LUND UNIVERSITY

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Cover:
Schematic representation of microgels and of their organization in dense suspension as described in D. Paloli, P. S. Mohanty , J. J. Crassous , E. Zaccarelli and P. Schurtenberger, Fluid-Solid Transition in Soft-Repulsive Colloids, Soft Matter 2013, 9, 3000 (Highlighted as front cover in Soft Matter, 11, 2013).By Jerome Crassous.

INTRODUCTION

The division of Physical Chemistry is part of the Linnaeus research environment Organizing Molecular Matter (OMM, www.omm.lu.se) together with members from the Theoretical Chemistry and Biochemistry divisions. The OMM environment was formally established in 2006, when it received an unusually long-term – 10 years – Linnaeus grant of 7.5 MSEK annually from the Swedish Research Council to support the research program proposed by the environment. There are only a few Linnaeus environments in Sweden, 20 of which were established in 2006, followed by some more in 2008. In 2006, OMM was the only Linnaeus environment created in chemistry, and the only Linnaeus environment at the Science Faculty of Lund University. Thus, the Linnaeus grant is a very prestigious grant, offering a long-term economic base for developing OMM as a coherent research environment.

The strategy, from the very beginning in 2006, was to use a significant part of the Linnaeus grant to recruit new faculty and to support young scientists in the beginning of their careers. Furthermore, as the environment spans a broad range of competences, we have worked very actively to stimulate collaborations combining different relevant competences in the research projects supported by the Linnaeus grant. This means in practice that two or more senior scientists with complementary expertise engage themselves in a project and co-supervise a PhD student or post-doctoral fellow. This way of working has proven to be very fruitful and has allowed us to tackle more complex research problems. To stimulate creativity, exchange of ideas and cross-disciplinary collaborations it is important to create meeting places. A joint seminar series, and joint PhD courses within the environment, have contributed significantly. However, very important was also the co-localization of the Physical and Theoretical Chemistry divisions when we moved to newly renovated offices and labs in 2010, including a common coffee/lunch room, just next to the Biochemistry division. This co-localization has led to many spontaneous informal meetings and discussions that probably would never have taken place otherwise. Within the Physical Chemistry division we today identify ourselves more or less completely with the OMM environment, which has brought tremendous vitality and renewal to our activities.

In 2011, it was time for the mid-term evaluation of the Linnaeus environments, with a site visit by an external panel of experts taking place in February 2012. The site visit, as well as the self-evaluation and report that we had to produce in advance, were very useful as they allowed us analyze our own work and put it into perspective. The panel was very impressed and pleased with our achievements, the way we work and how we are organized. Shortly before the summer we received the formal decision from the Research Council that they will continue to support us at an unchanged level until the end in 2016.

Discussions have begun concerning the fate of this environment beyond 2016. Given the success of the OMM environment, one should consider ways in which it can continue to prosper. However, a continuation is by no means automatic. There has to be a critical evaluation, and new concrete visions have to be formulated. Creating and maintaining a cross-disciplinary environment, like the OMM, requires specific funding. It will be a challenge in the years to come to identify the ideas and the support on which a new program, or programs, can be based.

Ulf Olsson
Chairman of the board of OMM
February 2013.

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.

Studies of model systems

Cardiolipin in model membrane systems (Contact person: Gerd Olofsson)

Cardiolipin is a phospholipid abundant in the inner mithocondrial membrane, where it is considered important in determining structure as well as membrane potential. It has been shown as a signaling molecule in apoptosis, and changes in concentration or composition of cardiolipins have been related to a number of different diseases and pathological conditions, including Parkinson's disease, ageing, heart failure and cardioskeletal myopathy. Cardiolipin differs from most other lipids in that it has four acyl chains. It has a dimeric structure consisting of two phosphatidylglycerols connected with a glycerol backbone. Thus, the cardiolipin molecule can carry two negative charges. The molecular structure with bulky hydrophobic chains and highly charged headgroups imply the formation of inverted or normal structures with negative or zero curvature, which is also highly relevant for the highly curved membrane structures in mitochondria.

It is clear that the membrane potential and curvature as well as the association with proteins and other biomolecules strongly depend on lipid charge. The acidic properties of the two identical phosphate groups should therefore be important for the biological function and the molecular organization in self-assembled structure. Indeed, there are contradictions in the literature regarding the titration and charge of the cardiolipin molecule. In the present project, we aim at characterization of cardiolipin pKa value. We also explore the phase behavior in pure cardiolipin systems as well as in mixture with other phospholipids. We use synthetic lipids with different chain length and saturation, and study these systems at different ionic strength and pH by means of calorimetry. (Gerd Olofsson, Marie Grey, Emma Sparr).

Self-Association and Interactions in Model Protein Solutions
(Contact person: Malin Zackrisson Oskolkova)

Some proteins self-associate forming dimers, and trimers etc., the reason for this behavior, i.e. its biological relevance, is yet to be clarified. Lactoferrin, also known as Lactotransferrin is a relatively large globular protein consisting of about 700 amino acids and a molecular weight of 80 kDa. This generic protein serves many functions in the body, and is found in milk, saliva, tear fluid and nasal secretions. More importantly, it plays a major role in the immune system especially for infants where it serves as an antibacterial agent. If one simply views proteins as polyelectrolytes one would not expect the removal of one of the charges to determine the energy of the system. This however is what is found in several studies of globular proteins. In the case of Lactoferrin, a dimer formation was found recently, by computer simulations when the pH was increased, approaching isoelectric conditions (pI=9.4). Moreover, The dimerization is found to be stereo-specific i.e. a charged patch at the surface of a protein gives rise to, under certain conditions, a highly complementary physical bond between two protein molecules. A purification and concentration protocol has been worked out producing monomeric Lactoferrin with a well-defined background, in terms of pH and ionic concentration. At low pH, under dilute, ideal conditions we see from static light scattering (SLS) monomeric Lactoferrin with a molecular weight in perfect agreement with the literature value. This was further supplemented by measurements of the form factor by SAXS. Upon increasing pH, still dilute, ideal concentrations, we observe an increase in the apparent hydrodynamic radius and of the apparent molecular weight, signaling the onset of dimerization. (Paula Sofia daSilva, Weimin Li, Manja Behrens, Björn Persson, Mikael Lund (Division of Theoretical Chemistry), Malin Zackrisson Oskolkova).

Polymer-grafted Core-Shell Colloidal Particles

(Contact person: Malin Zackrisson Oskolkova)

Having a polymer grafted onto particles creates a core-shell structure, a particle structure, commonly found in various industrial applications as well as in fundamental research. We have developed and characterized such a water-based colloidal system where the particle shell consisting of a PEG corona is chemically grafted onto a polystyrene core. The nature of the polymer used in the shell-layer dictates the particle interactions, which range from hard-sphere repulsive, found under good solvent conditions, to attractive in poor solvent conditions. The attraction is readily tuned by increasing the temperature due to the temperature sensitivity of PEG. The polymer-graft-induced attractions are found to be concentration dependent, the reason is yet unknown. Furthermore, Core-shell particles with a fluorinated core are now being synthesized and characterized. The fluorination serves to match the index of refraction of the solvent i.e. water, cancelling or minimizing the attractive Van der Waals (VdW) forces, normally always present in common systems. Now instead, the steric contribution to the interactions is dominating. This facilitates the study of the detailed nature of steric stabilization and destabilization and the role of VdW interactions. (Jeanette Ulama (Physical Chemistry, Göteborg University), Johan Bergenholtz (Physical Chemistry, Göteborg University), Malin Zackrisson Oskolkova).

Surface adsorption versus bulk aggregation of colloidal particles

(Contact person: Lennart Piculell)

In order to test recent theoretical predictions, we are setting up experimental studies of model liquid dispersions of spherical colloidal particles in contact with a flat solid surface, which is made of the same material as the particles. The particle-particle and particle-surface attractions are then increased by increasing the concentration of an added polymer depletant. Recent theoretical work by Per Linse and Håkan Wennerström has shown that in such a situation, for purely geometric reasons, the particles should adsorb to the infinite flat surface before phase separation occurs in the bulk. Ellipsometry, QCM and AFM are used to study the surface phenomena. (Samia Ouhajji, Lennart Piculell, Tommy Nylander, A. Philipse (University of Utrecht)).

On the ripening of solids (Contact person: Ulf Olsson)

Growth of nanoparticles is investigated by use of dynamic light scattering and transmission electron microscopy. Crystalline and amorphous nanoparticles are prepared from the drug compounds felodipine, bicalutamide and linaprazan. The crystalline nanoparticles are found to be in the nanometer range and polydisperse. However, neither of the crystalline systems display any change over time and no Ostwald ripening is observed over 10 weeks. Contrary, the amorphous nanoparticles prepared from felodipine show rapid growth, in correspondence with Ostwald ripening, in a matter of minutes after preparation, under the same stabilizing conditions as the crystalline nanoparticles. The amorphous system is also found to be polydisperse, though the polydispersity decrease with time. (Manja Annette Behrens, Ulf Olsson Urban Skantze and Lennart Lindfors (AstraZeneca R&D Mölndal)).

Oil-water electrochemistry in microemulsions (Contact person: Ulf Olsson)

We have investigated the effect of so-called potential determining salts, which are composed of a hydrophilic and a hydrophobic ion, on the phase behavior of microemulsions stabilized by nonionic surfactants with PEO headgroup. These salts strongly affect the phase behavior of the microemulsions through the induced electrostatic interactions. We observed that hydrophilic cations with hydrophobic anions lower the phase inversion temperature, while hydrophobic cations with hydrophilic anions increase the phase inversion temperature. Poisson-Boltzmann calculations and NMR measurements show that these salts preferentially dissociate across an oil/water interface, i.e. the oil and water domains in the microemulsion obtain opposite charge. Correspondingly, a potential drop is created across the surfactant film, and back to back diffuse double layers are formed in the oil and water phases. Repulsive long range interactions between thin surfactant-water lamellae in oil were observed using SAXS. (Ulf Olsson and Christoffer Johans (Aalto University, Finland)).

Micelles and their environment – wide q-range neutron diffraction studies to probe molecular interactions essential in mesoporous silica formation
(Contact person: Viveka Alfredsson)

In this project we investigate molecular interactions in systems giving rise to mesoporous silica material. The interaction between a cationic surfactant and a variety of counterions, including a silica model (a small and stable silica molecule) has been investigated with wide q-range neutron diffraction at ISIS (UK). The aim is to get an atomistic picture of the cationic micelle with its counterions and water molecules. The diffraction data will be interpreted through a modelling process that produces 3D atomistic configurations. (Emelie Nilsson, Karen Edler (University of Bath and guest Professor at Lund University), Sven Lidin (CAS, LU), Olle Söderman and Viveka Alfredsson).

