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Oral Presentations

Abstract #1

Electrostatic Assembly of Binary Nanoparticle Superlattices Using Protein Cages

Binary nanoparticle superlattices are periodic nanostructures with lattice constants much shorter than the wavelength of light and could be used to prepare multifunctional metamaterials. Such superlattices are typically made from synthetic nanoparticles and although biohybrid structures have been developed incorporating biological building blocks into binary nanoparticle superlattices remains challenging. Protein-based nanocages provide a complex yet monodisperse and geometrically well-defined hollow cage that can be used to encapsulate different materials. Such protein cages have been used to program the self-assembly of encapsulated materials to form free-standing crystals and superlattices at interfaces or in solution. Here, we show that electrostatically patchy protein cages—cowpea chlorotic mottle virus and ferritin cages—can be used to direct the self-assembly of three-dimensional binary superlattices.[1] The negatively charged cages can encapsulate RNA or superparamagnetic iron oxide nanoparticles and the superlattices are formed through tunable electrostatic interactions with positively charged gold nanoparticles. Based on cryogenic transmission electron microscopy and small-angle X-ray scattering data, Gold nanoparticles and viruses form an AB8fcc crystal structure that is not isostructural with any known atomic or molecular crystal structure and has previously been observed only with large colloidal polymer particles. Gold nanoparticles and empty or iron oxide nanoparticle-loaded ferritin cages form an interpenetrating simple cubic AB structure (isostructural with CsCl). Such magnetic assemblies can modulate efficiently spin–spin relaxation times of surrounding protons in water by enhancing the spin dephasing and consequently provide contrast enhancement in magnetic resonance imaging (MRI). We also show that stimuli-responsive superlattice structures can be achieved using optically degradable dendrons and protein cages.[2,3]

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Abstract #2

Spontaneous Changes of Bilayer Topology Observed in Surfactant Mixtures with Small-Angle Neutron Scattering (SANS)

The self-assembly in mixtures of an anionic and a cationic surfactant has been investigated with SANS. In regions where bilayer aggregates predominate, we observe the following sequence of changing bilayer topology: vesicles (Genus g = 0) -> disks (g = 1) -> perforated bilayers (g = 1 + number of holes), as the influence of electrostatics is reduced with increasing electrolyte concentration and decreasing surface charge density. We are able quantify that the fraction of disks, in mixtures of vesicles and disks, increases as an increasing amount of the inert salt NaBr is added to the solutions. Likewise, perforated bilayers are, for the first time, directly observed by means of fitting SANS data with an appropriate model. Our results from the SANS data analysis indicate that perforated bilayers do form, in mixtures of oppositely charged surfactants, beyond the regime where intact bilayers are present, and not in connection with the transformation from micelles to bilayers as has previously been suggested. The sequence of topological changes is rationalized in terms of an increasing saddle-splay constant as the influence from electrostatics is decreased.

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Abstract #3

Phospholipid bicelles for membrane protein solubilization investigated by SAXS

Mixed phospholipid micelles are widely applied in NMR studies of membrane proteins in solution, as they can solubilize them and be aligned in the magnetic field. Mixing of dihexanoyl phosphatidyl choline (DHPC) and dimyristoyl phosphatidyl choline (DMPC) in certain ratios leads to the formation of anisotropic micelles, called bicelles. It has been proposed that the DMPC molecules with relatively long C14 hydrocarbon tails constitute a flat bilayer, whereas the DHPC molecules with shorter C6 tails form the rim of the bicelles [1,2]. Thus, according to this idealized picture, the DMPC/DHPC ratio determines the size of the bicelles. Although SAXS [3,4] and SANS [5,6] data have previously been published for this system, only limited analysis in terms of a geometric model for the shape of the bicelles has been done for SANS data [5,6], and no modeling has been performed for SAXS data. In this work, SAXS data were collected for a wide range of DMPC/DHPC ratios. Solutions applied for NMR measurements with 30 wt% were diluted to avoid structure factor effects in the SAXS patterns. Dilution with pure solvent, however, leads to an increased DMPC/DHPC ratio in the micelles, as DHPC has a relatively high solubility. Dilutions with solutions of different DHPC concentrations were performed to find the concentration which does not lead to a change in the micelle composition. For the correct concentration, the structure factor effects decrease upon dilution, whereas the form factor does not change. The SAXS data reveal a relatively complex phase diagram as a function of DMPC/DHPC ratio with different morphologies of the aggregates, which do not follow the suggested trends for the ideal bicelle model.

