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Cover:
Illustration of a solution of capsomers and oppositely charged polyions containing single capsomers and nearly completed self-assembled T1 viruses composed of 20 capsomers and short polyanions. A capsomer is modeled by 20 fused spheres (yellow) making its triangular form and possesses sites of short-range interaction (small green and white spheres) and cationic charges (small blue spheres), whereas a polyanion is composed of 10 charged segments (small red spheres). The self-assembly do not appear when the polymeric counterions are exchanged to monomeric ones. (By Ran Zhang.)

INTRODUCTION

Getting ready for the future

On January 1, 2011, it became my turn to take over as head of the Physical Chemistry division, and I now wish to take the opportunity to reflect on the year that has passed in this edition of our Annual Report. It has been an exciting year, and a year when we in various ways have been busy getting our team in place and ready for the future. Within the group we have to deal with consequences of the fact that a fair few of us have become 60 years old or older. And in our immediate surroundings, the developments of the large scale facilities MAX IV and ESS affect us profoundly. There we wish to assume key roles, both as users and as a resource laboratory for other international users in the area of "soft matter".

Literally, we are now in place at Kemicentrum. In 2011, at long last, we could leave the last of our old rather run-down offices and labs to move into newly renovated ones. This means that we completed a process that we began planning no less than six years ago, going through many different prospective locations and architectural plans on the way. We are quite happy with how it all turned out in the end, and it felt good to install the many new instruments that we have recently acquired in our new labs. And one particularly nice aspect with the move is that we are now co-located with Theoretical Chemistry, sharing with the theoretical chemists not only scientific collaborations, but also a coffee room and our cherished coffee breaks.

On the staff side, 2011 was no less significant. This was the year when our newly recruited senior scientists Peter Schurtenberger, Anna Stradner and Malin Oskolkova Zackrisson really settled in. This significant addition to our division was further reflected in a quite large number of junior scientists that joined us in 2011: Carin Hagsten, Saskia Bucciarelli, Solmaz Bayati and Emelie Nilsson as PhD students, and Samuli Ollila, Ran Zhang, Lucía Casal, Martin Medebach and Jérôme Crassous as postdocs/researchers. With more to come. This was also the year when both Emma Sparr and Viveka Alfredsson became full professors at Physical Chemistry - a quite significant improvement of the gender balance among our senior scientists. And very important for our future was also the recruitment of new technical and administrative staff to Physical Chemistry. Christopher Hirst and Maria Södergren are our new full-time engineers, and Ingrid Nilsson has joined us on part-time to strenghten the administrative side.

In late October, we decided to celebrate the fact that we now have our team in place by inviting all our PhD alumni to a half-day reunion. Many helped with this event, but special thanks are due to Viveka, Patrik Knöös and Majlis Larsson who did a great job in organizing the reunion and tracking down as many as possible of our former PhD students. A good crowd of ca. 40 alumni came, representing all generations of PhD students since Björn Lindman took the chair in Physical Chemistry in 1978. The alumni were given tours our of our new facilities and also took part in group discussions with our present PhD students. This was actually our third PhD reunion, suitably on the 10th anniversary of the first one in 2001. Of course, we ended the reunion with a dinner party. Here we all took the opportunity to express our deep gratitude to Ingegerd Lind and Lennart Nilsson, both retiring in 2011, for their long and invaluable services to the Physical Chemistry division.

A challenge that our team faces in the very near future is the mid-term evaluation, taking place in 2012, of the center of excellence “Organizing Molecular Matter” (OMM), a center that we share with most of Theoretical Chemistry and with Sara Linse’s group at Biochemistry. OMM receives a 10-year “Linnaeus grant” from VR. In preparation for the evaluation we have worked hard during 2011 to write a report that summarizes our achievements during the first 5 years of OMM’s existence, and that also outlines our plans for the remaining years. This work has been useful in many ways. We were pleased to see that we had actually achieved most of what we set out to do in our original application. It was also good to be prompted to think again about our future goals and how to best use OMM as an instrument to reach these goals. And in the discussions and meetings around these issues, we have had several spontaneous positive comments, not least from our PhD students and postdocs, on how valuable it is to be part of a larger research environment that works actively together on defining and achieving such common goals.

Lennart Piculell

RESEARCH PROJECTS

Theoretical work - Statistical mechanics

Structural properties of polar liquids (Contact person: Per Linse)

The long-range structural properties of liquids composed of molecular dipoles are a question of long-standing interest within many fields of chemistry and physics. The long range of the dipole-dipole interaction makes the structure of dipolar systems notoriously difficult to probe using computer simulations, although many techniques have been proposed to overcome these problems. Within the present project, we combine the use of dielectric continuum theory with computer simulations to try to elucidate some fundamental properties of polar liquids. The theoretical analysis is based on electrostatic fluctuation formulas obtained using dielectric continuum theory. These describe the magnitude of the fluctuating electric multipole moments within spherical volumes inside a polar liquid, as a function of the radius of the volume and the dielectric constant of the fluid. The predictions from these formulae are compared with the results of computer (Monte Carlo and molecular dynamics) simulations of strongly polar liquids. The project is aimed at i) elucidating how accurately the structure and energetics of these liquids are described by dielectric continuum theory, and ii) investigating the accuracy of different schemes used to handle the long-range electrostatic interactions in computer simulations.

The research during 2011 was devoted to the study of how using periodic boundary conditions (PBCs) to handle the long-range electrostatic interactions in a polar system affects the structure and energetics of the system. To this end, a simple dielectric model describing the anisotropic solvation due to the PBCs was developed, relating the magnitude of electric multipole fluctuations to the lattice interaction energy for particular multipoles. The predicted linear relation between the magnitude of the fluctuations, quantified through an “apparent” dielectric constant, and the lattice interaction energy was shown to agree excellently with simulation results for a simple polar model system. (Joakim Stenhammar, Gunnar Karlström and Per Linse.)

Dielectric behavior of dipolar liquids (Contact person: Per Linse)

A long-standing challenging property of dipolar liquids is their attenuation of Coulomb interaction between ions and how that depends on the orientational structure of the fluid. Extensive Monte Carlo simulations have been performed to address two central questions: (i) development of a novel approach to extract the dielectric property of a molecular polar fluid and (ii) the effect of the retardation on the orientational structure, which is coupled to the dielectric response of the dipolar fluid.

Furthermore, the influence on the short-range packing in dipolar fluids by molecular shape and by additional higher order electrostatic moments has been investigated by molecular dynamic simulations. The dipole polarization was found to decrease as the particles were elongated parallel to the dipole and to increase for elongation perpendicular to the dipole, eventually forming a nematic order. The addition of a quadrupole lead to a reduction of the polarization, and the influence of an axial octupole was weaker and more complex. Both a decrease and an increase of the polarization is possible depending on the relative dipole–dipole and octupole–octupole interaction strength and the relative direction of the symmetry axes of the moments. These observations were attributed to the different parity of a dipole and a quadrupole and the same parity of a dipole and an axial octupole under reflection. In addition, further insights into the formation of dipole polarization were obtained. Short polar and long equatorial radii and strong dipole–dipole interaction are particle properties that promote a fluid with a high dipole polarization. (Per Linse and Gunnar Karlström.)

Polyelectrolyte complexes (Contact person: Per Linse)
Structural properties and the topology of polyelectrolyte complexes formed by a long polyion and shorter and oppositely charged polyions of varying length in solution have been investigated under different conditions by Monte Carlo simulations using a coarse-grained model. The extension of individual polyions has been characterized by their radius of gyration, whereas the composition and the internal topological structure of the complexes by their net charge and a novel analysis describing how the shorter polycations link to monomers of the longer polyanion, respectively. Conditions have been found at which the polyanion and a given number of polycations form distinguishable complexes differing in (i) the polyanion conformation and (ii) the fraction of polycations being in extended and collapsed states. Thus, at equilibrium these polyelectrolyte complexes display a stepwise variation of the degree of intracomplex disproportionation of the polycations (also referred to as a intrachain segregation), the appearing of an intracomplex disproportionation in agreement with previous theoretical predictions. The coexistence of different polyelectrolyte complex structures appeared at charge equivalence for PA with 30 monomers and beyond charged equivalence for a longer polyanion. A broad polyanion size distribution and a bimodal polycation size distribution appeared as a consequence of the coexistence of different polyelectrolyte complex structures. (Per Linse, Rita Dias and Alberto Pais (University of Coimbra, Portugal).)

Portal for statistical-mechanical computation and software (Contact person: Per Linse)
Through the web-portal www.fkem1.lu.se/sm, launched 2003, softwares for solving general problems in mainly statistical mechanics are accessible. The softwares were primarily developed as research tools, but have frequently been used in advanced undergraduate classes and in national PhD courses. From the web-portal, further information about each software can be obtained, reference manuals and sample input files can be retrieved, and the softwares can be executed for test purposes. The software's are:

DIELEC is a software for calculation of the electrostatics in the presence of spherical dielectric discontinuities. First version 2008.

MOLSIM is a package of four integrated and general programs for molecular dynamics, stochastic dynamics, and Monte Carlo simulation for molecular, colloidal, and polymer systems, including polarizable potentials, with extensive static and dynamic analyses. With contributions from Anna Akinchina, Fredrik Carlsson, Samuel Edgecombe, Yoshikatsu Hayashi, Niklas Källrot, Björn Linse, Vladimir Lobaskin, Thomas M. Nymand, Alberto Pais, Jurij Rescic, Stefanie Schneider, Marie Skepö, Joakim Stenhammar, Anders Wallqvist, and Per-Olof Åstrand. First version 1990. Parallel version employing MPI since 1997.

OZ is a software for solving the Ornstein-Zernike equation with a closure (MSA, PY, HNC, RY, ZH, and RHNC) for systems with central forces. First version 1985.

PB is a software for numerically solving the one-dimensional Poisson-Boltzmann equation for different boundary conditions and symmetries. First version 1982.

PGSE is a software for simulation of pulse gradient spin echo attenuations for spins diffusing in restricted spaces of different symmetries with permeable walls. First version 1993.

POLYMER is a software for solving lattice mean-field models containing a mixture of solvents and polymers for homogeneous (Flory-Huggins theory) and heterogeneous (Scheutjens-Fleer theory) solutions extended to polymers possessing internal degrees of freedom. First version 1991.

During 2011, MOLSIM has been extended with the smooth particle mesh Ewald sum to more efficiently handle long-range interactions for large systems.

Field theory applied to systems with dielectric discontinuities. (Contact person: Per Linse)

Aqueous solutions of charged spherical macroions with variable dielectric permittivity and their associated counterions are examined within the cell model using a field theory and Monte Carlo simulations. The field theory is based on separation of fields into short- and long-wavelength terms, which are subjected to different statistical-mechanical approximations. The simulations were performed by using a new, accurate, and fast algorithm for numerical evaluation of the electrostatic polarization interaction. The field theory provided counterion distributions outside a macroion in good agreement with the simulation results over the full range from weak to strong electrostatic coupling. A low-dielectric macroion leads to a displacement of the counterions away from the macroion. (Leo Lue (University of Strathclyde, UK) and Per Linse.)

Project completed in 2011.

Colloidal suspensions (Contact person: Per Linse)

Structure of charge-stabilized colloidal dispersions has been studied through a one-component model using a Yukawa potential with density-dependent parameters examined with integral equations theory and Monte Carlo simulations. Partial thermodynamic consistency was guarantee by considering the osmotic pressure of the dispersion from the approximate mean-field renormalized jellium and Poisson-Boltzmann-cell models. The colloidal structures could be accurately described by the Ornstein-Zernike equation with the Rogers-Young closure by using the osmotic pressure from the renormalized jellium model. Although we explicitly show that the correct effective pair-potential obtained from the inverse Monte Carlo method deviates from the Yukawa shape, the osmotic pressure constraint allows us to have a good description of the colloidal structure without losing information of the system thermodynamics. Our findings are corroborated by primitive model simulations of salt-free colloidal dispersions. (R. Castaneda-Priego, J. C. Mixteco-Sanchez (University of Guanajuato, Mexico)), V. Lobaskin (University College Dublin, Ireland), L. F. Rojas-Ochoa (Cinvestav-IPN, Mexico) and P. Linse.) Project completed in 2011.

Studies of model systems

Physico-chemical behavior of aqueous systems containing DNA, proteins and amphiphiles. (Contact persons: Dan Lundberg and Björn Lindman)

The behavior of systems where DNA coexists with both proteins and amphiphiles is of great biological importance. Most notably, there are indications that interactions between the lipid portions of the cell nucleus with chromatin, which is a DNAprotein complex, are involved in organization of the chromatin and regulation of gene expression. Another example is the finding that the inclusion of proteins in DNA-lipid complexes for gene therapy can greatly enhance the transfection efficiency. The aim of this project is to gain an improved understanding of the physicochemical behavior of such systems. Of particular interest is the structure and composition of aggregates and complexes formed by the components and a multitude of techniques are applied for characterization of these. The work is focused on three classes of systems: 1) model systems of well-characterized proteins, DNA and different types of amphiphiles,

2) systems containing nucleosome core particles (NCPs), i.e. the basic unit of chromatin, which consist of DNA wrapped around a core of eight histone proteins, and different types of amphiphiles, and 3) complexes comprising plasmid DNA, amphiphiles and certain proteins that have been evaluated with regards to their efficiency in transfection experiments. (Dan Lundberg, Karin Schillén, Viveka Alfredsson, Daniel Topgaard, Björn Lindman, Maria da Graça Miguel (University of Coimbra), Henrique Faneca (University of Coimbra), Maria C. Pedroso de Lima (University of Coimbra), Lars Nordenskiöld (Nanyang Technological University), Nikolay Korolev (Nanyang Technological) and Nikolay Berezhnoy (Nanyang Technological).)

Diffusive transport in responding membranes (Contact persons: Tahereh Mokthari and Emma Sparr)

A responding membrane is defined as a barrier membrane that cannot be described by a simple permeability constant, but which barrier properties can be altered in response to changes in its environment. The permeability of such a membrane depends on the gradient of the diffusing substance, and on variations in other membrane gradients. This can have implications for transport in biomembranes (e.g., the humans skin), release of drugs from formulations, as well as the formation of interfacial films in amphiphilic systems.

In this project, we study the coupling between transport, structure and gradients in responding membranes. One interesting example of this is molecularly ordered films that can form spontaneously at the interface between air and solutions of lipid vesicles or micelles composed of surfactant and polymer. An important observation is that film formation occurs only in dry air, which implies that the osmotic gradient across the interfacial layer is crucial for the formation of the film, and that the stable film is present during steady-state conditions rather than under equilibrium conditions. We recently treated the mechanisms for the formation of such ordered interfacial films in binary systems in a theoretical model (figure), and we now work on extending this to also cover ternary systems. We also explore the mechanisms for the formation of these responding interfacial films under steady-state conditions using a range of different experimental techniques, including null ellipsometry, sorption microbalance and small-angle X-ray scattering. (Emma Sparr, Tahereh Mokthari, Håkan Wennerström, Karen Edler (University of Bath, guest professor Physical Chemistry, LU) and Christoffer Åberg.)

How small polar molecules protect membrane systems against osmotic stress (Contact person: Emma Sparr)

Urea, under the name of carbamide, and glycerol are standard major components of skin lotions. They are claimed to act as “moisturizers” with seems to imply that have the effect of binding water in excess to what would be the case without the presence of these compounds. Compounds such as urea, glycerol and similar polar substances occur naturally in many organisms to regulate osmotic pressure and to prevent cell damage due to freezing or drying. The question addressed in the project concerns the molecular mechanism(s) behind the role of urea and glycerol in these contexts.

