CONTENTS

Cover:

Confocal fluorescence microscopy images of phospholipid bilayers supported by gallium phosphide nanowires. The bilayers are labelled with a rhodamine phospholipid (red). The vertical nanowires are laterally arrayed in various patterns on the surface.

By Aleksandra Dabkowska, Cassandra S. Niman, Gaëlle Piret, Henrik Persson, Hanna P. Wacklin, Heiner Linke, Christelle N. Prinz, and Tommy Nylander.

REFORMULATION

More and more often, innovation is mentioned alongside education and research as part of the central mission for a university. Accordingly, the current strategic plan for Lund University states as its goal to achieve "the highest quality in education, research and innovation and collaboration with the society around us". So, we should ask ourselves: How can the division of Physical Chemistry best contribute to innovation and collaboration with the society around us?

At Physical Chemistry we have since decades been involved in a large number of fruitful collaborations with industrial companies, big and small, in Sweden and abroad. Typically, the really successful cases are those where a project carried out at Physical Chemistry provides a fundamental understanding that is then used by an industrial researcher to create an innovation which makes a real difference in a specific context. If there is a single heading describing these innovations, this would be formulations: personal care formulations, pharmaceuticals, laundry detergents, paints, inks, food... To us who work with colloid and interface science, it is clear that ours is the science that can transform formulation work from an art into a science. And all of us who teach colloid and interface science find it natural to illustrate the usefulness of our subject with examples from everyday formulations that we may find in a kitchen, a bathroom or a garage.

Sweden is traditionally quite strong in colloid and interface science research and teaching, so it is rather remarkable that formulation science, as a generic branch of applied science, is not established here. This is in contrast to leading EU countries, such as the UK and France, where one finds employment ads asking for formulation scientists. Moreover, formulation science is more important than ever, for a number of reasons. Environmental concerns and the quest for sustainability create a pressure to generally minimize the use of chemicals and to replace those that are environmentally questionable with alternatives that are low-toxic and based on renewable resources. This calls for extensive "reformulation" of many common products. On top of this, the global competition regarding new innovative formulated products is increasing.

In the late spring of 2013, there was a call from VINNOVA (the Swedish Governmental Agency for Innovation Systems) and the Swedish Energy Agency to propose national so-called Strategic Innovation Areas. The idea with this ongoing large-scale activity, which addresses all industrial sectors, is to identify the most important strategic areas for Sweden where industry, the public sector and academia should collaborate to boost research, development and innovation. The identified strategic areas should have the potential to "create conditions for international competitiveness and to find sustainable solutions to global societal challenges". In response to the call, an initiative was taken by a group of Swedish scientists, including myself, to create an agenda for strategic reformulation research and innovation. The response from academia, research institutes and companies across application areas in Sweden was immediate and overwhelming. Together we almost managed to launch, in less than a year, a large national programme with substantial government support in the area. So, it is encouraging that the strategic importance of (re)formulation science for future innovation in large sectors of Swedish industry is now recognized by key government agencies such as VINNOVA.

To be continued!

Lennart Piculell
May 2014

RESEARCH PROJECTS

Theoretical work - Statistical mechanics

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. 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 2013, all softwares have been converted from static to dynamic memory allocation for more efficient use of memory and easier installation.

Spherical dielectric boundaries (Contact person: Per Linse)

Rapidly convergent expressions for the Green's function of the Poisson equation for spherically symmetric systems, where the dielectric constant varies discontinuously in the radial direction, were derived. These expressions were used in Monte Carlo simulations of various electrolyte systems, and their efficiency was assessed. The simulations were performed on six types of systems having either (i) a uniform surface charge distribution, (ii) a uniform volume charge distribution, or (iii) mobile ions, which were neutralized by mobile counterions. With only the leading term of the expansion included, a precision of the polarization energy of $0.005kT$ or better was achieved, which is smaller than the statistical uncertainty of a typical simulation. The inclusion of the dielectric inhomogeneity lead to a 2.5-fold increase of the computational effort, which is modest for this type of model. The ion density distributions were investigated for different dielectric conditions. These spatial distributions were discussed in terms of the importance of (i) the direct mean-field Coulomb interaction, (ii) the surface charge polarization at the dielectric discontinuity, and/or (iii) the change in the attractive Coulomb correlations. (Leo Lue (University of Strathclyde), Per Linse.)

Multigraft polymers in solution (Contact person: Per Linse)
Multigraft polymers comprise a subclass of branched polymers where more than one side chain is attached to each node (branching point) of the main chain. We have investigated structural properties of single multigraft polymers under good solvent conditions by Monte Carlo simulations, employing a flexible bead–spring model. Beside the grafting density, denoting the linear density of grafted side chains, we have introduced the concept of branching density, denoting the linear density of nodes. At high branching density, both the branching density and the branching multiplicity controlled the structure of the side chains, whereas at lower branching density only the branching multiplicity influenced the side-chain structure. The spatial extension of the main chain and side chains as a function of side-chain length and grafting density was analyzed using scaling formalism. The dependence of the main-chain extension on side-chain length, branching density, and branching multiplicity could be collapsed on a universal curve upon relevant rescaling. Multigraft polymers with equal number of side-chain beads but unequal numbers and lengths of side chains displayed unconventional bending properties. Few and long side chains gave rise to a still relative low locally stiffness but considerable long-range rigidity, whereas more numerous and shorter side chains lead to a higher local stiffness but to a smaller long-range rigidity. (Daniel Angelescu (Romanian Academy), Per Linse.)

Dynamics of polymer adsorption (Contact person: Per Linse)
Adsorption of uncharged homopolymers in good and theta solvents onto planar surfaces from solution at various chain flexibility and polymer--surface attraction strengths has been investigated by using a coarse-grained bead--spring polymer model and simulation techniques. Equilibrium properties of the interfacial systems have been obtained from Monte Carlo simulations by monitoring the bead and polymer density profiles, the number of adsorbed beads and polymers, the components of the radius of gyration perpendicular and parallel to the surface as well as tail, loop, and train characteristics. The adsorption process starting with a polymer-free zone adjacent to the surface was examined by Brownian dynamic simulations. At equilibrium, the adsorbed amount increased upon increasing chain stiffness and upon worsening of the solvent condition, and the structural characteristics depended also on the chain stiffness and solvent condition. The initial adsorption was diffusion controlled, but soon it became governed by the probability of a polymer to be captured by the surface attraction. Flexible polymers became flattened after attaching, but their final relaxation mechanism involved an increased perpendicular extension with fewer adsorbed beads and longer tails driven by the surface pressure originating from the surrounding adsorbed polymers. This structural rearrangement became more prominent at worsening of the solvent condition. Finally, the integration time denoting the adsorption time for adsorbed polymers to become fully integrated into the adsorbed layer and the residence times of integrated polymers were analyzed; in particular, the latter became longer with increasing chain stiffness and shorter upon worsening of the solvent condition. (Project completed.)

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 (PG) 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 situation, and study these systems in different solution condition by means of calorimetric studies combined with structural characterization. (Gerd Olofsson, Marie Grey, Emma Sparr.)

Anisotropic patchy protein-protein interactions

(Contact person: Malin Zackrisson Oskolkova)

In this project we are investigating the effect of anisotropy or patchiness on protein-protein interactions, using detailed Metropolis Monte Carlo computer simulations in combination with static light scattering and SAXS. The Monte Carlo simulations are combined with static light scattering (SLS) measurements of the second viral coefficient to provide insights into the origin of patchy, attractive protein interactions. We use Lactoferrin as our model protein, which has been predicted to display anisotropic attractive interactions and the calculated values of protein-protein interactions from the simulations leads to a good quantitative agreement with the experimental data, without any adjustable parameters. The molecular origin of the attraction is found to be a combination of a highly directional electrostatic contribution, a local charged patch, and van der Waals attraction. This gives rise to two competing electrostatic effects acting over different length scales, which is seen as an anomalous dependence in the virial coefficient as a function of electrolyte concentration. Currently the effect of the anisotropy on the phase diagram is being explored. (Weimin Li, Maxim Morin, Manja Behrens, Björn Persson (Division of Theoretical Chemistry), Mikael Lund (Division of Theoretical Chemistry), Malin Zackrisson Oskolkova.)

Polymer mediated interactions of PEGylated colloids

(Contact person: Malin Zackrisson Oskolkova)

In this project we have investigated how steric interactions, by surface-grafted PEG polymer on colloidal particles, translates into effective attractions and its effect on the static structure, phase behavior and dynamics. In particular, the interrelation between attractions, aggregation and a hidden fluid-fluid transition. These PEGylated particles differ from the commonly used non-aqueous systems for which crystallization in the polymer shell acts to trigger the attractions. Here, this water-based system offers a more controlled approach where the solvent quality for PEG is varied and found to smoothly regulate the interactions. From a quantitative analysis of small-angle neutron scattering data we can extract the effective attraction and locate an otherwise hidden spinodal line in the phase diagram, which is found in close proximity of the region where the system visibly aggregates. In contrast to what is commonly assumed, the effective attraction is found to depend on particle concentration at high volume fractions and the attraction is no-longer pairwise additive. This aspect should serve as impetus for further studies of graft-mediated interactions.

Furthermore, Core-shell particles with a fluorinated core are now being synthesized and characterized using Cryo-TEM. 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. (Marcel Ollila, Jeanette Ulama (Physical Chemistry, Göteborg University), Johan Bergenholtz (Physical Chemistry, Göteborg University and Physical Chemistry, Lund University), Malin Zackrisson Oskolkova.)

Surface adsorption versus bulk aggregation of colloidal particles

(Contact person: Lennart Piculell)

We are studying 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. This prediction is verified ty 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, Viveka Alfredsson.)

How lipid membrane are protected 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. In seeds and plants, a class of protein named dehydrins are also present to protect agains dehydration.

The question addressed in the project concerns the molecular mechanism(s) behind the role of the osmolytes and dehydrins in membrane systems under osmotic stress. By studying model lipid systems using a range of methods such as sorption calorimetry, sorption balance, X-ray diffraction/scattering and NMR we aim to unravel how the presence of different polar molecules and dehydrins interacts with phospholipid bilayers. We have previously studied urea and glycerol. In on-going studies, we explore the influence of dehydrins as well as other small polar molecules such as monosacharides, TMAO and PCA. (Dat Pham, Jenny Andersson, Emma Sparr, Håkan Wennerström, Pia Harrysson (Stockholm University), 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 DNAprotein complex, are involved in organization of the chromatin and regulation of gene expression. Another example is the finding that the inclusion of proteins in DNA-lipid complexes for gene therapy can greatly enhance the transfection efficiency. The aim of this project is to gain an improved understanding of the physicochemical behavior of such systems. Of particular interest is the structure and composition of aggregatesand 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, Anna Carnerup, John Janiak, Karin Schillén, Viveka Alfredsson, Daniel Topgaard, Björn Lindman, Maria da Graça Miguel, Henrique Faneca and Maria C. Pedroso de Lima at University of Coimbra, Coimbra, Portugal; Lars Nordenskiöld and Nikolay Korolev, Nanyang Technological University, Singapore.)

Drying interfaces (Contact person: Emma Sparr)
At the interface between two regions, for example the air–liquid interface of a lipid solution, there can arise non-equilibrium situations. In most cases, the condensed phase is not in equilibrium with the vapor phase, and as a consequence there will be evaporation of water and possible also other volatile components. There might also be dissolution of compounds from the gas phase into the solution. This non-equilibrium situation implies several simultaneous transport processes across the interfacial layer separating the condensed and the gas phases, which in turn can have consequences on the molecular organization in the interfacial layer. In systems containing of self-assembling amphiphilic molecules or colloidal suspensions, there is then a possibility of transport-generated interfacial phase separation. This is an apparent possibility in laboratory experimental studies of amphiphilic and colloidal systems. Similar conditions also exist in living systems, with obvious examples found in the lipid tear film formed on our eyes, which prevent evaporation and dry eyes, and the membrane system in the alveoli of the lung. In this study, we explore the underlying mechanisms of transport-generated interfacial phase separation using a combination of surface together with theoretical modelling solving diffusion equations. (Emma Sparr, Tahereh Mokthari, Håkan Wennerström, Karen Edler (University of Bath), Christoffer Åberg (University College Dublin).)

