Neutron Scattering Group Early Career Meeting

15–16 January 2026
Engineers House, Bristol, UK

ASTRAL SYSTEMS

EUROPEAN SPALLATION SOURCE

NEUTRONS FOR SOCIETY

Science and Technology Facilities Council
ISIS Neutron and Muon Source

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ASTRAL SYSTEMS

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Neutron Science for a Sustainable World

ESS (European Spallation Source ERIC) is a research facility under construction in Lund, Sweden, with its Data Management and Software Centre in Copenhagen, Denmark. When completed, ESS will be the world's most powerful accelerator-based neutron source to study the structure and behaviour of matter from the atomic to the macroscopic level.

Every year, thousands of researchers from academia and industry will use the ESS facility to learn more about materials and biological systems, unlocking discoveries and driving innovative solutions to tackle global challenges, from energy to healthcare and sustainability.

Built by 13 countries, ESS is Europe's flagship big-science project, with technical components developed at more than 40 European research institutes and contributions of know-how from more than 100 laboratories and experts worldwide.

ESS *Road to Science*

2003 Concept design of ESS finalised

2009 Decision to site ESS in Lund (SE), with Data Management & Software Centre in Copenhagen (DK)

2010 ESS becomes a publicly held company

2013 ESS Technical Design Report completed

2014 Start of construction

2022 Civil construction completed

2025 Accelerator commissioned (Beam on Dump)

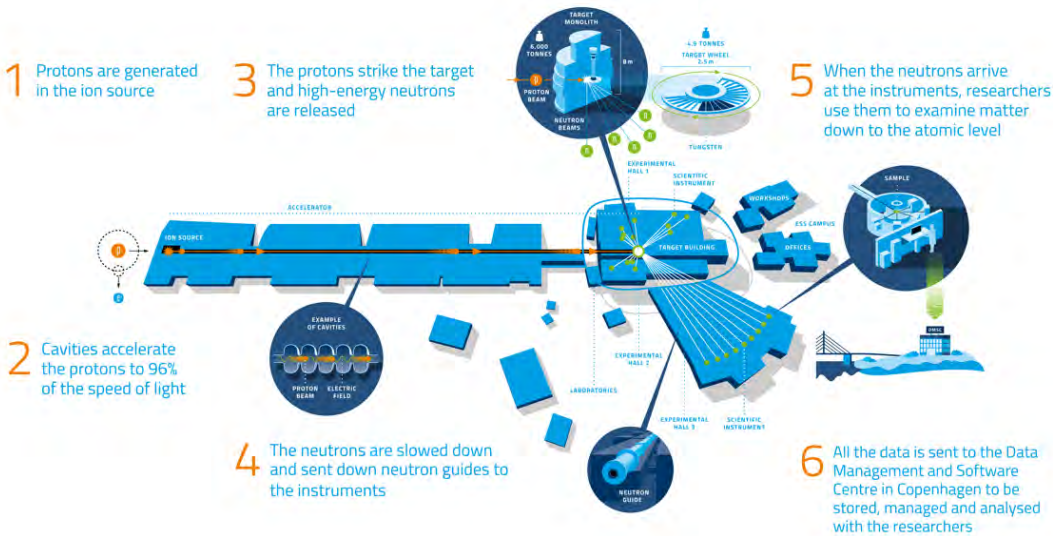
2026 First neutrons – the proton beam strikes the target for the first time

2027 First scientific experiments

2028 Transition to steady state operations

How ESS works

Research with neutrons is complementary to other techniques, providing insights thanks to the capabilities of going deep into materials and straight through metals. Neutrons have a high sensitivity to light elements like for example hydrogen, which is important in biological systems, and lithium, present in battery processes. Neutrons are non-destructive and therefore particularly suitable for fragile samples. All these and more properties make neutron science a powerful tool for sustainable solutions, driving innovation in medicine, chemistry, transportation, energy and more.



NEUTRONS FOR SOCIETY

ILL News @ IOP
Neutron Scattering Early Career Meeting

The Institut Laue-Langevin (ILL) is a world leader in neutron science and technology. Its high-flux reactor delivers the most intense neutron beams to the largest instrument suite in the world, serving a large community of researchers – both academic and industrial – in key areas such as health, energy, the environment, quantum materials and information technologies.

In 2025, ILL operated for 126 days, enabling 1800 researchers to perform 1400 experiments. The reactor will start operating again in late March delivering three cycles (~170 days) in 2027 and each of the coming years.

Each year there are two proposal deadlines in mid-February and mid-September. Rapid access can be requested at any time for full experiments (DDT access) and short measurements (EASY access). For more information on beam time access see www.ill.eu/for-ill-users/applying-for-beamtime/type-of-beamtime-access.

ILL provides an ideal research environment for early career researchers, with funded access to world class instruments enabling collaboration with international partners and expert instrument scientists. ILL also funds and hosts PhD students (see for example www.ill.eu/careers/all-our-vacancies/phd-recruitment/propose-a-phd-project) and is involved in numerous, European, Marie Curie, PhD and postdoc programmes.

