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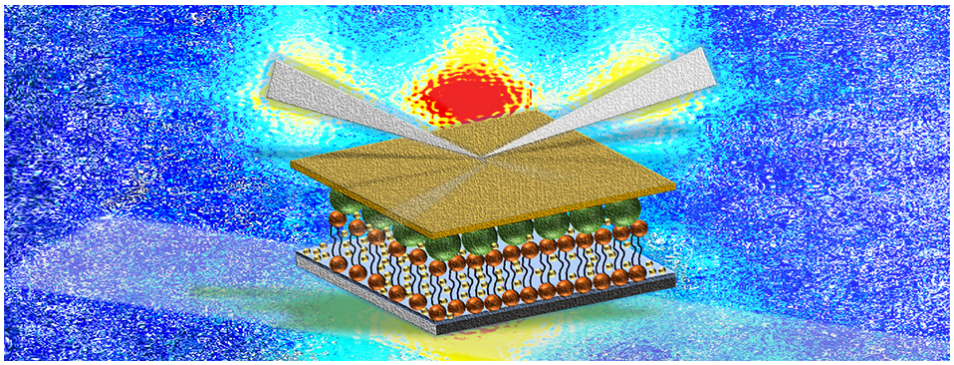

Buch der Abstracts

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Curvature induced phase separation in lipid bilayers: A structural and compositional perspective

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Curvature induced phase separation in lipid bilayers: A structural and compositional perspective
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The cellular membranes posses a range of different type of curvatures, with many biological processes occurring under curvature as high as 1/R = 1/20 nm-1. There is experimental evidence that curvature should induce phase separation in lipids mixtures including those with melting points above and below the experimental conditions [1–3], and for lipid mixtures containing low and high intrinsic curvature lipid types [4]. Such knowledge is based on fluorescence microscopy or molecular simulation data and little does it reflect the actual lipid composition or the structure of such membranes. The correlation between nanoscale membrane curvature and phase separation is a crucial point for understanding of membrane functionality. That is pivotal across a spectrum of applications, encompassing drug delivery and beyond.
In the present study, the curvature-induced phase separation for lipid mixtures containing low (phosphatidylcholine) and high intrinsic curvature (cardiolipin) lipid types was investigated by neutron reflectometry. The distinctive aspect of neutron reflectometry lies in its capability to reveal coexisting planar and curved model membranes, whereas small-angle neutron scattering allows us to study membranes with single curvature.
Here the "diffracting scaffolds"formed by SiO2 nanoparticles (NPs) ranging from 200 to 50 nm in diameter [5] were used to deposit a continuous, supported lipid bilayer (SLB) on both the SiO2 NPs and the flat regions in between these NPs [6]. In the given work, a clear compositional difference was shown between planar and curved regions of the nanoSLB prepared by solvent depletion as well as vesicle fusion methods. Moreover, selective lipid deuteration provided direct evidence of a curvature degree effect on lipid phase separation, which is critical for membrane functionality, as well as a very first characterization of the structure of the coexisting flat and curved bilayers. These models and protocols are now available to study a range of systems that will enable mapping the relationship between biological function and membrane structure under curvatures that are relevant in membrane biophysics.

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Neutron Scattering as diagnostic tool to investigate the molecular interactions at lipid nano-biointerfaces

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Biointerfaces describe the areas of making contact with biological environments, such cells, tissues, living organisms, bio(macro)molecules or organic/inorganic materials. Nano-biointerfaces are being mimicked by various models which allow studying important components of cell-life, hence permitting to reproduce various structural conditions [1], such as the architecture of plasma or bacterial membranes to monitor their interactions with guest molecules, the vesicle fusion intermediates, as well as the tubular cell-to-cell communicational connections.
The investigation of the structural organization and the molecular interactions occurring at the nano–biointerfaces level in controllable manner remains challenging due to analytical complexities and limitations. In this context, Neutron Scattering techniques represent powerful tools to shed light onto molecular features of functional nano-biointerfaces and their function with guest molecules, such as ions, proteins and peptides, oligonucleotides, antibodies and/or nanoparticles, thus involved into many molecular recognition processes.
Here, an overview of the main results obtained through Small-Angle Neutron Scattering (SANS) and Neutron Reflectometry (NR) measurements will be presented to show the powerful opportunity offered by them to describe the structural organization of lipid nano-biointerfaces biomimicking plasma or outer membranes of Gram(-) bacteria [2]. In this way, the type of nano-biointerfaces, such as lipid vesicles or supported lipid bilayers, as well as the nature and relative content of lipids, such as zwitterionic or anionic bi- or multi-chained phospholipids, sterols/hopanoids and lipopolysaccharides (LPS), resulted decisive in influencing the interaction with different bioactive molecules like antimicrobial peptides and oligonucleotides involved into specific biorecognition processes [2]. SANS and NR analyses allowed to shed light on the molecular interactions and binding affinity with specific portions (i.e., hydrophobic or hydrophilic region) of each lipid molecule, thus contributing to define the mechanisms occurring at molecular level and, consequently, the functional activity of such biomolecules.

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Timescales of Cell Membrane Fusion Mediated by SARS-CoV2 Spike Protein

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We investigated the SARS-CoV2 membrane fusion timescale by means of small-angle neutron scattering (SANS) using hydrogen/deuterium contrast variation. After the successful production of virus-like vesicles and human- host-cell-like vesicles we were able to follow the fusion of the respective vesicles in real-time. This was done using deuterated and protonated phospholipids in the vesicles in a neutron-contrast matched solvent. The vesicles were identical apart from either the presence or absence of the SARS-CoV2 spike protein. The human host-cell-like vesicles were carrying an ACE2 receptor protein in all cases. In case of the absence of the spike protein a fusion over several hours was observed in agreement with literature, with a time constant of 4.5 h. In comparison, there was not time evolution, but immediate fusion of the vesicles when the spike protein was present. Those two figures, fusion over several hours and fusion below 10 s corresponding to the absence or presence of the spike protein allow an upper-limit estimate for the fusion times of virus-like vesicles with the SARS-CoV2 spike protein of 10 s. This very fast fusion, when compared to the case without spike protein it is a factor of 2500, can also help to explain why infection with SARS-CoV2 can be so effective and fast. In order to access very short timescales we also performed continuous flow experiments, which support the stopped flow and static experiments. This fusion process could be strongly influenced by a promising drug candidate, which inhibited the fusion process.
In addition to the time-resolved contrast matching SANS experiments we also performed neutron-spin echo experiments to investigate the dynamics of the membrane during the fusion process, which show an increased diffusion constant in the size regime of the spike protein.
Studying spike protein variants using our method may explain differences in transmissibility between SARS-CoV2 strains. In addition, the model developed here can potentially be applied to any enveloped virus.

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NR determination of the structural profile of asymmetric myelin membranes and their interaction mechanism with Myelin Basic Protein (MBP)

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Myelin, an asymmetric multilamellar membrane enveloping axons, comprises alternating extracellular and cytoplasmic leaflets [1]. Structural alterations in the myelin sheath, particularly demyelination, are indicative of various inflammatory neurological disorders, such as Multiple Sclerosis (MS) [2]. Experimental autoimmune encephalomyelitis (EAE) serves as a recognized animal model for MS, characterized by significant changes in the overall myelin lipid composition [3]. Previous studies have reported an approximate asymmetric lipid composition in both native and EAE leaflets [4]. This study focuses on generating flat asymmetric myelin membranes, suitable for Neutron Reflectometry (NR) analysis. Employing the Langmuir-Blodgett and Langmuir-Schaeffer techniques, we successfully adsorbed asymmetric bilayers onto silica wafers.
Our findings reveal that the asymmetric myelin membranes demonstrate minimal differences in Scattering Length Density (SLD) when using non-deuterated lipids. However, deuterated lipids, such as d45-cholesterol, significantly enhance the detection of asymmetry. The addition of Myelin Basic Protein (MBP) shows preferential adhesion to the cytoplasmic leaflet, with higher concentrations on asymmetric membranes. Notably, MBP adheres less to EAE-modified membranes compared to native ones. The thickness of the MBP layer is reduced upon binding to EAE myelin, suggesting deeper protein penetration and membrane swelling.

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Dynamical heterogeneity in the model brain lipid membrane due to NSAIDs

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Nonsteroidal anti-inflammatory drugs (NSAIDs) are one of the most prescribed drugs for their analgesic, antiplatelet, anti-inflammatory, and antipyretic properties. NSAIDs have a strong propensity to alter the structure and dynamics of lipid membranes [1-2]. However, pure model membranes are too simple to represent a complex cell membrane. Hence, it is necessary to study a model membrane system mimicking the composition of a cell membrane. Here, we have prepared brain lipid (BLs) unilamellar vesicles (BLs-ULVs), extracted from the porcine brain tissues, physiologically a relevant model membrane system. We have studied the impact of NSAIDs aspirin (Asp), diclofenac (Diclo), and ibuprofen (Ibu), at varying concentrations on the dynamics of BLs using quasielasitc neutron scattering (QENS) and neutron spin echo (NSE). Normalized QENS spectra show that Asp, Diclo, and Ibu induce the highest QE broadening at 30, 10, and 20 mol%, respectively. QENS spectra are described by two Lorentzian corresponding to slow lateral and fast internal motion. The half width half maxima corresponding to lateral, Γlat, and internal, Γint, motions show unique behavior for each NSAID. The lateral motion follows Fickian diffusion and the internal motion is described by localized translational diffusion [3]. NSE spectra are described by Zilman and Granek model [5]. Modulus of bending rigidity (κkBT) BLs-ULVs rises in the presence of Asp. Whereas, κkBT of BLs-ULVs decreases at 30 mol% Diclo and increases at 20 mol% Ibu. This suggests that Asp hinders, at all concentrations, and Diclo promotes the membrane fluctuations at 30 mol%. Ibu suppresses the membrane fluctuations only at 20 mol%. This study shows that NSAIDs affect short and long range dynamics uniquely at different concentrations.