By studying lipid - mixed solvent systems using a range of methods such as sorption calorimetry, sorption balance, X-ray diffraction/scattering and nuclear magnetic resonance it is possible to unravel how the presence of urea and glycerol interacts with phospholipid bilayers. The major conclusions are: i) urea and glycerol shows a near ideal mixing with water in the lipid lamellar systems. ii) The presence of urea or glycerol has only a minor effect on the gel to liquid crystal transition temperature in the presence of excess solvent. iii) Under conditions of fixed lipid to urea (or glycerol) ratio the transition to a gel state occurs at lower relative humidities than for pure aqueous systems. The "moisturizing" effect of urea and glycerol is, based on these investigations, due to a suppression of a liquid crystal to gel/solid transformation that otherwise would occur under dry conditions. (Agnieszka Nowacka, Emma Sparr, Håkan Wennerström, Daniel Topgaard, Fátima Costa-Balogh (Coimbra university, Portugal) and Lars Wadsö (Building Materials, LTH).) Project completed in 2011.

Polymerization in structured media (Contact person: Ola Karlsson)

The long-term goal of this project is to study polymers that resemble biomacromolecules in their structure and function. To that end, we study polycondensation reactions in dispersed aqueous systems at ambient or slightly elevated temperatures. The incorporation of active chemical functionalities through polymerization in structured dispersed media will produce new types of polymer. The polymerization reactions that result in such materials include multifunctional monomers, which are often amphiphilic by nature. In order to facilitate the formation of specific molecular sequences, a detailed control of the polymerization loci is a necessity, and the partitioning of the reaction components in the various phases during reaction is crucial. Initially, we study the solubility of the active components and the complex formation between them. We also study how the reaction kinetics are affected by the distribution of the reaction species and by the particle size of the dispersed phase. The project is run in co-operation with MIP Technologies AB, Lund. (Johanna Bailey, Ola Karlsson, Lennart Piculell)

Soluble complex salts of surfactant ions and polymeric counterions: Composite macromolecular self-assembly (Contact Person: Karin Schillén)

The aim is to understand the physical chemistry of soluble complex salts in aqueous solution and the intermolecular interactions involved. A complex salt is defined as the neutral salt of surfactant ions (aggregated into highly charged micelles) that interact with a polyelectrolyte chain, which in turn acts as a large counterion (the polyion). The complex salts consist of polyacrylate (PA^{-}_{y}) and cationic $C_{16}TA^{+}$ surfactant ions, denoted $C_{16}TAPA_{y}$, where y is degree of polymerization. At high water contents, the investigated complex salts exhibit miscibility gaps that consist of co-existing phases: a concentrated phase (either cubic or hexagonal internal structure) and a less concentrated phase. In order to make the complex salts soluble, PEO-containing nonionic surfactants of the type C_iE_j are added. The phase studies on systems containing $C_{16}TAPA_{y}$ complex salts in water mixed with either $C_{12}E_5$ or $C_{12}E_8$ are carried out by visual inspection of the samples and by using small-angle X-ray scattering (SAXS). They reveal that the solubilization of the complex salts increases with increasing PEO-chain length of the nonionic surfactant. To gain further insight of the dissolution process, isothermal titration calorimetry (ITC) is employed. Thereafter, in the one-phase region, the solution properties of the self-assembled complex salt structures (e.g. their size effect of polyion and PEO lengths and their co-existence with pure nonionic surfactant micelles) are investigated by using dynamic light scattering (DLS), self-diffusion NMR and SAXS. Another study concerns the complex salts composed of polyacrylates, C_iE_j surfactants and ester-based cleavable cationic surfactants, where the effect of pH on the release of polyion is studied mainly using NMR. Finally, nanoparticles with different internal structure (hexagonal or bicontinous) have been prepared from $C_{16}TAPA_{6000}$ and $C_{12}E_5$ and are now currently being investigated using DLS, SAXS in combination with cryo-TEM. (John Janiak, Karin Schillén, Lennart Piculell, Gerd Olofsson, Dan Lundberg, M. Tomšič (University of Ljubljana, Slovenia), V. Pavel and L. Galantini (University of Rome "La Sapienza", Italy).)

Associative Polymer-Polymer and Polymer-Surfactant Systems: Phase Behaviour and the Influence of Chemical Reactions (Contact person: Lennart Piculell)

Polymer-surfactant pairs that associate strongly and separate out as a concentrated phase from an aqueous solution are extensively used to create water-insoluble materials, or surface coatings, with controllable properties. Two properties that are interesting to control are the water content and the packing of the surfactant aggregates in the concentrated phase. The control parameters are the detailed chemistry of the components, as well as their concentrations and proportions in the mixture. This project follows two lines of activity. One is concerned with systematic studies of the phase behavior of mixtures of associating pairs in water, using the minimum number of components to simplify the interpretation. We investigate nonionic pairs of polyacrylic acid and PEO-PPO-PEO triblock copolymers, as well as conventional cationic surfactants mixed with "complex salts" of cationic surfactant ions having acrylate-based copolymers as counterions. We study the effect of polymer length and polyion charge density for the structures formed in the concentrated phase, as well as the possibility to "redissolve" the concentrated phase by additions of excess surfactant. We also compare with simple model calculations in an attempt to extract the main physical mechanisms. The other line of research concerns using chemical reactions to modify the phase behavior. For this purpose we use surfactants containing either degradable cationic betaine esters as surfactant ions, or polymerizable acrylate ions as counterions. In both cases, we compare the outcome of the degradation or polymerization reactions with predictions from the appropriate equilibrium phase studies, where the effects of replacing one (reactant) component with another (product) component is readily apparent. (Salomé dos Santos, Charlotte Gustavsson, Lennart Piculell, Ola Karlsson, Per Linse, Maria da Graça Miguel (University of Coimbra) and Dan Lundberg (University of Coimbra).) Project completed in 2011.

Porous surface layers through deposition of structured polymer-surfactant particles (Contact person: Lennart Piculell)

A porous surface layer can function as a semi-permeable barrier, as a depot for material to be released from the pores, or as a size-selective adsorbent for substances in a surrounding fluid phase. For all these functions, it is of importance to control the size of the pores, their geometry, and their orientation (for non-spherical pores) relative to the surface. As one part of the larger SSF program "Porous surface layers through polymer-assisted deposition", this project investigates the making of porous polymer-surfactant particles from associating polymer-surfactant pairs, which are then deposited at a surface through a destabilizing mechanism. The deposition strategy is closely related to that commonly used in laundry and personal care applications to deposit particulate matter through "coacervating" polymer-surfactant formulations. The particles are made either by direct mixing or by polymerizing surfactant counterions (with or without cross-linkers) in solution, and are later studied by DLS, SAXS and cryo-TEM. The correct conditions for surface deposition of the particles (in a controlled fashion) will be studied by ellipsometry and AFM. (Charlotte Gustavsson, Lennart Piculell, Ola Karlsson and Viveka Alfredsson.)

Self-assembly in melts of block copolymer-based systems created by supramolecular interactions (Contact person: Lennart Piculell)

For an A-*b*-B diblock copolymer, the thermodynamic incompatibility between A- and B-blocks drives a microphase separation in the melt state where alternating A-rich and B-rich microdomains appear in order to minimize the contact between dissimilar A- and B-blocks, resulting in a variety of self-assembled structures. Similarly, self-assembled miscible melt mixtures between A-*b*-B diblock copolymers and homopolymers or block copolymers can be obtained by dissolving the latters in the segregated microdomains of the former.

It is the aim of the present project to explore melt self-assembly of systems that are created by supramolecular interactions (including ion-ion and ion-dipole interactions and hydrogen bonds) between, on the one hand, the segments of one of the blocks of a parent block copolymer (the polar segments of poly(styrene)-*b*-poly(methacrylic acid), PS-*b*-PMAA, or its lithium neutralized form PS-*b*-PMALi) and, on the other hand, the corresponding constituent segments of (i) cationic surfactants (alkyltrimethylammonium type), (ii) non-ionic surfactants (alkyl-ethylene oxide C_XE_Y type), (iii) a homopolymer (sodium poly(styrene sulfonate), PSSNa), and (iv) block copolymers (composed of poly(ethylene oxide), PEO, and poly(propylene oxide), PPO, blocks). In (i) the molecular architecture of the system can be envisaged as an A-*b*-(B-*graft*-C) block copolymer in which micro- and nanophase separations (between A- and (B-*graft*-C)- blocks and between B and C segments within (B-*graft*-C)-block, respectively) occur simultaneously, resulting in a variety of structure-*in*-structure two-scale hierarchical self-assemblies. In (ii)-(iv) the systems feature block copolymer-based blends in which miscibility is achieved by attractive interactions between the constituent elements of the system. (Mehran Asad Ayoubi, Lennart Piculell, Ulf Olsson, Bo Nyström and Kaizheng Zhu (University of Oslo) and Kristoffer Almdal (Micro- and Nanotechnology, DTU).)

Cellulose dissolution (Contact person: Björn Lindman)

The dissolution of cellulose is important for a number of industrial processes and several solvents and mixtures have been tested. On the basis of an examination of the intermolecular interactions in cellulose novel approaches to cellulose dissolution are attempted. It is found that for aqueous systems the presence of amphiphilic compounds can facilitate dissolution as well as prevent re-association. It is also found that kinetic parameters are important in control cellulose systems and that anomalous temperature effects are encountered, similar to the case of several other nonionic polymers. (Björn Lindman, B. Medronho (Coimbra), L. Stigsson (KIRAM), G. Karlström and A. Holt (Theoretical Chemistry, Lund Univ.).)

Controlling the phase behavior of polyion-surfactant ion complex salts by cyclodextrins (Contact person: Björn Lindman)

We have previously shown that cyclodextrins can be used to decompact single DNA molecules that were compacted by cationic surfactants. Additionally, macroscopically phase separated DNA-surfactant complexes were shown to be dissociated at sufficient cyclodextrin concentrations. In this study we look at the phase behavior of concentrated ternary systems of polyion-surfactant ion complex salt and cyclodextrins to deepen our knowledge on these interactions. Various parameters, such as polyion hydrophobicity and length, surfactant chain length, as well as salt dependence and type of cyclodextrin is addressed. Preliminary results from a system containing DNA-DTA:2-HP-β-CD:water shows a rich and very interesting phase behavior. These studies are both of biological and biotechnological interest and may also be interesting for other industrial applications.(Ulf Olsson, Azat Bilalov, Jonas Carlstedt and R. S. Dias (University of Coimbra, Portugal).)

Coulomb fission (Contact person: Per Linse)

Delayed asymmetric Coulomb fission in size-selected molecular dication clusters has been recorded for the first time. Observations on $(NH_3)_n^{2+}$ clusters show that fragmentation accompanied by charge separation can occur on a microsecond time scale, exhibits considerable asymmetry, and involves a kinetic energy release of ~0.9 eV. The fission process has been modeled by representing the fragments as charged dielectric spheres and the calculated maximum in the electrostatic interaction energy between the fragments gives a good account of the measured kinetic energy release. A simple kinetic model shows that instrumental factors may contribute to the observation of asymmetric fragmentation. (Per Linse and Guohua Wu, Xiaojing Chen, and Anthony J. Stace (University of Nottingham, England).)

Understanding ultra-dense microgel suspensions (Contact person: Peter Schurtenberger)

Cross-linked microgels are a particular interesting class of colloids with tunable size and softness that creates particle properties situated between classical hard spheres and soft-polymeric systems. Due to their soft-repulsive nature, microgels can be packed to an effective volume fraction feff much above closed packing fcp, with enormous consequences for the resulting structural and dynamic properties. In our project we aim at: 1) Understanding the particle size and structure as a function of the effective volume fraction far into the ultra-dense region feff >> fcp, using mainly small angle neutron scattering combined with advanced contrast variation schemes. 2) Understanding structural ordering and dynamics of microgel dispersions at high volume fractions using confocal laser scanning microscopy and scattering techniques. Here we also use the charge density as an additional and tuneable parameter to combine long-range electrostatic interaction with the intrinsic short-range soft repulsion from the cross-linked polymer network in order to probe complex equilibrium crystalline structure as predicted the theory of ionic microgels. (Priti Mohanty, Divya Paloli, Jerôme Crassous, Christos Likos (University of Vienna) and Peter Schurtenberger.)

Flexibility and conformation of giant dendronised polymers (Contact person: Peter Schurtenberger)

In recent years an interesting new class of polymers and polyelectrolytes has been developed, the so-called dendronized polymers. The unusual structure of these polymers with their tight and highly branched layer around the backbone has raised fundamental questions in polymer science, which all have their origin in the influence of the layer on the conformation and rigidity of the backbone. We investigate the effect of the dendrons on the chain stiffness, and look at the influence of charge and solvent on the cross-sectional conformation, the flexibility, and on the interchain correlation at higher densities using SANS, SAXS and light scattering. (Sebastian Lages, Peter Schurtenberger, Dieter Schlüter (ETH Zurich, Switzerland) and Reinhard Siegel (University of Fribourg, Switzerland.)

Phase behavior, structure and dynamics of anisotropic model colloids
(Contact person: Peter Schurtenberger)
Colloids are convenient model systems to study classical condensed matter problems such phase transitions, dynamical arrest, or nucleation and crystallization phenomena. Here we aim at a fundamental understanding of the phase behavior, structure and dynamics of concentrated suspensions of anisotropic particles. We focus both on structural anisotropy in ellipsoidal particles, as well as on the effects of an additional anisotropic component in the interaction potential between particles that can be generated using magnetic particles or particles with a magnetic core. (Ilya Martchenko, Jérôme J. Crassous and Peter Schurtenberger.)

The nature of the glass transition in microgel suspensions (Contact person: Peter Schurtenberger)
The main aim of this project is to study the phase behaviour of concentrated suspensions of Poly(N-isopropylacrylamide) (PNIPAM) microgel particles. PNIPAM particles are very interesting as they show a thermoresponsive size, where the particle swells at low and collapses at high temperatures. The size and thus the effective volume fraction of the particles can therefore be changed through a variation of the temperature. Here we use PNIPAM microgels as convenient model systems to investigate the glass transition that occurs at volume fractions » 0.6. We also look at the influence of the intrinsic softness of these particles on dynamical arrest, and investigate the nature of the dense phases that exist at high densities. We use confocal laser scanning microscopy that allows us to track the particles in real time and determine quantities such the pair correlation function or the mean square displacement of the particles as a function of effective volume fraction. (Divya Paloli, Jerôme Crassous, Priti Mohanty, Emanuela Zaccarelly (University La Sapienza Rome, Italy), Christos Likos (University of Vienna) and Peter Schurtenberger.)

Temperature-responsive supramolecular structures based on γ-cyclodextrin and polymers containing PNIPAAM chains (Contact person: Karin Schillén)
Pseudopolyrotaxanes or inclusion complexes are supramolecular assemblies formed by a linear molecule (e.g. a polymer chain) and several ring shaped molecules such as cyclodextrin (CD). Pseudopolyrotaxanes are widely studied because the structure of the assembly can readily be tuned by means of the solution conditions as well as the molecular architecture. A precise control of such supramolecular structures by using external stimuli and the understanding of the involved mechanism is a challenge for the design of smart nanomaterials. CDs are cyclic oligosaccharides formed by glucopyranose units. They have a truncated cone shape with a hollow cavity, which may incorporate

more or less hydrophobic solutes such as surfactants or polymer chains. Several CDs rings can thread a polymer chain assuming either a compact or loose structure depending on the nature of the CD. In this project, we investigate the inclusion complex formation between γ-CD and polymers containing thermoresponsive poly(N-isopropylacrylamide) (PNIPAAM) chains in solid state, in solution, at silica/liquid interfaces and at silica particle surfaces. Both PNIPAAM-diblock copolymers and PNIPAAM homopolymers have been studied so far. When temperature approaches the lower critical solution temperature of PNIPAAM, the CD molecules dethread. The experimental techniques employed are ^{1}H-NMR, Fourier transform infrared spectroscopy, synchrotron radiation powder X-ray diffraction, steady-state fluorescence spectroscopy, differential scanning calorimetry, static and dynamic light scattering and cryo-transmission electron microscopy. The surface properties of the PNIPAAM-diblock copolymer systems are investigated using ellipsometry, neutron reflectivity and quartz crystal microbalance with dissipation techniques. Furthermore, in a related project, the formation of coacervate core micelles of cationic and anionic PNIPAAM copolymers are studied using DLS and isothermal titration calorimetry. (Solmaz Bayati, Karin Schillén, Giuseppe Lazzara (University of Palermo, Italy), Tommy Nylander, Gerd Olofsson, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway), Viveka Alfredsson and Richard Campbell (ILL, France).)

