50 years of D11

Report of Contributions

Contribution ID: **1** Type: **poster contributions**

Longitudinal Conical Magnetic Structure in Scandium doped M-type Barium hexaferrite

M-type barium hexaferrites (BaM) has attract a lot of attention due to their multiferroic and other functional properties [1, 2]. We have investigated the doped M-Type Barium hexafer-rite, BaFe12-xTxO19, where T = Sc with x = 2.5. The structural and magnetic properties were characterized using XRD, VSM and Neutron diffraction measurements. XRD analysis reveals that the samples are in single phase with space group P63/mmc. Magnetization data reveal interesting behavior, Zero-field cooling (ZFC) and field cooled warming (FCW) curves in temperature range of 5 K to 750 K indicate several transitions for the Scandium doped com-pound. Transitions observed at lower temperatures indicate antiferromagnetic order. Tem-perature dependence neutron diffraction measurements performed at a wavelength of, λ = 2.315 Å, in the temperature range 3 K – 300 K, analysis of neutron data reveals non-collinear magnetic order at the lowest temperature. Magnetic satellite reflections start appearing at low angles on decreasing of temperature, refinement of this magnetic reflection indicates the presence of conical magnetic structures at low temperatures. This shows that the direc-tion of magnetic moments, when compared with the parent compound, is no longer along the hexagonal c-axis. Magnetic structures for the Scandium doped with doping concentra-tion x = 2.5 is analyzed and presented in details.

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Co-authors: Prof. SIRUGURI, vasudeva (UGC-DAE CSR Mumbai Centre, BARC CAmpus); Prof. SURESH, K. G. (Indian Institute of Technology, Bombay India)

Presenter: Dr GUPTA, Surbhi (Indian Institute of Technology, Bombay, India)

Session Classification: Poster session/Wine and Cheese evening

Contribution ID: **2** Type: **Invited speakers**

How SANS reveals the nanostructure and moisture interactions of wood cell walls

Monday, 26 September 2022 11:40 (25 minutes)

Wood is an abundant biological material with various technical applications ranging from sustainable building materials to advanced functional materials made of nanocelluloses. The structure of wood cell walls is hierarchical, consisting of well-oriented, elongated units from the molecular level to the macroscale. Our picture of the complex composite-like structure of wood cell walls and its interactions with water has become more accurate during the past decade, and results obtained with small-angle neutron scattering (SANS) have played an important part in this development.

SANS can be used to observe the structure of wood cell walls from the level of cellulose microfibrils (diameter 2-3 nm) to microfibril bundles (diameter 10-20 nm) and above. It detects the moisture-induced swelling of the microfibril bundles, which can be analysed using the WoodSAS model [1]. This model allows also determining the diameter of microfibril bundles in the wet state, without cutting the cell walls [2]. We have subsequently used SANS for *in situ* experiments investigating the drying behavior of wood [3] and the exchange of liquid water within the fibrillar structures [4]. All of these studies were based on SANS experiments carried out at D11.

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Co-authors: Mr ZITTING, Aleksi (Aalto University); Dr SCHWEINS, Ralf (Institut Laue-Langevin); Prof. RAUTKARI, Lauri (Aalto University)

Presenter: PENTTILÄ, Paavo (Aalto University)

Session Classification: Talks

Contribution ID: **3** Type: **poster contributions**

Limoncello and the art of mixing water and oil

Whoever tried to prepare homemade mayonnaise, knows how much energy input the formation of water/oil emulsions require. In addition to that, in order to provide stability to the emulsion, the presence of components which stabilize the system are required. This role is played by some of proteins and the lecithin contained in the egg yolk, for the case of mayonnaise. In most of other emulsions, surfactants and polymers are used to prov ide stability to the emulsion.

In a different approach, meta-stable emulsions can be prepared when three liquids, two partly miscible liquids (water and oil) and a common solvent, such as ethanol, are mixed. Close to the phase-separation boundary, strong composition fluctuations take place. In this portion of the phase diagram, called 'Ouzo region', the formation of 100-1000 nm sized oil rich domains are found. The name
'Ouzo' derives from the famous Greek liquor, which exhibits a typical opalescence when diluted with water, due to the formation of anethole (the oil) rich droplets.

In this contribution, we focus on Limoncello, the famous Italian liquor based on lemon essential oils. In contrast to similar, 'Ouzo-like' systems, Limoncello shows and exceptional stability. Small-angle neutron scattering was used to probe the microscopic structure of Limoncello, revealing the presence of self-emulsified submicrometer small droplets, whose size shows only little variation in a large range of composition and temperature. These findings open two fundamental questions to be addresses in forthcoming studies: what are the physical forces leading to the formation of oil domains with such an exceptional size and what is the mechanism guaranteeing a long term stability to Limoncello systems.

ACS Omega 2018, 3, 11, 15407-15415

Primary author: Dr CHIAPPISI, Leonardo (Institut Laue Langevin)

Presenter: Dr CHIAPPISI, Leonardo (Institut Laue Langevin)

Session Classification: Poster session/Wine and Cheese evening

Contribution ID: **4** Type: **poster contributions**

Neutron scattering and reflectivity to study the stability of foams in a multi-scale experiment

Liquid foams are non-equilibrium multi-scale soft structures. Moreover, the foamability of a surfactant solution as well as the metastability of the foam are still difficult to predict. In order to better understand the physico-chemical factors that affect the aging of foams at different length scales, a new columnar device was developed. It enables the simultaneous data collection from a small-angle neutron scattering (SANS) diffractometer, from an optical camera and an electrical conductivity meter. In order to evaluate the potentiality of this device, a foam from a mixture of the nonionic alkylether BrijO10 surfactant and of the sodium dodecyl sulfate (SDS) anionic surfactant was generated in D2O and analyzed as a function of time.
The volume of the foam, its liquid fraction and the radius of the foam bubbles as a function of time (obtained by image analysis and conductivity processing) are macroscopic information, necessary for foam lifetime characterization but not sufficient. SANS analysis is known to provide useful information at the nano-scale, on the structure of the inter-bubble film or the surfactant self- assemblies trapped within the foam. However, to extract this information over a large structural range and in order to be able to compare the various structural features (the specific surface area, the liquid fraction, the film thickness) determined from different techniques, we have for the first time performed a quantitative analysis - in absolute scale - of the scattering data.
The analysis of nano- and macroscopic information obtained simultaneously enabled us to better understand the correlation between the mechanisms of drainage, ripening and coalescence involved at the different scales in the aging of the foam.

Primary authors: CHIAPPISI, Leonardo; DIAT, Olivier; BAUDUIN, Pierre (CEA - ICSM); LAMOLINAIRIE, Julien

Presenter: LAMOLINAIRIE, Julien

Session Classification: Poster session/Wine and Cheese evening

Contribution ID: **5** Type: **Invited speakers**

Micelle structure and composition: the contribution from SANS (remote)

Tuesday, 27 September 2022 15:15 (25 minutes)

Surfactant self-assembly is an important phenomenon in a wide range of processes and applications. SANS has played a central and key role in developing our understanding of surfactant self-assembly. From the early 1980's D11 has been the leading and pioneering SANS instrument for such studies. Three key issues from some the early studies on D11, associated with micelle models, the complementarity of SANS and neutron spin echo, and the application of shear alignment, and which are still relevant and important to current studies, will be revisited. The contribution of more recent studies of mixed surfactant self-assembly will be reviewed, with a particular emphasis on three aspects: the role of surfactant molecular structure in manipulating the micelle structure, the complex evolution of structures that can arise in mixtures, and the emerging importance of biosurfactants.

Primary author: PENFOLD, Jeff (ISIS, STFC and PTCL, Oxford)

Presenter: PENFOLD, Jeff (ISIS, STFC and PTCL, Oxford)

Session Classification: Talks

Contribution ID: **6** Type: **Invited speakers**

Exploring the influence of nanoparticles on the polymer chain conformation: from solution to nanocomposites

Monday, 26 September 2022 14:25 (25 minutes)

Adding nanoparticles (NPs) to polymer solution or melt is an efficient strategy to improve the macroscopic polymer behavior (viscosity, mechanical reinforcement...) and design hybrid macromolecular materials with enhanced properties. Among the vast literature dealing with NPs and polymer, one fundamental question arises: do NPs modify the global and local polymer chain conformation? Such issue is highly relevant since chain conformation is a central concept in polymer science and its description is essential for understanding the physical and dynamical properties of polymers. While in solution there is a general consensus on chain collapse, it is more controversial in melt for which chain swelling, contraction or no perturbations have been observed.

Small-Angle Neutron Scattering (SANS) can directly answer this question thanks to the Zero Average Contrast (ZAC) method, which is an elegant approach to cancel out the scattering of the NPs by using an appropriate amount of hydrogenated and deuterated polymer in order to only measure the signal of a single polymer chain. Then, the analysis of the scattering spectra gives a radius of gyration from which we can deduce if the polymer contracts, swells or remains unperturbated in the presence of NPs. By investigating the behavior in both solution and melt, we can also figure out if there is a connection between chain conformation in solution with NPs and chain conformation in nanocomposites without solvent. During this talk, I will first present SANS results on both systems (polymer nanocomposites (PNCs) and polymer solution) and show the influence of NP size (from 1 nm to 20 nm), NP concentration and nature of NP/polymer interaction (attractive or repulsive) on the Rg evolution. Then, I will also address the influence of NPs on the chain deformation to get more insights into the mechanical reinforcement in PNCs. For the latter study the D11 spectrometer played a primordial role to access the stretched chain form factor.

Primary author: JOUAULT, Nicolas (Sorbonne-Université, Laboratoire PHENIX)

Presenter: JOUAULT, Nicolas (Sorbonne-Université, Laboratoire PHENIX)

Session Classification: Talks

Contribution ID: **7** Type: **Invited speakers**

Electrostatic Self-Assembly in Solution: Structure, Function and Switching

Tuesday, 27 September 2022 09:50 (25 minutes)

With regard to the increasing need for sustainable energy, developing strategies to exploit solar energy become more and more important. Inspired by natural systems it is highly promising to self-assemble building blocks into functional supramolecular units.
Electrostatic self-assembly leads to nanoscale shapes ranging from spheres and cylinders over vesicles to networks. Key to a targeted structure design is to fundamentally understand structure directing effects. In this regard, crucial insight has been gained from small-angle neutron scattering (SANS) at D11@ILL, alongside with other methods such as static and dynamic light scattering (SLS, DLS), atomic force microscopy (AFM), spectroscopy, zeta-potnatial measurements and isothermal titration calorimetry (ITC). Structure directing effects encoding the supramolecular nanoscale structure, in particular the particle particle size and shape on a 10-100 nm level, will be discussed. In particular, thermodynamics and the interplay of interaction forces are key to connect the molecular building block features with the nanoscale assembly properties.
In addition, we describe light-triggered size and shape changes of electrostatically self-assembled supramolecular nanostructures, following different strategies. This route for the conversion of light into structural and mechanical effects is promising for applications in drug delivery, nanosensors and solar energy conversion.

Primary author: GRÖHN, Franziska (Friedrich-Alexander-Universität Erlangen-Nürnberg)

Presenter: GRÖHN, Franziska (Friedrich-Alexander-Universität Erlangen-Nürnberg)

Session Classification: Talks

Contribution ID: **8** Type: **Invited speakers**

Understanding dipeptide-based hydrogels

Monday, 26 September 2022 14:50 (25 minutes)

Small angle scattering is a really useful technique to understand the self-assembly of a range of *N*-functionalised dipeptides. These form micellar structures at high pH and gels at low pH. Gels with different properties can be formed by controlling the micellar species present prior to gelation, for example by changing the counter-ion, by the addition of salts or by a heat-cool cycle. To understand all of this, we have used small angle neutron scattering, for example using contrast matching approaches to understand the molecular packing and rheo-SANS to follow the gelation process with time.

Primary authors: ADAMS, Dave; Dr DRAPER, Emily; SCHWEINS, Ralf; Prof. SEDDON, Annela (University of Bristol)

Presenter: ADAMS, Dave

Session Classification: Talks

Contribution ID: **9** Type: **Invited speakers**

Self-Assembly in Deep Eutectic Solvents

Tuesday, 27 September 2022 14:50 (25 minutes)

Deep eutectic solvents (DES) are promising novel solvents obtained through the complexation of a halide salt such as choline chloride with a hydrogen bond donor such as urea or glycerol, enabling them to be tuned for particular properties, including low toxicity and sustainability. They are of increasing interest to replace organic solvents in applications from synthesis to pharmaceutical formulations. We have found that polar DES will support amphiphile aggregation and so are undertaking a systematic study to correlate the unique hydrogen-bonded nanostructure of DES with surfactant phase behaviour in these solvents. We have used a range of scattering techniques, including small angle scattering and reflectivity as well as measurements of critical micelle concentration, rheology and thermal properties to study micellization in these media. These investigations have shown that DES can promote amphiphile self-assembly but alter surfactant phase behaviour significantly compared to that in water, offering control over micelle morphology, as the solvent components can be tuned to be interacting or non-interacting with the surfactant, altering the micelle shape. In ternary DES, containing both urea and glycerol as hydrogen bond donors, the interaction of cationic and anionic surfactant headgroups with these solvent components are strikingly different. In addition, despite the highly ionic nature of DES, surfactant counterion binding is also surprisingly important in controlling micelle shape, and the micelles appear to show electrostatic interactions as the surfactant concentration is increased. This presentation will discuss our results and try to draw conclusions on the important factors controlling amphiphile behaviour in these interesting novel solvents.