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Abstract #4

Kinetics of structural reorganizations in multilamellar photosynthetic membranes monitored by small angle neutron scattering

Most photosynthetic organisms have evolved highly organized multilamellar membrane systems, thus increasing the efficiency of light capturing. In higher plants, the photosynthetic pigment–protein complexes are embedded in the thylakoid membranes, which are located in the chloroplast, and are surrounded by an aqueous matrix, the stroma. The membrane systems exhibit a large structural flexibility, as evidenced by our structural investigations, allowing the system to adapt to changes in environmental conditions. It is well-known from electron microscopy that the thylakoid membrane is organized into closely appressed (regularly stacked) flattened vesicles, the granum thylakoids, and non-appressed stroma lamellae interconnecting the grana stack. We have performed transmission small-angle x-ray and neutron scattering on thylakoids freshly isolated from spinach or pea and suspended in an aqueous medium under near physiological conditions. A broad peak at q* ~ 0.02 Å-1 correponds to a repeat distance, RD, of 294 Å±7 Å in spinach and 345 Å±11 Å in pea (RD = 2π/q*). The repeat distance is strongly dependent on the osmolarity and the ionic strength of the suspension medium, as demonstrated by varying the sorbitol and the Mg++-concentration (Posselt et al, 2012). The repeat distance decreases when illuminating the sample with white light. The change is reversible and using time-resolved SANS we have investigated this effect on a seconds-to-minutes time scale (Nagy et al, 2011, Nagy et al, submitted). The structural changes observed are associated with functional changes, as e.g. evidenced by the observation that addition of an uncoupler prohibits the light-induced structural changes, strongly indicating that the light-induced changes are driven by the transmembrane proton gradient.

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Abstract #5

Coherent X-ray photons for studies of condensed matter.

Coherent X-ray sources provide novel opportunities for imaging and dynamics experiments in materials and condensed-matter science. In the presentation I will discuss examples of soft-matter studied by photon correlation spectroscopy with coherent X-rays (XPCS). Particularly, non-equilibrium dynamics and non-ergodic behavior can be addressed using an area detector. The similarities between aging phenomena in gels and glasses and the role of internal stresses are discussed. Advanced analysis allows the calculation of two-times correlation functions and higher-order correlation functions characteristic of non-Gaussian dynamics. An outlook to the possibilities provided by fully coherent X-ray laser sources is given.

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Abstract #6

Understanding the dynamics in concentrated protein solutions: a combination of neutron spin echo and dynamic light scattering experiments

While dynamical arrest and glass formation in suspensions of colloidal hard spheres at high densities is understood quite well by now, very limited information is available for the interplay between dynamical arrest and phase separation/critical phenomena close to the critical point for short range attractive particles. Here we will discuss the results of experimental investigations of the interplay between critical phenomena and dynamical arrest in concentrated solutions of the lens protein GammaB-crystallin. This globular protein has been identified as one that closely resembles the phase behaviour of colloidal particles interacting via a temperature-dependent short-range attractive potential and exhibits a liquid-liquid phase separation that is metastable with respect to the liquid-solid phase boundary. We use a combination of 3D static and dynamic light scattering, small-angle x-ray scattering and neutron spin echo measurements to study the structural properties as well as the collective and self diffusion of the protein at the relevant length and time scales as a function of temperature at concentrations close to and above the critical concentration. With dynamic light scattering we indeed find very different divergence of the characteristic decay time of the intermediate scattering function along the critical isochore and along isochores at higher concentrations, with a clear signature of critical slowing down along the former, and dynamical arrest caused by the presence of an attractive glass transition along the latter. This scenario is supported by neutron spin echo measurements, which allow us to probe the local self diffusive motion of the individual proteins. We discuss our results in view of our current understanding of the phase behavior of particles with short range attractions, and make links to the role that GammaB-crystallin plays in lens diseases that are ultimately linked to the attractive interactions of this protein.