Particle adsorption (Contact person: Per Linse)

A model for the adsorption of colloidal particles on a planar surface is analyzed by using a thermodynamic chemical equilibrium model and Monte Carlo simulations. Central to this investigation are that (i) particles and surface are considered to be of the same material, and (ii) the particle–surface and particle–particle interactions are related using the Derjaguin approximation using a surface–surface square-well potential as a basis. Thereby, all interactions within the system are characterized by the *same* parameters, and hence the difference between particle adsorption on the surface and particle aggregation in bulk is *solely* due to geometrical effects. Equilibrium constants for the different binary associations are calculated from the interaction potentials enabling a direct comparison between predictions based on a chemical equilibrium model and on computer simulations with no adjustable parameters. As the interaction gradually is made more attractive for a given particle concentration, we find the following sequence of events: (A) a weak particle adsorption to the surface, (B) particle association on the surface forming a denser single adsorbed layer, (C) formation of a second adsorbed layer on the surface, (D) multiple adsorbed layers on the surface, and (E) bulk phase separation. There is a semi-quantitative agreement between the predictions of the equilibrium model and the results of the simulations. The equilibrium model calculations facilitate a conceptual understanding of the *competition* between association on a surface and in bulk. Our study is relevant both for understanding processes where colloidal particle adsorption is used to modify surface properties and also for the understanding of heterogeneous versus homogeneous nucleation. (Per Linse and Håkan Wennerström.)

Arrested spinodal decomposition in soft particle suspensions (Contact person: Peter Schurtenberger)

Microgels are cross-linked colloidal particles with a network structure, which undergo solvation changes in response to the application of an external stimulus such as temperature, pH or electrolyte concentration. In this project, depletion interactions induced by the presence of a non-adsorbing polymer in a microgel system (PNIPAM cross-linked with MBA) are studied. The aims are to investigate the interplay between phase separation and dynamical arrest in concentrated suspensions, to locate the arrest line in the phase diagram, and to study the applicability of the Extended Law of the Corresponding States (ELCS) in these systems. The microgels are used as a versatile model system where the effective volume fraction can conveniently be changed via a change in temperature. In order to perform these studies, a combination of techniques such as 3D cross-correlation light scattering, ultra-small angle light scattering, small-angle x-ray and neutron scattering, confocal laser scanning microscopy and rheology are used to characterize the structural and dynamic properties of the system as a function of the strength of the interaction and the volume fraction of the particles. (Marc Obiols Rabasa, Priti Mohanty, Divya Paloli, Jerôme Crassous and Peter Schurtenberger.)

Ionic microgels as model systems for dipolar fluids (Contact person: Peter Schurtenberger)

Ionic microgels are intriguing soft colloids with an effective pair potential that crosses over from Yukawa-like at large distances to a much softer repulsive interaction at short distances. Here we describe the effect of an additional anisotropic dipolar contribution to colloids with such “ultra-soft” interactions. We use an alternating electric field to induce a tunable dipolar contribution, and study the resulting particle self-assembly and phase transitions in-situ with confocal laser scanning microscopy. (Priti Mohanty, Anand Yethiray (Memorial University, St. John’s, Canada), Christos Likos (University of Vienna, Austria) and Peter Schurtenberger.)

Asymmetric Catanionic Surfactants (Contact person: Ulf Olsson)

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 anusual miscibility gap within the lamellar phase, which has previously been observedonly in a few particular systems. With the addition of an alkane, the lamellar phase is transformed into a water-in-oil droplet microemulsion with spherical, weakly charged droplets of low polydispersity. Using small angle neutron scattering we study the longrange droplet-droplet interactions which depend on the concentration dependent effective droplet charge. (Bruno Silva (Porto University), Per Linse, Ulf Olsson and Eduardo Marques (Porto University).)

Living polymers and living networks (Contact person: Ulf Olsson)

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). In a living polymer system made of reverse, slightly water swollen, lecithin micelles in cyclohexane, the stress relaxation time is around an hour. Hence, the zero shear viscosity is unusually high. The long relaxation times also allow for studying the entangled system’s response to fast deformations. Here, the stress strain relationship is similar to that of rubbers. Above a certain critical strain the entangled micellar network fractures, and the micelles align in the flow direction. (Ulf Olsson, R. Angelico, L. Ambrosone and A. Ceglie (Campobasso), G. Palazzo (Bari), L. Gentile, C. Olivieri (Cosenza) and K. Mortensen (Risø, Denmark).)

Lamellar phase rheology and shear-induced formation of multi-lamellar vesicles (Contact person: Ulf Olsson)

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 tates. Oriented (“single crystal”) lamellar phases still contain equilibrium defects that give them a relatively high shear viscosity and in addition make them viscoelastic. In a Couette cell, magnetic resonance chemical shift imaging has shown that the lamellarto-onion transition takes place homogeneously throughout the sample, while in the onion-to-lamellar transition, the lamellar phase first forms at the inner rotor and the growth of that phase propagates through the gap. (Ulf Olsson, B. Medronho (Coimbra), M. Miguel (Coimbra), C. Schmidt (Paderborn), M. Imai (Tokyo), Y. Suganuma (Tokyo), P. Galvosas and P. Callaghan (University of Wellington), L. Gentile and C. Oliviero Rossi (Univ. of Calabria).)

PIT and PIC emulsificaiton (Contact person: Ulf Olsson)

In this project we re-examine the phase inversion temperature (PIT) emulsification process using model ternary nonionic surfactant/water/oil systems. This is a low-energy method that uses a physicochemical drive to produce very fine oil/water emulsions in the absence of high shear flows. We find that successful emulsification depends on two conditions. First, the mixture must be stirred at low speed throughout the whole process: this makes it possible to produce emulsions at surfactant concentrations that are too low to form an equilibrium microemulsion. Second, the stirred mixtures must be heated above a threshold called the clearing boundary (CB) and then quenched to lower temperatures. The clearing boundary is determined experimentally by a minimum in the turbidity of the stirred mixture, which results from solubilization of all the oil into swollen micelles. This matches the emulsification failure boundary corresponding to the condition $R^*C_0=1$, where R* is the spherical radius that results from the oil/surfactant composition for monodisperse spheres and C_0 is the spontaneous spherical curvature of the surfactant monolayer. Thus, we show that such cycles do not need to cross the PIT. In fact, sub-PIT cycles and cross-PIT cycles give exactly the same result. These conditions lead to emulsions that have a narrow size distribution and a mean diameter controlled by the oil/surfactant ratio. The typical range of those diameters is 20-100 nm. Moreover, these emulsions have an excellent metastability, in contrast with emulsions made with shorter oil and surfactant molecules. In the phase inversion composition (PIC) method, typically an oil-surfactant mixture is suddenly mixed with a large amount of water to produce an O/W emulsion. A key molecular event here is surfactant hydration. Also in this process a clearing boundary can be identified. However, the PIC mechanism, and its corresponding sequence of events, is significantly different from the PIT mechanism. The PIC mechanism involves as a fundamental step the formation of a separate oil phase. As a consequence of this separation a unimodal size distrubution of the final emulsion is not possible, as it is in PIT emulsification. (Ulf Olsson, K. Roger and B. Cabane (ESPCI, Paris)

Pickering Emulsions (Contact person: Ulf Olsson)
Pickering, or particle stabilized, emulsions have a number of interesting properties. When the particles are properly chosen, they are essentially irreversibly adsorbed at the oil-water interface, which, as a consequence, inhibits Ostwald ripening. In this project we investigate the properties of silica coated particles and their potential for stabilizing W/O emulsions. Furthermore, we want to develop a method to measure the strength of particle adsorption at the oil-water interface. (Ulf Olsson and Y. Sakazaki (Pola Chemical Industries INC, Yokohama).)

Experimental methodologies

Diffusive transport of multivalent ions in cartilage (Contact person: Olle Söderman)
Articulate cartilage is a complex material, composed of collagenous fibers, and cells called chondrocytes, all of which are embedded in a firm gel-like ground substance. The chondrocyte cells produce proteoglycans which bind to hyaluronic acid, forming large highly hydrophilic aggregates. These aggregates are entangled with each other and with the collagen fibrils forming what can best be described as a hydrogel that sits within the collagen network. In the general accepted model of the morphology of cartilage, the collagen fibrils associate into columnar structures that extend outward from the bone. The protoeglycans are highly charged due to the presence of sulfate and carboxylic groups.

The break-down of cartilage results in a lowering of the concentration of the proteoglycans. It has been suggested to use $(Gd\text{-}DTPA)^{2-}$ as a contrast n MRI to monitor the concentration of proteoglycans and therefore the state of the cartilage. In healthy cartilage the concentration of $(Gd\text{-}DTPA)^{2-}$ will be low, while in damaged cartilage it would be high leading to T1-contrast in MRI.

There are some fundamental questions in this context. What is the dynamics of the Gdcomplex in cartilage? How does one quantify the T_1 contrast in terms of the state of the cartilage? On the experimental side, NMR diffusometry and micro imaging techniques will be performed on model system of cartilage made from gel-forming polymers as well as on actual in-vitro samples of cartilage will be undertaken.

Theoretical studies on diffusion of large negative divalent ions in models of healthy and damaged cartilage will be carried out. These include Brownian Dynamics simulations, which possibly will be complemented by Dynamic Density Functional Theory calculations. (Jenny Algotsson, Daniel Topgaard, Olle Söderman, Jan Forsman (Division of Theroetical Chemistry, LU) and Jonas Svensson and Leif Dahlberg (Department of Radiation Physics and the Joint and Soft Tissue Unit at UMAS, Malmö).)

Polymer-surfactant interaction at liquid interface (Contact person: Tommy Nylander)

The project aims to understanding of the nature of the interaction between polyelectrolytes and oppositely charged surfactants at interfaces in relation to the bulk phase, with particular attention to non-equilibrium effects. We study polyelectrolyte systems of relevance for commercial products such as shampoos and fabric conditioners, but also model systems such at cationic dendrimers and anionic surfactants. We have demonstrated that the choice of sample preparation methods can have a profound effect on the state of the interface for chemically equivalent samples. This is particularly apparent in the phase separation region, where the extent of aggregation in the bulk solution on relevant time scales is affected by the polymer/surfactant mixing process, which in turn the structure and composition of the interfacial layer. The studies include experimental studies using ellipsometry, QCM-D, neutron reflectometry and light scattering as well as theoretical modeling. (Marianna Yanez, Tommy Nylander, Lennart Piculell, Per Linse, Richard Campbell (ILL, France), Katrin Tonigold (Ulm University), Imre Varga and Róbert Mészáros (Eötvös Loránd University, Budapest; Hungary).)

Solid-state NMR methods for amphiphile systems (Contact person: Daniel Topgaard)

Several types of intermolecular interactions, e.g., steric, electrostatic, and hydrophobic, affect the dynamic behavior of large molecules in a crowded system. NMR offers a unique possibility of resolving different molecules and molecular sites even in rather complex mixtures. For colloidal systems with reduced molecular mobility and sample heterogeneity on the nano- to micrometer scale, solid-state NMR methods with magic-angle spinning are required for extracting high-resolution spectroscopic information. Dynamic and site-resolved information can be correlated in multidimensional experiments. The experimentally determined parameters have simple geometrical definitions and can be estimated using theoretical approaches such as molecular dynamics simulations. The NMR methods are applied to a series of colloidal systems including cationic surfactants with mono-, oligo-, and polymeric counterions, nonionic surfactants with poly(ethylene oxide) or glucoside headgroups, DNA-lipid assemblies, and synthetic analogs of the lipid mixtures in the stratum corneum. (Agnieszka Nowacka, Tiago Ferreira, Samuli Ollila, Daniel Topgaard, Emma Sparr, Gunnar Karlström and Olle Söderman.)

Diffusion NMR/MRI methods for biological tissues (Contact person: Daniel Topgaard)

Molecular transport by diffusion is a crucial process for the function of biological tissues.

Diffusion NMR and MRI are powerful methods for non-invasively studying molecular motion on the micrometer length scale and millisecond time scale. By following the self-diffusion of molecules in a cellular system, information about structure and dynamics on the cellular scale can be obtained. Within this project we design new diffusion NMR/MRI protocols for estimating parameters such as the diffusion coefficient of the intracellular medium, cell membrane permeability, microscopic anisotropy, and the length scale at which an inhomogeneous medium start to appear homogeneous. The structure of biological materials, or the transport behavior of molecules within these materials, can often be mimicked by carefully designed colloidal model systems such as emulsions, gels, and liquid crystals. The new methods are first tested by simulations, subsequently applied to colloidal model systems, simple cellular systems and excised tissue, and finally implemented in the context of medical MRI. (Stefanie Eriksson, Daniel Topgaard, Olle Söderman, Markus Nilsson, Jimmy Lätt, Freddy Ståhlberg (Medical Radiation Physics), Stina Oredsson (Biology) and Samo Lasic (Colloidal Resource).)

Isothermal multi-channel microcalorimeters for use as monitors of biological and technical processes and in thermodynamics (Contact person: Ingemar Wadsö)

Isothermal microcalorimeters are used in thermodynamics and as general analytical tools, especially as monitors of biological systems and technical processes. The technique has several important properties but has also some weak points, in particular a low sample throughput and difficulties in interpreting the calorimetric signal for complex processes. Our instrument development work concentrates on these problems.

Isothermal microcalorimeters are normally twin instruments, where one vessel is used for measurements and one serves as a reference. In multi-channel instruments several samples can be measured simultaneously. In order to facilitate interpretation of the calorimetric signals specific analytical sensors can be positioned in the vessels.

Presently, work involves development of two different multi-channel microcalorimeters: a 12-channel instrument primarily intended for use as a “bio-activity monitor” and a 10-channel instrument for use in thermodynamic measurements, and as a general process monitor, over a wide temperature range, 0-150 °C.

The 12-channel design is based on an erlier 48-channel instrument (cf. AR 2007), which primarily was intended for use in screening experiments around 37 °C, involving cell-drug interactions. The new instrument has larger vessels and is designed use, over a wide temperature range, as a monitor for microbial activity in soil, animal (human) cells, tissues and small animals.

The 10-channel instrument is designed for use as a “platform” for different reaction vessels intended for thermodynamic measurements in the temperature range of 0-150 °C. Tests are conducted by use of simple static vessels, useful for stability measurements and as process monitors. Later, more advanced vessels (of types that we earlier developed for use with our twin instruments), will be added to the system: stirred vessels which allow injection of liquids, gases or solid reagents, introduction of light and the incorporation of analytical sensors, e.g. electrodes.

