12TH INTERNATIONAL MEETING OF THE SPANISH SOCIETY ON NEUTRON TECHNIQUES

13-15 JULY 2026 BILBAO

BOOK OF ABSTRACTS

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PLENARY

PL.1. Studying Soft Matter and Bioscience Systems with Neutrons

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Neutron scattering is a powerful technique for studying a wide variety of soft matter and biological systems as it can be used to determine both spatial and temporal information of multicomponent systems at the nanoscale.

The Soft Matter and Life Science Communities exploit both diffraction and spectroscopic techniques such as small-angle neutron scattering (SANS), neutron reflectometry (NR) and quasi-elastic neutron scattering (QENS) to study a broad range of systems across a large size and time regime.

Examples include comparing water dynamics in human cancer and non-cancer tissues [1], harnessing carbon dioxide as a green solvent (see Fig. 1) [2], studying supramolecular interactions in a MOF [3] and unlocking the molecular mechanism of rare antibiotics [4].

In recent years, the number of proposals requesting time to study both soft mater and life science systems have grown and the complexity of the experiments proposed has also increased. It is likely that this trend will continue as these areas of science are well supported by both the UK's Modern Industrial Strategy [5] as well as by the ISIS Science Strategy.

Current science highlights from the ISIS Neutron and Muon Source will be discussed as well as a taste of the new science to come.

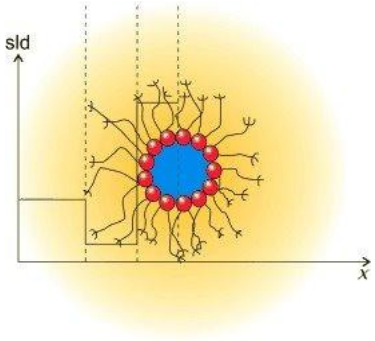

Fig.1: Schematic of a water in carbon dioxide microemulsion droplet, the structure of which can be studied via SANS.

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PL.2. Li-ion Batteries: a gateway to new compounds and new structures

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For improving lithium ion batteries, finding new electrode materials, determining their structure and being able to follow their structural evolution on charge and discharge is essential and powder diffraction is a method of choice. In this talk, I will present the strategy we use at the lab “Chimie du Solide et Energie” at Collège de France (Paris) to get useful information from diffraction experiments on battery materials, and how important a rigorous analysis of these data is for a reliable characterization. My talk will be illustrated by examples based on neutron and X-ray powder diffraction both in the field of electrode materials and ionic conductors, the developments of the latter being an important step towards the development of safe all-solid-state batteries. Lastly, it will be shown that other communities – e.g. solid state physicists- may benefit from research in materials for batteries with the discovery of compounds presenting interesting magnetic properties.

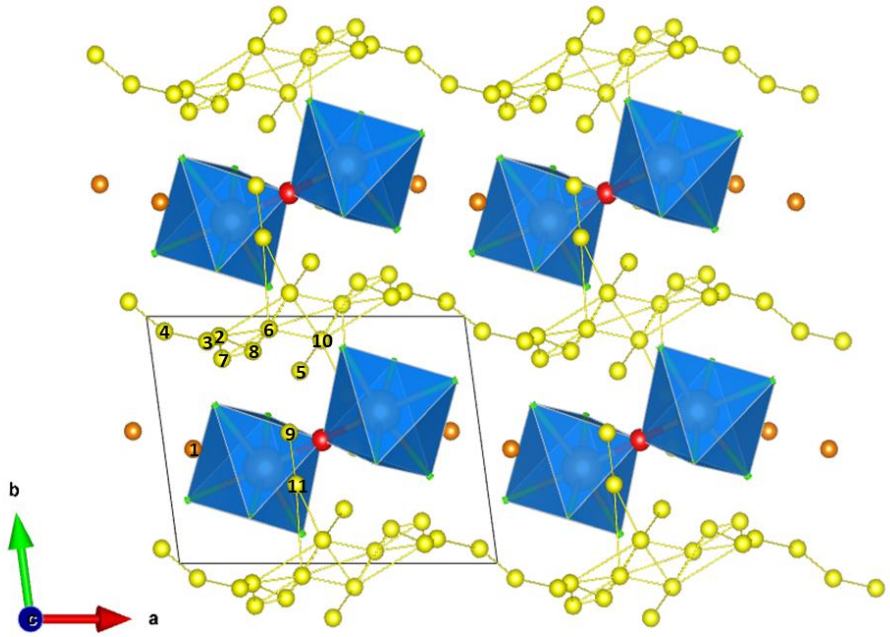

Fig.1: Illustration of the Li conduction paths in $Li_2Ta_2OCl_{10}$ [1]

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PL.3. Neutron Scattering with Polarization Analysis: New Insights into Collective and Self Dynamics of Liquids and Glass-forming Systems

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There is no doubt about the unique capabilities of neutron scattering to characterize structural and dynamic properties of matter. Particularly important is the potential, playing with isotopic labelling, of accessing different correlation functions (collective, self) or 'isolating' the signal of a given component or molecular group in a complex system. However, the coexistence of coherent and incoherent contributions to the scattered intensity is, in most of the situations, unavoidable. These contributions can only be separated by applying polarization analysis. The recent implementation of this capability in spectrometers, in particular in the case of PLET at ISIS with sub-meV resolution, opens the possibility of investigating problems / systems that could not be approached in a rigorous way until now. One of them is the question of the collective dynamics of liquids and glass-forming systems in the mesoscale or intermediate length scales region, i. e., at length scales larger than the intermolecular ones but not yet in the hydrodynamic regime. First PLET experiments provided new insight on this intriguing problem on water (H-bonded liquid) and tetrahydrofuran (van der Waals liquid) [1,2]. Those investigations were extended to other molecular liquids like glycerol, propylene carbonate, tributyl phosphate, 2-ethyl-1hexanol or squalane [3-5], in order to proof the universality of the phenomenology found. To do this, Neutron Spin Echo results on protonated and deuterated counterparts of the molecules were analyzed in a combined way as proposed in Ref. [6]. The procedure followed allows to deduce in a good approximation the coherent and incoherent contributions. For the data interpretation, the synergetic use of molecular dynamics simulations was crucial [7]. Here we present an overview of all these studies, which clearly show a universal non-dispersive mode as the predominant relaxation channel for density fluctuations at the mesoscale.

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KEYNOTE

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K.1. Neutron Scattering as a Tool to Study Spin Textures in Magnetic Nanomaterials

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Understanding the complex magnetic microstructure of nanomaterials—and its connection to bulk magnetic behavior—requires the complementary strengths of experimental characterization and computational modeling. Among the available techniques, magnetic small-angle neutron scattering (SANS) is particularly powerful, as it provides direct access to intricate spin textures on mesoscopic length scales (~1–1000 nm) deep within the bulk of magnetic materials [1]. Extensive SANS studies have revealed a wide variety of nonuniform spin configurations in nanostructured magnets, ranging from quasi-uniform and canted states to vortex-like and core–shell-type arrangements [1], underscoring the remarkable diversity of nanoscale magnetic textures. In parallel, micromagnetic simulations have become indispensable for predicting mesoscale spin structures and their corresponding scattering signatures. These simulations account for key factors such as particle size and shape, structural defects, and competing magnetic interactions that govern the magnetic ground state of nanoscaled systems. In this combined theoretical and experimental talk, we discuss neutron-scattering signatures associated with several characteristic features of the magnetic microstructure in nanomaterials. These include dipolar-energy-driven vortex states in magnetic nanoparticles [2]; the influence of the Dzyaloshinskii–Moriya interaction [3] and surface anisotropy [4]; characteristic signatures arising from hopfion textures [5]; the observation of scaling [6]; and the experimental observation of a recently predicted spin-disorder-induced angular anisotropy in the polarized neutron-scattering cross section [7] (see Fig. 1).

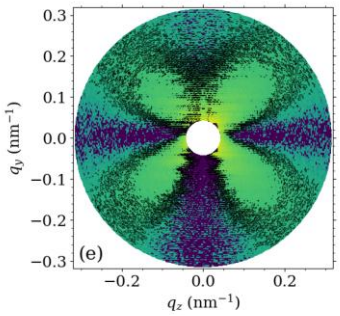

Fig.1: Spin-disorder-induced angular anisotropy in the polarized SANS cross section.

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K.2. From Molecular Vibrations to Energy Materials: Insights from Inelastic Neutron Scattering

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High-energy inelastic neutron scattering (INS) is a vibrational spectroscopy technique that is complementary to more conventional methods such as Raman and infrared spectroscopy. Its unique capabilities arise from the properties of neutrons, which are electrically neutral particles possessing a magnetic moment. Its sensitivity to all types of atomic motion makes it a powerful tool for detailed studies of the vibrational modes of materials, particularly hydrogen-containing materials.

IN1-Lagrange is an instrument dedicated to the study of atomic excitations in complex materials, located on the hot neutron source at the Institut Laue-Langevin. The instrument is unique at the ILL in combining a wide energy range (1–1000 meV), high count rates, and flexible energy resolution over a broad energy-transfer range. These characteristics open up new opportunities for spectroscopic investigations of complex materials.

In this presentation, I will discuss several examples illustrating the use of INS in energy-related materials. Applications will include gas separation in metal–organic frameworks (MOFs) [1], the characterisation of acid sites and adsorbed molecules in zeolites [2], and hydrogen and methane storage in mesoporous carbons [3,4].

Finally, I will introduce a new setup for IN1-Lagrange that will enable simultaneous Raman and INS measurements. The combination of both techniques will provide complementary information on molecular and lattice vibrations, allowing a more complete interpretation of complex spectral signatures in functional materials.

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K.3. New opportunities for Neutron Imaging at the Institut Laue-Langevin

L. Helfen [1,*], A. Tengattini [1,2], A. Fedrigo [1], J. Shen [1], B. Lukić [1], N. Kardjilov [3], K. Buckley [1], B. Giroud [1], E. Ruiz-Martinez [1]

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The Institut Laue-Langevin (ILL) has engaged in the process of considerably increasing the instrumentation dedicated to transmission imaging techniques available to the neutron user community. The upgrade of the established neutron and x-ray tomography instrument NeXT [1] (located at the former D50 port on a curved cold neutron guide) added monochromators and advanced contrast modes (such as grating interferometry and polarised imaging), as well as greater flexibility concerning experimental conditions and space for bulky sample environments. The monochromatic side-station MoTo was included to provide monochromatic tomography (to reduce beam-hardening artefacts) and advanced contrast modes with usually long scanning times. In 2025, The instrument PorTo (portable tomograph) was commissioned on ILL's PF1B port and provides increased access to high-resolution neutron imaging. Finally, the thermal neutron imaging station ThRILL is under construction in the reactor building to address very fast imaging as well as larger samples for typical engineering applications where increased penetration power and high flux for *operando* imaging is needed.

This presentation introduces the different imaging instruments available (or foreseen) at the ILL and gives an overview of their (expected) experimental capabilities and conditions. Examples from typical application fields will be shown to outline their attractiveness in different areas of science and engineering.

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K.4. From Static Structures to Molecular Movies: Time-Resolved Crystallography at X-ray Free-Electron Lasers

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Understanding how matter evolves in space and time is a central challenge across physics, chemistry, biology, and materials science. While conventional diffraction methods provide detailed structural information, many functional processes including catalysis, phase transitions, charge transfer, ligand binding, and allosteric regulation, are inherently dynamic and often occur on ultrafast timescales. X-ray Free-Electron Lasers (XFELs) have emerged as transformative research infrastructures capable of probing these transient phenomena with unprecedented temporal and spatial resolution. By delivering ultrashort femtosecond X-ray pulses, XFELs enable diffraction measurements before radiation damage occurs, allowing the study of matter under near-native and non-equilibrium conditions. Among XFEL methodologies, Time-Resolved Serial Femtosecond Crystallography (TR-SFX) has become a powerful approach for visualizing structural dynamics in crystalline systems. By combining reaction triggering, such as optical excitation or rapid mixing, with serial diffraction measurements, TR-SFX enables direct observation of transient intermediates and reaction pathways from femtoseconds to seconds. Although pioneered in structural biology, these methods are increasingly applied to chemical and materials sciences. XFELs are highly complementary to neutron and synchrotron techniques. While XFELs reveal ultrafast structural changes and short-lived intermediates, neutrons provide unique sensitivity to hydrogen atoms, magnetic phenomena, and collective motions. Together with spectroscopy and simulations, these approaches offer a powerful framework for connecting structure, dynamics, and function across multiple scales. This lecture will provide a multidisciplinary introduction to XFELs and TR-SFX and discuss how their integration with complementary techniques is advancing our ability to generate experimentally derived molecular movies of complex systems.

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K. 5. Polarized neutron diffraction for the study of novel (and not so novel) quantum materials

J.A. Rodríguez Velamazán [1,*], S. Vial[1], N. Qureshi [1], O. Fabelo[1]

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The study of novel (or, in some cases, rebranded) quantum materials requires the use of non-conventional neutron diffraction techniques, which give valuable - and sometimes crucial - insight into the subtleties of the magnetic structures that these materials may present. In this talk, we will illustrate the contribution of polarized neutron diffraction techniques, such as spherical neutron polarimetry and half-polarized neutron diffraction, to the investigation of this kind of systems, with examples concerning the emerging topics of altermagnetism [1] and ferrotoroidic materials [2,3].

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K.6. Neutron scattering for study bio-macromolecules

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Misfolded proteins and peptides can form insoluble and highly stable specific aggregates, called amyloid fibrils. Such aggregates are related to various neurodegenerative diseases. Using some model proteins, there have been a variety of studies aiming to understand the mechanism of amyloidosis and to develop detection methods at an early stage to prevent fibril´s formation and/or to decompose mature amyloid fibrils. Knowing how the amyloid formation occurs in general and the effect of different agents on amyloid formation/destruction can drive the development of more efficient anti-amyloid agents. Moreover, detailed structural/morphological information may help to tune the properties of complex systems with bio-macromolecules. In this regard, we performed a comprehensive analysis of amyloid fibrils formation, with an emphasis on studying changes in proteins structure and dynamics during amyloids formation by applying different neutron scattering methods in our investigation.

It is well known that neutron scattering is unique and powerful method for structural and dynamic study of various multicomponent systems. During the talk our neutron scattering studies of bio-macromolecules will be presented. Thus, I will start from small-angle neutron scattering investigation of the amyloids structures and effect of different anti-amyloids agents on the inhibition/destruction of the amyloids. Then some reflectometry experiments for the interface study will be presented. And finally, our recent attempt to study changes in the protein dynamics during amyloid fibril formation and description of the inhibition/destruction effects of anti-amyloids agents on protein amyloids by quasi-elastic neutron scattering will be discussed. And then correlation between the structural, fluorescence and computer simulation data with the dynamic of protein molecules will be presented.

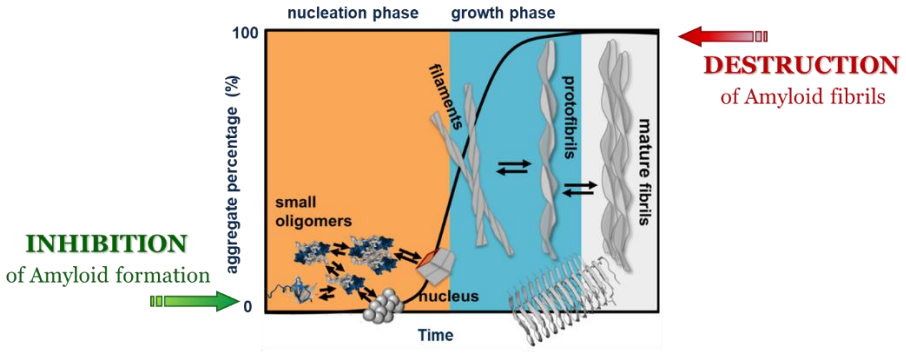

Fig.1: Effect of additives on protein amyloids inhibition and destruction

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ORAL PRESENTATIONS

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O.1. Toroidicity as a route towards non-volatile quaternary memory in antiferromagnets

N. Qureshi[1,*], A. Painganoor[1,2], M. C. Larsen[2], M. Ravn-Feld[2], K. Beauvois[3], J. A. Rodríguez-Velamazán[1], D. Vaknin[4], P. Steffens[1], R. Toft-Petersen[2,5], N. B. Christensen[2]

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Magnetoelectric materials couple magnetic and electric properties and are promising candidates for future data storage applications. While strong coupling between the two order parameters leads to cross-switchability, the separate actuation enables four different polarization states offering prospects for a quaternary memory device, an attractive high-density memory concept, especially in the post-Moore-law era. However, most reported systems rely on composite materials combining multiple components, and typically include at least one ferro- or ferrimagnetic phase that is sensitive to stray fields.

Here, we present a study on a bulk single-crystal of antiferromagnetic and ferrotoroidic $LiNi_{0.8}Fe_{0.2}PO_4$ in which a spontaneous tilt of the head-to-tail spin configuration leads to the presence of four different magnetic domains. Ferrotoroidicity—the fourth ferroic order [1] alongside ferromagnetism, ferroelectricity and ferroelasticity—is a key ingredient in the domain selection.

In this study, polarized neutrons provide the central experimental probe. We employ Spherical Neutron Polarimetry (SNP) which reveals microscopic information about the magnetic domain formation and has been particularly powerful in the investigation of magnetoelectric domains [2]. SNP is furthermore sensitive to toroidal domain populations and has previously enabled the demonstration of toroidal moment control in $LiFeSi_2O_6$ [3] and $Cs_2FeCl_5 \cdot D_2O$ [4] when cooling in a conjugate field **E** x **H**. Here, we extend the binary to quaternary domain control: In $LiNi_{0.8}Fe_{0.2}PO_4$ the axis and sense of the neutron spin rotation—as detected by SNP—bears the fingerprint of each of the four possible magnetic domains. Our results highlight a potential route towards the realization of high-density data storage devices based on single-phase antiferromagnetic materials [5].

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O.2. Unravelling Buried Interfaces: Using Neutron Reflectometry to Optimize Interphase Design and Mitigate Device Degradation

M. Salado[1,2*], L. Huang[3], V. Petrenko[1,2], M. Forsyth[3], A. Le Brun[4], T. Saerbeck[5] and J. M. Porro[1,2]

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Neutron reflectometry (NR) is a paramount analytical technique for characterizing multilayer devices and interfaces, offering sub-nanometer structural information as a function of depth along the surface or interface. Unlike X-ray techniques, which often struggle with the low scattering length density (SLD) of organic compounds, NR is highly sensitive to light elements. Moreover, the contrast between hydrogen and deuterium allow us to track the evolution and distribution of specific organic components within a complex multi-layered film.