Primary author: EDLER, Karen (Lund University)

Presenter: EDLER, Karen (Lund University)

Session Classification: Talks

Contribution ID: **10** Type: **Invited speakers**

The 1980s and the first D11 modernistion program

Monday, 26 September 2022 09:00 (25 minutes)

D11 was conceived and designed by Konrad Ibel, Werner Schmatz and Tasso Springer and became operational in 1972 shortly after ILL's first neutron beams became available. Soon after a high angle data bank (D11B) was added by Gernot Kostorz for studying diffuse scattering. The first few years were devoted to many pioneering experiments in the fields of polymers, materials, metallurgy as well as structural biology. In parallel rapid progress was made in software development (Ron Ghosh) although the fundamental design of the instrument remained constant. In the early 1980s at Oak Ridge Wally Koehler had built a 30m SANS instrument whose novel feature was having the 2-dimensional detector mounted on a trolley inside the tube. This was a major motivation for us to initiate a whole series of modifications to modernise D11. A new detector tube was installed with the detector moving inside on a trolley, the instrument control system underwent a major renewal, sample changers and beam stops were automated new sample environments introduced and old ones improved . In my talk I will attempt (within the constraints of 40 years memory) to describe the evolution of D11 in these early years and to show some examples of the data obtained.

Primary author: TIMMINS, Peter (ILL retired)

Presenter: TIMMINS, Peter (ILL retired)

Session Classification: Talks

Contribution ID: **11** Type: **Invited speakers**

Contribution of SANS and particularly of D11 on the understanding of thermoreversible gelation

Wednesday, 28 September 2022 11:15 (25 minutes)

Being among the first users of D11, I will give during my talk an outlook of the topics I investigated with this SANS camera. My first use of D11 dates back to Mai 1975 for studying the chain conformation in a crystalline polymer, namely isotactic polystyrene (iPS). Unlike polyethylene, that was studied simultaneously by other group of scientists, iPS did not display any isotopic segregation so that the single chain behaviour could be determined. We showed that the chain conformation depends on the crystalline growth rate with respect to the polymer viscosity. The chains fold completely in single crystals grown from dilute solutions while there is an alternation of folded parts and amorphous part in the bulk state. Our studies in polymer thermoreversible gels displaying fibrillar morphology have shown that the chain possesses a persistence length much larger that observed in the usual flexible state. We could show that this is due to helical stabilization through the formation of polymer/solvent molecular compounds. We could further show that a larger persistence length appears as a prerequisite for the formation of polymer thermoreversible gels.
We also investigated hybrid polymer thermoreversible gels/self-assembled systems. We could highlight the encapsulation of a bicopper complex by polymer fibrils, or the sheathing of polymer fibrils by self-assembled nanotubes.

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Primary author: GUENET, Jean-Michel (CNRS Institut Charles Sadron)

Presenter: GUENET, Jean-Michel (CNRS Institut Charles Sadron)

Session Classification: Talks

Contribution ID: **12** Type: **Invited speakers**

Dendrimers and Small-angle Neutron Scattering: History and Perspectives

Tuesday, 27 September 2022 10:50 (25 minutes)

Dendrimers are synthetic macromolecules having a defined architecture. Starting from a trifunctional monomer (generation 0), subsequent generations are connected to this initial core from which in a treelike structure results. Small-angle neutron scattering (SANS) has been extremely useful for the characterization of these molecules since it allows us to change the contrast through mixtures of deuterated and protonated solvents. In this way, SANS served for a full characterization of dendrimers set up of flexible [1] or stiff molecular units.[2, 3] Moreover, a SANS-study of flexible dendrimers with partially deuteration of the endgroups led to the unambiguous conclusion that these dendrimers have a dense core, that is, the endgroups fold back to a certain extend.[4] Another feature revealed by SANS in conjunction with modeling by molecular dynamics is the soft interaction of flexible dendrimers in solution.[5-7]
In this lecture we will review this work and its extension to more recent systems including DNA-based, charged dendrimers. We will demonstrate that, in the latter case, the generation number, the salt concentration and the flexibility between different generations serve as physical control parameters to tune the softness of the dendrimer interactions.[8] Finally, we will show how a combined effort between synthesis, theory and SAXS-measurements reveals that suitably engineered, hybrid dendrimers have recently led to the experimental verification of cluster crystals,[9] a novel state of matter, 20 years after its original theoretical prediction.[10]

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Primary authors: Prof. LIKOS, Christos (Faculty of Physics, University of Vienna); BALLAUFF, Matthias (Institut fuer Chemie und Biochemie, FU Berlin)

Presenter: BALLAUFF, Matthias (Institut fuer Chemie und Biochemie, FU Berlin)

Session Classification: Talks

Contribution ID: **13** Type: **Invited speakers**

Hard problems in soft matter - a not quite random walk through 30 years of soft matter research with neutrons (remote)

Monday, 26 September 2022 14:00 (25 minutes)

The small-angle instruments at ILL have been instrumental for our soft matter research during the last 30 years. I will illustrate this with a number of research projects where SANS has been key in elucidating structural properties of various soft matter systems, covering diverse topics such as the formation of polymerlike micelles, the kinetics of the micelle-to-vesicle transition, gel structures formed in an arrested spinodal decomposition in solutions of globular proteins, and the response of soft microgels to high packing densities. Particular attention will be given to the importance of interdisciplinary interactions and the role of computer simulations when attempting to interpret and understand results obtained with complex soft matter systems.

Primary author: SCHURTENBERGER, Peter (Lund University)

Presenter: SCHURTENBERGER, Peter (Lund University)

Session Classification: Talks

Contribution ID: **14** Type: **Invited speakers**

Multiscale micro-architecture of pore space in rocks: size, shape, deformation and accessibility (remote)

Monday, 26 September 2022 16:45 (25 minutes)

The interface between rock matrix and pore space in sedimentary rocks is rough over seven orders of magnitude of the linear scale, from sub-nanometers (nearly molecular) to centimeters. Since the early 1980's, pore-matrix roughness has often been described using the framework of Mandelbrot's fractal geometry and the corresponding mathematical formalism for correlation functions; this formalism has been applied to successfully model the power-law SANS and SAXS results for many types of sedimentary rocks (e.g. sandstones, shale, carbonates and coal). P.W. Schmidt first established the connection between pore-size distribution (as an alternative expression of roughness) and the power-law dependence of small-angle scattering intensity, and within a decade, the vast world of fractals in natural porous media was revealed.
Small-angle scattering is uniquely suited to microstructural geological applications, given its capacity to provide volume-average nano- and microstructural information, and its sensitivity to the chemical composition of pore content. In the early days, the crucial issue was the extent of the Q-range (hence the pore sizes). The capacity to study pore sizes was limited by the small-Q limit of the longest-base SANS instrument D11; this range was then greatly improved in 1997, following the construction of a Bonse-Hart type USANS instrument by M. Agamalian. Since that time, pore sizes ranging from sub-nanometeres to approximately 20 micrometers can be investigated using SANS-USANS. The capability of long base SANS instruments using wavelengths of ca. 5 Å to provide overlap with USANS data in the region around Q≈10-3 Å-1 has been crucial to the elimination of multiple scattering, a problem specific to strong scatterters (like most rocks), and inescapable for the modern lens-geometry and TOF SANS instruments. Technical developments resulting in low background noise of modern SANS detectors have enabled precise insight into the nano- and sub-nanometer scale regions, which led to the discovery of the ubiquitous phenomenon of gas condensation in the nano-pores of shales and carbonates. Similar results have been obtained for coal and aerogels.
A seminal step occured with the gradual development of SANS and USANS contrast matching capability, delivered by high pressure gas environmental cells, which offered significant progress compared to the use of deuterated liquids in earlier contrast matching experiments. This made it possible to independently characterise the total porosity, specific surface area and pore size distribution for porous spaces that are accessible and inaccessible to penetrating fluids (greenhouse gases in particular). Significantly, for a great majority of measured rocks, the roughness of the matrix - pore interface of the accessible pores turned out to be less accentuated than that of the inaccessible pores. This provided an interesting insight into the long-standing fundamental question of the origin and temporal persistence of porosity in rocks; in addition to the antisintering mechanism proposed by M. Cohen, the reactive transport of brine through the rock matrix likely plays a significant role. The recently added uniaxial stress capability enabled SANS and USANS measurements under simulated pressure conditions encountered in unconventional shales subjected to hydraulic fracturing. The results showed that the porosity response to simulated well-management is complex: it is both pore-size-dependent and thermal-maturity dependent. Armed with these capabilities, small angle neutron scattering has become a mainstream tool in petrology and geology on the nano- and microscale, applied in tandem with electron microscopy, gas adsorption measurements, mercury intrusion porosimetry and SAXS-USAXS .

Primary author: RADLINSKI, Andrzej (University of Warsaw)

Presenter: RADLINSKI, Andrzej (University of Warsaw)

Session Classification: Talks

Contribution ID: **15** Type: **Invited speakers**

D11, the stimulus for early biology at ILL

Monday, 26 September 2022 09:25 (25 minutes)

Following a period of strong development of the contrast variation method using H2O/D2O exchange on physical-chemical and readily available soluble protein samples,D11 hosted a number of challenging experiments in biology—in particular on protein-nucleic acid interactions. Important results were obtained on the inner structures of plant viruses, ribosomes and chromatin. A study of aminoacyl-tRNA synthetases interactions with their tRNA substrates established in-beam structural biochemistry on D11.

Primary author: ZACCAI, Joseph

Presenter: ZACCAI, Joseph

Session Classification: Talks

Contribution ID: **16** Type: **poster contributions**

Unravel the structure of meat analogues using SANS

The current, unsustainable meat industry makes a growing number of meat consumers turn to plant-based meat alternatives (PBMAs). To facilitate the transition towards a (partly) plant-based diet with its health, environmental and ethical benefits, the demand for an accurate reproduction of meat-like structure, texture and mouthfeel in PBMAs is pressing. High Moisture Extrusion Cooking (HMEC) is one of the methods to produce PBMAs starting from raw material powders. During HMEC, mixtures of plant proteins (e.g. soy, pea or wheat), dietary fiber and fat undergo heat- and flow-induced denaturation and subsequent plastification and texturization. The key to reproduce meat-like structures are the plastification and texturization which take place in a cooling die attached to the end of extruder. However, the "black-box" characteristics of the extrusion process including the cooling die make the understanding of the texturization process difficult. Small Angle Neutron Scattering (SANS) and complementary (scattering) techniques are a promising tool to unravel the mechanism of PBMA structurization. Here, we show the results of SANS measurements on different PBMA recipes. We employed contrast variation to elucidate the role of the different components in the texturization of PBMAs. We also provide insight into our plans to perform in-situ SANS with a customized neutron-transparent cooling die. Crucially, this setup will help shed light on the plastification and texturization mechanism throughout the entire cooling process of extrusion. Based on our results, we expect to obtain a detailed insight into the texturization of plant proteins in food processing and thereby to pave the way towards a more sustainable nutrition.

Primary authors: GUAN, Tong; MATSARSKAIA, Olga; Prof. FISCHER, Peter (ETH Zuerich); Dr ZYCHOWSKI, Lisa (Planted Foods AG)

Presenter: GUAN, Tong

Session Classification: Poster session/Wine and Cheese evening

Contribution ID: **17** Type: **poster contributions**

A Computational Model for Interpolyelectrolyte Complexes

Advances in modern polymer science allow to create evermore complex self-assembled structures, which are driven mostly by using electrostatic and hydrophobic forces. An example of such a system are multicompartment interpolyelectrolyte complexes (MIPECs) to be obtained by combining appropriate copolymers of opposite charge and which are stabilized by a hydrophilic corona [1]. These water-soluble colloids of 50-200 nm size combine different solubilisation properties, functionalities, and variable mesoscopic structure that make them interesting for example in the field of drug delivery. The structure of the MIPECs have been already studied e.g. by Small Angle Neutron Scattering (SANS) [2]. However, a detailed description of the architecture and appropriate modeling of the data is still missing. In this poster, we will present a computational model which can describe the existing SANS data and offer further structural insights from the model parameters.