Colloidal biology

Amyloid interaction with lipid membranes

(Contact persons: Emma Sparr and Sara Linse)

The starting point of this project was the recent realization that lipid membranes apparently play pivotal roles in the pathogenesis of the protein misfolding disorders, e.g., Alzheimer´s and Parkinson´s diseases. An increasing amount of evidence suggests that the process of fibril formation in vivo and the mechanism of toxicity involve membrane interactions. The objective of the project is to explore the basic principles of how aggregating amyloid protein influence the lipid membrane barrier and the underlying interactions between the aggregating protein and the lipid membrane. We use recombinant Aβ and α-synuclein produced in Escherichia coli, which allows us to perform large scale amyloid formation assays with good statistics where the aggregation process is followed in means of thioflavin T fluorescence. The lipid membranes are introduced in the system as unilamellar vesicles (see figure). One important goal of the present project is to further the understanding on how the aggregating amyloid protein can influence the membrane barrier properties and thus affect the transport of the protein itself as well as other substances. We have shown that no diffusive transport of α-synuclein can occur over a pure model membrane and moreover, that membrane interaction requires presence of negatively charged lipids. Continuing these studies we now focus on more complex biological membranes and their interaction with α-synuclein to further elucidate transport and uptake pathways using different biophysical techniques, including monolayer techniques, confocal microscopy on giant unilamellar vesicles, NMR, ellipsometry, QCM-D, neutron reflectivity and electron microscopy. (Erik Hellstrand (Division of Biophysical Chemistry, LU), Marie Grey, Emma Sparr, Agnieszka Nowacka, Daniel Topgaard, Sara Linse and Martin Lundqvist (Division of Biochemistry and Structural Biology, LU), Patrik Brundin (Wallenberg Neurocenter, LU), Ronald Melki (Laboratoire d'Enzymologie et Biochimie Structurales, CNRS, Gif-sur-Yvette, France), Marie-Louise Ainalem (ESS AB) and Tommy Nylander.)

Condensing DNA with cationic dendrimers: means of controlling aggregate morphology and membrane penetration (Contact person: Tommy Nylander)

Dynamic light scattering, cryogenic TEM and steady-state fluorescence spectroscopy are utilized to investigate the interaction between cationic poly(amido amine) (PAMAM) dendrimers and double stranded DNA. This systematic study reveals how the size, composition and morphology of aggregates formed between DNA and PAMAM dendrimers are affected by dendrimer size and charge. In gene therapy one often utilizes vehicles with the ability to condense DNA and thereby protect DNA against degradation, transport DNA across membranes as well as regulate gene expression. One such compacting agent is dendrimers. We have found that the compacting agent not only condenses the DNA chain, but can also on its one be transported across a model membrane. This might help the complex to be transported across the membrane. We are investigating the conditions, such as membrane and dendrimer properties, under which this occurs using ellipsometry, QCM-D, neutron reflectometry and different fluorescence techniques. (Marie-Louise Ainalem (ESS AB), Syma Khaled (University of Southampton), Anna Carnerup, John Janiak, Viveka Alfredsson, Tommy Nylander, Dan Lundberg and Karin Schillén.)

DNA gel particles and cross-linked DNA gels (Contact person: Björn Lindman)

Through an interfacial diffusion mechanism DNA particles were prepared and studied with respect to internal structure and DNA release. A large difference in internal structure between different DNA conformations for surfactant systems point to the role of hydrophobic interactions. Release properties of the gel particles, which can be manufactured in the size range from 100 nm to mm, are investigated. DNA gel particles are made from mixtures of DNA with cationic surfactants, proteins and polymers and also for other polymers. 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. The release of DNA and incorporated proteins are investigated, in particular related to triggering release. (Björn Lindman, Carmen Morán (Univ. Barcelona), Diana Costa (Univ. Beira Interior) and Maria Miguel (Coimbra University).)

Structure and Self-Assembly of Viruses (Contact person: Per Linse)

Studies of the packaging of DNA inside viral capsids using a density functional theory have been performed. Of special interest is to investigate the liquid-crystalline transition in the spherical capsid and elucidate possible conformation transitions of DNA in confined geometry. In more detail, a density functional theory of the spatial distribution or biaxial nematic order of polymers of arbitrary length and rigidity inside a spherical cavity is proposed. The local order of different chain segments is considered as an alignment to a spatially varying director field of cylindrical symmetry. The steric interactions are taken into account in the second virial approximation. Polymer density and orientational order distributions inside the spherically cavity are the principal results. It was found that short and flexible polymers are located at the center of the sphere and are orientationally disordered. Upon increasing polymer length and/or polymer rigidity, the location of the polymer is continuously shifted towards the surface of the spherical cavity and the polymer segments become gradually more aligned. Parameters have been selected to model the behavior of genomes in spherical viral capsids.

In addition, we have initiated examination of the self-assembly of charged capsid subunits in the presence of oppositely charged polyions by molecular dynamics simulations. The subunits were modeled as rigid trapezoidal bodies with positive charges localized on one side and the polyions as charged beads connected with harmonic bonds. Conditions were established under which no self-assembly appear without polyions present and self-assembly appear with polyions present as appearing many ssRNA containing viruses. Currently, we are mapping conditions for successful capsid formation. (Ran Zhang, Nikolay N. Oskolkov, Per Linse and Alexei R. Khokhlov (Moscow State University).)

The skin as a barrier to molecular diffusion (Contact persons: Sebastian Björklund and Emma Sparr)

The skin separates very different environments. Under normal conditions, there is a substantial gradient in water between the water-rich inside of the body from the dry outside. This leads to a variation in the degree of hydration along the skin and changes in this gradient may affect the structure and function of skin. Similarly, the skin is exposed to other gradients in, e.g., metabolic gases, temperature, pH, applied drugs etc. In this study we raise the questions: How do changes in these gradients across skin affect its permeability? In a recent study, we have shown that the permeability of the skin barrier increases abruptly at low water gradients, corresponding to high degrees of skin hydration, and that this effect is reversible. The results are explained on basis that the skin is a responding membrane, for which small changes in the environment can lead to major changes in membrane structure, which in turn affect its transport properties. This phenomenon is highly relevant to drug delivery applications due to its potential of temporarily opening the skin barrier for transdermal delivery of drugs and subsequently closing the barrier after treatment.

The main goal of this project is to couple stratum corneum barrier properties to stratum corneum lipid structure, and to explore how this is affected by, e.g. hydration, “moisturizers”. These studies aim to understand how molecular diffusive transport occurs through the SC and thus how it can be affected. We aim at the characterization of the lipid component of the stratum corneum and intact stratum corneum under varying conditions, using NMR and sorption calorimetry. This is combined with transport studies of different drugs across intact stratum corneum in the presence several gradients. (Emma Sparr, Agnieszka Nowacka, Daniel Topgaard, Johan Engblom (Biofilms; Malmö university), Krister Thuresson (Hemocue), Lars Wadsö (Building materials, LTH), Joke Bouwstra (Leiden university), Vitaly Kocherbitov (Malmö University), Véronique Burnier (L’ORÉAL, Paris) and Bernard Cabane (ESPCI, Paris).)

Understanding concentrated protein solutions (Contact person: Anna Stradner)

The main objective of this project is to measure and understand intermolecular interactions in concentrated protein solutions and mixtures. We use a combination of different scattering methods (SANS, SAXS, Static and Dynamic Light Scattering, Neutron Spin Echo experiments), and compare the results with the predictions from numerical simulations. We in particular investigate the influence of interactions and so-called crowding effects on the diffusion of proteins. (Saskia Bucciarelli, Mikael Lund, Giuseppe Foffi (EPFL, Switzerland), George Thurston (Rochester Institute of Technology, USA), Peter Schurtenberger and Anna Stradner.)

On the submicellar structure of casein micelles and their aggregation behavior (Contact person: Tommy Nylander)

This work aims to relate the nano- and microscopic structures formed in milk based products to macroscopic effects such as gel strength and syneresis. The substructure of the casein micelle will be revealed by using model systems systematically built up by the different components, by mainly using light scattering, small angle neutron scattering (SANS) with contrast matching using perdeuterated proteins and cryo-TEM. In order to reveal the aggregation process of casein micelles we are using SESANS (Spin-Echo-Small-Angle-Neutron-Scattering), which allows following the formation of structure at a wide length scales from 10nm-20µm. The objective of the study is to reveal the substructure and aggregation process of casein micelles and the relation between the two. (Sofie Botegård (ESS AB), Tommy Nylander, Marie Paulsson (Food Technology), Carl Holt (University of Glasgow) and Wim Bouwman (University of Delft).)

Supramolecular structures of bile salt derivates in aqueous solutions (Contact person: Karin Schillén)
Surfactants prepared by chemical modification of bile salts, e.g. sodium cholate derivatives, show a rich self-assembly in aqueous solution. The supramolecular structures formed range from small micelles, networks of thin threads (homogenous fibers), tubules, long (on the μm-mm length scale) rod-like objects ("poles") to twisted ribbon-like structures. The formation of these assemblies depends on the kind of modification, pH and temperature. The temperature response is particularly interesting since it is fast and reversible. Cryo-TEM, circular dichroism, synchrotron SAXS and light scattering techniques are employed to explore these various morphologies and the driving force of their formation. The formation of tubules occurs around body temperature and the tubules are further investigated using water-diffusion NMR. (Karin Schillén, L. Galantini and V. Pavel (University of Rome "La Sapienza", Italy) and Daniel Topgaard.)

Interaction between RNA and lipid membranes (Contact person: Emma Sparr)
In the living system, RNA (ribonucleic acid) is present in an environment that contains many substances, which can 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 interaction with hydrophobic species in the environment, e.g. lipids in the cell membrane and in the cell nucleus. We aim at revealing the basic features of RNA–lipid interactions. We study the adsorption of nucleic acids to lipid bilayers and monolayers with varying properties, and tune the assembly of RNA duplexes and RNA cuboids at deposited bilayers. The systems are studied by means of several experimental techniques, including calorimetry, ellipsometry, quartz crystal microbalance (QCM-D), neutron reflectometry, fluorescence microscopy and monolayer techniques. (Agnes Michanek, Emma Sparr, Tommy Nylander, Luc Jaeger (University of California, Santa Barbara, USA) and Fredrik Höök (Chalmers).)

Peptide folding (Contact person: Per Linse)
A new two-state polymer folding model is proposed, in which the folding of a stiff helical polymer is enabled by allowing for short sequences of coils connecting shorter and separated helices. The folding is driven by short-range attraction energy among stacked helices and is opposed by the free-energy cost of forming coils from helical monomers. Principal outcomes of the model are equilibrium distribution of the number of helices and their length in helical polymers. The proposed model is applied to α-helical polyalanine. The distribution of the number of α-helices as a function of number of alanine residues is fitted to corresponding result from molecular dynamics simulation employing an all-atom potential model with very good agreement. The influence and significance of the fitting parameters and possible use of the two-state folding model are discussed. (Per Linse and Peter Palenčár and Tomáš Bleha (Slovak Academy of Science).) Project completed in 2011.

Studies of osteopontin and casein self-assembly in the context of biomineralisation: applications in food, health and biomaterials (Contact person: Tommy Nylander)
Many biofluids are super saturated with respect to hydroxyapatite (HA) by forming complexes between phosphopolypeptides/phosphoproteins and amorphous calcium phosphate (ACP). The purpose is to maintain the integrity of bones and teeth without mineralising the surrounding soft tissues. Our long-term goal is to provide a unified

model of the structure and mechanism of the formation of the complex between ACP and different phosphorylated proteins/peptides, based on the hypothesis that the process is controlled by protein self-assembly. The structures of composite materials comprising phosphopolypeptides and calcium phosphate with very different neutron scattering length densities are well suited to being studied by neutron scattering and diffraction methods. We will use NMR techniques to study the formation of these composites as well as interfacial techniques to study their interfacial behavior of relevance for biomineralization. In combination with recombinant phosphoprotein expression and isotope labelling, novel nano-, micro- and macro-structures will be fabricated and their size and medium resolution substructures determined. (Susana Teixeira, Sam Lenton & Giuseppe Zaccai (ILL), Carl Holt (University of Glasgow), Tommy Nylander & Daniel Topgaard.)

Peptide self-assembly (Contact person: Ulf Olsson)

The development of modern peptide chemistry has opened for the possibility of custom peptide synthesis that allows for systematically investigating the relationship between a specific oligopeptide molecular structure and the macroscopic phases and structures formed in such systems. Understanding the assembly behavior of peptides is important in not only designing nanomaterials for a desired functionality but also for combating neurodegenerative diseases such as Alzheimer and Parkinson's disease which are strongly associated with an accumulation of amyloid forming peptides in the brain. In this newly started project we focus initially on the self-assembly behavior of short simple and synthetic petides, AnK, where n is varied in the range 4-10 (A=alanine, L=lysine). These peptides allows for a systematic investigation of e.g. the hydrophobicity and peptide length on the self-assembly behavior.

A6K in water forms very long hollow nanotubes with a (monodiperse) diameter of 52 nm, for concentrations above a critical aggregation concentration, cac≈11 %. Because of the large aspect ratio, the nanotubes form a nematic phase or a hexagonal phase. Work is now proceeding to investigate the self-assembly behavior of the analogue peptides A4K, A8K, and A10K. (Celen Cenker, Ulf Olsson, Malin Zackrisson, Mikael Lund (Division of Theoretical Chemistry), S. Bucak (Istanbul), I. Hamley (Reading) and V. Castelletto (Reading).)

DNA-lipid complexes (Contact person: Ulf Olsson)

Systems containing DNA, cationic cosolutes and phospholipids have a broad biological and biotechnological significance. For example, in the cell nucleus of eukaryotic cells, there is an intricate interplay between DNA, cationic proteins and lipids self-assembling into complex structures. This self-organisation is still far from being understood and in particular concerning the role of the lipids present. Important transfection agents are based on a mixture of cationic amphiphiles (surfactants of lipids) and neutral zwitterionic lipids. Understanding the interaction between the zwitterionic lipids and DNA would give a better basis for designing lipoplex formulations for transfections. In view of this significance we investigate the aqueous phase behavior of the "complex salt" DNA-amphiphilic cation (e.g. dodecyl trimethyl ammoinium (DTA)) when mixed with various lipids. The ternary DNA-DTA/water/lecithin system shows a rich phase diagram with several liquid crystalline phases. Of particular interest is the first observation of a DNA containing bicontinuous cubic phase. (Björn Lindman, Ulf Olsson and A. Bilalov (Kazan State Technological University).)

Molecular matter for specific functions

Hydrophobically modified polymers in pharmaceutical tablet formulations (Contact person: Lennart Piculell)

Hydrophobically modified polymers are water-soluble polymers that contain a small proportion of strongly hydrophobic functionalities attached to the polymer backbone. Such polymers are not traditionally used as excipients in pharmaceutical drug tablets. In this project, we study how the hydrophobic modification as such, and the possible presence of other amphiphilic molecules such as surfactants, affect the drug release properties of tablets made from hydrophobically modified poly(acrylic acid). Importantly, the added amphiphilic molecules affect the water solubility of the hydrophobically modified polymer, which in turn affects the tablet erosion and the drug release. Detailed time-resolved information on the tablet dissolution is obtained from NMR Chemical Chift Imaging. (Patrik Knöös, Lennart Piculell, Marie Wahlgren (Food Technology) Stefan Ulvenlund and Daniel Topgaard.)