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Abstract #7

Interaction of protein and hyaluronan at interfaces

Small-angle neutron scattering and neutron reflectometry have been used for structural studies of proteins and polysaccharide adsorbed on various surfaces. The surfaces involved are: anionic hydrophobic polystyrene latex, cationic sapphire, and anionic hydrophilic silica. Hydrophobic latices will bind strongly to any hydrophobic molecule, including proteins. We have studied two blood proteins (human serum albumin and myoglobin) and their interactions with latex nanoparticles using small-angle scattering. The other two types of surfaces were used in reflection experiments. For sapphire crystals, the isoelectric point is typically found to occur at pH~9, meaning that the sapphire surface is positively charged at pH<9. Negatively charged polysaccharides could be bound by electrostatic interactions on sapphire in this pH range. Polysaccharides could not be adsorbed on silica surfaces, but one could couple them to silica using silane chemistry. The main focus has been on the interaction of human serum albumin (HSA) and hyaluronan (HA). These two biological macromolecules are the most abundant components in synovial fluid, and are considered to play an important role in the reduction of friction. Understanding the behaviour of the major components of synovial fluid can help understand lubrication of joints. Using small-angle scattering, we observed HSA adsorption on anionic polystyrene latex that reaches a plateau at a HSA concentration of 4 mg ml−1. The adsorption reaches a maximum at the isoelectric point of HSA. This is due to the minimum in the solubility of the protein in the aqueous buffer, the reduced electrostatic barrier between the protein and the particle, and the decreased repulsion between the molecules in the interfacial layer. The myoglobin adsorption does not reach a plateau, but increasing the bulk concentration of the protein increases both the layer thickness and its thickness distribution. HA at several concentrations and chain lengths did not bind to the latex, either alone or together with HSA at pH above the isoelectric point for HSA (pH≥4.8). However at lower pH (3.9), where HSA and HA are oppositely charged, an increase of layer thickness was observed when low molecular mass HA (≤150 kDa) was introduced to the system. Increasing the concentration of short chain HA increased the layer thickness, although no significant binding was observed for longer HA chain lengths. This suggests that the electrostatic interaction between the protein and the HA is weaker than the hydrophobic adsorption of HSA on latex. Neutron reflection experiments showed the structure of HA, both adsorbed on sapphire by electrostatic interactions and covalently grafted on silica to be a diffuse layer. HSA penetrates into both types of HA layers and binds strongly to both grafted and adsorbed HA but only at a pH≤4.8. In this pH range, the HSA molecules are positively charged and are in turn bound to the anionic HA layers.

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Abstract #8

Decay of correlations in inhomogeneous fluids probed by x-rays

According to liquid-state theory, the asymptotic decay of ordering at fluid interfaces is governed by the decay of the bulk pair correlations. Surprisingly, this has recently been observed in surface-force experiments for slit widths as narrow as two particle diameters [1]. On the other hand, such narrow confinement is known to induce strongly anisotropic, non-bulklike pair correlations in dense fluids [2]. Here, we address this topic by studying the bulk and interfacial structure of a colloidal suspension using small-angle x-ray scattering and x-ray reflectivity, respectively [3].

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Abstract #9

Scattering from Complex Systems

The problems of interest in soft matter and colloid science increasingly involve heterogeneous and complex systems. This represents a challenge to those designing new sources and new instrumentation. This talk will present a view of the sort of systems that will become routinely studied using small angle scattering with some specific examples including the structure of casein micelles, magnetic nanoparticles for cancer treatment, and emulsion explosives.

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Abstract #10

Using Neutrons to understand the hydration process in dental cement pastes

It would be ideal if there was only one cement for all clinical situations: A cement that can be easily mixed and go through its setting reaction either quickly for a single crown or restoration, or could be adjusted to set slower in more delicate cementation cases. Alas, this “holy grail” is not available, and to develop a more effective way of controlling the hydration process of dental cements it is important to know how the dynamics of the liquids involved in the curing process changes as the paste hardens and the pore structure develops. To better understand how the dynamics of the liquid used in the hydration process in dental cement is modified when confined and relate the results get to durability properties QENS experiments on 3 types of dental materials have been carried out. Here I will present results from elastic fixed window experiments carried out using two different neutron backscattering instruments on three Glass-Ionomer cements consisting of a liquid (water or two polymeric chains) and a powder component. Glass-Ionomer cements belong to the family of dental cements considered as an acceptable alternative to amalgam in dentistry. The evolution of the elastic intensity observed during the first 24 hours of the hydration process using the IRIS spectrometer located at the ISIS Facility (UK) revealed that, in a resolution window of few picoseconds, the amount of bound hydrogen present in the amorphous structure increases faster in the cement paste where a polymeric chain is used as a liquid in comparison to a paste where the liquid is water. In addition, the same type of data collected in the nanosecond time scale using the high-resolution backscattering instrument located at the ILL (France) seems to indicate the same behavior.

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Abstract #11

Control of Order and Disorder in Binary Dispersions of Colloidal Particles

Mixtures of colloidal particles of essentially two different sizes are commonly used in technological applications such as film formation on surfaces, paper coatings, etc. A number of phenomena are commonly experienced, for example, if the larger particle size is denser than the smaller, sedimentation of the larger species occurs and if one set of particles is less dense than the medium, creaming can occur. More subtle changes in rheology due to the presence of small particles are also reported [1]. Hard spherical particles and even dried latex have been used as simple models to understand packing (e.g. [2]). Dispersed latex particles provide an excellent model system for study of mixtures with long range interactions and we will report changes in structure that are observed when concentrated monodisperse, charged particles that on their own would form crystals are mixed. Recent data from small-angle neutron scattering measurements with Sans2d, with mixtures of different size labeled particles in different solvents allows the partial structure factors to be determined. Both latices had interaction potentials of about 35 mV. On their own, each species show diffraction from ordered structures. Even raw data clearly shows that the Bragg peak in the mixture is preserved for the small particles but is lost for the large particles. Further data that provides information for a range of concentrations and size ratios will be presented. The results suggest that the small particles, by screening the interactions of the large particles cause 'melting'. Theoretical model that extend beyond the calculations of purely liquid structures [3] are needed.