This top-down, coarse-grained model presents micelles of hydrophobic chains as spherical particles confined into a spherical region composed of the IPEC. This simplistic model allowed us to use Molecular Dynamics (MD) simulations to rapidly sample the configurations of the system. The obtained scattering intensities revealed the lack of a fractal behavior [3] and the confinement shape. Moreover, we will show that by considering a third different Scattering Length Density (SLD) we can realistically model the scattering contribution of the confined region and obtain a realistic model of our system. This structural model then was tested on experimental SANS data obtained from complexes of oppositely charged microemulsion droplets and polyelectrolytes.

Primary authors: PREVOST, Sylvain (Institut Laue-Langevin); CZAKKEL, Orsolya; GRADZIELSKI, Michael; CHAMCHOUM, Matteo; SIMON , Miriam

Presenter: CHAMCHOUM, Matteo

Session Classification: Poster session/Wine and Cheese evening

Contribution ID: **18** Type: **Invited speakers**

Fighting Gravity on D11

Monday, 26 September 2022 17:35 (25 minutes)

To use the minimum q of a SANS instrument we require the longest collimation and detector distances combined with the longest wavelength. This combination maximizes how much gravity curves the neutron beam and how much the beam is spread due to the range of wavelengths. D11 is the only gravity limited SANS instrument in the world where at minimum q gravity prevents any transmission through the collimation above a certain wavelength and the beam also falls off the bottom of the detector. To solve these problems initially the use of a prism was employed providing a refracted angle to counter the fall in gravity. This worked in principle but suffered from absorption and scattering from the prism material and was limited to very small beams. Inspired by the horizontal reflectometer FIGARO, a reflective surface of one of the guides in the collimation was found to be able to undo the effects of gravity without the beamsize restriction. Combined with a lens, this allowed a minimum q of 7x$10^{-5} Ang.^{-1}$ to be measured. A scientific example of a system that would profit from this minimum q will be presented.

Primary author: CUBITT, Robert (ILL)

Co-authors: Dr SCHWEINS, Ralf (ILL); Prof. LINDNER, Peter (ILL); Dr FORGAN, Ted

Presenter: CUBITT, Robert (ILL)

Session Classification: Talks

Contribution ID: **19** Type: **poster contributions**

A Small-Angle Scattering study of the behaviour of polyelectrolytes in organic media

Polyelectrolytes are a class of material that have appealed to researchers in many different areas owing to their versatility and potential applications. The existing studies mostly deal with their behaviour in aqueous solutions due to their lack of solubility in other media. Here we have utilized carboxymethyl cellulose (CMC), which is widely available as a sodium salt, NaCMC. The solubility of CMC in organic media was enhanced by replacing the hydrophilic Na+ with the hydrophobic tetrabutylammonium (TBA^+) counterion. In this study, a series of SANS and SAXS measurements were conducted to explore the behaviour of TBACMC by determining the correlation length (ξ) as a function of concentration (c) and solvent dielectric constant (ε). We have combined these techniques with rheology to determine other properties such as the overlap (c*) and entanglement (c_e) concentrations in the different solvents. It was found that c* and c_e scale as $\approx \varepsilon^{-1}$ and $\approx \varepsilon^{0}$ respectively. Also, conductivity measurements were conducted to determine the degree of uncondensed counterions (f) in the different media. We are trying to utilize the knowledge of f to explain the deviation observed in SANS and SAXS behaviour in some of the systems. It is observed that in solvents with a higher dielectric constant, a greater deviation between SAXS and SANS results is observed, presumably due to the higher values of f and the difference in the origin of contrast for the two techniques (the polyelectrolyte backbone (SAXS) and the counterion (SANS)).

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In addition, a better understood polystyrene sulfonate (PSS) system with the same hydrophobic counterion has been explored using SANS. Owing to the low polydispersity obtainable in TBAPSS, we have also used it to study the effect of degree of polymerization (N) on properties such as c* in different solvents. These explorations allow us to draw parallels between the CMC and PSS systems and to expand our understanding of the polyelectrolytes.

Primary authors: Mr GULATI, Anish (RWTH Aachen University); Dr LOPEZ, Carlos G. (RWTH Aachen University)

Presenter: Mr GULATI, Anish (RWTH Aachen University)

Session Classification: Poster session/Wine and Cheese evening

Contribution ID: **20** Type: **Invited speakers**

Soft Quasicrystals - a D11 discovery

Wednesday, 28 September 2022 10:50 (25 minutes)

Quasicrystals are a peculiar state of order, which is fundamentally different from classical ordered crystalline states. Discovered in 1982 for MnAl-alloys, it has since then been found for more than 100 different metal alloys.

In a 2009 D11 summer nightshift we discovered a micellar phase showing an unusual SANS-pattern with 12-fold rotational symmetry. When published in 2011, it was the third ever reported non-metallic dodecagonal quasicrystalline phase. Non-metallic quasicrystals have since then been found also for block copolymers, nanoparticles, colloids, or fullerenes. This indicates that quasicrystals are a quite common state of matter.

We have since then shown by X-ray and neutron scattering experiments as well as MD-simulations that particles with soft repulsive interactions form a distinct set of two- and three-dimensional quasicrystalline states with 8-, 10- and 12-fold rotational symmetry. We investigated quasicrystals formed by block copolymers, nanoparticles and colloids covering length scales from 10 nm to 500 μm. We observe surprisingly good agreement between the predicted and observed quasicrystalline structures and their stability regions in 2D- and 3D-phase diagrams. We further show that all so far reported non-metallic quasicrystals including dendrons, star and block copolymers, nanoparticles, polymer-grafted nanoparticles, colloids, mesoporous silica as well as BaTiO3-, fullerene, and organo-framework monolayers can be derived from this set of quasicrystalline structures. Furthermore, we demonstrate a direct link between non-metallic quasicrystals derived from repulsive potentials and metallic quasicrystals derived from attractive potentials. We show that the existence of two intrinsic length scales is essential for the formation of both non-metallic and metallic quasicrystals, facilitating locally high coordination and thereby optimizing sphere packing.

Primary authors: Dr DULLE, Martin (Forschungszentrum Jülich); Dr JURCZYK, Tobias (Forschungszentrum Jülich); Dr GRUHN, Thomas (Universität Bayreuth); FÖRSTER, Stephan (Forschungszentrum Jülich)

Presenter: FÖRSTER, Stephan (Forschungszentrum Jülich)

Session Classification: Talks

Contribution ID: **21** Type: **poster contributions**

Method to simultaneously probe the bulk modulus and structure of soft compressible objects using SANS

An object's bulk modulus quantifies its resistance to an isotropic compression. For soft deformable colloids the bulk modulus must be known to predict their response to crowding. Here, we will present a new approach to obtain partially-deuterated, high molecular weight polyethylene glycol (dPEG), which is used to exert osmotic stress on soft objects [1,2]. In this study, microgels were used as a model system for soft compressible spheres and their bulk modulus is determined by means of small-angle neutron scattering with contrast matching. By partial deuteration the scattering length density of the dPEG was matched in pure heavy water. Consequently, no contribution of the osmotic stress polymer is measured during the scattering experiments, and the form factor of the microgels was directly measured. Furthermore, in addition to the total radius, the variation of the different parts of the microgels can be also measured as a function of the external osmotic stress. Therefore, using this method the different elasticity along a single particle, such as viruses, can be determined directly.

[1] J. E. Houston, L. Fruhner, A. de la Cotte, J. Rojo González, A. Petrunin, U. Gasser, R. Schweins, J. Allgaier, W. Richtering, A. Fernandez-Nieves and A. Scotti, *Science Advances*, 2022, **8**, eabn6129

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Primary authors: HOUSTON, Judith (ESS); SCOTTI, Andrea; SCHWEINS, Ralf

Presenter: HOUSTON, Judith (ESS)

Session Classification: Poster session/Wine and Cheese evening

Contribution ID: **22** Type: **Invited speakers**

Small angle scattering: scaling cross-sections and widening the q-window to answer scientific questions

Monday, 26 September 2022 11:15 (25 minutes)

We will recap published and unpublished work initiated on D11, D17 and D1B with J.B. Hayter: what happens at low-q and high-q for common and uncommon ionic micelles made from self-assembled amphiphiles in a given solvent?

In the standard SAS range, the Hayter-Penfold decoupling procedure work well for all ionic micelles investigated as long as the chain length is not too short or too long.

As suggested by Luzzati, the absolute scale was crucial to go beyond wild shape fitting of a broad peak with unphysical parameters: from then, the micellar growth controlled by the area per molecule in the lateral equation of state was understood.

But there are still fully open questions, even after 50 years of active X-ray/neutron work on "simple" systems that were not fully understood last century, even for systems where an apparent implicit consensus on unproven facts are favored by the absence of absolute scale and comparison of the results with models.

We will give three examples:

- At high-q, in the range 0.4 $Å^{-1}$ to 0.6 $Å^{-1}$, there is only very few published work about localization of methyl end-groups and this only for saturated aliphatic chains.[1]
- At low-q, there is sometimes an elusive intensity upturn following q^{-1} or q^{-2}:[2] this may be related to flexible necklaces of "flocculated" micelles with threadlike images in electron microscopy, common in the case of magnetic nanoparticles, as suggested by J.B. Hayter and R. Pynn.[3] Their domain of existence as a function of ionic strength is not yet identified.
- there are several observation of non-spherical micelles close to cmc. Theoreticians don't believe experimentalists observations because it is contradictory with elastic theory. We suggest that taking the chain packing as well as the head elastic contributions with one parameter, and not only one with two unphysical bending constants of a molecular film, may solve this long-standing scientific problem.

As always, a broad q window and comparing data on absolute scaled with different predictive models lead to solid scientific progress beyond multiparametric fitting with or without Fourier transforming the data.

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Primary author: ZEMB, Thomas

Presenter: ZEMB, Thomas

Session Classification: Talks

Contribution ID: **23** Type: **poster contributions**

Modeling of flexible biomolecular complexes in solution small-angle scattering

We outline a modeling scheme for calculating the scattering profiles from complex biological samples, such as multi-domain membrane proteins with intrinsically disordered regions and embedded in phospholipid nanodiscs. The scheme bases itself on a hybrid of classical form factor based modeling and the well known spherical harmonics-based formulation of small-angle scattering amplitudes.

We demonstrate the utility of this modeling scheme through a recent example of a structural model of the growth hormone receptor membrane protein in a nanodisc. We investigate how the scattering profiles from the complex would appear under different scattering contrasts. For each contrast situation we discuss what structural information is contained and the related consequences for modeling of the data.

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Co-authors: Dr PEDERSEN, Martin Cramer (University Of Copenhagen); Prof. ARLETH, Lise (University of Copenhagen)

Presenter: Ms BARCLAY, Abigail (University of Copenhagen)

Contribution ID: **24** Type: **poster contributions**

Surfactant-free microemulsions: how molecular dynamic reflects nano-structuration

Mixtures of simple molecules may lead to complex systems with unforeseen properties of particular interest such as reactivity or solubility. This is the case of aqueous solutions of alcohol and oil, typically found in all kind of liquors, cosmetics or solvents for liquid-liquid extraction.

The archetypal case of this family is the ternary mixture of water, ethanol and octanol. Its phase diagram presents a biphasic region with a critical point (Upper Solution Critical Temperature) close to which a strong nanostructuration of the liquid can be observed. In the biphasic region, this emulsion was termed Ouzo effect, following the greek beverage, commonly observed when the 40 \% alcohol liquor is quickly diluted with water. In the monophasic state, a ''pre-Ouzo" region has also been evidenced [1], extending between identified frontiers around the critical point (see Fig. 1, [2]). The structuration is also characterized by a structure factor presenting an Ornstein-Zernike behaviour, indicating the presence of aggregates of the order of 100 molecules similar to a micro-emulsion formed by a ternary water-poor mixture of octanol and ethanol and water, surrounded by a surface excess of ethanol that is immersed in a binary water-ethanol solution saturated with a low quantity of octanol.

In this system, we investigated, using QENS and various isotopic mixtures, the relaxation dynamic of each component along different composition lines crossing the phase diagram. The evolution of the diffusion coefficient is measured over a wave vector ranging from \(0.05 {\AA}^{-1}\) to \(0.6 {\AA}^{-1}\), bridging the scale from characteristic droplet size to molecular distances, i.e. from collective to individual dynamics.

We will show how the dynamics also reflect the (nano)structural organisation.