Phase separation, adsorption behavior and delivery capacity of polyelectrolytes and oppositely charged surfactants at surfaces (Contact person: Lennart Piculell)

An enhanced surface adsorption is typically obtained from dilute mixtures of a polyelectrolyte and an oppositely charged surfactant under conditions when there is a bulk associative phase separation in the mixture. This phenomenon is used in everyday products (e.g., shampoos, laundry detergents) that are specifically designed to produce deposited surface layers. Often the phase-separation and enhanced deposition can be obtained by a simple dilution process. The same process can also be used to deliver some additional substance to the surface together with the polyion-surfactant ion complexes. The aim of the present project is to investigate the deposition of polyion-surfactant ion complexes, and the co-deposition of added particles, from such complex formulations onto different model surfaces, and to link the deposition behavior with the characteristics of the phase separation in the bulk solution. As an example, the co-deposition of emulgated silicone oil droplets onto hydrophilic and hydrophobic surfaces has been studied for formulations containing anionic surfactant and cationic polymers of varying hydrophobicity. A combination of techniques is used: in-situ ellipsometry, QCM and neutron reflectometry to investigate the adsorption behavior, phase studies and turbidity measurements to look into the bulk properties and dynamic light scattering to determine the size of soluble/dispersed aggregates. (Asger B. Petersen, Maryline Clauzel, Tommy Nylander, Lennart Piculell, E. Johnson, R. Panandiker and M. Sivik (Procter & Gamble, Cincinnati).)

Associative effects of polyacrylates in surfactant systems (Contact person: Björn Lindman)

Effects of surfactants on the rheology of water-soluble polymers are investigated as a function of charge density, cross-linking and hydrophobicity. The delicate balance between restoring hydrophobic interactions and osmotic swelling can be critically controlled by small concentrations of surfactants, which can change the viscosity by several orders of magnitude. (Björn Lindman, Filipe Antunes (Coimbra University), Hans-Martin Haake and Björn Klotz (Cognis/BASF, Düsseldorf).)

Preparation of Calcium Alginate Nanoparticles Using Water-in-Oil (W/O) Nanoemulsions (Contact person: Ulf Olsson)

In this project, a procedure for the preparation of calcium alginate nanoparticles in the aqueous phase of water-in-oil (W/O) nanoemulsions is developed. Emulsions are produced from mixtures of nonionic surfactant, alkane, and aqueous solutions of up to 2wt % sodium alginate by means of the phase inversion temperature (PIT) emulsification method. This method allows the preparation of finely dispersed emulsions without a large input of mechanical energy. With alginate concentrations of 1-2 wt % in the aqueous phase, emulsions showed good stability against Ostwald ripening and narrow, unimodal distributions of droplets with radii <100 nm. Gelation of the alginate is induced by the addition of aqueous $CaCl_2$ to the emulsions under stirring and particles formed are collected using a simple procedure based on extraction of the surfactant on addition of excess oil. The final particles are characterized using cryo-transmission electron microscopy (cryo-TEM) and dynamic light scattering (DLS). They were found to be essentially spherical with a homogeneous interior and their size was similar to that of the initial emulsion droplets. The herein presented "low-energy" method for preparation of biocompatible nanoparticles has the potential to be used in various applications, e.g. for the encapsulation of sensitive biomacromolecules. (Alexandra H. E. Machado, Dan Lundberg, António J. Ribeiro (Coimbra University), Francisco J. Veiga (Coimbra University), Björn Lindman, Maria G. Miguel (Coimbra University) and Ulf Olsson.)

Cleaning technology in high temperature food processing - from fundamental understanding to sustainable and safe food processing (Contact person: Tommy Nylander)

Food products are heat treated in order to assure the food safety and to increase the shelf life of the product. An unwanted consequence of the thermal treatment is the formation of a deposit, fouling, onto exposed surface of the processing equipment. The challenge is to remove these deposits within minimal time and without using excessive amount of energy, water and chemicals. The key question that this work aims to answer is which mechanisms dominate and limit the efficiency during cleaning of deposits in process equipment for dairy or dairy based products. Focus will be to answer the question in relation to different: process parameters, detergent properties and deposit compositions and structures. The final vision is to establish a classification map that enables tailor made and optimized cleaning routines based on deposit composition, deposit structure, detergents and cleaning mechanisms. This scientific PhD project, granted within the Cross-disciplinary food research Programme by FORMAS and VINNOVA, will be followed by applied projects at Tetra Pak Processing Systems where the results will be verified in full scale for further implementation into new processing solutions. (Tommy Nylander, Fredrik Innings (Tetrapak AB), Christian Trägårdh and Marie Paulsson (Food Technology) and Niklas Lorén (SIK AB, The Swedish Institute for Food and Biotechnology Structure and Material Design).)

Understanding the dissociation of pharmaceutical salts (Contact person: Daniel Topgaard)

Active pharmaceutical ingredients (API) are active chemicals used in the manufacture of drugs. APIs poor solubility in water leads to many problems in the pharmaceutical industry, one of the biggest being the poor uptake in vivo. Many of the APIs that are manufactured today are formulated as salts with a suitable counter-ion instead of in its free form. Such salts are often found to have a higher transient solubility in biologically relevant fluids, with enhanced uptake in the body. The problem is that these API salts are very sensitive to water, and at a certain water activity a given salt will dissociate to its free form. The central questions of the project are when and how the pharmaceutical salt dissociates in the presence of moisture, and how this process influences the physical and chemical stability of solid dosage forms. The dissociation is studied with newly developed solid-state nuclear magnetic resonance spectroscopy methods giving information on molecular mobility and phase behavior at the relevant moisture contents. (Sanna Gustavsson, Daniel Topgaard, Stefan Ulvenlund and Johan Reimer.)

PNIPAAM-modified SBA-15 (Contact person: Viveka Alfredsson)
In this project we incorporate a thermoresponsive polymer (PNIPAAM) into a mesoporous silica host (SBA-15) with the aim of forming a functional material where the uptake can be monitored via a temperature change. The polymer is synthesized by atom transfer radical polymerization inside the host and covalently linked to the silica framework. The composite material is characterized primarily by sorption techniques, N_2 and Ar sorption as well as water sorption calorimetry. (Nina V. Reichhardt, Tommy Nylander, Beate Klösgen (SDU, Denmark), Vitaly Kocherbitov (MaH, Malmö), Freddy Kleitz and Remy Guillet-Nicolas (Université Laval, Canada), Matthias Thommes (Quantachrome, USA) and Viveka Alfredsson.)

Porosity Control of a mesoporous silica material (Contact person: Viveka Alfredsson)
The well-known mesoporous silica SBA-15 has a complicated porous system consisting of both ordered primary mesopores and unordered intrawall pores of various sizes (but smaller that the primary mesopores). In this project we seek to control the porosity by fine-tuning the formation events and targeting particular formation steps while conserving other important material characteristics. The porosity is studied with N_2 sorption, water sorption calorimetry and high resolution Scanning Electron Microscopy. (Nina V. Reichhardt, Tomas Kjellman, Motolani Sakeye and Jan-Henrik Smått (Åbo Akademi, Finland), Mika Lindén (Ulm University, Germany), Vitaly Kocherbitov, MaH), Osamu Terasaki (KAIST, Republic of Korea) and Viveka Alfredsson.)

Formation of SBA-15 and deposition of mesoporous silica particles (Contact person: Viveka Alfredsson)
We investigate the principal molecular and colloidal interactions in the formation process of SBA-15. The particle size and/or morphology are controlled by fine-tuning the formation events of the particles. We aim to deposit well-defined particles of mesoporous silica with a preferential orientation on a substrate. Initially a stable colloidal dispersion of the mesoporous silica particles should be obtained by influencing the colloidal stability of the particles. The particle dispersion will be used for deposition on a number of modified surfaces. Valuable techniques are Scanning Electron Microscopy, Elipsometry and Spin/dipcoating. This project is part of the SSF financed project "Porous surface layers through polymer-assisted deposition". (Tomas Kjellman, Håkan Wennerström, Karen Edler (University of Bath, UK) and Viveka Alfredsson (and other members of the SSF group).

Formation of mesoporous silica by structure-directing with cationic surfactants (Contact person: Viveka Alfredsson)
We have initiated a project aimed at systematically investigating the formation of mesoporous silica using the basic synthesis methodology with cationic surfactants (e.g. CTACl) as structure directors. We will investigate the means to control the structure by systematic alteration of the packing parameter of the surfactant complexes. (Emelie Nilsson, Sven Lidin (CAS, LU), Olle Söderman, Karen Edler (University of Bath, UK) and Viveka Alfredsson.)

Formation of mesoporous silica by the CSDA-approach (Contact person: Viveka Alfredsson)
We are investigating the structural response of the final silica material as a consequence of altering the phase characteristics of the structure directing surfactant by different means. The silica material is formed via the co-structure directing agent (CSDA) method described by Che et al. This method has proven to be particularly versatile for obtaining a large variety of mesostructured silica materials. (Ruiyu Lin, Shunai Che (Shanghai Jiaotong University, China) and Viveka Alfredsson.)

Model membranes on nanostructured sensing supports (Contact person: Tommy Nylander)
This project aims to study the mechanism of formation and structure of complex lipid bilayers, a lipid composition that mimics biological membranes (i.e composed of several lipid types) on a variety of substrates including structured surfaces consisting of nanowire forests. This will allow membranes with tailored properties to be developed for applications in key membrane processes, such as antimicrobial peptide activity, protein interactions, and DNA transfection. We will investigate the use of nano-wire “forests” developed by Lars Samuelson’s group at Solid State Physics, Lund University as a support for free standing lipid bilayers and means to sense membrane mechanical properties, such as lateral stress, as well as biomolecular interactions and activity with and in the membrane. Financed by OMM and nmC@Lund. (Tommy Nylander, Aleksandra Dabkowska, Emma Sparr, Heiner Linke and Christelle Prinz (Solid State Physics) and Hanna Wacklin (ESS AB).)

Controlled deposition of lipid liquid crystalline nanoparticles to obtain biofunctional surfaces (Contact person: Tommy Nylander)
Investigation of non-lamellar nanoparticles formed by dispersion of self-assembled lipid liquid crystalline phases is stimulated by their many potential applications in science and technology; resulting from their unique solubilizing, encapsulating and space-dividing nature. Our aim is to control the interfacial behavior of lipid liquid crystalline nanoparticles (LCNPs) at surfaces to facilitate the exploitation of such systems for a number of potentially interesting uses, including preparation of functional surface coatings and uses as carriers of biologically active substances. We have shown that LCNPs can form well-defined layers at the solid-liquid interface with a structure and coverage that is determined by the interplay between self-assembly properties of the lipids and lipid surface interactions, respectively. Financed by Swedish Foundation for Strategic Research. (Tommy Nylander, Debby Chang, Fredrik Tiberg (Camurus AB) and Justas Barauskas (Vilnius University).)

Low interfacial tension microemulsions for practical applications (Contact person: Ulf Olsson)

The high solubilization capacity and the ultra low interfacial tension exhibited by microemulsions make them desirable for a broad range of applications including enhanced oil recovery, soil and aquifer remediation, consumer and pharmaceutical formulation, chemical reaction media and nanoparticle preparations. In this project we investigate various microemulsion formulations, targeted for practical applications, combining phase diagram and interfacial tension studies. Systems studied include ionic surfactant in combination with oppositely charged hydrotropes with the aim to optimize the overall surfactant efficiency. (Ulf Olsson, I. Kayali and K. Qamhieh (Al-QudsUniversity, Jerusalem), L. Bemhert and R. Strey (University of Köln).)

SCIENTIFIC INSTRUMENTATION

Surface techniques

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 Ψ and Δ, 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).

A spectroscopic ellipsometer, Horiba UVISEL-ER-AGAS Spectroscopic Ex-Situ Ellipsometer for the FUV-VIS-NIR Range with Automatic Goniometer and Motorised Mapping Stage that allow determination of the thin film properties within the spectral range from 190-2100 nm was purchased in 2010. The spectroscopic ellipsometer incorporates phase modulation technology to characterize polarization changes at high frequency (50 kHz), and without any mechanical movement. The Uvisel is equipped with a Multi Channel System for Parallel Spectra Acquisition for kinetic studies of thin films within the spectral range from 190 to 810 nm. The instrument is equiped with measuring cells for measurements at the solid-liquid and air-liquid interface under controlled conditions. (Sponsored by The Knut and Alice Wallenberg Foundation.)

Quartz crystal microbalance with dissipation monitoring (QCM-D) (Contact person: Tommy Nylander)

The instrument is from Q-Sense fitted with E4 and E1 module and is able to collect, both the dissipation and the resonance frequency of a quartz crystal. These data can be used to follow the formation of thin films (nm) such as proteins, polymers and cells onto surfaces, in liquid by using a flow system at controlled temperature. The advantage with measurements at several frequencies and the dissipation is that we can determine the adsorbed film is rigid or water-rich (soft). The instrument is equipped with a Q-Sense Ellipsometry Module (for the Q-Sense E1 system), which enables simultaneous QCM-D and ellipsometric measurements on the same substrate. Thus we can determine both the adsorbed amount and the water content in adsorbed layer.

(Sponsored by The Knut and Alice Wallenberg Foundation.)

Scanning probe microscope (Contact person: Emma Sparr)

A XE-100 AFM system from ST Instruments (Park systems) was purchased in 2011. The instrument can be operated to image topography and friction on small and medium size samples both in air and in liquid. The instrument consists of completely decoupled XY & Z scanners by using flexure guided scan system for all three axes, closed/open-loop scan, XY flexure scanner with zero background curvature, motorized

Z stage, motorized focus stage, precision motorized XY sample stage and direct on-axis optics. The system also include high resolution digital CCD camera with digital zoom. (Sponsored by The Knut and Alice Wallenberg Foundation.)

Surface force apparatus (SFA) (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.)

Surface film balance (Contact persons: Tommy Nylander and Emma Sparr)
Three different equipments optimized for different purposes: 1) 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. 2) 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. 3) A 20 ml Langmuir micro-trough from Kibron. The equipment include surface pressure sensor, a window in the bottom of the trough for microscopy, a temperature control plate, and a multiwall plate for surface pressure measurements. (Sponsored by Crafoord Foundation and Per-Eric and Ulla Schyberg's foundation.)

Surface tension (Contact person: Tommy Nylander)
The Drop and Bubble Shape Tensiometer PAT-1 from SINTERFACE, Germany, allows measuring quite a number of interfacial properties. In addition to the properties of a standard drop and bubble instruments it allows, surface and interfacial tension of liquids, static and dynamic contact angle according to the sessile drop method, surface rheological studies to measure the dilational elasticity and viscosity, fast oscillations with extra module ODBA-1, 0.1 s resolution over a period of seconds up to days and an injection system that allows adding another solution to an already formed drop. (Sponsored by The Knut and Alice Wallenberg Foundation.)

Scattering techniques

Dynamic and static light scattering (DLS and SLS) goniometer system (Contact person: Karin Schillén)
The laser light scattering goniometer system from the ALV Gmbh, Langen, Germany, is a measuring system for simultaneous angular dependent determination of DLS and SLS. The CGF-8F compact based system includes CW Helium-Neon (He-Ne) gas laser (632.8 nm with a output of 22 mW), laser beam focusing optics including a laser beam attenuator and a Glan laser polarizer prism, a goniometer with a rotary table with the angular range of about 20° to 150°, a cell housing with an cylindrical quartz vat (filled with a refractive-index matching liquid, toluene), a fiber optical near-

monomodal detection system (with a possible depolarized light detection), a detection unit comprises of two matched avalanche photodiodes that is put in a pseudo-cross correlation arrangement. For the DLS measurements using photon correlation spectroscopy, the latest ALV-7004 multiple tau digital correlator is utilized to produce the time pseudo-cross correlation function of the scattered intensity. It has an initial real sampling time of 25 ns and a lag time range that extends from 25 ns to up to 54975.6 s, which makes it possible to detect particle sizes from 1 nm up to about 5000 nm. The temperature range of the vat is –12 °C to +140 °C (if the refractive index matched liquid changed) and is controlled to ± 0.01 °C by a F32 Julabo heating circulator. In addition, also included in the overall set-up, is a differential refractometer with one He-Ne laser from ALV for the determination of refractive index increments necessary for the SLS experiments.