During this talk, I am going to explain two cases of study in the energy field where in situ NR was applied. First related to energy storage such as sodium metal batteries to investigate how mixed-cation ionic liquid electrolytes modulate the electrical double layer (EDL). More specifically, how incorporating larger phosphonium cations (P_{1444}^+) facilitates a significantly higher concentration of Na^+ ions and coordinated FSI^- anions at the electrode surface. This structural shift directly promotes more favourable kinetics for solid electrolyte interphase (SEI) formation, resulting in a fivefold increase in cycling lifespan and reduced polarization.

Similarly, in the field of perovskite solar cells, NR was used to unravel the degradation mechanisms triggered by humidity and temperature. By selectively deuterating cations like FAI or MABr, it has been able to distinguished between the stability of different organic compounds. NR profiles demonstrated that moisture ingress causes an irreversible stratification of the film: FAI tends to accumulate near the surface, while MABr and PbI_2 accumulate at the substrate interface. Furthermore, NR confirmed that mesoporous TiO_2 layers enhance structural stability by mitigating this stratification, providing a clear pathway for optimizing device architectures for real-world conditions. Ultimately, NR serves as a bridge between nanoscale interfacial architecture and macroscopic device performance, proving essential for the design of stable, next-generation energy technologies.

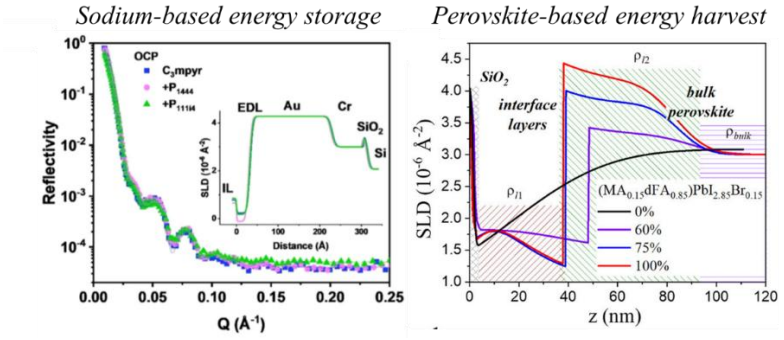

Fig.1: (a) NR curves for electrolytes/electrode interfaces at OCP. (b) Neutron SLD profiles of the $MA_{0.15}/dFA_{0.85}$ on Si, for different humidity conditions.

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0.3. Resolving Polymer Dynamics in Dipolar Glass Systems

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Dipolar glass polymers (DGPs) are promising high-dielectric materials because their polar side groups can reorient under an electric field, enhancing polarization [1]. However, their dielectric response results from overlapping molecular motions, from localized dipole rotations to cooperative segmental dynamics, making interpretation difficult. In many applications, these materials are used as thin films or nanostructured layers, where confinement can strongly modify molecular mobility. Here, confinement and selective deuteration are used as complementary strategies to study molecular dynamics in two representative DGPs: poly(2-(methylsulfonyl)ethyl methacrylate) (PSO_2MA) and poly(2-cyanoethyl methacrylate) (PCNMA) (Fig. 1) [2]. Protonated and selectively deuterated polymers were synthesized by RAFT polymerization, and nanoconfined samples were prepared by infiltration into anodic aluminum oxide (AAO) templates [3]. Broadband dielectric spectroscopy (BDS) was used to analyze secondary and segmental relaxations, while elastic fixed-window scans (EFWS) on the FOCUS neutron spectrometer were employed to detect motions of specific hydrogen-containing groups. BDS reveals clear sub-glass secondary relaxations in both systems, associated with motions of sulfone and nitrile side groups, together with the higher-temperature α-relaxation related to cooperative backbone motion. In addition, nanoconfinement further modifies the dielectric response of both polymers, highlighting the role of restricted geometry and polymer-surface interactions. Neutron scattering shows that deuteration is an effective tool to separate these contributions. In PSO_2MA, a first dynamical process near 180 K appears in all isotopic variants, indicating motions of the methyl group attached to the sulfone unit. Additional processes at higher temperatures are assigned to side-chain and backbone mobility. In PCNMA, where this methyl group is absent, the first relaxation shifts to higher temperature, reflecting different local dynamics. Backbone-deuterated samples also display clear signatures of the glass-transition region, helping to distinguish local from segmental motions.

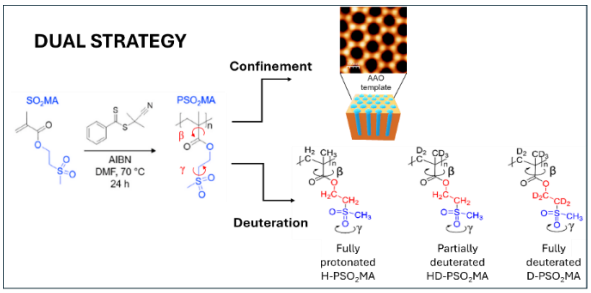

Fig.1: Two complementary strategies used to investigate molecular dynamics DGPs: nanoconfinement and selective deuteration.

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O.4. The role of the lipid helper in LNP structure, composition, and how protein corona forms

Marite Cardenas

Fundacion Biofisika Bizkaia
Ikerbasque Foundation

Lipid nanoparticles (LNPs) are the leading delivery platform for mRNA therapeutics, yet their structural evolution upon exposure to biological fluids remains poorly understood. Here, we employ small-angle neutron scattering (SANS) with contrast variation and selective deuteration to resolve the internal structure and lipid distribution of LNPs before and after incubation with serum proteins. By selectively deuterating individual lipid components, we distinguish the spatial organization of the ionizable lipid, cholesterol, PEGylated lipid, and helper lipid within the nanoparticle ultra strcutre. Our results reveal that the helper lipid plays a central role in defining the shell structure of LNPs, governing both its thickness and compositional organization. Critically, variations in helper lipid identity directly modulate the extent and kinetics of protein corona formation, with downstream consequences for LNP restructuring upon serum exposure. LNPs formulated with different helper lipids exhibit distinct structural rearrangements. These findings establish a mechanistic link between the initial lipid shell structure, mediated by the helper lipid, and the biological fate of LNPs in protein-rich environments. Our work demonstrates that SANS provides unique, label-free access to the nanoscale structural transitions that conventional techniques such as dynamic light scattering or cryo-TEM cannot resolve in situ, and highlights helper lipid selection as a rational design lever for controlling protein interactions and preserving LNP integrity in vivo.

O.5. Reorientational dynamics across a solid–solid transition in tetrachloro-*m*-xylene studied by quasielastic neutron scattering

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Orientationally disordered molecular crystals, or plastic crystals, retain long-range translational order while allowing molecular reorientations, making them model systems to study the coupling between molecular mobility, local ordering and crystallographic symmetry [1,2]. Tetrachloro-*m*-xylene (TCMX), a hexasubstituted benzene derivative, was previously considered to transform directly from its low-temperature orientationally (in-plane) disordered phase to the liquid [3]. Here, differential scanning calorimetry and powder X-ray diffraction reveal a weak but reproducible solid–solid transition at 437 K, from a monoclinic phase II to an orthorhombic phase I [4].

We carried out QENS measurements using complementary instruments: OSIRIS (at ISIS) and IN16B (at ILL) to study the reorientational dynamics of TCMX. Fixed-window scans show that molecular reorientations progressively enter the instrumental time window on heating, with a clear change near the II → I transition. Full QENS spectra are well described by a single dominant reorientational process in both phases [4].

The relaxation times obtained from OSIRIS and IN16B follow a common Arrhenius trend, showing that the activation energy remains essentially unchanged through the phase transition. Moreover, the elastic incoherent structure factor is well reproduced by a six-site jump model, consistent with discrete 60° in-plane jumps around the pseudo-sixfold molecular axis. Molecular dynamics simulations support this picture and show that the transition originates from the loss of weak orientational correlations between neighbouring molecular columns, restoring higher symmetry in phase I without changing the underlying rotational mechanism.

TCMX therefore provides a rare example of a disorder–disorder solid-state transition in which the high-symmetry phase emerges from a collective reorganization of orientational correlations, while the underlying 60° reorientational jumping mechanism remains essentially unchanged.

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O.6. Neutrons for conservation of stone materials and organic based artefacts in cultural heritage. The project nanoHERCULES.

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The conservation of our cultural heritage (CH) is of utmost and ever increasing importance. Considerable effort has been devoted to better understand the degradation processes and to find new techniques for conservation and restoration tailored to materials relevant to CH applications. The variety of materials in use as well their intrinsic complexity (composite nature, multifunctionality...) poses a challenge to scientists and conservators working in this area. Often validation of materials and formulations is limited to laboratory tests; the development of technologies for large-scale applications may highlight new problems, particularly when seeking long-term solutions. In the last years, nanoparticles (NPs) of earth-alkaline metal hydroxides were proposed for conservation of stones materials and for wood de-acidification, but their use presented a lot of limitation due to the synthesis method: they generally require organic compounds (no health compatible), and multi-step, time and energy-consuming procedures, with low specific yields of production and high costs, limiting them to niche uses or on very small areas. Prof. G. Taglieri patented [1] a new one-step process of synthesis of NPs overcoming many of the problems associated with previous procedures. The new protocols combine synthesis of highly dispersed NPs (few tens of nano-meters), in water, with higher reactivity, stability and deeper penetration into damaged materials, produced on large scale and feasibility to modify and optimise functionality. The innovative NPs are tailored to enhance compatibility, sustainability and long-term preservation, restoration and consolidation, on a large scale, of decorative architectural surfaces (stones, mortars, stuccos, mural painting and frescos), and of organic materials, such as ancient paper and wooden artefacts (shipwrecks, statues, ancient tools and utensils). We used neutron tecniques, as small angle neutron scattering, to study the NPs directly in suspension (in terms of shape, size, size distribution and solvent interaction and aggregation state), to drive their production on large scale, for curative and preventive eco-friendly treatments for waterlogged wood and stones materials. Furthermore, we used neutron diffraction and neutron tomography to investigate the substrates and the changes after NPs treatment. We investigated mortars and stones from the new excavation of Colosseum (Fig.1) and from the Greek theatre of Agrigento and ancient wood from shipwreaks of Gallo-Roman period. I will present the main results of our study together with the perspectives of using neutrons in our project, recentely funded: nano-HERCULES **nano**-particles for **HER**itage and **CUL**ture in **E**nvironmental **S**ustainability).

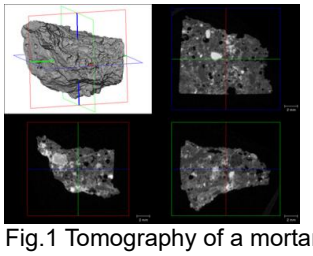

Fig.1 Tomography of a mortar from the floor of Colosseum

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O.7. Is there a new magnetic phase in MnSi, known as the B phase, at low temperatures?

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In cubic chiral magnets, Dzyaloshinskii-Moriya (DM) interactions within the chiral crystal structure result in diverse magnetic textures, including skyrmion lattices (SkL) and chiral soliton lattices, which hold promise for spintronic and magnonic devices. Among these, MnSi has been extensively studied due to the SkL formation in the so-called "A-phase" just below T_c [1]. Recently, it was suggested theoretically that at low temperatures (T), the conical helimagnetic (CH) and forced-ferromagnetic (FFM) phases in MnSi might not be directly connected but separated by another SkL phase, possibly metastable, or a new phase of *unknown* nature near the critical magnetic field (B_c) [2]. The theoretical prediction of the new SkL phase at low T is in good agreement with the experiments reported in MnSi and Cu_2OSeO_3 [3,4]. On the other hand, by using careful ac susceptibility measurements at low temperature, we determined the magnetic phase diagrams of oriented crystals of MnSi [5]. A new unexpected region, termed "B-phase", was observed when the magnetic field was applied along the main diagonal <111>.

To clarify the nature of the "B-phase", we performed small-angle neutron scattering (SANS) measurements at TAIKAN in J-PARC and transverse field (TF)-μSR experiments at TRIUMF. At low temperatures and fields near B_c, SANS patterns revealed two peaks along the horizontal axis, corresponding to the magnetic Bragg peaks of the CH state. Notably, no diffraction peaks indicative of a six-fold-symmetric SkL were observed. Meanwhile, μSR results showed a distinct internal magnetic field distribution in the "B-phase", different from those in the CH or FFM phases, suggesting that the "B-phase" could involve a reorientation of Mn helices within the unit cell.

In the presentation, we will discuss these SANS and μSR findings in detail and their implications for understanding the spin texture in the "B-phase".

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O.8. Producing an optimal accelerator-based clinical neutron beam for Boron Neutron Capture Therapy.

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Boron Neutron Capture Therapy (BNCT) is an emerging experimental cancer therapy with strong potential for the treatment of diffuse, infiltrative, and poor-prognosis tumours, where conventional therapies still face major limitations [1]. BNCT combines biological and physical selectivity through the administration of a boron-10-enriched radiopharmaceutical that preferentially accumulates in tumour cells. Subsequent local irradiation with low-energy neutrons induces the nuclear reaction $^{10}B(n,\alpha)^{7}Li$, producing high-LET alpha particles with cellular-range penetration depth, enabling the selective destruction of tumour cells while preserving surrounding healthy tissue [2].

Within this framework, the Chair “Neutrons for Medicine” at the University of Granada (UGR) has developed an innovative neutron production technology based on advanced high-heat-dissipation Li targets for accelerator-based BNCT systems [3] and a beam shaping assembly that produces a epithermal neutron beam which accomplished all IAEA recommendations [4].

A new collaboration between UGR and the Accelerator-Based BNCT team at the *Laboratoire de Physique Subatomique et de Cosmologie* (LPSC, Grenoble, France) aims to experimentally validate the thermal dissipation capability and structural robustness of the developed target under realistic irradiation conditions [4]. Experimental validation will be performed using the LPSC high-power electron beam irradiation facility, specifically designed for BNCT neutron target testing. With respect to the beam shaping assembly (BSA), a proof of concept of the moderation by means of sinterized MgF2 has been performed at MONNET (JRC Geel) [5]. These works represent a significant step toward the development of reliable accelerator-based neutron sources for medical applications and is expected to advance the technology toward prototype demonstration in a relevant operational environment.

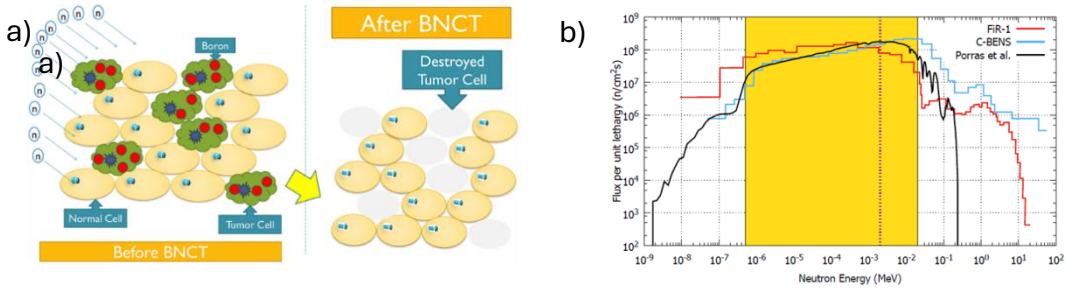

Fig. 1: a) Schematic representation of cells selectively enriched with ^{10}B: (a) before and (b) after BNCT. b) Spectrum from the BSA compared to facilities in Japan (C-BENS) and Helsinki (FiR-1).

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O.9. Definitive Mapping of Correlated and Uncorrelated Defectivity in Zr(IV)-MOFs studied by means of High-Resolution X-Ray and Neutron Diffraction

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The high connectivity of Zr(IV)-MOFs allows them to accommodate significant linker and cluster defects in their structures. Such defectivity can be non-correlated – with minor impact on XRD- and long-range correlated—generating distinctive XRD-signatures.[1] For example, in UiO-66, correlated cluster defects give rise to super-structural reflections associated with a symmetry reduction. However, linker or combined linker–cluster correlated defectivity have not been investigated by diffraction yet. Analogous group–subgroup relationships due to correlated defectivity have been reported for Zr-MOF constructed from C_4-linkers *(i.e. MOF-801)* or porphyrin linkers *(i.e. PCN-224)*.[2]

In this study, we address the combined quantification of correlated and non-correlated linker and/or cluster defectivity in UiO-66, MOF-801 and PCN-224 via XRD and ND.[3] For the studied families, a series of materials have been synthesized by modulating defectivity. Rietveld analyses were performed under three initial scenarios: (I) **high-symmetry, non-correlated defectivity**: average linker defects were quantified by refining the occupancy of the crystallographic independent linker; (II) **fully correlated linker-defectivity - low-symmetry model**: one crystallographic independent linker is fully vacant while the other is fully occupied; and (III) **combined correlated and non-correlated low-symmetry model:**, the occupancies of both crystallographic independent linkers are refined. Four are the main conclusions of the analysis. (I) the quality of the fitting when combining non-correlated and correlated defectivity is better in comparison with the fittings obtained from non-correlated or fully correlated defectivity (Fig. 1). (II) as the weight of the contribution of the linkers increases in the models, the quantification of the occupation factors of both crystallographic-independent linkers is more accurate. (III) for non-activated samples there is a strong correlation between the fitting of the solvent species and the occupation of the linkers; and, (IV), the XRD data do not allows detecting differences on the linker occupancies of the studied materials. All in all, in this study, we offer the tools and the protocols to accurately map the correlated and uncorrelated defectivity in Zr(IV)-MOFs that can be applied to analogue reticular materials.

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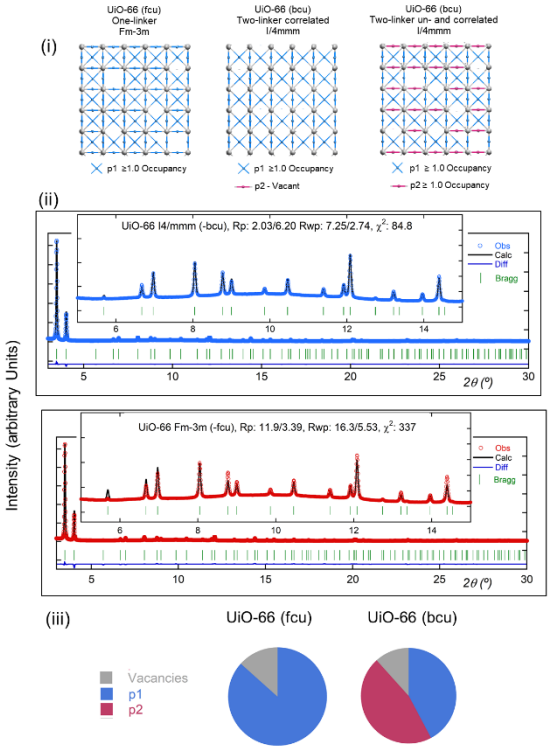

Figure 1. (i) Simplification of the models for UiO-66. (ii) Comparison of the fitting for the low and high-symmetry models. (iii) Occupancy factors for the linkers obtained from the fittings.