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

Small, water-soluble molecules with low vapor pressure can act to protect lipid membranes against osmotic stress. Such compounds, called osmolytes, occur naturally in many organisms to regulate osmotic pressure and to prevent cell damage due to freezing or drying. For example, urea, glycerol and pyrrolidone carboxylic acid (PCA) are a part of the Natural Moisturizing Factor in human skin, and are also used in skin care products. The question addressed in the project concerns the molecular mechanism(s) behind the role of the osmolytes 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 NMR it is possible to unravel how the presence of different osmolytes interacts with phospholipid bilayers. We have previously studied urea and glycerol. It was discovered that both glycerol and urea stabilize the liquid crystalline bilayers at low relative humidities (down to 75% RH at 27 C), whereas for the pure DMPC–water system, a solid gel phase is induced at 93% RH. This demonstrates the protective effect of glycerol and urea against osmotic stress. The observation that glycerol and urea have a similar effect on the lipid phase behavior under dry conditions, and that they stabilize the fluid bilayer structure that is it formed together with the lack of evidence of specific interactions between the lipids and glycerol or urea, implies a general mechanism. In on-going studies, we explore the influence of other small polar molecules on lipid bilayer systems, focusing on monosacharides, TMAO and PCA. (Dat Pham, Emma Sparr, Håkan Wennerström, Daniel Topgaard, Lars Wadsö (Building Materials, LTH), Roland Netz (FU-Berlin, Germany)).

Effect of electrostatic interactions on the casein-PEO phase diagram in the colloid limit (Contact person: Anna Stradner)

Here we explore the possibility to create solid-like (food) gels whose structural and mechanical properties can be varied and tailored over an extremely large range in a very controlled way through an arrested spinodal decomposition process. We exploit the use of a polymer-induced depletion interaction between food colloids such as casein micelles to tune the interparticle interaction strength and range and thus play with the interplay between spinodal decomposition and gel formation. We use aqueous mixtures of casein micelles and a low molecular weight poly(ethylene oxide) for a proof of concept and investigate the possibility to create gels with well-defined structural and mechanical properties. We investigate the phase diagram of casein–PEO mixtures and the resulting equilibrium and non-equilibrium structures using diffusing wave spectroscopy and confocal laser scanning microscopy. (Najet Mahmoudi (University of Fribourg, Switzerland), Peter Schurtenberger, Anna Stradner).

Interactions and phase behavior of aqueous colloid – polymer mixtures and the influence of charges (Contact person: Anna Stradner)

We investigate the use of depletion interactions to tune the interaction potential between colloids and the resulting phase behavior and the microstructure of the states that form. We use a combination of a well-defined colloid with tunable charge density and an added water-soluble polymer. We synthesize appropriate model core shell colloids consisting of a polystyrene core and an added shell that provides electrosteric stabilization. Small-angle neutron scattering combined with contrast variation techniques is used to obtain detailed information about the particle structure and the interparticle interactions. We add water-soluble polymers to create a mixed potential that we tune through appropriate variations of the ionic strength and polymer concentration. We investigate the resulting plethora of equilibrium and non-equilibrium states as a function of the strength and range of the two dominating contributions to the mixed potential, the depletion induced attraction and the soft screened Coulomb repulsion. We compare the experimentally determined phase diagrams with theoretical predictions and characterize the resulting microstructures and their dynamics through a combination of spin-echo small-angle neutron scattering (SESANS), small-angle neutron (SANS) and x-ray (SAXS) scattering and diffusing wave spectroscopy over a large range of length and time scales. (Kitty van Gruijthuijsen (University of Fribourg, Switzerland), Remco Tuinier (Utrecht University, The Netherlands), Marco Heinen (Heinrich Heine Universität Düsseldorf, Germany), Gerhard Nägele (FZJ, Jülich, Germany), Wim Bouwman (University of Delft, The Netherlands), Marc Obiols-Rabasa, Anna Stradner).

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 DNA-protein 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 person: 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, 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).

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 and 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 water-insoluble 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. In order to make them soluble, PEO-containing nonionic surfactants (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 SAXS. They revealed 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. The solution properties of the composite self-assembled structures based on $C_{12}E_8$ and a polyion of varying length (y=25 or 6000) in the L_1 phase were investigated using dynamic light scattering (DLS) and SAXS. Within the same project, nanoparticles with bicontinuous cubic or hexagonal internal structure have been formed by dispersing PAA_{6000}, $C_{16}TAOH$ and $C_{12}E_5$ in water. Their internal ordering was identified by SAXS. The particles have a well-defined, long-time stable (> one month) size and carry a positive net-charge according to DLS, cryo-TEM and electrophoretic mobility measurements. The micellization of two water-soluble complex salts consisting of cationic $C_{16}TA^+$ surfactant ions and copolyions constituted by a poly(methacrylate) main chain randomly grafted with oligo(oxyethylene) side chains has also been studied. The thermodynamically stable aggregates formed at a distinct critical micelle concentration were investigated by DLS, NMR self-diffusion and steady-state fluorescence spectroscopy and surface tension measurements. In another project, soluble aggregates of PA-$_y$ (y=25 and 160), the hydrolyzable cationic surfactant decyl betainate (DB) and $C_{12}E_8$, have been characterized using ^{1}H NMR and NMR self-diffusion measurements. The fraction of the released PA-$_y$, which is controlled by pH, was followed as well as the rate of polymer release by monitoring the extent and the rate of DB hydrolysis, respectively. (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)).

Porous surface layers of structured polymer-surfactant assemblies 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 structured self-assembled polymer-surfactant layers from associating polymer-surfactant pairs. New methodologies are being developed to produce water-swellable, but water-insoluble polymer-surfactant layers through direct application of mixtures or through surface polymerization. The structures of the layers can be controlled by choice of the polymer and/or the surfactant(s), and by control of the water activity in the medium surrounding the layer. The structures obain correspond to those found in studies of the bulk phase behavior of the corresponding concentrated mixtures. SAXS and GISAXS are used to study the surface structures. (Charlotte Gustavsson, Lennart Piculell, Ola Karlsson, Viveka Alfredsson, Karen Edler, and Joaquim Li).

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. The present project explored 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 CXEY 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, Kristoffer Almdal (Micro- and Nanotechnology, DTU), Bo Nyström and Kaizheng Zhu (University of Oslo) and Alexei Khokhlov (Moscow State University/Russian Academy of Science)).

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.)).

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 (NH3)n2+ 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)).

Soft particles at ultra-high densities (Contact person: Peter Schurtenberger)

Cross-linked microgels are an interesting class of colloids with tunable size and softness that creates particle properties situated between classical hard spheres and soft-polymeric systems. Ionic microgels are particularly 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. Due to their soft-repulsive nature, microgels can be packed to an effective volume fraction ϕ_{eff} much above closed packing ϕ_{cp}, with enormous consequences for the resulting structural and dynamic properties. In our project we aim at:

1) Understanding the particle size, structure and the effective interaction potential as a function of the particle crosslink density, number of charges and effective volume fraction far into the ultra-dense region $\phi_{\mathrm{eff}} >> \phi_{\mathrm{cp}}$, using mainly small-angle neutron scattering combined with advanced contrast variation schemes and computer simulations.

2) Understanding structural ordering and dynamics of microgel dispersions at high volume fractions using confocal laser scanning microscopy and scattering techniques. Here we particularly focus on the influence of the charge density to combine long-range electrostatic interactions with the intrinsic short-range soft repulsion from the cross-linked polymer network in order to probe complex equilibrium crystalline structure as predicted by the theory of ionic microgels.

(Priti Mohanty, Sofi Nöjd, Divya Paloli, Jerôme Crassous, Emanuela Zaccarelli (University La Sapienza Rome, Italy), Christos Likos (University of Vienna, Austria), Peter Holmqvist and Gerhard Nägele (Forschungszentrum Jülich, Germany), 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. (Peter Schurtenberger, Sebastian Lages, Dieter Schlüter (ETH Zurich, Switzerland) and Reinhard Siegel (German University in Cairo, Egypt)).

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.

We investigate the structural and dynamic properties of magnetic ellipsoidal particles in the presence of an external magnetic field using a combination of small-angle x-ray scattering, differential dynamic microscopy and magnetometry. (Ilya Martchenko, Jérôme J. Crassous, Ann Hirt (ETH Zurich, Switzerland), Vincent Martinez and Wilson Poon (University of Edinburgh, UK) 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. We combine these experiments with rheological measurements and diffusing wave spectroscopy to access local and macroscopic viscoelastic properties, and perform systematic computer simulations to explore the link between the particle structure, the interaction potential and the resulting structural and dynamic properties. (Divya Paloli, Jerôme Crassous, Priti Mohanty, Emanuela Zaccarelli (University La Sapienza Rome, Italy) and Peter Schurtenberger).

Amphiphilic Block Copolymers – Their Formation of Supramolecular Structures with Cyclodextrin and Interaction with Other Amphiphilic Macromolecules in Aqueous Solution and at Solid/Liquid Interfaces (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). 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. 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. Finally, the formation in water of complex coacervate core micelles consisting of cationic and anionic PNIPAAM copolymers and interaction with CD is studied as a function of temperature and concentration using light scattering and calorimetry techniques in combination with turbidity measurements. (Solmaz Bayati, Karin Schillén, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway), Tommy Nylander, Gerd Olofsson, Viveka Alfredsson, Giuseppe Lazzara (University of Palermo, Italy) 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).

Depletion interactions in soft particle suspensions

(Contact person: Peter Schurtenberger)

Microgels are responsive cross-linked colloidal particles with a polymeric 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 fraction of small microgel particles in a suspension of large microgels (PNIPAM cross-linked with MBA) are studied. Microgels are used as a versatile model system where the effective volume fraction and the strength and shape of the interaction potential 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 is used. We characterize the effective interaction potential USS(r), ULL(r), and USL(r) between the particles, where the subscripts S and L stand for small and large particles, respectively, from measurements of the pair correlation functions g(r) combined with computer simulations. We then investigate the phase diagram and determine the structural and dynamic properties of the system as a function of temperature, mixing ratio and volume fractions of small and large particles. (Marc Obiols Rabasa, Priti Mohanty, Emanuela Zaccarelly (University La Sapienza Rome, Italy) and Peter Schurtenberger).