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The Influence of Charge on the Interaction Between Intrinsically Disordered Proteins and Phospholipid Membranes: A Neutron Reflectometry Examination of α-Synuclein and Synaptobrevin-2

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Intrinsically disordered proteins (IDPs) are a class of proteins that do not have a defined three-dimensional structure but may fold if a binding partner is present. In our current research we focus on the interaction of two neuronal IDPs with bio-membranes where binding to the membrane induces configurational changes or folding:
α-Synuclein (αSyn) is associated with various neurogenerative disorders, including Parkinson's disease, which is characterized by fibril formations in the human brain. αSyn plays an important role

in synaptic vesicle trafficking and is involved in membrane interactions [1]. NMR and molecular dynamics (MD) simulation revealed that αSyn can interacts with the membrane by forming α-helices at its N-terminus, which include a kink in the helical structure. The fraction of αSyn in the bound α-helical state at the N-terminal increases with the amount of charged lipids in the membrane [2], while the disordered C-terminal region remains disordered. Interaction of αSyn with differently charged lipid bicelles was measured by Circular Dichroism (CD) Spectroscopy at SOLEIL and showed increasing of α-helical structure for charged membranes.
Synaptobrevin-2 (Syb2) is a vesicle-associated integral membrane protein. Syb2 plays an important role in vesicular membrane fusion at the neuronal synapse by participating in the dynamic formation of the SNARE complex. Syb-2 anchors with a short transmembrane region (TMR) to the membrane and has a large intrinsically disordered soluble region (1-96) which shows a gradually increasing rigidity from the N to C terminus that correlates with an increase in lipid binding affinity [3].
Further characterization of αSyn and Syb2 with membrane interactions using neutron reflectometry revealed insights into the protein's configuration both within the membrane and in the adjacent solution. We examined membranes with varying charge compositions to understand how different lipid environments influence the protein's behavior.

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Biomimetic interfaces to unveil the cell internalization mechanisms of extracellular vesicles

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Biomacromolecules, when approaching cell surface, can see different exposed chemical groups with a variety of possible spatial organization, depending on local plasma membrane composition and on intra- and extra-cellular environmental conditions. We develop experimental biomimetic interfaces in the form of dispersed aggregates in solution or of single supported bilayers, mimicking different cellular interfaces, suitably to be investigated by complementary scattering and reflectometry of neutrons and X-rays, calorimetry and FT-IR, to study their thermotropic behavior and structure upon interaction with incoming molecules. Lately, following our previous investigation [1][2][3], we could deepen the molecular details of plasma membrane interaction of extracellular vesicles (EV) of different origin. EV are nanosized vesicles secreted from all kind of cells, responsible of cell-cell communication [4]; there are widely investigated for diagnostic purposes, since their molecular cargo is specific of the originating cells, but their mechanisms of interaction with the plasma membrane of recipient cells are still hotly debated and hard to disentangle [5]. Our study reveals that the interaction extent, details at the molecular level, kinetics and the effects on target membrane lipid mobility are strictly dependent on EV origin as well as on the target membranes composition. Our approach has clear implications on the possibility to intervene and modulate EV internalization routes by targeting specific domains at the plasma cell membrane and, as a consequence, on the development of EV-based therapies.

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The Interaction of Styrene Maleic Acid Copolymers with Phospholipids in Langmuir Monolayers, Vesicles and Nanodiscs

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The self-assembly of amphipathic copolymers with phospholipids in aqueous solution results in the formation of 'nanodiscs' containing a planar segment of phospholipid bilayer encapsulated by a polymer belt. Recent studies have reported that lipids rapidly exchange between both nanodiscs in solution and external sources of lipids e.g. [1]. There are, however, outstanding questions regarding precise details of polymer-lipid interactions, the factors influencing lipid exchange and the structural effects of such exchange processes. Here, we structurally investigate the influence of membrane charge on free polymer interaction, and the impact of polymer chemistry on the propensity of nanodiscs undergo lipid exchange [2]. This was performed using two implementations of neutron reflectometry (NR): a traditional structural approach to examine the detailed location and amount of polymer incorporated in the lipid layers in order to understand the structures formed at equilibrium, and a novel compositional, time-resolved approach to investigate the changes in surface excess of both lipid and polymer during the interaction. We show that both free polymer and SMALP (styrene-co-maleic acid lipid particles) nanodiscs are surface active and disassemble when adsorbed to a clean air-water interface. In the presence of a pre-existing monolayer, the polymer embeds throughout the monolayer, the extent of which is governed by the net monolayer charge. Finally, we demonstrate that nanodiscs stabilised by three different polymers will exchange both lipids and polymer with a monolayer. These results demonstrate the dynamic nature of nanodiscs which interact with the local environment and are likely to deposit both lipids and polymer at all stages of use.
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Magnetic Nanocaps: Impact of Curvature on Structural and Magnetic Properties of Thin Films

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Magnetic nanocaps, formed by depositing Co/Pd multilayers on highly ordered arrays of silica nanospheres, present a promising area of study due to their unique properties. This research focuses on fabricating and characterizing these nanocaps and comparing them to films deposited on

flat silicon substrates. Using an advanced drop-casting method, we prepared two-dimensional arrays of silica nanospheres with diameters of 50 nm and 200 nm [1]. The curvature of these nanospheres induced lateral variations in film thickness, affecting the material properties. Structural analysis using X-ray reflectivity and Grazing Incidence Small Angle X-ray Scattering (GISAXS) revealed the curvature-induced morphology. Magnetic measurements via SQUID indicated distinct properties, including low coercivity and altered anisotropy axis direction, compared to flat films. Depth-resolved magnetization profiles were determined using Polarized Neutron Reflectivity (PNR). Additionally, Grazing Incidence Small Angle Neutron Scattering (GISANS) was employed to investigate in-plane lateral magnetic fluctuations. GISANS provided detailed information on the spatial distribution and correlations of magnetic domains within the nanocaps, revealing how the curvature and thickness variations influence magnetic interactions at the nanoscale. This comprehensive study correlates the magnetic and structural properties of thin films with varying thicknesses and nanosphere radii, enhancing our understanding of curvature's impact on nanostructure formation and magnetic behavior, and guiding the design of functional magnetic materials for technological applications.

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Functionality from topological insulating films and interfaces: electronic, magnetic, thermoelectric

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The discovery of the topological phases of matter sparked a renaissance in solid-state physics, however the broader applications to materials engineering are still in their infancy. The three-dimensional topological insulators offer a particularly simple new paradigm for developing unique functionality which relies on exploiting surfaces and interfaces via nanoarchitectural design.

I will give a brief introduction to the field of topology in materials, and the relation to the crystallographic space groups. I will then give some tangible experimental examples of interface-induced functionality in topological insulating Sb2Te3, MnBi2Te4 and Bi2Te3 ultra-thin films [1-6]. I will discuss how the topological features can lead to enhanced electronic, magnetic and thermoelectric properties. The interplay between the classical crystal and magnetic order parameters is critical in these materials, and glass transitions have important consequences for the electronic properties. For example, the delicate van der Waals crystals are highly sensitive to electron and ion beam irradiation [1,2,5], which can be used to deliberately drive glass transitions and spatially control the topological invariant toggling between $\mathbb{Z}2 = 1 \longrightarrow \mathbb{Z}2 = 0$ at a threshold disorder strength [1]. Controlled glass transitions are also important in the search for elusive higher order amorphous topological insulators predicted by theory. For accurate characterisation of crystalline parent phases, however, non-destructive characterisation techniques are critical.

To enable accurate, non-destructive characterisation of electron and spin density with atomic resolution, neutrons and X-ray scattering have some intrinsic advantages. I will focus on how surface sensitive neutron and X-ray techniques, including polarised neutron reflectometry, have led to new insights into the classical crystal and magnetic order-disorder transitions, and their concomitant electronic quantum transitions.

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Unveiling the mechanisms of hydrogen induced phase transitions in nickelate films

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An increasing number of studies are showing the possibility of tuning the electronic properties of functional materials via an unconventional dopant: hydrogen. In correlated oxide interfaces, and especially in rare-earth nickelates, hydrogen-induced reversible electronic and structural phase transitions have been uncovered [1-2]. Neutron and x-ray scattering methods are without doubt one of the best way to characterize in a non-destructive and non-local way these systems. Here we will show the multi-stage phase transformation observed at room temperature for $LaNiO_3$ upon exposure to hydrogen gas. Electrical transport shows a subsequent metal-insulator-metal transition. We will present the results of in situ neutron reflectometry, which allowed us to distinguish and quantify oxygen depletion, hydrogen incorporation, and lattice expansion (Figure 1). These are all different mechanisms that can explain the electronic modification of the host layer. In addition to the neutron measurements, we will present results from in situ synchrotron x-ray diffraction and x-ray absorption, which helped to understand the reaction with hydrogen and its effects on the Ni valence. This work highlights the need of combining appropriate complementary techniques to correctly identify the source of modifications induced by hydrogen exposure in complex systems such as transition metal oxides.

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Magnetic correlations in ion implanted metamaterials probed by neutrons

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Investigating the magnetism at interfaces with designed periodic modulation of the magnetization —known as magnetic metamaterials—has recently gained significant attention [1]. Such structures provide platforms for fundamental studies of order and dynamics at the mesoscale, as well as having potential applications such as computation [2]. The magnetism in these materials can be studied by real space techniques, such as magnetic microscopy employing polarized photon beams or scanning probe techniques. All these techniques have in common that they are local while the collective behavior of these metamaterials may be studied with scattering techniques offering complementary information. Neutrons are directly sensitive to the magnetic induction in materials and reflectometry allows to extract the magnetisation depth profile accross surfaces and interfaces [3], while off-specular and grazing incidence scattering [4] allows the study of lateral correlations on orders of length scales from nm up to around 100 μm.
In this work, we present a feasibility study performed on a new generation of magnetic metamaterials, produced using an additive approach based on ion implantation [5][6]. The resulting metamaterial architectures comprise chemical patterns on otherwise flat films, where the implanted species induce magnetism to a paramagnetic host matrix. By employing an electron beam lithography process, we define the lateral implantation patterns. We then characterize the implanted magnetization profiles using polarized neutron reflectivity (PNR) and present lateral magnetic order information through a grazing incidence small-angle neutron scattering (GI-SANS) measurement protocol.