(Sponsored by the former Swedish Natural Science Research Council, NFR, and by Knut and Alice Wallenbergs Stiftelse, KAW.)

Instrument for dynamic and static light scattering and electrophoretic mobility measurements (Contact person: Karin Schillén)

For convenient DLS and SLS measurements along with determination of electrophoretic mobility (or zetapotential) in both aqueous and non-aqueous dispersions, a Zetasizer Nano ZS from Malvern Instruments Ltd, Worshestershire, UK, is available. The instrument measures DLS and SLS at a set angle of 173° using the NIBS technology. The accessible particle-diameter range is 0.3 nm – 10 µm in concentrations up to 40 % (w/v) depending on sample and the molecular weight range is $980–2\cdot10^7$ g/mol. The zetapotential measurements in the conductivity range of 0-200 mS/cm are performed at 17 ° using M3-PALS technology (particle diameters from 3.8 nm to 100 µm). The instrument is equipped with a 4 mW He-Ne laser (wavelength of 632.8 nm) with an automatic laser attenuator that allows for measurements at sample transmissions ranging from 100 % to 0.0003 %. The detection unit comprises an avalanche photodiode. The temperature range of the instrument is 2–90 °C. (Sponsored by The Crafoord Foundation.)

Multi-angle static light scattering desktop instrument (Contact person: Karin Schillén)

For characterization of molecular weight and studies of conformation changes or association processes in macromolecular systems, a multi-angle laser light scattering 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 (632.8 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 aqueous solvents but batch analysis may also be performed.

(Sponsored by NFR.)

3D Light scattering instrument (Contact person: Peter Schurtenberger)

The instrument from LS Instruments is used for simultaneous dynamic and static light scattering with transparent and turbid samples. It is equipped with a HeNe laser light source, wavelength λ_0= 632.8nm and a maximum power of 35 mW. The sample is filled into cylindrical glass cells of a diameter of 3, 5 or 10 mm or 10 mm square cells and placed in the temperature controlled index-matching bath. The scattered light is detected within an angular range of 15 to 140° by two efficient Avalanche Photo Diodes and processed by a Flex correlator in a 3D cross-correlation configuration. In aqueous samples we have access to scattering vectors $0.0034 \leq q \leq 0.025$nm-1.The apparatus is equipped with a sample goniometer to characterize non-ergodic samples.

Multi-angle 3D-goniometer system (Contact person: Peter Schurtenberger)
The instrument allows time-resolved measurements of dynamic and static light scattering in transparent and turbid samples using the technique of 3D cross-correlation at four angles simultaneously. The apparatus is equipped with a diode-pumped solid-state laser (wavelength $\lambda_0 = 532$ nm) with a maximum power of 200 mW. The sample is filled into cylindrical glass cells of a diameter of 3, 5 or 10 mm or square cells with diameter 10 mm and placed in the temperature controlled index-matching bath. The scattered light is detected within an angular range of 10 to 150° by two photomultiplier tubes at each angle and processed by a Flex correlator in a 3D cross-correlation configuration. Thus four intensity correlation functions are obtained simultaneously, one for each scattering angle measured. In aqueous samples we have access to scattering vectors $0.0027 \leq q \leq 0.031$ nm-1.

Ultra small angle light scattering (USALS) (Contact person: Peter Schurtenberger)
The instrument is used for simultaneous dynamic and static light scattering at ultrasmall angles using a CCD camera. The scattered light is detected from 0.3° to 6°, corresponding to length scales from a few hundred nanometers to a fraction of a millimetre. Time resolved static measurements with a time resolution of approx. 100 msec. Multispeckle correlation functions are processed in real-time, thereby allowing measurements of a set of intensity autocorrelation functions at different q-values using measurement times that are comparable to the longest correlation time. A multitau correlation scheme is adopted (delay time space quasi-lograrithmically), requiring thereby less data storage and processing time. This allows one to calculate time- and pixel-averaged correlation functions in real time. Multiple exposure times are used in order to optimize the mean intensity level for all scattering vectors. The instrument is equipped with a HeNe laser light source with a wavelength of 632.8nm and a maximum power of 35 mW. The sample is filled into squared glass cells with path lengths ranging from 10 µm to 1 mm and placed in a temperature-controlled sample environment. The instrument is designed to study both ergodic and non-ergodic samples.

Diffusive wave spectrometer (DWS) (Contact person: Peter Schurtenberger)
The instrument is used for characterization of extremely turbid samples and is equipped with diode-pumped solid-state laser (wavelength of 660 nm) with a maximum power of 70 mW. The apparatus is implemented with a “Two-Cell Echo Technique” which allows reducing measurement times down to only a few minutes even for slowly relaxing and solid-like materials. The sample is filled into squared glass cells of 1 – 10 mm and placed in a temperature controlled sample environment (15-70 °C). The scattered light is detected with two efficient Avalanche Photo Diodes in transmission and processed by a multi-tau/linear correlator using pseudo-crosscorrelation as well as echo measurements. Also possible are experiments using backscattering geometry as well as CCD camera-based multispeckle measurements. The equipment runs with a powerful software solution (LS-Instruments, Fribourg, Switzerland) for data acquisition

and analysis (combined correlation-echo measurements, single-, multi-speckle analysis, user defined multi-run scripts, online microrheology analysis and full data access).

Electrophoretic light scattering (Contact person: Peter Schurtenberger)
A Zetasizer Nano Z instrument from Malvern Instruments Ltd, Worshestershire, UK, is available for eletrophoretic mobility (or zetapotential) measurements in both aqueous and non-aqueous dispersions using M3-PALS technology. The required particle diameter ranges from 3.8 nm to 10 µm with concentrations up to 40 % (w/v) depending on sample. A conductivity range from 0 to 200 mS cm^{-1} is required. The instrument is equipped with a 4 mW He-Ne laser (wavelength of 632.8 nm) with an automatic laser attenuator that allows for measurements at sample transmissions ranging from 100 % to 0.0003 %. The detection unit comprises an avalanche photodiode. The temperature range of the instrument is 2-90 °C.

Small/wide angle X-ray spectrometer (SAXS and WAXS) (Contact person: Peter Schurtenberger)
This instrument combines a X-ray focusing optics with a block collimator which produces an intense, monochromatic primary beam. The primary beam is focused through the sample allowing fast measurements of the scattering pattern, even from samples with low contrast. The scattering signal is detected by a CCD camera for SAXS and a 2D imaging plate detection system for WAXS. The apparatus is implemented with a SAXSess camera using a X-ray generator (PANalytical, PW 3830) with a sealed copper tube. The X-ray generator offers a maximum power of 4.0 kW and an operating range of 20-60 kV and 10-100 mA. A Göbel mirror and a Kratky block collimation system (line-shaped beam) is used to convert the divergent polychromatic X-ray beam into a focused line shaped beam of Cu-Kα radiation. Holders for liquid and solids are available. The instrument design makes it possible to investigate particles length scales from 0.25 nm (thanks to the wide angle extension system) up to 40 nm. Thus, q values range from ≤ 0.077 nm^{-1} (corresponding to a Bragg value ≥ 82 nm) up to ≈ 8 nm^{-1} (SAXS) and ≈ 29 nm^{-1} (SWAXS).

Nuclear magnetic resonance (NMR)

(Contact person: Daniel Topgaard)

Bruker Avance II spectrometers operating at 200 and 500 MHz are available at Physical Chemistry. Both spectrometers are equipped for high-performance diffusion studies. The 500 MHz has accessories for microimaging, solid-state, and high-resolution magic-angle spinning experiments. The instruments are equipped as follows:

Bruker Avance II 500

Magnet: 11.7 T / 500 MHz, 54 mm UltraShield

Probes: TXI 5mm XYZ-Gradient (1H/13C/15N), BBO 5mm XYZ-Gradient (31P-15N/1H), multinuclear DIF-30 and MIC-5 (1H, 2H/1H, 7Li/1H, 23Na/1H, 13C/1H, 31P/1H), H/X CP-MAS 4mm (1H/31P-15N), H/X CP-MAS 2.5mm (1H/31P-15N), TXI HR-MAS 4mm Z-Gradient (1H/13C/31P)

Bruker Avance II 200

Magnet: 4.7 T / 200 MHz, 89 mm

Probes: BBO 10mm (31P-15N/1H), DIF-25 5mm (1H)
(Sponsored by VR/KFI.)

Microscopy

Optical microscopy (Contact person: Emma Sparr)
The division has a Zeiss Axioplan Universal microscope equipped with differential interference contrast and a High Resolution Microscopy Camera AxioCam MRm Rev. 3 FireWire, Illuminator HBO 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, AxioVision 4 together with the Macintosh-based image analysis software.

(Sponsored by FRN and Crafoord Foundation.)

Confocal microscopy (Contact person: Peter Schurtenberger)
This instrument allows recording brilliant, high-resolution images to illustrate morphological features of fixed or slowly moving samples as well as monitoring high-speed dynamic processes by fast time-course studies. The equipment is implemented with five true spectral confocal channels simultaneously with a prism spectrometer for high transmittance and tunability. Illumination regimes are switchable in microseconds for fast dynamic measurement and the beam can be split instantly for new dyes or laser lines. The apparatus mounts up to 2 channels for spectral FLIM allowing resolved fluorescence life-time imaging and 3 laser lines: a HeNe laser (543 and 633 nm), an Argon laser (458, 476, 488 and 514 nm) and an IR (800 to 1100 nm). A fast resonant scanner (50 frames/sec at 512 x 256 pixels) and a non-resonant scanner (1400 lines/sec) are also implemented. The objective is mounted on a piezo-stage for fast z-scanning (50 frames/sec at 256 x 128 pixels). (Sponsored by The Knut and Alice Wallenberg Foundation.)

Transmission electron microscopy with cryo facilities (Contact person: Viveka Alfredsson)
The national Centre for High Resolution Electron Microscopy (nCHREM) at the Department of Chemistry has two transmission electron microscopes. The Philips CM120 BioTWIN Cryo is a microscope dedicated for cryo-imaging. It is operated at 120 kV. The BioTWIN objective lens gives high contrast and the resolution is 0,34 nm. The microscope is equipped with an energy filter imaging system (Gatan GIF 100) and digital multiscan CCD cameras (Gatan 791). There is an Oxford CT 3500 Cryoholder and transfer system. The JEOL3000F is an analytical high-resolution transmission electron microscope with a field-emission electron source and an operating accelerating voltage of 300kV. The microscope is equipped with video-rate camera, and a 2 x 2 k CCD camera for HR image recording. The structural resolution is 0.17 nm in conventional mode, and 0.13 nm in STEM mode with high-angle annular detector. The microscope has an Oxford XEDS system and a Gatan Imaging Filter (2 x 2 k) for analysis of chemical composition with a spatial precision below 1 nm. Specialised holders for specimen transfer at liquid nitrogen temperature, insitu heating, scanning tunneling microscopy with simultaneous TEM viewing etc are available. The microscope can be remote-controlled via Internet via a portable knobset. More information about nCHREM can be found at http://www.materialkemi.lth.se/nchrem/index.html. (Sponsored by NFR, Crafoord Foundation and Knut and Alice Wallenberg foundation.)

Calorimetry

Differential scanning calorimeter (DSC) (Contact person: Emma Sparr)

A VP-ITC Differential Scanning Microcalorimeter with a Pressure Perturbation Calorimetry accessory from MicroCal (GE Healthcare) was purchased in 2010. This is a sensitive microcalorimeter for samples in solution. The instrument has an active cell volume of ca 0.5 ml, and it operates for temperatures between –10ºC to +130ºC. The cells consists of non-reactive Tantalum 61™ for excellent chemical resistance, and they are fixed-in-place for reproducible ultrasensitive performance with low maintenance. The systems uses a Peltier element for precise temperature control. It allows for user selectable temperature scan rates (0ºC to 90ºC per hour upscans), enabling for studies of fast or slow transition processes. (Sponsored by The Knut and Alice Wallenberg Foundation.)

Isothermal titration calorimeters (ITC) (Contact persons: Emma Sparr and Gerd Olofsson)

* A VP-ITC Isothermal Titration Microcalorimeter from MicroCal (GE Healthcare) was purchased in 2010.This is an ultrasensitive microcalorimeter for samples in solution. The instrument has an active cell volume of ca 1.4 ml, and it operates for temperatures between 2ºC to 80ºC. The cells consists of non-reactive Hastelloy® for excellent chemical resistance, and they are fixed-in-place for reproducible ultrasensitive performance with low maintenance. The system includes precision liquid delivery system for accurate and reproducible injections and user-selectable mixing speeds to match sample conditions. (Sponsored by The Knut and Alice Wallenberg Foundation.)

* Isothermal titration microcalorimeter 2277 TAM Thermal Activity Monitor System.

Reaction calorimeter (Contact person: Ola Karlsson)

The energy released as heat by a process is directly proportional to the rate of reaction and by monitoring the reaction in a calorimeter detailed kinetics can be revealed.

In 2011 we got a Chemical Process Analyser CPA202 from Chemisens. It is a high precision factory pre-calibrated calorimeter made in Hastelloy C276 with a useful volume of 10 – 180 ml, which can be continuously varied during experiments. The temperature range for experiments is -50 °C to + 200 °C and it is possible to operate in a pressure range from vacuum up to 20 bars. The temperature resolution for an experiment is 0.001 °C and the power resolution is 0.001 Watt in the standard reactor and in the so called HighSens Reactor, which can be used for e.g. adsorption kinetics, crystallization, dissolution of tablets and micellization it is possible to perform studies with a power resolution of 0.1mW at a volume of 10 -180 ml. (Sponsored by The Knut and Alice Wallenberg Foundation.)

Sorption calorimeter (Contact person: Gerd Olofsson)

A double twin isothermal microcalorimeter for the simultaneous determination of sorption isotherms and differential sorption enthalpies of vapors on solids. The instrument is developed in-house by L Wadsö and N Markova.

Rheology

Rheometers (Contact person: Ulf Olsson)

A Physica UDS 200 stress controlled rheometer. Various cone and plate geometries with Peltier temperature control. A Couette geometry and a double gap measuring device, both in stainless steel, temperature controlled by circulated thermostated water.

An Anton Paar MCR301 stress controlled rheometer equipped with additional transparent tools (plate-plate and cone and plate geometries) to allow for simultaneous small angle light scattering or microscopy detection.

Advanced rheometric expansion system (ARES) (Contact person: Peter Schurtenberger)

The Advanced Rheometric Expansion System (ARES) is a true strain-controlled instrument, where the application of strain and the measurement of stress are separated. The sample is subjected to either a dynamic (sinusoidal) or steady shear strain deformation, and then the resultant torque expended by the sample in response to this shear strain is measured. The motor applies shear strain; the transducer measures torque. Strain amplitude and frequency are set by the operator, with the actual sample deformation determined by the measured motor, and transducer, displacement. The instrument is implemented with the transducer 1 K FRT (torque range 0.004 – 20.0 g•cm and normal force range 2.0 – 2000.0 gmf). The operational temperature range is between -30°C and 150°C with temperature stability at thermal equilibrium of ±0.1 °C, which is controlled with a Peltier system. The actual available geometries are: cone and plate (50 mm, 0.04 rad, 25 mm, 0.04 rad), plate and plate in (50 mm) and couette (16.5 mm bob, 17 mm cup and 32 mm bob and 34 mm cup).

Spectrophotometers

UV-Vis spectrophotometer (Contact person: Maria Södergren)

A Cary 300 Bio UV-Vis spectrophotometer with 4-position automatic cell holder with temperature sensor, stirrer and connected water bath was purchased in 2007.