Ionic microgels as model systems for dipolar fluids

(Contact person: Peter Schurtenberger)

Ionic microgels are intriguing soft and deformable colloids. Here we study 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. We also use small-angle neutron scattering from hydrogenated microgels as tracer particles in a dispersion of contrast-matched deuterated particles with identical size and charge density to obtain the particle size and structure as a function of effective volume fraction and field strength. We perform dynamic light scattering and differential dynamic microscopy in the presence of the electric field to learn more about the dynamics of the self-assembled structures. These experiments are complemented by dielectric spectroscopy to obtain the full frequency dependence of the dielectric response of the particles, and computer simulations of soft dipolar particles. (Priti Mohanty, Sofi Nöjd, Anand Yethiray (Memorial University, St. John's, Canada), Christos Likos (University of Vienna, Austria), Jan Dhont (Forschungszentrum Jülich, Germany) and Peter Schurtenberger).

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)).

Experimental methodologies

Raman dynamic light scattering – bringing chemical specificity to DLS

(Contact person: Peter Schurtenberger)

Dynamic light scattering (DLS) is a convenient and widely used technique for the investigation of particle diffusion and particle size characterization. An extension to Raman scattering, which is able to distinguish chemically different species, could open up a wide field of new applications. In mixtures, the diffusion coefficients for different components could be resolved without special labeling, and an analysis of cross correlation of different Raman lines would contain the information if different species diffuse together and are thus attached to the same particle.

In this project we develop a novel approach Raman dynamic light scattering (RDLS). While a simple implementation where DLS is performed on a single Raman line is clearly out of reach due to the low Raman intensities, a Fourier transform approach (like e.g. in Fourier transform infrared (FTIR) spectroscopy) based on an interferometer results in a sufficiently high intensity at the detector since all Raman lines as well as the Rayleigh scattering contribute to the signal. The single line autocorrelation functions and cross correlation functions are obtained from a set of correlation measurements at different settings of the interferometer by suitable Fourier analysis. The aims of the project are the implementation, the proof of principle, and applications of the described Fourier transform dynamic Raman scattering. (Martin Medebach, Reinhard Siegel (German University in Cairo, Egypt) and Peter Schurtenberger).

Diffusive transport of multivalent ions in cartilage

(Contact person: Olle Söderman)

Articular 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-DTPA)2- as a contrast in MRI to monitor the concentration of proteoglycans and therefore the state of the cartilage. In healthy cartilage the concentration of (Gd-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 Gd-complex in cartilage? How does one quantify the T1 contrast in terms of the state of the cartilage? On the experimental side, NMR diffusometry and micro imaging techniques are applied on model system of cartilage made from gel-forming polymers as well as on actual in-vitro samples of cartilage.

In addition, computer simulations on a model system of cartilage with the aim of going beyond the use of an ideal Donnan equilibrium approach in the analysis of experimental data pertaining to distribution of (Gd-DTPA)2 from MRI-data are performed.

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, Emma Sparr, Gunnar Karlström , Olle Söderman and Daniel Topgaard).

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

Model Membranes on Novel Sensing Support (Contact person: Tommy Nylander)

As nanowires (NWs) gain momentum in biological applications, it is becoming increasingly important to understand the molecular interactions at these sophisticated interfaces. Membrane-mediated processes play a key role in many biological functions and supported lipid bilayers are excellent model systems for the study of membranes and membrane-integrated proteins. Furthermore, for many cell organelles, membranes are curved. With this in view, we recently developed a hybrid system consisting of membrane-like phospholipid bilayers supported by NW forests, which allows the formation of bilayers with controllable curvature as a matrix for biomolecular interaction. We seek to use the hybrid system to monitor membrane processes, including mechanical properties of the membrane and interactions with biomolecules. This work is funded by the nmC@LU together with the Organizing Molecular Matter (OMM) Linné Centre of Excellence as well as Carl Tryggers Stiftelse. (Tommy Nylander, Aleksandra Dabkowska, Christelle Prinz (Solid State Physics, LU), Heiner Linke (Solid State Physics, LU), Hanna Wacklin (ESS AB) and Emma Sparr).

Protein Structure and Interactions Involved in Antigen Presentation
(Contact person: Malin Zackrisson Oskolkova)

In the responsive immune system major histocompatibility complex class I (MHC I) proteins plays a key role in the recognition of intracellular pathogens (virus and cancer). The main task of the MHC-I proteins is to present antigens, which may impose a hazard to the cell. The antigen processing and loading onto MHC-I molecules takes place in the intracellular environment, when the antigen-MHC-I complex is transferred to the cell surface for detection by circulating CD8 + T cells. The mechanism of this antigen presentation involves the formation of a so-called MHC-I peptide-loading complex (PLC) where several proteins are involved. One of these proteins, which help to stabilize, facilitate and edit the peptide-loading complex, is Tapasin, a chaperone transmembrane protein. We are interested in investigating the solution structure and behavior of Tapasin in a first step to understand the connection between its biological function and solution structure. The project is done in collaboration with Kajsa M. Paulsson, head of the Antigen Presentation group at the Faculty of Medicin. (Weimin Li, Kajsa M. Paulsson (Experimental Medical Science, Faculty of Medicin) and Malin Zackrisson Oskolkova).

Scanning SAXS study of bone fracture healing (Contact person: Ulf Olsson)

Callus formation is a critical step for successful fracture healing. Bone fractures require proper mechanical fixation of the fracture ends for successful healing to occur. However, still about 5-10% of all fractures lead to delayed healing or non-union. Bone morphogenetic proteins (BMPs) alone or combined with bisphosphonates have been shown valuable in the treatment of fracture non-unions. BMPs stimulate callus formation and the rate of remodeling and bisphosphonates reduce the resorption of the newly formed callus. Hence, they may alter the quality of the forming bone. To date, very little is known about the effect of the drugs on the forming callus composition and mineral structure. In this project we collaborate with the group of Hanna Isaksson at the division of Solid Mechanics and the Department of Orthopedics on the characterization of bone fracture healing using scanning SAXS. Combined with FTIR microscopy, that reports on spatial distribution of bone composition, it is found that while the investigated drugs stimulate callus formation, they do not seem influence the callus structure and composition. (Sebastian Lages, Ulf Olsson, Hanna Isaksson (Division of Solid Mechanics and Department of Orthopaedics), Magnus Tägil (Department of Orthopaedics) Mikael Turunen and Jukka Jurvelin (Kuopio, Finland), Ana Labrador (MAX IV laboratory)).

Cataract formation and eye lens transparency (Contact person: Anna Stradner)

The understanding of protein solutions, their dominant interactions and their complex phase behavior is an important topic that has greatly profited from the well established experimental and theoretical toolbox of colloid physics. Initially, these developments were primarily driven by attempts to better understand and improve protein crystallization. However, issues of interparticle interactions, aggregation, cluster formation and dynamical arrest in protein solutions have to be seen in a broader context. Understanding interparticle interactions in protein solutions is for example of central importance to gain insight into the origin of protein condensation diseases such as Creutzfeldt Jakob, Alzheimer, Parkinson or cataract. In this project we study the structural and dynamic properties of concentrated eye lens protein solutions and mixtures with the long-term goal of shedding light on the molecular origins of cataract formation, still the major cause of blindness worldwide.

We primarily use scattering experiments (light, neutron and x-ray scattering) as well as phase diagram determination and rheological measurements together with course grained computer simulations based on colloidal models to achieve a quantitative understanding of protein interactions in the eye lens. (Saskia Bucciarelli, Lucia Casal-Dujat, Bela Farago (ILL Grenoble, France), Giuseppe Foffi (EPFL, Switzerland), George Thurston (Rochester Institute of Technology, USA), Corinne Jud (University of Fribourg, Switzerland), Mikael Lund, Peter Schurtenberger and Anna Stradner).

Observing casein micelles on their way to yogurt (Contact person: Anna Stradner)

Food science and technology have started to enormously profit from parallel developments made in colloid and materials science. In this project we study the yoghurt making process where skim milk is acidified and the casein micelles are subsequently starting to aggregate and form a gel. We use our unique set of light scattering tools such as multi-angle 3D cross correlation measurements to follow the pH-induced structural changes of the casein micelles under ‘natural’ conditions, i.e. without the need to highly dilute the highly turbid skim milk samples. We exploit an analogy to classical colloids undergoing a sol-gel transition, which allows us to disentangle pH-dependent self-assembly of the casein micelles and the resulting interparticle interaction potential. We complement these experiments with small-angle neutron and X-ray scattering, which provide us with additional important information on a more local level such as the density distribution inside a casein micelle. The overall aims of the project are a critical test of the colloid analogy to a complex food system such as self-assembled casein micelles, and a comprehensive understanding of the different pH-dependent events that are going on during the yoghurt formation. (Christian Moitzi (University of Fribourg, Switzerland), Peter Schurtenberger and Anna Stradner).

Amyloid interaction with lipid membranes (Contact persons: Emma Sparr)

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 or supported bilayers.

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 in isolated exosomes. We also study the position of the associated protein in the bilayer to further characterize the interaction. Another important focus of our study is to elucidate when lipid-protein co-aggregation occurs, and how presence of lipids influence the aggregates formed.

In this project we explore 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, Sara Linse, Agnieszka Nowacka, Daniel Topgaard, Martin Lundqvist (Division of Biochemistry and Structural Biology, LU), Patrik Brundin (Wallenberg Neurocenter, LU), 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: 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. Such changes in structure was recently demonstrated by means of NMR for skin lipids and protein components. This responding behavior to control molecular transport 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 (SC, the upper layer of skin) barrier properties to SC molecular structure, and to explore how this is affected by, e.g. hydration, "moisturizers" and penetration enhancers. These studies aim to understand how molecular diffusive transport occurs through the SC and thus how it can be affected. We characterize the lipid and protein components in intact stratum corneum using NMR and sorption calorimetry and X-ray diffraction. This is combined with transport studies of different drugs across intact stratum corneum in the presence several gradients. (Sebastian Björklund, Dat Pham, 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)).

Molecular crowding: towards a better understanding of concentrated protein solutions and mixtures (Contact person: Anna Stradner)

There is an increasing awareness that a quantitative understanding of the cellular machinery requires considerable advancement of our current understanding of concentrated (or crowded) protein mixtures present in the cytosol.