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Functional magnetic thin films and heterostructures / **39**

Hydrogen absorption and spin reorientation in Pt/Co/Pt and Pd/Co/Pd

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Pt/Co/Pt and Pd/Co/Pd heterostructures with perpendicular magnetic anisotropy (PMA) are traditionally used for magnetic recording to achieve high magnetic data storage density. PMA can be tuned by e.g. thin film thickness, strain, ion bombardment or temperature. Recently, it has been shown that the absorption of hydrogen in the heavy metal modifies the interfacial spin-orbit coupling and hence reduces the PMA.[1-3] As a result, reversible and non-destructive toggling of the

easy axis of magnetization between in-plane and out-of-plane orientation at room temperature was demonstrated in a Co/GdOx all-solid-state device for magnetic hydrogen sensing.[4]

Polarized neutron reflectivity is an effective tool for studying the hydrogen uptake and its impact on the magnetic properties in PMA systems.[2, 5] Recently, resonance enhanced polarized neutron reflectometry (RNR) has proven to be a quantitative method for the determination of the hydrogen concentration with with a possible time resolution in the sub second (or few 10 millisecond) to few seconds regime. [6]
In this contribution we report the results of RNR experiments on hydrogen uptake in a Pt/Co/Pt trilayer sandwiched by 25 nm Nb layers on MgO(001) substrates fabricated by molecular beam epitaxy. Furthermore we discuss the differences in Pt/Co/Pt and Pd/Co/Pd trilayers with respect to their magnetic properties and hydrogen uptake.

Functional magnetic thin films and heterostructures / **25**

Magnetic chirality in superconducting/ferromagnetic heterostructures: insight via polarized GISANS

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The coexistence of different order parameters can lead to exotic new quantum phenomena. In hard condensed matter materials, their interplay often generates magnetic chiral structures with correlations on the nanometer and mesoscopic length scale, which can be explored by polarization-analyzed Small-Angle-Neutron-Scattering (SANS) in bulk systems, and by its surface-sensitive counterpart Grazing-Incidence-SANS (GISANS) in thin film structures. Thin film Nb/FePd exhibits coexisting superconducting and ferromagnetic phases, affecting both the superconducting and the magnetic order around its superconducting Tc [1,2]. While around Tc in Nb the superconducting state is confined above the domain walls of FePd, the superconducting state itself is affecting the width wDW of magnetic domain walls in FePd [1].
Although a Dzyaloshinskii–Moriya Interaction (DMI) leading to magnetic chirality is not expected in the L10-structured FePd, its domain walls obtain a preferred chiral direction, unveiled by polarized GISANS. An extensive study combining GISANS, circular-dichroism X-ray Resonant Magnetic Scattering (CD-XRMS), and Density Functional Theory (DFT), yields unique insight into the chiral wall formation and its origin.
At the ESS, neutron polarization analysis will be supported on many instruments [3], and together with a wide range of sample environments will enable pioneering science projects. Based on the above-mentioned science case using polarized GISANS, I will additionally present the impact from instrumentational and data reduction aspects.

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Functional magnetic thin films and heterostructures / **16**

Polarized neutron reflectometry on vertical and lateral magnetic domains in thin films

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Polarized neutron reflectometry (PNR) offers the possibility to resolve structural and magnetic morphologies of heterostructures and their interfaces as a function of depth with sub-nm resolution. In addition, lateral structures such as magnetic domains in the μm scale are accessible with off-specular scattering. This talk discusses two examples of functional thin films in which the formation of magnetic domains plays an important role.
The first example investigates the vector magnetization profile in high-anisotropy rare-earth alloys combined with soft magnetic Fe thin films. Such heterostructures form prime examples of exchange spring (ES) materials possessing high magnetizations and high magnetic anisotropy [1]. This promises a range of applications in logic circuits, sensor and magnetic storage technologies with high magnetic stability and durability. We use PNR to quantify the proximity coupling in $SmCo_5$/Fe and $NdCo_5$/Fe bilayers grown on Cr-buffered MgO substrates. Strong spin-flip signals of the neutron reflectometry as a function of field quantify the extension of moment canting away from the applied field towards the $SmCo_5$ interface. The case of $NdCo_5$/Fe is particularly intriguing due to its giant magnetocaloric effect and a spin-reorientation transition observed at 255 K [2]. PNR, recorded as a function of temperature and magnetic field orientation, shows a spiral moment configuration forming between the low and high temperature states.
In the second example, we investigate the lateral domain pattern of He-ion bombarded exchange bias thin films. Such artificially designed magnetic domain textures on micrometer length scales with controllable magnetization configurations present suitable templates for lab-on-a-chip applications, optically active surfaces, and biosensor devices [3]. Due to the absence of topographic height variations, guided positional control of magnetic particles is achieved solely from magnetic stray fields emerging from the domain walls of adjacent domains [4]. Polarized neutron scattering is used to resolve lateral periodicities, magnetization directions and disordered moments of the domains [5]. The measurements reveal crucial details about the magnetic pattern and the ordering of domain walls. The magnetic evolution is monitored during field cycling, providing a full picture of the magnetic configuration.

Functional magnetic thin films and heterostructures / **50**

Molecular Beam Epitaxy at JCNS for precise interface control in heterostructures and nanostructures

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Thin film heterostructures are essential in modern device development, offering a platform for manipulating interfacial effects. Molecular Beam Epitaxy (MBE) is an indispensable technique for the

growth of high-quality epitaxial films, heterostructures, and nanostructures. It enables precise control over the composition, thickness, and structure of materials and has led to the discovery of a wide range of complex interface behaviors; including two-dimensional electron gases (2DEGs), quantum confinement, magnetism, superconductivity, and topological insulators. These interface effects result in unique electronic, optical, and magnetic properties, making them of interest for both fundamental research and technological applications.
JCNS operates two MBE systems: An oxide MBE at JCNS-2 in Jülich, and an MBE at MLZ in Garching. Both systems are available to JCNS scientists, with the Garching instrument also available to a broader scientific community through a proposal system for thin film growth.
Here we highlight ongoing projects using our MBE facilities: Variable (perpendicular magnetic anisotropy) PMA in FePd, magnetite on Nb-doped strontium titanate, Co/Pd multilayers on silica nanospheres, and multilayers of oxide and non-oxide ferromagnets and metals for skyrmion lattices and other magnetic textures.
Additionally, x-ray and neutron scattering experiments on MBE-grown structures are powerful tools for investigating complex interfaces; enabling probing of structural, magnetic and electronic properties with high resolution. This can lead to new insights into the behavior of electrons, phonons, and spin waves in these systems, and help to elucidate the underlying physical mechanisms. The unique positioning of our MBE instruments provides scientists from Jülich, Garching and beyond the opportunity to grow thin film systems for neutron and x-ray experiments.

Functional magnetic thin films and heterostructures / **34**

Structural, magnetic and electrical properties of oxygen-deficient La(0.6)Sr(0.4)CoO(3-δ) thin films

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Controlled oxygen release or uptake in complex oxides can induce changes of the crystal structure and simultaneously of the magnetic and electrical properties. Consequently, a systematic control of the oxygen stoichiometry can enable potential applications in spintronics, solid oxide fuel cells and catalysts. In La0.6Sr0.4CoO3-δ (LSCO) the gradual oxygen release triggers a phase transition from the initial ferromagnetic (FM) perovskite (PV) structure to an oxygen vacancy layered antiferromagnetic (AFM) brownmillerite (BM) structure.
We have studied LSCO thin films fabricated by pulsed laser deposition (PLD). In situ x-ray diffraction during thermal annealing reveals the topotactic phase transition of the LSCO thin films, which can be attributed to the release of oxygen and ultimately the transition to a coherently ordered BM phase. By comparing the magnetic and electronic properties of the sample at different oxygen deficient states, we demonstrate that the magnetic and electronic transitions are apart from the structural phase transition [1].
Using in situ polarized neutron reflectometry (PNR) measured at the MR reflectometer (SNS/Oak Ridge), we explore the nuclear scattering density (nSLD) and quantify the change in oxygen stoichiometry and the magnetization of the LSCO film during annealing. The PNR data shows a significant decrease of nSLD for the annealed film indicating a reduction in oxygen concentration. The oxygen stoichiometry is found to vary from La0.6Sr0.4CoO3 before annealing to about La0.6Sr0.4CoO2.5 for annealed films. We find that disordered oxygen vacancies forming in the initial phase of annealing quickly govern the magnetic properties of the film by triggering a FM to AF transition [1].

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Functional magnetic thin films and heterostructures / **47**

Investigation of the structural and magnetic properties of the interface in Fe3O4/TiO2-Nb:STO heterostructures

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The Fe_3O_4/Nb:STO system has gathered significant attention due to its potential application in spintronics and memristors. The interface between Fe_3O_4 and Nb:STO plays a crucial role in determining the overall electronic and magnetic properties of the system. We present an investigation of a 30 nm Fe_3O_4 thin film on a TiO_2 terminated Nb-doped $SrTiO_3$ (TiO_2-Nb:STO) substrate deposited by pulsed laser deposition (PLD), focusing on the buried interface using Polarized Neutron Reflectometry (PNR), X-ray Magnetic Circular Dichroism (XMCD), and X-ray Reflectometry (XRR).

Our study utilizes XRR to assess the structural properties, including roughness and density variations, across the interface. PNR is employed to probe the magnetic depth profile. The combination of these techniques reveals a 1 unit cell (u.c.) γ-Fe_2O_3 interlayer between the Fe_3O_4 thin film and the Nb:STO substrate and a 2 u.c. γ-Fe_2O_3 surface layer. XMCD provides element-specific magnetic information throughout the entire system, confirming the total thickness of γ-Fe_2O_3 to be 3 u.c.

The results reveal significant modifications in the magnetic and structural properties at the buried interface, driven by interactions between the Fe_3O_4 film and the TiO_2-Nb:STO substrate. Specifically, the presence of the γ-Fe_2O_3 interlayer and surface layer affects the magnetic coupling of the system.

