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Front page picture:

A three-dimensional reconstruction of ellipsoidal colloids forming a tubular structure in the presence of a field.

Ref.: Crassous, J. J.; Mihut, A. M.; Wernersson, E.; Pfeiderer, P.; Vermant, J.; Linse, P.; Schurtenberger, P.; Nature Communication 2014, 5:5516.

MOVING TO LUND

When having been asked to write an introduction to the Annual Report 2014, my first reaction was that it felt a bit strange to do this as a newcomer. My second reaction was surprise when I realized that this occasion also marks already the beginning of the 5th year as a member of Physical Chemistry, which means I'm not really a newcomer anymore. And finally, my third reaction then was to take this as an opportunity to write a totally personal account of the scientific life within our division, which however will hopefully also be helpful to potential future collaborators, for whom this report is also written.

Having already spent half a year at the division as a postdoc in 1984 (!), and having had several collaborations with members from Physical Chemistry since then, I did of course have a reasonably sound basis for what to expect from my future new work environment when I decided in 2010 to accept an offer for a faculty position and move to Lund at a rather late stage in my scientific career. Nevertheless, after having worked for more than 20 years as an independent researcher and faculty member at the ETH Zurich and the University of Fribourg in Switzerland, in an environment where I knew the rules and how to get along and organize the necessary support to conduct my research, there was also a feeling of tension below the surface of the general excitement that goes along with such a big move. How would I cope with the situation that I once again was a newcomer, unknown to most of the national scientific community outside my own research field, and having to find out again how national and regional funding agencies work? And how different would the academic habits be, and how easy the integration into my new environment after having been shaped and molded by the academic and scientific life in Switzerland and the US?

It turned out that the move to Lund worked much more smoothly and successfully than anticipated. The highly collaborative spirit of the division, which becomes apparent when looking at the list of collaborators in the different projects summarized in this Annual Report, played a major role here. For somebody used to having to deal with individual "kingdoms" centered on large chairs in classical university departments, this came as a new and wonderful experience. Moreover, the existing Linnaeus center of excellence OMM (Organizing Molecular Matter) also helped enormously, as it not only created an ideal research environment for interdisciplinary soft matter research, but also allowed for previous recruitments of young faculty members and provided start-up support for myself. As a result, we now have a very lively research activity at our division where areas such as colloidal biology and colloid-based condensed matter research have been considerably strengthened, as becomes once again evident from this Annual Report.

After these first five years, things have settled. The initial excitement has partly been replaced by a (very positive) feeling of content routine operation, and I feel we have reached a steady state that resembles life in a well functioning marriage. This of course also means that one starts to realize that not everything is perfect, and that there is room for improvement. This is partly connected to the underlying funding structure at Swedish universities, which in our case requires obtaining major long-term funds such as the soon finishing OMM project in order to continue with our current research operation. Having received a large multi-PI research project supported by the Knut and Alice Wallenberg foundation for five years, which has just started on the 1st of July this year, means we are making progress. But it is clear, that major efforts are required by everybody to maintain research life at Physical Chemistry on the same level as before. Despite these few shortcomings, however, there always remains the feeling of having the privilege to work in a highly stimulating environment that I can only recommend to all potential collaborators that will read this Annual Report...

Peter Schurtenberger

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. The software's are:

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

MOLSIM is a software for atomistic and coarse-grain modeling of molecular, colloidal, and polymer systems, with extensive static and dynamic analyses, employing molecular dynamics, stochastic dynamics, and Monte Carlo simulation techniques. With contributions from Anna Akinchina, Fredrik Carlsson, Samuel Edgecombe, Yoshikatsu Hayashi, Pascal Hebbeker, Niklas Källrot, Björn Linse, Vladimir Lobaskin, Thomas M. Nymand, Alberto Pais, Jurij Rescic, Stefanie Schneider, Marie Skepö, Joakim Stenhammar, Anders Wallqvist, Jos van Rijssel, Erik Wernersson, 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 2014, MOLSIM has undergone a large structural reorganization simplifying its use, been extended to handle concave particles of arbitrary shape, and got an enhanced capacity of dynamic analyses. The ideas behind the software MOLSIM have been developed and presented in a research publication. (Jurij Rescic (University of Ljubljana) and Per Linse.)

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. Moreover, the accuracy of a splitting theory, based on dividing the electrostatic interaction into long and short wavelength contributions and applying different approximations on the two contributions, has been assessed against simulation results. The splitting theory works best for the case where the dielectric constant of the confining sphere is equal to or less than that of the surrounding medium. (Leo Lue (University of Strathclyde), and Per Linse.)

Multigraft polymers in solution (Contact person: Per Linse)

Complexes formed by one charged and branched copolymer with an oppositely charged and linear polyion have been investigated by Monte Carlo simulations. A coarse-grained description has been used, in which the main chain of the branched polyion and the linear polyion possess the same absolute charge and charge density. The spatial extension and other structural properties, such as bond-angle orientational correlation function, asphericity, and scaling analysis of formed complexes, at varying branching density and side-chain length of the branched polyion, have been explored. In particular, the balance between cohesive Coulomb attraction and side-chain repulsions resulted in two main structures of a polyion complex. These structures are (i) globular polyion core surrounded by side chains appearing at low branching density and (ii) extended polyion core with side chains still being expelled at high branching density. The globule-to-extended transition occurred at a crossover branching density being practically independent of the side chain length. Moreover, the properties of the complexes were investigated for variable electrostatic attraction between the polymers. The complexes were relatively intact for the fractional charge $\frac{1}{2}$, but at smaller charges considerable structural changes appeared. (Daniel Angelescu (Romanian Academy) and Per Linse.)

Studies of model systems

Emulsion Coarsening (Contact person: Ulf Olsson)

Two coarsening mechanisms of emulsions are well established: droplet coalescence (fusion of two droplets) and Ostwald ripening (molecular exchange through the continuous phase). Here we demonstrate the existence of a third mechanism, contact ripening, which operates through molecular exchange upon droplets collisions. A contrast manipulated small angle neutron scattering experiment was performed to isolate contact ripening from coalescence and Ostwald ripening. The key parameters have been identified through a kinetic analysis using dynamic light scattering and

monodisperse nanoemulsions. Contact ripening is accelerated by increasing the concentration of droplets but hindered by repulsions between droplets and highly hydrated cohesive films. These parameters can be tuned to control the magnitude of this exchange/coarsening mechanism, which is essential for both emulsion formulation and delivery of hydrophobic ingredients. (Kevin Roger, Ulf Olsson, Bernard Cabane (ESPCI, Paris), Ralf Schweins (ILL, Grenoble).)

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 have been combined with static light scattering (SLS) measurements of the second virial coefficient to provide insights into the mechanism of patchy, attractive protein interactions. We use lactoferrin as model protein, since it was 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, using no adjustable parameters. The molecular origin of the attraction could be explained as 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 second virial coefficient as a function of electrolyte concentration (Li et al., JPhys. Chem. B, 2015). Similar salt dependence has been observed in various proteins which points to a more general mechanism. Currently the effect of the attraction anisotropy on the scattering pattern is being explored. (Weimin Li, Björn Persson (Division of Theoretical Chemistry), Mikael Lund (Division of Theoretical Chemistry), Johan Bergenholtz and Malin Zackrisson Oskolkova.)

Polymer mediated attractive interactions of PEGylated colloids

(Contact person: Malin Zackrisson Oskolkova)

In this project we investigate 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. PEGylated particles differ from the commonly used non-aqueous systems for which crystallization in the polymer shell acts to trigger the attractions. This water-based system offers a more controlled approach where the solvent quality for PEG is varied and found to smoothly regulate the interactions (Zackrisson Oskolkova et al., RCS Advances, 2015). From a quantitative analysis of small-angle neutron scattering data we can extract the effective attraction. 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. (Jeanette Ulama (Physical Chemistry, Göteborg University), Johan Bergenholtz (Physical Chemistry, Göteborg University and Physical Chemistry, Lund University), Giuseppe Foffi (University of Paris-Syd) and 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 has been verified by ellipsometry for uncharged model systems (hydrophobically modified silica particles and silica surfaces in cyclohexane) and, also, for charged silica particles and surfaces in water. QCM and AFM are also used to study the surface phenomena. (Samia Ouhajji, Gerda Kamsma, Lennart Piculell, Tommy Nylander, A. Philipse and Remco Tuinier (University of Utrecht).)