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. Project completed in December 2013. (Johanna Bailey Jönsson, Ola Karlsson, Lennart Piculell.)

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

The aim is to understand the physical chemistry of soluble complex salts in aqueous solution and the intermolecular interactions involved. A complex salt is defined as the neutral salt of surfactant ions (aggregated into highly charged micelles) that interact with a polyelectrolyte chain, which in turn acts as a large counterion (the polyion). The complex salts consist of polyacrylate (PA^-_y) and cationic $C_{16}TA^+$ surfactant ions, denoted $C_{16}TAPA_y$, where y is degree of polymerization. At high water contents, the investigated complex salts exhibit miscibility gaps that consist of co-existing phases: a concentrated phase (either cubic or hexagonal internal structure) and a less concentrated phase. In order to make the complex salts soluble, PEO-containing nonionic surfactants of the type C_iE_j are added. The phase studies on systems containing $C_{16}TAPA_y$ complex salts in water mixed with either $C_{12}E_5$ or $C_{12}E_8$ are carried out by visual inspection of the samples and by using small-angle X-ray scattering (SAXS). They reveal that the solubilization of the complex salts increases with increasing PEO-chain length of the nonionic surfactant. To gain further insight of the dissolution process, isothermal titration calorimetry (ITC) is employed. The soluble complex salt aggregates of $C_{16}TAPA_{25}$ or $C_{16}TAPA_{6000}$ and $C_{12}E_8$ are characterized in dilute aqueous solution in terms of size, structure and composition by dynamic light scattering (DLS), SAXS and self-diffusion NMR. In a related study, thermoresponsive and stable nanoparticles consisting of PA^-_{6000}, $C_{16}TA^+$ and $C_{12}E_5$ with either bicontinuous cubic or hexagonal ordered interior have been prepared and characterized by DLS, SAXS, cryo-transmission electron microscopy and electrophoretic mobility measurements. (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).)

Structured surface layers of polymer-surfactant assemblies

(Contact person: Lennart Piculell)

A surface layer that contains both hydrophobic and hydrophilic domains can function as a semi-permeable barrier, as a depot for material to be released from the different domains, or as an absorbent of substances in a surrounding fluid phase. For all these functions, it is of importance to control the size of the domains, 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. Direct application of ethanolic polyion-surfactant ion “complex salts” on a surface, followed by evaporation of the ethanol, has proven to be an easy method to coat hydrophobic as well as hydrophilic surfaces with polymer-surfactant assemblies. The structures of the layers can be controlled by choice of the polymer and/or the surfactant, by added cosurfactants, and by control of the water activity in the medium surrounding the layer. The structures obtained correspond largely to those found in studies of bulk systems of the same compositions as the surface layers. SAXS is used to study the surface structures. (Charlotte Gustavsson, Lennart Piculell, Joaquim Li and Karen Edler.)

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. Project completed. (Mehran Asad Ayoubi, Lennart Piculell, Ulf Olsson, Alexei Khokhlov (Moscow State University/Russian Academy of Science), Bo Nyström and Kaizheng Zhu (University of Oslo) and Kristoffer Almdal (Micro- and Nanotechnology, DTU).)

Cellulose dissolution (Contact persons: Björn Lindman and Ulf Olsson)

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. Scattering techniques and NMR are used to characterize that state of cellulose in solution. (Björn Lindman, Ulf Olsson, Daniel Topgaard and B. Medronho, L. Alves and M. Miguel (Coimbra).)

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 $\phi eff >> \phi cp$, 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 Schurtenberger.)

Flexibility and conformation of giant dendronised polymers

(Contact person: Peter Schurtenberger)

In recent years an interesting new class of polymers and polyelectrolytes has been developed, the so-called dendronized polymers. The unusual structure of these polymers with their tight and highly branched layer around the backbone has raised fundamental questions in polymer science, which all have their origin in the influence of the layer on the conformation and rigidity of the backbone. We investigate the effect of the dendrons on the chain stiffness, and look at the influence of charge and solvent on the cross-sectional conformation, the flexibility, and on the interchain correlation at higher densities using SANS, SAXS and light scattering. (Sebastian Lages, Peter Schurtenberger, Dieter Schlüter (ETH Zurich, Switzerland), 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. We compare the experimental results with those obtained by computer simulations. (Ilya Martchenko, Jérôme J. Crassous, Per Linse, Erik Wernersson, Ann Hirt (ETH Zurich, Switzerland), Vincent Martinez and Wilson Poon (University of Edinburgh, UK), 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, Jérôme Crassous, Priti Mohanty, Emanuela Zaccarelly (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 14 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.) (Project completed.)

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 $U_{SS}(r)$, $U_{LL}(r)$, and $U_{SL}(r)$ 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, Emanuela Zaccarelly (University La Sapienza Rome, Italy), 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 "ultrasoft" 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. We finally study the effect of particle anisotropy by using also ellipsoidal core-shell microgels. For these systems we also perform extensive computer simulations. (Jérôme J. Crassous, Priti Mohanty, Sofi Nöjd, Per Linse, Erik Wernersson, Anand Yethiray (Memorial University, St. John's, Canada), Christos Likos (University of Vienna, Austria), Jan Dhont (Forschungszentrum Jülich, Germany), Peter Schurtenberger.)

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 states. 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).)

Magnetic particles (Contact person: Per Linse)
Fluids of spherical colloids possessing an off-centered embedded magnetic dipole were investigated by using Monte Carlo simulations. Systems of colloids with different strength and direction of the embedded dipole moment confined in a 2D space without and with external magnetic field applied were considered. The fluids were characterized by radial distribution functions, angular distribution functions, cluster data, and energetic data. In the absence of an external field, the colloids form dimers and trimers at sufficiently large magnetic moment without tendency of forming chains of colloids as appearing in systems with particles possessing a central magnetic dipole. In the presence of an external field, chains of colloids aligned in a zigzag fashion were formed for a field parallel to the plane of the particles, whereas the colloidal ordering were suppressed in the presence of a field perpendicular to that plane. The findings agree surprisingly well with recently experimental observations on fluids containing spherical polymer colloids with embedded single-domain magnetic hematite cubes. (Stefano Sacanna (New York University), Albert P. Philipse (Utrecht University), Alexei Abrikossov, Per Linse.)

Brush polymers at solid surfaces (Contact person: Per Linse)
A series of cationic diblock copolymers, poly(*N*-isopropylacrylamide)$_{48}$-*block*-poly((3-acrylamidopropyl)trimethylammonium chloride)$_X$, abbreviated as PNIPAAM$_{48}$-*b*-PAMPTMA^+_X, with $X = 0, 6, 10, 14$ and 20 have been synthesized, and their adsorption onto silicon oxynitride from aqueous solution has been investigated using dual polarization interferometry. The polymer adsorption was modeled by using a lattice mean–field theory, and a satisfactory consistency between theory and experiments was found in terms of surface excess and layer thickness. Both theory and experiments show that the adsorption is limited by steric repulsion for $X < X_{max}$ and by electrostatic interactions for $X > X_{max}$. Modeling demonstrates that significant surface charge regulation occurs due to adsorption. Both the nonionic and cationic block exhibit nonelectrostatic affinity to silicon oxynitride and thus contribute to the driving force for adsorption, and modeling is used for clarifying how changes in the nonelectrostatic affinity affects the surface excess. The segments of the nonionic and cationic blocks seem less segregated when both have a nonelectrostatic affinity to the surface compared to the case where the segments had no surface affinity. Adsorption kinetics was investigated experimentally. Two kinetic regimes were observed: the adsorption rate is initially controlled by the mass transfer rate to the surface and at higher coverage limited by the attachment rate.

Furthermore, we have investigated structural and thermodynamic properties of surface-grafted layers of model 'bottle-brush' polymers by Monte Carlo simulation. The polymers consisted of a longer main chain densely grafted with shorter side chains, of which the latter have some degree of affinity to the surface. Our focus is on the effect of the side-chain surface affinity on the brush properties, which we study in terms of compression isotherms spanning a broad range of grafting densities. For low grafting densities, side-chain adsorption causes the polymers to spread on the surface. As the grafting density is increased, the layer goes through a 'pancake-to-brush' transition to form a brush with the main chains aligned perpendicular to the surface. We find that side-chain adsorption is decisive for the structure of dilute layers and in the transition region, but has little influence on the properties of dense brushes. The close relation between compression and adsorption isotherms is discussed, and the implications of side-chain adsorption for the ability of the polymer to form a dense brush are investigated. This analysis suggests that side-chain surface affinity alone will not give rise to 'brush of bottle-brushes' layers by adsorption of polymers from solution, in agreement with recent experimental results. (Alexander Shovsky, Andra Dedinaite, and Per M. Claesson (KTH), Stefan Knohl (Chemnitz University of Technology), Kaizheng Zhu, Anna-Lena Kjøniksen, and Bo Nyström (University of Oslo), Erik Wernersson, Per Linse.)

Temperature-responsive supramolecular structures based on γ-cyclodextrin and polymers containing PNIPAAM chains (Contact person: Karin Schillén)

Pseudopolyrotaxanes or inclusion complexes are supramolecular assemblies formed by a polymer chain, which is threaded by several cyclodextrin (CD) molecules. CDs are cyclic oligosaccharides with a hollow cavity. In this project, we investigate the inclusion complex formation between γ-CD and diblock copolymers containing thermoresponsive poly(N-isopropylacrylamide) (PNIPAAM) chains in solid state, in solution, at silica/liquid interfaces. When temperature approaches the lower critical solution temperature of PNIPAAM, the CD molecules dethread. The experimental techniques employed are 1H-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. In a related project, the formation of coacervate core micelles of cationic and anionic PNIPAAM copolymers in dilute aqueous solution is studied using dynamic and static light scattering, differential scanning calorimetry and small angle X-ray scattering. (Solmaz Bayati, Karin Schillén, Giuseppe Lazzara (University of Palermo, Italy), Tommy Nylander, Gerd Olofsson, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway), Viveka Alfredsson, Richard Campbell (ILL, France).)

The interaction between PEO-PPO-PEO triblock copolymers and bile salts

(Contact person: Karin Schillén)

The long-term aim of this project is to investigate the possibility of using nonionic triblock copolymers of poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO) instead of ion exchange resins in the therapy of bile acid diarrhea. Bile acids are biological surfactants with a rigid four-ring system, not completely hydrophobic because of the presence of some hydroxyl groups, joined to a carboxylic head by an alkyl chain. In this project, physiochemical studies of the interaction between the bile salts, typically sodium glycodioxycholate (NaGDC), and PEO-PPO-PEO copolymers of various block lengths are carried out by means of dynamic and static light scattering (DLS and SLS), small angle X-ray scattering (SAXS), differential scanning calorimetry (DSC) and self-diffusion NMR. The experimental results obtained for the first system studied ($EO_{20}PO_{69}EO_{20}$ [P123] with NaGDC) reveal that the interaction process at constant copolymer concentration present three bile salt concentration regimes. At low bile salt concentrations, bile salt monomers associate with the copolymer micelles forming a large copolymer-rich complex that becomes increasingly charged upon increasing NaGDC concentration. At intermediate concentrations, small bile salt rich-P123 complexes coexist with the larges complexes, which start to disintegrate. At high bile salt concentrations (depending on the temperature), the small bile salt rich-P123 complexes are the dominant species in the system. Investigation of the dependence of the bile salt-copolymer interaction on added salt, relative copolymer block lengths and type of bile salt are planned as well as small angle neutron scattering experiments. (Solmaz Bayati, Karin Schillén, Gerd Olofsson, L. Galantini (University of Rome "La Sapienza", Italy).)

Experimental methodologies

Raman dynamic light scattering – bringing chemical specificity of 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), Peter Schurtenberger.)