Hard-soft interfaces / **20**

The neutron reflectometer Super ADAM at ILL

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SuperADAM is an angle dispersive neutron reflectometer operated as Swedish CRG instrument at the Institute Laue-Langevin, Grenoble (France). The instrument offers very high resolution and polarization and is optimized for the study of interfaces and thin films with an emphasis on small magnetic moments. The instrument allows to record and analyze off-specular and grazing incidence small angle scattering (GISANS). Beam time is allocated via ILL proposals and an internal competitive Swedish call for beam time applications. To complement the high-resolution the beam line has been upgraded by a second end station using a shorter wavelength. This offers higher flux and a larger q-range and allows surface diffraction studies. Both end station can be operated in parallel.
In this presentation we will summarize the capabilities of the beam line, including relevant parameters, as well as scientific examples form the past years. Those range from self-assembled particle templates over the study of lipid membranes to exchange interactions in magnetic thin films. We will also provide a perspective for method developments related to the instrument and potential future upgrades and relevant scientific questions.

Hard-soft interfaces / **17**

Rheo-NR to study the ordering of soft polymer crystals at the solid-liquid interface

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Soft crystalline structures are of great importance in many applications that improve human life on a day-to-day basis. Some examples include engineering of human tissue constructs [1]. They are particularly suitable in this environment because of their good biocompatibility and low toxicity as well as their tunable viscoelastic properties. The exact formulation can be varied by variables, such as temperature or ionic strength, to achieve desired properties. Soft crystals have a complex microstructure; therefore, a detailed understanding of how molecular and crystalline structure influence their viscoelasticity is of large interest. One example for polymers forming soft crystals in solution are polyethylene-glycol(PEG)-polypropylene-glycol(PPG)-PEG triblock copolymers, which can self-assemble into micelles in aqueous solution. The bulk properties of such systems have been extensively studied by rheology and scattering experiments, most notably by Small-Angle Neutron Scattering (SANS) [2]. However, close to an interface the structure differs from the bulk, which is less well studied.
In this work we employ in situ-Rheo-Neutron Reflectometry (Rheo-NR) to get insights into the effect of shear on the near surface structure of micellar crystals close to solid substrates [3]. We systematically study the ordering process of the triblock polymer Pluronic F127 in aqueous solution. Rheological parameters, such as shear rate, are found to have a decisive impact on the specular scattering intensity of the 111-Bragg peak as well as the off-specular scattering. A low shear rate seems to support alignment of the lattice planes along the interface, whereas high shear rates result in melting of the crystal. For temperatures near the thermo-gelling point and low shear rates, a coexistence of cubic close packing and hexagonal close packing could be observed, which disappears with higher shear rates. Apart from shear we study the influence of surface energy and temperature on the near surface order. A highly hydrophobic surface and a highly hydrophobic surface cause better alignment, whereas a surface of intermediate hydrophobicity shows worse alignment.

Hard-soft interfaces / **43**

Neutron reflectometry from interacting soft interfaces and not-so-thin films

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Interactions between soft interfaces occur in our daily life and in numerous wet technological contexts. They also influence the functions of biological entities like membranes. Understanding the character of such interactions often requires detailed insights into the structure of the interfaces and their response to the interaction. Neutron reflectometry is an ideal tool for the characterization of interfaces in close proximity. The experiments and the subsequent analysis benefit from controlled interaction conditions with homogeneous surface separations over large areas. In practice, however, one is often confronted with scenarios involving lateral heterogeneities or scenarios in which the interaction distance varies strongly with the surface chemistry or with time. Interaction scenarios or evaporating films with surface separations on the order of several micrometers pose a particular modeling challenge. We use various strategies to extract structural information from thin-film systems with such challenging characteristics.

Industrial applications & Emulsions / **57**

Tuning cellulosic functional materials and processing using neutron techniques

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Various engineering material concepts can be fabricated from cellulose. The starting point can be the cellulose polymer, nanoscale intermediates such as cellulose nanofibers (CNFs), and macroscopic cellulose fibres extracted from plants. The material concepts exhibit good mechanical performance, unique hierarchical structuring and various functional properties, making them suitable for various applications, such as barrier coatings in organic electronics and substrates for functional layers. Neutron-based characterisation techniques offer a versatile toolbox for further developing these material concepts and a set of examples will be discussed.
In power transformers, pressboard made from pure, unbleached cellulose fibres offers superior dielectric and mechanical properties. The key to enhancing its performance and efficiency lies in optimising the manufacturing process. Neutron imaging can play a crucial role in investigating the industrial process and the changes induced by processing [1].
Neutron scattering techniques complement imaging by providing detailed insights into the nanostructure and porosity of cellulose films. These methods are particularly useful in studying the packing density and surface characteristics of spray-coated CNF films, which are essential for their application in conductive and transparent coatings. Understanding the relationship between CNF morphology and film porosity is crucial for developing functional coatings and optimising the embedding of functional layers [2].
In conclusion, neutron imaging and scattering techniques are invaluable tools for advancing the development of cellulose-based materials for energy-related applications. By offering a deeper understanding of the material properties and manufacturing processes, these techniques enable the optimisation of cellulose for high-performance electrical insulation and other energy storage and conversion applications, contributing to a more sustainable future.

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Industrial applications & Emulsions / 18

Structure of industrially relevant sp2 carbon using wide Q-range neutron total scattering: From bitumen to batteries via benzene

Autor Tom Headen[1]

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Beyond crystalline graphite, planar sp2 hybridized carbon can make a wide array of different structures and therefore materials: From geologically formed asphaltenes, to new synthetic materials such as carbon nanotubes. Many of these materials are non-crystalline, making non-ambiguous structural determinations is therefore difficult. In this talk we will outline the combined use of wide Q-range total scattering, H/D isotopic substitution and classical molecular simulation to make progress in characterizing the structure in these industrially relevant materials.
We have studied the simplest sp2 carbon molecular liquids, the aromatics such as benzene, using Empirical Potential Structure Refinement (EPSR) methods. This reveals a complex mixture of local structures resulting from a delicate balance of different intermolecular interactions, rather than just archetypal pi-pi stacking [1]. We have pushed this approach to larger lengthscales using data from the NIMROD instrument at ISIS, with a simultaneous Q-range of 0.02-50Å⁻¹, allowing us to study the complex solvation structure of carbon nanotubes in amide solvents [2]. A molecular dynamics simulation-based approach has been extended to a considerably more complex set of aromatics, the asphaltenes, a heavy component of crude oil and bitumen, with a propensity to precipitate in oil recovery and refining. Simulations show a close match to the neutron scattering data, apart from at the lowest Q-range explored by NIMROD, due to the limited simulation size [3]. Finally, we will present recent operando studies of hard-carbon battery anodes on NIMROD. These promising materials comprise disordered nano-graphic domains allowing sodiation within the graphitic regions and nano-pores. The wide simultaneous Q-range of NIMROD affords a unique view of subtle changes at the atomistic and pore-scale during charge and discharge.

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Industrial applications & Emulsions / 56

Sustainable food emulsion systems explored with neutron scattering and spectroscopy

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Food emulsions may be either stabilized by amphiphilic milk-based or sustainable plant-based proteins, which affect the interfacial and emulsion stabilization mechanisms on a macro- and microscale of length and time. To understand these mechanisms in detail different length scales from molecular to macroscopic distances as well as time dependent mechansims need to be investigated.
Neutron scattering techniques provide insight into such emulsions on these length- and time-scales depending on the technique used. Combining structural information on molecular length scales from small angle x-ray and neutron scattering (SAXS and SANS) with time dependent neutron spin echo spectroscopy (NSE) allows to expand our understanding towards intermolecular interactions within the interface. These interactions are linked to the emulsion stability –the elastic properties of the protein or protein/phospholipid stabilized oil/water interface on molecular length scales.

Neutron and x-ray scattering techniques which broaden the classical characterization of food emulsions are introduced. Results from emulsions stabilized with b-lactoglobulin as a representative milk protein, and different plant-based proteins, are presented and discussed. Contrast variation by deuteration of some components of the emulsions is applied to focus on the interfacial region, relying on the uniqueness of neutrons. Connecting these emerging results with classical characterizations such as interfacial tension or viscoelasticity assist in understanding the complex mechanisms of interfacial stability, and may contribute to a knowledge driven development of sustainable food emulsions.

Industrial applications & Emulsions / **30**

Innovation in automotive coatings

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A coating in general serves two purposes, protection of the coated substrate and decoration of the coated object. Modern automotive coatings consist of multiple layers with each layer specialized to provide protective or appearance properties to the overall coating. The formulation of a single layer can easily contain dozens of individual components. The main component of an organic coating however is a mixture of polymers called binder or resin in coating technology. Therefore, polymer science has a major impact on the performance and innovation of organic coatings. The physical and chemical properties of the binders provide the required properties for e.g. corrosion or physical protection, chemical resistance or dispersion and orientation of embedded pigments. It could be argued that polymers are the main influence on the final properties of the coating. The current interest in E-mobility and focus on environmental performance has shifted the traditional topics of coatings research in recent years. Restriction to components currently used in coatings technology drive innovation towards alternative raw materials and innovative curing chemistry. The bioeconomy has increased research into biobased feedstocks and the need for energy efficient systems has renewed the interest in functional surfaces.

Industrial applications & Emulsions / **13**

An overview of the latest developments in the field of neutron supermirrors

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Efficient neutron transport through neutron guides is the basis for the high performance of modern neutron scattering instruments. The combination of special guide profiles and high reflectivity supermirror coatings allows the properties of the neutron beam to be tailored to the needs of the experiment. In addition, a variety of substrate materials (different glasses, different metals, silicon) offer extended possibilities in terms of precision, shielding and lifetime.
Recently, new concepts for focusing (nested mirror optics) and wide-angle polarisation analysis (tWAPA) have been developed, using advanced supermirror technology in new sophisticated geometric arrangements. In our presentation we will report on the state of the art and the latest developments in these areas at SwissNeutronics. In particular, we will demonstrate the capabilities and performance of neutron guides made from metallic substrates with highly reflective supermirror coatings. Similar coatings are used on very thin silicon substrates. Such substrates are used to build compact Nested Mirror Optics (NMO) [1], which make it possible to transfer the high brilliance of modern neutron sources to experiments or to focus large beams with defined phase space (beam size and divergence) on very small samples. In addition to neutron beam transport and focusing, polarising supermirror coatings are often used in special configurations such as
V-cavities to polarise the incident neutron beam and polarising benders in the transmission geometry. These devices are simple to use, easy to align and maintenance free. These advantages are highly appreciated for polarisation analysis of scattered neutrons, where devices capable of covering a large solid angle are required. This is realised by the tWAPA (Transmission Wide Angle Polarisation Analyzer) [2] concept.