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O.10. Impact of Si–Ge Substitution on the Magnetic Ordering and Magnetocaloric Performance of *$Tb_2Co(Si,Ge)_2$* Intermetallics

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Understanding the relationship between magnetic ordering and magnetocaloric performance is essential for the development of efficient magnetic refrigerants. In this work, we investigate the structural, magnetic, and magnetocaloric properties of the Sc_2CoSi_2-type (C2/m space group, N 12) intermetallic compounds Tb_2CoSi_2 and Tb_2CoGe_2, with particular focus on the effect of Si–Ge substitution. Magnetization measurements combined with neutron diffraction studies reveal that replacing Si with Ge expands the unit cell and strongly modifies the magnetic interactions.

Tb_2CoSi_2 exhibits a paramagnetic (PM) to ferromagnetic (FM) transition at T_C = 198 K, followed by spin reorientation at T_m = 75 K and an antiferromagnetic (AFM) transition at T_N = 13 K. In contrast, Tb_2CoGe_2 undergoes a PM to AFM transition at T_N = 126 K before evolving into an FM-like state at T_M = 66 K. Neutron diffraction confirms Tb_2CoSi_2 is an *ac*-plane collinear ferromagnet below T_C (C2'/m magnetic space group), while Tb_2CoGe_2 is an *ac*-plane collinear antiferromagnet below T_N. Upon application of an external magnetic field, Tb_2CoGe_2 exhibits a metamagnetic transition from an AFM state to a mixed collinear FM+AFM state. Both compounds show complex non-collinear ferro-antiferromagnetic ground states.

A highly desirable "table-like" magnetocaloric effect over a wide temperature range is observed in both compounds, which is essential for an efficient Ericsson-cycle based refrigeration system. For a field change of 5 T, the peak entropy change $|\Delta S_M^{pk}|$ reaches 4.45 J/kg·K for Tb_2CoGe_2. These results highlight Si-Ge substitution as an effective mechanism for tuning magnetic properties in this intermetallic family to optimize performance for N_2 and H_2 gas liquefaction.

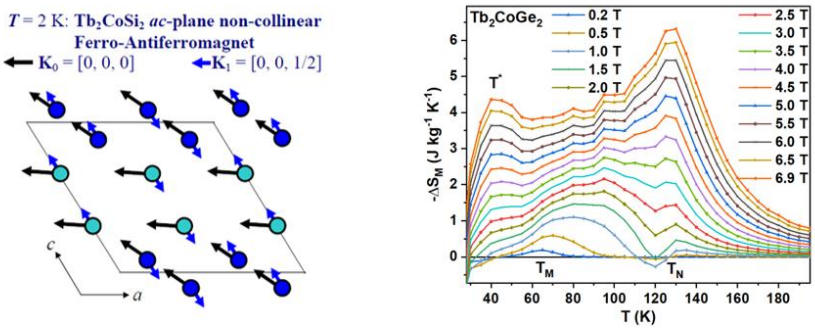

Fig.1: (Left) Unit cell representation of the *ac*-plane amplitude modulated non-collinear ferro-antiferromagnet with $\mathbf{K}_0$ and $\mathbf{K}_1$ wave vectors at 2 K. (Right) Magnetic entropy change $-\Delta S_M$ of Tb_2CoGe_2 for selected $\mu_0\Delta H$ from 0.2 T to 6.9 T.

O.11. Structural disorder and lithium diffusion pathways in lithium halide solid electrolytes

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All-solid-state lithium batteries require solid electrolytes combining high ionic conductivity with chemical and mechanical stability.[1] Lithium halides have recently emerged as promising candidates due to their wide electrochemical stability window and compatibility with high-voltage cathodes.[2] However, the structural factors governing lithium transport in these materials remain poorly understood, particularly in mechanochemically synthesized compounds where significant disorder may be present.[3, 4]

We investigate a series of lithium halides including Li_2ZnCl_4, Li_2MgCl_4, Li_2ZrCl_6 and related mixed cation and mixed-halide compositions obtained via partial Br substitution. The materials are synthesized using mechanochemical routes that enable rapid formation of crystalline phases at low temperatures. Their structural properties are examined using high-resolution synchrotron and neutron powder diffraction combined with Rietveld refinement to determine the average crystal structure, cation distribution, and lithium site occupancies.

Additional insight into the local structure is obtained from total scattering measurements and pair distribution function (PDF) analysis. For Li_2ZnCl_4, Rietveld refinement indicates a normal spinel-type framework, however, PDF analysis reveals deviations from the ideal average structure at short length scales, suggesting local distortions and disorder within the halide framework.

Furthermore, partial substitution of Cl by Br systematically modifies the lattice parameters and local coordination environment, providing a means to tune the structural landscape for lithium migration. Bond-valence energy landscape calculations based on the refined structures identify low-energy Li^+ diffusion pathways connecting octahedral sites via tetrahedral intermediates.

These results demonstrate how combined powder diffraction and total scattering approaches can elucidate both average and local structural features governing lithium-ion transport in halide solid electrolytes.

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O.12. Comparison of Spin depths profiles in Ta-Buffered and Unbuffered Co/Pt thin films via polarized neutron reflectometry: Impact on All-Optical Switching

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The relationship between the magnetic depth profile and All-Optical Switching (AOS) [1] performance in Co/Pt-based multilayers is investigated. While the variation of layer thickness and the introduction of buffer layers like Ta significantly alter AOS behavior, the underlying magnetic profile remains critical to understanding this phenomenon. To address questions regarding magnetic dead layers, cobalt magnetic moment conservation, and induced Pt magnetization [2], we employed Polarized Neutron Reflectometry (PNR), a non-destructive technique sensitive to the magnetic profile of thin films. In the case of Ta/[Co(1)/Pt(1)]x2 (thicknesses of layers indicated between parenthesis, in nm) the results revealed the presence of a superficial glass phase on the substrate and significant intermixing between the Co and Pt layers, leading to higher SLD values in the cobalt layers than nominal. Magnetic analysis at high fields (0.7 T) showed that for Ta/[Co(1)/Pt(1)]x2, the second Co layer is significantly more magnetic than the first, with magnetization penetrating adjacent Pt layers due to intermixing or proximity effects. Samples without buffer Ta, [Co(1)/Pt(1)]x2 and [Co(2)/Pt(1)]x2, show similar magnetization in both Co layers. However, [Co(2)/Pt(1)]x2 also shows magnetization in the Co layers at low field (5 mT) which is indicative of magnetization tilted to the in-plane. When correlating these profiles with AOS performance, it was observed that sample [Co(2)/Pt(1)]x2 only exhibited thermal demagnetization. Conversely, Ta/[Co(1)/Pt(1)]x2 showed the most efficient AOS, suggesting that a single effective magnetic layer with higher magnetization or fewer magnetic layers overall improves AOS efficiency.

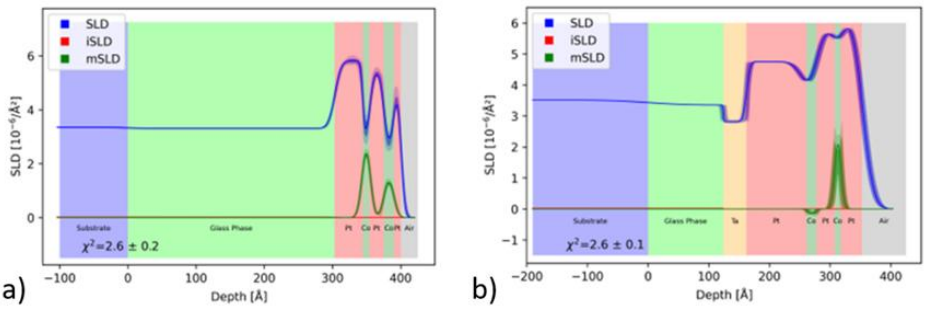

Fig.1: SLD and magnetic SLD profiles of [Co(1)/Pt(1)]x2 (a) and Ta/[Co(1)/Pt(1)]x2 (b) samples

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F1. ARGITU, the Spanish Proposal for a High-Current Accelerator-driven Neutron Source

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ARGITU is the Spanish proposal for a neutron facility aiming at the service of the Spanish (and international) scientific community.[1] The ARGITU source consists of a pulsed proton beam accelerator with an energy of 50 MeV, a pulse width of 1.5 ms and a period of 30 Hz. The proton beam hits a beryllium target, generating neutrons that are moderated at the desired thermal and cold energy ranges to supply neutrons to a selected suite of scientific instruments. With these technological features, and considering the broad science portfolio of the community, a neutron instrument suite formed by five scientific instruments is hereby proposed.[2] A thermal powder diffractometer, a horizontal reflectometer and a small angle scattering instrument will provide a complete structural characterization of materials probing length scales along several orders of magnitude. Additionally, an imaging instrument that includes capability to carry out irradiation and activation analysis experiments will cover the needs of industry and cultural heritage. Finally, a time-of-flight backscattering spectrometer will probe dynamics of molecules and protons through a wide timescale range. With this instrument suite, ARGITU is envisioned to contribute actively to the European landscape in neutron science, unfolding new developments in neutron instrumentation, training students and hence paving the future of neutron research.

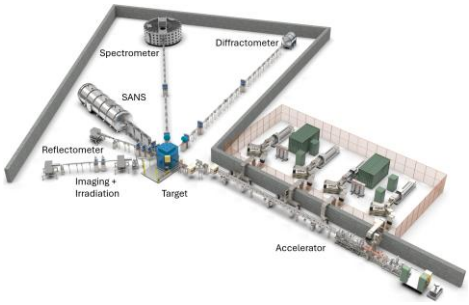

Fig.1: Layout of the ARGITU facility

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O.13. Photocurable carbonaceous composites with tunable piezoresistive response

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Photocurable polymer nanocomposites are emerging as promising materials for flexible and printed piezoresistive sensors, enabling rapid processing and tunable multifunctional properties [1]. However, achieving a controlled balance between electrical sensitivity, mechanical stability, and curing efficiency remains a major challenge, requiring a deep understanding of structure-processing-property relationships across multiple length scales [2].

In this work, carbon nanotubes (CNT) and reduced graphene oxide (rGO) are incorporated into two UV-curable matrices with distinct mechanical behaviour, an elastic polyurethane acrylate (SPOT-E) and a rigid bio-based acrylated epoxidized soybean oil (AESO), to tailor their piezoresistive performance. Photopolymerization studies reveal strong curing inhibition induced by CNT at low loadings due to optical shielding, whereas rGO enables curing at higher concentrations. Neutron scattering techniques provide key insights into the origin of these behaviors. Small-angle neutron scattering (SANS) shows that CNT form open entangled conductive networks, while rGO develops denser platelet-based aggregates. Quasielastic neutron scattering (QENS) reveals that these nanostructures directly influence polymer segmental dynamics after curing, leading to homogeneous rigid networks in SPOT-E and heterogeneous, mobility-enhanced regions in AESO at high filler contents. These multiscale effects govern the electromechanical response: SPOT-E/CNT composites exhibit stable and repeatable signals with low gauge factors (GF < 1), suitable for durable sensing, whereas AESO/rGO systems achieve high sensitivity (GF ≈ 50) due to network disruption under strain [3].

Overall, this work demonstrates that controlling filler morphology and matrix interactions through a multiscale structure–property framework is essential to rationally design photocurable composites with tailored piezoresistive performance.

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O.14. Simple-collinear 30° off–*c*-axis ferromagnetic structure of GdFeSi

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Magnetic refrigeration at cryogenic temperatures has attracted significant interest as an energy-efficient alternative to conventional gas liquefaction technologies. In this context, RFeSi intermetallic compounds (R = rare-earth element) have emerged as particularly promising candidates thanks to (I) their second-order magnetic phase transitions occurring between 10 and 150 K and (ii) the large magnetic moment of the R^{3+} ion [1-4]. In this work, the magnetic structure and magnetocaloric properties of melt-spun GdFeSi ribbons were investigated by combining short-wavelength powder neutron diffraction (PND) and magnetic measurements. The analysis indicates that the magnetic order originates exclusively from the Gd sublattice, with magnetic moments tilted 30(6)° with respect the c-axis, while the Fe sublattice remains non-magnetic due to strong Fe–3d/Si–3p hybridization. The Gd ordered moments increase from 5.7(3) μ_B at 90 K to 7.2(2) μ_B at 2 K, in excellent agreement with magnetization data and theoretical Brillouin function [5-7]. The magnetocaloric effect was evaluated, showing a maximum value of the isothermal magnetic entropy change of 8.3 J kg^{-1} K^{-1} around the Curie temperature under an applied field change of 5 T, close to the mean-field prediction. These findings underscore the essential role of neutron diffraction in resolving the magnetic structure of GdFeSi that would otherwise remain elusive or difficult to determine using other techniques, while simultaneously validating the functional properties of this material.

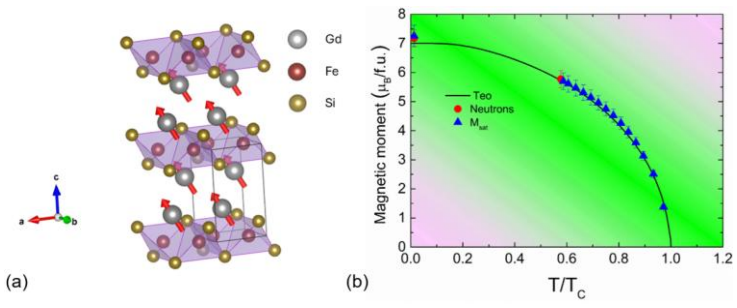

Fig.1: (a) Magnetic cell for GdFeSi ribbons. (b) Temperature dependence of the magnetic moment of the Gd sublattice.

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O.15. Neutron and X-ray Scattering for Probing Protein–Membrane Interactions and Peptide Self-Assembly

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A central question in molecular biophysics is how proteins and peptides recognize, remodel, and assemble at biological membranes. We address it by combining neutron and X-ray scattering—neutron reflectometry (NR), small-angle neutron scattering (SANS), grazing-incidence X-ray diffraction (GIXD) and SAXS—with atomic force microscopy (AFM) and light scattering, to resolve the structure and dynamics of interfacial systems under near-physiological conditions. This approach has been applied to endocytic adaptor proteins, viral fusion peptides, and biofunctional nanomaterials.

In clathrin-mediated endocytosis, NR on supported bilayers and GIXD on Langmuir monolayers reveal how AP2 and CALM bind PtdIns(4,5)P2-rich membranes through distinct but cooperative mechanisms. AP2 undergoes conformational transitions that regulate cargo recognition [1], while CALM clusters PtdIns(4,5)P2 and inserts an N-terminal amphipathic helix that softens and bends the bilayer [2,3], modulating lipid order and curvature to drive vesicle formation.

For SARS-CoV-2 fusion peptides (FPs), NR and XRR combined with GIXD shows self-assembly into spiral fibres that disrupt cholesterol-rich domains, supporting a "loaded-spring" fusion mechanism [4]. NR further demonstrates that calcium ions trigger deep FP insertion across the host membrane, a re-orientation step essential for viral entry [5]. Exploiting the same assembly, these peptide spirals can serve as templates for metallic nanostructures [6].

Overall, these results highlight how neutron and X-ray scattering uniquely access buried, sub-nanometre structure and dynamics at soft interfaces, delivering biological insight and design rules for biomimetic materials.

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O.16. Role of Fe, Co and Cu addition in the structural and magnetic properties of Ni-Mn-Ga Magnetic Shape Memory Alloys

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Magnetic Shape Memory Alloys (MSMAs) have been attracting attention due to their applicability in solid-state refrigerators, sensors and actuators, arising from their magnetocaloric and magnetostrictive effects. These effects steam from a huge magnetostructural coupling allowing the magnetic-field induced martensitic transformation from a low temperature, low symmetry phase (martensite) to a high temperature, high symmetry one (austenite). Consequently, both the structural and magnetic properties and their transitions play a critical role in these functional responses.[1]The strong correlation between composition, structure and magnetic properties in magnetic shape memory Heusler alloys is well established. Doped Ni-Mn-Ga alloys are particularly compelling due to their high compositional tunability.[2] Within this context, the present work explores the role of Co, Fe and Cu substitution on the crystal structure and magnetic behaviour of three series of alloys ($Ni_{51}Mn_{29-x}Ga_{20}Co_x$, $Ni_{51}Mn_{29-x}Ga_{20}Fe_x$, $Ni_{50}Mn_{25-x}Ga_{25}Cu_x$). Via Powder Neutron Diffraction (PND), the symmetry and atomic site occupancies of the austenitic and martensitic phases were disclosed. The structural differences were linked to the observed evolution of martensitic transformation temperature (Fig. 1a) -which increase with Co and Cu substitution but decreases with Fe- and to the atomic distribution, correlated with a change in the predominant type of magnetic exchange interaction (Fig. 1b), thereby affecting the magnetic coupling. While Fe and Co doping enhance ferromagnetic interactions, Cu atoms provoke the opposite effect, promoting antiferromagnetic ones.

The results established a clear correlation between dopant concentration, transition temperatures and type of magnetic exchange interactions. Moreover, they underscore the distinct effect associated with each dopant, providing valuable insight into the mechanism behind the fine tuning of the actuation temperature range via compositional variations.

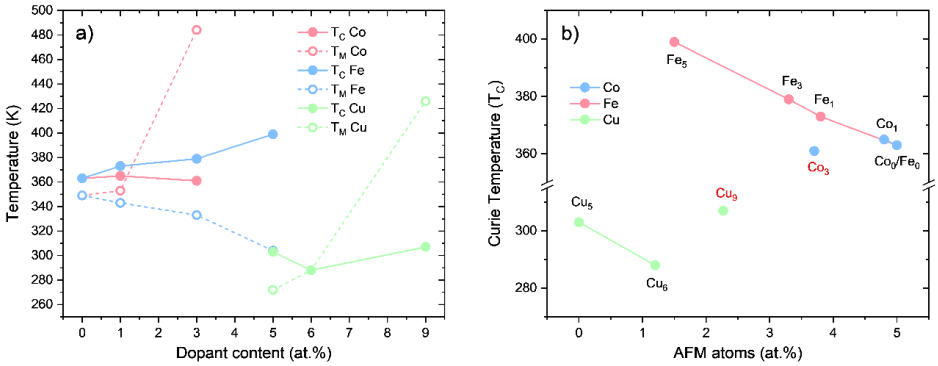

Fig.1: (a) Evolution of T_C and T_M (b) Correlation of the percentage of atoms interacting antiferromagnetically with the evolution of the T_C^A (sample name in black) and T_C^M (sample name in red)

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12TH INTERNATIONAL MEETING OF THE SPANISH SOCIETY ON NEUTRON TECHNIQUES
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O.17. Water layers on a virus – scanning probe microscopy & neutron reflectometry

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Many natural protein surfaces [1] are in contact with air of variable humidity [2]. This is crucial for the transmission of many viruses, which must "survive" for a certain time (minutes to years) at low humidity in air or on surfaces. What is the role of adsorbed water layers?