The main objective of this project is thus to measure and understand intermolecular interactions in concentrated protein solutions and mixtures as well as their dynamics. 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 focus on the influence of interactions and so-called crowding effects on the diffusion of proteins. (Saskia Bucciarelli, Lucia Casal-Dujat, Bela Farago (ILL Grenoble, France), Giuseppe Foffi (EPFL, Switzerland), George Thurston (Rochester Institute of Technology, USA), Mikael Lund, Sara Linse, 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, SAXS at MAX IV laboratory 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), Ulf Olsson 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 we study how interaction affect the phase behavior, which in turn provide information of how and where the interaction takes place. For this purpose, we investigated a set of model membrane systems with varying charge density and with fluid or solid acyl-chains together with RNA or DNA of different size and degree of base pairing. We use small single-stranded and doublestranded oligonucleotides (RNA), tRNA and long DNA. Model lipid membrane systems are zwitterionic, anionic, as well as cationic lipids. The system are studied with several techniques, including calorimetry, ellipsometry, quartz crystal microbalance (QCM-D), Neutron reflectometri, fluorescence microscopy and monolayer techniques. (Agnes Michanek, Emma Sparr, Tommy Nylander, Luc Jaeger (University of California, Santa Barbara, USA) and Fredrik Höök (Chalmers)). Project completed in 2012.

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 and 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. Because of the large aspect ratio, the nanotubes form a nematic phase or a hexagonal phase. The nanotube walls are crystalline and the tube formation involves crystaI growth processes including oriented fragment attachments. Increasing the peptide concentration, close packing is obtained and there is a first order phase transition to a lamellar phase with the peptide now forming planar bilayers. Increasing the number of hydrophobic alanines to A8K and A10K, aggregation begins at lower peptide concentrations. Also, they do not aggregate into tubes. Instead they form fibrils, a few 100 nm long, with a rectangular cross section on ca. 8 nm x 4 nm. (Çelen Cenker, Ulf Olsson, Malin Zackrisson Oskolkova, Mikael Lund (Division of Theoretical Chemistry), S. Bucak (Istanbul), I. Hamley and V. Castelletto (Reading), Paul Bomans, Heiner Friedrich and Nico Sommerdijk (Eindhoven), Burcu Dedeoglu and Viktorya Aviyente (Istanbul) and Theyencheri Narayanan (ESRF, Grenoble)).

DNA-lipid complexes (Contact person: Ulf Olsson)

Systems containing DNA, cationic co-solutes 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 compound DNA-amphiphilic cation (e.g. dodecyl trimethyl ammoinium (DTA)) when mixed with various surfactants or lipids. A review of the work was published in Soft Matter 2012. The compounds, like DTADNA are water insoluble because the amphiphilic counterions self-assemble into micelles acting like highly charged macro-ions. However, by the addition of -cyclodextrin, that forms strong 1:1 inclusion complexes with surfactants, the DTA+ ions can be dispersed without micelle formation and DTADNA can be solubilized. As part of a joint post-doc collaboration, involving Bruno Silva, we also collaborate with the group of Cyrus Safinya at UC Santa Barbara. Here, complexation/precipitation is investigated using a combination of cationic and PEG-lipids including the effect of salt. In this project, we discovered that if the liposomes's membrane is functionalized with a long hydrophilic polymer (such as PEG2K, for steric protection from the immune system), the formation of CL-DNA particles becomes pathway-dependent in brine, close to physiological conditions. If DNA and the cationic liposome are mixed in water, onions with a large number of alternating layers (ca. 20 layers) of lipid bilayer and DNA are formed, and almost independent of the amount of PEG2K. If these onions are transferred to brine, their structure is kept. Conversely, if liposomes and DNA are mixed in the presence of brine (150 mM NaCl), different regimes are obtained, depending on the amount of PEG2K and liposome membrane charge density. At low PEG2K surface coverage and high membrane charge density, CL-DNA complexes form, but with a small number of layers (typically less than 5). At high PEG2K coverage and low membrane charge density, despite some aggregation between DNA and liposomes, complexation barely occurs. (Björn Lindman, Ulf Olsson, Bruno Silva, Azat Bilalov and Alexey Krivtsov (Kazan State Technological University), Claudia Schmidt (Paderborn), Cyrus Safinya, Youli Li, Ramsey Majzoub and Chia-Ling Chan (University of California Santa Barbara)).

Molecular matter for specific functions

Dynamics in SBA-15 formation - morphology variations.

(Contact person: Viveka Alfredsson)

In this project we follow, in real-time using small angle and ultra-small angle x-ray scattering/diffraction, the formation of different morphologies of the 2D hexagonal structure of SBA-15. Synthesis of SBA-15 can yield particles with a variety of morphologies but with conserved structure. Well-defined morphologies such as hexagonal plates, short rods, "rice-shaped grains", long rods and toroids can be obtained from very similar synthesis conditions. (Tomas Kjellman, Julien Schmitt and Marianne Impéror-Clerc (University Paris-Sud, France) Karen Edler (University of Bath and guest Professor at Lund University), Adrian Rennie (Uppsala University) and Viveka Alfredsson).

Following the nucleation and growth of a material using cryogenic transmission electron microscopy (Contact Person: Viveka Alfredsson)

Cryogenic TEM is used as a tool to visualize the early stages of formation of a chiral mesoporous structured material. (Juanfang Ruan (presently at Osaka University, Japan), Ruiyu Lin, Shunai Che (Shanghai Jiaotong University) and Viveka Alfredsson).

Investigation of growth and association of siliceous colloidal flocs with cryogenic-TEM (Contact Person: Viveka Alfredsson)

Mesoporous SBA-15 grow by association of colloidal flocs. In this project we follow using cryogenic TEM, DLS SEM how the flocs aggregate. Using a number of "interventions" during the synthesis we aim at targeting the function of the stabilizing brushes in order to identify the cause of the (transient) colloidal stability. (Juanfang Ruan (presently at Osaka University, Japan) Tomas Kjellman, Yasuhiro Sakamoto (Osaka Prefecture University, Japan) and Viveka Alfredsson).

Project completed in 2012.

Nanoparticle-protein interactions – towards understanding cellular response to nanoparticles (Contact person: Peter Schurtenberger)

In this project we investigate and model interactions between nanoparticles and proteins in serum and cellular environments. We characterize their properties (size, polydispersity, surface charge density etc.) and the resulting interaction potential and particle stability as a function of solvent conditions (pH, ionic strength).

We study the interactions of these particles with a set of model proteins covering a representative array of protein sizes and charges. We investigate the fate of the particles in a crowded mixture of proteins, thus mimicking the interaction of nanoparticles with the cell cytoplasm. Experimentally, we combine several scattering techniques (Static and dynamic light scattering, depolarized light scattering, small-angle x-ray and neutron scattering, confocal and electron microscopy), various labeling schemes that allow for the detection of complex formation, and numerical simulations. (Marc Obiols Rabasa, Lucia Casal-Dujat, Alke Fink (University of Fribourg), Peter Schurtenberger).

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 shift 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, Tommy Nylander, Lennart Piculell, E. Johnson, P. Ellingson, B. Schubert, N. Vega (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 CaCl2 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)

Water sorption isotherms of calcined SBA-15-1 (red), acid treated

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, N2 and Ar sorption as well as water sorption calorimetry. (Nina V. Reichhardt (presently at Henkel, Germany), 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).

Project completed in 2012.

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 N2 sorption, water sorption calorimetry and High Resolution Scanning Electron Microscopy. (Tomas Kjellman, Nina V. Reichhardt (presently at Henkel, Germany), Motolani Sakeye and Jan-Henrik Smått (Åbo Akademi, Finland), Mika Lindén (Ulm University, Germany), Vitaly Kocherbitov, MaH), Osamu Terasaki (KAIST, Republic of Korea) Shunjuke Asahina (JEOL, Tokyo and Tohoku University, Japan) and Viveka Alfredsson).

Finding a protocol for adsorbing disc-like mesoporous silica particles with the pores parallel to the surface normal (Contact person: Viveka Alfredsson)

In this project the aim is to deposit mesoporous silica particle with controlled orientation onto a support surface. We work with a modified version of the well-known 2D hexagonal silica material denoted SBA-15. In this material primary mesopores are oriented in parallel with the surface normal. It is generally difficult to form a layered silica surface with pores in this orientation, typically the pores will orient along the underlying support surface. In our synthesis protocol disclike particles are formed in a well-characterized process and our aim is to take advantage of the shape and/or growth behavior in order to deposit the particles with the desired orientation.

We have been following two main tracks in this sub-project, (i) adsorbing the mesoporous particles on a surface, and, (ii) controlling the porous properties of the material.

The project is part of the SSF-program "Porous surface layers formed through polymer-assisted deposition". (Tomas Kjellman (PhD student), Prof. Viveka Alfredsson (PI), Dr Karen Edler (guest Professor at Lund University), Prof. Håkan Wennerström and other members of the SSF group at Physical Chemistry).

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).

The role of the co-structure directing agent in the formation of mesostructured silica. (Contact person: Viveka Alfredsson)

One synthesis strategy of mesoporous silica utilizes a so-called co-structure-directing agent believed to serve as a link between the silica network and the structure-directing amphiphile. This synthesis strategy, discovered and developed by Shunai Che and her group in Shanghai, has proven to be very versatile and a large number of structures can be obtained by small variations of the synthesis parameters. In this project we are investigating the molecular interactions involved and the role of the co-structure-directing agent. (Ruiyu Lin, Karen Edler (University of Bath and guest Professor at Lund University), Lennart Piculell, Shunai Che (Shanghai Jiatong 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 anglesandthus, 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 ALV/DLS/SLS-5022F, 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 15° to 150°, a cell housing with an cylindrical quartz vat (filled with a refractive-index matching liquid, cis-decahydronaphtalene, decaline), 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, an ALV-7004 multiple tau digital correlator with an initial real sampling time of 25 ns and 4 x 312 channels covering ≈12 decades in lag time is utilized to produce the time pseudo-cross correlation function of the scattered intensity. This make it possible to measure 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 ALV/DR-1 differential refractometer with a He-Ne laser for determination of refractive index increments (dn/dc) necessary for the determination of molar masses by SLS experiments. The limited accuracy of the refractive index is ≤ 2 x 10-6 refractive index units. (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 zeta potential) 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 980–2107 g/mol. The zeta potential 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: Marc Obiols-Rabasa)

The instrument from LS Instruments is used for simultaneous dynamic and static light scattering with transparent and turbid samples. It incorporates the 3D cross-correlation technology for eliminating the contributions from multiple scattering. It is equipped with a 3D modulation unit, which implements the newest development to increase signal-to-baseline and leads to an almost four-fold improvement in the cross-correlation intercept compared to standard 3D technology. The instrument is equipped with a HeNe laser light source, wavelength $\lambda 0= 632.8$nm and a maximum power of 35 mW. Samples can be measured in cylindrical glass cells (with 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 an upper sample goniometer to characterize non-ergodic samples.