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Industrial applications & Emulsions / 41

Interdiffusion of polymer and water in waterborne polymer latex films

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Waterborne latex films, obtained from the dispersion of latex particles are of particular interest due to the non-content of volatile organic compounds (VOC), often mandatory under environmental legislation.1 However, abrupt water penetration inside the films restricting their lifespan and deteriorating the shining of the coating. In order to prepare efficient and solvent-free coatings with the low glass-transition temperature (Tg < the drying temperature) but with higher mechanical strength, we have integrated hydrophilic layers (Acrylic acid/ Poly(acrylamide)) around the hydrophobic cores (mixture of Methyl methacrylate and Butyl acrylate) and also hard shell around the soft core in the latex film. Latex particles with different morphology (hairy layer variants and core-shell particles) have been synthesized using emulsion polymerization.2 Polymer latex films have been prepared in the next step by evaporating water in a thermo-humidistatic chamber at temperature 25 oC. The structure formation of polymer latex films in the dry state (crystallinity) and in re-swelled state

(change in crystallinity and whitening or blushing) have been studied to propose a recipe for the preparation of efficient latex coatings. The Small-Angle Neutron Scattering (SANS) study shows the FCC-like structure formation by the latex film, which become more organized with the inclusion of the hydrophilic shell. The hydrophilic shell also promotes the formation of the homogeneously water-swollen film and slows down the development of water "pockets", preventing the deterioration of the latex film over time. On the other hand, the inclusion of hard shell protects the latex films from water whitening and provides additional mechanical strength. The interdiffusion between the latex particles has been analyzed by mixing H/D polymers. The transfer of polymer chains through interparticle boundaries that vanishes the crystalline structure and results in a formation continuous material.

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Industrial applications & Emulsions / **38**

Self-Assembly of the biosurfactant rhamnolipid in concentrated aqueous solutions studied with SAXS and SANS

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Research on the physico-chemical properties of microbial biosurfactants is a very active field as these compounds are of increasing interest to industry due to their enhanced biodegradability and their derivation from renewable sources [1]. To achieve the goal of replacing existing surfactant formulations with this greener alternative, a solid knowledge of the latter's properties is required.
In this contribution, we present investigations on the self-assembly of the biosurfactant di-rhamno-di-lipid (Rha_2-$C_{10}C_{10}$) in concentrated aqueous solutions. We used a combination of Small-Angle X-ray (SAXS) and Neutron (SANS) Scattering to elucidate the structural evolution of the rhamnolipid micelles up to concentrations of 50 wt.%, taking advantage of the different contrasts detected by the two scattering techniques.
Most previous studies in literature have focused on very dilute rhamnolipid concentrations to not have to deal with interaction effects when analysing the scattering data [2]. In order to shed light on the self-assembly of rhamnolipids also in highly concentrated systems, we used the Generalised Indirect Fourier Transformation (GIFT) [3] technique to separate the micellar form factor and the structure factor describing the interaction between them with a minimum of a priori knowledge of the structure. We found that globular micelles dominate the phase behaviour over a surprisingly large surfactant concentration range and that the transition to a hexagonal (H_1) liquid crystalline mesophase occurs almost instantly.

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Industrial applications & Emulsions / **55**

Polysaccharide-based nano-/micro-gels for the food sector

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Polysaccharides, as major components of natural origin, have garnered extensive attention and utilization across diverse fields, including the nutritional manufacturing sector. Due to their advantageous properties such as safety, stability, biocompatibility, biodegradability and nontoxicity, polysaccharide-based complex systems have a significant potential in the fields of cosmetics, pharmaceutics and food engineering. Microencapsulation of active ingredients such as flavors, antioxidants, vitamins, and lipids into biopolymer nano-/micro-gels offers greater bioavailability, effectiveness, lower toxicity, and more lasting stability than conventional formulations. Therefore, understanding the physicochemical properties of these micro- and nanogels, as well as their encapsulation and release ability under various conditions, is crucial for optimizing their use in the food sector.

In our study we present *k*-carrageenan and *λ*-carrageenan-based nanogels obtained as a result of electrostatic coassembly with BSA protein as macro-ionic crosslinking agent. Such systems are of interest as carriers for bioactive ingredients, therefore we compared the microstructure of unloaded and VD3-loaded gels under various pH and temperature conditions applying scattering (LS, SAXS, SANS) and spectroscopic (FTIR, CD, Fluorimetry) techniques.

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Charge Density Waves that Guide Critical Composition Fluctuations

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Binary liquids may show critical composition fluctuations if the temperature and composition are close to the critical point. When adding ionic surfactants (or antagonistic salts) the whole system gets dominated by the ions that are arranged locally in lamellae that display the charge density waves. The domains only fluctuate along the surfaces in 2 dimensions on short time scales. Only at longer time scales of milliseconds, the charge density waves take over and the third dimension springs to life. Many details of the system 3-methyl pyridine / heavy water and sodium tetraphenylborate support this view.

Binary fluids are interesting in many aspects such as electrolytes in batteries or fuel cells and electrolyzers. But also applications as skimming where the liquids are separated may be interesting. Thus, the fundamental understanding of binary fluids may support enhanced applications in the near future.

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Neutrons as key technique for a better understanding of lithium and post-lithium batteries

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Li-ion batteries are key players for the energy transition and help decrease greenhouse emission owing to their storage ability. But batteries are also very complex electrochemical systems that deserve an in depth characterisations to understand their limitation during cycling. Indeed, batteries are constantly under further development and employing new type of chemistry and materials that needs to be investigated during operation i.e., in operando mode.
Neutron powder diffraction (NPD) is a technique of choice to investigate structural changes, especially for light elements like lithium. Developing an electrochemical cell dedicated to operando neutron diffraction measurements is challenging due to the large amount of electroactive materials needed and due to the incoherent neutron scattering with hydrogen, highly contributing to the background.
We report here an optimal cylindrical cell based on 18650 design1-3: i) the casing is made of transparent TiZr alloy4 and ii) several grams of active materials per electrodes. Additionally, we modified several set-up on D19 neutron diffraction beamline at ILL enabling the investigation of the electrochemical cell during relaxation processes giving information about diffusion. NCM811 vs. graphite was selected as promising full-cell battery due to the high energy density expected with this electrode couple. Figure 1 represents the neutron diffraction patterns evolution of both phases along the first (de)lithiation. As can be seen both the stages in graphite lithiation (peak (002)) and the insertion reaction of NCM811 (peak (003)) can be easily followed and analysed by mean of Rietveld refinement.
In another example, we used neutron imaging to follow the Li diffusion processes by using Li isotopes 6Li and 7Li. By monitoring fast charge behaviour in Li-rich cathode materials vs. Li metal, we demonstrated that the electrode engineering is a key parameter to optimise to allow fast charging protocol. Coupling experimental data to modelling reveals the hindrance of several Li transport pathway for electrocoupling fast charge and high-power features. Similar examples will be presented on solid state batteries.

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Building better batteries with insights from neutrons

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Since their introduction in 1991, lithium-ion batteries have become the popular choice for power sources in consumer electronics. Furthermore, as they have achieved a tremendous boost in their performance in the last decades, they are being increasingly employed in electrical vehicles and grid-scale energy storage systems as well. However, there is still room for improvement in terms of life expectancy, safety, cost, energy storage capabilities and interfacial stabilities. In this regard, understanding fundamental aging mechanisms that lead to capacity fade in Li-ion batteries becomes important to design batteries with improved components for performance enhancement.
With help of several examples, this presentation will reveal how different aging contributors such as loss of electrochemically active Li, active material degradation, and Li metal deposition can be detected using neutrons and conventional lab-based methods. For each of these cases, I will demonstrate how we optimized electrode design with feedback from obtained data and enhanced cell performance by positively affecting key parameters such as lifetime, charging rate, energy density, interfacial stability, and safety.
For example; using anodes containing mesocarbon microbeads instead of needle coke graphite we obtained faster charging capabilities and a longer lifetime [1]; by coating electrodes with polymers we achieved interfacial stability and obtained superior cycling performance [2]; by using Co-free

cathodes and extending the operating voltage limits, we achieved both reductions in costs and increase in energy densities compared to conventional cathodes [3]; by incorporating silicon in anodes, we obtained increased energy densities compared to conventional anodes [4].

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Small-angle scattering analysis of capillary rise in micro- and meso-porous carbons

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Numerous applications of nanoporous materials require their pores to be filled with liquids. In spite of its huge technological importance, the conditions for the wetting of nanometer-sized pores and its phenomenology are still poorly understood. Here, we report on time-resolved synchrotron small-angle scattering experiments performed during capillary rise of water in carbon xerogels. These materials are widely used for electrochemical applications, in battery, surpercapacitor, or fuel-cell electrodes. Their structure consists in molecular-sized micropores coexisting with larger mesopores about 10 nanometers across.

The time- and space-resolved scattering and data reveal a two-step wetting process whereby water first diffuses into molecular-sized micropores, and this is followed by the imbibition of the meso-pores. A Cassie-Baxter analysis shows that the presence of water in the micropores is central as it turns the meso-pores from being hydrophobic to hydrophilic. Based on so-calculated contact angles, the overall nanometer-scale wetting kinetics is found to be quantitatively captured by macroscopic physical concepts.