Primary authors: MALAYIL KALATHIL, Firoz; PLAZANET, Marie (Laboratoire Interdisciplinaire de Physique); HOFFMANN, Ingo; Prof. ZEMB, Thomas (CEA ICSM); ALBA-SIMIONESCO, Christiane

Presenter: MALAYIL KALATHIL, Firoz

Contribution ID: **25** Type: **poster contributions**

Time-Resolved Light-Tunable Nanoparticles by Electrostatic Self-assembly

Electrostatic self-assembly is a well-known technique to form nearly monodisperse nanoparticles using coulombic interactions between oppositely charged species in the aqueous phase. In this study, the opposite charges originate from cationically charged polyelectrolytes and multivalent organic counterions. Self-assembly of these charged, multi-responsive building blocks leads to forming a wide range of shapes, for example, spheres, rods, ellipsoids, cylinders, etc. Various external triggers such as pH, light irradiation, and charge ratio could be used to tune these electrostatic self-assembled structures.

In the present work, small-angle neutron scattering (SANS) plays a crucial role in determining the formation mechanisms and structure-directing effects. As a model system, a divalent azo dye (AY38, Acid Yellow 38) and cationic polyamidoamine (PAMAM) dendrimers were used as the key components to construct self-assembled structures in aqueous solution. The isomerization capability of AY38 and pH-responsiveness of the dendrimers make them suitable candidates to alter the size and shape of self-assembled particles through light irradiation and degree of protonation. In particular, the preparation method has been modified to gain insight into the formation mechanism (see Scheme). Slow assemblies' growth was observed time-dependently whilst the dye-molecules reconverted to the trans-isomer. A home-built device is designed to analyze the structural changes using in-situ UV irradiation on the SANS instrument. Various complementary methods are used towards understanding the formation and restructuring mechanism, especially dynamic and static light scattering (DLS/SLS), zeta potential, isothermal titration calorimetry (ITC), and UV/Vis spectroscopy.

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Primary authors: GROEHN, Franziska; Dr SCHWEINS, Ralf (ILL); AGARWAL, Mohit

Presenter: AGARWAL, Mohit

Contribution ID: **26** Type: **Invited speakers**

D11: a fantastic instrument for conservation, restoration and the study of ancient technologies in Cultural Heritage

Monday, 26 September 2022 17:10 (25 minutes)

Artefacts of interest in cultural heritage (CH) are often rare, precious, manifolds and complexes and their secrets are difficult to disclose.
The D11 instrument at Institut Laue Langevin (ILL) is a very unique instrument to investigate CH samples and their history. D11 uses: neutrons that are a no-destructive probe and the small angle neutron scattering (SANS) technique covering four decades in Q, i.e. it is able to investigate dimensions between the Å to some hundreds of microns, a very interesting range of investigation for complexes systems as those of interest in CH. Furthermore the fact that with neutrons we can investigate light elements and to use contrast methods to make in evidence some specific part of the systems makes D11 the best and very versatile instrument for these kind of studies. We will present here three applications of D11 to CH systems: a study on ancient paper to shade light on the mechanisms of the paper degradation 1; a study of the porosity of ancient ceramic and how it is related to a specific technique of production and the historical context [2]; a study of the characteristics of nanoparticles of alkaline earth hydroxide to drive their production on large scale, for curative and preventive eco-friendly treatments of waterlogged wood [3].

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Presenter: MONDELLI, Claudia (CNR-IOM-OGG)

Session Classification: Talks

Contribution ID: **27** Type: **poster contributions**

Towards a Comprehensive Picture of Temperature-responsive Elastin-like Peptides

Elastin-like peptides (ELPs) mimic the hydrophobic repeat units of elastin, a protein rendering biological tissues such as lung, ligaments and blood vessels elastic. ELPs collapse hydrophobically upon crossing a lower critical solution temperature (LCST). Due to their stimulus-responsive properties, ELPs are of interest for many application areas including biomaterials, protein purification and drug delivery. However, a comprehensive mechanistic characterisation of the static and dynamic aspects of the collapse has not yet been obtained. By combining SANS, QENS, molecular dynamics simulations and selective deuteration, we investigate the temperature response of selectively deuterated ELPs. Here, we focus on the SANS data which reveal differences in the behaviour of short and long ELPs. In agreement with simulations, a shift towards more compact ELP structures with increasing temperature is observed. Based on our results, we aim at establishing a framework for the investigation of stimulus-responsive molecules and materials.

Primary authors: MATSARSKAIA, Olga (ILL); MOROZOVA, Tatiana (ILL); WEHBE, Zeina (ILL); WALDIE, Sarah (U Malmö); GARCÍA, Nicolas A. (U Nacional del Sur); KOZA, Michael M. (ILL); MOULIN, Martine (ILL); LAUX, Valérie (ILL); HAERTLEIN, Michael (ILL); FORSYTH, Trevor (ILL); BARRAT, Jean-Louis (ILL); ROOSEN-RUNGE, Felix (U Malmö)

Presenter: MATSARSKAIA, Olga (ILL)

Contribution ID: **28** Type: **poster contributions**

Understanding how coacervation of two viral proteins drives the formation of membrane-less compartments

Rabies virus (RABV) causes fatal encephalitis in human. At the cellular level, infection by RABV induces the formation of cytoplasmic inclusion bodies called Negri's bodies, which have the properties of liquid-like compartments (Nikolic et al. 2017) formed by phase separation and constitute viral factories (Nikolic et al. 2016). The expression of two viral proteins, the nucleoprotein (N) and the phosphoprotein (P), in cultured cells proved to be sufficient to reproduce phase separation and the formation of Negri body-like compartments (Nikolic et al. 2017).

We reconstitute the liquid-liquid phase separation with purified hydrogenated N as well as hydrogenated and deuterated P proteins in the prospect of using small-angle neutron scattering experiments to probe the relative arrangement of biomacromolecules in these densely packed microphases.

To decipher the physico-chemical principles underlying protein-induced liquid-liquid phase separation leading to the self-coacervation of these proteins into membraneless compartments, particularly in the context of viral infection by certain RNA viruses, SANS and SAXS measurements were performed at the Institut Laue-Langevin (ILL) and ESRF. We will present results obtained for proteins in dilute conditions away from phase separation at various ionic strengths as well as over a wide range of concentrations and temperatures, to introduce our proposed mechanism of protein-protein interaction that leads to a fully reversible macroscopic phase transition but only a partially reversible protein quaternary structure.

Primary authors: Mrs BOUCHAMA, Fella; CUELLO, Gabriel Julio; Prof. ZEMB, Thomas (CEA ICSM); JAMIN, Marc (Université Grenoble Alpes)

Presenter: Mrs BOUCHAMA, Fella

Contribution ID: **29** Type: **Invited speakers**

Kinetics Pathways of Block Copolymer Self-assembly in Solution: transitions, logarithmical relaxations, molecular exchange and effect of crystallinity

Tuesday, 27 September 2022 09:25 (25 minutes)

Self-assembled systems are generally highly dynamic structures characterized by molecular exchange, fluctuations and fusion/fission and morphological transitions. Examples include micelles formed by synthetic surfactants and block copolymers as well as lipid membranes. Despite their importance in technological and biomedical applications, the kinetic pathways associated with the formation and molecular transport of such self-assembled nanostructures are generally poorly understood. Time-resolved small-angle X-ray/neutron scattering (TR-SAXS/SANS) is powerful technique 1 that allow non-equilibrium kinetic processes such as nucleation processes [2,4] and morphological transitions [3,5] to be followed with structural resolution over time scales starting from a few milliseconds. Neutrons have the additional advantage of facile contrast variation through H/D substitution schemes, which also allow equilibrium processes such as molecular exchange and diffusion to be studied without perturbation [1,6-8].
In this presentation we will address the basic kinetic pathways found in block copolymer micelles formed by amphiphilic self-assembly. We will address both equilibrium and non-equilibrium kinetics and argue that the understanding of kinetic pathways can be utilized to manipulate and design the physical properties of self-assembled systems. The mechanism of molecular exchange in block copolymer micelles that was tediously studied at D11 in the early 2000s and the rather dramatic effect of polydispersity will be discussed in detail . Furthermore, we shall discuss the role of confinement and crystallinity on the stability and molecular transport processes in semi-crystalline micelles [8,10] and telechelic polymer micelles [11,12] and discuss the relevance to biological systems and biomedical applications.

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Primary author: LUND, Reidar

Presenter: LUND, Reidar

Session Classification: Talks

Contribution ID: **30** Type: **Invited speakers**

SANS Crystallography

Monday, 26 September 2022 12:05 (25 minutes)

Soon after the advent of High-Tc superconductors, it became clear that that important information could be obtained by observing the lattice of quantised flux lines in these and other unconventional and conventional superconductors. This meant that SANS scattering patterns contained Bragg peaks had to be analysed. I will compare the state of the art of early experiments with what is available today to investigate flux line lattices and other mesostructures, including Bayesian analysis and quasi-monochromatic (as on D11) versus TOF SANS techniques.

Primary author: FORGAN, Edward M

Presenter: FORGAN, Edward M

Session Classification: Talks

Contribution ID: **31** Type: **poster contributions**

Structure and interaction of surface charged polymeric micelles

Soft colloids are ubiquitous in synthetic and biological material as e.g. vesicles, dendrimers, microgels, polymer-grafted nanoparticles, micelles, star polymers and certain proteins. They display a dual character between a polymer and the archetypical hard sphere colloid. Due to this hybrid nature, soft colloids macroscopically show interesting structural 1 and dynamical [2] properties resulting from its unique microscopic structure. Flow behavior of crowded solutions, (visco-) elastic properties of jammed states as gels and glasses and finally (crystal) structure and stability of other highly ordered phases [3] crucially depend on "softness", which is intimately related to the details of molecular structure.

We established micelles formed by n-alkane-PEO-OH amphiphilic block copolymers as an easy and elegant model system to tailor colloidal softness [4]. Parameters to tailor the "softness" start on a microscopic level by selecting the chemical nature of the hydrophobic block, by varying the solvophobic-to-solvophilic block ratio 1, the absolute block molecular weights [2], polydispersity of the hydrophobic block [3], and/or the interfacial tension [4].

In the present work, we introduce surface charges on the micelles resulting in electrostatic interactions in addition to the inherently present steric repulsion. The charges are implemented by oxidation of the terminal hydroxy group of the PEO block into a carboxy group by means of Bobbitt's salt [5]. Since carboxylic acids are weak acids, the number of charges on the particles depends on pH. The range and strength of the electrostatic repulsion can be easily modified by varying the effective number of charges via change in pH and/or ionic strength. Thus, the structural properties of micellar solutions can be effectively adjusted.

Here we present a study on the intra- and interparticle structure of C28-PEO5k-COOH polymer micelles in D2O over a broad range of concentrations by SANS as a function of the number of surface charges and ionic strength. We demonstrate that the micellar form factor remains the same independent of the number of charges. However, in contrast to neutral micelles, the charged micelles typically reveal structure factor contributions even at very dilute concentration, arising from the dominating long-range electrostatic repulsion. Structure factors in the liquid state are analyzed using established effective interaction potentials [7]. By increasing the concentration a liquid to crystal transition is observed for all systems, but for charged micelles at a much lower concentration compared to the uncharged micelles.

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Presenters: Dr TEA, Lingsam (FZ-Juelich GmbH); Dr WILLNER, Lutz (FZ-Juelich GmbH)

Contribution ID: **32** Type: **poster contributions**

SANS contrast variation for the localization of anionic dyes in DTAB-micelles

Aqueous solutions of dye and surfactant are of major significance in industrial applications such as textile dyeing, wastewater-treatment and cosmetics. Hence, numerous studies investigating dye-surfactant interaction were performed.1 Changes in the UV/vis absorption spectrum of the dye upon surfactant-addition induced assumptions about the polarity of the environment of the dye and its location within the surfactant micelle. However, these assumptions have yet to be confirmed with measurements that unambiguously reveal a) size and shape of the dye-surfactant aggregate and b) the location of the dye within the aggregate.
Small-angle scattering (SAS) provides answers to the first question. Concerning the investigation of dye-surfactant aggregation with SAS, only one publication describing the aggregation of an anionic dye and cationic surfactants is known to us. Here, worm-like or cylindrical aggregates were described.[2] For an unambiguous localization of the dyestuff within the micelles, as it is addressed in the second question, contrast variation in small-angle neutron scattering (SANS) needs to be employed.
We studied the interaction of two commercial, anionic azo dyes (**Blue** and **Red**) with the cationic surfactant dodecyltrimethylammoniumbromide (**DTAB**) in an aqueous, alkaline buffer solution. These azo dyes self-assemble in the absence of surfactant. Whereas **Blue** forms dimers, **Red** self-assembles to higher aggregation numbers in the employed buffer. At a given dye concentration, addition of **DTAB** leads to a change in the absorption spectrum of the dye, indicating a redistribution of intermolecular interactions. Using SANS, we were not only able to determine shape and size of dye-surfactant aggregates, but also to locate the dye within the dye-surfactant micelle employing contrast variation by isotopic substitution of h34-**DTAB** with a mixture of d25-**DTAB**/d34-**DTAB**. We will present SANS-data that reveal the formation of oblate ellipsoids, cylinders or flexible cylinders from **Blue** and **DTAB**, dependent on **Blue**/**DTAB**-ratio, and data showing the formation of prolate ellipsoids or cylindrical structures from **Red** and **DTAB**. In all cases, the dye was found to be located on the outside of the surfactant micelle.