For more ILL news, to sign up for the newsletter, and to find us on social media, see www.ill.eu.

ISIS Neutron and Muon Source

The ISIS Neutron and Muon Source is a world-leading centre for multidisciplinary research at the Rutherford Appleton Laboratory, on the Harwell Campus in Oxfordshire.

Our suite of over 30 neutron and muon instruments gives unique insights into the properties of materials on the atomic scale.

UKRI Science and Technology Facilities Council

ISIS Neutron and Muon Source

www.isis.stfc.ac.uk

- Over 3000 user visits a year, covering science areas including energy and clean growth, advanced manufacturing and materials, life sciences and healthcare and quantum matter.
- Over 550 PhD students visiting each year for experiments
- Annual Springboard awards for Early Career Researchers
- Biannual student meetings, and an annual whole-community user meeting attended by 300 people
- Training schools and online training resources

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Photos: STFC

Programme

Thursday 15 January 2026

09:30 Coffee and Registration

10:00 Welcome and Introduction

10:15 Flash Presentations (all participants)

11:40 Coffee Break

Sponsored Presentations

12:00 ISIS neutron and muon source for ECRs
Rosie de Laune, ISIS Muon and Neutron Source, UK

12:15 Compact Fusion Neutron Facilities: Supporting Research and Medical Isotope Development Today
Daniel Scoon, Astral Systems, UK

12:30 Supporting the Next Generation of Researchers at ESS
Raquel Costa, European Spallation Source, Sweden

12:45 Lunch and Networking

13:30 Keynote 1: This Wasn't the Plan (How I started in Neutron Scattering)
Adam Clancy, University College London, UK

14:30 Development Activity

16:00 Tea Break

16:30 Networking Activity

18:00 Reception

20:30 Close

Friday 16 January 2026

08:30 Coffee

09:00 Keynote 2: Lipid-based nanoparticles for drug delivery: Uncovering relationships between structure and function
Margaret N. Holme, Chalmers University of Technology, Sweden

Scientific Presentations – Session 1

10:00 The Upgrade of the TOSCA Spectrometer at ISIS
Sam Lambrick, ISIS Neutron and Muon Source, UK

10:20 Balancing life and death with proteins: A protein-protein interaction at the mitochondrial membrane investigated with neutron reflectometry
Sophie Ayscough, Ill-Institut Max Von Laue-Paul Langevin, France

10:40 Software for inelastic neutron scattering simulations
Adam Jackson, Science and Technology Facilities Council, UK

11:00 Coffee Break

Scientific Presentations – Session 2

11:40 Novel synthesis route and characterization of low polydispersity hydroxypropyl cellulose nanogels
Mónica Ledesma-Motolinía, University of Florence, Italy

12:00 Cross-validation of neutronic activation codes with a neutron scattering module irradiated by a compact DD neutron source
Hugo Dominguez-Andrade, University of Bristol, UK

12:20 Neutron Scattering Across Disorder and Frustration in Metal–Organic Frameworks
Luis Leon, University of Cambridge, UK

12:40 Lunch

Scientific Presentations – Session 3

13:30 Invited: Exploring Molecular Endofullerenes with Neutron Scattering and Finding a Career Path
Mo Aouane, European Spallation Source inc, Sweden

14:00 FlowSAS: Resolving 3D Small-Angle Scattering in Flowing Complex Liquids
Wouter Grünewald, Paul Scherrer Institute, Switzerland

14:20 Design of new, amine-rich, double hydrophilic block copolymers by copolymer modification and their use to form PolyIon Complex micelles studied by scattering techniques
Elena Andreea Palade, Institut Laue Langevin (ILL), France

14:40 NeXT 2.0, MoTo and Imaging at ILL
Alessandro Tengattini, Institut Laue Langevin (ILL), France

15:00 Tea Break

Scientific Presentations – Session 4

15:30 Invited: A Case for Good Simulation To Complement Neutron Scattering: A p-QENS Example
Andrew McCluskey, University of Bristol, UK

16:00 Muti-Scale Dynamic Study on Nanostructured Ionic Liquids
Shurui Miao, Department of Chemistry, University of Oxford, UK

16:20 Impact of mRNA structures on the interaction with lipids and nanoparticle formulation properties
Nga Man Cheng, University of Nottingham, UK

16:40 Lost in Translation: Simulation-Informed Bayesian Inference for Quasi-Elastic Neutron Scattering
Harry Richardson, University of Bristol, UK

17:00 Event Close

Keynote Presentations

This Wasn't The Plan (How I Started Neutroning)

Adam Clancy[1]
[1]University of Bristol, UK

As a nanomaterials chemist, neutron scattering came quite late into my career – originally as a collaborator, then an extra pair of hands during beamtime, and finally snowballing into a major part of my groups research. In this talk I'll show you the outsider's view of neutron scattering, and how I started using this toolkit to understand the (nano)things close to my heart. Beyond the cool experiments and unique insights QENS, TNS, and INS have given me, it also shows how pushing beyond your scientific comfort zone, overlapping diverse fields, and bringing your uncommon expertise to a new table can lay the groundwork for building an academic career.