Diffusive transport of multivalent ions in cartilage (Contact person: Olle Söderman)

Articulate cartilage is a complex material, composed of collagenous fibers, and cells called chondrocytes, all of which are embedded in a firm gel-like ground substance. The chondrocyte cells produce proteoglycans which bind to hyaluronic acid, forming large highly hydrophilic aggregates. These aggregates are entangled with each other and with the collagen fibrils forming what can best be described as a hydrogel that sits within the collagen network. In the general accepted model of the morphology of cartilage, the collagen fibrils associate into columnar structures that extend outward from the bone. The protoeglycans are highly charged due to the presence of sulfate and carboxylic groups. The break-down of cartilage results in a lowering of the concentration of the proteoglycans. It has been suggested to use (Gd-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), 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 nonionic surfactants with poly(ethylene oxide) or glucoside headgroups, lipid/cholesterol membranes, synthetic analogs of the lipid mixtures in the stratum corneum, and lung surfactant extracts. (Daniel Topgaard, Sanna Gustavsson, Dat Pham, Jenny Andersson, Emma Sparr, Tiago Ferreira, Olle Söderman, Samuli Ollila, Johan Reimer, Stefan Ulvenlund (CR Competence).)

Diffusion MRI methods development (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 experimental protocols for estimating parameters such as cell shape, orientation, and membrane permeability. 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 and Freddy Ståhlberg (Lund BioImaging Center), Samo Lasic and Karin Bryskhe (CR Development), Carl-Fredrik Westin (Harvard Medical School), Hans Knutsson (Linköping University).)

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), 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 Medicine. (Weimin Li, Kajsa M. Paulsson (Experimental Medical Science, Faculty of Medicin), 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 (Université Paris-Sud, France), George Thurston (Rochester Institute of Technology, USA), Corinne Jud (University of Fribourg, Switzerland), Mikael Lund, Peter Schurtenberger, 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, Anna Stradner.)

Amyloid interaction with lipid membranes (Contact person: Emma Sparr)
Amyloid protein aggregation is associated with over 30 known diseases in humans. In amyloid plaques associated with several amyloidogenic diseases, tightly associated lipids

have been identified. For several of the amyloid disorders, protein aggregation has also been associated with membrane disruption in cells and in model lipid systems. In this project, we investigate interactions between aggregating amyloid proteins and lipid membranes, and we explore the basic principles of the amyloid-lipid coaggregation.

The proteins Aβ and α-synuclein are found in the protein aggregates characteristic for Alzheimer and Parkinson disease, respectively. In this project, we study interactions between the amyloid proteins α-synuclein Aβ (M1-40) or Aβ (M1-42) and lipid membranes. We use model membranes with varying lipid compositions, and biological membranes in isolated exosomes. We study protein-lipid co-aggregation, membrane association and the consequences of protein-lipid interaction on aggregation kinetics and membrane intergrety. In this project we explore different biophysical techniques, including PT ssNMR, confocal microscopy on giant unilamellar vesicles, fluorescence correlation spectroscopy, fluorescence spectroscopy, QCM-D, neutron reflectivity and cryo-TEM. (Ricardo Gaspar, Erik Hellstrand (Division of Biophysical Chemistry, LU), Marie Grey, Aleksandra Dabkowska, Agnieszka Nowacka, Daniel Topgaard, Sara Linse (Division of Biochemistry and Structural Biology, LU), Emma Sparr, Chris Dunning and Patrik Brundin (Wallenberg Neurocenter, LU), Marie-Louise Ainalem (ESS AB), Tommy Nylander, Chris Dobson (Cambridge University, UK).)

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. (Marianna Yanez, Marie-Louise Ainalem (ESS AB), Syma Khaled (University of Southampton), Anna Carnerup, John Janiak, Viveka Alfredsson, Tommy Nylander, Dan Lundberg, 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)
The role of the genome in the assembly of icosahedral viral capsids has been investigated by molecular dynamics simulation of a coarse-grained model, in which the capsomers carry explicit charges and the polynucleic acid is represented by a bead-spring chain. The co- assembly process was contrasted with the self-assembly of uncharged capsomers. In the co- assembly, the capsomers first associated to the polyion and then rearrange into a capsid, whereas the self-assembly proceeded through a spontaneous nucleation and growth of partial capsids. The polyion backbone stiffness was found to have a significant effect on the co- assembly process; polyions of intermediate flexibility gave the fastest and most faithful assembly process. Addition of a small amount of monovalent salt also improved both speed and fidelity of the co-assembly process. Moreover, the capsid assembly process in terms of cluster size development and encapsulation efficiency was investigated by employing different polyion topologies from linear to dendritic ones. With increased branching degrees of the polyion, the encapsulation process is significantly steered to the formation of icosahedral T1 capsids. The dendritic polyions were entirely encapsulated in an ordered capsid structure for all the designed polyion/ capsid charge ratios considered. (Ran Zhang, Erik Wernersson, Per Linse.)

The skin as a barrier of molecular diffusion (Contact person: Emma Sparr)
The human skin is a large (ca. 2 m2) membrane that separate regions with profoundly different properties. This implies that several simultaneous transport processes occur across a non-equilibrium system. The skin is a vital organ, and its outer layer, stratum corneum (SC) forms the barrier that prevents from desiccation and protects against the uptake of hazardous chemicals. SC also highly attractive as a target for directed and controlled delivery of drugs.

We aim at a characterization of the material properties of the SC by coupling macroscopic SC barrier properties to its molecular structure and dynamics. The SC is a sophisticated barrier in that behaves as a responding membrane, and diffusional transport can be regulated by changes in the skin environments. One example is the abrupt increase in SC permeability at high degrees of SC hydration. This penetration enhancement is taken advantage of in transdermal drug delivery, and it is called "occlusion effect". Through a complementary experimental and theoretical approach, we have provided a molecular explanation to this effect.

The skin is regularly exposed to osmotic stress due dry and cold climate of the external environment. In the skin, the osmolytes are referred to as the natural moisturizing factor (NMF). We investigate how osmolytes as well as other polar, apolar and amphiphilic molecules influence the molecular properties of SC components and the macroscopic barrier properties of the skin. We characterize the lipid and protein components in intact stratum corneum using natural abundance PT ssNMR, sorption calorimetry and X-ray diffraction. This is combined with transport studies of different drugs across intact stratum corneum in the presence several gradients. (Dat Pham, Sebastian Björklund, Emma Sparr, Daniel Topgaard, Johan Engblom (Biofilms; Malmö University), Krister Thuresson (Hemocue), Lars Wadsö (Building materials, LTH), Joke Bouwstra (Leiden University), Vitaly Kocherbitov (Malmö University), Bernard Cabane (ESPCI, Paris), Katarina Ekelund (LeoPharma, Copenhagen).)

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, Marc Obiols-Rabasa, Johan Bergenholtz, Bela Farago (ILL Grenoble, France), Olaf Holderer (Juelich Centre for Neutron Science (JCNS), Germany), Simon Poblete (FZ Juelich, Germany), Roland Winkler (FZ Juelich), Gerhard Gompper (FZ Juelich), Jan Dhont (FZ Juelich), Giuseppe Foffi (Université Paris-Sud, France), George Thurston (Rochester Institute of Technology, USA), Mikael Lund, Sara Linse, Peter Schurtenberger, Anna Stradner.)

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, Daniel Topgaard.)

RNA assemblies at model lipid membranes (Contact person: Emma Sparr)

Nanostructured 3D assemblies of RNA are determined by the formation of specific interactions between constituent nucleotides, while changes in the salt environment can be explored to control the folding and assembly of the 3D structure. In this project, we take advantage of electrostatic interactions to form and control the supra-molecular assembly of negatively charged 3D RNA polyhedrons on cationic and mixed zwitterionic/cationic fluid lipid bilayers. We use complementary surface techniques, inluding combined QCM-D and ellipsometry and fluorescence recovery after photobelaching (FRAP), and we study the RNA polyhedrons self-assembly at the bilayer scaffold. The understanding of RNA assembly at lipid surfaces may have important implications for the development of functional composite lipid/nucleic acid nano-architectures that may be used as nano-devices, diagnostic tools or therapeutics in nanotechnology, nanomedicine and synthetic biology. (Aleksandra Dabkowska, Tommy Nylander, Emma Sparr, Fredrik Höök (Chalmers), Luc Jaeger (University of California, Santa Barbara).)

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 and Giuseppe Zaccai (ILL), Carl Holt (University of Glasgow), Tommy Nyland, 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.

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

Lung surfactants (Contact person: Emma Sparr)
The alveolar surface is lined by film of submicron thickness between the epithelial cells and the alveolar lumen with the main function to lower the surface tension. The aqueous bulk structure of this layer consists of lipid bilayers forming lamellar bodies (LB:s) and tubular myelin (TM), and two hydrophilic proteins in the outside water; SP-A and SP-D. We are studying the interfacial and bulk structure of and phase transitions in this lung surfactant extracts and model systems using ssNMR, SAXS/WAXS, ellipsometry, monolayer techniques and cryo-TEM. Another aspect of the project is the diffusion in through the interfacial lipid membrane with complex structure that implies a diffusional permeability that is different for hydrophilic and hydrophobic substances. (Jenny Andersson, Tommy Nylander, Marcus Larsson (Lund University Hospital), Daniel Topgaard, Emma Sparr.)

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. (Project completed.) (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 microscope (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.)

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, 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 tablet swelling/dissolution behavior and the drug release from 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 molecular transport of various species (water, surfactant, a hydrophilic model substance) into and out of the swelling tablet is obtained from NMR Chemical Chift Imaging, giving clear evidence of the consequences of the presence or absence of hydrophobic association for these molecular transport processes. (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 persons: Tommy Nylander and 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. 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. The aim of the present project is to provide fundamental understanding of the kinetics of this process by combining models of kinetics with experimental data by obtained by using surface techniques such as neutron reflectometry and ellipsometry as well as scattering techniques to reveal the changes in composition at the interface versus time. (James Holdaway, Tommy Nylander, Lennart Piculell, E. Johnson, R. Panandiker and M. Sivik (Procter & Gamble, Cincinnati), 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 2 wt % sodium alginate by means of the phase inversion temperature (PIT) emulsification method. This method allows the preparation of finely dispersed emulsions without a large input of mechanical energy. With alginate concentrations of 1-2 wt % in the aqueous phase, emulsions showed good stability against Ostwald ripening and narrow, unimodal distributions of droplets with radii <100 nm. Gelation of the alginate is induced by the addition of aqueous $CaCl_2$ to the emulsions under stirring and particles formed are collected using a simple procedure based on extraction of the surfactant on addition of excess oil. The final particles are characterized using cryo-transmission electron microscopy (cryo-TEM) and dynamic light scattering (DLS). They were found to be essentially spherical with a homogeneous interior and their size was similar to that of the initial emulsion droplets. The herein presented "low-energy" method for preparation of biocompatible nanoparticles has the potential to be used in various applications, e.g. for the encapsulation of sensitive biomacromolecules.

(Project completed.) (Alexandra H. E. Machado, Dan Lundberg, António J. Ribeiro (Coimbra University), Francisco J. Veiga (Coimbra University), Björn Lindman, Maria G. Miguel (Coimbra University), 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), Niklas Lorén (SIK AB, The Swedish Institute for Food and Biotechnology Structure and Material Design).)

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. (Project completed.) (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.)

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), 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), 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 $\lambda 0$= 632.8nm 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 $0.0034 \le q \le 0.025$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 $0.0027 \le q \le 0.031$ 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 oC). 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 $Å^{-1}$.

NMR

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 instrument has accessories for microimaging, solid-state, and high-resolution magic-angle spinning experiments. (Sponsored by VR/KFI.)