Fluorescence spectrophotometer (Contact person: Emma Sparr)

A Cary Eclipse Fluorescence spectrophotometer for fluorescence, phosphorescence or chemi/bio luminescence was purchased in 2007. The instrument includes both 4-position automatic cell holder with temperature sensor, stirrer and connected water bath as well as a microplate reader. Equipment also include the automated polarizer accessories. (Sponsored by the Crafoord foundation.)

COLLABORATIVE RESEARCH PROGRAMS

Organizing Molecular Matter

(Contact person: Lennart Piculell)

In 2005, the Swedish Research Council (VR) launched a call for proposals of collaborative research efforts from strong Swedish research environments with the prospect of long-term (10 years) "Linnaeus support". A group of nineteen senior researchers from the divisions of Physical Chemistry, Theoretical Chemistry and Biophysical Chemistry at the Department of Chemistry, Lund University, responded with a proposal called Organizing Molecular Matter (OMM). The program was accepted and was operational from June 2006, with a funding of 7.5 MSEK from VR and 1 MSEK from Lund University. The OMM research program, which can be found together with accounts of ongoing research at the OMM website (http://www.omm.lu.se), focuses on intermolecular interactions and their manifestations in a liquid environment. The interplay between theory and experiment is an essential feature of the program. The theoretical basis for the description of intermolecular interactions and their consequences are treated using quantum chemical calculations and statistical mechanical simulations. Carefully selected model systems are studied experimentally, and an important part of the experimental studies is an ongoing improvement of methods. A final part of the program is to apply the understanding obtained in the basic studies for solving applied problems both in the biophysical/molecular biology field and in the industrial area. By the end of 2010, a total of 23 new PhD and postdoctoral projects had been initiated within OMM, and each of these projects typically involves two or more OMM scientists. OMM also contributes substantially to the salaries of four young senior scientists. In addition, OMM organizes a series of weekly seminars, occasional workshops, and two annual meetings.

SSF–"Porous surface layers through polymer-assisted deposition"

(Contact person: Håkan Wennerström)

This project started in July 2009 and is a five-year research programme financed by the Swedish Foundation for Strategic Research (SSF). The goal of the program is to develop a method for a controlled deposition of mesoporous colloidal particles on surfaces and to apply the method on three types of porous particles. The basic strategy is to gradually destabilize an initially stable colloidal dispersion to achieve surface deposition rather than bulk aggregation. For this we use a potentially phase separating polymer to achieve colloidal stability/instability. The transition stability-instability should be smooth, which allows for an ordered equilibrium deposition layer. In one project we model theoretically the process to identify useful tuning parameters. In one experimental project flat mesoporous silica particles are deposited on a surface to give micrometer thick layers with pores of well defined size and orientation. Such layers can be used for separating small solutes from larger ones through a diffusional membrane transport. Another application is in tapes with a graded porous layer to be used as precise meters for relative humidity. In a third project we deposit porous liquid crystalline particles. Such particles can be loaded with an enzyme producing an enzymatically active surface coating. The fourth project aims at synthesizing soft mesoporous gel particles through in situ polymerization. In a surface layer of the particles the porosity can respond to changes in the properties of the bulk liquid such as pH or salt content. Porous responsive surface layers have a large potential in drug formulation. (L. Piculell, P. Linse, B. Lindman, V. Alfredsson, T. Nylander and H. Wennerström.)

SoftComp

(Contact person: Peter Schurtenberger)

Softcomp is a Network of Excellence (NoE) with the aim to establish a knowledge base for an intellegent design of functional and nanoscale soft matter composites. Since December 2009 it has a durable structure organized as a Consortium, which is self-financed by the partners. It supports research visits between partner institutions, and organizes and supports a number of schools, lab courses, workshops and conferences.

European Soft Matter Infrastructure (ESMI)

(Contact person: Peter Schurtenberger)

Free access to soft matter infrastructure, synthesis facilities, first-class instrumentation and a fast supercomputer is offered by the new EU project ESMI. ESMI consists of three main parts:

- TransNational Access - ESMI provides (free of charge, travel and accommodation included) access to the offered infrastructure (full range of synthesis facilities, a comprehensive set of specialized experimental techniques, fast supercomputer and theoretical support for data interpretation) to researchers or research teams. An Online Proposal Submission System will be available under the ESMI web portal. Experimental access will be coordinated through Physical Chemistry (Peter Schurtenberger)
- Networking: A dissemination and educational plan will be implemented to foster a culture of cooperation between research infrastructures and scientific communities
- Joint Research Activities - A number of research projects are funded to improve the existing infrastructure.

Biopolymers based surfactants - stabilization and functionalization of particles and surfaces

(Contact person: Björn Lindman)

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.

BIOCONTROL

(Contact person: Tommy Nylander)

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 biomimetic 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 program comprising (bio) physicists, biologists, (bio)chemists, surface chemists and computational biologists. (T. Nylander, V. Alfredsson) (http://biocontrol.tau.ac.il)

NordForsk Network

(Contact person: Tommy Nylander)

Nordic Milk Science Initiatives, 2008-2011 (NordicMilk Network). Research within dairy science has a long tradition in the Nordic and Baltic countries and the level of the research has been on high international standard. Recent research has revealed in cow's milk many protective components and their derivatives displaying a range of bioactivities. The research has been focused on product and process development directly related to the traditional use of the milk raw material. This also involves health and nutritional aspects as well as linking the genetic variants of the milk components to the product quality. This project joins multidisciplinary research groups from five Nordic countries and two Baltic countries who are working on milk compounds related to health and technological aspects. This project will join high know-how in chemical, analytical, technological, structural, in vitro studies and human clinical studies related to milk compounds. https://portal.mtt.fi/portal/page/portal/www_en/Projects/Nordicmilk.

Division of Surface Chemistry of the Swedish Chemical Society

(Contact person: Lennart Piculell)

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. From 2011, the scope of the division was widened to include also materials chemistry. The main activity of the Division is to organize an annual conference. The theme of the Symposium in 2011, held in Lund, was "Soft and Hard Materials", with contributions addressing topics such as biomineralization, nanocellulose films, nanoparticles, biomedical applications and new functional devices. Karin Schillén and Ulf Olsson took part in the program committee, while Jenny Algotsson, Celen Cenker, Charlotte Gustavsson, Sanna Gustavsson, Tomas Kjellman, Marianna Yanez and Lennart Piculell were on the local organizing committee. Peter Schurtenberger, Mehran Asad Ayoubi and Lennart Piculell gave oral presentations at the symposium.

Strategic Research Areas at Lund University

nmC@LU is a interdisciplinary research environment in nanoscience. One focus of the multi-disciplinary Nanometer Structure Consortium at Lund University (http://nano.lth.se) is on materials science and synthesis. Viveka Alfredsson, Tommy Nylander, Ulf Olsson are associated with this program. Multipark is a i translational program that ranges from pre-clinical research to studies on the life situation of patients with Parkinson's disease (www.med.lu.se/multipark). Emma Sparr is associated partner in this program, participating in subproject dealing with biophysical studies of protein-membrane interactions.

CONFERENCES, TRAVELS AND SEMINARS

Björn Lindman gave plenary lectures at the *International Conference in Advanced Materials and Nanotechnology (ICAMN-2011)* in Kathmandu, Nepal; at *Zellcheming: Cellulose Symposium 2011* in Wiesbaden, Germany; at the *EPNOE 2011 Polysaccharide conference* in Wageningen, the Netherlands. He gave keynote and invited lectures at the *STEP meeting on Shaping polysaccharides* in Maribor, Slovenia; at *The 4th Asian Conference on Colloid and Interface Science (ACCIS 2011)* in Tainan, Taiwan; at the workshop on *Phase Transformations and Novel Materials* in Obergurgl, Austria; at the *symposium celebrating 90 years of the Physical Chemistry Department* at Åbo Akademi in Åbo, Finland; at the *AkzoNobel Nordic Prize Symposium* in Stenungsund, Sweden and at *The workshop on Mapping the detailed composition of Surface-Absorbed Protein Layers on Biomaterials and Nanoparticles*, in Dublin, Ireland. He also gave lectures at the *COST D36 – final meeting* in Fuengirola, Spain and at the *Joint Meeting of D43 Workgroups 2-6* in Madrid, Spain. He also attended the *24th Conference of the European Colloid and Interface Society (ECIS)* in Berlin, Germany and the *4th Iberian Meeting on Colloids & interfaces* in Porto, Portugal. During the year Björn Lindman visited a number of universities and other research centers and in most cases he presented a lecture. The institutions visited included: Nanyang Technological University, Singapore; Cognis/BASF Research Center, Düsseldorf, Germany; Alberto Culver research center, Chicago, Instituto de Química Avanzada de Catalunya CID-CSIC, Barcelona, Spain, University of Porto, Portugal; Kazan Technological University, Kazan, Tatarstan, Tatastan Academy of Science, Kazan, Henkel Research Center, Düsseldorf, Beiersdorf, Research Center, Hamburg; Akzo Nobel Surface Chemistry, Stenungsund, Sweden; Faculty of Pharmacy, University Complutense, Madrid, Spain, Norwegian Technical University, Trondheim, Åbo Akademi, Finland, Royal Institute of Technology, Stockholm, Max-Planck Institute, Potsdam, Uppsala University, AkzoNobel Research Center, Slough, UK, University of Barcelona, Spain, Dyrup Research Center, Copenhagen, MidSweden University, Sundsvall. Björn Lindman was visiting professor at the Department of Chemistry, Coimbra University, Portugal and at Nanyang Technological University, Singapore.

Peter Schurtenberger held an invited plenary lecture at the *SoftComp Annual Meeting* in Crete, Greece. He also held invited keynote lectures at *Nanotech 2011* in Boston, USA and at *Trends in Nanotechnology* in Teneriffa, Spain. He held invited lectures at the workshop on *European Spallation Source - Perspectives for the Development of Bio-, Medical- and Material Science in the Oresund Region* in Copenhagen, Denmark; at the *International Workshop on Modern Light Scattering Technologies* in Karlsruhe, Germany; at the ESS Neutron Instrument Design School in Lund, Sweden; at the *First Annual NBIA Meeting on ESS Science* at the Niels Bohr International Academy in Copenhagen, Denmark; at the *International Workshop on Modern Light Scattering Technologies* in Fribourg, Switzerland and at the *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden. Finally he held invited seminars at the following Universities and Industry Research Centers: Freiburg Institute of Advanced Science in Freiburg im Breisgau, Germany; at the University of Copenhagen in Copenhagen, Denmark; at the Hemlholtz Zentrum Berlin in Berlin, Germany; at the MPI for Colloid and Interface Research in Golm, Germany; at Novo Nordisk Park in Måløv, Denmark and at the University of Tübingen in Tübingen, Germany.

Håkan Wennerström held a seminar at Pufendorfinstitutet, Lund and gave a lecture at the symposium *Hydration of nanostructured and biological materials* in Malmö, Sweden.

Lennart Piculell gave an oral presentation at the *25th ECIS symposium* in Berlin, Germany and an invited lecture at the symposium *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden.

Per Linse gave an invited oral presentation at *BIT's 1st Annual World Congress of Microbes-2011* in Beijing, China.

Tommy Nylander gave an invited talk at *FYF Member days*, YKI, Institute for Surface Chemistry. He gave an invited talk at the *Rideal award symposium for Robert K. Thomas* organized by SCI's Colloid and Surface Chemistry Group and the RSC's Colloid and Interface Science Group. He gave one invited overview talk at a workshop for PhD students and researchers at the Center for Bioengineering and Biotechnology, China University of Petroleum in Beijing, China. He also gave an invited talk at *Italian-Swedish workshop on Nanoscience and Medical Technology* held at the Institute for Surface Chemistry Stockholm, Sweden. He presented a poster at *European Conference on Neutron Scattering* in Prague, Czech Republic, and gave an oral presentation at the international workshop *Geometry of Interfaces* in Primošten, Croatia. He also gave an invited talk at Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. Tommy Nylander co-organised *Neutrons in Biology and Biotechnology* in ILL-Grenoble, France.

Viveka Alfredsson gave invited talks at the *Frontiers of silica research* in Göteborg, Sweden and at the *2nd Korea-Sweden and International Workshop* at KAIST in Daejeon, Korea.

Karin Schillén gave a poster presentation at *XXV European Colloid and Interface Society Conference* in Berlin, Germany.

Emma Sparr participated in the delegation of *Young Scientists at World Economic Forum of the New Champions* in Dalian, China (by nomination by the Royal Swedish Society).

Anna Stradner gave invited keynote lectures at the *12th Trends in nanotechnology International Conference (TNT2011)* at the Canary Islands, Spain, and at the *NSTI Nanotech Conference, 2011* in Boston, USA. She gave an invited seminar at the University of Massachusetts, Amherst, Department of Chemistry in Massachusetts, USA and gave an oral presentation at *NordForsk Network of Dairy Structures – Health and Functionality Workshop* in Kaunas, Lithuania.

Daniel Topgaard gave an invited lecture at the *11th International Conference on Magnetic Resonance Microscopy*, Beijing, China and presented a poster at *Neutrons in Biology and Biotechnology 2011* in Grenoble, France. He also held a seminar at the *Update Workshop on LU ESS MaxIV partnership* in Lund, Sweden.

Malin Oskolkova Zackrisson was nominated as young researcher by the Science faculty to attend and present her research at *LMK idéforum 2011* in Björkliden, Sweden.

Per Linse, Jurij Rescic, Guphua Wu, Xiaojing Chen, and Antony Stace presented a poster at the *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden.

Marc Obiols Rabasa gave talkes at the *8th Nordic Workshop on Scattering from Soft Matter* in Kjeller, Norway and at the *25th Conference of the European Colloid and Interface Society* in Berlin, Germany. He also held a seminar at the Institute of Advanced Chemistry of Catalonia (IQAC-CSIC) in Barcelona, Spain.

Jérôme Crassous presented posters at the *Particles 2011 Meeting, Stimuli Responsive Particles and Particle Assemblies* in Berlin, Germany and gave a talk at *SoftComp Annual Meeting* in Crete, Greece.

Debby Chang gave an oral presentation at *Geometry of Interfaces conference* at Primosten, Croatia. She gave an invited talk at the division of Biomedical Laboratory Science and Technology at Malmö University, Sweden. She also presented posters at the scientific meeting *BILL2011-Bilayers* at the Institut Laue-Langevin in Grenoble, France and at the *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden.

Priti Mohanty gave an invited lecture at the *15th Swedish Neutron Scattering Society Meeting* in Gothenburg, Sweden. He also gave invited seminars at the Dept. of Physics and Phys. Oceanography Memorial University of Newfoundland, St. John's in Canada; at the Condensed matter division, Institute of Physics in Bhubaneswar, India and at the Department of Physics, University of Vienna in Vienna, Austria. He presented posters at the 8th *Liquid Matter Conference* in Vienna, Austria, at the *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden and at the *Swiss Soft Days VI* in Zürich, Switzerland.

Alexandra Machado gave an oral presentation at the *UK Colloids 2011: An International Colloid and Surface Science Symposium* in London, UK and presented a poster at the *AAPS Annual Meeting and exposition* in Washington, USA.

Celen Cenker gave a talk at the *8th Nordic Workshop on Scattering* in Kjeller, Norway.

Jenny Algotsson presented a poster at the symposium *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden.

Jonas Carlstedt gave an oral presentation at the *XXV European Colloid and Interface Society Conference* in Berlin, Germany.

John Janiak presented posters at *XXV European Colloid and Interface Society Conference* in Berlin, Germany and at the *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden.

