Uppsala, Sweden, XX ECIS, Budapest, Hungary and 6th Surface and Colloid Symposium, Lund, Sweden.

Fatima Costa gave an oral presentation at XX ECIS, Budapest, Hungary and presented a poster at 6th Surface and Colloid Symposium, Lund, Sweden

Samuel Edgecombe presented posters at the 6th International Symposium on Polyelectrolytes, Dresden, Germany and 6th Surface and Colloid Symposium, Lund, Sweden.

Niklas Källrot presented a poster at XX ECIS, Budapest, Hungary.

Cecilia Leal delivered oral presentation for Prof. Safinya's lab in the University of California Santa Barbara, and at the CPISNAC workshop, Dublin.

Peter Linton gave an oral presentation at 3rd Scandinavian workshop on Scattering from Soft Matter, Uppsala, Sweden and presented a poster at 5th International Mesostructured Materials Symposium, IMMS2006, Shanghai, China.

David Löf gave an oral presentation at XX ECIS, Budapest, Hungary. David made a 2 month research visit to Institute of Physical Chemistry, University of Graz, Austria.

Luis Pegado presented a poster at 6th Surface and Colloid Symposium, Lund, Sweden.

Pauline Vandoolaeghe gave oral presentation at 3rd Scandinavian Workshop on Scattering from Soft Matter, Uppsala, Sweden, Food Colloids 2006, Montreux, Switzerland, Refsans User Workshop, Munich, Germany, 12th IACIS, Beijing, China and SOFTILL, Grenoble, France and presented a poster at 6th Surface and Colloid Symposium, Lund, Sweden

Christoffer Åberg gave an oral presentation at XX ECIS, Budapest, Hungary and presented a poster at 6th Surface and Colloid Symposium, Lund, Sweden.

Marie-Louise Örberg gave oral presentations at the CIPSNAC meeting in Dublin, Ireland as well as at the NEONUCLEI meetings in Penacova, Portugal and Munich, Germany. Marie-Louise also presented posters at the 3rd Scandinavian Workshop on Scattering from Soft Matter in Uppsala, at the ILL Soft Matter User Meeting in Grenoble, France and at the 6th Annual Surface and Colloid Symposium in Lund.

FINANCIAL SUPPORT

For the fiscal year 2006, the department had a turnover of ca 36.6 million SEK. From the University we obtained 14.9 million of which 1.2 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 11.6 million SEK, We also received 3.3 million SEK from The Swedish Foundation for Strategic Research (SSF), which is an important funding agency for supporting novel research ventures in Sweden. We are grateful for support from private industry, directly and via their foundations, amounting to ca. 3.4 million. Finally, we received 3.4 million SEK from The European Commission.

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 was 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. For the period 2006-2009 Björn Lindman is President of the International Association of Colloid and Interface Scientists (IACIS). He was also the committees for the PhD theses of Mónica Rosa and Filipe Antunes, Coimbra University. Björn Lindman was invited to Toulouse to evaluate the CNRS Laboratory IMRCP, Université Paul Sabatier.

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 innovation group (Idérådet), Lund University and chairman of he Liquids Board of the European Physical Society.

Ulf Olsson was chairman of the board of undergraduate studies, board member of the Swedish Neutron Scattering Society, member of a review panel for the Committee for Research Infrastructure of the Swedish Research Council, and member of the evaluation committee of the thesis of Filipe Antunes, Coimbra University

Olle Söderman is vice dean at the Science faculty for the period 2006-2009, member of the Science Faculty Board and chairs the Undergraduate Training Committee of the faculty. Olle served as opponent for Kai Grythe at the University of Oslo.

Per Linse served on the PhD thesis committee for Jérémie Gummel, CEA, Saclay, Paris, France and Elisbet Horvath, KTH, Stockholm, Sweden. He was also member of the Chemical Engineering panel at the Swedish Research Council.

Lennart Piculell was the director of the Center for Amphiphilic Polymers (CAP) until the center ended in June 2006. 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 is a member of the board of the Department of Chemistry at Lund University and a member of the board of the Division of Surface Chemistry of the Swedish Chemical Society. He served as an external examiner at the thesis defense of Marit Sletmoen, Norwegian University of Science and Technology, Trondheim, Norway and as a member of the grading committee at the thesis defenses of Lidia Elfstrand, Food Technology, Lund University and Charlotte Trotzig, Polymer and Materials Chemistry, Lund University.