Our model system is the classical Tobacco Mosaic Virus TMV, the first and best characterized virus, whose particles contain only RNA and coat protein, and present a very well defined nanotubular shape [3,4,5]. TMV can assemble into densely packed liquid-crystal-like structures. We simplified the system to a monolayer adsorbed on a solid surface [6], which is suspected to be the case for transmission by touching, a process that is familiar from mammalian virus transmission ("droplet nuclei" on surfaces).

Water absorption and adsorption are notoriously difficult to characterize [2]. We here show that combining atomic force microscopy methods [1,2,3,6] with cold neutron reflectometry, carried out at the FIGARO beamline of ILL Grenoble, allows to approach systems as complex as adsorbed virions. Our preliminary result is the presence of an ultrathin water layer (<2nm) on the hydrophilic protein coat at intermediate to high humidities (40 to 80% relative humidity), and a "pool" of water, extending between the virus particles at very high humidities (80%) close to bulk condensation.

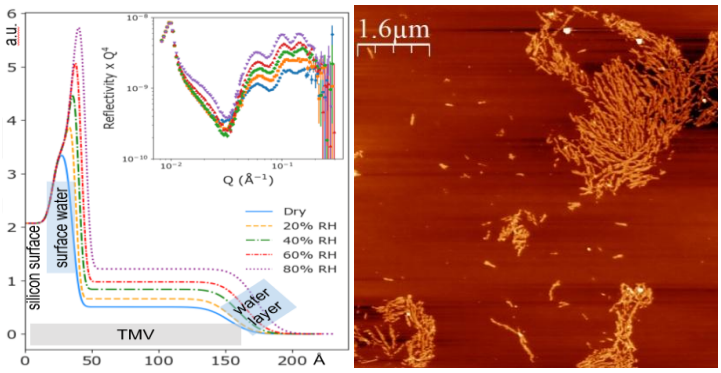

Fig.1: Neutron reflectometry curves (inset), model, and AFM scan after neutron irradiation. Tobacco Mosaic Virus (300 nm long rods, 15 nm height) adsorbed on oxidized silicon. RH=relative air humidity.

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O.18. Evolution at the nanoscale of magnetic clustering of the Griffiths-like phase in magnetocaloric $Tb_{5-x}La_xSi_2Ge_2$

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The increasing complexity of magnetic phase diagrams, often involving coexisting and competing phases as well as disordered states such as spin glasses and Griffiths-like phases (GP), highlights the need for a deeper understanding of the microscopic mechanisms governing magnetism in advanced materials. GP [1] have been identified in a wide range of technologically relevant systems, including transition metal oxides, Heusler alloys and rare-earth intermetallics, underscoring their universal character. Among them, the $R_5(Si_xGe_{1-x})_4$ family stands out due to its remarkable magnetoresponsive properties, closely linked to its intrinsically complex nanostructure [2]. In particular, giant magnetocaloric $Tb_{5-x}La_xSi_2Ge_2$ alloys with small La substitutions exhibit an unconventional regime where a cluster spin-glass state (CSG) coexists with a GP within the paramagnetic region, reflecting a subtle interplay between disorder, magnetic correlations and slow dynamics [3–5].

Here, we continue investigating the nanoscale evolution of magnetic clustering in the GP phase of the x = 0.075 compound, focusing on the relationship between spatial correlations and slow magnetic dynamics as a function of temperature. By combining macroscopic magnetic characterization, ageing protocols and small-angle neutron scattering (SANS), we provide direct insight into the formation, growth and interaction of nanometric magnetic clusters above the ferromagnetic transition [6]. Correlation lengths of 1–5 nm above the freezing temperature are, in the present work, discussed from the magnetic correlation function C(r) data, derived from SANS intensity. A phenomenological model based on ferromagnetic clusters with intercluster interactions within the paramagnetic matrix is proposed to explain the observed re-entrant glassy behavior. We will also discuss ongoing efforts to access relaxation processes governing this critical window of disordered magnetism, namely the unexplored GSG–GP regime, using neutron-based techniques. This may well serve for evaluations on other nanoscale magnetic systems.

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O.19. Elucidating the nanostructure of screen-printed high-resolution gas sensors using neutron scattering

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Volatile organic compounds (VOCs) pose significant risks to indoor air quality and industrial safety. Addressing these risks requires the development of sensors that combine high sensitivity and selectivity, with scalability and low production costs, an ongoing challenge in the field. Printing technologies offer a practical route to scalable, cost-effective sensor fabrication. Selectivity can be enhanced by engineering materials with stronger and more specific interactions with target gases, as well as by employing sensor arrays coupled with machine learning techniques[1]. Sensitivity, in turn, can be enhanced through optimization of the sensor's electronic components, particularly the transducer. In this context high-resolution interdigitated (IDT) electrodes can be screen-printed onto sensing films to fabricate highly sensitive and miniaturized chemoresistive gas sensors with improved sensitivity (Fig. 1a)[2].As for material selection this work proposes, a flexible, room-temperature sensing platform based on printable poly(vinylidene fluoride) (PVDF) composite films incorporating chemically diverse ionic liquids (ILs). ILs offer high ionic conductivity, thermal and chemical stability, low volatility, and non-flammability, making them well-suited as active sensing materials. However, their liquid nature poses significant processing challenges. This issue is addressed encapsulating ILs in PVDF, this way combining them with the chemical and mechanical stability of PVDF, nanoparticle-free inks compatible with scalable additive manufacturing can be obtained.

Additionally, the observed, specific polymer-IL interactions enable a selective detection of structurally similar VOCs — acetone, isopropanol, and ethanol— that could not have been achieved with pure IL sensors. To investigate how the different specific IL-polymer interactions notably affect the nanostructure of the PVDF matrix, the composite films have been characterized by small-angle neutron scattering (SANS) (Fig 1 b)[3]. The interplay between IL content and distribution with the functional sensing performance will be presented and discussed.

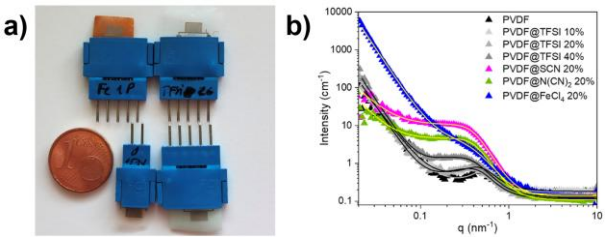

Fig.1: a) Chemoresistive sensors. b) SANS curves of the samples.

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O.20. Neutron Scattering Insights into Structure and Disorder in Functional Oxides

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Inorganic oxides, such as scheelites (ABO_4) and perovskites (ABO_3), are highly relevant classes of functional materials due to their diverse physical and electronic properties, with applications in photocatalysis,[1] solid-state ionic conduction,[2,3] and ferroelectrics.[4] Optimizing their functionality requires detailed understanding of their structural features and tunability, as even subtle symmetry changes can significantly influence material behaviour.

Many of these compounds undergo phase transitions near their operational temperatures, making it crucial to determine the nature and tunability of these transformations. In addition to symmetry-breaking distortions in the average crystal structure, correlated local distortions and disorder can emerge over short length scales, leading to significant differences between local and average structures. Understanding these effects is essential for establishing robust structure–property relationships.

Neutron scattering techniques play a key role in this context, owing to their high sensitivity to light elements such as oxygen and their ability to probe both long-range and local structure. In particular, neutron powder diffraction and total scattering enable direct investigation of the anionic sublattice and its disorder, which is often inaccessible to X-ray-based methods.

This presentation will highlight selected examples where neutron diffraction and total scattering, combined with complementary techniques, provide insight into complex phase transitions in scheelite- and perovskite-type oxides. Emphasis will be placed on the role of anion sublattice disorder, the stereochemical activity of lone-pair cations, and the use of chemical substitution to tune the structural energy landscape of these materials.[5–10]

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O.21. The Interplay of Temperature, Magnetic Field, and Pressure on the First-Order Magnetoelastic Phase Transition in $Fe_{49}Rh_{51}$ Bulk Alloy

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Near-equiatomic Fe–Rh alloys undergo a first-order magnetoelastic phase transition (FOPT) between antiferromagnetic (AFM) and ferromagnetic (FM) states near room temperature. This transition is accompanied by a 1% expansion of the unit-cell volume, while the B2 crystal structure is preserved, and gives rise to giant multicaloric effects [1,2]. Despite its relevance, the origin of this transition is not yet fully understood, and contradictory interpretations still reported in the literature [1]. A deeper understanding of the FOPT is essential not only for reproducing the remarkable properties of Fe–Rh in less expensive alloys, but also for optimizing their functional response. In this work, we carried out a comprehensive neutron diffraction investigation of a bulk $Fe_{49}Rh_{51}$ alloy under different internal and external stimuli, including temperature, magnetic field, and hydrostatic pressure. Neutron thermo-diffraction at 0-T and 8-T applied magnetic field allowed us to track the magnetic structure over a wide temperature range and to correlate it with the structural response (see Fig. 1) [2]. Magnetization measurements indicate that the applied magnetic field favours the FM phase lowering the transition temperature of the transformation to a rate of –9.1 K/T. The structural change during the FOPT, followed through the isothermally evolution of the lattice parameter under applied magnetic field up to 10 T, exhibits the same shift toward lower temperatures as observed in magnetization measurements. However, these results depict that in the AFM phase the magnetic field affects only the magnetic order and not the structural one. Conversely, the application of hydrostatic pressure shows that the structural transformation requires higher temperatures to be completed (see Fig. 1), thus favouring the AFM phase. The compilation of these results allowed us to propose a plausible mechanism of the origin of the FOPT, leading to the conclusion that both the magnetic and lattice structures define the conditions for the phase transition, while the trigger is provided by the magnetic order.

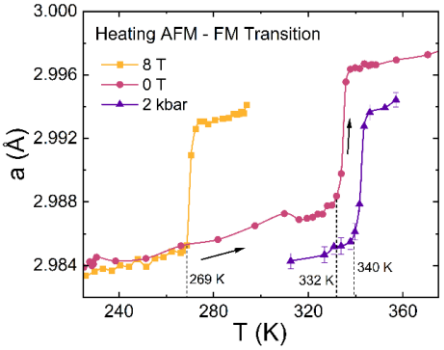

Fig. 1. Thermal evolution of the lattice parameter of $Fe_{49}Rh_{51}$ measured under different conditions—without external stimulus, under applied magnetic field, and under hydrostatic pressure—illustrating the corresponding shifts in the transition temperature.

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O.22. Structural relaxation in complex liquids with non-covalent interactions

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The glass transition is one of the most intriguing phenomena in solid state and soft matter physics, where the use of Neutron Scattering Techniques has been extensive. Starting from an equilibrium state, upon decreasing temperature, the molecular mobility of glass- forming materials progressively decreases until, at some point, equilibrium cannot be maintained on the time scale of the cooling rate, resulting in vitrification. This arrest of molecular dynamics accompanied by the transition from an equilibrium to non-equilibrium state is known as the glass transition phenomenon. The slowing down of the dynamic mechanism eventually leading to the glass transition is commonly studied by neutron scattering by following the decay of the coherent scattering function S(Q,t) at the maxima of the static structure factor, what is generally referred as 'structural relaxation'. On the other hand, among various dynamic processes that whose arrests leads to the glass transition is traditionally referred as the 'alpha relaxation' when studied by macroscopic relaxation techniques as dielectric spectroscopy of rheology.

Recently it has been shown that the presence of non-covalent interactions in relatively simple glass forming systems can lead to complex macroscopic relaxation response, where the identification of the dynamics related to the glass transition become controversial [1-4]. Moreover, the presence of non-covalent interactions can sometimes induce some supramolecular organization leading to the emergence of new structural correlations at different characteristic lengthscales [5-8]. In such cases the decay of density fluctuations at different length scales might occur by distinct mechanisms requiring a broader perception for the concept 'structural relaxation'.

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O.23. Post synthetic amine modification of MIL-101(Cr): Effects on water distribution and methane hydrate formation in confined nanospace

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Methane is considered a promising transitional fuel due to its high energy density and lower CO_2 emissions compared to conventional hydrocarbons. In addition to its role as an energy source, a significant fraction of methane is naturally stored in the form of gas hydrates, crystalline structures in which water molecules form cages that encapsulate gas under specific pressure and temperature conditions [1].

Porous materials have been widely explored to enhance methane hydrate formation [2], with metal–organic frameworks (MOFs) offering exceptional control over pore structure and surface chemistry. Among them, MIL-101 stands out due to its high surface area, large pore volume, and chemical stability, as well as its capacity for post-synthetic functionalization. In this work, methane hydrate formation is investigated in MIL-101 and its amine-functionalized derivatives prepared using alkylamines of different chain lengths, hexylamine and dodecylamine [3].

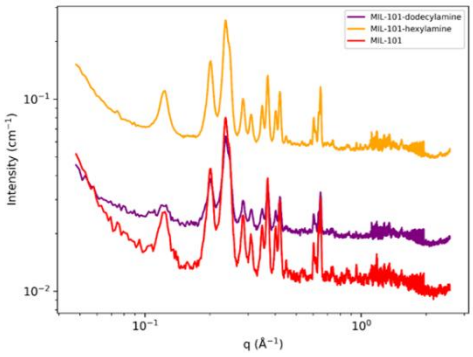

Figure 2: SANS scattering profiles I(q) as a function of q for MIL-101 and its functionalized derivatives, MIL- 101–

Neutron-based techniques were employed to characterize the materials. Inelastic neutron scattering (INS), performed at IN1-Lagrange, was used to probe the vibrational properties of the dry MOF and to analyze differences in the spectra with the aim of understanding the location and environment of the amine groups within the framework. Small-angle neutron scattering (SANS) and neutron diffraction, conducted at D16, were applied to analyze structural features and determine changes in the unit cell before and after water incorporation. These results provide insight into the influence of pore functionalization and water distribution on hydrate formation, contributing to the design of advanced materials for methane storage and transport.

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O.24. Protein Adsorption on Self-Polarized β-PVDF Ultrathin Film by Neutron Reflectometry

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Stimuli-responsive materials are essential for properly mimicking the dynamics of tissue microenvironment, where protein adsorption dictates biological activity and cellular response. In this context, electroactive polymers such as poly(vinylidene fluoride) (PVDF) are particularly attractive due to their piezoelectric properties. [1] This study aims to fabricate self-polarized ultrathin PVDF films and investigate their influence on protein adsorption, as was done recently for micron-sized PVDF films. [2] The ultrathin (<10 nm) self-polarized β-PVDF films were fabricated via Langmuir–Blodgett (LB) deposition. The film thickness was tuned by varying the number of deposited layers, affecting the nanoscale morphology of PVDF from fibrillar to spherulitic structures (Fig. 1a).

The adsorption of extracellular matrix proteins, collagen and fibronectin, on PVDF-coated substrates was analysed by quartz crystal microbalance, revealing concentration-dependent viscoelastic properties. Furthermore, neutron reflectometry (NR) provided detailed insights into the nanoscale structure of the interfaces, confirming a layered structure and enabling determination of scattering length density profiles. Notably, NR analysis demonstrated that fibronectin forms a less dense and more diffuse layer compared to collagen (Fig. 1b-c), suggesting distinct adsorption mechanisms and molecular packing.

In conclusion, despite some nonhomogeneous PVDF layer formation, the LB method enables the fabrication of self-polarized ultrathin PVDF films with tunable properties, demonstrating strong potential for controlling protein–surface interactions in advanced piezoelectric biomaterials.

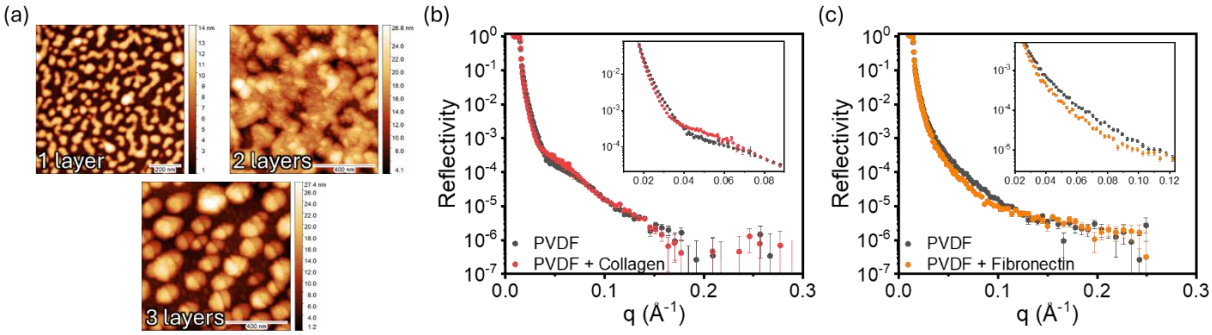

Fig.1: (a) Representative AFM topographical images of one, two and three layers of PVDF. NR reflectivity data for the PVDF layer before and after (b) collagen and (c) fibronectin adsorption in D_2O.

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12TH INTERNATIONAL MEETING OF THE SPANISH SOCIETY ON NEUTRON TECHNIQUES
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I1. MIRACLES, the Time-of-Flight Backscattering Spectrometer at the European Spallation Source

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MIRACLES is the Spanish contribution to neutron scientific instrumentation for the European Spallation Source.[1,2] MIRACLES will be the spectrometer with the highest energy resolution at the start of the ESS user program.[3] The chopper cascade can leverage the long pulse provided by the ESS source allowing a tunable energy resolution of the instrument, from δE = 2 μeV (highest-resolution mode) to δE = 45 μeV (highest-flux mode) with the concomitant capability of probing a wide range of molecular and atomic timescales, ranging from the nanosecond to the picosecond. The instrument is optimized for quasielastic neutron scattering (QENS) experiments around the Si(111) backscattering reflection with a wide dynamic range of $\Delta E \approx \pm 500$ μeV. Moreover, MIRACLES will also be able to carry out inelastic neutron scattering (INS) experiments scanning an energy range of ~ 20 meV. After completing the phase for conceptual and system design, the project is currently in the construction and installation phase, and hot commissioning and user program is planned to start in 2028. From there, it is envisioned that the MIRACLES science program will unfold new opportunities in neutron spectroscopy, being capable to disentangle complex dynamics over a wide timescale range to obtain a complete picture of polymeric and biological systems, drug delivery, and energy materials.