Bruker Avance II 500

Magnet: 11.7 T / 500 MHz, 54 mm UltraShield

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

Bruker Avance II 200

Magnet: 4.7 T / 200 MHz, 89 mm

Probes: BBO 10mm (31P-15N/1H), DIF-25 5mm (1H)

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 61TM 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 calorimeters (ITC)
(Contact persons: Emma Sparr and Gerd Olofsson)
* A VP-ITC Isothermal Titration Microcalorimeter from MicroCal (GE Healthcare) was purchased in 2010. This is a ultrasensitive microcalorimeter for samples in solution. The instrument has an active cell volume of ca 1.4 ml, and it operates for temperatures between 2°C to 80°C. 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 include precision liquid delivery system for accurate and reproducible injections and user-selectable mixing speeds to match sample conditions. (Sponsored by the Knut and Alice Wallenberg Foundation.)
* Isothermal titration microcalorimeter 2277 TAM Thermal Activity Monitor System.

Reaction calorimeter (Contact person: Ola Karlsson)
The energy released as heat by a process is directly proportional to the rate of reaction and by monitoring the reaction in a calorimeter detailed kinetics can be revealed. In 2011 we got a Chemical Process Analyser CPA202 from Chemisens. It is a high precision factory pre-calibrated calorimeter made in Hastelloy C276 with a useful volume of 10 – 180 ml, which can be continuously varied during experiments. The temperature range for experiments is -50°C to +200°C and it is possible to operate in a pressure range from vacuum up to 20 bars. The temperature resolution for an experiment is 0.001°C and the power resolution is 0.001 Watt in the standard reactor and in the so called HighSens Reactor, which will be used for e.g. adsorption kinetics, crystallization, dissolution of tablets and micellization it will be 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 -30oC and 150oC with temperature stability at thermal equilibrium of ±0.1 oC, 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.

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.

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.)

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

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.

Division of Surface and Materials Chemistry of the Swedish Chemical Society

(Contact persons: Viveka Alfredsson and 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 conference in 2013, held in Stockholm, was a one-day meeting focusing on the trends in surface and materials chemistry "Green and sustainable surface and materials chemistry". Viveka Alfredsson and Lennart Piculell are serving as members of the board.

Strategic Research Areas and 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.

EU FP7-PEOPLE-2013-ITN – BIBAFOODS Network

(Contact person: Tommy Nylander)

This project was granted during autumn 2013 and will start 1 February 2014. The "BIopolymer BAsed FOOd Delivery Systems" (BIBAFOODS) network will train young researchers for the advancement of food science and technology, by providing them with the complementary skills necessary to develop the future sustainable food industry and entrepreneurial skills crucial for creating biotechnological food oriented start-up companies. This collaborative training network will combine the complementary training capabilities of each individual partner institution to improve the trainees' chances for employment and promote health and welfare in the EC by providing the capability to develop novel functional foods. The scientific focus of the research training is on colloidal delivery systems to protect and deliver active components via foods, resulting in novel functional foods. The development of these systems is to be based on only food-grade ingredients and upon economical feasible processes. The hypothesis is that the materials and coatings can be made responsive to the external chemical conditions and therefore suitable for controlled releases targeted at a desired stage during food processing or at a specific point during digestion of the food, e.g. in the intestinal tract. This will involve probiotic bacteria and enzymes that are liberated and allowed to be active in a controllable way. The ultimate successful materials ensure stability of the active component during long term storage prior to food production, during food production or during digestion, but at the same time liberating the active component at the right point. The behaviour and interaction of the delivery systems will be studied by simulation of gastric and intestinal conditions and by implementation in food production and formulation into probiotic products. BIBAFOODS will train 14 young researchers distributed among 11 industrial and academic partners, among them Physical Chemistry, Lund University.

CONFERENCES, TRAVELS AND SEMINARS

Jérôme Crassous gave an oral presentation at the International Soft Matter Conference in Rome, Italy.

Aleksandra Dabkowska gave an invited lecture at the ESS Science Day in Malmö, Sweden. She also contributed a talk at the Neutrons and Life Science meeting (Lund, Sweden) and presented posters at 4th Scandinavian Meeting on Amyloid Proteins and Disease (Lund, Sweden) and the "Global Challenges – Opportunities for Nanotechnology" workshop (Venice, Italy).

Charlotte Gustavsson gave an oral presentation at the 14th European Student Conference on Colloid and Interface Science in Potsdam, Germany. Another oral presentation was given at the 27th Conference of European Colloid and Interface Society in Sofia, Bulgaria.

Patrik Knöös gave an oral presentation at Formula VII in Mulhouse, France.

Weimin Li presented a poster at the conference 4th Scandinavian Meeting on Amyloid Proteins and Disease in Lund, Sweden.

Ruiyu Lin presented a poster at the conference 8th International Mesostructured Materials Symposium in Awaji, Japan and at the workshop on Transmission Electron Microscopy in Antwerp, Belgium.

Björn Lindman gave plenary lectures at the 11th Conference on Colloid and Surface Chemistry in Iasi, Romania; at the IVth International Conference on Colloid Chemistry in, Moscow; at the conference Fine Chemicals in Nanjing, China; at the International Conference on "Surface Science and Nanotechnology in Biomedical, Pharmaceutical and Engineering Systems" (ICON-NANO 2013), in Nadiad, India. He gave invited lectures at Ekmandagarna, Stockholm, the workshop "Synthesis, Kinetics and Catalytic Aspects of Biocolloids", in La Valetta, Malta, the workshop "Balance of Interactions in condense matter systems", Nicosia, Cyprus, the AVANT Institute symposium on formulations and polymers in Paris, the WWSC workshop in Stockholm, the 5th Asian Conference on Colloid and Interface Science, Bagdogra, India. 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: Procter&Gamble Research Center, Singapore; Procter&Gamble Research Laboratories, Cincinnati; Nanyang Technological University, Singapore; Chemical & Biological Engineering Dept., University at Buffalo, Buffalo, NY; Lappeenranta University of Technology, Lappeenranta Finland; Materials Science, CSIRO, Melbourne; Oslo University; University of North Bengal, Darjeeling, India; Dharmsinh Desai University, Nadiad, Gujarat, India; Sun Pharmaceutical Industries Ltd, Tandalja, Vadodara, Gujarat, India; Institute of Chemical Technology (Deemed University), Matunga, Mumbai, India; MidSweden University, Sundsvall, Sweden; Royal Institute of Technology, Stockholm; BASF Research Center, Düsseldorf, Germany; Elkem Research Laboratories, Kristiansand, Norway; Åbo Akademi University, Finland; School of Chemical Engineering, Nanjing University of Science and Technology, China. Furthermore, Björn Lindman was visiting proefessor at Nanyang Technological University, Singapore.

Adriana Mihut gave an oral presentation and presented a poster at the International Soft Matter Conference in Rome, Italy.

Priti Mohanty gave an oral presentation at the conference Physics of Complex Colloids in Ljubljana, Slovenia.

Emelie Nilsson presented a poster at the 8th International Mesostructured Materials Symposium at Awaji Island, Japan.

Tommy Nylander gave invited plenary lectures at European Colloid and Interface Society Meeting in Sofia, Bulgaria as well as at American Chemical Society meeting in Indianapolis, USA. He gave oral presentations at ”The Impact and Future Directions of Scattering Techniques in Soft Matter – Symposium honoring Prof. Jeff Penfold”, University of Oxford, UK; International Conference on Neutron Scattering, Edinburgh, UK as well as at the ISIS/DIAMOND workshop Emerging Themes in Analysis of Grazing Incidence Small Angle Scattering, Coseners House, Abingdon, UK. He also gave invited talks at University of Cagliari, Sardinia, Italy; University of Napoli, Italy; and Technical University Munich, Germany.

Sofi Nöjd presented a poster at the 14th European Student Colloid Conference, Potsdam-Golm, Germany.

Marc Obiols-Rabasa gave oral presentations at the SoftComp Annual Meeting in Rimini, Italy, and at the Swedish Neutron Scattering Society Meeting in Uppsala, Sweden. He also gave an invited lecture at the Department of Pharmacy, University of Copenhagen in Copenhagen, Denmark.

Ulf Olsson attended the Annual Nordic workshop on Scattering from Soft Matter in Copenhagen and the International Soft Matter Conference in Rome. He gave an invited talk at the Gruppo Italiano Discussione Risonanze Magnetiche in Bari, Italy. He also visited and presented seminars at Universidad Complutense in Madrid and the University of Delaware.

Quoc Dat Pham gave an oral presentation at the workshop From Molecule to Man! – Topical Research in the Malmö-Lund area at ASA Herrgård.

Lennart Piculell gave lectures at the Soft Matter Symposium in Wageningen, the Netherlands (invited), the 11th Conference on Colloid and Surface Chemistry, Iasi, Romania (plenary) and the AkzoNobel Nordic Prize Symposium in Stenungsund, Sweden (invited).

Karin Schillén presented two posters at the International Soft Matter Conference, in Italy, Rome.

Peter Schurtenberger gave an invited keynote lecture at Formula VII International Workshop in Mulhouse, France, and he also gave invited lectures at the following international conferences, workshops and summer schools: workshop on “SAXS and coherent X-ray scattering” in Marstrand, Sweden; International Workshop on Modern Light Scattering Technologies, Leeds, England; Neutron Spin Echo Science Case Meeting, Düsseldorf, Germany. Peter Schurtenberger also gave the following invited seminars at universities and industry research centers: FredagsFåtöljen Seminar, Faculty of Science, Lund University; Nanometer Structure Consortium Retreat Workshop, Frostavallen, Sweden; Royal Swedish Academy of Science visit at ESS, Lund, Sweden; Soft Matter Physics Seminar, University of Leeds, Leeds, England; CMPS research school in molecular protein science, Röstånga, Sweden; BASF, Ludwigshafen, Germany; Young Academy of Sweden meeting, Lund, Sweden; Society of Chemistry and Physics Vienna (CPG), Vienna, Austria.

Bruno Silva presented posters at: the Biophysical Society Meeting in Philadelphia, USA; the International Soft Matter Conference in Rome, Italy; and SAXS and Coherent X-ray Scattering Workshop (for discussing the first SAXS beamline on MAX IV) in Marstrand, Sweden.

Emma Sparr gave an keynote lecture at the International Soft Matter conference (ISMC) in Rome, Italy, and invited lectures at the workshop "From molecule to man – Topical research in the Malmö-Lund area (Asa, Sweden) and at the workshop "Ett möte mellan klinik och teknik kring vår gemensamma gränsyta: huden" (Lund, Sweden). Emma Sparr also held an oral presentation at the ESS symposia Neutrons in Biology (Lund Sweden), and a poster presentation at the 4th Scandinavian Meeting on Amyloid Proteins and Disease (Lund, Sweden).

Anna Stradner gave invited lectures at the 10th Nordic Scattering Workshop on Soft Matter (NSSM 2013) in Copenhagen, Denmark, and at a visit of the Royal Swedish Academy of Sciences to the European Spallation Source ESS and MAX IV in Lund, Sweden. She also gave an invited seminar at the Technische Universität Wien, ViCoM (Vienna Computational Materials Laboratory) in Vienna, Austria and contributed with an oral presentation at the SoftComp Annual Meeting in Rimini, Italy.

Daniel Topgaard gave invited lectures at the conferences 12th International Conference on Magnetic Resonance Microscopy at Fitzwilliam College, Cambridge, UK, and EUROMAR 2013 in Hersonissos, Crete, Greece University, USA, as well as the workshops Imaging of Cognitive Functions at Center for Languages and Literature, Lund University, and Double-PFG Workshop 2013 at Jukkasjärvi IceHotel, Sweden. He also gave seminars at Swedish NMR Center, Göteborg, and Laboratory of Mathematics in Imaging, Harvard Medical School, Boston, USA.

Ingemar Wadsö gave an invited lecture at the Ulm-Freiberger Kalorimetrietage 2013 in Ulm, Germany.

Marianna Yanez gave an oral presentation at the Symposium Neutrons in Life Science, ESS in Lund and presented a poster at the International Conference on Neutron Scattering in Edinburgh, Scotland.

Malin Zackrisson Oskolkova attended the Annual Soft Matter Conference, held in Rimini, Italy, and gave an oral contribution. She also attended the 4th Scandinavian Meeting on Amyloid Proteins and Disease, held in Lund, and the Soft Matter Conference, held in Rome, Italy, with poster contributions.