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Presenter: MUELLER, Wenke

Contribution ID: **33** Type: **poster contributions**

Polyoxometalate-rich complex micelles for functional mesoporous materials

50 YEARS OF D11
Poster Abstract

Introduction

The newly developed Polyion complex (PIC) micelles have unparalleled significance in the construction of functionalized and ordered mesoporous materials. MesoPIC micelles are fabricated through the electrostatic complexation between a charged double hydrophilic block copolymer (DHBC) and an oppositely charged polyelectrolyte. The formation and deformation of these micelles could be controlled by physico-chemical proceedings such as a pH change, a property of predominant importance in templeting agents employed for the preparation of ordered mesoporous materials. The immense study of PIC micelles has opened a new array of opportunities in front of us. We are currently working on two different protocols, employing the MesoPIC process.

Protocol 1:

In this procedure, functionalised Polyion complex (PIC) micelles, fabricated through the electrostatic complexation between a charged double hydrophilic block copolymer (DHBC) and an oppositely charged polyelectrolyte, functions as structuring agent for the construction of porous materials. Hence, the primary aim of the strategy would be to synthesise DHBCs, with well controlled degree of polymerisation. Secondly, the focus would be the functionalisation of the DHBC synthesised. The functional DHBC envisaged, PEO-b-POMs, will contain a poly(ethyleneoxide) block and a block grafted with polyoxometalates (POMs). POMs are metal anionic nanoclusters with promising properties, especially as catalysts or UV-absorbers. This method will permit the direct formation of porous organised materials, functionalised with POMs at the pore surface.

Protocol 2:

In the giant novel complex micelles (Complex PIC Micelles) developed through this novel means, inorganic clusters exhibiting various structural and functional properties, referred to as Polyoxometalates (POMs), functions as the core and the DHBC builds the periphery. POMs employed for the initial studies are Pospho- and Silicotungstic acid. Preliminary analysis of the Complex PIC Micelles through DLS/SLS, confirm them to be giant structures, with a radius of approx. 45 nm. SAS would be employed for understanding these micelles in more detail. Knowing the structure and shape of the micelles prepared would be key, for the efficient use of them in order to construct mesoporous materials, with potential application in catalysis and UVAdsorption

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Presenter: Mr UNNIKRISHNAN, Ananthapadmanabhan (PhD Student)

Contribution ID: **34** Type: **Invited speakers**

Using SANS to explore multi-Q magnetic phases in quantum materials

In quantum materials, interactions between unpaired electrons can lead to the formation of complex magnetization textures, that themselves generate novel quantum effects ripe for exploitation in applications. When the periodicity of these textures are incommensurate with the host crystal lattice, SANS can play the key role in both their observation, and the efficient characterization of their phase diagram as function of various thermodynamic parameters. Of particular interest are magnetization textures that modulate along more than one direction simultaneously, the so-called multi-Q structures. In the last decade, multi-Q structures have been shown to possess novel topological properties. Consequently, SANS continues to be an indispensable tool in the search for new multi-Q phases in a variety of systems. Here, I will highlight our recent work in this area done using the SANS instruments at the ILL, in particular at the hard matter SANS beamline D33. This beamline combines the high flux of the ILL, with flexible sample environment and beam polarization analysis options to make this instrument a most attractive choice for this research area.

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Presenter: WHITE, Jonathan (Paul Scherrer Institute, Switzerland)

Session Classification: Talks

Contribution ID: **35** Type: **Invited speakers**

Structural evolution of temperature-responsive polysaccharide-block-polypeptide copolymers

Tuesday, 27 September 2022 11:40 (25 minutes)

Linking polysaccharides and polypeptides together leads to fully biocompatible copolymers with unique properties for healthcare applications: not only they are fully biodegradable, but also they offer specific recognition and docking properties to membrane receptors of biological cells. Moreover, the two blocks can respond to external stimuli, such as pH, temperature, or the presence of specific molecules. Although they are both hydrophilic, the solubility in water of the polypeptide block can differ from that of the carbohydrate part, leading to compartmentalized supramolecular aggregates such as core-corona spherical or cylindrical micelles, or vesicles.[1,2] Accordingly, they are ideal candidates as novel nano-carriers for drug delivery. This work reports a structural study performed by SANS in fall 2018 at the ILL on the D11 spectrometer, where we deciphered the phase behavior (in temperature and concentration) of diblock copolymers made of a thermosensitive elastin-like polypeptide (ELP) block,[3] tethered to various hydrophilic carbohydrate blocks: PEG, dextran, hyaluronan, and a short oligosaccharide (laminarihexose).[4]

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Presenter: SANDRE, Olivier (CNRS / Université de Bordeaux / Bordeaux INP)

Session Classification: Talks

Contribution ID: **37** Type: **poster contributions**

Dynamic cluster formation, viscosity and diffusion in monoclonal antibody solutions

Antibodies play an essential role in the immune response of mammals. Monoclonal antibodies (mAbs) are particularly relevant for therapeutic approaches due to their high specificity and versatility. The pharmaceutical challenge is to formulate highly concentrated antibody solutions to achieve a significant therapeutic effect, while minimizing their viscosity and keeping it under the subcutaneous injectability limit 1, thus rendering the drug administration to patients less difficult and painful. Since the understanding of macroscopic viscosity requires an in-depth knowledge on protein diffusion and dynamic cluster formation [2,3], we study the self-diffusion of five mAbs of the IgG1 subtype (produced and characterized at Lonza AG) in aqueous solution as a function of the type of antibody and of their concentration, by quasi-elastic neutron scattering (QENS) and small angle neutron scattering (SANS). QENS allows to determine unambiguously the hydrodynamic mAb cluster size [4] and to gain information on the internal mAb dynamics, while SANS has been crucial to obtain information on sample structure and on the nature of interactions occuring among mAb molecules. The instruments employed for data collection are the spectrometer IN16b (ILL) and D11 (ILL).

Complementary information is provided by molecular dynamics (MD) simulations and rheology measurements.

As a reference, we use polyclonal antibody (IgG from bovine serum) solutions [5], thus obtaining a comprehensive picture of mAb diffusion.

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Contribution ID: **38** Type: **poster contributions**

Probing the micro- and meso-structure of activated carbons with SANS

Activated carbons are among the most widely employed materials in catalysis, either as supports or as catalysts on their own. The reasons of their success are mainly their low cost and their elevated specific surface area (SSA), which is enlarged by the activation process (i.e., the treatment of a char precursor at high temperature in the presence of either a chemical agent, e.g. phosphoric acid, or steam), resulting in the development of a complex porosity. The morphology of these micro- and mesopores, together with their spatial organization, is crucial to understand the catalytic properties of activated carbons.

Despite several studies have addressed the issue of pore shape of activated carbons, contradictory results were obtained. As reported by Kurig et al.,1 not only the widely accepted slit model is suited for describing their pores, as spherical or cylindrical shapes can show better agreement with experimental data. Defining the shape of the carbon platelets entails similar issues. Despite the idea of activated carbons as a collection of graphitic platelets of variable extension has been widely accepted for a long time, the relevance of fullerenic carbon domains has significantly increased in the last years.2,3 Finally, even though plenty of papers can be found addressing the pore shape in activated carbons, very few works are addressing the problem of the three-dimensional organization of the pores in space. The heterogeneity and defective character exhibited especially by industrially activated carbons implies that determining the hierarchical organization of the pores is a challenging task.

In the past years, our team has investigated the structural and surface properties of many activated carbons exploiting an unusually high amount of different techniqyes.2,4–6 By coupling together insights from this multitude of methodologies, we were able to shed light on composition, identity and amount of functional groups, size and shape of carbon domains, etc. The only piece we miss to complete the puzzle is the knowledge about the size and shape of the pores together with their organization on the mesoscale. This contribution is intended to present the first steps moved by our team in the characterization of porosity in activated carbons employing SANS.

This work focuses on two activated carbons of wood origin: CwA is physically activated with steam, while CCh is chemically activated with phosphoric acid. Previously collected data pointed out that the two samples differ in both structure and surface properties.

SANS patterns of the same two samples were collected during a preliminary experiment on D11. The two patterns exhibit clear differences, suggesting that they feature two distinct morphologies on the micro and mesoscale as well as possible different hierarchical organization of pores. Further experiment and advanced modeling will be required to assess these points.

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Contribution ID: **39** Type: **poster contributions**

Interaction of Prohibitin with the inner of mitochondrial membrane

Prohibitins (PHB) are highly conserved heterodimeric proteins composed of two subunits PHB1 and PHB2 arranged to make a multimeric ring at the inner mitochondrial membrane 1. They play a crucial role in premature cellular ageing, tumour suppression, cell cycle regulation, apoptosis, and mitochondrial homeostasis via their function in the intermembrane space (IMS) of mitochondria (between the inner and outer membranes).
Despite the essential role of this complex, little is known regarding its molecular structure and arrangement within the membrane. Initial reports suggest that the formation of the prohibitin complex is influenced by the action of cardiolipin (CL), which is involved in maintaining a particular shape and curvature of the inner mitochondrial membrane [2].
The two main aims of this project are to (i) characterize the interaction between the N-terminal helices of PHB (NT-PHBx) with the membrane and establish a possible synergy of the two PHB homologues, and (ii) understand the role of cardiolipin in this interaction.
To answer these questions, we employ both interface and bulk techniques on simplified model systems, using synthetic peptides corresponding to the transmembrane domains of PHB (NT-PHB, 20-24 residues long), and synthetic or natural mixtures of lipids. As interfacial techniques exploring the solid/liquid interface, we apply Neutron Reflectometry (NR) and Quartz-crystal microbalance with dissipation monitoring (QCM-D). As bulk techniques are used to extruded liposomes we employ Small-Angle Scattering by X-rays and Neutrons (SAXS, SANS).
NR and QCM-D preliminary results suggested a higher tendency of NT-PHB1 of insertion into the membrane in the presence of CL, while NT-PHB2 can remove lipid from the bilayer in absence of CL. Due to the amphipathic character, NT-PHB2 seems to puncture the membrane.
SANS is employed to evaluate the in-solution structure, studying the effect of the peptides on the vesicles, and focusing on the liposomes. Preliminary SANS results show that the peptide induces fusion of the vesicles, from multilamellar to unilamellar vesicles, indicating a tendency of the peptides to disrupt the membrane.

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Contribution ID: **40** Type: **poster contributions**

Hierarchical self-assembly of surfactants and cyclodextrins: from inclusion complexes to responsive supramolecular aggregates

Cyclodextrins (CD) are cyclic oligosaccharides formed by α-(1-4)-D-glucopyranoses linked units. Their unique shape and the presence of a cavity provide particular physicochemical properties, including the ability to form host-guest complexes 1. Cyclodextrin-surfactants host-guest complexes are a flourishing research field due to the availability and diversity of surfactants and the tendency to self-organize into highly ordered structures [2]. Among many surfactants, polyoxyethylene alkyl carboxylic acids (CiEjCH2COOH) are attractive surfactants to integrate these systems as guests due to their pH and thermo-responsiveness [3]. In the last years, a multi-level assembly involving complex building blocks ordering has raised strong interest in many scientific areas. The lattice self-assembly of inclusion complexes relies on strong and directional intermolecular interactions between the CDs involving a delicate balance of forces, producing rigid and complex structures [4].

The formation of inclusion complexes and thermodynamics of complexation of α-CD and β-CD with C12E5CH2COOH and C12E10CH2COOH in aqueous solutions was studied by densitometry and isothermal titration calorimetry (ITC), and a comprehensive structural investigation was conducted by small-angle neutron scattering (SANS), differential scanning calorimetry (DSC) and microscopy. The spontaneous formation of the host-guest complexes and their assembly as building blocks of large supramolecular aggregates with rich structural behaviour was verified.
The results pointed to a remarkable dependence of the structures on the mixing ratio, concentration of the components, and temperature. In addition, by exploring the pH responsiveness property of the surfactants, it was possible to fine-tune the structures and, therefore, control the self-assembly process. The formation of well-layered structures exhibited long-range order in the most concentrated systems with the ionized surfactant, at high pH, featuring multilayered hollow cylinders, whereas rhomboidal crystalline plates are obtained in nonionic systems, at low pH [4]. The analysis also allowed an insight into the effect of the number of ethylene oxide units and CDs features in the formation and topology of the novel aggregates.