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 against 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 monosaccharides, 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, 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), Wim Bouwman (University of Delft, The Netherlands), Marc Obiols-Rabasa, Anna Stradner.)

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).)

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 system 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 system, 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, Håkan Wennerström, Karen Edler (University of Bath), Kevin Roger (Univ Toulouse, France).)

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, Manja Behrens, Joel Hagman, Christian Moestrup Jessen, Daniel Topgaard, B. Medronho, L. Alves, M. Miguel (Coimbra).)

Colloids with complex interactions: from model atoms to colloidal recognition and bio-inspired self-assembly (Contact person: Peter Schurtenberger)

In this ERC Advanced Grant Project we follow nature's strategies and make a concerted experimental and theoretical effort to study, understand and control self-assembly for a new generation of responsive colloidal building blocks. We investigate the influence of anisotropy in shape and interactions on phase behavior and self-assembly in colloidal suspensions and mixtures. Using responsive particles we implement colloidal lock-and-key mechanisms and then assemble a library of "colloidal molecules" with well-defined and externally tunable binding sites using microfluidics-based and externally controlled fabrication and sorting principles. We use them to explore the equilibrium phase behavior of particle systems interacting through a finite number of binding sites, and subject recently developed theoretical models and computer simulations to a critical test. In parallel, we will exploit them and investigate colloid self-assembly into well-defined nanostructures. We combine molecule-like colloidal building blocks that possess directional interactions and externally triggerable specific recognition sites with directed self-assembly where external fields not only facilitate assembly, but also allow fabricating novel structures. (Jérôme J. Crassous, Adriana Mihut, Linda Månsson, Maxime Bergman, Antina Ghosh, Per Linse, Emanuela Zaccarelli (University La Sapienza Rome, Italy), Peter Schurtenberger.)

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 $\text{C}_{16}\text{TAPA}_y$, 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 $\text{C}_{16}\text{TAPA}_y$ 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 is employed. The soluble complex salt aggregates of $\text{C}_{16}\text{TAPA}_{25}$ or $\text{C}_{16}\text{TAPA}_{6000}$ 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 (Colloidal Resource, Lund, Sweden), Matija Tomšič (University of Ljubljana, Slovenia), Viorel N. Pavel and Luciano Galantini (University of Rome "La Sapienza", Italy).) (Project completed.)

Structured surface layers of hydrated 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 hydrated liquid-crystalline polymer-surfactant layers from associating oppositely charged 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 complex salt assemblies. The surface layers swell, but do not dissolve, in water, and the structures of the layers can be controlled by choice of polyion, surfactant ion and added co-surfactant, and they also respond to the humidity of surrounding air, and to solutes such as salts, acids, surfactants and polymers in a surrounding aqueous solution. Detailed SAXS studies of the liquid crystalline structures give both kinetic and equilibrium information, and confirm that the structures largely correspond to those found in studies of bulk systems of the same compositions. (Charlotte Gustavsson, Lennart Piculell, Joaquim Li, Marc Obiols-Rabasa, Karen Edler.)

Phase behavior, dynamics and directed self-assembly of anisotropic model colloids

(Contact person: Peter Schurtenberger)

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, or with an external alternating electrical field.

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.

We also study the effect of particle anisotropy and external polarizing electrical fields with soft ellipsoidal core-shell microgel particles using a combination of confocal laser scanning microscopy and computer simulations. (Jérôme J. Crassous, Adriana Mihut, Ilya Martchenko, Per Linse, Erik Wernersson, Ann Hirt (ETH Zurich, Switzerland), Vincent Martinez and Wilson Poon (University of Edinburgh, UK), Jan Vermant (ETH Zurich, Switzerland), Peter Schurtenberger.)

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, Maxime Bergman, Emanuela Zaccarelli (University La Sapienza Rome, Italy), Peter Schurtenberger.)

Magnetic particles (Contact person: Per Linse)

Structure of quasi-2d solutions of dipolar superballs in the fluid state has been determined by Metropolis Monte Carlo simulations without and with the presence of an external field. Here, the superballs resemble cubes but possess rounded edges. Examination has been made for three different dipole directions with respect to the superball principal axes and at several magnitudes of the dipole moment. At a small dipole moment, the superballs are translationally and orientationally disordered, and the dipoles become partially orientationally ordered in the presence of the field parallel to the plane of the superballs. At a large dipole moment, chains of superballs are formed, and the chains become parallel in the presence of the field. The chains remain separated for the dipole in the 001-direction and form bundles for the 011- and 111-directions. The different structures obtained for the different dipole directions are interpreted in terms of how compatible the dipole-dipole interaction is with the cube-cube interaction at short separation for the different directions of the dipole moment. Hence, the structural richness appears from an interplay of the different symmetries of a cube and of the field of a dipole. (Albert P. Philipse (Utrecht University) and Per Linse.)

Understanding and exploiting soft and anisotropic interactions in colloidal suspensions (Contact person: Peter Schurtenberger)

We investigate structural and dynamic properties of colloidal particles with a soft repulsive interaction potential, and study self-assembly without and with externally applied fields. The project follows the well-established tradition of using colloids as model systems in condensed matter research to unravel basic phenomena such as phase transitions, crystallization and glass formation. Here we extend this approach to responsive soft particles such as Poly(*N*-isopropylacrylamide) microgels with tunable and directional interactions. We address the following key points:

- (1) We use responsive neutral microgels to re-investigate recently developed approaches to disentangle glass and jamming transitions in soft particle systems.
- (2) We extend the previous work to ionic microgels and develop a quantitative description of the interaction potential of ionic microgel particles with and without an

applied electric field.

(3) We use them as a convenient model system for an investigation of crystallization, melting and domain growth processes and develop analogies to classical materials such as alloys.

(4) We employ structured arrays of nanowire electrodes to generate complex electrical fields in order to fabricate novel 2d and 3d structures through field-directed self-assembly and templated growth of various ionic microgel-based core-shell nanoparticles.

(Jerôme Crassous, Priti Mohanty, Sofi Nöjd, Jasper Immink, Divya Paloli, Peter Holmqvist, Anand Yethiray (Memorial University, St. John's, Canada), Emanuela Zaccarelli (University La Sapienza Rome, Italy), Christos Likos (University of Vienna, Austria), Jan Dhont (Forschungszentrum Jülich, Germany), Peter Schurtenberger.)

Inclusion complex formation between thermoresponsive PNIPAAm diblock copolymers and cyclodextrin at solid/liquid interfaces

(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 at silica/liquid interfaces. Ellipsometry, neutron reflectivity and quartz crystal microbalance with dissipation techniques are employed to study the surface properties under different conditions, such as with the presence of CD, at different temperatures and with copolymers of different PNIPAAm block lengths. (Solmaz Bayati, Karin Schillén, Tommy Nylander, Aleksandra Dabkowska, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway), Giuseppe Lazzara (University of Palermo, Italy) and Richard Campbell (ILL, France).)

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).)

Brush polymers at solid surfaces (Contact person: Per Linse)

Thermo-responsive polymer layers on silica surfaces have been obtained by utilizing electrostatically driven adsorption of a cationic-nonionic diblock copolymer. The cationic block provides strong anchoring to the surface for the nonionic block of poly(2-isopropyl-2-oxazoline), referred to as PIPOZ. The PIPOZ chain interacts favorably with water at low temperatures, but above 46 °C aqueous solutions of PIPOZ phase separate as water becomes a poor solvent for the polymer. We explore how a change in solvent condition affects interactions between such adsorbed layers, and report temperature effects on both normal forces and friction forces. To gain further insight, we utilize self-consistent lattice mean-field theory to follow how changes in temperature affect the polymer segment density distributions and to calculate surface force curves. We find that with worsening of the solvent condition an attraction develops between the adsorbed PIPOZ layers, and this observation is in good agreement with predictions of the mean-field theory. The modeling also demonstrates that the segment density profile and the degree of chain interpenetration under a given load between two PIPOZ-coated surfaces rise significantly with increasing temperature. (Junxue An, Xiaoyan Liu, Andra Dedinaite and Per M. Claesson (KTH), Françoise M. Winnik (University of Montreal) Per Linse.)