Lipid-based nanoparticles for drug delivery: Uncovering relationships between structure and function

Margaret N. Holme[1]
[1]Chalmers University of Technology, Sweden

Lipid nanoparticle (LNP) delivery vectors comprise a broad class of lipid-based particles with diameters of 10s to 100s of nanometres. They include biologically [1] and synthetically derived vesicles, as well as LNPs with ionisable lipids [2] such as those employed in the COVID-19 vaccines, and have shown huge promise as delivery vectors for nucleic acids [3] and other therapeutic moieties. Due to the variety of possible cargoes, target cells, and therapeutic applications, a "one size fits all" approach to designing LNPs is insufficient. There has therefore been intense focus on developing LNPs tailored to specific applications.

The structures of LNPs are dictated by the way their constituent lipids self-assemble. This depends on both their chemical composition and formulation method. Additionally, LNP structures can rearrange in response to their local environment in the body, and characterising these self-assembly properties is crucial for understanding how LNPs behave during formulation and upon interaction with cells. Furthermore, this knowledge can be applied to inform design of optimised LNPs for medical applications [4].

In our group, we approach the question of LNP structural characterisation by combining small angle neutron scattering (SANS) with complementary techniques such as cryo-transmission electron microscopy, Raman spectroscopy, light scattering, surface techniques and small angle X-ray scattering (SAXS). Together, combinations of these techniques provide information about particle ensemble averages as well as single particle-level characterisation [5]. This is of particular importance since it is known that LNP formulations are often heterogeneous mixtures of different particle sub-populations, which may each behave differently in cells. In this lecture I will highlight examples from our work

applying SANS in combination with other techniques to uncover LNP morphology and sub-population analysis, and discuss how combining this with studies in cells can help to uncover structure-function relationships for various LNP formulations.

[1] Armstrong JP, Holme MN, Stevens MM. *ACS Nano* 11, 69 (2017).
[2] Han X, Zhang H, Butowska K *et al. Nat Commun* 12, 7233 (2021).
[3] Cárdenas M, Campbell RA, Yanez Arteta M, Lawrence MJ, Sebastiani F, *Curr. Opin. Colloid Interface Sci* 66, 101705 (2023).
[4] M. Ojansivu et al, Adv. Mater., 37 (2025), 2419538.
[5] V. Nele et al, Langmuir, 35 (2019), 6064-6074.

Sponsored Presentations

ISIS neutron and muon source for ECRs

Rosie de Laune[1]
[1]Isis Neutron and Muon Source, UK

I plan to introduce the facility and what we currently offer to early career researchers but then open for discussion on what else we could be doing.

Compact Fusion Neutron Facilities: Supporting Research and Medical Isotope Development Today

Daniel Scoon[1]
[1]Astral Systems

Astral Systems, a Bristol-based fusion neutron generator company Start-Up, is unlocking a complimentary service to larger National facilities to the Neutron community. Astral have developed and are ready to provide DD neutron source to the community today, demonstrated by providing irradiation services for UK universities and UKAEA.

Astral are opening a new DT Facility, operated within the vicinity of Bristol, ready to provide DT Irradiations to support cancer care research through the production of medical radioisotopes not currently produced in the UK, while offering researchers access to neutron irradiations for materials testing, and collaborative research opportunities.

Supporting the Next Generation of Researchers at ESS

Raquel Costa[1]
[1]European Spallation Source (ESS), Sweden

This presentation outlines how the European Spallation Source (ESS), as a European research infrastructure, supports Early Career Researchers from a facility-level perspective. It introduces the ESS context, highlights who our ECRs are and what ESS offers them in terms of access, training, collaboration, and scientific environment, and presents current initiatives alongside future directions. The talk also outlines the ambition to strengthen doctoral training at ESS through a more structured programme developed in partnership with universities.

Invited Speaker Presentations

Exploring Molecular Endofullerenes with Neutron Scattering and Finding a Career Path

Mo Aouane[1]
[1]European Spallation Source Eric, Sweden

Molecular endofullerenes, with atoms or small molecules trapped inside C60 carbon cages, are a remarkable example of 'particles in a box'. They invite basic questions: What happens to a molecule when it is confined in such a tiny space? How does it move compared to when it's free? In this talk, I'll share how neutron scattering has helped answer some of these questions. Along the way, I'll share a few scientific results from these studies. I'll also reflect briefly on how encountering these experiments early on, as a student at ILL, inspired me to work more closely with instrumentation — leading me from research to a career supporting other scientists at facilities like ISIS and then focus on instrument building at ESS.

A Case for Good Simulation to Complement Neutron Scattering: A p-QENS Example

Andrew McCluskey[1]
[1]University of Bristol, UK

Quasi-elastic neutron scattering and classical molecular dynamics simulations are highly complementary methods, covering the same time and length scales. Therefore, it is necessary that we understand fully the accuracy of the simulations that we have performed and how these may be correlated with neutron spectroscopy measurements. In this work, I will present a Bayesian scheme for estimating the self-diffusion coefficient from a single simulation trajectory with high statistical efficiency and accurately estimating the uncertainty in the predicted value [1]. I will then discuss how this approach may be used to find the collective-diffusion coefficient and the relevance of this measurement to QENS measurements with polarisation analysis. Throughout this seminar, I will introduce kinisi, a software package developed to improve the analysis of molecular dynamics simulation [2].