In an additional approach, the addition of chitosan to the system revealed a novel parameter for self-assembly control. The polymer addition affects the specific inclusion complexation forces, long-range electrostatic interactions, and dispersion forces within the supramolecular aggregates, influencing the CD-CD hydrogen bonding network.

This work delivers a thermodynamic and structural complementary approach that allows designing supramolecular aggregates of the desired properties with potential applications in a variety of formulations.

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Contribution ID: **41** Type: **poster contributions**

Time dependent kinetic measurements reveal a metastable intermediate phase during protein crystallization processes

The understanding of protein crystallization is of great interest for many areas of biological research. Examples include drug delivery of crystalline substrates and structural biology, which relies on diffraction-quality crystals. Some crystallization pathways are characterized by a one-step process and can be described by classical nucleation theory (CNT). However, for different systems, several steps are visible in the crystallization process resulting in an insufficient description of the crystallization process by CNT. These cases require a more detailed investigation to obtain a comprehensive picture of the underlying mechanisms. Bovine β-lactoglobulin (BLG) in the presence of the divalent salt $CdCl_2$ is characterized by a rich phase diagram. The protein solutions become turbid after crossing a first threshold salt concentration c^* upon further increasing the salt concentration, the solutions become less turbid but not completely clear again (pseudo-c^{**}). Near pseudo-c^{**}, crystallization follows a nonclassical process with a metastable intermediate phase (MIP). Here we explore the MIP in detail with a focus on the structural evolution and the growth kinetics of the MIP prior to crystal nucleation. We present a systematic study using real-time SANS, optical microscopy and neutron backscattering (NBS) to study the protein crystallization process in the presence of a MIP.
Real-time SANS measurements on D11 show that a correlation peak develops inside the MIP, and its peak position shifts to higher q-values with time (see Figure), finally stabilizing at a characteristic length scale of $d_{MIP} \approx 84$ Å. The area of this peak (proportional to the amount of MIP in the sample) first increases with time, reaches a maximum, and then decreases quickly upon crystallization due to consumption by crystal growth. The evolution of the correlation peak indicates a "preordering" nature of the MIP as precursors of crystal nucleation, which lowers the nucleation barrier for subsequent crystallization. These results on structural evolution and the role of MIPs during a nonclassical crystallization process may be relevant for other fields ranging from structural biology to pharmacology.
Literature: R. Maier et al.: "Protein Crystallization from a Preordered Metastable Intermediate Phase Followed by Real-Time Small-Angle Neutron Scattering" Cryst. Growth Des. 2021, 21, 12, 6971−6980

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Contribution ID: **42** Type: **Invited speakers**

Evolution of a HP-SANS cell and its upgrade with a periodic pressure jump unit for soft matter studies

Tuesday, 27 September 2022 11:15 (25 minutes)

Motivated by the patented idea of using scCO2-microemulsions as a starting material for the production of polymer nanofoams 1, we developed a new high-pressure cell together with Ralf Schweins and Peter Lindner in 2006. We were able to demonstrate its functionality in a first test SANS experiment at D11 in March 2007. In this and a series follow-up experiments we could show that scCO2-microemulsions containing water, supercritical carbon dioxide and fluoro-surfactants show similar properties as "classical" water/oil microemulsions [2]. However, using carbon dioxide, one exiting feature of scCO2-microemulsions is, that the solvent quality of scCO2 and hence the overall microemulsion properties, are tuned simply by adjusting pressure. Moreover, due to its large sapphire windows, we were also able to use the HP-SANS cell to study the dynamics of scCO2-microemulsions using NSE [3]. Further, in another study, we discovered that substituting cyclohexane with small amounts of scCO2 allows significant reductions in environmentally harmful fluorinated surfactants. Applying systematic contrast variation SANS, we were able to relate this effect to the formation of a depletion zone of cyclohexane near the fluorinated amphiphilic film [4]. Last but not least, we upgraded the high-pressure SANS cell with a periodic pressure jump system as part of the TISANE project. By combining this unique setup with time-resolved SANS, we were able to elucidate not only the kinetics of pressure-induced structural changes in scCO2-microemulsions [5], but also unravel the swelling kinetics of N-n-propylacrylamide-based microgels using periodic pressure jumps [6].
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Presenter: SOTTMANN, Thomas

Session Classification: Talks

Contribution ID: **43** Type: **poster contributions**

Heavy Metal (Gd - Er to U) loaded Nanoparticles for Indirect Radiation Therapy IRT of Cancer with Photons and Neutrons – SANS, (A)SAXS, Spectroscopy and Treatment Tests

Indirect radiation therapy IRT of cancer uses heavy metals as specific absorbers and local converters of external radiation into cell toxic secondary products, e.g. free radicals. The IRT principle can be applied with neutron and hard X-ray/ gamma photon radiation. Both can be focused by tomographic irradiation methods. The local radiotherapy effect can be enforced, if the heavy element can be deposited specifically in the tumor region by metal nanoparticles.
We have developed three kinds of biocompatible heavy metal nanoparticles: heavy metal liposomes, metal entrapping porous polymers (patent, PLGA), and lanthanide loaded magnetic nanoparticles, e.g.5% Gd, Er in Fe3O4. All metal carriers depicted a size of 100 - 200 nm for high load, bio-compatibility, and upper size limit < 0.5 µm, which avoids embolic problems.
The heavy metal load was adapted to the therapeutic sources according to their radiation spectrum and the human body transmission. For IRT with cold neutrons the optimized result was a double metal loading with Gd and excess Erbium, where the Erbium specifically catches the high energy photons (MeV) from the neutron capture of Gadolinium and converts them to soft X-rays and free radicals over Auger electrons, acting locally at the tumor site. For monochromatic synchrotron radiation (60-120 keV) and clinical LINAC sources Lanthanides of (A>65, Gd-Lu) and heavier elements (Pt, Au, Bi, U) were identified for suitable high body transmission at E > 60keV) by their high K-electron absorption energy and absorption coefficient (“white line” absorption).
The structure and metal load of the heavy metal nanoparticles for IRT, produced at GMP conditions, was investigated by a combination of SANS and DLS at ILL-D11, gamma spectros-copy at ILL-GAMS4-PN3 and by (A)SAXS at ESRF-ID01, DESY and BESSY-9T. Therapy tests with dummies, cancer cell cultures, pig tissue and tumor-rats where performed with neutrons at ILL-D22 with EMBL/CIBB Grenoble, with LINAC-source photons at the radiooncology clinics Gutenberg University Mainz, and monochromatic synchrotron photons at ESRF-ID17 with BioMedical facility BMF. The development resulted in a palliative treatment method for primary glioblastoma, which may be developed to a permanent healing method for other cancer types.

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Contribution ID: **44** Type: **not specified**

Structure Dynamics of the Energy Conversion Proteins ATP-Synthase and F1ATPase: From SANS at ILL-D11 to time resolved SAXS during reaction cycle at ESRF-ID02

Bio-energy converting membrane proteins couple the transport of material across a membrane, e.g. protons, with the reversible formation or cleavage of an energy rich chemical bond (ATP). Thus local energy is stored and available in the cell lumen or tissue, by temporal energized protein state.

The most common energy transfer protein ATP-Synthase (M = 500 000) and its catalytic head F1ATPase was studied by SANS at ILL-D11, -D22 and FZ Jülich, and SAXS at DESY Hamburg, ELETTRA Trieste and ESRF-ID02 and –ID01. Already the SANS of bacterial F1ATPase starting 1978 at ILL-D11 (fig. a) and DESY-EMBL depicted a highly organized but flexible hollow structure of segregated subunits, which results in SANS and SAXS side maxima. The structure is dynamic, as the side maxima change position and height by functional changes of the enzyme. Details were resolved by crystallography of resting F1ATPase by Walker (Noble award 1997). But the mechanism of reversible energy conversion in the ATP reaction cycle remains unknown.

Our studies of the flexible structure of F1ATPase and ATP-Synthase in detergent solution with SANS at ILL-D11 and D22, and SAXS at DESY, ELETTRA and ESRF depicted rearrangements of the subunit complex upon regulatory states and inhibition, e.g. by temperature, pH and azide. ATP-Synthase was reconstituted into liposomes, and with Bacteriorhodopsin or caged acids for light-induced energization. After the very first SANS of D-contrast matched proteo-liposomes with ATP-Synthase at FZ Jülich, our studies in energized liposomes, at membrane ΔpH>1 by time-resolved SANS at ILL-D22 depicted temporal energetic structure changes by Rg-changes.

The structure dynamics of the F1ATPase in the reaction cycle was investigated by time resolved SAXS upon ATP activation by stopped-flow, and flash photolysis (caged ATP). A tour through EU-synchrotrons lead from first success at ELETTRA Trieste to ESRF-ID02, and contributed later to the DESY-PETRA P12 setup. Fig.c depicts cyclic dynamics of working F1ATPase in subsequent ATP reaction cycles at 1013 ph/s with He-jet cooling, triggered by stopped-flow mixing (Rg-changes T-depended). The results could trigger the development of novel energy conversion materials with improved efficiency, e.g. chimeric polymer-protein systems.

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Presenter: Dr NAWROTH, Thomas (Gutenberg University Mainz)

Contribution ID: **45** Type: **poster contributions**

Drug-Lipid Structure Development upon Oral Drug Delivery in simulated Intestine - Time resolved SANS and DLS

The active substance resolution in oral application of badly soluble drugs of the BCS classes 2 and 4 depends on the drug interaction with micelles and liposomes formed from bile and pharmaceutical formulation in the duodenum part of the small intestine. During the passage of the second duodenum half, i.e. after bile influx, the native and drug lipid nanoparticles depict a sequence of structure conversions from 1 nm micelles to 100 nm liposomes, additionally to cholesteric phase particles of some 10 µm size. The success of the pharmaceutical product depends on the kinetic and structural interaction with the different lipid phases, forming the uptake-competent drug-excipient complex. At ILL-D11 we have developed a method of time resolved estimation of those wide size spectrum particle samples by parallel application of SANS and DLS, both with time resolution of the suspensions in a model system (Gastro-Intestinal Simulator GISim). The dynamic sample, which represents the fluid in the second half of the Duodenum after influx of bile, was produced by rapid mixing of pre-diluted bile ("FeSSIF") with drug-lipid suspension in buffer solution (transfer medium TM), forming the late intestinal fluid "FaSSIF" with a stopped-flow device (HiTech Scientific UK). The sample is injected into a flow-through SANS cuvette (2 mm). A trigger signal starts the SANS detection film at D11, and the estimation of the DLS sequence film by a controller. The SANS and DLS beams meet at the same point of the flow cell. The SANS operates in transmission (foreward scattering. 0-30°), but the DLS in backscattering mode (173°, non invasive back scattering "NIBS" from the front 100 µm sample layer) using a dual beam projecting DLS device (ProSpecD, Nanovel). By the novel method intermediates during the structural transition of the intestinal fluid upon addition of pharmaceutical solution were detected. The particle size scale was extended by the method combination to 1nm – 100µm in parallel, in this case of micelles, liposomes and cholesteric particles. The method is used for the study of pharmaceutical nanoparticles.

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Presenter: Dr NAWROTH, Thomas (Gutenberg University Mainz)

Contribution ID: **46** Type: **poster contributions**

Structure Detail Resolution of Pharmaceutical Drug Carriers by Contrast Variation: Deuterium-SANS and (A)SAXS

Pharmaceutical nanocarriers are complexes composed of frame materials, e.g. lipids or polymers, and medically active materials, such as bio-chemical drugs or biological agents, e.g. proteins or mRNA. The structure is the key to the medical application and safety. The formulation depends on the application pathway, which may be oral (tablets, capsules), pulmonary (inhalation), intramuscular (tissue injection), parenteral (blood injection), or intracranial (brain injection). Success, patient security and structure issues increase in this sequence.

The structure determination by solution scattering and imaging of neutrons and synchrotron X-rays is enforced by specific component labeling by contrast variation, i.e. deuteration in SANS, magnetic material scattering, or heavy metal scattering, absorption and fluorescence (ASAXS, imaging), in combination with DLS as µm size range extension. The neutron contrast variation of pharmaceutical and bio-medical samples in solution follows two strategies: solvent deuteration, mostly with D2O, or material deuteration, e.g. of lipids, proteins or mRNA.

We have investigated the structure and development of pharmaceutical nanocarriers in original form (static) and upon simulated application (dynamic, space-time resolved) by contrast labeling via selective deuteration and lanthanide complexes. The studies were done by SANS (ILL-D11, MLZ-KWS2), and SAXS, ASAXS (DESY-EMBL-P12, ESRF-ID01, BESSY-SAXS-9T) with lipid and polymer frame carriers and surface modification by an artificial protein shell for specific biotargeting, e.g. in cancer therapy. The application of the complementary neutron and synchrotron X-ray methods combines the detection of deuterated lipids and mRNA without radiation damage with high resolution scattering, focusing and flux.