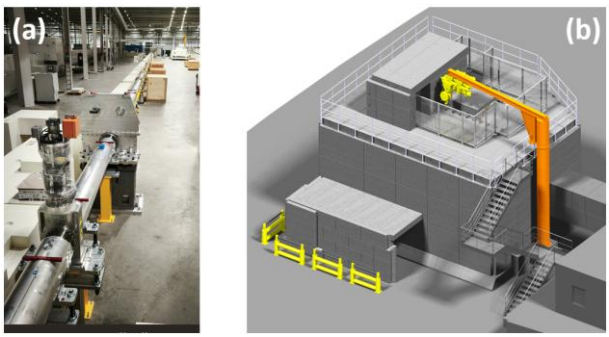

Fig.1: (a) Beamline and (b) Experimental Station of the MIRACLES Spectrometer

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O.25. Zero and Negative Thermal Expansion in Tb_2Fe_{17} alloy Investigated by Neutron Diffraction

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Neutron diffraction is a powerful tool that allows not only the characterization of magnetic structures but also provides access to spin-lattice coupling phenomena, including magnetovolume effects. These effects may manifest as anomalous variations of the lattice parameters with temperature and a strong dependence of the magnetic phase transition temperature (T_C) on pressure [1,2]. To investigate the origin of the magnetovolume anomalies in the Tb_2Fe_{17} alloy crystallizing in the non-conventional $R\bar{3}m$ rhombohedral structure, we have performed neutron diffraction experiments under varying temperature and pressure conditions. This compound is ferrimagnetic below T_C and exhibits a strong pressure dependence of T_C, with $dT_C/dP \approx -46$ K/GPa [3]. Additionally, it exhibits a remarkable zero thermal expansion (ZTE) below 300 K and negative thermal expansion (NTE) between 300 K and T_C = 408 K, as shown in **Fig. 1**. These behaviors are related to the critical dependence of magnetic exchange interactions on the interatomic distances of the Fe dumbbell atoms [4,5]. Such properties are of great interest for sensors and devices requiring resistance to thermal shocks.

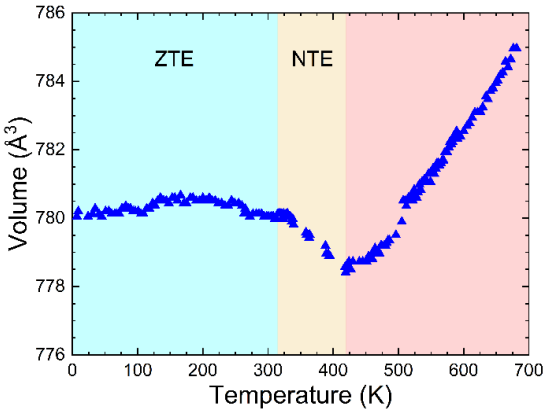

Fig.1. Volume cell as a function of the temperature for Tb_2Fe_{17} alloy.

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O.26. Neutron scattering study of polysaccharide hydrogels with magnetic–piezoelectric bi-fillers

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Multi-component hydrogels with functional fillers are promising materials for biomedical applications, where macroscopic properties are governed by nanoscale structure [1]. In this work, polysaccharide-based hydrogels incorporating magnetic and electroactive bi-fillers were usefully synthesized and studied. The systems are based on covalently crosslinked methacrylated hydroxypropyl guar (HPG-MA) hydrogels loaded with Fe_3O_4 nanoparticles and poly(L-lactic acid) (PLLA) piezoelectric microspheres (Fig1a). The spatial organization, size distribution, and aggregation state of magnetic nanoparticles (MNPs) within the polymer network play a key role in determining the response of magneto-active systems. The hydrogels were characterized using complementary techniques (scanning electron microscopy for morphology, vibrating sample magnetometry for magnetic properties, magnetorheology for mechanical behavior, magnetic response tests, hyperthermia measurements, and in vitro cytocompatibility studies, among others). Small-angle neutron scattering (SANS) method was used to investigate the nanostructure of complex multicomponent hydrogels with different fillers. Performed SANS measurements reveal a hierarchical structure arising from the coexistence of the polymer network and MNPs aggregates (Fig1b). Scattering data were successfully fitted using the Beaucage model indicating the presence of complex multi-level structural organization of MNPs into mass-fractals inside the composites. Obtained size of single MNPs is consistent with SEM results. In contrast, neat polymer hydrogel was well described using the classical “gel_fit” model in SasView program providing a correlation length (mesh size of the crosslinked network). These results highlight the capability of SANS to resolve hierarchical organization inside the complex hydrogels and MNPs aggregation in complex soft-matter systems, providing structural insight relevant for the design of functional hydrogels. Overall, these results demonstrate that these “smart” hydrogels exhibit strong potential for biomedical applications.

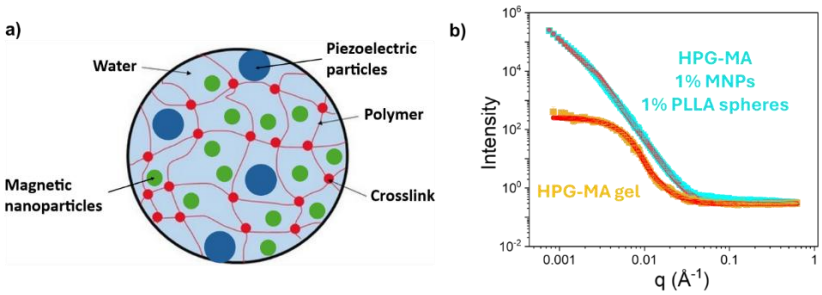

Fig.1: (a) Scheme of the multi-component hydrogel structure. (b) SANS curves and corresponding fits of neat HPG-MA hydrogel and HPG-MA/MNPs/PLLA composite.

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O.27. Tuning Polymer Dynamics with Dipolar Side Chains

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Polymer dynamics are strongly governed by the chemical nature of side chains, which influence segmental mobility, relaxation behavior, and macroscopic properties such as the glass transition temperature (T_g) and mechanical performance [1]. In particular, polar and dipolar functional groups introduce additional intermolecular interactions, including dipole-dipole interactions and hydrogen bonding that constrain chain motion and broaden the spectrum of relaxation times [2]. These effects span multiple length and time scales, ranging from localized molecular motions to cooperative segmental dynamics, making their experimental separation and interpretation especially challenging. Although polymers with high dipolar content are promising for energy applications, their high T_g-s often restrict experimentally accessible timescales. In this context, poly(tetrahydrofuran-*ran*-epichlorohydrin) (P(THF-*ran*-ECH)) serves as an ideal model system [3]. Its relatively low T_g enables the investigation of both fast segmental motions and slower cooperative relaxations over a broad temporal window, allowing comprehensive analysis without the limitations imposed by slow dynamics near or below T_g. In the present work, a comprehensive experimental investigation combining differential scanning calorimetry (DSC), broadband dielectric spectroscopy (BDS), and neutron scattering techniques, including time-of-flight (ToF) and neutron spin echo (NSE), was performed to clarify the effect of different dipolar functional groups on the dynamics of P(THF-*ran*-ECH)-based copolymers. DSC experiments reveal that the T_g increases with the dipolar moment of the functional group (Fig. 1A). Consistently, BDS measurements show that the α-relaxation shifts toward longer relaxation times depending on the nature of the modified functional group, reflecting a progressive restriction of segmental mobility (Fig. 1B). In addition, ToF and NSE studies demonstrate that fast localized motions on the tens-of-picoseconds timescale are only moderately affected by side-chain chemistry, whereas slower cooperative segmental motions on the nanosecond timescale are strongly influenced by the polarity of the substituents (Fig. 1C), in agreement with the trends observed by DSC and BDS.

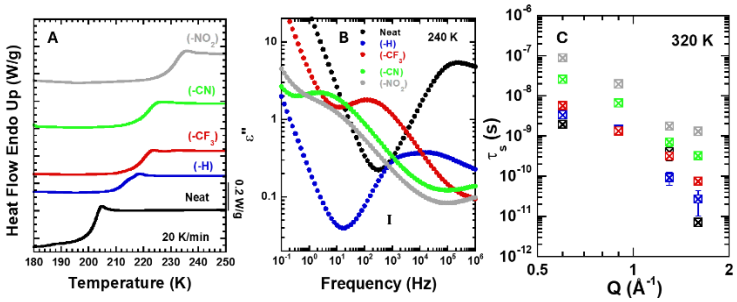

Fig. 1: A) DSC heating scans, B) isothermal ε″ spectra, and C) the relaxation times (τ_s) corresponding to hydrogen motions derived from NSE data of the neat copolymer (black) and its functionalized derivatives: -H (blue), -CF_3 (red), -CN (green), and -NO_2 (grey).

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O.28. The antiferromagnetic transition of β-Fe_2O_3 iron oxide

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Iron oxide's phases are well known multifunctional materials for many technological applications. The ubiquitous Iron (III) Fe_2O_3 oxide is a canonical polymorphic example. At ambient pressure, the best-established crystalline polymorphs are α-Fe_2O_3 (hematite), γ-Fe_2O_3 (maghemite), ε-Fe_2O_3, and β-Fe_2O_3, while pressure treatment can stabilize additional forms such as ζ-Fe_2O_3 [1]. Across these polymorphs, magnetic properties are largely controlled by exchange topology, magnetocrystalline anisotropy and electronic structure, without changing chemical composition.

Within this polymorph family, β-Fe_2O_3 is exceptional as, in sharp contrast to α-, γ-, and ε-Fe_2O_3, it is magnetically disordered at room temperature, and becomes antiferromagnetic below T_N ≈112 K (θ_C=-757 K) [2]. The magnetic structure of this polymorph had not yet been determined, being the only unsolved order of this family [1,3]. Here, we have investigated the Néel transition, the origin of frustration and the magnetic properties of nanosized β–Fe_2O_3 particles, with bixbyite-type cubic structure (Ia-3). We present the magnetic structure of β–Fe_2O_3, a noncollinear spin arrangement with commensurate propagation vector and a single active magnetic irrep [4]. The spins are also non-collinear within each of the two magnetic orbits of the magnetic configuration. The implications of the magnetic symmetry for its physical properties will be discussed, as well as the origin of magnetic frustration in this iron oxide polymorph. A deviation from ideal antiferromagnetic behavior below T_N has been previously invoked to account for a small net ferromagnetic component inferred from magnetization measurements.

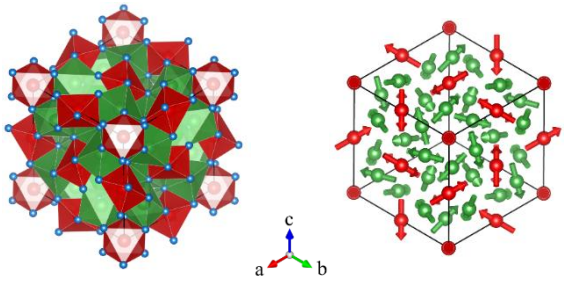

Fig.1: [111] projection of the crystal and magnetic structure of the cubic β–Fe_2O_3 iron oxide.

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O.29. Synergistic Effects between Ni Exsolution and B-site Doping in $SrMoO_3$ Perovskites for SOFC Applications

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The growing global energy demand and the need to reduce greenhouse gas emissions are driving the development of efficient technologies such as solid oxide fuel cells (SOFCs). Their performance strongly depends on the stability and catalytic activity of electrode materials, particularly at intermediate temperatures. Perovskite-type oxides are promising anodes due to their structural flexibility, redox stability, and mixed ionic-electronic conductivity.

$SrMoO_3$-based perovskites stand out for their good transport properties and stability under reducing conditions, although further optimization is needed to maintain high efficiency at lower temperatures. A key strategy to enhance their performance is B-site engineering through co-doping with a trivalent metal (e.g., Cr, Fe, Mn or Ga) and a transition metal prone to exsolution (e.g., Ni or Cu). The trivalent dopant promotes oxygen vacancy formation and structural stability[1,2], while the exsolvable metal enables the formation of catalytically active nanoparticles on the surface[3].

In situ exsolution is particularly effective: under reducing atmospheres, Ni-doped scheelite-type precursors transform into perovskites while generating metallic nanoparticles. Their size and distribution can be tuned via reduction conditions, improving catalytic activity, fuel oxidation, and long-term stability.

In this work $SrMoO_3$ perovskites are obtained by reduction of the "oxidized" $SrMoO_4$ scheelites (with Mo^{VI}). This transformation involves dopant migration, oxygen vacancy formation, and cation redistribution. In this work, $SrMoO_3$ samples doped with 10 at.% Fe and Ni were synthesized and analyzed by X-ray and neutron diffraction. Rietveld refinement confirmed the presence of exsolved metallic Ni.

The results demonstrate that B-site engineering enables controlled exsolution of well-dispersed nanoparticles, significantly improving electrochemical performance, with power densities above 663 $mW \cdot cm^{-2}$ at 850 °C under hydrogen. The evolution with temperature allows following *in-situ* the oxygen contents and displacement factors, tightly related to the performance in test SOFC cells.

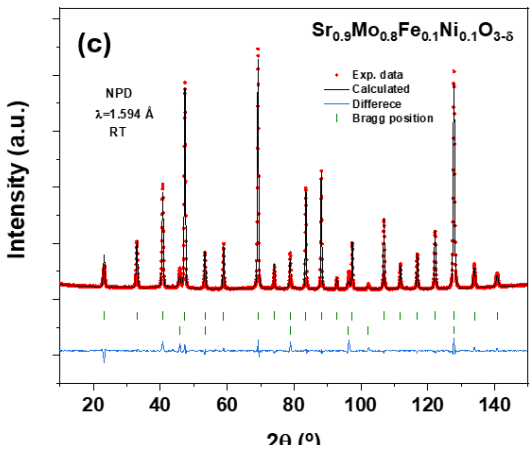

Figure 3. Rietveld refinement of $Sr_{0.9}Mo_{0.8}Fe_{0.1}Ni_{0.1}O_{3-\delta}$ diffractogram at RT. The second phase corresponds to Ni metal

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12TH INTERNATIONAL MEETING OF THE SPANISH SOCIETY ON NEUTRON TECHNIQUES
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O.30. Revealing the Structural, Magnetic, Transport, and Magnetocaloric Properties of High-Pressure Synthesized $R_xTi_2S_4$ (R = Fe, Ni) Sulfides

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Transition-metal chalcogenides with intercalated layered structures are interesting systems in material physics due to their attractive electronic and magnetic properties, with applications in electrochemical energy storage and conversion [1], thermoelectrics and magnetocaloric materials [2]. Herein, we studied in detail the structural, magnetic, and magnetocaloric properties of (Fe/Ni,Ti)-based sulfides with formula $R_xTi_2S_4$ (R = Fe, Ni), prepared by rapid high-pressure method under 3.5 GPa at moderate temperatures, starting from TiS_2 and Fe/Ni metals [3], which different compositions have been stabilized at decreasing temperatures in the range of 800–900 °C. The crystallographic features have been probed by a neutron powder diffraction (NPD) experiment at room temperature. FexTi2S4 compounds crystallize in a Heideite-type phase with space group C12/m1; the structure consists of layers of [TiS_6] octahedra sharing edges with Fe/Ni atoms located in between the layers, also in octahedral coordination, whereas $Ni_{0.8}Ti_2S_4$ crystallizes into a trigonal space group P3m1 (No. 164). Moreover, the NPD study unveils a discrete Fe/Ti inversion (<6%) at the TiS_2 layers. The surface chemistry from XPS at Fe 2*p* and Ti 2*p* core levels revealed the presence of Fe^{2+} in all samples, whereas the Ti main contribution mainly arises from the Ti^{3+} state, with a smaller contribution of Ti^{2+} and Ti^{4+} states. The magnetic properties stemming from Fe^{2+} and Ti^{3+} spins offer a complex scenario with antiferromagnetic interactions, characterized by a strongly negative Weiss constant, predominant for the Fe-rich phase $Fe_{0.42}Ti_2S_4$, combined with ferromagnetic-like interactions, leading to spin–glass or cluster–glass behavior. The coexistence of Ni^{2+} and Ni^{3+} in $Ni_{0.8}Ti_2S_4$ results on the competitive dynamic exchange interaction by electron hopping between Ni^{2+} (high-spin) and Ni^{3+} (low-spin) states due to magnetic frustration in the system. Lastly, magnetocaloric effect has been described for the three compounds, but especially for $Fe_{0.24}Ti_2S_4$ with a magnetic entropy change of 2.1 J/KgK (Fig 1c) and relative cooling power of 135.3 $J.kg^{-1}$, depicting a remarkable temperature stability for magnetic refrigerators.

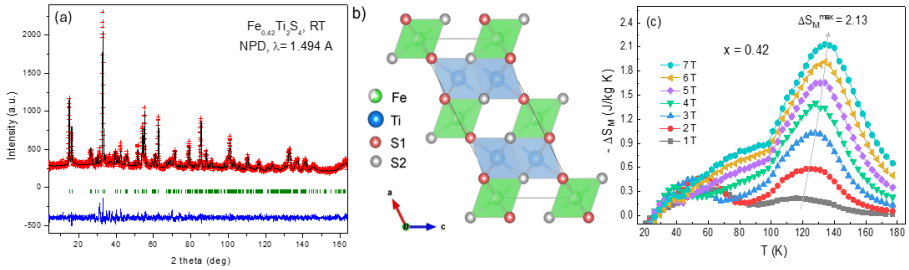

Fig.1: (a) Rietveld refinement plot from NPD data, (b) 3D view of the crystal structure, and (c) temperature-dependent magnetic entropy change ($-\Delta S_M$) for the $Fe_{0.42}Ti_2S_4$ sample.