Self-organized structures of oppositely charged PNIPAAm diblock copolymers in aqueous solution (Contact person: Karin Schillén)

Self-organized structures are formed in water by electrostatic attraction between two oppositely charged poly(N-isopropylacrylamide) PNIPAAm diblock copolymers, which are mixed at 1:1 charge ratio. The copolymers have the same lengths of the PNIPAAm and the charged blocks. We use dynamic and static light scattering, turbidimetry, small angle X-ray scattering, 2D- or NOESY-nuclear magnetic resonance, cryo-transmission electron microscopy, electrophoretic mobility and DSC measurements to investigate the effect of temperature and total concentration on the aggregation behavior. (Solmaz Bayati, Karin Schillén, Bo Nyström and Kaizheng Zhu (University of Oslo, Norway) and Jan Skov Pedersen and Beatrice Plazzotta (Aarhus University, Denmark).)

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 and hypercholesterolemia. Bile salts 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, physicochemical studies

of the interaction between the anionic 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, small angle X-ray and neutron scattering in combination with differential scanning calorimetry. The experimental results reveal that the bile salt interacts with the copolymers forming, at low bile salt concentrations, a large copolymer-rich complex by association of NaGDC monomers to the block copolymer micelle. The micelle disintegrates upon increasing the concentration of bile salt passing different aggregation states. The dependence of added salt and the type of bile salt on the bile salt-copolymer interaction is under investigation. (Solmaz Bayati, Karin Schillén, Gerd Olofsson, Luciano Galantini (University of Rome “La Sapienza”, Italy) and Kenneth D. Knudsen (Institute for Energy Technology, Kjeller, Norway).)

Experimental methodologies

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

Articulate cartilage is a firm gel-like complex material, composed of collagenous fibers and cells called chondrocytes. 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 proteoglycans 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.

Finally, a theoretical framework for the transport and concentration of ions in cartilage starting from a non-equilibrium situation is developed. This forms the basis for numerical calculations based on the finite element method. (Jenny Algotsson, Daniel Topgaard, Olle Söderman, Peter Jönsson, Jan Forsman (Division of Theoretical 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 as 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 soft matter

(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 earlier 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 that and its biological function. 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 Medicine), Malin Zackrisson Oskolkova.)

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 coarse grained computer simulations based on colloidal models to achieve a quantitative understanding of protein interactions in the eye lens. (Saskia Bucciarelli, Tommy Garting, Najet Mahmoudi, Lucia Casal-Dujat, Bela Farago (ILL Grenoble, France), Cristiano de Michele (La Sapienza, Rome), Francesco Sciortino (La Sapienza, Rome), Giuseppe Foffi (Université Paris-Sud, France), George Thurston (Rochester Institute of Technology, USA), Mikael Lund, Peter Schurtenberger, Anna Stradner.)

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).)

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 α -synuclein is found in the protein aggregates characteristic for Parkinson disease. In this project, we study interactions between α -synuclein 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 integrity. 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, Aleksandra Dabkowska, Sara Linse (Division of Biochemistry and Structural Biology, LU), Chris Dunning & Patrik Brundin (Wallenberg Neurocenter, LU), Tommy Nylander, Ulf Olsson, Daniel Topgaard, Celine Galvagnion (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 own 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 Alfreðsson, 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, and Per Linse.) (Project completed.)

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. Diffusional transport across SC can be regulated by changes in the skin environments. One example is the abrupt increase in SC permeability at high degrees of SC hydration, called occlusion effect. Through a complementary experimental and theoretical approach, we have provided a molecular explanation to this effect.

We investigate how different classes of small molecules used as penetration enhancers or moisturizers influence the molecular properties of SC components and the macroscopic barrier properties of the skin. We also study the differences between healthy and diseased SC. We characterize the lipid and protein components in intact stratum corneum using natural abundance PT ssNMR and sorption techniques. 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), Lars Wadsö (Building materials, LTH), Joke Bouwstra (Leiden 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, Tommy Gating, Najet Mahmoudi, Lucia Casal-Dujat, Marc Obiols-Rabasa, Johan Bergenholtz, Bela Farago (ILL Grenoble, France), Olaf Holderer (Jülich Centre for Neutron Science (JCNS), Germany), Jin Suk Myung (FZ Juelich, Germany), Roland Winkler (FZ Jülich), Gerhard Gompper (FZ Jülich), Jan Dhont (FZ Jülich), 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 userface techniques, including combined QCM-D and ellipsometry and fluorescence recovery after photobleaching (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, Agnes Michanek, Tommy Nylander, Emma Sparr, Fredrik Höök (Chalmers), Luch Jaeger (Univ California, Santa Barbara).) (Project completed in 2014.)

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 Nylander, Daniel Topgaard.)

Peptide self-assembly (Contact person: Ulf Olsson)

The development of modern peptide chemistry has opened for the possibility of custom peptide synthesis that allows for systematically investigating the relationship between a specific oligopeptide molecular structure and the macroscopic phases and structures formed in such systems. Understanding the assembly behavior of peptides is important in not only designing nanomaterials for a desired functionality but also for combating neurodegenerative diseases such as Alzheimer and Parkinson's disease which are strongly associated with an accumulation of amyloid forming peptides in the brain. In this newly started project we focus initially on the self-assembly behavior of short simple and synthetic peptides, AnK, where n is varied in the range 4-10 (A=alanine, L=lysine). These peptides allow 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 (monodisperse) 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 crystal 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 (monodisperse) diameter of 52 nm, for concentrations above a critical aggregation concentration, $c_{ac} \approx 11$ %. 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, Mikael Lund (Division of Theoretical Chemistry), S. Bucak (Istanbul), Paul Bomans, Heiner Friedrich and Nico Sommerdijk (Eindhoven), Burcu Dedeoglu and Viktorya Aviyente (Istanbul), Theyencheri Narayanan (ESRE, Grenoble).)

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), Tiago Ferreira (Martin Luther universität Halle-Wittenberg, Germany), Emma Sparr.)

Molecular matter for specific functions

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, Sandor Balog and Alke Fink (University of Fribourg), Peter Schurtenberger.) (Project completed.)

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 Shift 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.) (Project completed.)

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 this 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).)

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 (SİK AB, The Swedish Institute for Food and Biotechnology Structure and Material Design).)

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).)

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 disc-like 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.)

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).)

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).)

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.)

Alternative Diesel Fuel (Contact person: Ulf Olsson)

Alternative fuel from renewable resources has been receiving increased attention worldwide due to the expected depletion of fossil fuel and the environmental hazardous nature of emissions associated with its combustion. Diesel exhaust poses one of the major health hazards to human. The particulate matter or soot and the nitrogen oxide compounds released directly to the environment can cause serious health problems. Vegetable oils, being renewable, with similar energy content to diesel, can be a viable alternative fuel. However, due to their high viscosity, they can't be injected directly without engine modifications. Reducing viscosity can be achieved through the trans esterification process, in which the oils react with alcohol, commonly methanol, to yield the corresponding fatty methyl ester, known as biodiesel. The produced biodiesel has many attractive properties. It is compatible with diesel, renewable and it produces lower emission of greenhouse gases and pollutants like soot and polycyclic hydrocarbons. On the other hand, some technical problems associated with its usage, like the poor low temperature properties and the increased NO_x exhaust emissions still need to be solved.

The phase behavior of water, diesel, limonene and ethanol was investigated at ambient temperature using single nonionic alkyl poly glycol ethers (C_{14}E_3). Visual inspection as well as cross polarizers were used to detect transparency and anisotropy. Ternary phase diagrams were determined. Combustion experiments using a 4-cylinder diesel engine were carried out. Isotropic water in diesel microemulsion region (L_2) and anisotropic liquid crystalline region (LC) were found with all combinations. Increasing the ratio of limonene to diesel reduced the microemulsion region while the presence of ethanol increased it on the expense of the LC region. Combustion tests performed on a selected formulation from the ternary phase diagram of water, diesel, ethanol and C_{14}E_3 revealed substantial reduction of soot, NO_x and CO_2 emissions compared to neat diesel. (Ibrahim Kayali, Ulf Olsson, Khawla Qamhieh.)