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Abstract #12

Valuing inelastic neutron scattering in pharmaceutical formulation science: A headache free alternative

The physicochemical properties of pharmaceutical formulations are of primary interest when determining structure-activity relationships in lead drug optimization processes. Knowledge of the active chemical structure, solubility, dissolution rate, affinity and thermodynamic stability of the pharmaceutical drug is crucial in drug development as these are the primary factors affecting efficient drug delivery. Inadequate characterisation can prove extremely costly and often fatal (Lipitor, Crixivan, Ritonavir and others). We explore the use of inelastic neutron scattering in assessing the dynamical behavior of the polymorphic forms of model peptide systems such as N-(4-hydroxyphenyl)ethanamide (paracetamol) and for the first time reporting on the relaxation dynamics of paracetamol form II under pressure measured in the picosecond time scale. We attempt to expose an atomistic understanding of the physicochemical and dynamical properties under pressure but also hints to the activity of the hydrogen bonded functional groups uniquely identified by inelastic neutron scattering.

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Abstract #13

Development of a stealth carrrier-system for SANS studies of membrane proteins

The lipid bilayer compartmentalizing the cell harbors some of the most important proteins. These proteins are not water soluble and require complex isolation protocols to enable their biochemical and biophysical studies. Reconstitution into bilayer mimicking carriers, such as Nanodiscs, is necessary to ensure stability and function (Bayburt et al, 2002). The Nanodisc carrier system is a phospholipid bilayer stabilized by two amphipathic protein belts which has shown a large potential as a platform for structural investigations of membrane proteins using Small-Angle Scattering (SAS) (Skar-Gislinge et al, 2010). Still, the Nanodisc itself contributes to the measured scattering intensity in a highly non-trivial fashion and needs to be explicitly accounted for in the analysis of the scattering data (Skar-Gislinge et al, 2011). A way to circumvent the added complexity is to carefully tune the deuteration levels in the phospholipid bilayer and the surrounding amphipathic belts. This approach allows for the assembly of a specifically deuterated, i.e. a “Stealth” carrier-system that is virtually invisible to neutrons, leaving only the incorporated membrane protein visible. Small-angle neutron scattering (SANS) can then be directly used to determine the low-resolution structure of membrane proteins and their complexes using contrast variation . The theoretical deuteration levels needed for full “invisibility” vary for the different parts of the Nanodisc complex and even differ for the different parts of the phospholipid bilayer alone. Here we present that the specific deuteration required can be achieved through bacterial expression in deuterated media. Furthermore we show that selective labeling of the lipid bilayer can be regulated during lipid synthesis through careful design of the bacterial growth conditions.

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Abstract #14

Electronic structure and dynamics of molecular systems investigated with soft X-rays

Most fundamental questions regarding the function of complex molecular systems are related to local electronic and dynamic properties of the different molecular building blocks. Core-resonant soft X-ray spectroscopy and scattering has for a long time allowed access to local electronic structure and electron dynamics (on the fs-timescale of the core hole decay), however, been restricted to artificial sample conditions under UHV. In recent time the application of soft X-ray spectroscopy, in particular when applied in photon-in-photon-out mode, has successfully been extended to the investigation of molecular systems in relevant chemical environments, i.e. the liquid phase under ambient conditions. MAX IV will provide unprecedented possibilities in terms of resolution and signal strength and availability of the necessary sample environments for this type of investigations.

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Abstract #15

Nano- to microscale characterization of betonite clay with microbeam small-angle x-ray scattering and microtomography