Nanoparticles / **15**

Magnetization distribution in core/shell magnetic nanoparticles

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In single-domain nanoparticles (NPs), magnetic anisotropy significantly influences crucial properties in crafting magnetic nanocrystals for high-density data storage or medical purposes[1]. Success

in designing systems to fulfill these applications requires a fine tune in the magnetic properties of the NPs, which is directly related to the control of the composition and morphology of the system. In particular, the development of fabrication techniques of systems with complex architecture, such as core/shell or even onion-like multiphase NPs, gives new degrees of freedom to tune specific physical-chemical properties by combining materials with different compositions and magnetic characteristics and providing new perspectives for their potential applications. Another original yet uncommon strategy is boosting the magnetic anisotropy via anchoring magnetic spin crossover (SCO) molecules on the particle surface[2,3,4]. However, the characterization with traditional and affordable techniques is challenging, and the spatial probe is necessary to unveil nuclear and magnetization fluctuation at the nm length scale. Within this contribution, I will present our latest results on different core/shell NP systems. In this context, I will demonstrate the magnetic small-angle neutron scattering technique as a unique and powerful tool for elucidation of the nanoscale magnetization with a spatial resolution[5,6], allowing us to uncover and disentangle the magnetization within these complex nanostructured materials. Firstly, I will present the changes in magnetization within the 2 nm ferrimagnetic shell in the FeO/Fe_3O_4, $CoO/CoFe_2O_4$ core/shell NPs and explore the influence of the core's magnetic state below and above the Néel temperature on the shell's magnetization response. Later, I will focus on the more complex NP system with a ferromagnetic core of ε-Fe_3N and an oxidic shell layer of unknown stoichiometry Fe_xO_y, revealing the unexpected magnetic response of the oxidic shell. Finally, I will introduce a novel core/shell system with a ferrimagnetic $CoFe_2O_4$ core and NH_2-functionalized iron-triazole SCO molecule as a shell, emphasizing the core's coupling and influence on the SCO's response.

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Multi-responsive nanostructured materials for the targeted delivery of anticancer agents

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Novel, multifunctional nanoparticles and hydrogels that exhibits a unique set of properties for the effective treatment of cancer are presented. The materials are comprised of polypeptidic and polyethylene oxide polymers that are a non-cytotoxic polymer. The amphiphilic hybrid materials assemble in aqueous media to form micelles or vesicles, comprised of an outer hydrophilic corona of PEO chains, and a pH- and redox- responsive hydrophobic layer based on poly(L-histidine) (PHis) and poly(L-cystein) (PCys). Due to the presence of the thiol groups of PCys, a crosslinking process was achieved further stabilizing the nanoparticles (NPs) formed. Dynamic Light Scattering, Static Light Scattering and Transmission Electron Microscopy were utilized to obtain the structure of the NPs. Moreover, the pH- and redox-responsiveness in the presence of the reductive tripeptide of

glutathione (GSH) was investigated at the empty as well as the loaded NPs. The ability of the synthesized polymers to mimic natural proteins was examined by Circular Dichroism, while the study of zeta potential revealed the "stealth"properties of NPs. The anticancer drug doxorubicin (DOX) was efficiently encapsulated in the hydrophobic core of the nanostructures and released under pH- and redox- conditions that simulate the healthy and cancer tissue environment. It was found that the topology of PCys significantly altered the structure as well as the release profile of the NPs. Finally, in vitro cytotoxicity assay of the DOX-loaded NPs against three different breast cancer cell lines showed that the nanocarriers exhibited similar or slightly better activity as compared to the free drug, rendering these novel NPs very promising materials for drug delivery applications.
Hybrid-polypeptidic materials formed injectable in situ forming quickly self-healing hydrogels, responsive to alteration of pH and increase of temperature. The connection between the alteration of secondary structure of the polypeptides with the viscoelastic behavior was revealed by means of Rheology and Circular Dichroism. Small-Angle Neutron Scattering and Scanning Electron Microscopy were employed to shed light to the structure of the polymers and how it affects their rheological properties. The results suggest that these biomaterials have the potential to be used in a number of bioapplications like drug delivery.

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Time-resolved USAXS and contrast-modified SANS probing ZnO nanocluster formation and mesopore-induced solvent segregation

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Scattering methods such as small-angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) are well established as powerful techniques to investigate the structure of nanoscale objects. The usefulness of these methods for elucidating the role of confinement in catalysis, which is the main goal of the Collaborative Research Center 1333, is demonstrated by two recent studies. In the first, we investigated the formation of ZnO nanoparticles, which plays a crucial role in the formation of mesoporous ZnO inverse opals, by time-resolved USAXS [1]. The USAXS/SAXS data and complementary TEM images clearly show that heating of the precursor solution initiates the formation of small ZnO nanoparticles that assemble into clusters. Quantitative analysis of the scattering data provided the underlying kinetics of this process, which consists of continuous nucleation followed by autocatalytic growth. In the second, contrast variation SANS was used to study the influence of confinement of ordered mesoporous silica materials (OMS) on the inner-pore segregation of a dioxane/for¬mic acid mixture used in Ru-catalyzed formic acid dehydrogenation to yield CO2 and H2. Molecular dynamics simulations and preliminary catalysis results indicate that segregation of this binary mixture indeed occurs in cylindrical pores with a diameter of 7.7 nm, leading to the inhibition of the catalyst due to a higher formic acid concentration at the pore surface. It will be shown whether the quantitative analysis of the contrast variation SANS data can confirm this separation [2].
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Nanoparticles / 33

Impact of Coating Type on Structure and Magnetic Properties of Biocompatible Iron Oxide Nanoparticles: Insights into Cluster Organization and Oxidation Behaviour

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Superparamagnetic iron oxide nanoparticles (SPIONs) are promising nano-vehicles for biomedical applications such as drug delivery, imaging, and magnetic hyperthermia. However, one of the limitations of these systems is their tendency to agglomerate, which has a direct impact on the efficiency of their performance. One way to overcome this limitation is to apply a coating during synthesis. In this work, we have investigated the effect of three biocompatible coatings on controlling the agglomeration of iron oxide nanoparticles. The biocompatible coatings used are sodium citrate, (3-aminopropyl)triethoxysilane (APTES), and dextran. The structural and magnetic properties of the coated nanoparticles are characterized using various experimental techniques, including cryogenic transmission electron microscopy (cryo-TEM), magnetometry, Mössbauer spectroscopy, and small-angle X-ray and neutron scattering. The results show that the coatings effectively stabilize the nanoparticles, and lead to clusters of different sizes which then modifies their magnetic behaviour due to magnetic inter-particle interactions. We also investigated the oxidation kinetics of the nanoparticles prepared with the various coating materials as a function of time to characterize the oxidation behaviour and stability. This research provides valuable insights into the design of an optimized nanoparticle functionalization strategy for biomedical applications.

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Inelastic Neutron Scattering: A technique to probe the soul of magnetic nanoparticles.

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During the last decades, we have dived into the fascinating pool of 4f intermetallic ensembles of nanoalloys. With a strong magnetic moment, these ensembles constitute the best case examples alloys to unveil modifications in RKKY interactions and crystalline electric field (CEF) driven by the

size reduction to the nanoscale. Chiefly focused in binary alloys, in the form RM2, being R = Tb, Nd, Gd (magnetic), and M = Cu, Al, Y, La (non-magnetic), we have been able to elucidate the existence of two different symmetry environments, one ascribed to the magnetic moments located within the core, which mostly retain the bulk-like properties, and a second one, connected to the surface magnetic moments, where the less-symmetric and more distorted environment alters the magnetic coupling [1], [2]. Indeed, the existence of two different symmetry environments leads to a dual spin dynamics, with also a possible modification of the actual role of the CEF at the mesoscopic scale, both essential matters, as they determine the energy levels, i.e., the basic support of the material properties. As a matter of fact, the streamlined experimental technique capable of probing such excitations is inelastic neutron scattering (INS), which imposes a limitation to magnetic nanoparticles (NPs), as large amounts (≈10g) are needed to get a reliable signal-to-noise ratio. Using ball-milling, we mastered the production of crystalline RCu2 NPs, where the antiferromagnetic bulk state is retained at the core, being lost at the surface. Equipped with these NPs, we dived, for the first time, into their soul.

In this talk, we will address how we depicted the energy level splitting in both TbCu2 and NdCu2 nanoalloys using INS [3], [4]. By varying the temperature, we surveyed the different magnetic regions of those NPs, probing both crystalline electric field and collective magnon excitations. Our results show how neutrons can be a game changer in the investigation of spin dynamics in magnetic NPs, as a powerful tool to depict their underlying physics.

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Spin Correlations in Assemblies of Iron Oxide Nanoparticles

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In recent decades, analyzing complex, disordered systems posed a challenging yet highly rewarding endeavor in the field of physics [1]. One intriguing area of investigation involves spin disorder [2], particularly in the context of magnetic nanoparticles. They exhibit a reduced saturation magnetization compared to their bulk counterparts that is the result of a substantial degree of spin disorder occurring close to the particle surface. Polarized SANS with longitudinal polarization analysis (POLARIS) is a powerful technique to distinguish between spin configurations in nanoscale materials [3]. Whereas correlated spin canting near the particle surface was revealed in arrangements of nanoparticles [4,5], non-correlated spin disorder has been reported throughout non-interacting nanoparticles [6,7]. These observations indicate that interparticle interactions might play a pivotal role for the formation of correlated surface spin canting.

In this contribution, we will present our work on the effect of decreasing interparticle distances, correlated with increasing dipolar interactions, on the magnetic morphology of iron oxide nanoparticles. By pyrolysis treatment of self-organized nanoparticle arrangements, a systematic increase of packing densities in nanoparticle assemblies was achieved and related to increased superparamagnetic blocking temperatures. We will present the results of a POLARIS experiment (D33/ILL) on the magnetic morphology of nanoparticles with varying interparticle interactions.

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Nanoparticles / **45**

Disentangling anisotropy contributions in Mn-mixed ferrite nanoparticles

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The macroscopic physical properties of magnetic nanoparticles rely on magnetic anisotropy, and their understanding is fundamental to the design of magnetic materials for different applications[1]. Magnetic anisotropy is influenced by the shape, crystal structure, surface effects, and interactions. Macroscopic magnetic measurements, such as DC magnetization and AC susceptibility, allow us to overview the macroscopic physical properties and gain knowledge on the total effective magnetic anisotropy[2]. The investigation of all the contributions to the total effective anisotropy is challenging but extremely important for the design of the material and the deep comprehension of all the microscopic phenomena that drive the resulting macroscopic properties. Due to the sub-atomic resolution, small-angle polarised neutron scattering (SANSPOL) is a powerful tool for investigating surface anisotropy and microscopic phenomena[3]. In this contribution, we will show the impact of the Mn-doping level in cobalt ferrite nanoparticles (10(1) nm) on their magnetic properties. Nevertheless, the macroscopic magnetic responses of the Mn-mixed cobalt ferrite nanoparticles were inconclusive and inconsistent with changing Mn content[2]. However, I will demonstrate the versatility of SANSPOL and disentangle all anisotropy contributions of the total magnetic anisotropy of a series of Mn-mixed Cobalt ferrite nanoparticles with different Mn content but the same shape, size, and surfactant and correlate it with their macroscopic response. Ultimately, our work aims to clarify the complicated picture of magnetic anisotropy and offer insights into the design of magnetic materials.