Tommy Nylander is member of the advisory board of Journal of Colloid and Interface Science and Chemistry and Physics of Lipids.Tommy Nylander is member of the Permanent Expert Panel ("Beredningsgrupp") for Food at The Swedish Research Council for Environmental, Agricultural Sciences and Spatial Planning (FORMAS). Tommy Nylander was the faculty opponent on Matti Säily's PhD Thesis at University of Helsinki, Finland in January 2006 and on Indriati Pfeiffers PhD thesis at Chalmers University of Technology, Gothenburg, Sweden.

Gerd Olofsson was external examiner (opponent) for Angelica Hull's Ph D thesis defense, Karlstad University.

Karin Schillén was deputy member of the board of the Department of Chemistry. Karin served on PhD thesis committees for Anna Körner, Lund University and Charlotte Trotzig, Lund University.

Viveka Alfredsson was the faculty opponent on Teresa Czuryszkiewicz PhD Thesis at Åbo Akademi, Turku, Finland and served on PhD thesis committees for Peter Oleynikov, Stockholm University, Sweden.

HÅKAN WENNERSTRÖM 60 AND A WORKSHOP ON "ORGANIZING MOLECULAR MATTER"

Håkan became 60 in August and this was of course duly celebrated both in August and by a special symposium on November 18. It was a nice coincidence that Håkan within only a few weeks of his birthday received two outstanding awards. Firstly, he was the leader of the successful proposal which gave him and his colleagues in Lund a "Linné grant" from our research council (see elsewhere). Secondly, the European Colloid & Interface Society (ECIS) honoured him on its meeting in Budapest with its most prestigious award, the first Overbeek Gold Medal; we give ECIS's official motivation below.

The November symposium attracted a large number of Håkan's friends locally as well as nationally and internationally. The symposium was started by an overview by Björn Lindman on the development of surfactant science in Lund from its start 40 years ago, a start which included experimental ion binding studies by Håkan; it did not last long before Håkan's pioneering studies on electrostatic theory started. Björn Roos gave a survey on the developments of quantum chemical computations, with Håkan's early work in this area as a starting-point. Other contributors included Fennel Evans, Gordon Tiddy, Alexey Kabalnov, Per-Olof Westlund, Bernard Cabane and Göran Lindblom who amply illustrated how broad Håkan's scientific contributions have been. The success of Håkan as a teacher and mentor was illustrated by the presence at the symposium of many previous students and postdocs, now at important positions in the scientific world.

After the successful symposium we all went to Pelarsalen in the main university building for a splendid dinner, where several anecdotes from Håkan's scientific life were told (and some early historic tales corrected). Håkan's after-dinner talk thanking many of his colleagues and coworkers included many wise remarks on how to manage a laboratory and touched everyone. We all left with a wonderful memory of the day and feeling a deep gratitude to Håkan for his unselfish contributions to our careers.

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, 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 Christoffer Åberg. 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 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 advanced surface and colloid chemistry course is organized and taught by Lennart Piculell (main teacher) along with Tommy Nylander and Per Linse. It is given once a year during the fall semester, and is based on the book by Håkan Wennerström and Fennel Evans. The advanced physical chemistry course is also given once a year during the spring semester and is taught by Per Linse, Ulf Olsson and Daniel Topgaard. This course is focused on methodology and is divided into three parts: (i) Small angle scattering and light scattering (Ulf), (ii) NMR (Daniel), 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.

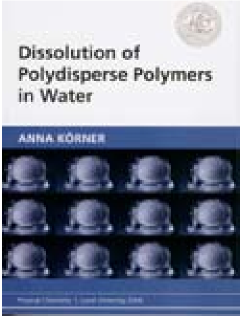
On the graduate level most senior members of the department also participate and organize various graduate courses, many of which have been given within the national research school in Colloid and Interface Technology, COLINTECH.

Björn Lindman was one of the teachers on the annual course on surfactants and polymers in aqueous solution, this year given in Lisbon and he also taught on courses at Coimbra University and Malmö University College

Lennart Piculell delivered 3 popular lectures at "Naturvetenskap- & teknikdagar för gymnasister".