Bentonite is a clay mixture composed primarily of montmorillonite and accessory minerals such as quartz, feldspar, and other silicates. Due to its swelling and water retention properties, bentonite has various uses in geotechnical engineering , e.g. as a component of drilling mud or as a liner material at landfills. These same properties also make compacted bentonite an attractive candidate for a buffer material in geological disposal of used nuclear fuel. Microstructurally, the water absorbing ability of bentonite is due to the nanostructure of its principal component: montmorillonite is a layered smectite clay, in which (negatively charged) alumino-silicate platelets alternate with interlayer cations (typically Na- or Ca-ions). Water is absorbed between platelets, causing the structure to swell in the direction perpendicular to the platelets (i.e. the crystallographic 001-direction). [1] We have used a novel experimental setup, which combines small-angle x-ray scattering (SAXS) with x-ray microtomography (XMT) in a home-lab setting, to investigate the effects of varying relative humidity on the nano- and microscale structure of purified Ca-montmorillonite and non-purified MX-80 bentonite samples (dry density ~1.6 g/cm3). The distance between platelets in montmorillonite is typically 10-20 Å, making SAXS an ideal tool for quantifying both the interlamellar distance and the thickness of the platelet stacks, or tactoids. In compacted clay, the tactoids exhibit significant preferred orientation, which can also be observed using SAXS. In the micrometer scale, XMT can be used to observe and quantify the orientation and size of microcracks that develop within the samples with decreasing relative humidity. The combined setup also allows us to target the beam used for the SAXS experiment to a specific location within the sample; we can thus correlate the preferred orientation seen in the SAXS pattern (a nanometer-scale feature) with the orientation of microcracks seen in the XMT scans (a micrometer-scale feature). The results indicate that uniaxial compaction tends to align the clay platelets perpendicular to the axis of compaction, and that microcracks tend to form parallel to the platelets as the sample is dried. The effect is much less pronounced in the MX-80 samples, where we presume the essentially incompressible accessory minerals disturb the stress field during compaction.

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Abstract #16

Intercalation and Retention of Carbon Dioxide in Synthetic Fluorohectorite Clay at near-ambient Conditions

We show using synchrotron as well as in-house x-ray diffraction methods that gaseous CO2 intercalates into the interlayer space of the synthetic smectite clay fluorohectorite at conditions close to ambient. The rate of intercalation is found to be dependent on the interlayer cation (Li+ or Na+ in this case), with about one order of magnitude increased rate in Li-fluorohectorite compared to Na-fluorohectorite. We further show that Li fluorohectorite is able to retain CO2 in the interlayer space at room temperature, which could have applications related to CO2 capture, transport and storage. De-intercalation starts occurring at temperatures exceeding 30 °C.

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Abstract #17

SAXS activities at the MAX IV Laboratory: Past, Present and Future

As highlighted by another talk at this workshop, the soft matter user community at the MAX IV Laboratory could utilize several experimental techniques/ beamlines. The focal point of the activities, however, is of course the SAXS station on the Cassiopeia beamline. It was preceded by a SAXS set-up on the multi-purpose beamline I711. Although very successful from the start in 2006 it was soon realized that this was not sufficient in either availability or performance. The much more powerful and dedicated 911:4 station was inaugurated in 2011 and has now been upgraded with a Pilatus 1M detector and will very soon also have an automatic sample handling system. This beamline is planned to be open for users as long as the MAX II storage ring is in operation to minimize any "dark" period before the new MAX IV facility will be open for users. At present 8 beamlines have been funded on the new MAX IV facility, the work on these has proceeded according to plans and the beamlines should in go operation 2015 (FemtoMAX) and 2016 (the remaining 7). It is foreseen that SAXS will an important technique in the NanoMAX experimental portfolio but a dedicated SAXS beamline is still not funded. The MAX IV Laboratory is planning to submit an application for the next round of VR/RFI applications in spring, 2013 asking for a funding for 3-5 full beamlines and/or a transfer package for beamlines existing at MAX II & III and additional endstations. A short-list compiled from the beamlines (or combinations/modifications) of the Strategic Plan presented for VR in 2012 has been produced and includes a SAXS and Hard X-ray Coherent Scattering beamline. This shortlist will be evaluated among the main MAX IV stakeholders in early 2013. In this presentation both the present activities as well as the process regarding beamlines on MAX IV will be presented.

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Abstract #18

The oligomerisation mechanism of a novel Insulin analogue with Protracted action revealed by SAXS analysis.

As an important part of the effort to improve diabetes treatment, insulin analogues with protracted action are developed in the pharmaceutical industry. A novel class of analogues facilitates a prolonged therapeutic profile by acylation at specific positions (1). Upon subcutaneous injection the protein oligomerises to form a depot of large soluble aggregates, which slowly release into the interstitial fluid.
Here we present a timeresolved analysis of the oligomerisation process of such an acylated insulin analogue, LysB29(Nεω-carboxyheptadecanoyl) des(B30) (2, 3). In vivo, the process is initiated upon subcutaneous injection, causing diffusion of phenol, which is part of the insulin formulation. We mimick this by passing the formulated analogue over a fast desalting column, and follow the oligomerisation process with a number of biophysical methods, most prominently small-angle X-ray scattering. We combine data from applying the HPLC system integrated with the SAXS camera at the SWING beamline at synchrotron SOLEIL. From this system, we have data both from size-exclusion purified intermediate oligomers, and time-resolved data from the developing oligomers. For the latter, the protein is separated from phenol (see figure below) which initiates oligomerisation and the protein is immediately transferred to the SAXS sample cell where data collection is inititated at defined time points after the onset of oligomerisation. We further analyse the data from complex mixtures of higher oligomers and combine with field flow fractionation, dynamic and multi-angle light scattering, circular dichroism, size exclusion chromatography, and crystallography.
Together, our analysis provides an insight to the oligomerisation of novel acylated insulin analogues.