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O.31. NSAIDs Induced Dynamical Heterogeneity in Brain Lipid Membrane Mimetics

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Non-steroidal anti-inflammatory drugs (NSAIDs) are predominantly prescribed drugs for their analgesic, anti-inflammatory, antipyretic, and antiplatelet effects. Higher dosage of NSAIDs is prescribed under chronic medical conditions leading to possible side effects. NSAIDs have shown strong propensity to alter the biophysical properties of the pure membrane mimetics which has drawn attention toward its impact on the plasma membrane. However, effects of NSAIDs on complex lipid membrane has rarely been explored. Here, we have prepared a unilamellar vesicles (ULVs) from the brain lipids (BLs), extracted from porcine brain tissues, representing physiologically a realistic membrane mimetic. We have studied effects of aspirin (Asp), diclofenac (Diclo) and ibuprofen (Ibu), at high molar concentration, on the BLs dynamics and BLs membrane fluctuations using QENS and NSE, respectively. Structural properties of BLs-ULVs are studied using small angle neutron scattering. It is found that Asp, Diclo, Ibu uniquely affects the local and long range lipid dynamics. The local BLs dynamics is described by motions on two time scales slow translational [1] and fast internal motion [2]. Fig. 1(a) shows typical fitted QENS spectra in presence of 30mol% Asp (Asp30). Variation of Γ_{int} and EISF, Fig. 1 (b) and (c) respectively, suggests faster internal motion at 30 and 10 mol%. Fig. 1(d) shows typical fits of NSE spectra in presence of Asp30. To understand the effect membrane fluctuations, NSE data is described using Zilmann and Granek model [3] and modulus of bending rigidity (κ_{kBT}) of BLs membrane is obtained at each NSAIDs concertation's. The rise in the κ_{kBT} is observed in presence of Asp at all concentration suggests Asp stiffens the BLs membrane. Whereas Diclo at highest concentration softens the BLs membrane promoting membrane fluctuations. In presence of Ibu, the κ_{kBT} increases at intermediate concentration. This study provides insights into the NSAIDs induced dynamics on the physiologically relevant model brain lipid membrane mimetics.

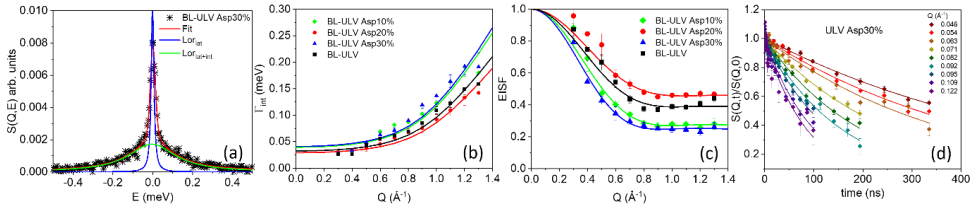

Fig.1:(a) QENS fitted spectra of BLs-ULVs at 30 mol% of Asp (b) Half width half maxima (Γ_{int}) and (c) Elastic incoherent structure factor corresponding to internal dynamics of BLs-ULVs at different mol% of Asp. (d) NSE fitted spectra corresponding to BLs-ULVs at 30mol% Asp.

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O.32. Bringing Mechanochemistry to the Neutron Beam: Set-up Development, Real-Time ND Monitoring, and the Scale Trade-off

M. Perfecto-Irigaray [1,2,*], I. da Silva [2], A. Mortazavi [2], C. Bull [2], G. Beobide [1], S. Pérez-Yáñez [1] and O. Castillo [1]

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Mechanochemistry has become a powerful alternative for synthesizing functional materials, yet fundamental reaction mechanisms often remain a black box. While *in situ* X-ray techniques provide invaluable insights, conventional *ex situ* sampling inherently alters the native reaction environment.[1] To achieve continuous and non-disruptive observation, this project leverages the unique high penetrating power and light-element sensitivity of neutrons for bulk real-time structural monitoring using neutron diffraction (ND). We present the design, evolution, and preliminary implementation of a bespoke mechanochemical reactor adapted for the General Materials Diffractometer (GEM) at the ISIS Neutron and Muon Source (RAL, UK). The set-up required re-engineering a commercial ball mill, stripping the original casing, and mounting the core assembly inverted to align with the neutron beam (Fig. 1a). Reactor material evolution involved balancing mechanical resilience and neutron transparency. This led to an adapted vanadium (*null matrix*) reactor with custom-machined V-balls, successfully eliminating container Bragg peaks.

Through iterative *ex situ* optimization, the set-up is being validated using systems of diverse chemical nature, including metal-organic frameworks (MOFs), polyoxometalates (POMs), perovskites, and co-crystals. Unlocking true bulk real-time monitoring represents a major challenge when using neutrons. Nevertheless, we successfully achieved a good signal-to-noise ratio by scaling up to 1-2 g of sample and captured the first continuous, real-time full phase formation of $Cs_6[Mo_7O_{24}]$ [2] from raw precursors (Fig 1b). While this proves the viability of the set-up, optimizing the *in situ* monitoring for the rest of the systems remains an ongoing task. We will openly discuss these current limitations, primarily the scale trade-off (balancing the high sample volumes required for neutron signal/statistics against mechanochemical energy demands and system evolution), as well as the time resolution and feasibility of the set-up depending on the nature of the system under study. Finally, we will also discuss the future work needed to establish a robust *in situ* platform for the broader user community.

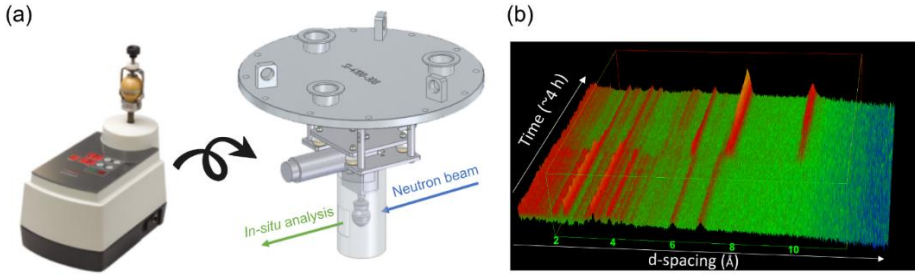

Fig.1: (a) Bespoke inverted ball mill set-up designed for the GEM sample tank. (b) *In-situ* ND mechanochemical synthesis monitoring of $Cs_6[Mo_7O_{24}]$ in GEM (bank 2).

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O.33. Magnetic order and magnetocaloric effect in $A_2MMn_3O_8$ hyperkagome spinels

L. Fernández-Gallego[1*], Á. M. Arévalo-López[2], S. Savvin[3,4], J. Prado-Gonjal[1], A. A. Tsirlin[5] and E. Solana-Madruga[1*]

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Hyperkagome spinel oxides of the $A_2MMn_3O_8$ family exhibit strong geometric frustration, making them promising candidates for magnetic refrigeration via the magnetocaloric effect (MCE) [1,2]. The 1:3 ordering of cations and vacancies at octahedral sites promotes highly degenerate spin states and complex exchange interactions [1]. Crucially, the specific ordering of cations at the tetrahedral positions induces a structural symmetry lowering that gives rise to a distinct space group, as illustrated in Figure 1a. Since the precise degree of structural order across these sites fundamentally modulates the resulting magnetic behaviour [3,4], resolving these precise distributions is key to optimizing magnetocaloric performance [2,3]. Therefore, high-resolution Neutron Powder Diffraction (NPD) is employed as the fundamental tool for both structural and magnetic characterization.

To this end, we investigate two different lithiated parent spinels from this family and their topochemically substituted child materials using low-temperature neutron thermodiffraction. Resolving the site-occupancy preferences and cation-vacancy distributions clarifies how the structural architecture dictates the competing exchange pathways inherent to the frustrated hyperkagome lattice. These insights elucidate how site symmetries and lattice configurations govern the onset of magnetic ground states and the resulting magnetocaloric properties in these complex systems.

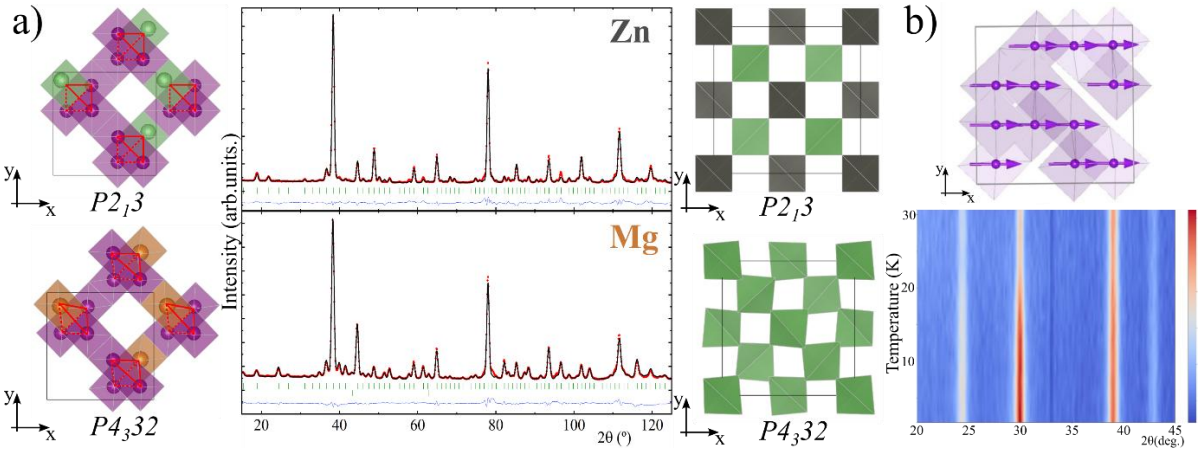

Fig.1: (a) High-resolution NPD refinements of $Li_2ZnMn_3O_8$ and $Li_2MgMn_3O_8$. Two layers of O_h and T_d cation ordering. O_h sites as building blocks of hyperkagome magnetic lattice are identified. (b) Refined magnetic structure of LMMO and magnetic intensity heat map in the 2 – 30 K range.

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O.34. Insights into the Local and Long-Range Structure of Metal-Doped ZIF-8 under CO_2 and CH_4 loading via Rietveld Refinement and Inelastic Neutron Spectroscopy

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Zeolitic Imidazolate Frameworks (ZIFs), specifically ZIF-8 [1], are premier gas separation candidates. While isostructural variants of ZIF-8 with other divalent metals are known, the structure allows as well the stabilization of Cu(II) and Fe(III) dopants. The mechanisms of stabilization of these ions at local structural level, as well as their impact on the "gate-opening" and gas adsorption remain intensely debated [2]. ZIF-8 features Zn(II) ions with tetrahedral coordination, while Cu(II) is usually square-planar or elongated octahedral and Fe(III) exhibits penta- or octahedral coordination environment [3]. This mismatch in their coordination preferences raises an open question: how do these ions accommodate within the ZIF-8 structure?

In this study we optimized Cu/Fe-doped ZIF-8 synthesis to try to elucidate that research-gap in the literature. After the synthesis, the materials were characterised using XRD, FTIR, TGA, UV-VIS, EPR and DRIFTS, which confirmed dopant stabilisation. Preliminary results indicate that these coordination differences are accommodated through the formation of localized imidazolate-linker defects and the integration of auxiliary water and hydroxyl ligands into the coordination sphere of Cu and Fe-dopants. In parallel, adsorption isotherms for N_2-77K, CO_2 (0ºC-40ªC) and CH_4 (0-40ºC) reveal that metal doping induces a second gate-opening event—shifting its activation pressure—while improving CO_2/CH_4 uptake and isosteric heat of adsorption versus parent ZIF-8. Bare and gas-loaded materials were evaluated via Neutron Diffraction (ND), Inelastic Neutron Spectroscopy (INS), and DFT. ND data (ILL-D1B, ISIS-WISH) were refined via Rietveld analysis (Jana2006). A rigid-body Im-linker model precisely determined linker orientations via X and Ψ rotational angles, isolating subtle framework distortions in doped samples. INS revealed significant phonon mode alterations, accurately reproduced by DFT models. Finally, under gas loading, INS and DFT simulations show CO_2 attenuates vibrational modes of the Im-linker methyl groups. Concurrently, the modes of CH_4 adsorbed in ZIF-8 and its variants reveal the pore environment heavily constrains their vibrational freedom. This study reveals how dopants with coordination environments that mismatch the Zn(II) coordination environment can become stabilised within the ZIF-8 structure; and the effect that this local structural distortion has on gas adsorption.

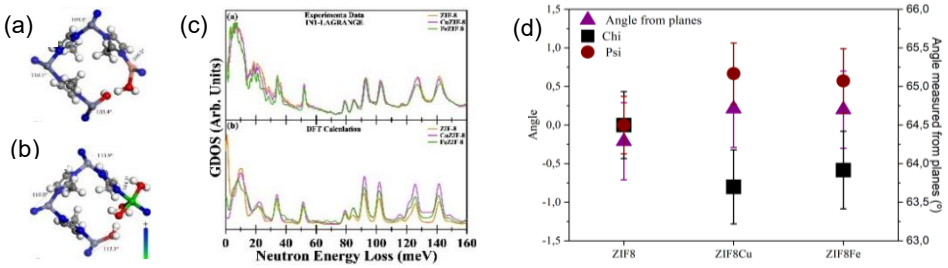

Fig.1: Coordination environments for the ZIF-8@Cu (a) and ZIF-8@Fe (b), INS spectra measured by means of IN1-LAGRANGE for ZIF-8, CuZIF-8, and FeZIF-8 (c-up), calculated INS spectra for ZIF-8, CuZIF-8, and FeZIF-8 (c-down) and variation in χ and ψ among the samples (d).

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O.34. Influence of water in the dynamics of a prototypical ionic liquid: Revisit of QENS results using molecular dynamics simulations

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In [1], we used quasielastic neutron scattering to systematically explore how the addition of water affects the dynamics of 1-butyl-3-methylimidazolium tetrafluoroborate. By combining backscattering and time-of-flight spectrometry and using H_2O and D_2O, we obtained a fairly complete picture of the dynamics of both the cation and the water at different water contents. However, the analysis and interpretation of quasielastic neutron scattering (QENS) data unavoidably relies on some approximations and assumptions. Here, we use molecular dynamics simulations to explore the effect of such approximations. Our simulated data are in reasonable agreement with the measured spectra, allowing us to assess how the model selected to fit the QENS spectra, as well as the presence of fast motions and coherent contributions, may affect the results concerning the centre-of-mass translational dynamics of the cation. The simulations also shed light on the origin of the mismatch between the self-diffusion coefficients obtained by QENS and by PFG-NMR for most ionic liquids, as well as for other viscous liquids.

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P.1. On the low transition magnetic transition of bulk and magnetosome magnetite

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Magnetite (Fe_3O_4) is a present on Earth and has been employed and studied since ancient times [1]. Presently, Fe_3O_4 nanoparticles, which retain the ferrimagnetic order, are widespread as biomedical agents and their production involve chemical routes [2], or more sparsely, natural ones (e.g. magnetosomes from magnetotactic bacteria) [3].

Even if there has been a considerable effort to elucidate the origin of the magnetic behaviour of magnetite, especially related to observation of the well-known Verwey transition, less attention has been paid to the temperature magnetic behaviour below such a transition. Effectively, low-temperature magnetic transitions (LTMT) are found at $T < 50$ K. To observe them, the quality of the samples should be high and die-hard susceptibility measurements are challenging in this temperature range. Seminal work conducted by H. Kronmüller and F. Walz in the 80s [4], among others [5, 6], proposed a model in which the electronic state of Fe^{2+} ions was crucial. Other viewpoints attribute the transition to electronic hopping of the conduction electrons. Unfortunately, these works only focus on macroscopic evidence. In this contribution we present detailed DC and AC susceptibility results combined with high resolution results obtained at ID22 in ESRF and preliminary neutron diffraction at XtremeD (ILL) in bulk and nanometric magnetite samples. The aim is to advance towards the microscopic understanding of the LTMT.

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P.2. Lipid bilayers membranes: Relevance of curvature in phase separation characteristics

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Understanding lipid membrane functionality is essential to appreciate and comprehend how cells behave and interact with their environment [1] [2]. Cellular membranes are inherently spherical, and this curvature is expected to influence lipid organization inducing phase separation in lipids as suggested by previous studies using different lipids combinations [3] [4].

Clarifying the relationship between nanoscale membrane curvature and lipid phase separation is therefore crucial. In this study, we employ nanoparticles (NPs) of different sizes (200, 100 and 60 nm) as a spherical scaffold to systematically modulate membrane curvature. The experimental strategy consists in two main steps. First, a compact nanoparticle monolayer is fabricated using a Langmuir-Blodgett trough (LBT) [5]. The uniformity and density of the NPs monolayer are characterized structurally by neutron reflectometry via small angle neutron scattering (SANS) [6], and atomic force microscopy (AFM).

Once the NPs support scaffold is established, lipid deposition is performed. The lipid system consists of cardiolipin (CL) and deuterated POPC (d-POPC). Vesicles composed of both lipids, CL predominantly in the inner layer and d-POPC in the outer layer, are prepared using the solvent depletion method, transitioning from an isopropanol solution to an aqueous environment. Then, these vesicles are deposited on top of the NP monolayer to form a flat and curved lipid layer [7]. Finally, fluorescence recovery after photobleaching (FRAP) measurements are conducted to evaluate membrane continuity and lipid. Fluoerescent dyes are incorporated into lipids to enable visualization of mobility. Upon photobleaching a defined region, fluorescence recovery is monitored to determine lipid diffusion pathways.

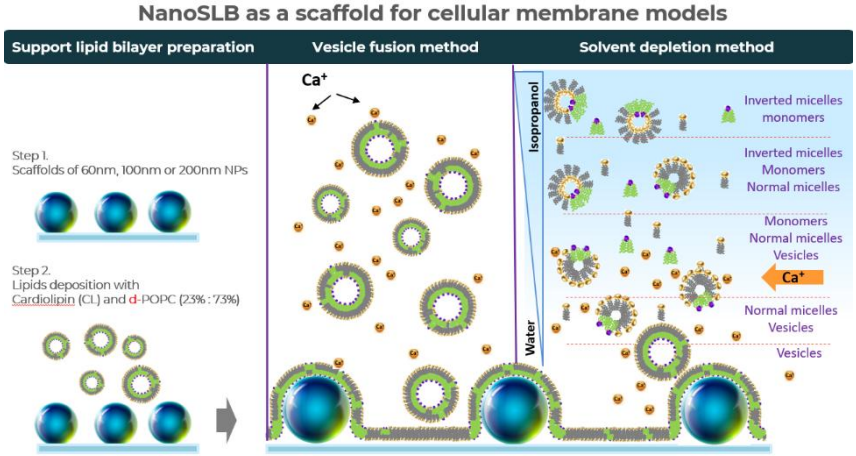

Fig.1: Procedure to obtain the lipidic layer

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P.3. Methyl Group Dynamics in the Conformational Flexibility of Methacetin

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The dynamics of functional groups in drug molecules play a crucial role in determining their medicinal and toxicological properties, particularly through their influence on molecular recognition and binding processes. In this work, we investigate the molecular dynamics and conformational flexibility of methacetin ($C_9H_{11}NO_2$), an acetamide derivative structurally related to paracetamol ($C_8H_9NO_2$) and phenacetin ($C_{10}H_{13}NO_2$). A combined approach employing inelastic neutron spectroscopy and density functional theory calculations is used to probe the relationship between crystal structure and internal molecular motions. The results demonstrate that subtle differences in crystal packing and hydrogen-bonding interactions give rise to multiple conformations, with methyl group reorientations playing a dominant role in the observed dynamics. These findings highlight the importance of integrating experimental and computational techniques to achieve a comprehensive understanding of structural dynamics in pharmaceutical compounds, with direct implications for rational drug design and optimization.