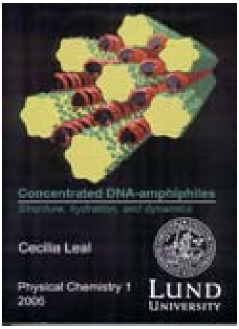
DOCTORAL THESIS

March 1, 2006
Anna Körner
Dissolution of Polydisperse
Opponent: Prof. Martin Malmsten, Uppsala University, Sweden



March 31, 2006
Joakim Balogh
Nonionic Microemulsions: Dependence on Oil Chain Length of the Surfactant Curvature Elastic Properties
Opponent: Prof. Reinhard Strey, Institut für Physikalische Chemie Universitet zu Köln, Germany

September 9, 2006
Cecilia Leal
Concentrated DNA-amphiphiles Structure, Hydration, and Dynamics
Opponent: Prof. Brad Chmelka, University of California, Santa Barbara, USA



AWARDS

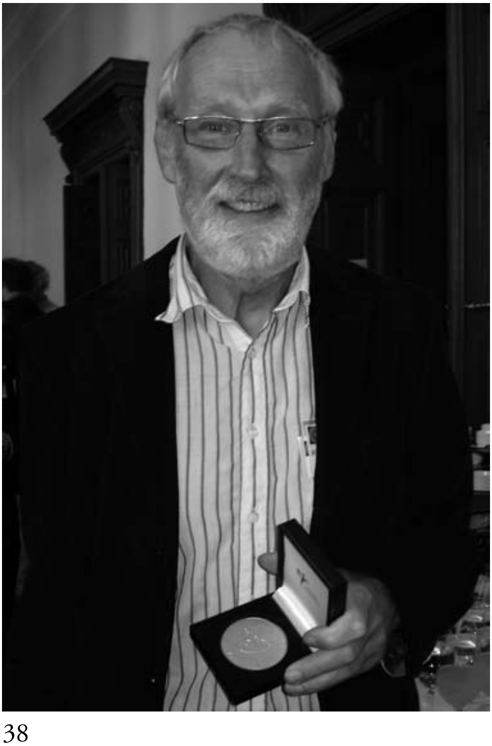
Björn Lindman received the Bror Holmberg Medal of the Swedish Chemical Society.

Emma Sparr recieved Per-Eric och Ulla Schyberg's Award

HÅKAN WENNERSTRÖM: OVERBEEK GOLD MEDAL WINNER 2006

Håkan Wennerstöm recived the very first Overbeek Gold medal at XX Conference of the European Colloid and Interface Society, Budapest, Hungary with the following prize motivation:

"Håkan Wennerström has a long and outstanding career in colloid science, with many contributions to different fields of the discipline. He was educated in Lund and first became a professor at Stockholm University, after which he returned to his Alma Mater in 1984 where he has been ever since. He is respected by the entire scientific community; the fact that he presently chairs the Nobel Prize committee can be seen as a token of this. Among his many achievements one should particularly mention his profound understanding – inspired by Overbeek – of charged interfaces. Not only did he develop this in many directions, e.g., into quantitative predictions for cmc's of ionic surfactants, but he was also among the first to point out the importance of ion correlations for ions of multiple valency, something which is now, many years later, generally recognized. Surface forces, which are at the heart of colloid science, were carefully analyzed by him for many different systems, such as those between lipid bilayers discussed in a classical paper with Israelachvili in Nature. But we do not only know Håkan as a scientist writing papers of exceptional quality, but also as a passionate and devoted teacher, who has disseminated his clear insights in ′The Colloidal Domain′, a book to be found on the desk of many scientists, professors and students alike. Following from the formal recognition and award of Overbeek himself last year, we are now proud to award him the very first Overbeek Gold medal."



MEMBERS OF THE DEPARTMENT

Scientists/Teachers

Viveka Alfredsson, associate prof.
Daniel Angelescu, postdoc
Tarek Awad, postdoc
Justas Barauskas, postdoc
Richard Campbell, postdoc
Parveen Choudhary, postdoc
Rita Dias, postdoc
Alfredo Gonzáles Pérez, 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.
Andreas Mohr, postdoc
Tommy Nylander, prof.
Gerd Olofsson, associate prof.
Ulf Olsson, prof.
Lennart Piculell, prof.
Gabriel Rata, postdoc
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.
Malin Zackrisson, postdoc

Technical-Administrative Personnel

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

Graduate students working on a Ph. D. Thesis

Joakim Balogh
Sanja Bulut
Samuel Edgecombe
Niklas Källrot
Anna Körner
Géraldine Lafitte
Cecilia Leal
Peter Linton
David Löf
Carin Malmborg
Markus Nilsson
Jens Norrman
Luis Pegado
Pauline Vandoolaeghe
Agnes Zettergren
Christoffer Åberg
Ingrid Åslund
Marie-Louise Örberg