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Poster / **26**

Time-dependent Gaussian field models for the analysis of structure and dynamics of fluctuating membranes

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The structure and fluctuations of membranes such as phospholipid vesicles or microemulsions is experimentally accessible with small angle neutron and x-ray scattering (SANS and SAXS) and neutron spin echo spectroscopy (NSE). A mathematical model is developed which jointly analyzes SANS, SAXS and NSE data within a single framework. As an example, scattering data from unilamellar vesicles [1] and from microemulsions [2] will be presented.

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Poster / 29

Correlation of the Structural and Magnetic Morphology of Nanoparticles

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Tailoring magnetic nanoparticles (MNPs) involves selecting the right combination of size, shape, and material, which is essential for creating various technological [1], biomedical [2], or environmental applications. To achieve optimal performance in a specific application, it is crucial to understand how the macroscopic characteristics of MNPs and their ensembles are related to their structural and magnetic properties. Despite the significant interest in MNPS, the magnetic morphology and spin structure pose pivotal challenges due to their inaccessibility by conventional macroscopic techniques. Nevertheless, the magnetic small-angle neutron scattering technique with incident beam polarization (SANSPOL) is a powerful technique for resolving magnetization distribution at the nm-length scale and thus disentangling the contribution of the spin disorder [3-4] or magnetization contribution from core and shell part of core@shell NPs [5].
In this contribution, we will show the impact of the chemical composition on the resulting magnetic structure of manganese (Mn)-doped ferrite MNPs. To do so, different doping levels of Mn into cubically shaped CoFe2O4 NPs with the same particle size ($\sigma_{log} < 10$ %) were perfectly achieved by the thermal decomposition method. Using SANSPOL experiments, we reveal the chemical homogeneity and magnetic morphology of the resulting NPs and show the dependence of the surface spin disorder on the chemical composition of nanoparticles.

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Poster / **10**

Neutron tools for detecting nano-second dynamics at interfaces

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Over the past three to four decades, the technique of grazing incidence small-angle scattering has gained widespread acceptance as a means to investigate nanostructures near the surface. While conventional X-ray methods involve directing the beam onto the sample from a vacuum, typically on a wafer, neutron-based approaches allow the beam to penetrate through a silicon wafer, thereby accessing buried near-surface structures. This capability facilitates the study of solid-liquid interfaces, crucial in fields like battery research, colloid science, and physics of complex fluid.

A recent advancement in grazing incidence neutron scattering involves the utilization of neutron spin echo (NSE) spectroscopy. This technique enables detailed examinations of the dynamics of microemulsions and lipid bilayers. By utilizing adjacent planar solid interfaces to confine the membranes of complex fluids, NSE reveals novel physics and mechanisms, unveiling unforeseen phenomena. Several examples showcasing specific unexpected features are presented.

Technically, our development includes a resonator designed to enhance the wave field within the fluid. This enhancement significantly boosts scattering intensities by allowing much higher intensities to pass through the sample. Additionally, at the SNS spallation source in Oak Ridge, a neutron prism is incorporated into the NSE setup to adjust for wavelength-dependent critical angles. This prism ensures a consistent and suitable depth resolution throughout the experiment.

Poster / **35**

Lithium Battery Electrodes Investigated by SANS

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Lithium batteries are ubiquitous in our daily lives, finding applications in cell phones, laptop computers, and automobiles. Each of these applications requires specific key features, such as increased capacity, compact size, rapid charging, and cost efficiency. Achieving these objectives involves material research that employs a diverse range of techniques to optimize each battery component, including electrode morphology, chemistry, and complex electrolyte formulations. Small Angle Neutron

Scattering (SANS) plays a crucial role in this context. SANS is an ideal technique for investigating the nanoscale structure of batteries and their essential components in situ, as it easily penetrates the entire compound. Many surface properties of the electrodes are thus accessible using SANS. I will present some examples of how SANS is employed in battery research: (a) Investigating a cathode material with a protective carbon layer [1], (b) Studying metal phosphide anodes in a discharge/charge cycle [2], (c) Analyzing the formation of a protective SEI (Solid-Electrolyte Interphase) layer within an aqueous electrolyte during battery operation [3]. These examples are complemented by other methods that further support the significant findings for practical battery applications.
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Poster / **52**

Investigation on the presence of magnetic skyrmions in SrIrO3/SrRuO3 bilayer Interface on SrTiO3

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Topological magnetic textures, known as magnetic skyrmions, hold significant promise for applications as nanoscale information components in logic and memory devices. These quasiparticles, characterized by their swirling spin configurations, exhibit unique advantages due to their stability, diminutive size, and the low current densities required for manipulation [1]. In transition metal oxides, electronic correlations between 4d and 5d oxides in bilayer forms induce strong spin-orbit coupling (SOC), facilitating the formation of magnetic skyrmions on the surface of $SrRuO_3$ (SRO). Stacks of $SrRuO_3/SrIrO_3$ (SIO) epitaxial layers integrate essential elements such as the Dzyaloshinskii-Moriya interaction (DMI), large perpendicular magnetic anisotropy (PMA), and spin-orbit torques (SOT) to stabilize magnetic skyrmions and enable their efficient current-driven motion. Bilayers of SRO/SIO are grown on TiO_2 terminated $SrTiO_3$ (STO) (001) substrates, where the growth of SRO is achieved via High Oxygen Pressure Sputtering (HOPS) and SIO via Molecular Beam Epitaxy (MBE). Precise control of film thickness is crucial to maintain the intrinsic properties of both materials and observe magnetic skyrmions. Therefore, we systematically vary the thickness of both the layers to optimize their magnetic properties, magnetoresistance and the Hall effect that includes ordinary Hall effect (OHE), anomalous Hall effect (AHE), and Topological Hall effect (THE). Given the challenges associated with directly observing skyrmions directly at the nano-meter scale in the real space, we employ the topological Hall effect as an indirect method to characterize magnetic skyrmions in ferromagnetic thin films[2]. For detailed interfacial and surface studies of the thin films, Polarized Neutron Reflectometry (PNR) and Grazing Incidence Small Angle Neutron Scattering (GISANS) will be performed. The expected results will test the hypothesis of the presence of ordered magnetic skyrmions and their contribution to the topological Hall effect in the bilayer oxide thin film, potentially advancing our understanding of skyrmion dynamics and their application in spintronics devices.
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Poster / **37**

Morphology-Controlled Synthesis and Characterization of Cobalt Ferrite Nanoparticles: Insights from SAXS and TEM

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Cobalt ferrite (CoFe2O4) nanoparticles have garnered significant attention due to their unique magnetic properties and potential applications in fields ranging from biomedicine to data storage. This study presents a systematic investigation of shape- and size-controlled synthesis of CoFe2O4 nanoparticles, focusing on spherical and cubic morphologies. We employed thermal decomposition method to synthesize nanoparticles with varying sizes.
The synthesized nanoparticles were characterized using a complementary approach combining Small Angle X-ray Scattering (SAXS) and Transmission Electron Microscopy (TEM). SAXS provided ensemble-averaged information on particle size distribution, shape, and interparticle interactions in solution, while TEM offered direct visualization of individual nanoparticles, confirming their morphology and size.
Our results demonstrate excellent control over nanoparticle shape and size, with SAXS data revealing distinct scattering patterns for spherical and cubic morphologies. Size distributions obtained from SAXS showed good agreement with TEM measurements, validating the complementary nature of these techniques.
This study highlights the effectiveness of combining SAXS and TEM for comprehensive nanoparticle characterization and underscores the importance of morphology control in tailoring the properties of CoFe2O4 nanoparticles for specific applications.

Poster / **53**

Tuning contact angle and colloidal stability by charge

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*Poster contribution
Self-assembled nanocrystal crystals of nanoparticles (NPs) offer the opportunity to create devices with collective properties from the individual NP building blocks. Applications in plasmonic, optoelectronic, catalysis, magnetic, phonon, biomedical and electrochemical devices with much improved performance are expected [1,2]. Large area 2D nanocrystals may be prepared by Langmuir type deposition, where particles are dispersed at a liquid/air interface and compressed by barriers to form close packed 2D nanocrystals. These can then be transferred onto solid substrates. The formed layer at the interface and its long-range order can be tuned by the particle size, surfactant shell properties, solvent interaction, charge, and magnetic moment of the particles among others. The fundamental science and optimization of this self-assembly is key to preparing large area functional devices at high throughput and low costs. One important parameter is the contact angle of the particles and the interface, which is related to the NPs affinity to adsorb at a fluid surface. Previous studies [3] and theory [4] suggests that the contact angle is dependant on the magnitude and sign of the charge of a single particle, since the air/water interface is believed to possess a negative charge. Also, a distance dependant out-of-plane force, pushing particles downwards and deforming the interface has been observed [3] because of the assymetric charge distribution of the particle surface in air and liquid medium. To add to this, we have tuned the charge magnitude and sign of negatively charged SiO2 nanoparticles by varying the amount of cationic surfactant coating. For these samples we aim to present results with neutron reflectometry, surface pressure-area isotherms, GISAXS and

UV-spectroscopy on the charge dependant contact angle, colloidal stability and long range order of films at the air/liquid interface and of transferred films to solid substrates.