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Abstract #19

Model-Independent Decomposition of SAXS Data from Heterogeneous Samples yield Solution Structure of the Intrinsically Oligomeric Protein PICK1

PICK1 is a 46 kDa cytosolic protein that plays an important role in regulation of excitatory neurotransmission in the brain through its involvement in AMPA receptor trafficking. It is proposed to form a homodimer, and the quaternary structure may play an important role in the function and regulation of PICK1. Lacking a crystal structure, we have used solution based Small Angle X-ray Scattering (SAXS) to determine the low-resolution quaternary structure. In contrast to other BAR domain proteins, PICK1, in addition to the dimeric fraction, has a significant tetrameric fraction. Since the samples were polydisperse, we developed a method to decompose the scattering data into dimeric and tetrameric components. By combining data from different samples it was possible to decompose the data without a priori assumptions about protein structure, other than the molecular mass. Through rigid body modeling, based on the BAR domain of the homologous protein Arfaptin and the crystallized PDZ domain of PICK1, a quaternary structure was determined. The domain arrangement is very similar to previously published structures of other BAR domain containing proteins, including SnX9 and Endophilin. Our data provide the first direct insight into the tertiary and quaternary structure of full-length PICK1, and we conclude that PICK1 is not in a configuration that fits previously published hypotheses explaining the auto inhibition as a mechanism in which the BAR domain is sterically hindered by the PDZ domains binding to the concave surface of the BAR domain.

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Abstract #20

Nano-composite hydrogels. A combined SAXS and SANS study.

Organic-inorganic hybrid materials have attracted attention since they can be tailored to combine the advantages of organic polymers with those of inorganic components yielding materials, which possess enhanced mechanical properties, chemical resistance, optical quality, and other useful properties, which arise from the synergetic interaction of the individual organic and inorganic constituents. Nature also combines different types of macromolecules in order to form gels with outstanding physical properties. One example is the lens, which projects the optical image on the retina together with the cornea. With the attempt to make a artificial composite material with mechanical properties, light transmission factor and refractive index that makes it suitable for implant of intraocular lens, we have studied a nano-composite material composed of hydrophobically-modified poly(ethylene glycol) (HM-PEG) and silica OCAPS nano-particles (Annaka et al. 2011 and 2012), using combined SANS and SAXS. The structural studies show that the polymers form a micellar network that order into a bcc-ordered phase when appropriate concentrated. The network structure easily aligns into mono or twin-domain texture upon shear. The OCAPS nano-particles are very well dispersed within water as well as within the polymer gel structure. The dispersion characteristics remain apparently unchanged upon loading into the micellar structure, but the different contrasts factors of SANS and SAXS also unambiguously show that the form factor of the micelles changes markedly upon OCAPS loading, convincingly showing that the OPACS nano -particles are located within specific regions of the micellar network structure.

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Poster Presentations

Abstract #21 (Poster)

The Potential of Scatter-Free Pinholes for SAXS Instrumentation

Parasitic scattering caused by apertures is a well-known problem in X-ray analytics, which forces users and manufactures to adapt their experimental setup to this unwanted phenomenon. Increased measurement times due to lower photon fluxes, a lower resolution caused by an enlarged beam stop, a larger beam defining pinhole-to-sample distance due to the integration of an antiscatter guard and generally a lower signal-to-noise ratio leads to a loss in data quality. In this presentation we will explain how the lately developed scatter-free pinholes called SCATEX overcome the aforementioned problems. We will show first measurements with SCATEX performed at home-lab small angle X-ray scattering systems and at synchrotron beamlines. The results will be compared to setups with conventional pinholes and scatterless Germanium slit systems. We will further present the latest SAXS instruments of Buker AXS, the N8 HORIZON and the NANOSTAR with METALJET X-ray source, in which scatter-free SCATEX pinholes are already integrated.