GUESTS

Almasy, Laszlo, Research Inst. for Solid State Physics and Optics, Hungary (S)
Almgren, Mats, Uppsala University, Uppsala, Sweden (S)
Barreleiro, Paula, Henkel KGaA, Duesseldorf, Germany (S)
Björnholm Thomas, University of Copenhagen, Denmark (S)
Brito, Rodrigo, University of Porto, Portugal (L)
Cabalero-Lago, Celia, Universidad de Vigo, Spain (L)
Cabane, Bernard, Laboratoire PMMH, ESPCI, Paris, France (S)
Chmelka, Bradley F., University of California Santa Barbara, US (S)
Ciunel, Kasia, TU-Berlin, Germany (S)
Clauzel, Maryline, Institut Charles Sadron, Strasbourg, France (S)
D'Errico, Gerardino, University of Naples "Federico II", Italy (S)
Deleu, Magali, Gembloux Agricultural University, Belgium
dos Santos, Salomé, University of Coimbra, Portugal, (L)
Edwards, Mark, Glaxo Smith Klein, UK (S)
Eeman, Marc, Gembloux Agricultural University, Belgium (L)
Esteban, Isabel, Universidad Nacional de Educación a Distancia, Spain (L)
Furo, István, KTH, Sweden (S)
Gargallo, Ligia, Pontificia University Catolica de Chile, Chile (S)
Heimburg, Thomas, University of Copenhagen, Denmark (S)
Jiang, Nan, Uppsala, Sweden (S)
Kinnunen, Paavo, University of Helsinki, Finland (S)
Kleitz, Freddy, Université Laval, Quebec, Canada (S)
Klitzing, Regine v., TU-Berlin, Germany (S)
Kristen, Nora, Basel, Switzerland (L)
Larsson, Kåre, Camurus Lipid Research Foundation, Sweden (S)
Lasic, Samo, University of Ljubljana, Slovenia (S)
Liu, Yaqian, BASF, Ludwigshafen (Rhein), Germany (S)
Lynch, Matthew, Procter & Gamble Company, Cincinnati, USA (S)
Malmsten, Martin, Uppsala University, Sweden (S)
Marques, Eduardo, University of Porto, Portugal, (S)
Matsuo, Goh, Hokkaido University, Sapporo, Japan (L)
Medronho, Bruno, University of Coimbra, Portugal (L)
Meszaros Robi, Hungary (S)
Muck, Joscha, Ludwig Maximilian Universität, München, Germany (S)
Neumann, Peter, BASF, Ludwigshafen, Germany (S)
Pairin, Cécile, Ecole Nationale Supérieure de Chimie de Paris, France (L)
Peron, Nicolas, Hungary (L)
Reisner, Walter, DTU, Copenhagen, Denmark (S)
Sakamoto, Yasuhiro, Stockholm University, Sweden (S)
Salvati, Anna, University of Florence, Italy (L)
Santos, Salomé, Portugal (L)
Santos, Tiago, University of Coimbra, Portugal (S)
Saveyn, Pieter, University of Ghent, Belgium (L)
Serra, Elias, CSIC, Madrid, Spain (L)
Shahram, Shafaei, University of Paderborn, Germany (S)
Silva Cláudia, University of Coimbra, Portugal (L)
Silva, Bruno, University Porto, Portugal (L)
van Stam, Jan, Karlstad University, Sweden (S)

Stepanek, Petr, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, (S)
Strey, Reinhard, Universität zu Köln, Germany (S)
Strumia, Miriam, Universidad Nacional de Córdoba, Argentina (S)
Szopko, Richard, University of Paderborn, Germany (S)
Takemasa, Makoto, Osaka City University, Osaka, Japan (L)
Teixeira, Cilaine, Universidad Autonoma de Barcelona, Spain (S)
Vaccaro, Mauro, University of Naples "Federico II", Italy (L)
Voncina Bojana University Maribor, Slovenia (L)

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

PUBLICATIONS

(1) Ambrosi, M.; Fratini, E.; Alfredsson, V.; Ninham, B. W.; Giorgi, R.; Lo Nostro, P.; Baglioni, P.
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WELCOME TO VISITORS

Dear Visitor,

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

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

To arrange a visit, you may contact an appropriate member of our department. Depending on the nature of the visit different arrangements may be made. Help with accommodation can be provided by Majlis Larsson. 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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