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Presenter: Dr NAWROTH, Thomas (Gutenberg University Mainz)

Contribution ID: **47** Type: **poster contributions**

Surface coating of Pharmaceutical Nanoparticles with SH-Proteins for Site-directed Drug Targeting and Radio-Therapy – Time-resolved SANS of Deuterium-matched Carriers

Nanoparticles circulating in the human blood depict a protein corona [Tenzer et al.]. This principle can be used for site specific drug targeting by receptor recognition after attachment of an artificial specific protein corona to drug loaded nanoparticles, lipoplexes, liposomes and polymers, which contain a protein-binding anchor component, and the therapeutic drug or mRNA.
We have studied the surface protein coating of PLGA polymer particles (w/o/w double emulsion) and liposomes bearing an activated binding thiol-component by coupling with proteins containing a SH-group. The Thiol-activated anchor component was synthetized from Amino-lipid, cholesterol or PLA-derivative (L. Krebs, Nanovel). The proteins for surface coating contained a SH-group by nature (BSA, HSA), or were equipped with this by conversion of a surface Lysine to a SH-derivative by Trout's reagent. The studied nanoparticle contained 2% of anchor group embedded in a host matrix of lecithin (DMPC, DOPC) or polymer (PLGA). The drug loads were hydrophobic drugs of the BCS classes 2 and 4 (Fenofibrate, Curcumin, Amphotericin B) or Lanthanide chelates (Gadolinium, Erbium, Lutetium -DTPA) as radiation absorber for indirect radiotherapy of cancer with photons (PT) or neutrons (NCT).
The drug nanoparticles were studied at ILL-D11 with SANS and DLS at site (same cuvettes). The particle structure details were distinguished by D2O-contrast variation. The protein surface coating process, i.e. the formation of a sulfur-bridge between activated anchor component and thiolated protein was studied with time resolved SANS of D2O-contrast matched PLGA nanoparticles with 2% activated PLA-anchor "P4". The size of the foam-like PLGA nanocarriers (100 nm) and the smaller proteins (BSA, SH-BSA, SH-Transferrin) required a SANS double shot strategy with cross-like distance changes (2m, 8m, 34m) after stopped flow mixing of the components (activated nanoparticle and protein solutions). As result the coupling was detected structurally in a time regime of 2h with sliding resolution. The result is important for the medical application, where the person and/or tissue specific protein or antibody coating can be attached to preformed drug/mRNA nanoparticles (stock) in the studied time window before the patient application.

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Presenter: Dr NAWROTH, Thomas (Gutenberg University Mainz)

Contribution ID: **48** Type: **not specified**

Funtionalized Lipid and Polymer Nanoparticles for BioMedical Application and Cancer Radiotherapy: Synthesis, SANS and DLS

Modular targeting materials bearing a specific ligand head can supply a cell or tumor receptor recognition to radiotherapy enhancers, hydrophobic drugs (BCS classes 2, 4) or mRNA, entrapped in nanoscaled drug carriers, e.g. liposomes, micelles and polymer particles. This drug / co-drug complex concept requires the synthesis of special modular targeting materials.
We synthesized targeting modifiers of oral drug nano-intermediates and parenteral drug loaded nanoparticles which consist of four structure domains (fig.1) with lipid or hydrophobic polymer anchors (Fig.1, left). The components are varied and optimized in a case specific manner. The nanoparticles, e.g. intestinal lipid-bile nanoparticles, biodegradable polymer (PLGA), lipid particles as well as the anchor domain are hydrophobic, while iron oxide can be included for bio-medical manipulation. With proteins as ligands, e.g. transferrin or albumin, the surface bound protein is transformed to an artificial membrane protein. The linker binds the ligand in two steps: adsorption and a fast covalent bond formation as terminal step. The hydrophilic spacer is essential for keeping the distance from the nanoparticles surface.
The nanoparticle anchor groups were amino-lipids (DMPE, Stearylamine), Cholesterol, and PLA derivatives with amino or carboxy headgroups. A thiol-linker was attached as S-S-dimer through diamino- and peptide spacers with DCCD catalysis. The synthesis strategy avoided expensive protective groups by two-side block synthesis, with late coupling of the halfes. Finally the S-S-dimer was cleaved before activation of the thiol-group for protein coupling by a sulfur bridge.
The structure of modified nanoparticles bearing 2% activated anchor was analyzed by dynamic light scattering DLS, neutron small angle scattering SANS with D2O-contrast variation and metal specific X-ray scattering ASAXS. The biomedical effect of the drug is proven in cell culture tests. The multi-targeting modification is applied to lanthanide loaded polymer nanoparticles (PLGA, patent of the Gutenberg-University) for indirect radiation therapy IRT and liposomes as fast development system.

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Presenter: Dr NAWROTH, Thomas (Gutenberg University Mainz)

Contribution ID: **49** Type: **poster contributions**

Parallel SANS/SAXS and DLS at nm - µm Scale: Quantitative and Experimental Strategy for Pharmaceutical Nanoparticles and Polymers

Biological, polymer and medical samples may depict a wide particle size spectrum from nm to µm scale. The particle structure in solution can be studied without radiation damage by SANS up to 1 µm size (ILL-D11, 30m distance, 15Å), and at high intensity by SAXS. The particle size distribution is available by dynamic light scattering DLS, while this requires with concentrated original samples of SANS and SAXS the application at backscattering (173°; NIBS , No-Invasive Back-Scattering) and focusing to the front layer of the sample to avoid multiple scattering and special optics.
At ILL-D11 we have developed a strategy, setup and theory for a quantitative SANS/SAXS-DLS coupling. The SANS/SAXS beam and the laser of DLS hit the same point of a quartz cuvette/capillary. The DLS laser beam (Tm00) is focused to the 100 µm front layer of the cuvette to avoid multiple scattering. The DLS size range is extended from the usual 5µm to >100 µm by a special long focus (150 mm) optics in a dual optical bench device (Nanovel ProSpecD). In structure dynamics applications SANS and DLS are operated time resolved (SANS-DLS film).
The evaluation of SANS and DLS data is done following the same principles and scaling: The raw DLS data IDLS(r) represent the amount of scattering yielded by the particle size spectrum r. Here the large particles are tremendously over-estimated by the dependence of IDLS(r) on r6. The evaluation of the contributions with respect to mass contribution Cm(r) requires a scaling according to the particle type, as usual in SANS and SAXS in the Guinier- and Kratky-Porod-plots for spherical, flat / liposomal or stick-type particles. A theory and formula set for quantitative DLS in parallel to SANS/SAXS with pharmaceutical nanoparticle examples, and optics setup calculation is presented.

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Presenter: Dr NAWROTH, Thomas (Gutenberg University Mainz)

Contribution ID: **50** Type: **Invited speakers**

Science Director's Welcome

Monday, 26 September 2022 08:45 (15 minutes)

Primary author: JESTIN, Jacques

Presenter: JESTIN, Jacques

Session Classification: Talks

Contribution ID: **51** Type: **Invited speakers**

Using X-ray and neutron scattering to analyze nanoparticles for drug and RNA delivery

Monday, 26 September 2022 09:50 (25 minutes)

Primary author: HAAS, Heinrich (BioNTech AG)

Presenter: HAAS, Heinrich (BioNTech AG)

Session Classification: Talks

Contribution ID: **52** Type: **Invited speakers**

Polarised neutron scattering from dynamic polarised nuclei.

Monday, 26 September 2022 10:50 (25 minutes)

It was in September 1972 when Konrad Ibel and myself put a solution of sperm whale myoglobin into the sample chamber of D11. To our great surprise it was after a few seconds of irradiation by thermal neutrons – I think the A-selector was not yet in place – when a beautiful central peak of scattered neutron intensity emerged on the screen, the first picture of neutron small-angle scattering with D11.

The was also the beginning of neutron small-angle scattering from macromolecules in mixtures of heavy water, D2O, and H2O. The large difference in the scattering lengths of the isotopes 1H (=H) and 2H (=D) has been beneficial for studies of composite structures like membranes, nucleoproteins, lipoproteins and viruses. The demand of beam time largely exceeded the time available at D11.

At the same time Hayter, Jenkins and White (Physical Chemistry Laboratory Oxford) came up with a method using the spin dependence of the interaction of polarised neutrons with polarised protons. The variation of the scattering length b with proton polarisation largely exceeds that obtained with isotopic substitution. No echo for a long time.

About a decade later, a growing interest of neutron scattering from dynamic polarised bulk protons in macromolecules developed, mainly triggered by the introduction of glassy hydrogenous substances as polarized target material in high energy physics (reviewed by Niinikoski, 2013). The selective depolarisation of dynamically polarised proton spins or deuteron spins by the method of adiabatic fast passage (AFP) in specifically deuterated ribosomal particles has been extensively used in polarised neutron small-angle scattering in collaboration with CERN (Knop et al. 1986, Willumeit et al. 1996). This method which became known as nuclear spin contrast variation has also found numerous applications in structural studies on polymers (Koghi et al. 1987, Glättli et al. 1989, Kumada et al. 2010). This work was done outside the ILL.

What about the evolution of proton polarisation at the onset of microwave irradiation? The answer could be interesting with radical proteins, like tyrosyl doped catalase. The study of free radicals of different size would help to find an answer. On that substantially enlarged basis a Swiss-French-German collaboration was established. The polarised target facility from PSI was temporarily installed at the instrument D22 of the ILL. In fact, the results from solutions of free radicals were quite clear. The creation of a local proton polarisation in the vicinity of an unpaired electron is followed by its diffusion into the bulk. The barrier confining the domain of local polarisation is identical with the molecular surface of small free radical molecules dissolved in a deuterated solvent. With larger free radical molecules an intramolecular magnetic spin diffusion barrier cannot be ignored.

Now let us turn to catalase. This enzyme converts hydrogen peroxide incredibly fast into water and oxygen. Replacing one of the hydrogens of the H2O2 by CH3CO this derivative is accepted by catalase like H2O2 but treated in a quite different way: first, the response is slow and, second, after some intermediate steps, one of its amino acids, tyrosine, is converted to a tyrosyl radical. The number of tyrosyl radicals created in this way is small, typically less than one among the 500 amino acids of one of the four subunits of catalase molecule. The contribution of a small domain of reasonably strong polarised protons near a tyrosyl radical to the polarisation dependent scattering intensity is expected to be small. The direction of DNP has been changed several thousand times in

order to obtain the polarisation dependent scattering intensity of only 1/1000 of the total intensity with a sufficient accuracy. The unpaired electron is probably that of the tyrosines fairly close to the centre of the catalase molecule (Zimmer et al. 2016).
A more sophisticated version of time-resolved neutron scattering using the inversion of the proton polarisation by AFP appears to confirm the existence of the tyr-369 radical in agreement with an earlier analysis of the EPR of tyrosyl doped catalase (Hautle et al. manuscript in preparation).

Primary author: STUHRMANN, Heinrich (retired)

Presenter: STUHRMANN, Heinrich (retired)

Session Classification: Talks

Contribution ID: **53** Type: **not specified**

Ever higher magnetic fields, ever larger magnetic structures (remote)

Monday, 26 September 2022 16:20 (25 minutes)

A magnetic field is one of the many tools that we can use to tune or adjust materials. In some cases, this is through the very direct coupling to atomic magnetic moments, giving rise to new structures. In other cases, the interaction is on the microscopic scale, for example, the rotation or growth of magnetic domains over a wide range of length scales. Some materials do not have direct magnetic degrees of freedom, but due to their shape can still respond to the direction imposed by a magnetic field. In this talk, I will show how this tool, the magnetic field can been used to control what appears in the small angle scattering domain.

Primary author: BLACKBURN, Elizabeth (Lund University)

Presenter: BLACKBURN, Elizabeth (Lund University)

Session Classification: Talks

Contribution ID: **54** Type: **not specified**

D11 & Small Angle Neutron Scattering – A Paradigm of ILL (remote)

Tuesday, 27 September 2022 09:00 (25 minutes)

D11 at the ILL Grenoble is an exceptional tool for diverse areas of European and worldwide science and technology. Its value stems from the pioneering work of Springer, Schmatz and Ibel, (1,2) and the quality of a sequence of "instrument responsibles", technicians and users since 1972. Long wavelength, well collimated neutron beams has been a success everywhere. I will touch on some pleasant examples of our experiences:

1973 at the start of biological work- Collagen and Tobacco Mosaic Virus- with Andrew Miller and Peter Timmins,
1974 the first spin echo instrument- with Ferri Mezei, -
1979 the Deuxieme Souffle,
2009 Saving a Figaro experiment with Jared Raynes, Peter Lindner,
2015 Australian High Court re. what is an emulsion ?-with Andrew Jackson,
20o22 Current USANS from Emulsions on Kookaburra, ANSTO with Liliana de Campo, Kevin Galvin.