SCIENTIFIC INSTRUMENTATION

Surface techniques

Ellipsometry (Contact person: Tommy Nylander)

The development of a high precision ellipsometer for time-resolved studies of thin adsorbed films has been successful and of great importance to several specific projects. The instrument allows precise and rapid measurements of the ellipsometric angles and thus, allowing unique studies of the evolution of both the thickness and density (refractive index) of adsorbed surfactant and polymer layers with time. The possibility of working at different wavelengths provides an additional source of information on complex systems as well as flexibility to optimize the optical contrast of the systems studied. Continued efforts are invested in upgrading this instrument to improve its potential for studies of fast interfacial processes occurring on the nanometer scale.

During 1998 we acquired an additional ellipsometer, an Optrel Multiskop (Optrel, Berlin Germany). This instrument has been fitted with sample cells to measure at the solid-liquid, liquid-liquid and liquid-air interfaces. Apart from doing null-ellipsometry we can also do imaging ellipsometry, Brewster Angle Microscopy, Surface plasmons as well as operate it in waveguide mode. (Sponsored by FRN).

A spectroscopic ellipsometer, Horiba UVISEL-ER-AGAS Spectroscopic Ex-Situ Ellipsometer for the FUV-VIS-NIR Range with Automatic Goniometer and Motorised Mapping Stage that allow determination of the thin film properties within the spectral range from 190-2100 nm was purchased in 2010. The spectroscopic ellipsometer incorporates phase modulation technology to characterize polarization changes at high frequency (50 kHz), and without any mechanical movement. The Uvisel is equipped with a Multi Channel System for Parallel Spectra Acquisition for kinetic studies of thin films within the spectral range from 190 to 810 nm. The instrument is equipped 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-decahydronaphthalene, 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 $\leq 2 \times 10^{-6}$ 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 μ m 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 μ m). The instrument is equipped with a 4 mW He-Ne laser (wavelength of 632.8 nm) with an automatic laser attenuator that allows for measurements at sample transmissions ranging from 100 % to 0.0003 %. The detection unit comprises an avalanche photodiode. The temperature range of the instrument is 2–90 °C. (Sponsored by the Crafoord Foundation.)

Multi-angle static light scattering desktop instrument

(Contact person: Karin Schillén)

For characterization of molecular weight and studies of conformation changes or association processes in macromolecular systems, a multi-angle laser light scattering instrument for SLS measurements is available. The instrument is a Dawn DSP-F MALLS photometer (Wyatt Technology Corp., Santa Barbara, California) equipped with a 5 mW He-Ne laser (632.8 nm). The intensity of the scattered light is measured using photodiodes at 18 different angles simultaneously. The instrument is connected to a gel permeation chromatography system for on-line molecular weight determinations in aqueous solvents but batch analysis may also be performed. (Sponsored by NFR.)

3D Light scattering instrument (Contact person: Marc Obiols-Rabasa)

The instrument from LS Instruments is used for simultaneous dynamic and static light scattering with transparent and turbid samples. It incorporates the 3D cross-correlation technology for eliminating the contributions from multiple scattering. It is equipped with a 3D modulation unit, which implements the newest development to increase signal-to-baseline and leads to an almost four-fold improvement in the cross-correlation intercept compared to standard 3D technology. The instrument is equipped with a HeNe laser light source, wavelength $\lambda_0 = 632.8\text{nm}$ and a maximum power of 35 mW. Samples can be measured in cylindrical glass cells (with a diameter of 3, 5 or 10 mm) or 10 mm square cells and placed in the temperature controlled index-matching bath. The scattered light is detected within an angular range of 15 to 140° by two efficient Avalanche Photo Diodes and processed by a Flex correlator in a 3D cross-correlation configuration. In aqueous samples we have access to scattering vectors $0.0034 \leq q \leq 0.025\text{nm}^{-1}$. 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 $\lambda_0 = 532\text{nm}$) with a maximum power of 200 mW. Samples can be measured in cylindrical glass cells (with a diameter of 3, 5 or 10 mm) or 10 mm square cells and placed in the temperature controlled index-matching bath. The scattered light is detected simultaneously at 4 angles within an angular range of 10 to 150° by two photomultiplier tubes at each angle, and processed in real time by a 8 channel Flex correlator in a 3D cross-correlation configuration. Thus four intensity correlation functions are obtained simultaneously, one for each scattering angle measured. In aqueous samples we have access to scattering vectors $0.0027 \leq q \leq 0.031\text{nm}^{-1}$.

Electrophoretic light scattering (Contact person: Marc Obiols-Rabasa)

A Zetasizer Nano Z instrument from Malvern Instruments Ltd, Worshestershire, UK, is available for electrophoretic 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.

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 0.30 to 60, 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.

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-K α 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 $\leq 0.077 \text{ nm}^{-1}$ (corresponding to a Bragg value $\geq 82 \text{ nm}$) up to $\approx 8 \text{ nm}^{-1}$ (SAXS) and $\approx 29 \text{ nm}^{-1}$ (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 $\approx 0.003 \text{ \AA}^{-1}$ up to $\approx 2.5 \text{ \AA}^{-1}$.

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 person: Emma Sparr)

* 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 2oC to 80oC. The cells consists of non-reactive Hastelloy® for excellent chemical resistance, and they are fixed-in-place for reproducible ultrasensitive performance with low maintenance. The system 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: Emma Sparr)

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

Rheology

Rheometers (Contact person: Ulf Olsson)

A Physica UDS 200 stress controlled rheometer. Various cone and plate geometries with Peltier temperature control. A Couette geometry and a double gap measuring device, both in stainless steel, temperature controlled by circulated thermostated water. An Anton Paar MCR301 stress controlled rheometer equipped with additional transparent tools (plate-plate and cone and plate geometries) to allow for simultaneous small angle light scattering or microscopy detection.

Advanced rheometric expansion system (ARES)

(Contact person: Peter Schurtenberger)

The Advanced Rheometric Expansion System (ARES) is a true strain-controlled instrument, where the application of strain and the measurement of stress are separated. The sample is subjected to either a dynamic (sinusoidal) or steady shear strain deformation, and then the resultant torque expended by the sample in response to this shear strain is measured. The motor applies shear strain; the transducer measures torque. Strain amplitude and frequency are set by the operator, with the actual sample deformation determined by the measured motor, and transducer, displacement.

The instrument is implemented with the transducer 1 K FRT (torque range 0.004 – 20.0 g•cm and normal force range 2.0 – 2000.0 gmf). The operational temperature range is between -30°C and 150°C with temperature stability at thermal equilibrium of ± 0.1 °C, which is controlled with a Peltier system. The actual available geometries are: cone and plate (50 mm, 0.04 rad, 25 mm, 0.04 rad), plate and plate in (50 mm) and couette (16.5 mm bob, 17 mm cup and 32 mm bob and 34 mm cup).

Spectrophotometers

UV-Vis spectrophotometer (Contact person: Maria Södergren)

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

Fluorescence spectrophotometer (Contact person: Emma Sparr)

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

COLLABORATIVE RESEARCH PROGRAMS

Organizing molecular matter

(Contact person: Emma Sparr)

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

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, V. Alfredsson, T. Nylander and H. Wennerström.)

Division of Surface and Materials Chemistry of the Swedish Chemical Society

(Contact person: Viveka Alfredsson)

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. Viveka Alfredsson is serving as member of the board.

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 intelligent 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.

Strategic Research Areas and Lund University

nmC@LU is an 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 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 started 1 February 2014. The “Blopolymer 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.

Avancell

(Contact person: Ulf Olsson)

Avancell is a research network with focus on cellulose involving scientists from Södra Skogsägarna, Swerea IVE, Lund University, Chalmers and Coimbra University. With combined efforts and research collaborations, the network focuses on the dissolution and regeneration of cellulose.

Biocatalytic functionalisation of hemicellulose from waste (BIOFUNC)

(Contact persons: Henrik Stålbrand (Biochemistry) and Tommy Nylander (Physical Chemistry))

Softwood hemicellulose (galactoglucomannan, GGM) is one of Sweden's major renewable resources that make up 25% of the wood. GGM is, however, currently discarded in industrial waste-streams and its potential is not sufficiently explored. In BIOFUNC we will develop sustainable processes to substitute GGM structure and thereby transform it to a versatile and excellent renewable resource for novel high-performance products with added value. For this purpose we will develop new biotechnical processes for GGM recovery and enzyme-aided conversion to added value products that replace existing non-renewable products, but also have entirely novel added functionality. The outcome will be novel surfactants and a new family of polymers with special functions (e.g. controlled degradability, cellulose/wood/surface adhesiveness, acrylate latex/emulsion stabilisation). Thus the enzymatic route enable production of these high-value GGM-derivatives from GGM recovered from a low-value stream. This framework project is funded by Swedish Strategic Research and coordinated by Prof. Henrik Stålbrand (Biochemistry).