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Abstract #22 (Poster)

SAXS at the MAX IV Laboratory

The dedicated and multipurpose I911-SAXS (Small-Angle X-ray Scattering) beamline at the MAX IV laboratory has been serving the user community since May 2011. After only one year and a half, the station is already oversubscribed. Now, there is a much higher demand of beam time than is available for peer-reviewed projects. So far, there have been successful measurements on a diversity of samples and setups mostly oriented to soft matter and protein in solution experiments. It is reassuring to see the first publications coming out. The current configuration of the beamline has been described in Labrador A. et al. J. Phys.: Conf. Ser. (2013) (in press). The accessible q-range (q = (4pi/lambda) sin(theta)) of a typical I911-SAXS setup is 0.01 1/Å - 0.3 1/Å but lower values (0.006 1/Å) or higher (2 1/Å WAXS set-up) can also be reached. The SAXS chamber design permits reaching even higher q values with isotropic scattering samples. The size of the focused beam is around 0.3x0.2 mm2(HxV). Measurements with a beam collimated down to 0.1x0.1 mmxmm have been performed with very small samples and also in experiments in which SAXS measurements are taken over a 2D area of the sample (mesh scan). A selection of fundamental SAXS sample environments has been available from day one: An in-vacuum flow-through capillary for solution scattering and several multiple positions sample-holders for solids (films and powders), gels or liquid samples in air. The temperature of the sample can be controlled in both cases. Other setups, brought by the users, are often installed and integrated in the beamline such us ultrasonic levitators, electrochemical cells or tensile test machine. The feedback from the user community is currently supporting further development of in situ and time resolved I911-SAXS experiments. A low noise, fast read-out pixel area detector (PILATUS 1M) has been acquired and commissioned recently and is now available for the user community.

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Abstract #23 (Poster)

Goal and Status of the SURF-project: Saxs-Uvvis-Raman-Fluorescence

In most research fields such as soft matter, biology, and protein research; an important link to establish is the relation between structure and function. To fully understand this relationship, we have built the first generation integrative characterization platform for complex systems, namely: SURF (Saxs-Uvvis-Raman-Fluorescence). The SURF platform provides simultaneously measurement and correlation of the information from Saxs, UV-absorption, Fluorescence and/or Raman. The latter correlation built from multivariate analysis enables complex behaviour (structure and chemistry) to be resolved. Additional benefits of the SURF are sample quality control and live experimental diagnostics. In this contribution, we present the 1st generation setup of the in-house developed SURF sample holder for solution scattering. In light of the 1st generation challenges and achievements, we also discuss the 2nd generation setup. The details of the design and performance of the 1st generation SURF-environment is highlighted through a series of test experiments as follows:

• Radiation damage study of BSA using SAXS and UV-VIS spectroscopy.
• Urea Unfolding of BSA using SAXS, UV-VIS and Raman spectroscopy.
• Assembly and stability of single wall carbon nano-tubes (SWNT) in SDS solution using SAXS, UV-VIS and Raman spectroscopy.

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Abstract #24 (Poster)

Instrumentation for Soft Matter at ESS

The ESS will be the world's leading long pulse neutron source, with 7 out of the first instrument suite of 22 expected to come operational in 2019. During the Pre-construction phase 2010-2012, the Instrument Design Update project has explored a range of instrument concepts for soft condensed matter studies including neutron reflectometry, small angle scattering, as well as spin-echo and quasi-elastic/inelastic neutron spectroscopy. The key instrument types and their applications within the science case and future perspectives for soft matter will be described.

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Abstract #25 (Poster)

Mechanism of cyclotide interaction and pore formation in lipid membranes

Cyclotides are a family of plant-derived circular proteins with potential therapeutic applications arising from their remarkable stability, broad sequence diversity, and range of bioactivities. Their membrane-binding activity is believed to be a critical component of their mechanism of action. We have studied the binding of the prototypical cyclotides kalata B1 and kalata B2 with bilayer membranes using a combination of dissipative quartz-crystal microbalance measurements and neutron reflectometry[1]. Our results show that initial binding to the membrane surface is followed by a gradual insertion and pore formation process consistent with a carpet-type mechanism, and provide a structural insight into how cyclotides exert their biological activities.

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Abstract #26 (Poster)

Tailoring a Soft X-ray SAXS Beamline to Soft Matter Research

At the synchrotron radiation facility BESSY II in Berlin, the Physikalisch-Technische Bundesanstalt (PTB) operates a four-crystal monochromator (FCM) beamline covering a photon energy range from 1.75 keV to 10 keV. This beamline was recently equipped with a large-area hybrid pixel photon counting detector, the PILATUS 1M from Dectris Ltd., tailored to operate directly in vacuum without any windows. Using the newly developed detector, the signal-to-noise ratio is significantly improved in comparison to a conventional CCD-based camera. Further, the full photon energy range of the FCM beamline is available for SAXS experiments with this detector, giving access to the absorption edges of biologically relevant elements like sulphur, phosphorus and calcium. Dimensional nanometrology, well established at the FCM beamline for nanoparticles, can thus be extended to soft matter materials. First measurements demonstrate the superior image quality of the new setup at photon energies down to 1.75 keV.