You may enjoy this seminar if you are interested in diffusion, applied mathematics, molecular dynamics simulations, or open-source software.

[1] A. R. McCluskey, S. W. Coles and B. J. Morgan, J. Chem. Theory Comput, 21(1), 79, 2025.
[2] A. R. McCluskey, A. G. Squires, J. Dunn, S. W. Coles and B. J. Morgan, Journal of Open Source Software, 9, 5984, 2024.

Contributed Talks - Scientific Presentations

Session 1

The Upgrade of the TOSCA Spectrometer at ISIS

Sam Lambrick[1]
[1]Isis Neutron and Muon Source, UK

The TOSCA spectrometer is a broadband indirect geometry spectrometer, with a particular sensitivity to and high-resolution in the chemical fingerprint region ħω = 50–200 meV (400–1600 cm−1), making it well suited to the study of molecular vibrations. TOSCA has been operating since 1998 and with a guide upgrade in 2017 providing a significant flux increase. To keep the instrument competitive and to further increase its scientific capabilities TOSCA is due for an upgrade of its secondary spectrometer (termed TOSCA-plus) as part of the ISIS Endeavour programme. The primary aim of the upgrade is to increase the detected flux (~ x10) by increasing the solid angle of the instrument's graphite analysers. However, introducing a spatially focusing analyser means deviation from the current ideal time/energy focusing of the geometry, thus requiring careful design to ensure there is no degradation in resolution. In order to investigate the impacts on both the resolution and signal of the proposed geometry Monte Carlo ray tracing simulations have been performed with the McStas package to compare the performance of TOSCA-plus to the current TOSCA setup.

Balancing life and death with proteins: A protein-protein interaction at the mitochondrial membrane investigated with neutron reflectometry

Sophie Ayscough[1], Luke Clifton[2], Jorgen Aden[3], Gerhard Groebner[3], and Hanna Wacklin-Knecht[4,5]
[1]Institut Max Von Laue-Paul Langevin, [2]ISIS Neutron and Muon Source, UK [3]Department of Chemistry, University of Umea, Sweden [4]Division of Physical Chemistry, Lund University, Sweden [5]European Spallation Source, Sweden

Mitochondria play a crucial role in apoptosis, a programmed mechanism of cell death. This mechanism is tightly regulated by proteins at the mitochondrial outer membrane (MOM). In apoptosis the pro-apoptotic Bax protein is attracted to the outer mitichondrial membrane (MOM), where it induces membrane leakage. [1] In healthy cells, Bax is neutralized by the anti-apoptotic Bcl-2 residing in the MOM.[2]

The complexity of the MOM system makes it difficult to obtain an overall picture of its organisation. However, preparation of planar lipid bilayers and analysis with neutron reflectivity (NR) and attenuated total reflection- fourier transform infrared spectroscopy (ATR-FTIR) can be used to identify the position of the two crucial proteins in respect to the membrane and to identify the kinetics of the interaction.

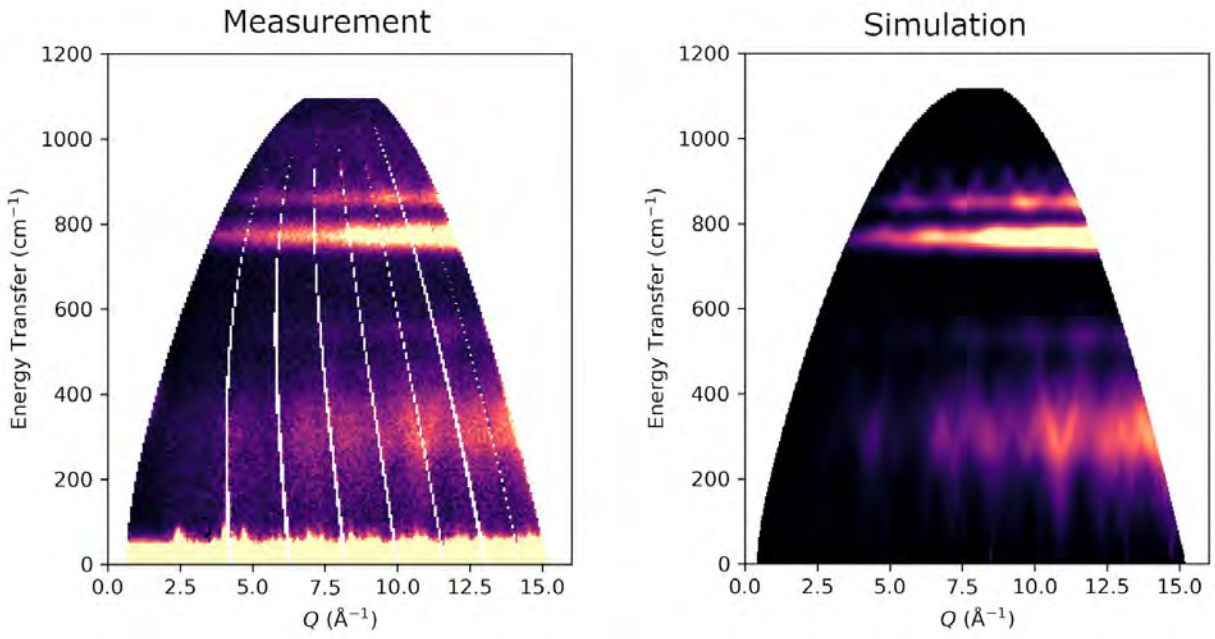
Our findings demonstrate that in the absence of Bcl-2, the Bax protein both inserts into the lipid bilayer and removes lipids, forming a lipid-protein complex on top of the original bilayer structure. However, our recent findings show that when Bcl-2 is reconstituted into lipid bilayers, Bax associates to the bilayer but does not insert into it or remove lipids. [3] Initially monomeric Bax associates to Bcl-2 followed by further sequestration of Bax to the surface. Our results provide the first structural evidence of Bcl-2 preventing membrane perforation by Bax as part of its anti-apoptotic mechanism.