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P.4. Topology-Controlled Dynamics and Phase Segregation in Bottlebrush Polymers

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Bottlebrush polymers differ from linear analogs in chain dynamics, self-assembly, and bulk properties due to dense side-chain grafting. This architecture suppresses entanglements and extends the backbone, producing more stretched conformations. These features modify segmental mobility, phase segregation, and nanoscale organization, with direct consequences for mechanical, transport, and dielectric behavior [1,2]. Understanding how topology and dipolar functionality control local dynamics is therefore essential for the rational design of advanced polymer materials. Here, a modular synthetic strategy is used to obtain two bottlebrush polymers (BPs) as building blocks for bottlebrush block copolymer (BBCP) self-assembly [3]. Polystyrene (PS) and poly(methyl sulfonyl methacrylate) (PSO_2MA) were selected as simple, immiscible model systems. PS serves as a nonpolar reference that promotes phase segregation, whereas PSO_2MA introduces high-dipole-moment sulfonyl groups, providing a polar counterpart with stronger local interactions [4]. Broadband dielectric spectroscopy (BDS) shows that both systems exhibit topology-dependent secondary relaxations, but with opposite trends (Figure 1A). For PS, the bottlebrush architecture leads to faster relaxation compared to the linear analog, while the activation energy remains similar or slightly higher, indicating that topology mainly enhances the frequency of local motions rather than lowering the energetic barrier, consistent with increased free volume and modified local packing. In contrast, PSO_2MA exhibits a shift of the secondary relaxation to higher temperatures upon grafting, reflecting restricted sulfonyl-group mobility due to stronger dipolar interactions and steric crowding. Neutron spin echo (NSE) experiments are underway to probe segmental dynamics at complementary length and time scales, enabling direct comparison with BDS and a more complete description of topology-dependent motion. In parallel, atomic force microscopy (AFM) reveals clear phase segregation and well-defined domain formation in PS/PSO_2MA-based blends, confirming their suitability as BBCP building blocks (Figure 1B). Overall, these results demonstrate that polymer topology is a key parameter for tuning local dynamics and nanoscale morphology, enabling the controlled design of self-assembled bottlebrush-based materials.

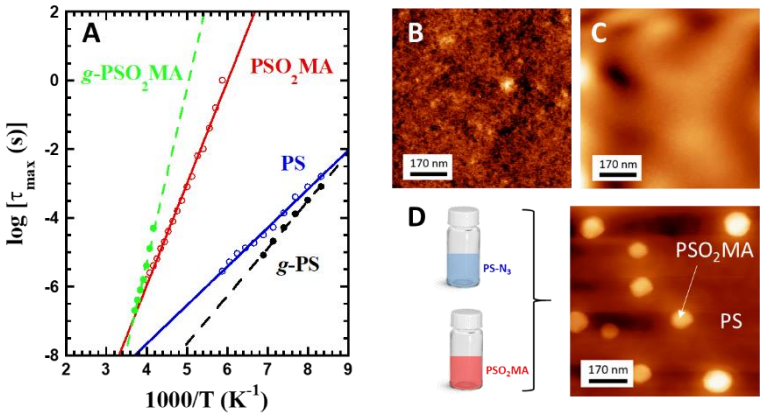

Fig.1: (A) BDS secondary relaxation of linear and bottlebrush PS and PSO_2MA. AFM images of PS (B) and PSO_2MA (C) homopolymers and phase-separated domains in PS/PSO_2MA blend thin films (D).

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P.5. Exploring Anisotropic Magnetocaloric Performance via Fe/Ti substitution in Ni–Co–Mn–ti heusler-type melt-spun ribbons

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In this work, a series of $Ni_{35}Co_{13}Mn_{35}Fe_xTi_{17-x}$ (x = 0, 1, 2, 3) ribbons were prepared using the melt-spinning technique. Thermodiffraction measurements performed at the D1B diffractometer of the Institut Laue-Langevin (ILL) confirmed a B2-type structure for the austenite phase. The analysis of the diffractograms revealed a highly texture along the (100) direction. For the Fe-free alloy (x=0) the coexistence of retained austenite and no-modulated orthorhombic martensite was observed. Additionally, the specific modulation of the martensite phase in the Fe-containing alloys (x = 1, 2, 3) is currently under further analysis. Macroscopic magnetic measurements of the melt-spun ribbons show that the magnetostructural transformation strongly depends on the Fe/Ti ratio, exhibiting a significant shift in the martensitic transformation (MT) temperature from 117 K to 318 K (fig. 1). Furthermore, these samples display a large change in magnetization ΔM during the MT, associated with the transition from the ferromagnetic austenite phase to the weak magnetic martensite phase. Another remarkable observation is that the thermal hysteresis in this family of compounds remains nearly constant, around 25 K. Additionally, the large shape anisotropy characteristic of melt-spun ribbons enables the exploitation of the rotational magnetocaloric effect, making these materials promising candidates for anisotropy-driven magnetic refrigeration applications.

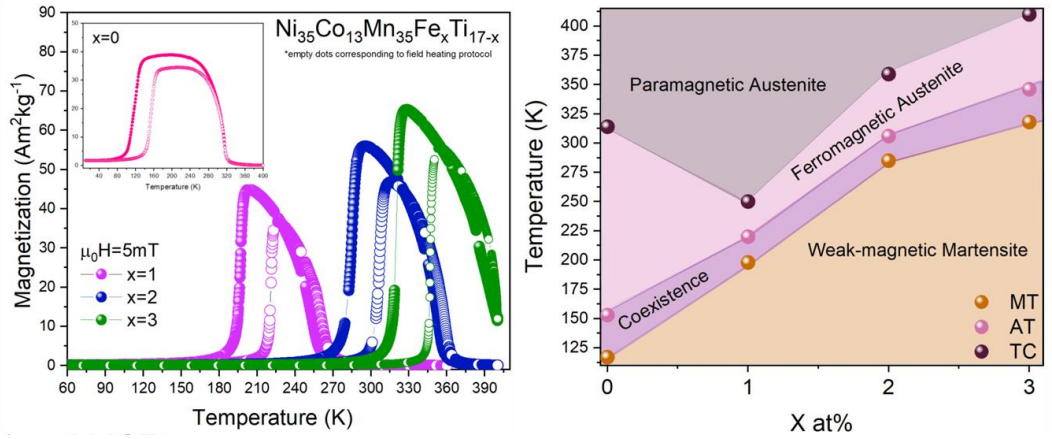

Fig.1: (left) Thermomagnetization curves of $Ni_{35}Co_{13}Mn_{35}Fe_xTi_{17-x}$ (x = 0, 1, 2, 3) ribbons. (right) Phase diagram of magneto-structural phases at low magnetic field.

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P.6. Inelastic Neutron Scattering Analysis of Silica Xerogels

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Silica xerogels have been used as sensing elements in fiber optic sensors to analyze vapors of water, acetone, butanamine, cyclohexane, dichloromethane, chloroform, or toluene [1-3]. The surface chemistry and the porous texture determine their response. Silica xerogels are inherently hydrophilic; consequently, water often interferes with the detection of volatile organic compounds. The incorporation of non-polar alkyl or aryl functional groups reduces this hydrophilic character, promoting the formation of ordered domains dispersed within an amorphous matrix. However, the exact structural nature of these domains remains an open question. Inelastic neutron scattering (INS) is a powerful tool for investigating atomic and molecular vibrations, particularly in hydrogen-rich materials. Neutron scattering experiments were performed using the IN1-Lagrange (Large Analyzer for Genuine Excitations) spectrometer, located at the hot source of the high-flux reactor at the Institut Laue-Langevin (ILL). INS spectra were recorded at 10 K over the 200–4000 cm^{-1} range.

Five hybrid xerogels were synthesized via the sol-gel process at 333 K (pH 4.5) using mixtures of tetraethoxysilane (TEOS) with 30% methyl-, ethyl-, propyl-, or phenyl-triethoxysilane (M/E/P/Ph-TEOS). In sol-gel chemistry, $R_xSi(OR')_{4-x}$ alkoxysilanes are frequently used, where R is a hydrolytically stable organic group (e.g., CH_3) covalently bonded to the polysiloxane network, and OR' is a hydrolyzable alkoxy group. Hydrolysis and polycondensation of these precursors yield organically modified SiO_2 xerogels. To gain insight into the structural properties of the modified SiO_2 xerogels, INS measurements were conducted to examine the vibrational bands associated with both the network bonds and the open-cage framework. Previous studies [4] have demonstrated the utility of this methodology for determining structural parameters in xerogels synthesized with varying proportions of precursors.

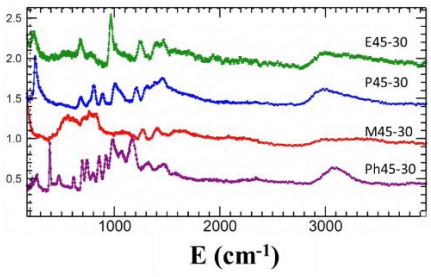

Figure: INS measurements corresponding to the different precursors TEOS and M/E/P/Ph-TEOS

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P.7. Vibrational spectroscopy of phenol absorption on functionalized Fe-C core-shell nanoparticles for water cleaning

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Multifunctional nanocomposites have been extensively studied for several decades. In this field, magnetic carbon nanocomposites stand out [1,2], and have demonstrated efficient performance in wastewater treatments as adsorption-desorption pollutant platforms, where phenol is one of the emerging contaminants with high toxicity for humans and the environment [3]. In this work, functional Fe-C core-shell nanostructured platforms have been designed for adsorption of phenol in contaminated water [4]. The synthesized magnetic nanocomposites are inserted in an aqueous solution containing phenol, whose content was measured as a function of time showing a complete removal of phenol in the first cycle. Nevertheless, this high efficiency reduces in the subsequent cycles (Figure 1a).

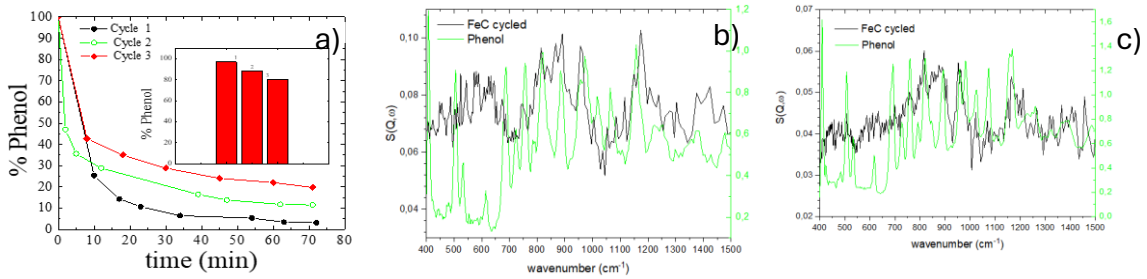

Fig. 1: a) Phenol concentration as a function of the contact time employing the Fe-C nanoadsorbents, b) inelastic neutron scattering measured at IN1-ILL and c) TOSCA-ISIS (phenol data from Ref. [5]).

FTIR and Raman spectroscopy measurements, despite showing good spectra, were inconclusive to demonstrate a deactivation mechanism. With the aim to shed light on the mechanism leading to the loss of phenol absorption efficiency, inelastic neutron scattering experiments were carried out at IN1-ILL (feasibility test EASY-1202) and at TOSCA-ISIS (RB2520567) in several phenol containing Fe-C samples, before and after phenol absorption and with or without water washing cycles. Preliminary analysis demonstrates the existence of at least two possible phenolic specific vibrations modes at around 885 and 1190 cm^{-1} corresponding to C_xH molecular out and in-plane-bends respectively [6], thus showing that some evidence of phenol-carbon interaction should be taken into account to justify the loss of phenol adsorption capacity after subsequent cycles; additionally, low energy vibrations point out to the possible formation of iron oxides (Figure 1, b and c).

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P.8. Magnetostructural evolution in Ni–Mn–Co–Ti metamagnetic shape memory alloys: a temperature-dependent neutron diffraction study

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All-d-metal Mn-based Heusler alloys have attracted considerable attention due to their functional properties, including magnetocaloric effects, giant magnetostrain, and magnetically driven phase transformations.[1-3] These phenomena are governed by d–d orbital hybridization, which stabilizes the martensitic transformation and controls magnetostructural coupling. In off-stoichiometric compositions, magnetic interactions can be tuned via chemical substitution, affecting the balance between ferromagnetic and antiferromagnetic coupling.[4]

Previous neutron diffraction studies on $Ni_{35}Mn_{45-x}Ti_{15}Co_{5+x}$ (x = 0, 2.5, 5, 7.5), obtained from melt-spun ribbons and powdered, showed a B2-type cubic austenitic phase (Fm-3m) and a non-modulated orthorhombic martensitic phase (Pnma). The austenitic lattice parameter decreases with Co content, while Co substitution promotes ferromagnetic interactions due to Mn/Co disorder. The largest magnetocaloric response occurs at intermediate Co content (x ≈ 5), highlighting the strong coupling between composition, magnetism, and structure

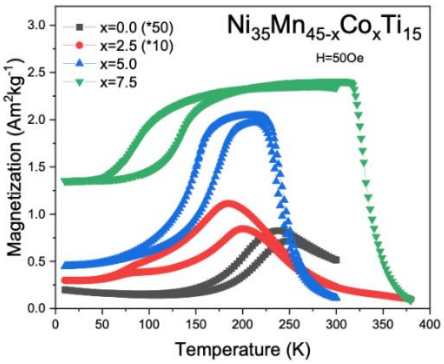

Figure 4: Thermomagnetization curves at different composition $Ni_{35}Mn_{45-x}Ti_{15}Co_{5+x}$ (x = 0, 2.5, 5, 7.5).

In this work, we extend these studies by performing a temperature-dependent neutron diffraction analysis to directly track the structural evolution across the martensitic transformation in order to monitor the phase coexistence and transformation kinetics. The main objective of this study is to determine how the lattice parameters, phase fractions, and structural symmetry evolve as a function of temperature, and to identify the presence of phase coexistence between austenite and martensite at low temperatures, in particular, the kinetic arrest phenomenon. Special attention is

given to the stability of the orthorhombic martensitic phase, possible deviations from ideal symmetry, and the correlation between structural changes and previously reported magnetic behavior.

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P.9. Mag2Pol: A user-friendly software for the analysis of powder and single-crystal diffraction data

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Addressing scientific challenges in complex materials often requires advanced analysis methods and the combination of multiple experimental techniques to obtain a consistent and comprehensive picture. The Mag2Pol software project [1] originated from the need to solve a specific problem [2] in the specialised field of Spherical Neutron Polarimetry [3]. Since then, it has evolved into a versatile and generally applicable program for the analysis of diffraction data from powder and single-crystal X-ray and (polarised) neutron experiments, covering both constant-wavelength and time-of-flight instruments, with a strong focus on user-friendliness and efficient workflows.

Mag2Pol integrates a wide range of features, including irreducible representations, magnetic (super)space groups, group-to-subgroup transformations, and rigid-body modelling, as well as tools for preparing, conducting, and analysing diffraction experiments. Combined with high-quality 3D visualisation of crystal and magnetic structures, enabling the export of publication-ready graphics, these capabilities make Mag2Pol a comprehensive standalone solution for the analysis of diffraction data.

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P.10. Microstructural evolution during crystallization process in Ni-Co-Mn-Sn and Ni-Co-Mn-In metamagnetic shape memory alloys

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Ni-based metamagnetic shape memory alloys (MMSMAs) are of particular interest due to the possibility of inducing the reverse martensitic transformation (MT) by applying a magnetic field. This feature opens up opportunities for their use in applications such as magnetic refrigeration and sensing, owing to the inverse magnetocaloric effect and giant magnetoresistance, respectively [1,2]. However, the poor mechanical properties of these alloys remain one of the main limitations for practical applications. To overcome these limitations, the incorporation of alloy powders into polymer matrices to form composites has been proposed as a promising alternative [3]. A detailed analysis of the powder can provide valuable insight into the influence of microstructure on both the martensitic transformation and the magnetic properties, enabling proper tuning of the functional behavior.

The structural evolution during the crystallization process after high-energy ball milling has been studied in Ni-Co-Mn-Sn and Ni-Co-Mn-In MMSMAs. In situ neutron thermodiffraction measurements reveal that crystallization begins around 500 K, evolving from an amorphous-like state to a nearest-neighbor ordered B2 phase At higher temperatures, a next-nearest-neighbor ordering process occurs, corresponding to the B2 to $L2_1$ transition at approximately 700 K. While the $L2_1$ phase in the Ni-Co-Mn-Sn system remains stable up to 1200 K, the Ni-Co-Mn-In alloy undergoes a second-order $L2_1$–B2 order–disorder transition at 850 K. On the other and, an anomalous behavior in the evolution of the lattice parameter associated with the B2–$L2_1$ transition is observed. Finally, the evolution of microstructural parameters, such as grain size and internal strain, as well as macroscopic strain, was determined from the diffraction patterns collected during crystallization.