Marianna Yanez presented a poster at the *5th European Conference on Neutron Scattering* in Prague in Czech Republic and at the S*oft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden.

Mehran Asad Ayoubi gave an invited oral presentation at *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden. He also gave an oral presentation at the *European Polymer Congress 2011* in Granada, Spain.

Johanna Bailey Jönsson, Lennart Piculell and Ola Karlsson presented a poster at the *IPCG Conference: Polymer Colloids* in Durham, New Hampshire, USA.

Patrik Knöös gave an oral presentation at the *European Student Conference* in Falkenberg, Sweden and presented a poster at the *Soft and hard materials. A Symposium on surface and materials chemistry* in Lund, Sweden.

Poster presentations were held at the *8th Liquid Matter Conference* in Wien, Austria by Joakim Stenhammar, Martin Trulsson, Håkan Wennerström, Per Linse and Gunnar Karlström.

Sebastian Björklund gave an oral presentation at the *Skin Trail Blazer Workshop* in Boston, Massachusetts, USA and a poster presentation at the *Gordon Research Conferences - Barrier Function of Mammalian Skin* in Waterville Valley, New Hampshire, USA.

Ilya Martchenko presented a poster at *Swiss Soft Days 6 & Annual Meeting* of the Swiss Group of Rheology at ETH Zürich in Zürich, Switzerland and gave a talk at the *8th Liquid Matter Conference* at the University of Vienna in Vienna, Austria. He also gave talks at events organized by Swedish Physical Society and University of Gothenburg and the University of Leoben in Leoben, Austria.

Divya Paloli gave a talk at the *SoftComp Annual meeting* in Crete, Greece.

EXTERNAL PROFESSIONAL ACTIVITIES

Björn Lindman was on the Advisory or Editorial Boards of Advances in Colloid and Interface Science, Current Opinion in Colloid & Interface Science, Fine Chemicals, Colloid&Polymer Science, The open Physical Chemistry Journal, and Journal of Dispersion Science and Technology. Björn Lindman is a member of The Royal Swedish Academy of Engineering Sciences, of The Royal Swedish Academy of Sciences, of the Academia das Ciências de Lisboa, the Portuguese Academy of Sciences and of The Royal Physiographic Society in Lund, and honorary corresponding member of Romaniae Scientiarium Societas. He is cofounder and honorary member of the European Colloid & Interface Society (ECIS). For the period 2006-2009 Björn Lindman was President of the International Association of Colloid and Interface Scientists (IACIS) and now acts as immediate-past-President. He was also evaluator of research and training networks and research programs for the European Commission as well as evaluator of research programs for Lundbeckfonden, Denmark. Björn Lindman was "first opponent" for the Ph D defence of Nils Opedal at the Norwegian Technical University, Trondheim.

Peter Schurtenberger was a member of the Swiss National Research Council, of the Liquids Board of the European Physical Society, of the Scientific Advisory Committee of the Swiss Light Source, of the ESS Science Board and the ESS Science Directorate, of the ESS SANS Scientific Advisory Panel. He was also a member of the Organizing Committee 11th European Summer School on "Scattering Methods Applied to Soft Condensed Matter", Bombannes, France and of the International Program Committee of the International Soft Matter Conference in Rome 2013. Peter Schurtenberger was Chairman of the Scientific Review Board of the European Soft Matter Infrastructure ESMI, coordinator of the Experimental Infrastructure and Member of the Program Executive Committee of ESMI and Chairman of the Review Panel of the Jülich Center for Neutron Scattering. He was also a member of the Network Governing Board and Chairman of the Experimental Platform of the European Network of Excellence SoftComp. He was on the Editorial Board of Colloid & Polymer Science, he was Section Editor on Current Opinion in Colloid and Interface Science and was om the Advisory Board (Kuratorium) on "Physik in unserer Zeit".

Lennart Piculell was section editor for the Polyelectrolytes section of "Current Opinion in Colloid and Interface Science", a member of the editorial board of "Soft Matter", and a member of the international organizing committee of the biannual "International Polyelectrolyte Symposia". He was a member of the board of the Department of Chemistry at Lund University 2006-2011, and the Chairman of the Division of Surface and Materials Chemistry of the Swedish Chemical Society. Lennart Piculell was also chairing the local organizing committee of the "Soft and Hard Materials" symposium, organized by Division of Surface Chemistry and Physical Chemistry, that took place in Lund in October. He was the director of the Linnaeus center OMM. He was the external examiner ("faculty opponent") at the PhD thesis defense of Martin Andersson, Uppsala, and a member of the examination committees at the PhD thesis defense of Anna Viridén, Chalmers, Göteborg and the licenciate thesis defense of Erdem Karabulut, KTH, Stockholm.

Tommy Nylander served as thesis examiner for the PhD theses of Josephine Corsi, University of Southampton, Southampton, UK, Alexander Shovsky, KTH, Royal Institute of Technology, Stockholm and Christian Rein, Copenhagen University, Copenhagen Denmark. He was a member of Formas (The Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning) standing evaluation committee for Products and processes based on renewable and recycled resources and the Swedish Research Council (VR) evaluation panel for Physical Chemistry, Biophysics and Theoretical Chemistry. He was member of the evaluation panel for beam time applications NIST Centre for Neutron Research, Gaithersburg, USA and ISIS, Rutherford Appleton Laboratory, Oxfordshire, UK. In addition he was evaluator of research proposals for BBSRC – Biotechnology and Biological Sciences Research Council, Australian Research Council and MIUR – Ministero dell'Istruzione, dell'Università e della Ricerca, Italy. Tommy Nylander was a member of the ESS Scientific Advisory Group.

Anna Stradner was a board member of the Swiss Neutron Scattering Society and a member of the Program Executive Committee of the European infrastructure project ESMI (European Soft Matter Infrastructure).

Ingemar Wadsö served as external examiner in professor appointment at University of Porto, Portugal and was a member of the Scientific Committee for XVII International Society of Biological Calorimetry and the Award Committee for the International Congress on Thermal Analysis and Calorimetry.

Emma Sparr was elected member in the Young Academy of Sweden. Emma Sparr was opponent for Raghu Sankar (SDU, Odense, Denmark)

Karin Schillén was a member of the board of the undergraduate studies in chemistry at the Department of Chemistry, LU.

Ola Karlsson was a member of the examination committee for Sofia Målbergs´ Ph.D. thesis, "Macromolecular Synthesis of Functional Degradable Aliphatic Polyesters and Porous Scaffold Design" at KTH, Stockholm, Sweden.

Olle Söderman served as a panel member in the Education Assessment Exercise (EAE). EAE was a project for evaluating the education carried out at the Royal Institute of Technology (KTH) in Stockholm.

Viveka Alfredsson was a member of two PhD students grading committees and participated in the Science Faculty election committee at Lund University. Viveka was a member of Council of the International Mesostructured Materials Association and a member of the department of Chemistrys´ (KILUs´) equality group. She was also a Deputy Member of the Board of KILU.

Ilya Martchenko was a juror at the 'International Young Physicists' Tournament, July 22-31, 2011 that received a dedicated support from Swedish Physical Society via Riktat stöd från Vetenskapsrådet project.

COURSES AND TEACHING

Members of the Division of Physical Chemistry are involved in a number of undergraduate courses and a number of our graduate students serve as teaching assistants on all courses given by the division. Karin Schillén is the head teacher in Physical Chemistry with the responsibility of organizing the teaching given by the members of the Division of Physical Chemistry.

The first year of chemistry studies at the Department of Chemistry consists of four 5-week chemistry courses (which are given both during the fall and the spring semesters), one 10-week course in mathematics and one 10-week course in physical chemistry. In the first basic chemistry course during the spring semester, Malin Zackrisson Oskolkova was involved in lectures and leading exercises and question hours, whereas Daniel Topgaard and Viveka Alfredsson gave the course during the fall semester. The topic of the first-year physical chemistry course is thermodynamics and quantum mechanics and it is based on the textbook of P. W. Atkins and J. De Paula "Atkins' Physical Chemistry". Karin Schillén is the main teacher for this course and she gave the lectures in thermodynamics together with Viveka Alfredsson, who also led the corresponding exercise sessions.

As regards higher courses, the division gives one basic course and one advanced Master course in surface and colloid chemistry and two Master courses in experimental physical chemical methods. The introductory colloid and surface chemistry course was taught by Ulf Olsson, Lennart Piculell, Håkan Wennerström and Stefan Ulvenlund. The advanced surface and colloid chemistry course, given during the fall semester, was taught by Emma Sparr (main teacher) along with Lennart Piculell, Håkan Wennerström, Per Linse, Tommy Nylander, and Peter Schurtenberger. This course is based on the textbook "The Colloidal Domain" by Fennell Evans and Håkan Wennerström. The additional two master courses were given during the spring semester by Daniel Topgaard (nuclear magnetic resonance, NMR, techniques) and by Ulf Olsson along with Tommy Nylander and Yngve Cerenius from MAX-lab (scattering methods). Furthermore, Björn Lindman taught courses at Coimbra University, Portugal and in-house courses for industry.

Several nationally and international Ph.D. courses were organized and/or taught by members of the division during the past year. In the spring semester Ulf Olsson continued to lead the Ph.D. course on advanced physical chemistry in collaboration with the Divisions of Theoretical Chemistry and Chemical Physics at the Department of Chemistry and the Department of Theoretical Physics. This course is based on the book "Physical Chemistry" by R. Stephen Berry, Stuart A. Rice and John Ross. Gerd Olofsson and Emma Sparr organized a four-day Ph.D. course "Calorimetric Methods with Basic Thermodynamics", within the frame of the Chalmers Soft Matter Graduate School, at Örenäs castle, Sweden. Ola Karlsson gave a lecture at this course. Viveka Alfredsson lectured at the PhD summer school on "From Soft to Hard Materials: Mesocrystals, self-assembly and non-classical crystallization" in Tynningö. Anna Stradner and Peter Schurtenberger organized and taught at a three-day Ph.D. course "Scattering Methods and Their Applications to Food Systems" within the NordForsk Network on Dairy Structures – Health and Functionality. A few Ph.D. students of the division were engaged as teaching assistants at this course. Moreover, Björn Lindman taught the national Ph.D. surface chemistry course at Marstrand, the international ECIS training course "Surfactants and Polymers in Aqueous Solution" in Potsdam. He was also one of the teachers at the annual course "Surfactants and Polymers in Aqueous Solution", this year given in Lisbon, and on an industrial course in Singapore. Björn Lindman and Tommy Nylander taught at the summer school "Molecular Engineering" at Utö, Finland.

Finally, Lennart Piculell gave his popular science lecture with the title "Edible and inedible gels" on three occasions for Swedish high school students visiting Lund University.

SEMINARS 2011

Synchrotron radiation, X-FELs and life science: the future is bright. Richard Neutze (Department of Chemistry, University of Gothenburg)

The supported bilayer as a platform for probing. Aleksandra Dabrowska (Kings College, London, England)

Towards understanding peptide self-assembly: a model system study. Celen Cenker (Physical Chemistry)

Structure Retrievement of Ordered Mesoporous Solids by Low Angle X-ray Diffraction. Wolfgang Schmidt (The Max Planck Insitut für Kohlenforschung, Germany)

Dendrimer cluster crystals. Dominic Lenz (Institute of Theoretical Physics, Heinrich-Heine-Universität, Düsseldorf, Germany)

Towards a responsive functional material: Modification of porosity and grafting of poly(N-isopropylacrylamide) in mesoporous silica SBA-15. Nina Reichhardt (Physical Chemistry)

The science and technology of full cells location. Jan Noolandi (Stanford University, US)

The development of a new hydrogel for tissue engineering. Jan Noolandi (Stanford University, US)

Simulation of physical gelation in telechelic polyelectrolyte solution. Ran Zhang (Physical Chemistry)

Self-Consistent Field Modeling of Moleculary Inhomogeneous Systems. Frans Leermakers (Physical Chemistry & Colloid Science, Wageningen University, the Netherlands)

Topological effects in entangled polymer networks. Nikolay Oskolkov (DTU Nanotech, Technical University of Denmark, Denmark)

Magnetic response of functionalized lipid bilayers. Joachim Kolbrecher (Laboratory for Neutron Scattering, Paul Scherrer Institut, Switzerland)

Atomistic simulation of skin lipids: effect of product ingredients. Ana Akashina (Unilever Discovery, Wirral, UK)

Confinement of lambda-phage DNAs by phospholipids walls. Carlos M. Marques (Institut Charles Sadron, Strasbourg Cedex, France)

Neutron methods in R&D. Hubert King (Exxon Mobile)

Ordering, Dynamics and Phase Transitions in Charged Colloids and Nanogel Dispersions. B.V.R. Tata (The Indira Gandhi Centre, India)

Biomimetic Control of Magnetite Shape and Morphology using Polyaminoacids. Seyda Bucak (Department of Chemical Engineering, Yeditepe University, Istanbul, Turkey)

Cubic Crystals from Cubic Colloids. Albert P. Philipse (Physical & Colloid Chemistry, Van't Hoff Laboratory, Utrecht)

Polarization transfer solid state NMR. Agnieszka Nowacka (Physical Chemistry)

Proteins and Polyelectrolytes: A Charged Relationship. Mathias Ballauff (Helmholtz Zentrum Berlin, Germany)

Light scattering experiments on concentrated suspensions. Martin Medebach (TU Berlin)

Using Photobleaching and Microfluidics to Study Mobility and Mechanical Properties of Lipid Bilayers. Peter Jönsson (Chalmers University of Technology)

Structure and function of the casein micelle. Carl Holt (University of Glasgow, United Kingdom)

Diffusion Dynamics of Gold Nanorods at a Liquid / Liquid InterfaceDiffusion. Tahereh Mokthari (Physical Chemistry)

In vitro and in vivo evalutations of targeted drug delivery using mesoporous silica nanoparticles as carriers. Mika Lindén (Department of Physical Chemistry, Åbo Akademi University, Finland)

Multicomponent self-assembly: MD simulations and NMR. Daniel Topgaard (Physical Chemistry)

A variational field theory approach for modeling charged colloidal solutions. Leo Lue (University of Strathclyde, United Kingdom)

DNA-loaded calcium alginate nanoparticles. Alexandra Machado (Physical Chemistry)

van der Waals interactions in classical systems. Joakim Stenhammar (Physical Chemistry)

Microphase separation in block copolymer melts. Mehran Asad Ayoubi (Physical Chemistry)

Cyclodextrins, surfactants and DNA. Jonas Carlstedt (Physical Chemistry)

Polyelectrolytes in solution. Sebastian Lages (Physical Chemistry)

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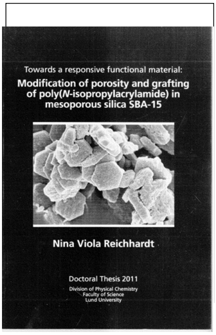
DOCTORAL THESIS

Nina Viola Reichhardt

Towards a responsive functional material: Modification of porosity and grafting of poly(N-isopropylacrylamide) in mesoporous silica SBA-15.

Opponent: Wolfgang N. Schmidt, Max-Planck-Institut für Kohlenforschung, Germany



Towards a responsive functional material:

Modification of porosity and grafting of poly(*N*-isopropylacrylamide) in mesoporous silica SBA-15

Nina Viola Reichhardt

Doctoral Thesis 2011

Division of Physical Chemistry
Faculty of Science
Lund University

MANUSCRIPTS SUBMITTED DURING 2011

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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, seminars 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 division 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 division. 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.

We recommend our visitors to fly to Kastrup Airport, Copenhagen. Then, take a train (frequency every 20 min.) from Kastrup Airport over the Öresund bridge directly to Lund railway station (takes approx. 45 min).

Visit the Kemicentrum website for further information:

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