[1] M. Lidman, BBA-Biomembranes 1858, 1288-1297 (2016).
[2] A. Mushtaq, Commun Biol 4, 507 (2021).
[3] S. Ayscough, Sophie E., et al., bioRxiv (2025)-in review.

Software for inelastic neutron scattering simulations

Adam Jackson[1]
[1]Science and Technology Facilities Council, UK

Inelastic neutron scattering measurement of phonons is a sensitive probe of chemical environment and complementary to optical methods of vibrational spectroscopy. However, the resulting spectra are not easy to interpret; to extract the best possible value from beamtime the ISIS facility supports software development for relevant simulation tools. The AbINS and Euphonic packages implement complementary methods of processing from ab initio or machine-learned simulations in the harmonic approximation. The ResINS library is in development to unify treatment of instrumental resolution across a variety of simulation methods and codes. Here we outline some available simulation methods, their limitations and the state of software development to make them accessible to facility users.



Session 2

Novel synthesis route and characterization of low polydispersity hydroxypropyl cellulose nanogels

Mónica Ledesma-Motolinía[1], Fernando Soto-Bustamante[1], Gavino Bassu[1], Jacopo Vialetto[1], and Marco Laurati[1]
[1]Department of Chemistry "Ugo Schiff", University of Florence, Italy

Thermoresponsive hydroxypropyl cellulose (HPC) nanogels were synthesized via a novel route of polymerization. In this study, the optimal surfactant concentrations and reaction temperature were identified by analyzing the solution dispersity of different HPC molecular weights. The required surfactant concentration of dodecyltrimethylammonium bromide (DTAB) is inversely related to the polymer's molecular weight, with higher molecular weights requiring lower surfactant concentrations. Nanogels were synthesized at twice the polymer critical solution temperature (LCST). Divinyl sulfone (DVS) was used to crosslink the polymer network structure. Under this novel route, HPC nanogels exhibited a low polydispersity index. The thermoresponsive behavior of HPC nanogels as a function of the crosslinker concentration was characterized by dynamic light scattering (DLS). The results indicated that as expected the average size decreased with increasing crosslinker molarity. Small-angle neutron scattering (SANS) was used to provide information about the internal structure as a function of the temperature, indicating significant deviation from the fuzzy sphere structure characteristic of PNIPAM microgels.

Cross-validation of neutronic activation codes with a neutron scattering module irradiated by a compact DD neutron source

Hugo Dominguez-Andrade[1,2], Alex Little[1], Tom Mooney[1], Rob Havel[1], Mahmoud Bakr[1,2], Alexandre Sureda Croguennoc[3], Juan Diego Iberico Leonardo[3], Robert Annewandter[2], Mark Gilbert[4], Tom Wallace-Smith[2], Tom Scott[1]
[1]University of Bristol, UK [2]Astral Systems, UK [3]IDOM, UK [4]UKAEA, UK

The University of Bristol in collaboration with Astral Systems and IDOM are being funded by UKAEA to study tritium breeding materials for fusion applications through a project called small scale experiments for tritium breeding (SSETB, codename Scorpio). Part of the project is the cross-validation of neutronic activation codes against experimental data acquired in Astral's irradiation facility in Bristol.

For this experiment, a "scattering module" was designed and built. This consists of a sandwich structure with several layers of HDPE plates. Intercalated between the HDPE layers, neutron activation foils of In and Au were placed in specific positions. Foils were also positioned at the front and the back for calibration purposes. The scattering module was placed in front of a DD neutron source (E = 2.45 MeV) with an intensity of I = 5 × 107 n/s for t = 50 h. The irradiation has concluded and now the whole irradiation ensemble (source + scattering module + neutron bunker) will be simulated with different

codes by different research teams. The codes that we are aiming to evaluate are: GEANT4, MCNP and OpenMC.