EXTERNAL PROFESSIONAL ACTIVITIES

Viveka Alfredsson served as deputy head of Physical Chemistry and deputy member of the board of KILU. She is also member of the executive council of the International Mesostructured Materials Association and the Division of Surface and Materials Chemistry of the Swedish Chemical Society. She is a member of the KILU equality group and sits on the board of “Lunds universitets gästhem”.

Ola Karlsson served as thesis examiner (opponent) for the PhD thesis of Ibon Iturralde Ugalde, the University of the Basque Country, San Sebastian, Spain.

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, 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). He was evaluator of research programs for Lundbeckfonden, Denmark and for national research councils.

Tommy Nylander served as thesis examiner (opponent) for the PhD theses of Amy Freund, University of Manchester, UK; Jes Dreier, University of Southern Denmark, Odense, Denmark; Stine Rønholt, Copenhagen University, Denmark; Nils Carlsson, Chalmers University of Technology, Gothenburg, Sweden. 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, Germany. In addition he was evaluator of research proposals for BBSRC – Biotechnology and Biological Sciences Research Council, Australian Research Council, MIUR – Ministero dell’Istruzione, dell’Universita e della Ricerca, Italy, Swiss National Science Foundation, Netherlands Organisation for Scientific Research.

Ulf Olsson was board member of the MAX IV Laboratory, and also served on the Science Advisory Committe of the Swiss spallation neutron source, SINQ. He also served on the review panel NT-5 at the Swedish Research Council, and in the grading committees of the PhD thesis of Mónica Muñoz Úbeda at Univesidad Complutense in Madrid, and Alexandra Machado at the University of Coimbra.

Lennart Piculell was section editor for the Polyelectrolytes section of Current Opinion in Colloid and Interface Science and a member of the international organizing committees of the biannual International Polyelectrolyte Symposia and the conference Formula VII, held in Mulhouse 2013. At Lund University he was a member of the Electoral Committee of the Faculty of Science and an appointed mentor for a PhD student at the Department of Biology. In June, he received a grant from VINNOVA to work out a national agenda for strategic innovation and research in the area of Formulation in Sweden. The work on the agenda, with the acronym ReForm, will be carried out from August 2013 to June 2014, and is led by an operating group consisting of Lennart Piculell, Martin Malmsten (Uppsala University) and Marie Wahlgren (LTH).

Karin Schillén was a Guest Editor of the Festschrift of Björn Lindman in Advances in Colloid and Interface Science.

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 12th European Summer School on "Scattering Methods Applied to Soft Condensed Matter" in Bombannes, France, member of the International Program Committee of the International Soft Matter Conference in Rome 2013, member of the International Program Committee of the 9th Liquid Matter Conference in Lisbon 2014, Editorial Board for Colloid & Polymer Science, Editorial Board for Soft Matter, and Section Editor folr Current Opinion in Colloid and Interface Science.

Emma Sparr was "first opponent" for the PhD defence of Andreas S. Lystvet at the Norwegian Technical University, Trondheim, Norway and faculty opponent for the PhD defence of Hanne Evenbratt at Chalmers. She also served on the PhD grading committee for Hanna Rydberg at Göteborg University. She was a member of the organizing committees of the annual meeting 4th Scandinavian Meeting on Amyloid Proteins and Disease (Lund, Sweden). During the year, Emma Sparr was member in a panel discussion on Creative environment organized by Kungliga fysiografiska sällskapet (shown at Swedish TV). She participated in evaluation interviews by Högskoleverket in their evaluation of Swedish Master programs in chemistry. Emma Sparr was member of the board of the Young Academy of Sweden from June 2013. At Lund University, she was the director of the Linnaeuscenter OMM.

Anna Stradner is a member of the International Advisory Board for the 28th European Colloid and Interface Society (ECIS) Conference 2014 to be held in Haifa, Israel. She is also a member of the Program Executive Committee of the European infrastructure project ESMI (European Soft Matter Infrastructure) as well as a member of the Faculty Search Committee at ETH Zürich/Switzerland for a Professor position.

Håkan Wennerström was chair in the jury for "The Chemistry for the Future Solvay Prize". "Rapporteur" for the thesis of Kevin Roger at the Ècole Superiuer de Physique et Chimie Industrielle, Paris.

Malin Zackrisson Oskolkova was part of a cross-disciplinary Advanced Study Group (ASG) at the Pufendorf Institute.

OUTREACH ACTIVITIES

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.

Emma Sparr was a teacher at a Summer research school for high school pupils “Forskarmöten” (arranged by the young academy of Sweden). She was part of a panel in a discussion on the theme “Why did you become a scientist and why should I?” at Värmdö gymnasium (Stockholm) together with, among others two of the 2013 Chemistry Nobel prize winners. She was part of an exchange program between the Swedish parliament and academic researchers in the young academy of Sweden. She wrote a book chapter in the book “Vägar till vetenskapen” (Santerus förlag 2013) with one ambition to inspire younger students in doing research, and she took part in the presentation of this book at “Bok och biblioteksmässan” (Göteborg). Emma Sparr presented her research at LeoPharma (Copenhagen, Denmark). She also gave popular science seminars within the seminar series “Lunchföredrag at Kemicentrum” at Lund Rotaryklubb.

AWARDS

Emma Sparr received the Hagberg Foundation 2013 prize (Kungliga vetenskapsakademien, KVA).

DISTINCTIONS

Peter Schurtenberger is Fellow of the Royal Society of Chemistry.

PATENTS

Surface protection of exposed biological tissues.

US 08461104 (also Europe, China, Japan)

Bengmark, S.; Larsson, K.; Lindman, B.; Andersson, R.

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 course in General and Analytical Chemistry during the spring semester, Malin Zackrisson Oskolkova was leading exercises and question hours, whereas Daniel Topgaard was lecturing and Malin and Viveka Alfredsson led the exercises 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 responsible for this course and she gave the lectures in thermodynamics together with Viveka Alfredsson, who also led the corresponding exercise sessions.

As regards higher courses, the Division gives one Bachelor 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 course in Surface and Colloid Chemistry, given during the fall semester, was taught by Emma Sparr (course responsible) along with Lennart Piculell, Peter Schurtenberger, Tommy Nylander, Anna Stradner and Erik Wernersson. This course is based on the textbook "The Colloidal Domain" by Fennell Evans and Håkan Wennerström. The other two Master courses were given during the spring semester, one on nuclear magnetic resonance techniques taught by Daniel Topgaard and one on scattering methods, which was taught by Malin Zackrisson Oskolkova (course responsible). Björn Lindman taught at the Ph.D. student course "Surfaces and Colloids" at Nanyang Technological University, Singapore. Also, he taught the Ph.D. course "Surfactants and Cellulose Polymers in Aqueous Solution" at Lappeenranta University of Technology, Lappeenranta and was teacher at the Ph.D. course on Surface Chemistry at Marstrand, Sweden. He was one of the teachers at the annual course on "Surfactants and Polymers in Aqueous Solution", this year given in Lisbon, and taught a course on the same topic for industry in Singapore. He also taught in-house courses for industry in Singapore, USA and Norway. Håkan Wennerström taught at a basic course in Surface and Colloid Chemistry.

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 2013

Joakim Stenhammar, School of Physics and Astronomy, University of Edinburgh, United Kingdom
Phase behaviour of self-propelled colloids

Fernanda Poletto, Institute of Chemistry, University of Campinas, Brazil
Tailoring polymeric-based and surfactant-base drug nanocarriers for treatment of parasitic diseases

Anand Yethiraj, Department of Physics & Physical Oceanography, Memorial University, St. John's, NL, Canada
Tunable hydrodynamics in oil droplet phases: from dipolar crystals to droplet breakup to turbulent energy cascades

Kevin Roger, Laboratoire de Physique et Mécanique des Milieux Hétérogènes & Laboratoire de Colloïdes et Matériaux Divisés, ESPCI, Paris, France
Self-Assembled Nanoemulsions through Physicochemical Methods

Peter Jönsson, Cambridge University, United Kingdom
Molecular nanomechanics and local stimulus of individual biomolecules on the surface of cells

Ben J Boyd, Monash Institute of Pharmaceutical Sciences, Monash University, Australia
Controlling structural transformation in self assembled lipid liquid crystals for drug delivery

Stefan Kuczera, Victoria University of Wellington, New Zeeland
RheoNMR observations of Wormlike Micelles

Bruno Silva, Division of Physical Chemistry, Lund University
Microfluidics with in-situ small-angle X-ray scattering: a tool to investigate soft matter dynamics

Melissa Sharp, European Spallation Source ESS, Lund
From polymers to proteins

Tomas Kjellman, Division of Physical Chemistry, Lund University
Mesoporous Silica SBA-15 - Formation, Modification and Application

Petrik Galvosas, Victoria University of Wellington, New Zeeland
Magnetic Resonance Pore Imaging as a novel tool for porous media characterization

Russel Crawford, Swinburne University of Technology, Australia
Novel approaches to prevent bacterial adhesion on medical implant materials

Maura Monduzzi, Dept. Scienze Chimiche e Geologiche, University of Cagliari, Italy
Soft and Hard Matter Drug Delivery Systems: Some Recent Results

Alex Evilevitch, Department of Biochemistry and Structural Biology, Lund University and Carnegie Mellon University, Department of Physics, Pittsburgh, PA, USA
Physical Chemistry of Viral Evolution

Maxim Morin, Lund University
Probing the Intermolecular interactions of Lactoferrin

OMM Minisymposium: Human interfaces – Structure and transport in the skin and in the lung alveolar lining layer
- Jenifer Thewalt, Simon Fraser University, Vancouver, Canada

Insights into stratum corneum barrier membrane organization from deuterium NMR
- Luis Bagatolli, Memphys, University of Southern Denmark, Denmark

Do liposomes penetrate skin?
- Sven Engström, Chalmers University of Technology, Sweden

Forming cubic and sponge phases with monoolein and its ether analogue: Phase studies, transdermal drug delivery formulations and biotech applications
- Marcus Larsson, Lund University

The first breath at the molecular level

Ilja Voets, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, the Netherlands
Hot proteins and cool crystals

Klaus Gawrisch, National Institutes of Health (NIH), USA
Elastic properties of polyunsaturated phosphatidylethanolamines influence rhodopsin function

Sebastian Björklund, Physical Chemistry, Lund University
Skin hydration - How water and osmolytes influence biophysical properties of stratum corneum

Tiago Ferreira, Physical Chemistry, Lund University
Structure and dynamics in amphiphilic bilayers NMR and MD simulations studies

Katarina Fromm, University of Fribourg, Switzerland
Clusters aggregates and cage compounds: From precursors for mixed metal oxides via catalysis to molecular magnets

Bernd Giese, University of Fribourg, Switzerland
Miner al Respiration. How peptides transport electrons over long distances

Katharina Fromm, University of Fribourg, Switzerland
Bioinorganic Chemistry of Silver: Interactions of silver with amino acids and peptides

Katharina Fromm, University of Fribourg, Switzerland
Agent Silver: with a License to Kill

Bernd Giese, University of Fribourg, Switzerland
Is DNA a Nanowire?