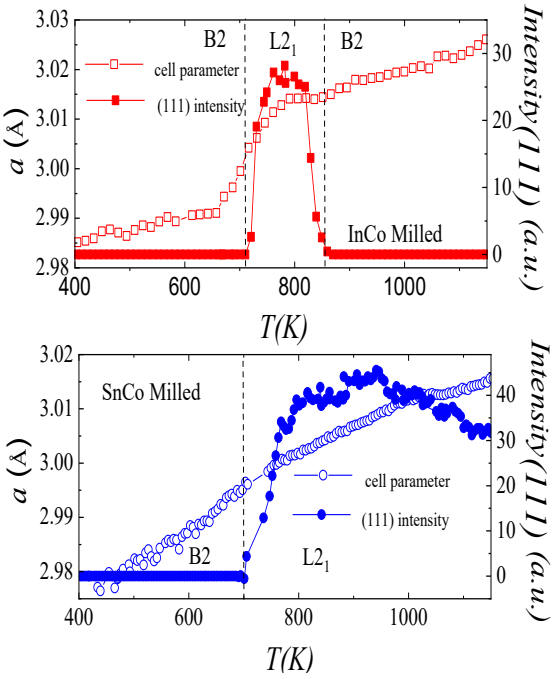

Fig.1: Cell parameter and degree of atomic order (intensity of (111) reflection) as a function of temperature of the cubic austenite for (a) Ni-Mn-Sn-Co and (b) Ni-Mn-InCo milled samples

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P.11. Design of a Novel Bio-Based Polymer matrix doped with expandable particles for battery shutdown applications

Cristian Mendes-Felipe[1], David Santos[1], June Herreros[1], Paola Crocomo[1], Ivan Bobrikov[2], Maksym Golub[3], Mohamed Zbiri[4], Dominika Zákutná[4,5], Kuno Schwärzer[6], Marco Sangermano[7], Jörg Pieper[3], Senentxu Lanceros-Mendez[1,8,9], Viktor Petrenko[1,8], Manuel Salado[1,8]

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The increasing energy density and operating voltage of lithium batteries have intensified safety concerns associated with thermal runaway, highlighting the need for electrolyte materials capable of actively preventing catastrophic failure. In this work, we developed a sustainable, bio-based polymer electrolyte with an integrated thermal shutdown function by combining acrylated epoxidized soybean oil (AESO) with reactive diluents and a highly concentrated EmimTFSI/LiTFSI electrolyte. Thermally expandable particles were incorporated into the polymer network to interrupt ion transport when exposed to elevated temperatures. The formulations, containing up to 90 wt.% electrolyte, were successfully processed by digital light processing (DLP), yielding free-standing and mechanically stable electrolyte membranes.

The relationship between composition, microstructure, and transport properties was investigated using complementary characterization techniques, including neutron diffraction, neutron imaging, small-angle neutron scattering (SANS), and quasielastic neutron scattering (QENS). These analyses revealed that increasing electrolyte content promotes the formation of interconnected electrolyte-rich domains that enhance ionic transport, although at the expense of greater polymer plasticization and structural heterogeneity. Upon heating above the activation temperature, the expandable particles induce significant morphological changes that disrupt conductive pathways, effectively reducing ionic transport and enabling a thermal shutdown response. This study provides new insight into how microstructural design governs ion transport and thermal responsiveness, offering a promising route toward safer and more sustainable solid-state electrolytes for next-generation lithium batteries

Figure 5. Thermo-responsive AESO/IBOA-ionic liquid polymer electrolytes with expandable microspheres

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P.12. New type of high-T_S magnetic spiral in layered YBCFO type perovskites

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Most spiral magnetoelectric multiferroics investigated in recent years are geometrically or exchange-frustrated magnets with low magnetic transition temperatures. The remarkable stability of the incommensurate spiral magnetic order in the layered structure of $YBaCuFeO_5$ [1] arises from an unconventional mechanism [2]. We have investigated the impact of tuning magnetic frustration on the spiral magnetic phases and related properties of these layered perovskites through different strategies [3-5]. Powder samples and single crystals were prepared and characterized by powder and single-crystal neutron diffraction using both unpolarized and polarized neutrons [6]. This simple layered structure appears as an effective platform for the development of functional spiral magnets operating at ambient temperatures.
Here, we report the identification and characterization of a new type of incommensurate spiral phase (spiral-2, with $\mathbf{k}_{S2}$ = (½, ½, ±q)) in doped $YBa(Cu,M)FeO_5$ (M divalent), characterized by a propagation vector distinct from that of spiral-1. Spiral-2 was observed beyond the magnetic triple point, previously considered the critical limit for the stabilization of chiral magnetic order in this structure [7]. This new spiral phase emerges from the collinear-2 commensurate magnetic order and can exhibit transition temperatures comparable to those of spiral-1, which develops from the collinear-1 phase. This finding expands the range of competing magnetic phases in layered perovskites with the YBCFO-type structure.

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P.13. Linking interphases' structure and optical response in CdS quantum dots: the role of SANS

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Colloidal quantum dots (QDs) are promising materials for light emission devices (LEDs) and optically pumped lasers application, thanks to their highly tunable optoelectronic properties. CdS is a promising gain media for OPLs, especially in the bulk nanocrystal regime [1], where the bandgap becomes independent of size. A major role on the stability of CdS in various environmental conditions, like solvent, temperature and humidity, is played by the ligands that passivate the QD. In this work, we probe the influence of ligand shells and ZnS coatings on optical properties of small sized CdS quantum dots by means of combination of UV–Vis absorption, steady-state and time-resolved photoluminescence, and transient absorption spectroscopy. In addition, despite cadmium strong neutron absorption challenging issues, we will conduct small angle neutron scattering (SANS) experiments to resolve the key interphases, such as the ligand/solvent interphase, exploiting contrast variation, to correlate the surface composition and morphology with experimental optical response and theoretical predictions, paving the way to the design of a quantum dot digital twin.

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P.14. Exploring low dimensional and frustrated magnets as magnetocalorics for efficient refrigeration

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In the context of cryogenic cooling, key for many applications as medical sensing, quantum technologies or H_2 liquefaction, our Low-MACER project [1] explores low dimensional and metamagnetic materials as potential magnetocalorics for efficient refrigeration.[2] With a combined theoretical and experimental approach, different target materials under study include highly frustrated lacunar spinels or layered/chain-like structures, such as hollandites.

In this communication we present preliminary results on the hollandite materials. Its structure (Figure 1a) contains double chains of edge-sharing octahedra connected through corners. This atomic arrangement originates zig-zag chains and thus, low-dimensional triangular based magnetic sublattices (highlighted in Figure 1b), which sets the playground for a strong geometric frustration. Modification of the chemical composition in $K_2M_{2+x}Ti_{6-x}O_{16}$ has proven a useful way towards modulation of the magnetic interactions, where the interplay between cation distribution and valence states [3] yields a means to control magnetic dilution and frustration effects.

On the other hand, the high pressure $A_2Cr_8O_{16}$ family of mixed valent Cr^{3+}/Cr^{4+} is presented. Transition metal oxides containing mixed valent cations often display rich electronic and magnetic phase diagrams, including metal insulator transitions, [4] charge ordering,[5] and unconventional magnetic ground states. [6] Here, the A = K and Rb ferromagnetic phases are shown. Neutron diffraction has proven essential for a full understanding of the structure-properties relationship, including high resolution structural characterization, magnetic structure determination and thermal evolution, and *in-situ* high-pressure experiments to explore phase transitions and magnetic phase diagrams.

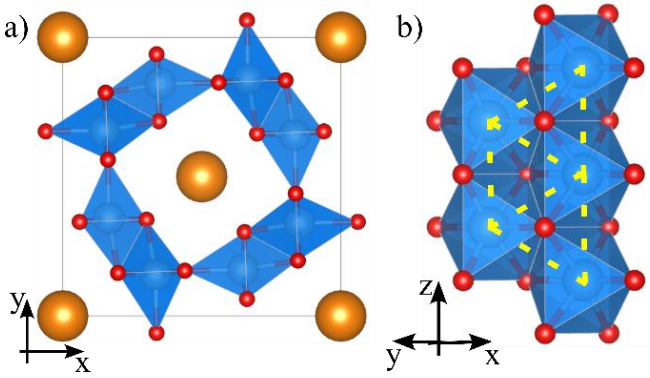

Fig.1: (a) top view of hollandite-type structure unit cell. (b) focused zig-zag double chains of $[BO_6]$ octahedra. Triangular magnetic sublattices highlighted with a dashed yellow line.

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P.15. Structural evolution and magnetic behaviour in the $La_{0.3}Ca_{0.7}Fe_{1-x}Cr_xO_{3-\delta}$ solid solution

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The $La_{0.3}Ca_{0.7}Fe_{1-x}Cr_xO_{3-\delta}$ solid solution represents a versatile class of functional materials where B-site substitution and oxygen deficiency facilitate the fine-tuning of electronic and magnetic properties. This system exhibits a remarkable structural evolution that governs its potential in SOFC and thermoelectric applications [1-2]. At low chromium contents (x < 0.5), the system stabilizes in the rhombohedral *R*3*c* (No. 161) phase defined by $a^-a^-a^-$ octahedral tilting and polar displacements [3]. As Cr content increases, the system undergoes a transition to an orthorhombic *Pnma* (No. 62) symmetry, signalling the emergence of the in-phase M_3^+ tilting component and a characteristic $a^-b^+a^-$ tilt pattern. [4]

Crucially, the interplay between these structural phases and the resulting modulation of p-type transport properties is directly driven by the Cr/Fe ratio and the associated defect chemistry. Since the distribution of cations and oxygen vacancies dictates the underlying exchange pathways and emergent magnetic correlations, resolving these orderings is essential to understand the symmetry-governed ground states. High-resolution Neutron Powder Diffraction (NPD) is therefore the fundamental tool for characterization, leveraging the significant contrast in neutron scattering lengths between Fe and Cr to uncover the structural origin of the physical properties in these complex oxides.

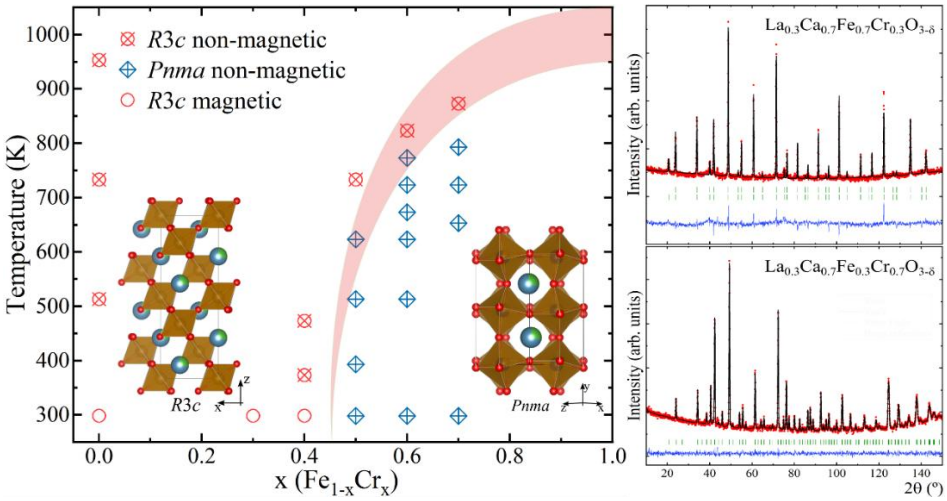

Fig.1: Structural evolution of $La_{0.3}Ca_{0.7}Fe_{1-x}Cr_xO_{3-\delta}$. (Left) Composition-temperature phase diagram. (Right) Rietveld refinements of the rhombohedral (*R*3*c*, top) and orthorhombic (*Pnma*, bottom) phases.

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P.16. Ammonia adsorption on small pore Ag-containing zeolites

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Ammonia is an industrially important compound due to its widespread use as a feedstock and its potential as an energy carrier [1,2]. However, it is also an atmospheric pollutant emitted from industrial activities and fossil fuel combustion, with adverse effects on both human health and the environment [3]. To mitigate ammonia emissions, selective catalytic oxidation (NH_3-SCO) over silver based catalysts, including zeolites (Ag-zeolites), has emerged as a promising approach [4,5]. Understanding NH_3 adsorption on Ag-zeolites is essential to elucidate its activation and conversion in catalytic processes, as well as to design improved materials for catalysis and gas sensing [6].

This work investigates NH_3 adsorption on small-pore Ag-zeolites (Ag-RHO, Ag-CHA with Si/Al ≈ 5 and Ag/Al = 0.5; Ag-LTA with Si/Al ≈ 5 and Ag/Al = 0.8) using inelastic neutron scattering (INS). INS spectra were recorded at 10 K on IN1-Lagrange (ILL, Grenoble) using sealed glass ampoules containing 1 NH_3/Ag. UV-Vis spectroscopy identified Ag^+ species in Ag-RHO, Ag^+ and Ag_n^+ clusters in Ag-CHA, and silver nanoparticles in Ag-LTA.

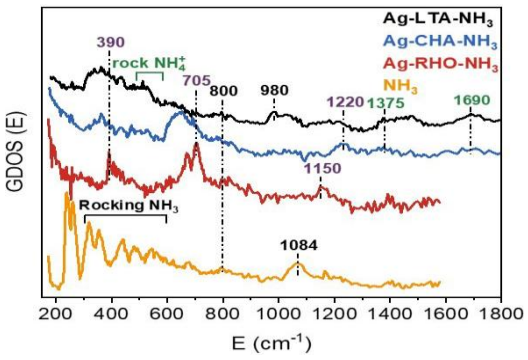

Fig.1: Normalized INS spectra of ammonia adsorbed on Ag-zeolites compared to ammonia. In Green NH_4^+ cations; in purple Ag-NH_3 complex.

Figure1 shows the INS spectra of the NH_3 adsorbed on the Ag-zeolites compared with pure ammonia, demonstrating the NH_3-Ag interaction. Spectra of NH_3 adsorbed on the three Ag-zeolites are different, in agreement of the occurrence of different silver species. The spectrum of the Ag-RHO-NH_3 sample is consistent with the formation of Ag^+-NH_3 complex. This species and NH_4^+ formed on the Brønsted acid sites are dominant in the Ag-CHA-NH_3. Meanwhile, NH_4^+ and NH_3 are mainly present in Ag-LTA-NH_3.

Thus, the results reported here allows concluding that the nature of ammonia species adsorbed on Ag-zeolites strongly depend on the Ag clustering and framework topology of the zeolites.

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P.17. Pressure-Dependent Nitrogenation of Nd-Based $ThMn_{12}$-Type Alloys for Rare-Earth-Lean Permanent Magnets

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The development of rare-earth-lean permanent magnets is a relevant strategy to reduce the dependence of the magnet industry on critical rare-earth elements and geographically concentrated supply chains. In this context, Nd-based $ThMn_{12}$-type compounds are being explored as alternatives to conventional $SmCo_5$ and $Nd_2Fe_{14}B$ magnets, since they contain a lower rare-earth fraction while retaining promising intrinsic magnetic properties. However, further improvement of their magnetocrystalline anisotropy is required for practical permanent magnet applications.

Nitrogenation is a suitable route to modify the crystal structure and enhance the magnetic performance of $ThMn_{12}$-type compounds. In this work, we investigate the nitrogenation process of Nd-based 1:12 alloys under different nitrogen pressures, focusing on the time evolution of the crystal structure during nitrogen uptake. Structural changes are analysed as a function of processing time and applied pressure in order to identify conditions that enable controlled nitrogen incorporation while preserving the $ThMn_{12}$-type framework.

The magnetic properties of the parent and nitrogenated compounds are compared to assess the effect of nitrogen insertion on the magnetic response. These results provide insight into the relationship between nitrogenation conditions, structural evolution and magnetic performance, contributing to the optimization of processing routes for rare-earth-lean permanent magnet materials.

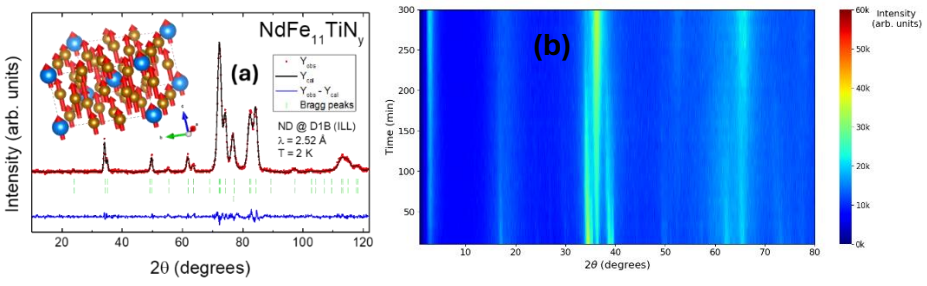

Fig.1: (a) Rietveld refinement of the neutron powder pattern for the $NdFe_{11}TiN$ alloy at T = 2 K (b) Time dependent powder neutron diffractograms taken at 723 K for the nitrogenation process performed during the isotherm, with P = 5 bar.

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P.18. Devil's staircase magnetic spirals in $Ni_{2-x}Co_xScSbO_6$

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Complex magnetic structures are of interest as frustrated systems and for coupling of magnetism to lattice distortions, which can give rise to multiferroics. Many frustrated systems show spiral magnetic structures, with incommensurate or commensurate (locked-in) propagation vectors. When these wave vectors vary systematically with a tuning parameter, a series of observed fractional states may follow staircase models.[1]

$Ni_{2-x}Co_xScSbO_6$ solid solution crystallises with the Ni_3TeO_6 (NTO) –type structure (Fig. 1a), in the polar *R3* space group. It is built up of stacked triangular magnetic sublattices, which induces a strong magnetic frustration. The Ni end member is reported as a spin-cycloidal [0k_y0] ferroelectric material,[2] and chemically-tunable commensurate helical spin structures [00k_z] were more recently reported for samples with x = 0.5, 1.0, 1.5 and 2.0, where k_z takes fractional *1/3n* values with *n* = 5, 6, 8 and 10, respectively. [3] These values arise from the spins lying along the 3-fold easy axes in the *ab* plane, likely driven by the strong electronic anisotropy of Co^{2+}. A collinear ferrimagnetic [000] phase coexists in the Co rich compounds.

Bulk magnetic characterisation shows sharp magnetic transitions at T_C~ 60 K for all samples, with wasp-wasted hysteresis loops and metamagnetic transitions at moderate critical fields < 2.5 T for all studied compounds with x ≤ 0.5. This behaviour reflects a more complex and field dependent spin order. Our neutron diffraction studies reveal x = 0.1 - 0.4 samples develop helical spirals with wavevectors described as a "harmless staircase" of k_z = *6/n* values. Both *6/n* and *1/3n* can be expressed as *6p/q*, which holds other members as *6/n*, *3/n*, *1/n* or *1/6n*, making this system a realisation of a "complete devil's staircase", where finite steps between compositionally modulated wavevectors are stable throughout the whole temperature range.[4] Neutron diffraction shows that the metamagnetic transition marks a *k*-flop from helical [00k_z] to cycloidal [k_x00] spin spirals, which gradually transform to a coexisting [000] collinear state (Fig. 1b).

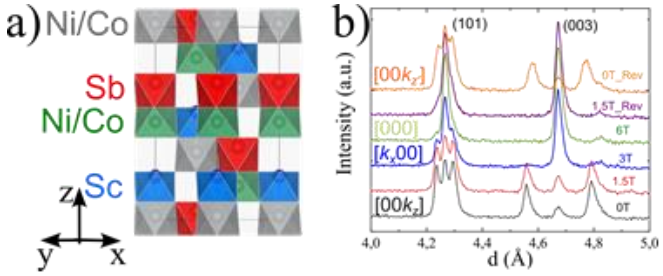

Fig.1: (a) *R3* structure of $Ni_{2-x}Co_xScSbO_6$. (b) Low temperature neutron diffraction scans of x = 0.2 under different magnetic fields.

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