Multi-angle 3D-goniometer system (Contact person: Marc Obiols-Rabasa)

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. Samples can be measured in cylindrical glass cells (with 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 simultaneously at 4 angles within an angular range of 10 to 150° by two photomultiplier tubes at each angle, and processed in real time by a 8 channel 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: Marc Obiols-Rabasa)

The instrument is used for simultaneous dynamic and static light scattering at ultra-small angles using a CCD camera as a position sensitive 2D-detector. The scattered light is detected from 0.3º to 6º, corresponding to length scales from a few hundred nanometers to a fraction of a millimeter. Time resolved static measurements can be performed 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-logarithmically), 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 square 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: Marc Obiols-Rabasa)

The instrument is used for the characterization of extremely turbid samples and is equipped with a diode-pumped solid-state laser (wavelength of 660 nm) with a maximum power of 70 mW. The apparatus implements a "Two-Cell Echo Technique" which allows to cover a very large range of time scales while reducing measurement times down to only a few minutes even for slowly relaxing or solid-like (non-ergodic) materials. Samples are measured in square glass cells with path lengths of 1 – 10 mm and placed in a temperature controlled sample environment (15-70 °C). The scattered light is measured in transmission with two efficient Avalanche Photo Diodes and processed by a multi-tau/linear correlator using pseudo-crosscorrelation. Also possible are experiments in backscattering geometry and CCD camera-based multispeckle measurements. The instrument is controlled and data is analyzed with a powerful commercial software solution (LS-Instruments, Fribourg, Switzerland) which allows for 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: Marc Obiols-Rabasa)

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. 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 (Kratky system)
(Contact person: Anna Stradner)

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).

Small/wide angle X-ray spectrometer, SAXS (pinhole system)

(Contact person: Anna Stradner)

This is a fully automated and remotely controllable Small Angle X-Ray Scattering instrument. The x-ray source is a high brilliance microfocus sealed tube with shaped multilayer optics, yielding a monochromatic high intensity beam at very low power. The beam shaping is initially handled by the shaped multilayer, and then further collimated by 3 sets of 4-bladed slits. The beam path is evacuated by an oil-free high speed pump allowing full pump-down to clean operating pressures in 4 minutes. The sample area comes with an XY-theta goniometer for alignment and positioning of samples for both transmission and grazing incidence work. The scattering signal is detected by a state-of-the-art pixelized solid state detector (synchrotron style), combining the best of single photon counting, dynamic range and robustness. The motion of the detector allows the user to make measurements over a very large q-range. The integrated data management (with detailed system information being carried over in date-headers interpretable by the data-reduction software) facilitates the task of monitoring, data-collection, data-reduction and data-interpretation.

Sample holders/stages available:

- Versatile ambient plate for disposable capillaries
- JSP capillary stage with temperature control
- WAXS capillary stage with temperature control
- Flow-through cell

The available q range extends from ≈ 0.003 $Å^{-1}$ up to ≈ 2.5 $Å^{-1}$.

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 multinuclear microimaging, solid-state, wideline, 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, 19F), H/X CP-MAS 4mm (1H/31P-15N), E-free CP-MAS 4mm (13C/31P/1H), H/X CP-MAS 2.5mm (1H/31P-15N), Wideline 5mm (25Mg-31P), 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).

In 2012, the system was upgraded with SMD Detection package FCS (high quantum efficiency, 2 APD). The system acquires and analyzes FCS and FCCS (Fluorescence Cross-Correlation Spectroscopy) data. Both methods focus on quantitative analysis of transport and binding processes.

(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 consist of non-reactive Tantalum 61™ for excellent chemical resistance, and they are fixed-in-place for reproducible ultrasensitive performance with low maintenance. The system uses a Peltier element for precise temperature control. It allows for user selectable temperature scan rates (0ºC to 90ºC per hour upscans), allowing studies of fast or slow transition processes. (Sponsored by The Knut and Alice Wallenberg Foundation.)

Isothermal titration calorimeter (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).

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 was 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: Emma Sparr)

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 is available under the ESMI web portal. Experimental access will be coordinated through Physical Chemistry (Peter Schurtenberger)
- Networking: A dissemination and educational plan has been 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 Nanoformulations Conference in Barcelona, Spain, and at the EuFoam Conference in Lisbon, Portugal. He gave keynote lectures at the IACIS Conference in Sendai, Japan, at the 5th International Conference on Applied Hair Science, Princeton, USA. He gave invited lectures at the workshop "Nano-biocolloidal materials and non-equilibrium self-assembly" in Barcelona, Spain, at the AkzoNobel Nordic Prize Symposium in Stenungsund and at the workshop on Cellulose, Regenerated Cellulose and Cellulose Derivatives in Örnsköldsvik, Sweden. 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; Universidade de Algarve, Faro, Portugal; MidSweden University, Sundsvall, Sweden; Royal Institute of Technology, Stockholm; BASF Research Center, Düsseldorf, Germany; Department of Chemistry, Princeton University, USA; Perstorp AB Research Center, Perstorp, Sweden; Dyrup Research Center, Copenhagen, Denmark; Elkem Research Laboratories, Kristiansand, Norway; Henkel Research Center, Düsseldorf, Germany; Lenzing Research Center, Lenzing Austria; Kao Research Laboratories, Wakayama, Japan; Procter&Gamble Research Laboratories, Kobe, Japan; Instituto de Química Avanzada de Catalunya CID-CSIC, Barcelona, Spain; Akzo Nobel Surface Chemistry, Stenungsund, Sweden; Norwegian Technical University, Trondheim; Åbo Akademi, Finland; University of Barcelona, Spain; MidSweden University, Sundsvall; School of Chemical Engineering, Nanjing University of Science and Technology, China; VTT Technical Research Centre of Finland, Helsinki. Björn Lindman was visiting professor at the Department of Chemistry, Coimbra University, Portugal, at Nanjing University of Science and Technology, China and at Nanyang Technological University, Singapore.

Håkan Wennerström gave invited lectures at a workshop on Discussions on hydration forces in Sofia, Bulgaria. He attended the conference on Self Assembly: From Biocolloids to nano-Engineering in Bifröst, Iceland and Faraday Discussion on Lipids and Mambrane Biophysics in London, UK, and an SSF organized "Program Conference" in Stockholm, Sweden.

Peter Schurtenberger gave invited lectures at the following international conferences, workshops and summer schools: Russell Berry Nanotechnology Institute Winter School in Nanoscience and Nanotechnology – HaGoshrim, Israel (2 lectures); 11th European School on Scattering Methods Applied to Soft Condensed Matter (2 lectures); Faraday Discussion 158 Soft Matter Approaches to Structured Food – Wageningen, The Netherlands; Association in Solution III Self-Assembly: From Bio-Colloids to Nano-Engineering – Bifröst University, Iceland; Biological & Pharmaceutical Complex Fluids: New Trends in Characterizing Microstructure, Interactions & Properties – Tomar, Portugal; The Emerging Science of Gastrophysics, An Interdisciplinary Symposium at The Royal Danish Academy of Sciences and Letters - Copenhagen, Denmark; Interdisciplinary Training for Young Scientists 2012, Training School from the Swiss National Science Foundation – Centre Löwenberg, Switzerland. Peter Schurtenberger also gave an invited keynote lecture at ACS National Meeting – San Diego, USA as well as an invited seminar at Physics Colloquium, University of Halle – Halle, Germany.

Anna Stradner gave an invited lecture at the 16th Swedish Neutron Scattering Society (SNSS) meeting in Stockholm, Sweden and at the International Conference on Molecular Crowding 2012: Chemistry and Physics meet Biology in Monte Verità, Switzerland as well as at the ECI (Engineering Conferences International) Association in Solution III: From Bio-Colloids to Nano-Engineering at Bifröst University, Iceland.

Ulf Olsson organized, together with Norman Wagner, University of Delaware, the 3rd Association in Solution Conference at Bifröst University, Iceland, within the framework of Engineering Conference International (ECI). The conference had all together about 60 participants from four different continents. Ulf Olsson also gave invited lectures at the Annual Fall Meeting of the Swiss Chemical Society at ETH, Zürich and at the 19th Ostwald Kolloquium in Berlin, and attended the 9th Nordic Workshop on Scattering from Soft Matter in Gothenburg. During the year, he also visited Yeditepe University, Carnegie Mellon University, the University of California Santa Barbara, and the Institut Charles Sadron at University of Strasbourg as part of research collaborations

Tommy Nylander presented an oral presentation at International Association of Colloid and Interface Scientists conference, IACIS2012, Sendai, Japan, ACS-meeting, San Diego, USA an invited plenary talk at International Food Colloids Conference, Copenhagen, Denmark and an invited lecture/ German Neutron Scattering Society Meeting, Jülich/GSI-Bonn, Germany. He also gave invited talks at Duke University, Durham NC, USA, UCLA, Los Angeles CA, USA and Aalto University, Espoo, Finland. Tommy Nylander took part in the The Partnering Nano Medicine Mission Tour to North Carolina and Boston, organized by Nanoconnect Scandinavia and Medion Valley Alliance .

Ingemar Wadsö gave a plenary lecture at XVII International Society of Biological Calorimetry Conference (ISBC) in Leipzig, Germany and an invited lecture at the meeting Living & Breathing Calorimetry, RSC Thermal Methods Group, at Ware, UK.

Emma Sparr gave an invited lecture at the Workshop Discussion on Hydration Forces in Sofia, Bulgaria and at the annual Biofilm workshop Hydration of Biomolecules and Biointerfaces in Malmö, Sweden. She also presented a poster at the Faraday Discussion 161 on Lipids and membrane Biophysics in London.

Daniel Topgaard gave a keynote lecture at the conference Magnetic Resonance in Porous Media 11 in the University of Surrey, UK, as well as invited lectures at the 4th International Conference on Porous Media at Purdue University, USA, the conference Materials for Tomorrow in Göteborg, and the workshop NMR in Heterogeneous Materials in Göteborg. He also gave seminars at Applied Physical Chemistry, KTH, Stockholm, and the Center for Language and Literature in Lund.

Malin Zackrisson Oskolkova attended the conference Science and Scientists @ ESS held in Berlin, Germany .

Patrik Knöös attended the International Symposium on Polyelectrolytes in Lausanne, Switzerland, in July, where he gave an oral presentation.

Saskia Bucciarelli gave a presentation at the SoftComp Annual Meeting 2012 in Crete, Greece and at the 11th European Summer School on Scattering Methods Applied to Soft Condensed Matter in Bombannes, France

Jenny Algotsson presented a poster at the 11th International Bologna Conference on Magnetic Resonance in Porous Media in Guildford, UK. She also gave an oral presentation at the 5th Nordic Meeting on Quantitative Imaging of Cartilage in Malmö, Sweden.