Jan Dhont, Forschungszentrum Jülich GmbH, Germany
The behaviour of rod-like colloids in shear flow

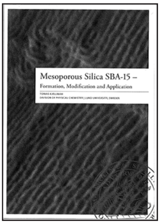
Adam Squires, University of Reading, United Kingdom
Soft and hard nanomaterials: from peptide fibrils and lyotropic liquid crystals to mesoporous electrodes

Christian von Corswant, AstraZeneca R&D, Mölndal, Sweden
Towards a mechanistic understanding of drug release from polymer coated pellets

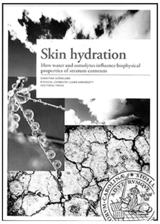
Kevin Roger, Laboratoire de Physique et Mécanique des Milieux Hétérogènes & Laboratoire de Colloïdes et Matériaux Divisés, ESPCI, Paris, France
The Ouzo effect: coalescence of repelling droplets can lead to monodisperse populations

Doctoral theses

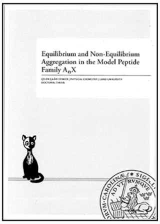
Tomas Kjellman
Mesoporous Silica SBA-15 - Formation, Modification and Application
Opponent: Professor Lennart Bergström, Stockholm University, Stockholm, Sweden


Mesoporous Silica SBA-15 –
Formation, Modification and Application
TOMAS KJELLMAN
DIVISION OF PHYSICAL CHEMISTRY | LUND UNIVERSITY, SWEDEN

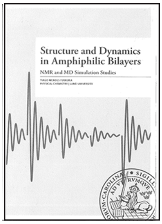
Sebastian Björklund
Skin hydration - How water and osmolytes influence biophysical properties of stratum corneum
Opponent: Professor Jenifer Thewalt, Department of Physics, Simon Fraser University, Vancouver, Canada


Skin hydration
How water and osmolytes influence biophysical properties of stratum corneum
SEBASTIAN BJÖRKLUND
PHYSICAL CHEMISTRY | LUND UNIVERSITY
DOCTORAL THESIS

Celen Cenker
Equilibrium and non-equilibrium aggregation in the model peptide family AnX
Opponent: Professor Martin Malmsten, Department of Pharmacy, Uppsala University, Uppsala, Sweden

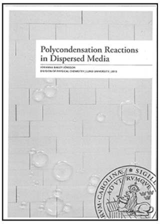

Equilibrium and Non-Equilibrium Aggregation in the Model Peptide Family A_nX
ÇELEN ÇAĞRI CENKER | PHYSICAL CHEMISTRY | LUND UNIVERSITY
DOCTORAL THESIS

Tiago Mendes Ferreira
Structure and dynamics in amphiphilic bilayers – NMR and MD simulation studies
Opponent: Dr. Klaus Gawrisch, Laboratory of Membrane Biochemistry and Biophysics, National Institute on Alcohol Abuse and Alcoholism, Maryland, USA


Structure and Dynamics in Amphiphilic Bilayers
NMR and MD Simulation Studies
TIAGO MENDES FERREIRA
PHYSICAL CHEMISTRY | LUND UNIVERSITY

Licentiate thesis

Johanna Bailey Jönsson
Polycondensation reactions in dispersed media
Opponent: Dr. Jan-Erik Jönsson, Dafo Fomtec AB, Sweden


Polycondensation Reactions in Dispersed Media
JOHANNA BAILEY JÖNSSON
DIVISION OF PHYSICAL CHEMISTRY | LUND UNIVERSITY | 2013

Publications

(1) Abrikossov, A.; Sacanna, S.; Philipse, A. P.; Linse, P.
Self-assembly of spherical colloidal particles with off-centered magnetic dipoles.
Soft Matter 2013, 9, 8904-8913.

(2) Albèr, C.; Brandner, B. D.; Björklund, S.; Billsten, P.; Corkery, R. W.; Engblom, J.
Effects of water gradients and use of urea on skin ultrastructure evaluated by confocal Raman microspectroscopy.
Biochim. Biophys. Acta 2013, 1828, 2470-2478.

(3) Asad Ayoubi, M.; Zhu, K.; Nystrom, B.; Almdal, K.; Olsson, U.; Piculell, L.
Micro- and nanophase separations in hierarchical self-assembly of strongly amphiphilic block copolymer-based ionic supramolecules.
Soft Matter 2013, 9, 1540-1555.

(4) Asad Ayoubi, M.; Zhu, K.; Nystrom, B.; Olsson, U.; Almdal, K.; Khokhlov, A. R.; Piculell, L.
Morphological Investigation of Polydisperse Asymmetric Block Copolymer Systems of Poly(styrene) and Poly(methacrylic acid) in the Strong Segregation Regime.
J. Polym. Sci., Part B: Polym. Phys. 2013, 51, 1657-1671.

(5) Bailey Jönsson, J.; Muellner, M.; Piculell, L.; Karlsson, O.
Emulsion Condensation Polymerization in Dispersed Aqueous Media. Interfacial Reactions and Nanoparticle Formation.
Macromolecules 2013, 46, 9104-9113.

(6) Bernin, D.; Topgaard, D.
NMR diffusion and relaxation correlation methods: New insights in heterogeneous materials.
Curr. Opin. Colloid Interface Sci. 2013, 18, 166-172.

(7) Bilalov, A.; Elsing, J.; Haas, E.; Schmidt, C.; Olsson, U.
Embedding DNA in surfactant mesophases: The phase diagram of the ternary system dodecyltrimethylammonium-DNA/monoolein/water in comparison to the DNA-free analogue.
J. Colloid Interface Sci. 2013, 394, 360-367.

(8) Björklund, S.; Engblom, J.; Thuresson, K.; Sparr, E.
Glycerol and urea can be used to increase skin permeability in reduced hydration conditions.
Eur. J. Pharm. Sci. 2013, 50, 638-645.

(9) Björklund, S.; Nowacka, A.; Bouwstra, J. A.; Sparr, E.; Topgaard, D.
Characterization of stratum corneum molecular dynamics by natural-abundance (13)c solid-state NMR.
PLoS One 2013, 8, e61889.

(10) Björklund, S.; Ruzgas, T.; Nowacka, A.; Dahi, I.; Topgaard, D.; Sparr, E.; Engblom, J.
Skin Membrane Electrical Impedance Properties under the Influence of a Varying Water Gradient.
Biophys. J. 2013, 104, 2639-2650.

(11) Crassous, J.; Casal-Dujat, L.; Medebach, M.; Obiols-Rabasa, M.; Vincent, R.; Reinhold, F.; Boyko, V.; Willerich, I.; Menzel, A.; Moitzi, C.; Reck, B.; Schurtenberger, P.
Structure and Dynamics of Soft Repulsive Colloidal Suspensions in the Vicinity of the Glass Transition.
Langmuir 2013, 29, 10346-10359.

(12) Crassous, J.; Millard, P.-E.; Mihut, A.; Wittemann, A.; Drechsler, M.; Ballauff, M.; Schurtenberger, P.
Giant hollow fiber formation through self-assembly of oppositely charged polyelectrolyte brushes and gold nanoparticles.
Soft Matter 2013, 9, 9111-9118.

(13) Dabkowska, A.; Lawrence, M. J.; McLain, S. E.; Lorenz, C. D.
On the nature of hydrogen bonding between the phosphatidylcholine head group and water and dimethylsulfoxide.
Chem. Phys. 2013, 410, 31-36.

(14) Dabkowska, A.; Talbot, J. P.; Cavalcanti, L.; Webster, J. R. P.; Nelson, A.; Barlow, D. J.; Fragneto, G.; Lawrence, M. J.
Calcium mediated interaction of calf-thymus DNA with monolayers of distearoylphosphtidylcholine: a neutron and Xray reflectivity study.
Soft Matter 2013, 9, 7095-7105.

(15) Dechezelles, J.-F.; Malik, V.; Crassous, J.; Schurtenberger, P.
Hybrid raspberry microgels with tunable thermoresponsive behavior.
Soft Matter 2013, 9, 2798-2802.

(16) Deleu, M.; Lorent, J.; Lins, L.; Brasseur, R.; Braun, N.; El Kirat, K.; Nylander, T.; Dufrene, Y. F.; Mingeot-Leclercq, M.-P.
Effects of surfactin on membrane models displaying lipid phase separation.
Biochim. Biophys. Acta, Biomembr. 2013, 1828, 801-815.

(17) di Gregorio, M. C.; Pavel, N. V.; Jover, A.; Meijide, F.; Tato, J. V.; Soto Tellini, V. H.; Vargas, A. A.; Regev, O.; Kasavi, Y.; Schillén, K.; Galantini, L.
pH Sensitive Tubules of a Bile Acid Derivative: a Tubule Opening by Release of Wall Leaves.
Phys. Chem. Chem. Phys. 2013, 15, 7560-7566.

(18) Eriksson, S.; Lasic, S.; Topgaard, D.
Isotropic diffusion weighting in PGSE NMR by magic-angle spinning of the q-vector.
J. Magn. Reson. 2013, 226, 13-18.

(19) Ferreira, T.; Bernin, D.; Topgaard, D.
NMR Studies of Nonionic Surfactants.
Annu. Rep. NMR Spectrosc. 2013, 79, 73-127.

(20) Ferreira, T.; Coreta-Gomes, F.; Ollila, S.; Moreno, M. J.; Vaz, W. L. C.; Topgaard, D.
Cholesterol and POPC segmental order parameters in lipid membranes: solid state (1)H-(13)C NMR and MD simulation studies.
Phys. Chem. Chem. Phys. 2013, 15, 1976-1989.

(21) Gentile, L.; Silva, B.; Lages, S.; Mortensen, K.; Kohlbrecher, J.; Olsson, U.
Rheochaos and flow instability phenomena in a nonionic lamellar phase.
Soft Matter 2013, 9, 1133-1140.

(22) Gibaud, T.; Zaccone, A.; Del Gado, E.; Trappe, V.; Schurtenberger, P.
Unexpected Decoupling of Stretching and Bending Modes in Protein Gels.
Phys. Rev. Lett. 2013, 110, 058303.

(23) Haberl, J. M.; Sanchez-Ferrer, A.; Mihut, A. M.; Dietsch, H.; Hirt, A. M.; Mezzenga, R.
Liquid-Crystalline Elastomer-Nanoparticle Hybrids with Reversible Switch of Magnetic Memory.
Adv. Mater. 2013, 25, 1787–1791.

(24) Hellstrand, E.; Grey, M.; Ainalem, M.-L.; Ankner, J.; Forsyth, V. T.; Fragneto, G.; Haertlein, M.; Dauvergne, M.-T.; Nilsson, H.; Brundin, P.; Linse, S.; Nylander, T.; Sparr, E.
Adsorption of α-Synuclein to Supported Lipid Bilayers: Positioning and Role of Electrostatics.
ACS Chem. Neurosci. 2013, 4, 1339-1351.

(25) Hellstrand, E.; Nowacka, A.; Topgaard, D.; Linse, S.; Sparr, E.
Membrane Lipid Co-Aggregation with α-Synuclein Fibrils.
PLoS One 2013, 8, e77235.

(26) Janiak, J.; Piculell, L.; Schillén, K.; Lundberg, D.
Responsive Release of Polyanions from the Soluble Aggregates Formed with a Hydrolyzable Cationic Surfactant, and a Nonionic Surfactant.
Soft Matter 2013, 9, 4103-4112.

(27) Johans, C.; Behrens, M.; Bergquist, K.-E.; Olsson, U.; Manzanares, J. A.
Potential Determining Salts in Microemulsions: Interfacial Distribution and Effect on the Phase Behavior.
Langmuir 2013, 29, 15738-15746.

(28) Karlsson, O.; Schade, B. E. H.
"Particle Analysis." In Chemistry and Technology of Emulsion Polymerisation, edited by Alex M. van Herk.
Oxford, UK: John Wiley & Sons Ltd, 2013.

(29) Kihlman, M.; Medronho, B. F.; Romano, A. L.; Germgard, U.; Lindman, B.
Cellulose Dissolution in an Alkali Based Solvent: Influence of Additives and Pretreatments.
J. Braz. Chem. Soc. 2013, 24, 295-303.

(30) Kjellman, T.; Alfredsson, V.
The use of in situ and ex situ techniques for the study of the formation mechanism of mesoporous silica formed with non-ionic triblock copolymers.
Chem. Soc. Rev. 2013, 42, 3777-3791.

(31) Kjellman, T.; Asahina, S.; Schmitt, J.; Imperor-Clerc, M.; Terasaki, O.; Alfredsson, V.
Direct Observation of Plugs and Intrawall Pores in SBA-15 Using Low Voltage High Resolution Scanning Electron Microscopy and the Influence of Solvent Properties on Plug-Formation.
Chem. Mater. 2013, 25, 4105-4112.