On this talk we are aiming to present the experimental data that was acquired during the irradiation and some preliminary simulation data.

Neutron Scattering Across Disorder and Frustration in Metal–Organic Frameworks

Luis Leon[1], Ludovic Jaubert[2], Guillermo Mínguez Espallargas[3], and Matthew Cliffe[1]
[1]University of Cambridge, UK [2]Université de Bordeaux, France [3]Universidad de Valencia, Spain

Metal–organic frameworks (MOFs) offer an exceptional platform for exploring unconventional magnetic states, providing access to magnetic lattices that are difficult or impossible to realize in dense inorganic materials. Their synthetic versatility allows the construction of both topologically disordered and geometrically frustrated networks, and neutron diffraction is a powerful probe for uncovering their magnetic behaviour.

We first consider the case of directly synthesized amorphous MOF glasses of composition Fe(im)2-x(bim)x (L. León-Alcaide et al., Nat. Commun. 2025, 16, 8783), showing that these materials form continuous random networks while maintaining a remarkably uniform Fe(II) local environment, an unusual combination not accessible in conventional inorganic glasses. Neutron scattering and magnetometry show that these systems behave as amorphous antiferromagnets dominated by nearest-neighbour Heisenberg interactions, exhibiting collective magnetism despite the absence of long-range order.

In contrast, we also examine a highly ordered yet strongly frustrated lattice: the centred pyrochlore network realized in the metal-azolate framework [Mn(II)(ta)2], previously identified as a classical spin-liquid candidate (R. P. Nutakki et al., Phys. Rev. Res. 2023, 5, L022018). Using powder neutron diffraction supported by simple magnetic models, we explore the exchange interactions and moment sizes that stabilize its possible ground states, mapping the parameter space compatible with classical spin-liquid behaviour.

Together, these studies illustrate how neutron diffraction provides unique insight into both disordered and frustrated magnetic frameworks in MOFs, highlighting the breadth of magnetic phenomena accessible in molecular materials.

Session 3

FlowSAS: Resolving 3D Small-Angle Scattering in Flowing Complex Liquids

Wouter Grünewald[1], Ashley Williams[1], and Viviane Lutz-Bueno[1]
[1]Paul Scherrer Institute, Switzerland

Complex fluids are ubiquitous in science and industry and include colloids, polymers and biological materials. Such systems alter their internal structure under the influence of external stresses and often display non-linear rheological behaviour. The response of the microstructure to shear flow is commonly studied using small-angle neutron scattering (SANS) coupled to a rheometer with a Couette geometry [1]. However, in common applications the flow fields can be more complex than simple Couette flow, and when the flow is three-dimensional this necessitates the measurement of the structure in three dimensions.

We have developed a measurement and data analysis protocol to obtain the 3D reciprocal space scattering of flowing liquids. Using programmable rotation stages, a capillary, flat flow channel or arbitrary other flow geometry can be rotated to acquire a SANS signal from different angles. The 3D reciprocal space scattering pattern can then be reconstructed from the set of projections by fitting a sum of spherical harmonic functions to the data [2]. Using this 3D pattern, the isotropic and anisotropic contributions to the scattering pattern can be decoupled, or a 2D slice can be taken to obtain SANS patterns that are not normally measurable, e.g. with the beam parallel to the flow in a capillary. This way, we gain a more complete understanding of the 3D structure of the liquid under flow.

[1] Eberle AP, Porcar L. Curr. Opin. Colloid Interface Sci. 2012;17(1):33–42.
[2] Liebi M, Georgiadis M, et al. Acta Crystallogr. A 2018;74(1):12–24.

Design of new, amine-rich, double hydrophilic block copolymers by copolymer modification and their use to form PolyIon Complex micelles studied by scattering techniques

Elena Andreea Palade[1], Ralf Schweins[1], Corine Gerardin[2], and Julien Schmitt[2]
[1]Institut Laue Langevin (ILL), France [2]Institut Charles Gerhardt (ICGM), France

Double hydrophilic block copolymers (DHBC), consisting of one neutral and one charged block with distinct chemical identities, have emerged as versatile agents for both structuring and functionalizing self-assembled nanomaterials. Under specific pH conditions, DHBC can form polyion complex (PIC) micelles in the presence of an oppositely-charged micellization partner. The reversible nature of micellization, governed by pH, enables the formation of well-defined mesostructured materials in the presence of silica. Subsequent pH variation removes the micellization partner, liberating the porosity while the DHBC remains embedded within the pore walls, giving intrinsic functionality to the resulting material.[1]

The present work aims to design intrinsically functional ordered mesoporous materials through a one-pot synthesis strategy employing an amine-rich DHBC. We developed a method to modify a previously synthesized parent polymer, P(OEGMEA)-b-P(AA), composed of a comb-like ethylene oxide-rich neutral block and an poly(acrylic acid) block, into an amine-rich DHBC, P(OEGMEA)-b-P(AA/NH2). Functionalization involved an initial activation reaction using N-(3-(dimethylamino)propyl)-N′-ethylcarbodiimide (EDC), 4-dimethylaminopyridine (DMAP), and N-hydroxysuccinimide (NHS), followed by amidation at pH 9 with N-Boc-ethylenediamine.[2,3] Optimization of this activation/amidation procedure was carried out with respect to reactant ratios and reaction pH.