Marc Obiols Rabasa gave an oral presentation at the Engineering Conferences International conference: Biological and Pharmaceutical Complex Fluids in Tomar, Portugal.

Jérôme Crassous presented a poster at the 9th Nordic Workshop on Scattering from Soft Matter in Gothenburg, Sweden and gave oral presentations at the ESS Symposium “The Future of Soft Matter SANS: Consequences for Sample Environment and Complementary Techniques” in Lund, Sweden; at the Softcomp Annual Meeting 2012 in Heraklion, Crete and at the conference Materials for Tomorrow in Gothenburg, Sweden.

Adriana Mihut-Crassous gave an oral presentation at the Softcomp Annual Meeting 2012 in Heraklion, Crete.

Ran Zhang attended the conference Workshop on Physical Virology in Trieste, Italy.

Manja A. Behrens gave an oral presentation at the 9th Nordic Scattering Workshop on Soft Matter in Gothenborg, Sweden. She presented a poster at the ECI (engineering conferences international) conference ‘Association in Solution III) in Bifrost, Iceland. She also gave an oral presentation at the International Small-Angle Scattering conference in Sydney, Australia

Ilya Martchenko gave oral presentations at the SoftComp Annual meeting 2012 in Heraklion, Grece and at the 9th Nordic Workshop on Scattering from Soft Matter in Gothenburg, Sweden.

Emelie Nilsson presented a poster at the conference Materials For Tomorrow in Gothenburg, Sweden.

Sebastian Björklund presented a poster at the Faraday Discussion 161 on “Lipids and membrane Biophysics” in London.

European Colloid and Interface Society (ECIS) conference 2012

The 26th Conference of the European Colloid and Interface Society in Malmö was organized by Lund University (Physical Chemistry (Tommy Nylander) and Solid State Physics (Christelle Prinz)) and Malmö Högskola (Thomas Arnebrant) on the 2-7 of September 2012.

Colloid and interface science is an interdisciplinary field that embraces many scientific disciplines, from nano-science, physics and chemistry to biology and medicine. Much of the fundamental knowledge on colloidal and interfacial processes have and will be key for the development of a sustainable processes. This was apparent from the breath of the participation in the 26th Conference of the European Colloid and Interface Society held in Malmö Sweden 2-7 September 2012. The meeting attracted 531 participants from 49 different countries around the world. The largest number of participants from outside Europe came from Japan. The conference was sponsored by 22 companies and organizations. We would specially point out the significant contribution provided by The Swedish Research Council for Environment Agricultural Sciences and Spatial Planning, FORMAS, as well as Camurus AB, a local small but growing drug delivery company in Lund, that was based on research carried out at the Department of Chemistry at Lund University. ECIS had 2 parallel sessions with keynote and contributed talks in addition to the two-day sessions devoted the two-day sessions devoted the COST action (CM1101). Of the delegates 68 had registered for the COST action of which 27 only took part in the COST action session. It should be noted that the COST action session was very well attended. Not only by persons that had registered for the session, but also from the ECIS delegates. The scientific program consisted of 9 ECIS sessions and 1 COST session. This program included 6 plenary talks including the Rhodia Prize Lecture and Overbeek Medal Lecture, 12 keynote lectures including the 2 in the COST session, and 118 oral contributed presentations including 26 in the COST session. The scientific program was divided in 10 sessions with oral presentations:

1. Interfacial Phenomena and Structures
2. Surfactants, Lipids, and Self-Assembly
3. Colloids and Colloidal Stability
4. Polymers, Biopolymers, and Polyelectrolytes
5. Hydration Phenomena
6. Nanostructured Materials
7. Biocolloids/Interfaces
8. Soft Matter Formulations
9. Neutrons and Synchrotron Radiation Revealing Colloidal and Interfacial Structure and Dynamics

C. COST action

In addition there were 3 poster sessions with almost 400 poster contributions. The social program included Max IV synchrotron construction site and the European Spallation Source ESS planned site in Lund. These represent the largest investments in research infrastructure in Europe. We are particularly happy for the large media coverage of the conference, with presence of some local newspapers, a report in Sydnytt, the regional TV channel and a special report on the Science Radio program on the national radio channel. On Friday afternoon, directly after the ECIS Conference, a symposium "Outlooks from strong traditions in Colloid and Interface Science" honoring one of the founding fathers of ECIS, Björn Lindman was held. This symposium attracted almost 200 participants.

Researchers from physical chemistry who participated at the conference:

Karin Schillén, Jenny Algotsson, Erik Wernersson, Solmaz Bayati, Adriana Mihut-Crassous, Jérôme Crassous, Marc Obiols Rabasa, Sebastian Björklund, Tahereh Mokthari, Dat Pham, Marie Grey and Marianna Yanez presented posters.

Björn Lindman, Emma Sparr, Saskia Bucciarelli and Marianna Yanez gave presentations.

EXTERNAL PROFESSIONAL ACTIVITIES

Lennart Piculell was section editor for the Polyelectrolytes section of Current Opinion in Colloid and Interface Science and a member of the editorial board of Soft Matter. He was a member of the international organizing committees of the biannual International Polyelectrolyte Symposia and the conference Formula VII, to be held in Mulhouse 2013. He was a member of the board of the Surface and Materials Chemistry Division of the Swedish Chemical Society, and a member of the Electoral Committee of the Swedish Chemical Society. At Lund University he was the director of the Linnaeus center OMM until June 2012, a member of the Electoral Committee of the Faculty of Science and an appointed mentor for a PhD student at the Department of Biology.

Peter Schurtenberger was a member of the Liquids Board of the European Physical Society, 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, chairman of the Jülich Centre for Neutron Scattering and FRM II Soft Matter Review Committee, member of the Network Governing Board and Chairman of the Experimental Platform of the European Network of Excellence SoftComp, member of the ESS Science Board and the ESS Science Directorate, member of the ESS SANS Scientific Advisory Panel, member of the Organizing Committee 11th European Summer School on Scattering Methods Applied to Soft Condensed Matter, Bombannes, France, member of the International Program Committee of the International Soft Matter Conference in Rome 2013, co-organizer of the ESS Science Symposium The Future of Soft Matter SANS, Lund, 2012, editorial Board, Colloid & Polymer Science and section Editor, Current Opinion in Colloid and Interface Science.

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 “docent” at Åbo Akademi, Finland. 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 during the year acted as immediate-past-President. He was evaluator of research programs for Lundbeckfonden, Denmark and for research councils. Björn Lindman was “first opponent” for the Ph D defence of Andreas L. Nenningsland at the Norwegian Technical University, Trondheim and faculty opponent for the Ph D defence of Per Dahlsten at Åbo Akademi University, Finland.

Olle Söderman served on the electorate that appointed members on the board of the Swedish Research Council and members of the Scientific Council for Natural and Engineering Sciences. Olle Söderman was appointed as Head of the Department of Chemistry from January 1, 2012.

Ulf Olsson was a member of the strategy group at the Science Faculty in Lund working on preparing the faculty for the upcoming large scale facilities, MAX IV and ESS. He was also a member of an advisory group within the Swedish Research Council dealing with issues related to neutron, synchrotron and X-ray free electron laser work. Ulf Olsson was a external examiner of the PhD thesis of Lauriane Lagarde, Institut

Charles Sadron at University of Strasbourg, France and of Nikolay Berezhnoy at Nanyan Technological University, Singapore. He also served as member of the Science Advisory Committee of the Swiss Spallation Source, SINQ, at the Paul Scherrer Institute, Switzerland.

Tommy Nylander served as thesis examiner (opponent) for the PhD theses of Chantelle Driever, University of Melbourne, Australia, Xiaona Jing, Copenhagen University, Copenhagen Denmark, Sanjeev Ranjan, Aalto University, Espoo, Finland, and Jessica Valle Orero, Ecole Normale Supérieure de Lyon, and ILL, Grenoble, France. He was a member of Formas (The Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning) standing evaluation committee for Resource efficient products and processes. He was member of the evaluation panel for beam time applications NIST Centre for Neutron Research, Gaithersburg, USA and ISIS, ISIS -Rutherford Appleton Laboratory, Oxfordshire, UK and chaired the panel for Biology at FRMII, Munich. 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'Universita e della Ricerca, Italy.

Viveka Alfredsson served as the assisting head of division of Physical Chemsitry. Viveka was a member of the executive Council of the International Mesostructured Materials Association and a member of the equality group of the department of Chemistry (KILU). She was also a Deputy Member of the Board of KILU. She was a member of the Swedish Research Council evaluation committee for Physical, Biophysical and Theoretical Chemistry. She is a member of the board for "Lunds Universitets gästhem".

Karin Schillén served on the PhD grading committees for Jens Uhlig, Chemical Physics, Lund University and for Shogo Takamuku, Polymer Technology, Lund University. Since 2009, she is also a member of the board of the undergraduate studies in chemistry at the Department of Chemistry, Lund University.

Anna Stradner was board member of the Swiss Neutron Scattering Society. Member of the Program Executive Committee of the European infrastructure project ESMI (European Soft Matter Infrastructure) and member of the Faculty Search Committee at ETH Zürich/Switzerland for a Professor position.

Emma Sparr is a member of the Young Academy of Sweden (initiated by KVA in 2011). She was leading the organization committee for an open workshop on "Practicing interdisciplinary science research" (Lund). open work She was a member of the examining board at the PhD defense of Jonathan Liljeblad (KTH, Stockholm).

Daniel Topgaard was a member of the examination board at the PhD thesis defenses of Matias Nordin at Chalmers, and John Janiak in Lund.

Ilya Martchenko was elected Treasurer of the International Young Physicists' Tournament and was juror at the 25th IYPT in Bad Saulgau, Germany. He was juror at the 14th AYPT in Leoben, Austria and at two events by Nationellt resurscentrum för fysik (LU) in Lund and Malmö.

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 in the laboratories. 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 and Emma Sparr were 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 and course coordinator for this course and she gave the lectures in thermodynamics together with Viveka Alfredsson, who also led the corresponding exercise sessions.

During the fall semester, a novel course in physical chemistry, drug delivery and formulations ("Galenisk och fysikalisk farmaci") was given as a joint course between the Physical Chemistry and the Food Technology divisions. Emma Sparr was the course coordinator. Teachers from the Division of Physical Chemistry were Emma Sparr and Malin Zackrisson Oskolkova.