(32) Kjellman, T.; Reichhardt, N.; Sakeye, M.; Smatt, J.-H.; Linden, M.; Alfredsson, V.
Independent Fine-Tuning of the Intrawall Porosity and Primary Mesoporosity of SBA-15.
Chem. Mater. 2013, 25, 1989-1997.

(33) Knöös, P.; Onder, S.; Pedersen, L.; Piculell, L.; Ulvenlund, S.; Wahlgren, M.
Surfactants modify the release from tablets made of hydrophobically modified poly (acrylic acid).
Results Pharma Sci. 2013, 3, 7-14.

(34) Knöös, P.; Topgaard, D.; Wahlgren, M.; Ulvenlund, S.; Piculell, L.
Using NMR Chemical Shift Imaging To Monitor Swelling and Molecular Transport in Drug-Loaded Tablets of Hydrophobically Modified Poly(acrylic acid): Methodology and Effects of Polymer (In)solubility.
Langmuir 2013, 29, 13898-13908.

(35) Koivuniemi, A.; Sysi-Aho, M.; Oresic, M.; Ollila, S.
Interfacial Properties of High-Density Lipoprotein-like Lipid Droplets with Different Lipid and Apolipoprotein A-I Compositions.
Biophys. J. 2013, 104, 2193-2201.

(36) Lidenmark, C.; Pettersson, T.; Karlsson, O.; Notley, S. M.; Norgren, M.; Edlund, H.
The adhesive behavior of extracted latex polymers towards silicon oxide and cellulose.
Int. J. Adhes. Adhes. 2013, 44, 250-258.

(37) Machado, A.; Lundberg, D.; Ribeiro, A. J.; Veiga, F. J.; Miguel, M. G.; Lindman, B.; Olsson, U.
Encapsulation of DNA in Macroscopic and Nanosized Calcium Alginate Gel Particles.
Langmuir 2013, 29, 15926-15935.

(38) Marques, E.; Silva, B.
"Surfactants, Phase Behavior." In Encyclopedia of Colloid and Interface Science, edited by Tharwat Tadros: Springer, 2013. 1290-1333.

(39) Marques, E.; Silva, B.
"Surfactant Self-Assembly." In Encyclopedia of Colloid and Interface Science, edited by Tharwat Tadros: Springer, 2013. 1202-1241.

(40) Medronho, B.; Andrade, R.; Vivod, V.; Ostlund, A.; Miguel, M. G.; Lindman, B.; Voncina, B.; Valente, A. J. M.
Cyclodextrin-grafted cellulose: Physico-chemical characterization.
Carbohydr. Polym. 2013, 93, 324-330.

(41) Mergenthaler, K.; Iqbal, A.; Wallentin, J.; Lehmann, S.; Borgström, M.; Samuelson, L.; Yartsev, A.; Pistol, M.-E.
Large-energy-shift photon upconversion in degenerately doped InP nanowires by direct excitation into the electron gas.
Nano Res. 2013, 6, 752-757.

(42) Mihut, A.; Crassous, J.; Dechezelles, J.-F.; Lages, S.; Menzel, A.; Dietsch, H.; Schurtenberger, P.
Towards smart self-assembly of colloidal silica particles through diblock copolymer crystallization.
Polymer 2013, 54, 3874-3881.

(43) Mihut, A.; Dabkowska, A.; Crassous, J.; Schurtenberger, P.; Nylander, T.
Tunable Adsorption of Soft Colloids on Model Biomembranes.
ACS Nano 2013, 7, 10752-10763.

(44) Mihut, A.; Sanchez-Ferrer, A.; Crassous, J.; Hirschi, L. A.; Mezzenga, R.; Dietsch, H.
Enhanced properties of polyurea elastomeric nanocomposites with anisotropic functionalised nanofillers.
Polymer 2013, 54, 4194-4203.

(45) Moran, M. C.; Nogueira, D. R.; Vinardell, M. P.; Miguel, M. G.; Lindman, B.
Mixed protein-DNA gel particles for DNA delivery: Role of protein composition and preparation method on biocompatibility.
Int. J. Pharm. 2013, 454, 192-203.

(46) Nowacka, A.; Bongartz, N.; Ollila, O. H. S.; Nylander, T.; Topgaard, D.
Signal intensities in (1)H-(13)C CP and INEPT MAS NMR of liquid crystals.
J. Magn. Reson. 2013, 230, 165-175.

(47) Nöjd, S.; Mohanty, P.; Bagheri, P.; Yethiraj, A.; Schurtenberger, P.
Electric field driven self-assembly of ionic microgels.
Soft Matter 2013, 9, 9199-9207.

(48) Olofsson, G.; Sparr, E.
Ionization Constants pKa of Cardiolipin.
PLoS One 2013, 8, e73040.

(49) Paloli, D.; Mohanty, P.; Crassous, J.; Zaccarelli, E.; Schurtenberger, P.
Fluid-solid transitions in soft-repulsive colloids.
Soft Matter 2013, 9, 3000-3004.

(50) Percebom, A. M.; Janiak, J.; Schillén, K.; Piculell, L.; Loh, W.
Micellization of Water-Soluble Complex Salts of an Ionic Surfactant with Hairy Polymeric Counterions.
Soft Matter 2013, 9, 515-526.

(51) Piculell, L.
Understanding and Exploiting the Phase Behavior of Mixtures of Oppositely Charged Polymers and Surfactants in Water.
Langmuir 2013, 29, 10313-10329.

(52) Pourmousa, M.; Wong-ekkabut, J.; Patra, M.; Karttunen, M.
Molecular Dynamic Studies of Transportan Interacting with a DPPC Lipid Bilayer.
J. Phys. Chem. B 2013, 117, 230-241.

(53) Rochette, C. N.; Crassous, J.; Drechsler, M.; Gaboriaud, F.; Eloy, M.; de Gaudemaris, B.; Duval, J. F. L.
Shell Structure of Natural Rubber Particles: Evidence of Chemical Stratification by Electrokinetics and Cryo-TEM.
Langmuir 2013, 29, 14655-14665.

(54) Sparr, E.; Millecamps, D.; Isoir, M.; Burnier, V.; Larsson, Å.; Cabane, B.
Controlling the hydration of the skin though the application of occluding barrier creams.
J. R. Soc. Interface 2013, 10, 20120788.

(55) Stenhammar, J.; Tiribocchi, A.; Allen, R. J.; Marenduzzo, D.; Cates, M. E.
A Continuum Theory of Phase Separation Kinetics for Active Brownian Particles.
Phys. Rev. Lett. 2013, 111, 145702.

(56) Topgaard, D.
Isotropic diffusion weighting in PGSE NMR: Numerical optimization of the q-MAS PGSE sequence.
Microporous Mesoporous Mater. 2013, 178, 60-63.

(57) Travaglini, L.; D'Annibale, A.; di Gregorio, M. C.; Schillén, K.; Olsson, U.; Sennato, S.; Pavel, N. V.; Galantini, L.
Between Peptides and Bile Acids: Self-Assembly of Phenylalanine Substituted Cholic Acids.
J. Phys. Chem. B 2013, 117, 9248-9257.

(58) Wadsäter, M.; Barauskas, J.; Nylander, T.; Tiberg, F.
Nonlamellar lipid liquid crystalline model surfaces for biofunctional studies.
Soft Matter 2013, 9, 8815-8819.

(59) Wadsö, L.; Karlsson, O.
Alkaline hydrolysis of polymers with ester groups studied by isothermal calorimetry.
Polym. Degrad. Stab. 2013, 98, 73-78.

(60) van Gruijthuijsen, K.; Obiols-Rabasa, M.; Heinen, M.; Nägele, G.; Stradner, A.
Sterically stabilized colloids with tunable repulsions.
Langmuir 2013, 29, 11199-11207.

(61) van Gruijthuijsen, K.; Tuinier, R.; Brader, J. M.; Stradner, A.
Phase behaviour of colloids with short-range repulsions plus nonadsorbing polymer chains.
Soft Matter 2013, 9, 9977-9982.

(62) Wang, H.; Alfredsson, V.; Tropsch, J.; Ettl, R.; Nylander, T.
Formation of CaCO3 Deposits on Hard Surfaces-Effect of Bulk Solution Conditions and Surface Properties.
ACS Appl. Mater. Interfaces 2013, 5, 4035-4045.

(63) Wennerström, H.
Scattering and diffraction described using the momentum representation.
Adv. Colloid Interface Sci. 2013.

(64) Wennerström, H.
Björn Lindman: Fifty years in science and technology.
Adv. Colloid Interface Sci. 2013.

(65) Wennerström, H.; Olsson, U.; Israelachvili, J. N.
Entropic forces between fluid layers.
Proc. Natl. Acad. Sci. U. S. A. 2013, 110, E2944-E2944.

(66) Wennerström, H.; Westlund, P.-O.
On Stern-Gerlach coincidence measurements and their application to Bell's theorem.
Physics Essays 2013, 26, 174-180.

(67) Wernersson, E.; Linse, P.
Spreading and brush formation by end-grafted bottle-brush polymers with adsorbing side chains.
Langmuir 2013, 29, 10455-10462.

(68) Xie, F.; Nylander, T.; Piculell, L.; Utsel, S.; Wagberg, L.; Åkesson, T.; Forsman, J.
Polyelectrolyte Adsorption on Solid Surfaces: Theoretical Predictions and Experimental Measurements.
Langmuir 2013, 29, 12421-12431.

(69) Yanez, M.; Eltes, F.; Campbell, R. A.; Nylander, T.
Interactions of PAMAM Dendrimers with SDS at the Solid-Liquid Interface.
Langmuir 2013, 29, 5817-5831.

(70) Zaccone, A.; Crassous, J.; Ballauff, M.
Colloidal gelation with variable attraction energy.
J. Chem. Phys. 2013, 138, 104908.

(71) Zackrisson, M.; Norrman, E.; Olsson, U.
Study of the micelle-to-vesicle transition and smallest possible vesicle size by temperature-jumps.
J. Colloid Interface Sci. 2013, 396, 173-177.

(72) Zhang, R.; Linse, P.
Icosahedral capsid formation by capsomers and short polyions.
J. Chem. Phys. 2013, 138, 154901.

(73) Zhang, R.; Wernersson, E.; Linse, P.
Icosahedral capsid formation by capsomer subunits and a semiflexible polyion.
RSC Adv. 2013, 3, 25258-25267.

(74) Znamenskaya, Y.; Sotres, J.; Gavryushov, S.; Engblom, J.; Arnebrant, T.; Kocherbitov, V.
Water Sorption and Glass Transition of Pig Gastric Mucin Studied by QCM-D.
J. Phys. Chem. B 2013, 117, 2554-2563.

Manuscripts submitted during 2013

Agzenai, A.; Lindman, B.; Alfredsson, V.; Topgaard, D.; Sánchez Renamayor, C.; Pacios, I. E.
In situ X-ray polymerization: From swollen lamellae to polymer-surfactant complexes.
J. Phys. Chem. B, 2014, 118, 1159–1167.

Ainalem, M.-L.; Bartles, A.; Muck, J.; Dias, R.; Carnerup, A.; Zink, D.; Nylander, T.
DNA compaction induced by a cationic polymer or surfactant impact gene expression and DNA degradation.
PLoS One, 2014, 9, e92692.

Angelescu, D. G.; Linse, P.
Monte Carlo Simulations of Multigraft Homopolymers in Good Solvent.
Macromolecules, 2014, 47, 415-426.

Arnebrant, T.; Nylander, T.; Miller, R.
The 26th Conference of the European Colloid and Interface Society held in Malmö, Sweden on 2–7 September 2012.
Colloids Surf., A, 2014, 442, 1-1.

Barauskas, J.; Christerson, L.; Wadsäter, M.; Lindström, F.; Lindqvist, A.-K.; Tiberg, F.
Bioadhesive Lipid Compositions: Self-Assembly Structures, Functionality, and Medical Applications.
Mol. Pharm., 2014, 11, 895-903.