The behavior of these modified DHBC in solution, with or without micellization partners, was investigated using scattering techniques, namely DLS and SAXS/SANS. These studies provided key insights into micellization conditions, enabling their application in synthesizing functional mesoporous materials.

[1] Baccile N. et al., Angew. Chem., Int. Ed. (2008), 47, 8433-8437.
[2] Unnikrishnan A. et al., Macromolecules (2025), 58 (10), 5110–5134.
[3] Mendes Alexandre M., M2 Internship (2025).

NeXT 2.0, MoTo and Imaging at ILL

Alessandro Tengattini[1], Lukas Helfen[1], Anna Fedrigo, and Emilio Ruiz-Martinez
[1]Institut Laue Langevin, France

NeXT-Grenoble is the neutron and X-ray tomograph born in 2015. This instrument has undergone a major upgrade to further expand the portfolio of contrast options, completed in September 2023. In May 2025 we are also commissioning MoTo, a Monochromatic Tomograph.

These works have improved the highest attainable spatio-temporal resolutions by increasing the maximum flux (expanding the accessible collimation ratios L/D) as well as by upgrading the range of

detectors. The simultaneous x-ray imaging has also been improved, passing from a 150 kV to a 300kV setup. An improved sample stack helps automate and expands the possibilities (in size/weight) of in-situ apparatus that can be easily installed on the instrument, as well as adding a laminography option.

MoTo is instead a new monochromatic (2.4Å) instrument that takes part of the beam from the same guide as NeXT but that can operate independently from NeXT, and tailored for grating interferometry and polarized neutron imaging.

This presentation will focus on recent results from NeXT and MoTo and show the plans for the construction of another two neutron imaging instruments at ILL.

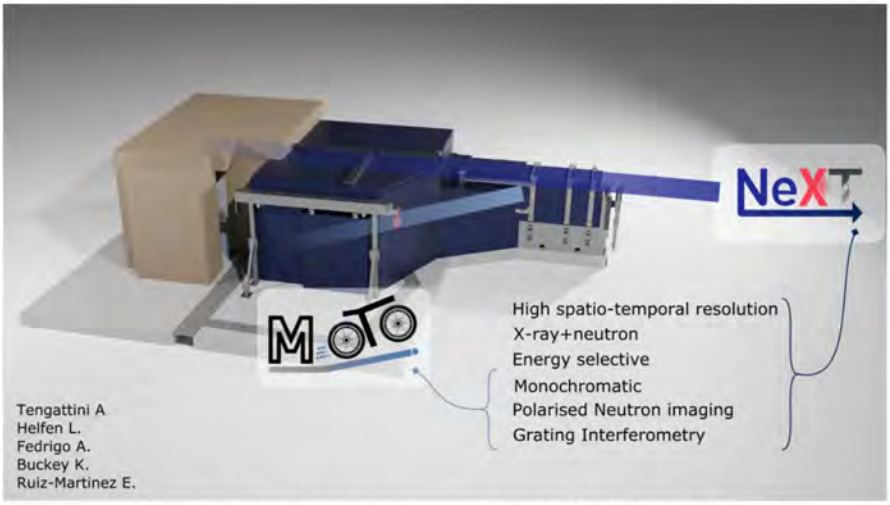


Figure 1. A schematic representation of NeXT and MoTo

Session 4

Muti-Scale Dynamic Study on Nanostructured Ionic Liquids

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Ionic liquids are a novel class of solvents with ultra-low vapour pressure and tunable liquid properties. Among them, protic ionic liquids (PILs) are particularly effective solvents for self-assembly of surfactants and lipids into micelles, vesicles, liquid crystals and microemulsions. This is exemplified by alkylammonium PILs, which are also cheap, easily prepared, and can be readily deuterated. Over the past decade, much has been learnt about the static structure of alkylammonium PILs, however, virtually nothing is known about their dynamics, both the single ion diffusion and the collective motion of clusters. This is due to the complex and disordered nature of liquid nanostructure, which is expected to display a range of dynamic behaviours on different time and length scales. In this study, we have examined ethanolammonium nitrate, ethylammonium nitrate and propylammonium nitrate, using a variety of dynamic techniques. We employed multi-contrast wide-angle neutron spin echo spectroscopy (WASP, ILL) to capture the nanosecond-millisecond relaxations across 0.1 – 1.4 ^Å-1, and pulse-field gradient NMR to track molecular diffusion. Combined with their known averaged liquid nanostructures, we have now characterized the static and dynamic nanostructure of three protic ionic liquids, carefully chosen to demonstrate different degrees of ordering, at multiple temperatures. This allows us to understand the structure-property relationship of alkylammonium PILs across a wide space and time scale, which has the potential to unlock the rational design of job-specific PIL-based solvent systems.