Many people have participated in other major work at ILL including John Hayter, Maurice Leslie, Graham Jenkin, Robert Thomas, Jeff Penfold, Ron Ghosh, Karen Edler. I am glad to acknowledge them.

(1) J. Mol. Bid. (1969) 41,231-236 Neutron Small-angle Scattering from Aqueous Solutions of Oxy- and Deoxyhaemoglobin R. SCHNEIDER, A. MAYER Physik-Department der Technischen Hochschule, Miinchen, Germany W. SCHMATZ, B. KAISER AND R. SCHERM Institut fiir Festktirper- und Neutronenphysik der Kernforschungsanluqe Julich, Germany (Received 15 November 1967, and in revised form 1 January 1969)
(2) Theory of a velocity focussing instrument for neutron small angle scattering" K Ibel, W. Schmatz, T Springer, Kernphysik und Kernchemie, Atomkernenergie 17, 13-18, 1971

Primary author: WHITE, John W.

Presenter: WHITE, John W.

Session Classification: Talks

Contribution ID: **55** Type: **not specified**

Interpreting simultaneous small-angle neutron scattering and reflection from surfactant stabilised air-water foams

Tuesday, 27 September 2022 12:05 (25 minutes)

Air-in-water foams stabilised by surfactants and polymers have been the subject of much recent debate due to their ubiquitous occurrence, desirable or otherwise. When examining such hierarchically structured and dynamic materials using neutron techniques, the complex patterns observed are often discussed in terms of a superposition of on- and off-specular scattering and reflectivity arising from the air/water interfaces and any (self-assembled) structures within the sample. Here, we present such data from foams stabilised by surfactant multi-layers comprising sodium lauryl ether sulfate/sodium dodecylsulfate blends in the presence of multi-valent salts (AlCl3, CaCl2). Concurrently, we demonstrate how the absolute intensities, the incoherent backgrounds and the transmissions can be used to determine the thickness of the liquid films within the beam, and thence, the liquid volume fraction in the foam. Together with literature data, and with additional contrast variation data, we re-interpret our previously published data and highlight some correlations between surface structure / composition and foam stability.

Primary author: GRIFFITHS, Peter Charles

Co-authors: MANSOUR, Omar; HILL, Christopher; ALBA VENERO, Diego; SCHWEINS, Ralf; DALGLIESH, Robert

Presenter: GRIFFITHS, Peter Charles

Session Classification: Talks

Contribution ID: **56** Type: **not specified**

Small-angle scattering from proteins: Crowding conditions and phase transformations (remote)

Tuesday, 27 September 2022 14:00 (25 minutes)

Protein solutions can exhibit rather complex behavior, in particular at high concentrations, i.e. “crowding” conditions.
For a comprehensive understanding of the structures,
from the molecular level to oligomers to larger-scale structures arising, e.g., in phase separating systems,
small-angle scattering plays a crucial role. This is also the basis for the interpretation of the associated dynamics
as well we kinetic effects. We discuss examples for the crucial role of small-angle scattering, particularly for the kinetics of phase transformations such as liquid-liquid phase separation and phenomena related to crystallization.

Primary author: SCHREIBER, Frank (University of Tübingen)

Presenter: SCHREIBER, Frank (University of Tübingen)

Session Classification: Talks

Contribution ID: **57** Type: **not specified**

D11 and the microgel's softness, a long standing story with a bright future

Tuesday, 27 September 2022 14:25 (25 minutes)

In this talk, I will discuss the fundamental contribution of small-angle neutron scattering - in particular of D11 - in the understanding of the properties of both individual microgels and of the macroscopic properties of microgel suspensions. We will discuss the use of SANS for the characterisation of the architecture of individual microgels. Then we will focus on the use of contrast variation to determine the microgel bulk modulus and the response of individual microgels to crowding.

Primary author: SCOTTI, ANDREA

Presenter: SCOTTI, ANDREA

Session Classification: Talks

Contribution ID: **58** Type: **Invited speakers**

The use of SANS in optimising pharmaceutical formulation

Wednesday, 28 September 2022 09:00 (25 minutes)

Nanosuspensions are sub-micron-sized colloidal dispersions of nano-sized drug particles stabilised by surfactant and/or polymer. Nanosuspensions are of considerable interest as a means of solving the problems of poor water solubility and low bioavailability exhibited by many drugs, and which pose significant challenges for the preparation of a medicine for patient use. Despite the fact that there are an increasing number of commercially available nanosuspensions, it is still not possible to make a rational selection of the stabilising polymer/surfactant. To gain this understanding we have performed small-angle neutron scattering (SANS) measurements in combination with isotopic substitution of the aqueous solvent on a range of drug nanosuspensions wet-bead milled in the presence of a number of different hydrophilic polymers of varying molecular weight and, in some instances, in the presence of surfactant. The layer thickness and amount of the absorbed polymer was determined to be insensitive to the molecular weight of the various polymers indicating that the adsorbed layer was lying relatively flat on the various drug particle surfaces. In contrast, however, SANS studies revealed that the amount adsorbed and the thickness of the polymer layer was dependent on both the nature of the hydrophilic polymer and the nature of the drug. The insensitivity of the adsorbed polymer layer to polymer molecular weight has important implications for the production of nanoparticles, suggesting that lower molecular weight polymers should be used when preparing nanoparticles by wet-bead milling, since nanoparticle formation is then more rapid but with no likely consequence as regards the physical stability of the resultant nanoparticles.

Primary author: LAWRENCE, Jayne

Presenter: LAWRENCE, Jayne

Session Classification: Talks

Contribution ID: **59** Type: **not specified**

Isotropic and anisotropic SANS from polymer systems

Wednesday, 28 September 2022 09:25 (25 minutes)

I will try to tell you a story about our hour after hour life – with mixture of stress and pleasure to be by the side of this beautiful leading machine, building a special relationship as D11 co-users, with different colleagues along my career. It actually started here!
This should cover different science cases, where D11 was useful in different ways: polymer gels, stretched polymers/reptation, stretched networks/rearrangements, sheared solutions, nanocomposites (stretched also…), polyelectrolytes, electrostatic complexes…This implied several local contacts invaluable support, too: Radulf, Robert, Peter, Adrian, Isabelle, Sylvain, and Ralf…

Primary author: BOUÉ, Fraançois (Laboratoire Léon Brillouin)

Presenter: BOUÉ, Fraançois (Laboratoire Léon Brillouin)

Session Classification: Talks

Contribution ID: **60** Type: **Invited speakers**

Visualisation of morphological changes in Soft Matter Systems via SANS contrast variation at the D11

Wednesday, 28 September 2022 09:50 (25 minutes)

The striking difference in the scattering length density of H and D offers a chance to vary or tune the neutron scattering contrast of selected components in complex systems while retaining the chemistry of the systems. Such contrast variation in turn provides unique opportunities for structural analysis in the field of Soft Matter not accessible to other scattering techniques like for instance to investigate the structure of particles in distinct matrices or to analyse the shape and distribution of a component or compartment within a particle. The present contribution reports on three typical examples of a successful application of the concept of contrast variation carried out with D-11. The first example presents a model analysis on aspects of cellular crowding via an investigation of the impact small colloidal particles at variable concentration exert on the size and shape of macromolecules in dilute solution. SANS demonstrated for the first time that small colloids induce a shrinking of the coil dimensions of macromolecules.1 The second example presents an investigation of double hydrophilic block copolyelectrolytes forming micelles at high and low temperature. SANS could locate the two blocks within the micelles at either temperature and revealed full inversion of the micelles along the temperature variation.2 The third example, establishing the most recent project, presents a study on mixed micelles formed from DTAB as a typical cationic surfactant and an anionic azo-dyestuff. SANS succeeded to locate the dyestuff within the co-assembly of the two components.

1. Kramer, T.; Schweins, R.; Huber, K. Macromolecules 2005, 38, 9783-9793
2. Carl, N.; Prevost, S.; Schweins, R.; Houston, J. E.; Morfin, I.; Huber, K. Macromolecules 2019, 52, 8759–8770

Primary author: HUBER, Klaus (Professor at University of Paderborn)

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Session Classification: Talks

Contribution ID: **61** Type: **not specified**

SANS studies of polymer structure in nanocomposites

Wednesday, 28 September 2022 11:40 (25 minutes)

As compared to other techniques of analysis of nanostructures, small-angle neutron scattering has always been way better in terms of design of special contrast situations, and worse for statistics due to inherently low flux. SANS beamlines at ILL, and in particular D11 dedicated to soft matter studies, have allowed to keep the first advantage, while providing excellent experimental conditions respect to, including with respect to flux.
In this talk, I will present some recent studies of polymer structure in nanocomposites. Such materials have striking mechanical and dynamical properties, in particular the dynamics of the polymer close to the nanoparticles has triggered a large body of experimental and theoretical studies. The possible slow-down of the polymer corresponds to higher moduli, and the percolation of any hard phase, particles or slowed-down polymer, has a strong impact on the macroscopic mechanical properties. If one wishes to specifically characterize the structure of the polymer, SANS is one of the best options. By blending hydrogenated and deuterated chains, while matching the filler silica nanoparticles, we have recently provided evidence for chain-mass dependent bulk or interfacial segregation, and modelling and experimental results will be critically reviewed. In a second study, we have characterized the particle dispersion by small-angle scattering and reverse Monte Carlo modelling, and used it to improve the determination of the thickness of the polymer interfacial layer seen by broadband dielectric spectroscopy. Both the general nanoparticle dispersion and the characteristic time of this interfacial layer has been shown to be tunable by surface modification, paving the way for a precise control of mechanical properties of polymer nanocomposites in the future.

Primary author: OBERDISSE, Julian

Presenter: OBERDISSE, Julian

Session Classification: Talks

Contribution ID: **62** Type: **not specified**

Small Angle neutron Scattering and Polymer science (remote)

Wednesday, 28 September 2022 12:05 (25 minutes)

50 years ago, polymers were well established materials, but there were a number of crucial questions open to relate molecular to material properties. It was already 50 years since Herman Staudinger had proposed that plastics were composed of long chain molecules and 20 years since Paul J. Flory described long chain molecules as random walks where dimensions increase as the scare root of mass. Both of these won Nobel prizes for their work and it was accepted that the material properties of plastics such as elasticity and viscoelasticity were determined by their long chain nature. However no direct experimental evidence for Staudinger and Flory had been observed. It was understood that small angle scattering would provide the link if a labelling technique were available. Given the large content of hydrogen, deuteration would be ideal if SANS instruments could provide a high enough count rate. Enter D11 and in 1973 the random walk nature of a single polymer molecule in a melt was demonstrated by several groups. Rapidly afterwards SANS experiments showed many other examples of the molecular basis for plastic behaviour such as the deformation and then relaxation of molecules in stretched samples.

Primary author: HIGGINS, Julia S.

Presenter: HIGGINS, Julia S.

Session Classification: Talks

Contribution ID: **63** Type: **Invited speakers**

Small-angle scattering from proteins: Crowding conditions and phase transformations

Protein solutions can exhibit rather complex behavior, in particular at
high concentrations, i.e. “crowding” conditions. For a comprehesive understanding of the structures,from the molecular level to oligomers to larger-scale structures arising, e.g., in phase separating systems,small-angle scattering plays a crucial role. This is also the basis for the interpretation of the associated dynamics as well we kinetic effects.

We discuss examples for the crucial role of small-angle scattering, particularly for the kinetics of phase transformations such as liquid-liquid phase separation and phenomena related to crystallization.

Primary author: Prof. SCHREIBER, Frank (University of Tübingen)

Presenter: Prof. SCHREIBER, Frank (University of Tübingen)

Session Classification: Talks

Contribution ID: **64** Type: **Invited speakers**

Isotropic and anisotropic SANS from polymer systems

I will try to tell you a story about our hour after hour life – with mixture of stress and pleasure to be by the side of this beautiful leading machine, building a special relationship as D11 co-users, with different colleagues along my career. It actually started here!
This should cover different science cases, where D11 was useful in different ways: polymer gels, stretched polymers/reptation, stretched networks/rearrangements, sheared solutions, nanocomposites (stretched also…), polyelectrolytes, electrostatic complexes…This implied several local contacts invaluable support, too: Radulf, Robert, Peter, Adrian, Isabelle, Sylvain, and Ralf…

Primary author: BOUÉ, Fraançois (Laboratoire Léon Brillouin)

Presenter: BOUÉ, Fraançois (Laboratoire Léon Brillouin)

Session Classification: Talks

Contribution ID: **65** Type: **not specified**

Conference photo

Monday, 26 September 2022 15:15 (10 minutes)

Session Classification: Talks