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 and Stefan Ulvenlund. The advanced surface and colloid chemistry course, given during the fall semester, was taught by Emma Sparr (course coordinator) along with Lennart Piculell, Per Linse, Tommy Nylander, Peter Schurtenberger and Karen Edler (University of Bath, England). 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, one on nuclear magnetic resonance techniques taught by Daniel Topgaard and one on scattering methods taught by Malin Zackrisson Oskolkova together with Ulf Olsson, Peter Schurtenberger and Yngve Cerenius (MAX IV laboratory). Björn Lindman taught courses on colloid chemistry and on medicinal physical chemistry at Coimbra University, Portugal; a course on colloids at School of Chemical Engineering, Nanjing University of Science and Technology, China; an advanced course on surfactants and polymers at the VTT Technical Research Centre of Finland; and in-house courses for industry.

During the past year, members of the division taught several national and international Ph.D. student courses. Björn Lindman taught at the courses "Surfaces and colloids" at Nanyang Technological University, Singapore; at the WWSC Winter Graduate School on "Interactions in multicomponent materials from trees. Towards innovative products" in Varberg, Sweden and at a course on colloids at the International Postgraduate Institute "Excellence PolyTech", Kazakh National Technical University, Kazakhstan. He was also one of the teachers at the course "Surfactants and polymers in aqueous solution", MidSweden University, Sundsvall, Sweden. Moreover, Gerd Olofsson and Emma Sparr gave lectures at the European Colloid and Interface Society (ECIS) Training Course "Thermodynamics and calorimetry of colloidal and biological cystems", Malmö, Sweden.

Erik Wernersson contributed to the development and teaching of the PhD course "Monte Carlo and Molecular Dynamics Tools" within the COMPUTE research school.

Emma Sparr and Lennart Piculell gave invited popular science lectures for the high school students at a "Chemistry fair" at Polhemskolan in Lund in May.

Finally, Lennart Piculell and Ulf Olsson gave popular science lectures with the titles “Edible and inedible gels” and “ESS och MAX IV och konsten att se små saker”, respectively, for Swedish high school students visiting Lund University.

Seminars 2012

Johan Bergenholtz, Physical Chemistry, Göteborg University.
Dissociation Dynamics of Colloidal Clusters.

Paula Sofia da Silva, FCTUC - Faculty of Science and Technology of University of Coimbra, Department of Biochemistry.
Self-assembly and Interactions of Lactoferrin.

Jennifer Chen Lee, NIH.
Protein-membrane interactions.

Christopher Dunning, Lund University.
Prion-like spread of alpha-synuclein in Parkinson’s disease.

Anna Stradner, Physical Chemistry, Lund University.
Reexamining the colloid analogy for casein proteins.

Robert Vacha, Cambridge/Prague.
Exocytosis of nanoparticles.

Tommy Nylander, Physical Chemistry, Lund University.
The lipid-aqueous interface beyond bilayers - curvature and lipids at interfaces.

Philip Kuchel, University of Sydney.
13C DNP NMR in kinetics of cellular systems.

Luca Monticelli, Inserm, Paris.
Simulating nanoparticles into membranes.

Nitash P Balsara, Department of Chemical and Biomolecular Engineering Environmental Energy Technologies and Materials Sciences Divisions Lawrence Berkeley National Laboratory, University of California, Berkerley.
All-Solid Lithium Batteries and the Clean Energy Landscape.

Erik Hellstrand, Biophysical Chemistry, Lund University.
Protein-Lipid Association and Aggregation in Neurodegenerative Disease.

Mehran Asad Ayoubi, Physical Chemistry, Lund University.
Self-assembly in Melts of Block copolymer-based Systems Featuring Supramolecular Interactions.

John Janiak, Physical Chemistry, Lund University.
Phase Behavior and Solution Properties of Aqueous Polyion-Surfactant ion Systems.

Andrew Jackson, European Spallation Source (ESS).
Explosives and Milk - Nanoscale to Microscale Structure.

Robert K. Thomas, University of Oxford.
How Not to Determine Surface Excess: A Century of Wasted Measurements?

Jan K.G. Dhont, Forschungszentrum Juelich.
Charged Colloids in Electric Fields and Thermal Gradients.

Dominique Massiot, CEMHTI-CNRS, Orléans.
Order and disorder in materials: from atomic to nanometer scale.

Andrew Nelson, Australia.
Studying kinetics in thin film systems using neutron reflectometry.

Prof Albert P. Philipse, Van ‘t Hoff Laboratory for Physical and Colloid Chemistry, Utrecht University.
Anisometric colloids.

Agnieszka Nowacka, Physical Chemistry, Lund University.
Polarization Transfer Solid-State NMR for Studying Soft Matter: From Surfactants to the Stratum Corneum.

Albert P. Philipse, Van ‘t Hoff Laboratory for Physical and Colloid Chemistry, Utrecht University.
Magnetic colloids.

Karen Edler, Department of Chemistry, University of Bath, United Kingdom.
Surfactant Templated Inorganic Films at the AirSolution Interface.

István Furó, Physical Chemistry, KTH.
Electrophoretic NMR.

Martin Medebach, Physical Chemistry, Lund Univeristy.
Two examples of heterodyne light scattering: Electrophoresis of concentrated colloidal suspension FT-Raman-Dynamic Light Scattering.

Erik Wernersson, Physical Chemistry, Lund University.
Molecular Modeling of Molecular Ions – Salty Tales from a Landlocked Country

Drew Parsons, Canberra, Australia.
Hydration and Ions.

Freddy Kleitz, Department of Chemistry, Laval University, Quebec City, Canada.
Functional Mesoporous Materials: From Material Synthesis to Application Perspectives.

Adriana Mihut, Physical Chemistry, Lund University.
Self-Assembly of Semicrystalline Diblock Copolymers in Selective Solvents: From Experimental Phase Map to Guided Colloidal Self-Assembly.

Eckhard Spohr, Universität Duisburg-Essen, Germany.
Computer Simulations of a Thermo-responsive Polymer in Aqueous Solution.

Jérôme Crassous, Physical Chemistry, Lund University.
Designing Composite Microgels with Varying Shapes and Functionalities: On the Road towards Supracolloidal Self-Assembly.

Jonas Gernandt, Uppsala University.
Phase separation within elastic hydrogels absorbing macroions.

Manja Behrens, Lund University.
Scattering studies of polymeric micelles and biological macromolecules

Pavlik Lettinga, Research Centre Jülich Institute of Solid State Research (IFF) Soft Matter Division, Jülich, Germany.
Dynamics and colloidal rods at rest and in external fields.

Marianne Impéror-Clerc, Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France.
Structure and Formation of Periodic Silica-based Templated Materials: Investigation using Small Angle X-Ray Scattering.

Patrik Knöös, Physical Chemistry, Lund University.
Monitoring the drug release from tablets made from hydrophobically modified poly (acrylic acid)

Jonas Carlstedt, Physical Chemistry, Lund University.
Tuning DNA-surfactant interactions with cyclodextrins.

Richard Campbell, Institute, Laue Langevin, Grenoble, France.
Impact of bulk non equilibrium effects on an oppositely charged polyelectrolyte/surfactant mixture at the air/water interface.

Tiago Ferreira, Physical Chemistry, Lund University.
Biomembrane models: NMR and MD simulations

Sebastian Björklund, Physical Chemistry, Lund University.
Biophysical characterization of the skin barrier

Joaquim Li.
Small angle X-ray scattering study of a drying colloidal film.

AWARDS

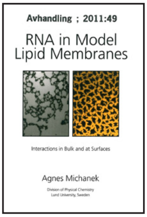
Dr Robert K. Thomas, FRS, from University of Oxford became Honorary Doctor at Science Faculty, Lund University 2012, due to his pioneering and outstanding work on using neutron reflection to study interfacial layer structures. He is long-time friend and collaborator of researchers in this field at Lund University, in particular Physical Chemistry where he has been involved in several PhD projects. We had also the pleasure to host him for sabbatical during October 2012.

DOCTORAL THESIS

Agnes Michanek

RNA in model lipid membranes – interactions in bulk and at surfaces.

Opponent: Professor George Attard, Department of Chemistry, University of Southampton, England



Avhandling ; 2011:49

RNA in Model Lipid Membranes

Interactions in Bulk and at Surfaces

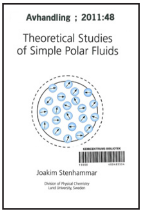
Agnes Michanek

Division of Physical Chemistry
Lund University, Sweden

Joakim Stenhammar

Theoretical Studies of Simple Polar Fluids.

Opponent: Professor Martin Neumann, Universität Wien, Austria



Avhandling ; 2011:48

Theoretical Studies of Simple Polar Fluids

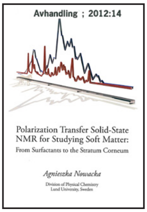
Joakim Stenhammar

Division of Physical Chemistry
Lund University, Sweden

Agnieszka Nowacka

Polarization transfer solid-state NMR for studying soft matter: From surfactants to the stratum corneum.

Opponent: Professor Dominique Massiot, CEMTHI, Orléans, France



Avhandling ; 2012:14

Polarization Transfer Solid-State NMR for Studying Soft Matter:
From Surfactants to the Stratum Corneum

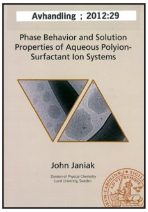
Agnieszka Nowacka

Division of Physical Chemistry
Lund University, Sweden

John Janiak

Phase Behavior and Solution Properties of Aqueous Polyion-Surfactant Ion Systems.

Opponent: Professor Bo Nyström, University of Oslo, Norway



Avhandling ; 2012:29

Phase Behavior and Solution Properties of Aqueous Polyion-Surfactant Ion Systems

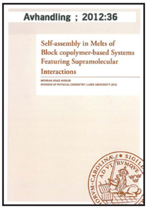
John Janiak

Division of Physical Chemistry
Lund University, Sweden

Mehran Asad Ayoubi

Self-assembly in Melts of Block copolymer-based Systems Featuring Supramolecular Interactions.

Opponent: Professor Nitash Balsara, University of California, Berkeley, USA



Avhandling ; 2012:36

Self-assembly in Melts of Block copolymer-based Systems Featuring Supramolecular Interactions

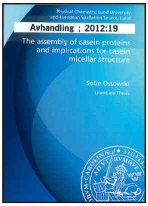
MEHRAN ASAD AYOUBI
DIVISION OF PHYSICAL CHEMISTRY | LUND UNIVERSITY 2012

LICENTIATE THESIS

Sofie Ossowski

The assembly of casein proteins and implications for casein micellar structure.