GERD OLOFSSON IN MEMORIAM

Sadly, Gerd Olofsson, a long-time member of our division with an extensive network of friends and colleagues in Sweden and abroad, passed away during 2014 at the age of 78.

Gerd Olofsson, born on a small farm in Vilhelmina in the far north of Sweden, was raised in Anundsjö, Ångermanland together with her seven sisters. The family lived under modest circumstances, but Gerd's parents, realizing that she had a good head for studying, made arrangements for her to study.

After graduating from secondary school ("studentexamen"), Gerd continued her education in Uppsala, where she became a Licentiate in Inorganic Chemistry in 1964 with Professor Ingvar Lindqvist as her supervisor. Gerd then continued her scientific research at the Thermochemistry Division of the newly formed Chemical Center in Lund, under the supervision of Professor Stig Sunner. Initially, her work was performed in close collaboration with Lindqvist. The intention was that Gerd would return to Uppsala, where Lindqvist planned to embark on thermochemistry research, but Gerd settled in Lund and did not return to Uppsala. In 1968, Gerd publicly defended her thesis in thermochemistry and then continued her research at the Thermochemistry Division. She soon started calorimetric investigations of problems within colloid and surface chemistry, often in close collaboration with colleagues at the Division of Physical Chemistry. Through her experimental skills and her analytical stringency, Gerd became recognized internationally as a leading expert, and she attracted a number of international guest researchers to Lund.

Gerd had a very large capacity for work, and her contributions to chemistry locally, nationally and internationally extended far outside of her own research. For many years she was the Chemical Center contact person for industry and other external relations. At the Division of Physical Chemistry, to which the Thermochemistry Group joined in 1995, Gerd got the unquestioned key role as an outstandingly efficient organizer and administrator of several large networks and ventures. Nationally, Gerd had a central role in the founding, in 2001, of the Section for Surface Chemistry at the Swedish Chemical Society, and she was appointed its first chair. During many years Gerd was active in IUPAC. She was elected to the Commission of Thermodynamics in 1987, where she was involved primarily in the standardization of international recommendations regarding thermodynamic data and nomenclature. Gerd's experience of scientific administration was taken to use in her tasks as the secretary of the Commission and, later, also the secretary of the IUPAC division of Physical Chemistry.

Naturally, Gerd had rich interests also outside of her profession. Her curiosity and appetite for travels brought her to many near and far places on the globe, where she always knew how to appreciate both nature and all kinds of culture. Her own garden in Södra Sandby, close to Lund, was a lovely oasis of ornamental and utility plants. Gerd's interest in playing golf most probably contributed to her characteristic physical fitness.

The picture of Gerd is, however, very incomplete without an attempt to describe her deeply appreciated personality. In every situation she saw what needed to be done, always with a consideration of the people involved and their needs. She was invaluable as mentor and creator of contacts. In her low-key, empathetic and altruistic way, but with a great integrity and firmness, she always supported us friends and colleagues, both in our professional roles and as the human beings and social creatures that we are. Gerd leaves a large void behind her.

CONFERENCES, TRAVELS AND SEMINARS

Viveka Alfredsson attended EMRS in Lille in May and gave an invited talk and also attended the ECIS conference in Cyprus in September and Realizing Reformulation in Lund in October. She gave invited lectures at Université Sud in Paris in October and in University of Ulm, Germany in December. She participated in a neutron scattering experiment at ISIS, UK, in June.

Jenny Algotsson gave an oral presentation at the 12th International Bologna Conference on Magnetic Resonance in Porous Media in Wellington, New Zealand.

Solmaz Bayati gave oral presentations at the 11th Nordic Workshop on Scattering from Soft Matter (NSSM) in Stockholm, Sweden and at the 20th International Symposium on Surfactant in Solutions in Coimbra, Portugal. She also presented her PhD-half-time seminar at the Division of Physical Chemistry.

Saskia Bucciarelli gave an invited presentation at the 18th annual meeting of the Swedish Neutron Scattering Society in Göteborg and an oral presentation at the 2nd “Research on Vertebrate Vision in Lund” meeting in Lund.

Stefanie Eriksson gave an oral presentation at the 12th International Bologna Conference on Magnetic Resonance in Porous Media in Wellington, New Zealand.

Peter Jönsson presented a poster at the ASMCS symposium Realizing reformulation in Lund, Sweden, and gave an invited lecture at Chalmers, Gothenburg, Sweden.

Ruiyu Lin gave an oral presentation at the 28th conference of the European Colloid and Interface Society in Limassol, Cyprus, and presented a poster at Realizing reformulation, a symposium on surface and materials chemistry in Lund, Sweden.

Björn Lindman gave plenary lectures at the Polymer networks and gels Conference in Tokyo, Japan and at the 4th International Mini-Workshop in Polymer and Surfactant Science, Look back to “Principles of Solution and Solubility” to honor the late Prof. K. Shinoda, Choshi, Japan. He gave a keynote lecture at the NANO-TR 10, Istanbul, Turkey and invited lectures at the workshop “Interactions in Colloidal Systems”, Berlin and the workshop “Particles at Liquid and Solid Interfaces: Fundamentals and Applications”, Genoa, Italy. He also attended the 26th Conference of the European Colloid and Interface Society (ECIS) in Limassol, Cyprus and the 20th Symposium on surfactants in Solution, Coimbra, Portugal. During the year Björn Lindman visited a number of universities and other research centers and in most cases he presented a lecture. The institutions visited included: Nanyang Technological University, Singapore; UNICAMP, Campinas, Brazil; MidSweden University, Sundsvall, Sweden; Laboratório Nacional de Nanotecnologia - CNPEM, Campinas, Brazil; Hokkaido University, Sapporo, Japan; University Sao Paulo, Brazil; Group of Colloid Physics, Sao Paulo State University, Sao Jose do Rio Preto, Brazil; Technische Universität Berlin; CNR-Istituto per l'Energetica e le Interfasi, Genova, Italy; University of Copenhagen, Denmark; Akzo Nobel Surface Chemistry, Stenungsund, Sweden; Chalmers University of Technology, Göteborg, Sweden; Södra Cell, Värö, Sweden; School of Science and Technology, Örebro University, Sweden; Royal Institute of Technology, Stockholm; Chiba Institute of Science, Choshi, Chiba, Japan; Tokyo University, Japan; Coimbra University, Portugal; Yeditepe University Ataşehir, Istanbul, Turkey; Tokyo Science University, Noda; Tokyo Science University, Katsushika; Tokyo Science University, Kagurazaka; LION Corporation Functional Materials Science Research Laboratories, Tokyo; Kazakh National Technical University, Almaty, Kazakhstan; Kazakh National University, Almaty, Kazakhstan; Delft University of Technology, Department of Chemical Engineering, Delft, The Netherlands; University of Florence, Italy. Björn

Lindman was Guest Professor at the Mid-Sweden University, FSCN - Fibre Science and Communication Network, and at Nanyang Technological University, Singapore.

Per Linse gave an oral presentation at the “Multiscale materials modelling” workshop in Uppsala, Sweden: Virus Self-Assembly Induced by Polyions; an oral presentation at the “Topical Meeting on Molecular Dynamics” in Copenhagen, Denmark: Virus Self-Assembly Induced by Polyions; an oral presentation at the “Aggregation and Clustering of Molecules” discussion meeting in Copenhagen, Denmark: Polyion-Induced Virus Assembly, attended a departmental seminar at University of Gothenburg: Virus Self-Assembly Induced by Polyions; and attended a departmental seminar at University of Gothenburg: Virus Self-Assembly Modelling.

Emelie Nilsson presented a poster at the conference of the European Colloid and Interface Society - ECIS 2014 in Limassol, Cyprus.