Impact of mRNA structures on the interaction with lipids and nanoparticle formulation properties

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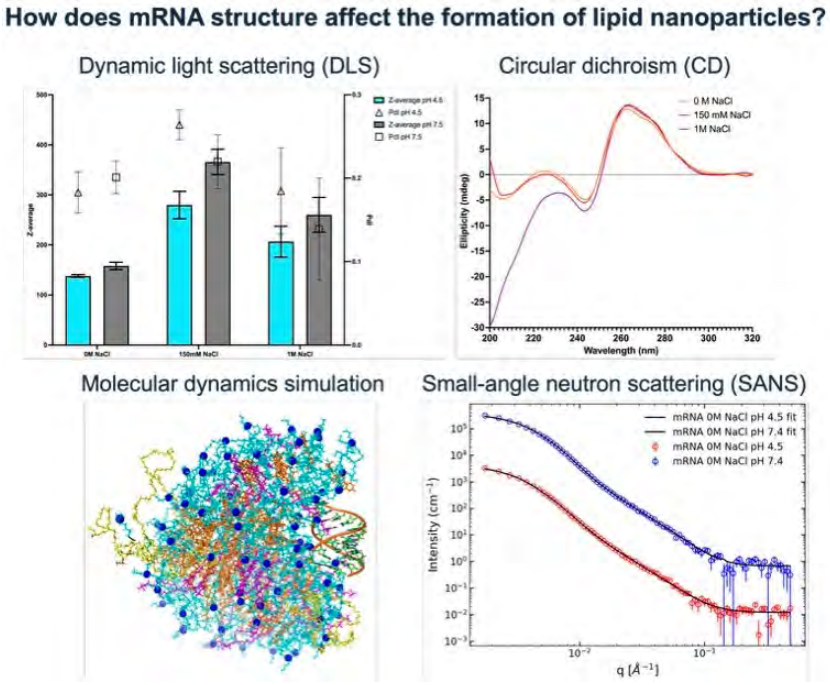
Messenger RNA (mRNA) technology allows the treatment of previously undruggable targets, broadening the range of treatable diseases. Its ability to encode therapeutic proteins and manipulate gene expression makes it a great candidate for treating diseases with known genetic profiles, such as cancer and infectious diseases (like COVID-19) 1. However, mRNA alone cannot be delivered to cells directly as it is highly susceptible to degradation by the endogenous nucleases, hence it must be packaged in a delivery vehicle. The most translatable approach is to encapsulate the mRNA in lipid nanoparticles (LNPs). LNPs are made up of four main components: cationic/ionisable lipid, helper lipid, cholesterol,

and PEGylated lipid, where they self-assemble into a lipid matrix 2,3. The wide variety for the lipid types and lipid ratios enable a diverse space to study the optimal formulation for targeted therapies. However, our fundamental understanding of how mRNA structure impacts the formation of LNPs and the lipid arrangement is poorly understood. These are important factors relating to uptake, endosomal escape, and cargo release. Utilising a combination of biophysical characterisation techniques and molecular dynamics simulation, we gain a deeper understanding of the interactions between lipids and mRNA at the molecular level. Our preliminary results show that altering the formulation condition for mRNA-LNPs affect the size and internal structure of the particles formed.



Lost in Translation: Simulation-Informed Bayesian Inference for Quasi-Elastic Neutron Scattering

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Quasi elastic neutron scattering (QENS) is a powerful experimental tool for the elucidation of molecular motions and has considerable potential as a means of experimentally validating machine learning interatomic potentials (MLIPs). However, extracting physical insight from QENS data is challenging: the inversion from measured spectra to dynamical mechanisms typically relies on analytical models that are frequently oversimplified, over-parameterised, and insufficiently discriminative. As a result,

traditional fitting approaches often struggle to distinguish between competing dynamical processes, limiting their usefulness for assessing MLIP performance.

Using liquid benzene as a benchmark system, we demonstrate the limitations of these traditional approaches in distinguishing distinct motions before introducing an integrated framework that combines molecular dynamics (MD) simulations with Bayesian inference to yield more robust analyses. MD simulations provide an ideal complement to QENS probing similar time and length scales, whilst offering truly atomistic resolution - albeit within the constraints of the approximate simulation force field. We first validate the accuracy of our simulations using model-agnostic methods before leveraging their atomistic resolution alongside Bayesian evidence estimation via nested sampling to guide experimental fitting.

Applying these methods, we empirically separate rotational and translational dynamics, quantify the influence of coherent scattering, and develop a mathematically rigorous model for benzene's anisotropic rotational motion. Through encoding the underlying physics into the analytical models and incorporating insights gained from simulation, we were able to identify individual rotational modes and reproduce experimental diffusion coefficients, laying the groundwork for improved quantification of the discrepancies between simulation forcefields and experimental measurements.

Notes

Neutron Scattering Group Early Career Meeting

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Engineers House, Bristol, UK

IOP Institute of Physics