Björklund, S.; Andersson, J. M.; Pham, Q. D.; Nowacka, A.; Topgaard, D.; Sparr, E.
Stratum corneum molecular mobility in the presence of natural moisturizers
Soft Matter, in press

Buell, A. K.; Galvagnion, C.; Gaspar, R.; Sparr, E.; Vendruscolo, M.; Knowles, T. P. J.; Linse, S.; Dobson, C. M.
Solution conditions determine the relative importance of nucleation and growth processes in α-synuclein aggregation
Proc. Natl. Acad. Sci. U. S. A., in press

Dabkowska, A.; Barlow, D. J.; Clifton, L. A.; Hughes, A. V.; Webster, J.; Green, R.; Quinn, P.; Lawrence, M. J.
Calcium-mediated binding of DNA to 1,2-distearoyl-sn-glycero-3-phosphocholine-containing mixed lipid monolayers.
Soft Matter, 2014.

Ferreira, T.; Topgaard, D.; Ollila, S.
Molecular conformation and bilayer pores in a nonionic surfactant lamellar phase studied with (1) h-(13)c solid-state NMR and molecular dynamics simulations.
Langmuir, 2014, 30, 461-469.

Gentile, L.; Behrens, M.; Balog, S.; Mortensen, K.; Ranieri, G. A.; Olsson, U.
Dynamic Phase Diagram of a Nonionic Surfactant Lamellar Phase.
J. Phys. Chem. B, 2014, 118, 3622-3629.

Haberl, J. M.; Sánchez-Ferrer, A.; Mihut, A. M.; Dietsch, H.; Hirt, A. M.; Mezzenga, R.
Light-Controlled Actuation, Transduction, and Modulation of Magnetic Strength in Polymer Nanocomposites
Adv. Funct. Mater., in press

Han, L.; Ohsuna, T.; Liu, Z.; Alfredsson, V.; Kjellman, T.; Asahina, S.; Suga, M.; Ma, Y.; Oleynikov, P.; Miyasaka, K.; Mayoral, A.; Diaz, I.; Sakamoto, Y.; Stevens, S. M.; Anderson, M. W.; Xiao, C.; Fujita, N.; Garcia-Bennett, A.; Yoon, K. B.; Che, S.; Terasaki, O.
Silica-Based Nanoporous Materials Revealed by Microscopy.
Z. Anorg. Allg. Chem., 2014, 640, 521-536.

Holt, C.; Lenton, S.; Nylander, T.; Sørensen, E. S.; Teixeira, S. C. M.
Mineralisation of soft and hard tissues and the stability of biofluids.
J Struct Biol, 2014, 185, 383-396.

Janiak, J.; Tomšič, M.; Olofsson, G.; Lundberg, D.; Piculell, L.; Schillén, K.
Soluble Aggregates in Aqueous Solution of Polyion-Surfactant Ion Complex Salts and a Nonionic Surfactant.
J. Phys. Chem. B, submitted

Kjellman, T.; Xia, X.; Alfredsson, V.; Garcia-Bennett, A. E.
Influence of microporosity in SBA-15 on the release properties of anticancer drug Dasatinib
Chem. Mater., submitted

Knöös, P.; Schulz, C.; Piculell, L.; Ludwig, R.; Gorton, L.; Wahlgren, M.
Quantifying the release of lactose from polymer matrix tablets with an amperometric biosensor utilizing cellobiose dehydrogenase.
Int. J. Pharm., 2014.

Lasic, S.; Szczepankiewicz, F.; Eriksson, S.; Nilsson, M.; Topgaard, D.
Microanisotropy imaging: quantification of microscopic diffusion anisotropy and orientational order parameter by diffusion MRI with magic-angle spinning of the q-vector.
Front. Physics, 2014, 2.

Linse, P.; Lue, L.
Green's function for a spherical dielectric discontinuity and its application to simulation.
J. Chem. Phys., 2014, 140, 044903.

Majzoub, R. N.; Chan, C.-L.; Ewert, K. K.; Silva, B.; Liang, K. S.; Jacovetty, E. L.; Carragher, B.; Potter, C. S.; Safinya, C. R.
Uptake and transfection efficiency of PEGylated cationic liposome-DNA complexes with and without RGD-tagging.
Biomaterials, 2014, 35, 4996-5005.

Malik, V.; Grobety, B.; Trappe, V.; Dietsch, H.; Schurtenberger, P.
A closer look at the synthesis and formation mechanism of hematite nanocubes.
Colloids Surf., A, 2014, 445, 21-29.

Michanek, A.; Dabkowska, A.; Jaeger, L.; Rabe, M.; Höök, F.; Nylander, T.; Sparr, E.
RNA origami at supported lipid bilayers
submitted

Mohanty, P.; Paloli, D.; Crassous, J.; Zaccarelli, E.; Schurtenberger, P.
Effective interactions between soft-repulsive colloids: Experiments, theory, and simulations.
J. Chem. Phys., 2014, 140, 094901.

Pomorski, T. G.; Nylander, T.; Cárdenas, M.
Model cell membranes: Discerning lipid and protein contributions in shaping the cell.
Adv. Colloid Interface Sci., 2014, 205, 207-220.

Siegel, G.; Ermilov, E.; Pries, A. R.; Winkler, K.; Schmidt, A.; Ringstad, L.; Malmsten, M.; Lindman, B.
The significance of lipid peroxidation in cardiovascular disease.
Colloids Surf., A, 2014, 442, 173-180.

Silva, B.; Majzoub, R. N.; Chan, C.-L.; Li, Y.; Olsson, U.; Safinya, C. R.
PEGylated Cationic Liposome - DNA Complexation in Brine is Pathway-Dependent.
Biochim. Biophys. Acta, Biomembr., 2014, 1838, 398-412.

Stenhammar, J.; Marenduzzo, D.; Allen, R. J.; Cates, M. E.
Phase behaviour of active Brownian particles: the role of dimensionality.
Soft Matter, 2014, 10, 1489-1499.

Ulama, J.; Zackrisson, M.; Bergenholtz, J.
Monodisperse PEGylated spheres: an aqueous colloidal model system.
J. Phys. Chem. B, 2014, 118, 2582-2588.

Wadsäter, M.; Barauskas, J.; Nylander, T.; Tiberg, F.
Formation of highly structured cubic micellar lipid nanoparticles of soy phosphatidylcholine and glycerol dioleate and their degradation by triacylglycerol lipase.
ACS Appl. Mat. Interfaces, 2014.

Wennerström, H.; Olsson, U.
The undulation force; theoretical results versus experimental demonstrations.
Adv. Colloid Interface Sci., 2014.

Zackrisson Oskolkova, M.; Ulama, J.; Stradner, A.; Bergenholtz, J.
Effective attractions and aggregation of PEGylated nanoparticles.
Langmuir, 2014.

PEOPLE

Scientists/Teachers

Viveka Alfredsson, Professor
Manja Behrens, Researcher
Johan Bergenholtz, Visiting Professor
Casal-Dujat, Lucia, Researcher
Jerome Crassous, Researcher
Aleksandra Dabkowska, Postdoc
Marie Grey, Researcher
James Holdaway, Postdoc
Andrew Jackson, Adjunct Associate Professor
Ola Karlsson, Adjunct Professor
Björn Lindman, Professor
Per Linse, Professor
Martin Medebach, Postdoc
Adriana Mihut, Researcher
Priti Mohanty, Researcher
Marc Obiols-Rabasa, Researcher
Tommy Nylander, Professor
Gerd Olofsson, Associate Professor Emerita
Ulf Olsson, Professor
Lennart Piculell, Professor
Karin Schillén, Professor
Peter Schurtenberger, Professor
Bruno Silva, Postdoc
Nicholas Skar-Gislinge, Postdoc
Emma Sparr, Professor
Joakim Stenhammar, Postdoc
Anna Stradner, Associate Professor
Olle Söderman, Professor
Fredrik Tiberg, Adjunct Professor
Daniel Topgaard, Professor
Stefan Ulvenlund, Adjunct Associate Professor
Maria Wadsäter, Postdoc
Ingemar Wadsö, Professor Emeritus
Håkan Wennerström, Professor
Erik Wernersson, Postdoc
Malin Zackrisson Oskolkova, Assistant Professor
Ran Zhang, Postdoc
Yana Znamenskaya, Researcher

Technical-Administrative personnel

Tomislava Andric, Economist
Christopher Hirst, Engineer
Majlis Larsson, Administrator
Helena Persson, Administrator
Maria Södergren, Engineer

Graduate students

Alexei Abrikossov
Jenny Algotsson
Jenny Andersson
Johanna Bailey Jönsson
Solmaz Bayati
Sebastian Björklund
Saskia Bucciarelli
Çelen Cenker
Stefanie Eriksson
Tiago Ferreira
Tommy Garting
Charlotte Gustavsson
Sanna Gustavsson
Carin Hagsten
Tomas Kjellman
Patrik Knöös
Weimin Li
Ruiyu Lin
Ilya Martchenko
Emelie Nilsson
Sofi Nöjd
Divya Paloli
Dat Pham
Marianna Yanez Arteta

Guests

Kazuhiro Ishikawa, Kao Corporation, Japan
Javier de Prada Lopez, Complutense University, Madrid, Span
Gavin Hazell, University of Bath, U.K.
Kevin Roger, ENS CACHAN/Université Paris XI, France

Christian von Corswant, AstraZeneca R&D Mölndal, Sweden
Niklas Bodén, Lund University
Max Morin, Lund University
Viktor Persson, Lund University
Nadine Verstappen, Wageningen University, Netherlands
Aaron Riede, Universität Konstanz, Germany
Marta Gubitosi, University of Rome, La Sapienza, Italy
Ricardo Gaspar, University of Coimbra, Portugal
Samira Mohseni, Lund University, Faculty of Engineering LTH
Bruno da Silva, University of Santa Barbara, U.S.A.
Jan Dhont, Forschungszentrum Jülich GmbH, Germany
Nicholas Skar-Gislinge, Novo nordisk AIS, Denmark
Katharina Fromm, University of Fribourg, Switzerland
Bernd Giese, University of Fribourg, Switzerland
Stefan Kuczera, Victoria University Wellington, New Zealand,
Klaus Gawrisch, Nat. Institutes of Health, Bethesda, U.S.A.
Hanna Bergenholtz
Albert Philipse, Utrecht University, Netherlands
Martin Malmsten, Uppsala University, Sweden
Jenifer Thewalt, Simon Fraser University, Vancouver, U.S.A.
Niklas Bodén, Lund University
Viktor Persson
Luigi Gentile, Univ. of Calabria, Cosenza, Italy
Maura Monduzzi, University of Cagliari, Italy
Daniel Abegao, University of Coimbra, Portugal
Karen Edler, University of Bath, U.K.
Joshua Avossa, University of Naples Federico the second, Italy
Ricardo Gaspar, University of Coimbra, Portugal
Fernanda Poletto, University Estadual de Campinas, Brazil
Petrik Galvosas, Victoria University of Wellington, New Zealand
Hayato Shiba, University of Tokyo, Japan
Melissa Sharp, ESS, Lund
Ting Liu, Carnegie Mellon University, Pittsburgh, U.S.A.
Wolfgang Schmidt, Max-Planck-Institut für Kohlenforschung, Germany
Claudia Weidenthaler, Max-Planck-Institut für Kohlenforschung, Germany
Youli Li, University of California, U.S.A.
Mona Koder Hamid
Anand Yethiraj, Memorial University, Canada
Gerda Kamsma, Utrecht University, Netherlands

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 Øresund Bridge directly to Lund railway station (takes approximately 35 min.).

Visit the Kemicentrum website for further travel information: www.kc.lu.se/english/visitors/directions

CONTACT INFORMATION

Division of Physical Chemistry
Department of Chemistry
P.O. Box 124
SE-221 00 Lund, Sweden
Telephone: +46 46 222 81 50
Fax: +46 46 222 44 13
www.physchem.lu.se

This report is produced by Helena Persson with kind assistance from Johan Reimer at the Department of Chemistry, LU.