Tommy Nylander gave an oral presentation at Neutrons in Foods, Paris, European Colloid and Interface Society Meeting, Cyprus and invited keynote talks at the Food Structure Conference, Amsterdam, The Netherlands, Surfactant in Solution Symposium, Coimbra Portugal, Swedish Neutron Scattering Society Meeting, Chalmers Gothenburg, Sweden, Bicontinuous Cubic Phases Conference, Noosa a satellite meeting to the 2014 International Biophysics Congress, Brisbane, at Chinese German workshop at Institute of Chemistry, Chinese Academy of Sciences, Beijing and a plenary talk at AutoOrg 2014, Sao Pedro, Brasil. He also gave invited talks at Bragg Institute, Ansto, Lucas Heights and Applied Maths Australian National Univeristy, Canberra Australia, Federal University of Rio Grande do Sul, Porto Allegre, and University of Campinas, Brasil.

Sofi Nöjd gave an oral presentation at the 11th Nordic Scattering Workshop on Soft Matter in Stockholm, Sweden. Another oral presentation was given at the 28th Conference of the European Colloid and Interface Society in Limassol, Cyprus. A poster was presented at Realizing Reformulation in Lund, Sweden.

Marc Obiols-Rabasa gave oral presentations at the 11th Nordic Workshop on Scattering from Soft Matter in Stockholm, Sweden, at the Annual SoftComp meeting in Heraklion, Greece, and at the ECI Conference Biological and Pharmaceutical Complex Fluids II in Durham, USA. He also gave an invited lecture at Institute Laue-Langevin (ILL) in Grenoble, France, one invited lecture at Anton Paar Nordic in Malmö, Sweden, and two invited lectures at UMR CNRS 5672, École Normale Supérieure de Lyon in Lyon, France. Marc Obiols-Rabasa also gave a poster presentation at the Realizing Reformulation, a Symposium on surface and materials chemistry in Lund, Sweden.

Ulf Olsson spent one month as invited visiting professor at Centre de Recherche Paul Pascal (CNRS) in Pessac, France. He attended the Workshop on Non-Equilibrium Complex Fluids and gave an invited talk at the Workshop on Non-Equilibrium Surfactant Solution, both at Tokyo Metropolitan University. He visited and gave seminars at the Physics Department, Tohoku University, Sendai, Japan, Kao Corporation, Tokyo and at the Chemistry Department at the University of Rome “La Sapienza”. He also attended the CNRS summer school “Soft Interactions in Biological and Biomimetic Self-Assemblies” in San Malo, France.

Lennart Piculell gave invited lectures at the 10th International Symposium on Polyelectrolytes 2014 in Ein Gedi, Israel, the 8th International Symposium on Molecular Order and Mobility in Polymer Systems in St.-Petersburg, and the Annual symposium on surface and materials chemistry in Lund, Sweden. He also presented a contributed lecture at the 20th International Symposium on Surfactants in Solution in

Coimbra, Portugal.

Karin Schillén gave an invited lecture at XXVIII European Colloid and Interface Society Conference, Limassol, Cyprus. She also held an oral presentation at the 20th International Symposium on Surfactants in Solution, Coimbra, Portugal and presented a poster at the 11th Nordic Workshop on Scattering from Soft Matter (NSSM), in Stockholm, Sweden.

Peter Schurtenberger gave invited keynote lectures at the Conference on “Neutron Characterisation in Fundamental and Applied Biotechnology” in Abingdon, UK, and at the 28th Conference of the European Colloid and Interface Society – Limassol, Cyprus, and he also gave invited lectures at the following international conferences, workshops and summer schools: the Workshop on “ESS and MAX IV – new opportunities in formulation research” in Lund, Sweden, two lectures at the 12th European School on “Scattering Methods Applied to Soft Condensed Matter”, Bombannes, France, the Workshop on Neutron Spin Echo at ESS in Copenhagen, Denmark, the Nordic X-ray Science Days, the NanoForum Connect, and the conference on Crystallography – Present and Future, all in Lund, Sweden. Peter Schurtenberger also gave the following seminars at Lund University: Physics with Neutrons and X-rays Seminar, Physics Seminar, Science Faculty Seminar.

Emma Sparr gave an invited lecture at the Berzelius days in Stockholm and at the conference Cutting Edge Biomolecular Sciences (Marstrand, Sweden). She gave an oral presentation at the International society for biological calorimetry conference XVIII ISBC Conference (Lund Sweden). Emma Sparr also gave an invited talk at the University of Cambridge (UK).

Anna Stradner gave invited lectures at the ECI (Engineering Conferences International) Biological and Pharmaceutical Complex Fluids II: Novel Trends in Characterizing Interactions, Microstructure and Rheology in Durham (North Carolina, USA) and at the Realizing Reformulation Conference in Lund (Sweden). She gave an oral presentation at the APS March Meeting 2014 in Denver (Colorado, USA).

Olle Söderman gave an invited lecture at the 20th International Symposium on Surfactants in Solution.

Daniel Topgaard gave invited lectures at the conferences XII International Conference on the Applications of Magnetic Resonance in Food Science: Defining Food by Magnetic Resonance (FOODMR 2014), Cesena, Italy, and Swedish NMR Meeting 2014, Gothenburg, Sweden, as well as the workshops NMR in Soft Matter, Durham University, UK; International symposium on Microstructures of Learning: Novel methods and approaches for assessing structural and functional changes underlying knowledge acquisition in the brain, Pufendorf Institute for Advanced Studies, Lund University, Sweden; NSF sponsored workshop: Physical, Engineering, and Biological Limits to Brain Measurements, Arlington, Virginia, USA; The 6th PRISM workshop. Diffusion coefficient by NMR and MRI: a novel approach to probe structures, interactions and to characterize complex systems, University of Rennes, France; Recent advances in cellulose nanotechnology research: Production, characterization and applications, Paper and Fibre Research Institute, Trondheim, Norway. He gave a contributed talk at the conference Magnetic Resonance in Porous Media 12 (MRPM12), Victoria University of Wellington, New Zealand. He also gave seminars at Center of functionally integrative neuroscience, Aarhus University, Denmark; Avancell 3 kick-off, Coimbra University, Portugal; Minisymposium on Formulation Science, Lund University, Sweden; Molecular Materials Research Community, University of Oulu, Finland; Medical Radiation Physics, Lund University, Sweden; and Department

of Chemistry, University of Bergen, Norway.

Ingemar Wadsö gave a lecture at the XVIII International Society for Biological Calorimetry Conference (ISBC) in Lund, Sweden.

Malin Zackrisson Oskolkova attended the Jülich Soft Matter Days, held in Bad Honnef, Germany and gave an oral contribution. She also gave invited talks at the Institute für Physikalische Chemie, RWTH Aachen University, Germany and at NovoNordisk, Copenhagen, Denmark. Malin Zackrisson Oskolkova attended a workshop on Biological Self-Assembly in St. Malo, France.

EXTERNAL PROFESSIONAL ACTIVITIES

Viveka Alfredsson was a member of the board of the International Mesosstructured Materials Association and the Division of Surface and Materials of the Swedish Chemical Society. She is a board member of “Lunds universitets gästhem”.

Peter Jönsson was on the advisory board for the graduate school ADMIRE at Lund University, Sweden.

Björn Lindman was on the Advisory or Editorial Boards of *Advances in Colloid and Interface Science*, *Current Opinion in Colloid & Interface Science*, *Fine Chemicals*, *Colloid & Polymer Science*, *The open Physical Chemistry Journal*, and *Journal of Dispersion Science and Technology*. Björn Lindman is a member of the Royal Swedish Academy of Engineering Sciences, of the Royal Swedish Academy of Sciences, of the Academia das Ciências de Lisboa, the Portuguese Academy of Sciences and of the Royal Physiographic Society in Lund, and honorary corresponding member of Romaniae Scientiarum Societas. He is “docent” at Åbo Akademi, Finland. He is cofounder and honorary member of the European Colloid & Interface Society (ECIS). Björn Lindman was “faculty opponent” for the Ph D defence of Argyro Kalaitzakis at Örebro university and for the Ph D defence of Nicholas Cervin at the Royal Institute of Technology, Stockholm.