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Abstract #27 (Poster)

Double Scattering - A simple approximation to include the effect of mild multiple scattering in model fitting

If the scattering from a sample that is ideally thin is described by a function, or form factor, P(Q) ,where Q is the momentum transfer equal to $(4\pi/\lambda) \sin(\theta/2)$, it is possible to make a simple approximation to the effects of mild multiple scattering by estimating two-fold scattering. If the change in the transmission of a sample due to coherent scattering is, Ts some simple approximations are possible. The probability of scattering, f is $(1 - Ts)$ and the probability of two-fold scattering, f squared, is approximately $(1 - Ts)2$. The double scattering will be distributed according to the same P(Q´) as the single scattering but the effective incident beam is displaced in momentum transfer. The intensity of double scattering, Id, that is observed at momentum transfer Q relative to the incident beam will arise from a self-convolution of P:

$Id = (1 - Ts)(1 - Ts) P(u)P(u-Q)du$ Eq. (1).

The single scattering is given by

$Is = (1 - Ts) P(Q)$ Eq. (2),

and the estimate for the observed total scattering is:

$It = Is + Id$ Eq. (3).

Equations 1 to 3 are incorporated readily in numerical data fitting procedures for a variety of models. The transmission Ts is distinct from the measured total sample transmission Tt which is used to correct the measured intensity for self-shielding, and contains contributions from incoherent scattering and from the cell and solvent. Ts has been left as a free parameter in fitting, but the results correspond approximately to the calculated values and to Monte Carlo estimations of multiple scattering in example cases. These programs are reasonably fast and useful to estimate the effects on models such as monodisperse spheres, rods and fractal aggregates where, with increasing concentration, marked smoothing of the scattering is observed.

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Abstract #28 (Poster)

Identification of crystal structure and orientation of a crystal of polystyrene latex

Charged latex particles can form highly ordered structures in dispersions that are mobile liquids which flow freely. There has been considerable interest in determining what factors influence the crystal structure and the orientation as well as possible defects. Drying may introduce defects and boundaries such as cell surfaces may influence the structure. In-situ observation with small-angle neutron scattering is thus a powerful tool to investigate these structures. Rotation of a single crystal sample is the best means to identify the structure of the crystal, as there are many Bragg peaks that occur at the same position in Q for hexagonal and cubic close packed structures. This contribution reports the study of a large (1 cm diameter, 2 mm thick) crystal formed from particles of 72 nm radius in a dispersion at 8.7% vol. that had a face centred cubic structure with a lattice parameter of 404 nm. This was identified by indexing a number of Bragg peaks and observing, for example, a change from 6-fold to 4-fold symmetry of the visible peaks on rotation by 45 degrees. The study allows us to investigate factors, such as sample flow and interface geometry that determine the alignment of the crystal. Control of the both the structure and orientation of crystals of colloids is important for applications that include templating photonic devices or preparation of magnetic arrays for storage devices. The study illustrates the advantage of a goniometer that permits eucentric rotation of a sample through large angles on a small-angle scattering instrument.

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Abstract #29 (Poster)

Electrostatic assembly of binary nanoparticle superlattices using protein cages

Binary nanoparticle superlattices are periodic nanostructures with lattice constants much shorter than the wavelength of light and could be used to prepare multifunctional meta-materials. Such superlattices are typically made from synthetic nanoparticles, and although biohybrid structures have been developed, incorporating biological building blocks into binary nanoparticle superlattices remains challenging. Protein-based nanocages provide a complex yet monodisperse and geometrically well-defined hollow cage that can be used to encapsulate different materials. Such protein cages have been used to program the self-assembly of encapsulated materials to form free-standing crystals and superlattices at interfaces or in solution. Here, we show that electrostatically patchy protein cages—cowpea chlorotic mottle virus and ferritin cages—can be used to direct the self-assembly of three-dimensional binary superlattices. The negatively charged cages can encapsulate RNA or superparamagnetic iron oxide nanoparticles, and the superlattices are formed through tunable electrostatic interactions with positively charged gold nanoparticles. Gold nanoparticles and viruses form an AB8fcc crystal structure that is not isostructural with any known atomic or molecular crystal structure and has previously been observed only with large colloidal polymer particles. Gold nanoparticles and empty or nanoparticle-loaded ferritin cages form an interpenetrating simple cubic AB structure (isostructural with CsCl). We also show that these magnetic assemblies can provide contrast enhancement in magnetic resonance imaging. http://dx.doi.org/10.1038/NNANO.2012.220 http://www.nature.com/nnano/journal/v8/n1/full/nnano.2012.220.html

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