Evaluation committee: Kell Mortensen, University of Copenhagen and Björn Bergenståhl, Lund University.



Physical Chemistry, Lund University
and European Spallation Source, Lund

Avhandling ; 2012:19

The assembly of casein proteins and implications for casein micellar structure

Sofie Ossowski

Licentiate Thesis

PUBLICATIONS

(1) Aben, S.; Holtze, C.; Tadros, T.; Schurtenberger, P.
Rheological Investigations on the Creaming of Depletion-Flocculated Emulsions.
Langmuir 2012, 28, 7967-7975.

(2) Algotsson, J.; Åkesson, T.; Forsman, J.
Monte Carlo simulations of Donnan equilibrium in cartilage.
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PEOPLE

Scientists/Teachers

Viveka Alfredsson, professor
Manja Behrens, post-doc
Lucia Casal, researcher
Debby Chang, post-doc
Jerome Crassous, post-doc
Alexandra Dabkowska, researcher
Karen Edler, guest professor
Marie Grey, post-doc
Kazuhiro Ishikawa, guest researcher
Christoffer Johans, post-doc
Ola Karlsson, adjunct professor
Alexey Krivtsov, post-doc
Sebastian Lages, post-doc
Björn Lindman, professor
Per Linse, professor
Dan Lundberg, post-doc
Martin Medebach, researcher
Adriana Mihut, researcher
Priti Mohanty, post-doc
Tahere Mokhtari, post-doc
Tommy Nylander, professor
Marc Obiols-Rabasa, researcher
Ger Olofsson, associate professor emeritus
Samuli Ollila, post-doc
Ulf Olsson, professor
Asger Bjorn Petersen, researcher
Lennart Piculell, professor
Horie Wataru, guest researcher
Karin Schillén, professor
Claudia Schmidt, guest professor
Peter Schurtenberger, professor
Bruno Silva, post-doc
Emma Sparr, professor
Anna Stradner, associate professor
Olle Söderman, professor
Fredrik Tiberg, adjunct professor
Daniel Topgaard, associate professor
Stefan Ulvenlund, adjunct associate professor
Maria Wadsäter, researcher
Ingemar Wadsö, professor emeritus
Håkan Wennerström, professor
Erik Wernersson, post-doc
Malin Zackrisson-Oskolkova, researcher
Ran Zhang, post-doc

Technical-Administrative Personnel

Tomislava Andric, economist
Christopher Hirst, engineer
Majlis Larsson, administrator
Maria Södergren, engineer

Graduate students

Alexei Abrikossov
Jenny Algotsson
Mehran Asad Ayoubi
Jonas Carlstedt
Johanna Bailey Jönsson
Solmaz Bayati
Sebastian Björklund
Saskia Bucciarelli
Celen Cenker
Stefanie Eriksson
Charlotte Gustafsson
Sanna Gustavsson
Carin Hagsten
John Janiak
Tomas Kjellman
Patrik Knöös
Weimin Li
Ilya Martchenko
Tiago Mendes Ferreira
Emelie Nilsson
Agnieszka Nowacka
Sofi Nöjd
Sofie Ossowski
Divya Paloli
Quoc Dat Pham
Joakim Stenhammar
Marianna Yanez Arteta

Guests

Manja Behrens	Danmark, iNANO Center Aarhus Universitet
Stefanie Eriksson Sverige	
Agzenai Ben Salem Yahya	Spanien, Univ. National de Educasion a Distancia
Georg Attard	England, University of Southampton
My Mattsson, dipl.worker BSc	
Jenny Andersson, dipl.worker MSc	
Caroline Eriksson, dipl.worker MSc	
Sofi Nöjd, dipl.worker MSc	Sverige, Lunds universitet
Adriana Mihut	Schweiz, University of Fribourg
Aadil Abbas, dipl.worker MSc	
Karen Edler	England, University of Bath
Erik Wernersson	Sverige, Göteborgs universitet
Aleksandra Dabkowska	England, Kings College London
Martin Neumann	Österrike, Universität Wien
Richard Campbell	Frankrike, Inst. Lau-Langevin, Grenoble
Marianne Imperor-Clerc	Frankrike, Université Paris-Sud
Pavlik Lettinga	Tyskland, Forschungszentrum Juelich GmbH
Julian Eastoe	England, University of Bristol
Marie Jehannin	Frankrike, Chimie-Paris Tech
Carolin Anderberg Haglund, BSc	
Jonas Gernandt	Sverige, Uppsala universitet
Alexey Krivtsov	Ryssland, Kazan State Technology University
Karen Edler	England, University of Bath
Freddy Kleitz	Kanada, Université. Laval, Quebec
Drew Parsons	Australien, Australien National Univ.,Canberra
Quoc Dat Pham	Vietnam, Nat.Univ.Saigon/Umeå universitet
Fredric Ericson	
Weimin Li	Kina
Albert Philipes	Holland, Van´t Hoff Lab., Utrecht University
Kevin Roger	Frankrike, ENS CACHAN/ Université Paris XI
Andrew Nelson	Australien, Bragg Inst., ANSTO
Priti Mohanty	Schweiz, University of Fribourg
Simon Aben	Tyskland, BASF Ludwigshafen
Roberta Pigliapochi, BSc	Italien, LM Mater, Bologna
Felix Eltes	
Linda Månsson, BSc	
Stefan Kuczera	Nya Zeeland, University of Wellington
Kevin Roger	Frankrike, ENS CACHAN/ Université Paris XI
Luigi Gentile	Italien, Univ. of Calabria, Cosenza
Karen Edler	England, University of Bath
Luc Jaeger	USA, University of California
Simon Aben	Tyskland, BASF Ludwigshafen

Felix Grewe	Tyskland, Universität Paderborn
Norman J. Wagner	USA, University of Delaware
Luciano Galantini	Italien
Christoffer Johans	Finland, Aalto University, Helsinki
Ricardo Gaspar,dipl.worker MSci	Portugal, University of Coimbra
Kazuhiro Ishikawa	Japan, Kao Corporation
Norah Heinz, erasmus	Tyskland
Alexey Krivtsov	Ryssland, Kazan State Technology University
Paula da Silva	Portugal, University of Coimbra
Marek Twardoch	
Masayuki Imai	Japan
Samia Ouhajji	Nederländerna, Utrecht University
Robert Thomas	England, University of Oxford
Maria Wadsäter	Danmark, University of Copenhagen
Martha Brennich	Tyskland, Georg-August-Univ. Göttingen
Jan Dhont	Tyskland, Forschungszentrum Juelich GmbH
Philip Kuchel	Australien, University of Sydney
Felix Grewe	Tyskland, Universität Paderborn
Hanna Bergenholtz, BSc	
Bo Nyström	Norge, University of Oslo
Luca Monticelli	Frankrike, INSERM, Paris
Nitash Balsara	USA, Berkeley, University of California
Gavin Hazell	England, University of Bath
Bill Price	Australien, Univeristy of Western Sydney

WELCOME TO VISITORS

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, foreign students and guest professors. Visitors are very important for us and help us to improve our level of research and education.

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. 35 min.)

Visit the Kemicentrum website for further travel information:
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This report is produced by Cecilia von Arnold Communication officer at the Department of Chemistry, LU

TELEPHONE LIST

Physical Chemistry
Department of Chemistry
P.O. Box 124
SE-221 00 Lund
Telephone. +46 46 2228150
Facsimile: +46 46 2224413
www.physchem.lu.se

Direct phone: +46 46 22+extention
E-mail adresses:
firstname.surname@fkem1.lu.se
(å,ä,ö= a,a,o).

Name	Phone no.
Aadil Abbas	046-2224504
Alexei Abrikossov	046-2223248
Viveka Alfredsson	046-2228155
Jenny Algotsson	046-2228249
Johanna Bailey Jönsson	046-2228154
Solmaz Bayati	046-2228216
Manja Behrens	046-2228188
Hanna Bergenholtz	046-2220112
Sebastian Björklund	046-2224682
Saskia Bucciarelli	046-2228234
Lucia Casal-Dujat	046-2228234
Celen Cenker	046-2228188
Jerome Crassous	046-2223677
Paula da Silva	046-2224812
Aleksandra Dabkowska	046-2228234
Karen Edler	0462228163
Stefanie Eriksson	046-2228249
Tiago Ferreira	046-2223247
Ricardo Gaspar	046-2224812
Marie Grey	046-2224682
Charlotte Gustavsson	046-2228154
Sanna Gustavsson	046-2223247
Carin Hagsten	046-2228158
Norah Heinz	046-2228148
Christopher Hirst	046-2224954
Kazuhiro Ishikawa	046-2224504
John Janiak	046-2228216
Christoffer Johans	046-2224504
Ola Karlsson	
Tomas Kjellman	046-2223332
Patrik Knöös	046-2228163
Alexey Krivtsov	046-2228163
Majlis Larsson	046-2228150
Weimin Li	046-2224504
Ruiyu Lin	046-2224812

Name	Phone no.
Björn Lindman	046-2228160
Per Linse	046-2228151
Ilya Martchenko	046-2223677
Martin Medebach	046-2228175
Adriana Mihut	046-2228175
Priti Mohanty	046-2223677
Emelie Nilsson	046-2223332
Tommy Nylander	046-2228158
Sofi Nöjd	046-2224812
Marc Obiols-Rabasa	046-2223677
Samuli Ollila	046-2228216
Gerd Olofsson	046-2228185
Ulf Olsson	046-2228159
Samia Ouhajji	046-2223332
Divya Paloli	046-2223677
Dat Pham	046-2224812
Lennart Piculell	046-2229518
Karin Schillén	046-2221439
Peter Schurtenberger	046-2228219
Bruno Silva	046-2228150
Emma Sparr	046-2221536
Joakim Stenhammar	046-2223248
Anna Stradner	046-2228214
Maria Södergren	046-2223489
Olle Söderman	046-2228603
Krister Thuresson	
Fredrik Tiberg	046-2228150
Daniel Topgaard	046-2228204
Stefan Ulvenlund	7075-21434
Maria Wadsäter	046-2220112
Ingemar Wadsö	046-2228180
Håkan Wennerström	046-2229767
Erik Wernersson	046-2223248
Marianna Yanez	046-2220112
Malin Zackrisson	046-2228185
Ran Zhang	046-2223248

LUND UNIVERSITY

WWW.PHYSCHEM.LU.SE

LUND UNIVERSITY
Physical chemistry

P.O Box 124
221 00 Lund
Phone: 046-222 81 50
www.physchem.lu.se