Tommy Nylander served as thesis examiner (opponent) for the PhD theses of Merete Bøgelund Munk, Murillo Longo Martins and Anna Maria Sulewska (Copenhagen University) as well as Jonas Bruun (DTU, Lyngby). He was member of the evaluation panel for beam time applications NIST Centre for Neutron Research, Gaithersburg, USA and ISIS, ISIS – Rutherford Appleton Laboratory, Oxfordshire, UK and chaired the panel for Biology at FRMII, Munich. In addition he was evaluator of research proposals for BBSRC – Biotechnology and Biological Sciences Research Council, Australian Research Council and MIUR – Ministero dell’Istruzione, dell’Università e della Ricerca, Italy as well as expert evaluator for EU Marie Skłodowska-Curie Actions “Individual fellowships”.

Ulf Olsson was board member of the MAX IV Laboratory, and also served on the Science Advisory Committee of the Swiss spallation neutron source, SINQ. He is the spokes person for the CoSAXS beamline project at MAX IV. He also served in the grading committees of the PhD thesis of Marta Gubitosi at the University of Rome “La Sapienza”.

Lennart Piculell is a 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. He is also a member of the AkzoNobel Nordic Prize Award Committee. At Lund University he was a member of the Electoral Committee of the Faculty of Science during 2014.

Karin Schillén served on the PhD grading committee for Louise Ovaskainen, Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm. She is the head teacher in Physical Chemistry. 2014 was Karin's final year as a member of undergraduate studies in chemistry.

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 SANS Scientific Advisory Panel, Member of the MAX IV CoSAXS Beamline Scientific Advisory Panel, Member of the Organizing Committee 12th European Summer School on "Scattering Methods Applied to Soft Condensed Matter", Bombannes, France, of the International Program Committee of the European Conference on Neutron Scattering ECNS in Zaragossa, Spain, 2015, and of the International Program Committee of the 9th Liquid Matter Conference in Lisbon 2014, and he was on the Editorial Board of the journals Colloid & Polymer Science and Soft Matter, and Section Editor of Current Opinion in Colloid and Interface Science. He is a member of the Royal Swedish Academy of Sciences, a fellow of the British Royal Society of Chemistry, and an honorary member of the European Colloid and Interface Society (ECIS).

Emma Sparr was chairing the organizing and scientific committees of the annual meeting on surface and material chemistry "Realizing Reformulation" held in Lund on October 22-24. Emma Sparr was member of the board of the Young Academy of Sweden until June 2014, and she was chairing the panel for electing new academy members 2014. Emma Sparr was in the panel for grant evaluation in physical, theoretical and analytical chemistry at the Swedish Research Council, and she was external reviewer for the Swiss research council. Emma Sparr served on the PhD grading committee for Maria Matson-Dzebo at Chalmers. At Lund university, Emma Sparr was the director of the Linnaeus center OMM.

Anna Stradner was a member of the International Advisory Board for the 28th European Colloid and Interface Society (ECIS) Conference 2014 (Limassol, Cyprus), member of the Program Executive Committee of the European infrastructure project ESMI (European Soft Matter Infrastructure) and member of the Search Committee for the Enzo Ferroni Award for a Young Scientist and the Technion Prize for a Young Scientist awarded at the 28th European Colloid and Interface Society (ECIS) Conference in Limassol, Cyprus.

Daniel Topgaard served as thesis examiner (opponent) for the PhD theses of Päivi Kekkonen, University of Oulu, Finland and Abduljelil Sultan Kedir, University of Bergen, Norway. He was evaluator of research proposals for the Danish Council for Independent Research and the Swedish Research Council.

Malin Zackrisson Oskolkova organized and led a public debate with Masters students within the course KEMM37 at Polhemsskolan, Lund. She is part of a newly formed Scandinavian network named NYNNes for young neutron users, with approved funding by Nordforsk.

OUTREACH ACTIVITIES

Lennart Piculell gave a popular science lecture with the title “Edible and inedible gels” for Swedish high school students visiting Lund University.

Emma Sparr participated in an exchange program between the Swedish parliament and academic researchers in the young academy of Sweden, and hosted a visit of a Parliament member at the Chemistry department. Emma Sparr gave a talk for high school pupils at Berzeliusdagarna and she performed experiments together with primary school pupils at Vårfruskolan. She also presented her research at LeoPharma (Copenhagen, Denmark) and she was involved in collaborative projects with LeoPharma and L'Oréal (France).

AWARDS

Emma Sparr received the Hagberg Foundation 2014 prize (Kungliga vetenskapsakademien, KVA).

DISTINCTIONS

Peter Schurtenberger is elected as a member of the Royal Swedish Academy of Sciences.

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 and Emma Sparr were leading exercises and question hours, whereas Daniel Topgaard was lecturing 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, Per Linse, Tommy Nylander, Anna Stradner and Peter Schurtenberger. This course is based on the textbook "The Colloidal Domain" by D. 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 on the Ph D student course in Surfaces and Colloids at Nanyang Technological University, Singapore and on a course on colloids at the International Postgraduate Institute "Excellence PolyTech", Kazakh National Technical University. Furthermore, Björn Lindman was one of the teachers at the annual course on Surfactants and Polymers in Aqueous Solution, this year given in Lisbon.

Malin Zackrisson Oskolkova was invited lecturer at MAX-lab in the MAXM06 course.

SEMINARS 2014

Kira Bartnik, Ludwig-Maximilians-Universität (LMU), Munich, Germany
Study of adsorption of the protein α -synuclein to lipid bilayers using QCM

Stefanie Eriksson, Physical Chemistry, Lund University
Illuminating microscopic anisotropic structures with diffusion NMR

Solmaz Bayati, Physical Chemistry, Lund University
Self-Organization in Dilute Block Copolymer Systems

Emanuel Schneck, Max Planck Institute of Colloids and Interfaces, Biomaterials Department, Potsdam, Germany
Influence of Glycolipids on Mechanics and Interactions of Membranes

Realizing reformulation – A symposium on surface and materials chemistry

Invited speakers:

- Thomas Arnebrant, Malmö University, Biofilm research center, Sweden
- Odille Aubrun-Sonneville, L'ORÉAL, France
- Vance Bergeron, Ecole Normale Supérieure de Lyon, France
- Lennart Bergström, Stockholm University, Sweden
- Joke Bouwstra, Leiden university, the Netherlands
- Katarina Edwards, Uppsala University, Sweden
- Anette Larsson, Chalmers University of Technology, Sweden
- Jayne Lawrence, King's college, London, UK
- Mika Lindén, University of Ulm, Germany
- Mariagrazia Marucci, AstraZeneca, Mölndal, Sweden
- Lennart Piculell, Lund University, Sweden
- Lovisa Ringstad, SP Technical Research Institute of Sweden, Sweden
- Mark Rutland, KTH Royal Institute of Technology, Sweden
- Anna Stradner, Lund University, Sweden
- Ishi Talmon, Technion-Israel Institute of Technology, Israel
- Fredrik Tiberg, Camurus, Sweden
- Christine Vauthier, University Paris Sud, France
- Peter Wilde, Institute of Food research, UK

Young scientists and AkzoNobel prize winners:

- Romain Bordes, Chalmers University of Technology, Sweden
- Hanna Dahlenborg, SP Technical Research Institute of Sweden, Sweden
- Sara Frykstrand, Uppsala University, Sweden
- Kevin Roger, Lund University, Sweden
- Yolanda Hedberg, KTH Royal Institute of Technology & Karolinska Institutet, Sweden
- Samuli Ollila, Aalto University, Finland

Saskia Bucciarelli, Physical Chemistry, Lund University

Structural and dynamic properties of concentrated eye lens protein solutions

Dikran Kesal, Technical University Berlin, Germany

Interaction of Lipid Bilayer Systems on Nanowire Arrays

Emelie Nilsson, Physical Chemistry, Lund University

Understanding the formation of mesoporous silica – the study of a model system

Sandrine Bouquillon, Université de Reims Champagne-Ardenne, Reims, France

Contributions of the biomass to dendrimer's and ionic liquid's fields

Sanna Gustavsson, Physical Chemistry, Lund University

Carbohydrate systems in the water-poor regime

Jenny Algotsson, Physical Chemistry, Lund University

A study of the transport and equilibrium distribution of an MRI contrast agent in a model system of articular cartilage

Marianna Yanez Arteta, Physical Chemistry, Lund University

Nanostructured surfaces created by the interactions of dendrimers and oppositely charged amphiphiles