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Poster / 40

A SANS design study for the HBS Science Demonstrator

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Aiming to develop a high-current accelerator-driven neutron source (HiCANS), the High Brilliance Neutron Source (HBS) project has extensively detailed its technical aspects in the conceptual and technical design reports [1][2]. The facility, based on a high-power linear proton accelerator delivering a 70 MeV proton beam with a peak current of 100 mA, is designed to supply three distinct target stations operating at different pulse frequencies. Each target station will provide pulses optimized for specific instrument groups, ensuring efficient use of the available beam and supporting a competitive suite of instruments.
A next step is the realization of an HBS Science Demonstrator, which aims to assess the scientific potential of HiCANS, providing a proton beam power of approximately 10 kW. It will feature a selection of highly demanded neutron instruments, among them a small angle neutron scattering (SANS) instrument. For this, we will present a conceptual design including ray-tracing Monte Carlo simulations using the software VITESS to optimize instrument parameters. Virtual experiments on select samples, representing typical use cases, will be used to quantify the instrument performance.

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Poster / 54

Port-GISANS: A portable GISANS booster for revealing the structure of complex interfaces

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Port-GISANS will be a module to enable grazing incidence small angle neutron scattering (GISANS) experiments for existing and future small-angle neutron scattering (SANS) instruments by improving flux and signal to noise ratio. This will allow GISANS experiments at ESS from day one on its SANS instruments. By focusing the incident flux on the sample and improving the signal-to-noise ratio Port-GISANS will enable high quality surface scattering experiments with neutrons addressing scientific questions which currently remain unsolved. The increase in flux has the potential to extend the applicability of GISANS for areas unfeasible today, such as single lipid membranes, which serve as benchmark here, as well as other weakly scattering or high background systems. Some systems of interest to highlight include curvature induced phase separation of biomembranes [1], responsiveness of lipid membranes to external stimuli in situ, such as exposure to light for photolipids [2], as well as the hydration and in-plane structure of DNA composites during encapsulation by protective shells [3], and micellar nanoreactors [4]. We aim to present simulation results of the performance of this device as well as simulations of the scattering from a realistic sample.

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Poster / **42**

Magnetic morphology of multishell nanoparticles

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The magnetism exhibited by magnetic nanoparticles (MNPs) is of intense research interest. These nanoscale materials exhibit complex magnetic behaviour, which is essential in the proposed applications, ranging from spintronics and catalysis to biomedicine, where they found their usage as contrast agents in imaging techniques or innovative cancer treatment (hyperthermia) [1]. For these purposes, broadly known iron oxide MNPs were thoroughly investigated in the past. However, we present a novel candidate, the ε-Fe3N, having unprecedented magnetic properties in bulk form, surpassing classical MNPs of iron oxides. In this contribution, we will present an in-depth characterization of passivated ε-Fe3N MNPs with a mean particle diameter of 17.2(2) nm. Unexpectedly, macroscopic magnetization measurements revealed low saturation magnetization (MS ≈ 40 emu/mg) compared to the bulk counterpart [2]. To sufficiently resolve the complex magnetic nature of passivated ε-Fe3N MNPs, the magnetic small-angle scattering with incident beam polarization at the D33 instrument at ILL [3] was employed to probe magnetic scattering fluctuations within MNPs. Finally,

we will show the radial distribution of nuclear scattering density, reveal the magnetic morphology of passivated ε-Fe3N MNPs, disentangle magnetization contributions from the magnetic core and shell, and ultimately discuss the resulting magnetic response of the MNPs.

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Poster / 21

SAGA: A surface scattering beam line for ESS

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Surface science has developed enormously over the last decades and interfaces play an increasing role in applications as well as many areas of science. This fact is in part related to new instrumental capabilities allowing to extract information with high resolution and sensitivity.
Neutron scattering methods offer unique opportunities, as the neutron is sensitive to light elements, low energy excitations and the magnetic induction. Surfaces and interfaces are studied with neutron reflectometry, which allows to extract density profiles along the surface normal. Lateral correlations can be studied by off-specular and grazing incidence small angle scattering (GISANS). However, sample volumes are small and neutron beams are comparably weak.
The European Spallation Source (ESS) will soon be commissioned and offer unprecedented brilliance for neutron scattering experiments. This offers a unique opportunity for the construction of a dedicated surface scattering beam line optimized for GISANS. In this presentation we summarize the scientific case and conceptual design of SAGA, which will be proposed as one of the instruments 16-22 at ESS. SAGA will offer high resolution to allow depth sensitive surface scattering studies and complement reflectometry and SANS capabilities at ESS. We propose a 65-70 m long instrument with a wavelength frame multiplication option for 1% wavelength resolution, including capabilities to measure neutron reflectometry. Once built the instrument will offer a platform to extract three-dimensional information on surface and near interface structures over a wide range of length scales. We submit this contribution on behalf of the SAGA consortium and will present the input from the working groups, focusing on the different aspects of the instrument specifications and design.

Poster / 46

Polarization analysis with 3He for functional interfaces

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Polarization analysis is a useful tool for probing magnetic order or disorder at interfaces. 3He spin filters are powerful because they can provide the 2D resolutions and high signal to noise needed to study such systems. A high performance in-situ polarized 3He polarization analyzer has been in user operation for over 10 years on MARIA (Magnetism reflectometer). More recently a similar analyzer has been commissioned for KWS-1 (SANS) with experiments at ISIS on ZOOM. We will present our unique in-situ polarizer devices and give some scientific examples of data obtained.

Poster / **48**

Anomalous magnetoresistance driven by interfacial proximity in superconductor/ferromagnet heterostructures

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Proximity effects (PE) are emergent phenomena that occur at the interfaces of appropriately designed superconductor (SC)/ferromagnet (FM) thin films heterostructures. PE arise due to the strong correlation and electronic competition in the antagonist phase materials. PE have potential applications in spin-triplet Josephson Junctions that involve the manipulation of fluxons, such as superconducting Qubits, for quantum computing [1–3]. Several types of PE were reported when considering heterostructures based on conventional SC and FM with either in-plane or perpendicular magnetic anisotropy (PMA). However, there are few contributions regarding PE in heterostructures based on high critical temperature (T_c) SC and FM with perpendicular magnetic anisotropy. $SrRuO_3$ (SRO) is a suitable FM candidate due to its strong PMA with narrow domain walls, high spin-orbit coupling, anomalous Hall and Berry effects, and excellent lattice match with the high-T_c SC $YBa_2Cu_3O_{7-x}$ (YBCO). We report magnetotransport results of epitaxial YBCO/SRO and SRO/YBCO heterostructures prepared on low miscut $SrTiO_3$ (001) single crystals by high oxygen pressure sputtering. We have observed intriguing proximity effects characterized by (i) a reduction in the SC T_c and (ii) an inversion of the magnetoresistance (MR) signal at the superconductivity onset. We suggest that the change in the MR signal is related to the competition between the FM and SC states within both samples. In addition, features in the MR curves that may be attributed to weak localization and antilocalization effects at the YBCO/SRO and SRO/YBCO interfaces were observed. Such features could be correlated to the high Ru deficiency in the SRO films and to a possible orbital reconstruction at the interfaces, which will be further investigated by synchrotron and neutron scattering techniques. This study enhances our understanding of the intricate relationship between magnetism and superconductivity in high-T_c SC/FM systems, illuminating potential future materials for quantum electronics.

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Poster / 59

Tuning the functionality of model lipid membrane with novel polymeric systems: a neutron scattering study

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The addition of synthetic polymers to lipid membranes has emerged as an effective route to modulate their properties and support them in performing biological functions [1]. The presence of polymers in the bilayer can alter the ordering and flip-flop activity of lipids, thus facilitating membrane permeation. In special cases, the addition of selected polymers results in membrane fracturing and the formation of peculiar structures (nanodiscs) that find useful applications for membrane proteins (MPs) handling in solution [2]. Despite the considerable fundamental and applicative interest, the molecular interactions between synthetic polymers and biological interfaces are yet not fully understood, and a rationale is lacking in the design of polymer structures aimed at supporting specific membrane tasks.
In this work, we investigate model lipid membranes as platform for the insertion of a novel class of polymers (alternating amphiphilic polymers or AAPs [3]) featuring unique characteristics and combining high chemical malleability with bio-compatibility, which make them a promising tool to investigate polymer-membrane interactions and optimize membrane activities. The structural modifications induced by the polymers have been investigated by experimental techniques including small-angle neutron scattering (SANS) and neutron reflectometry.

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The influence of the SARS-CoV-2 spike protein on red blood cells

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Almost 4 years into the Covid-19 pandemic, its repercussions go far beyond a simple respiratory infection. A current study estimates that more than 13 % of Covid-19 patients develop Long Covid

(LC) with symptoms such as shortness of breath, memory loss and, most prominently, a debilitating, chronic fatigue (CF). Similar post-viral complications (PVC) including CF have also been observed after other viral infections. Micro-blood clots including red blood cell (RBC) stacks (”rouleaux”) found in Covid-19 patients’ blood samples appear to contribute to LC/CF, e.g. by interfering with oxygen transport. Evidence suggests that the SARS-CoV-2 surface spike protein (”Spike”), which circulates in the bloodstream after a Covid-19 infection binds to RBC membranes [1] and triggers blood coagulation [2]. A detailed investigation of the structural aspects of spike protein binding to RBCs is the 1st part of this study: To address this question, we performed SAXS/ SANS experiments with RBCs at different ionic strength of the buffer solution and studied the effect of spike protein binding on cellular RBC properties. From the measured protein-protein structure factors we determined the intracellular hemoglobin concentration that is informative on morphological shape of the RBCs. Our results reveal a swelling of RBCs upon spike protein binding under all investigated conditions. Effectively, an osmotic counter pressure of around 50 mOsm is needed to counterbalance the swelling effect caused by the spike protein under physiological conditions. A 2nd part of our project zooms in on the role of the stiffness of biological RBC membranes and the effect of the spike protein on RBC membrane bending stiffness. We performed NSE experiments on liposomes prepared from entire RBC membranes and determined the RBC membrane bending modulus within the Zilman-Granek model. Our results demonstrate that RBC membrane stiffness is not affected by spike protein binding. However, an additional dynamic mode at low q-vectors could be observed in native RBC membranes that is suppressed upon pathological conditions induced by spike protein binding. Our study reveals molecular effects of spike protein binding on RBC membranes that affect cellular RBC properties which might lead to impaired oxygen transport and an increased thrombosis risk of Covid-19 patients.

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