Minisymposium: “Nanostructured interfaces: Formation, Properties and Applications”

- Robert K. Thomas, University of Oxford, UK:
Neutron Reflection from Layered structures at Surfaces
- Stefan Zauscher, Duke University, Durham-NC, USA:
“Living” Enzymatic Polycondensation Polymerizations: Towards new DNA Nanostructures
- Kell Mortensen, Niels Bohr Institute, University of Copenhagen, Denmark:
Hydrogels based on Molecular Self-assembly – Combined Studies of Structure and Rheology
- Fredrik Höök, Chalmers University of Technology, Gothenburg, Sweden:
Label-free biomolecular interaction analysis and single-molecule studies of cell-membrane mimics
- Andra Dédinaité, Royal Institute of Technology, Stockholm, Sweden:
The role of self-assembly structures in biolubrication
- Charlotte Gustafsson, Physical Chemistry, Lund University, Sweden:
Nanostructured responsive polymer-surfactant films on solid surfaces
- Richard Campbell, Institute Laue Langevine, Grenoble, France:
A non-equilibrium perspective on polyelectrolyte/surfactant mixtures at the air/water interface

Chris Evers, Van 't Hoff Laboratory for Physical and Colloid Chemistry, Debye Institute, Utrecht University, the Netherlands

Spontaneous Directionality in Anisotropic Floppy Colloids

Jasenko Gavran, Physical Chemistry, Lund University

Exploring folding conditions and stability of N-terminal region of tapasin

Tadashi Kato, Tokyo Metropolitan University, Japan

Re-Entrant Lamellar/Onion Transition with Varying Temperature under Shear Flow in a Nonionic Surfactant/Water System

Florian Nettesheim, DuPont

Structure and Rheology of carrageenan gels

Gerda Kamsma, Utrecht University, the Netherlands

Bulk aggregation versus surface adsorption of charged colloidal silica spheres on a surface of the same material in water

Maura Monduzzi, Dept. Scienze Chimiche e Geologiche, Cagliari University, Monserrato (CA), Italy

Proteins and electrolytes: Effects at the polar interface of ordered mesoporous silica

Jasper Immink, Utrecht University, the Netherlands

From crystals to gels: Phase behavior of charged binary thermosensitive microgel mixtures with adjustable hydrophobic interactions

Céline Galvagnion, University of Cambridge, United Kingdom

Lipid vesicles trigger α -syn aggregation by stimulating primary nucleation

Maxime Bergman, Wageningen University, the Netherlands

Studying depletion interactions in microgel systems

Caroline Anderberg Haglund, Physical Chemistry, Lund University

A Light Scattering and Calorimetry Study on the Interaction between PEO-PPO-PEO Triblock Copolymers and the Bile Salt Sodium Glycodeoxycholate

Giuseppe Foffi, Laboratoire de Physique des Solides, Université Paris-Sud 11, France

Arrested phase separation, can we arrest demixing? Introducing bigels.

Marcel Ollila, Physical Chemistry, Lund University

Phase behavior of PEGylated model core-shell colloids

Linda Månsson, Physical Chemistry, Lund University

Synthesis of Thermosensitive Colloidal Molecules Through Pickering Emulsions

Frank Scheffold, Department of Physics and Fribourg Center for Nanomaterials, University of Fribourg, Switzerland

The fascination of randomly packed spheres: from dense emulsions to photonic materials design

Pegah Nosrati Hefzabad, Physical Chemistry, Lund University

Characterization of Cellulose Dissolved in Aqueous Tetrabutyl Ammonium Hydroxide

Ellen Rieloff, Physical Chemistry, Lund University

Adsorption of Thermoresponsive Microgels to Lipid Membranes

Björgvin Hjörvarsson, Uppsala University, Sweden

Using scattering techniques to explore the nano-world

Gerda Kamsma, Utrecht University, the Netherlands

Adsorption versus bulk aggregation of silica spheres on a silica surface in an aqueous system

Volker Koerstgens, Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Germany

The combination of microfluidics and microGISAXS – in situ structural investigations at the solid liquid interface

Najet Mahmoudi, Physical Chemistry, Lund University

Proteins with intermediate-range depletion attraction: connecting structure and mechanics

Håkan Wennerström, Physical Chemistry, Lund University

Diffraction and Scattering

Håkan Wennerström, Physical Chemistry, Lund University

The Stern-Gerlach experiment

Samia Ouhajji, Utrecht University / Lund University

Surface adsorption versus bulk aggregation of particles and surfaces of the same material: An experimental study

Christine Dupont-Gillain, Université catholique de Louvain (UCL), Faculté de bioingénierie (AGRO), Institut de la matière condensée et des nanosciences (IMCN), Belgium

Understanding and controlling the assembly of collagen at interfaces

Patrik Knöös, Physical Chemistry, Lund University

**Water-swelling tablets based on hydrophobically modified poly(acrylic acid)–
Effects of amphiphiles on swelling and drug release**

Minisymposium on Formulation Science

A half-day open seminar presenting a variety of examples of problems and methods of interest in current formulation science.

- Peter Griffiths, University of Greenwich, UK
Bubbles, snot and slime
- Stefan Ulvenlund, Colloidal Resource, Lund
Formulating the future. The tricks of the trade of tomorrow's technology
- Emma Sparr, Physical Chemistry, Lund University
Controlling the skin barrier through topical formulations
- Anette Larsson, Chalmers, Gothenburg
Controlled release formulations based on cellulose derivatives
- Björn Bergenståhl, Food technology, LTH
How to please the consumers – formulation challenges in food science
- Daniel Topgaard, Physical Chemistry, Lund University
Magnetic resonance characterization of formulations

ESS and MAX IV – new opportunities in formulation research

A half-day open seminar for industrial and academic researchers.

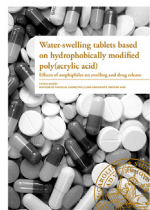
- Christoph Quitmann, MAX IV Laboratory, Lund University
MAX IV – A national resource for research & innovation
- Andrew Jackson, ESS, Lund
Nanoscale structural analysis with neutrons
- Heloisa N. Bordallo, Niels Bohr Institute, University of Copenhagen
Inelastic Neutron Scattering: A different approach to understand drug stability
- Marité Cárdenas, Nano science center, Department of Chemistry, University of Copenhagen
Film composition and its relevance in pharmacological formulations
- Sven Lidin, Materials Chemistry, KILU, LTH, Lund University
Simultaneous studies of structure at different length scales – requirements on equipment and sample
- Peter Schurtenberger, Physical Chemistry, KILU, Lund University
The stability and flow behavior of concentrated formulations– insight from x-ray and neutron scattering
- Adrian Rennie, Materials Physics, Department of Physics, Uppsala University
Understanding complex materials with x-rays and neutrons – realistic conditions and samples

DOCTORAL THESES

Patrik Knöö

Water-swelling tablets based on hydrophobically modified poly(acrylic acid) – Effects of amphiphiles on swelling and drug release

Opponent: Professor Peter Griffiths, University of Greenwich, United Kingdom



Marianna Yanez Arteta

Nanostructured surfaces created by the interactions of dendrimers and oppositely charged amphiphiles

Opponent: Professor Stefan Zauscher, Duke University, U.S.A.



Ilya Martchenko, Department of Physics, University of Fribourg, Switzerland

Magnetic colloidal ellipsoids

Thesis written under the supervision of Professor Peter Schurtenberger, Physical Chemistry, Lund University
External expert: Professor Jan Dhont, Forschungszentrum Jülich, Germany

PUBLICATIONS

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- (2) Ainalem, M-L.; Bartles, S.; 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, 3, e92692
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- (4) Angelescu, D. G.; Linse, P. Monte Carlo Simulations of Multigraft Homopolymers in Good Solvent *Macromolecules*, 2014, 1, 415-426
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- (6) 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*, 442, 1-1
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- (12) Bernin, D.; Steglich, T.; Roeding, M.; Moldin, A.; Topgaard, D.; Langton, M.
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- (14) Buell, A. K.; Galvagnion, C.; Gaspar, R.; Sparr, E.; Vendruscolo, M.; Knowles, T. P. J.; Linse, S.; Dobson, C. M.
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We recommend our visitors to fly to Kastrup Airport, Copenhagen. Then take a train 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

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