JDN 2022

Program & Abstract book

Journées de la
Diffusion
Neutronique

Biarritz, Nov 14-17, 2022

JDN PROGRAM 2022

The multidisciplinary conference JDN2022 is dedicated to new results, obtained using neutron scattering techniques, in various scientific domains representative of the whole French users community. We are also very pleased to announce that the Spanish Community will contribute to this edition. Five sessions will be organized:

A. Magnetism and Materials,
B. Soft Matter and Biology,
C. French Neutron Scattering Society (SFN) PhD prize,
D. Instrumentation,
E. News from the facilities,
F. Neutron Scattering Associations,
G. Molecular Modelling, Optical and Neutron spectroscopies,
H. Diffraction at the European Spallation Source (ESS).

Each session will be introduced by invited talks (40 min. plenary and 30 min. keynote), which will be followed by a series of oral communications (15 min.). Several poster sessions will also take place during the whole conference, with a Best Poster Award for a deserving young scientist. The sessions A to F will be held on Monday 14/11 and Tuesday 15/11 in the main conference room. **The sessions G and H will be held in parallel on Wednesday 16/11 morning and Thursday 17/11 morning** (the rooms of the sessions will be indicated on site).

On Wednesday afternoon, after some “free time”, a “Cesta Punta” session followed by an aperitif will be organized at the Biarritz Athletic Club from 5.30pm to 7.30pm. The transfer by bus will be organized at 5.30pm from the Domaine de Françon. The conference dinner will be organized on Wednesday evening.

PROGRAM

MONDAY, NOVEMBER 14th

12.00 - Registration and buffet
13.50 - Welcome and introduction

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Magnetic excitation spectrum of the unconventional superconductor UTe_2

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Study of magnetic epitaxial thin films using neutron diffraction

15.45 - A. Roll *(LLB, Saclay)* 12
Spin dynamics seen by Inelastic Neutrons Scattering in an 1D Fe superconducting compound

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Small-angle scattering studies of polymer and filler structures

17.10 - Keynote - L. Noirez *(LLB, Saclay)* 14
Collective effects in liquids: what scattering methods say and what it does not say

17.40 - F. Cousin *(LLB, Saclay)* 15
Controlled synthesis of gold nanoparticles in copolymers nano-molds by x-ray radiolysis: a coupled SANS/laboratory SAXS/synchrotron SAXS study

17.55 - M. Almeida *(ICPME, Thiais)* 16
Decorating tunable self-assembled nanostructures with PEG for stealth applications

18.10 - G. Meyer *(LiPhy, Grenoble)* 17
Insights into the microscopic mechanisms responsible for phase separation in a biphasic acidic solution for metallic ion extraction

18.25 - L. Lafon *(LPS, Orsay)* 18
Probing polymers adsorption under highly viscous flows using neutron reflectivity

18:40 - 20:00. Poster Session and welcome cocktail

20.00 - Dinner

Tuesday, November 15th

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Dynamically disordered solids across physical and chemical space

9.40 - Keynote - S. Lyonnard *(CEA/IRIG, Grenoble)* 20
Batteries/fuel cells TBA

10.10 - R. Cubitt *(ILL, Grenoble)* 21
Self-Organised Vortex Structures under the Influence of Current in Superconducting Niobium

10.25 - O. Demortier *(LLB, Saclay)* 22
Thermal conductivity of spinons in the 1D spin ½ cuprate $SrCuO_2$

10.40 - Coffee break

SESSION C - SFN PHD AWARD CEREMONY
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11.15 - C. Alba-Simionesco, presentation of the 2022 SFN PhD award

11.45 - SFN PhD Award Laureate

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Seeing the Chemistry in Biology

14.30 - C. Beck *(ILL, Grenoble)* 24
Time dependent kinetic measurements reveal a metastable intermediate phase during protein crystallization processes

14.45 - M. Napieraj *(LLB, Saclay)* 25
Monitoring digestion of protein gels: Neutron Small Angle Scattering and Dark Field Imaging completed with SAXS

15.00 - A. Nidriche*(ILL-Liphy, Grenoble)* 26
Using polarisation analysis to compare the dynamics of protonated and perdeuterated samples of proteins

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16.00 - Invited - U. Hansen *(ILL, Grenoble)* 28
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16.15 - Invited - N. Martin *(LLB, Saclay)* 29
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16.30 - F. Natali *(ILL, Grenoble)* 30
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16.45 - Invited - F. Ott *(LLB, Saclay)* 31
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17.20 - Institut Laue-Langevin, **J. Jestin**, ILL, Grenoble, France

17.40 - Laboratoire Léon Brillouin, **G. Chaboussant**, LLB, Saclay, France

18.00 - Fédération Française de la Neutronique, **M. Plazanet**, 2FDN, France

18.20 - Break

SESSION F - NEUTRON SCATTERING ASSOCIATIONS
CHAIR : P. LAUNOIS

18.30 - European Neutron Scattering Association, **N. Malikova**, France

18.45 - Spanish Neutron Scattering Society (SETN), **M.T. Fernandez-Diaz**, France

19.00 - General assembly of the French Neutron Scattering Society (SFN), **P. Launois**, France : annual report and financial statement, election of the new board members - Cocktail

20.30 - Dinner

WEDNESDAY, NOVEMBER 16th

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TOF powder neutron diffraction through the lens of quantum materials

9.45 - Invited - S. Capelli *(ISIS, UK)* 39
Single crystal neutron diffraction in time-of-flight

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11.00 - Invited - M. Feygenson *(ESS, Sweden)* 41
DREAM: Neutron powder diffraction at the ESS

11.45 - Invited - X. Fabrèges *(LLB, France)* 42
MAGiC: Polarized neutron diffraction at the ESS

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Cesta Punta, Cocktails and Tapas
20.00 - Conference dinner and Party

THURSDAY, NOVEMBER 17th

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9.30 - Keynote - M. Plazanet *(LiPhy, Grenoble)* 44
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10.00 - L. Karam *(ISM, Bordeaux)* 45
Second order optical response in poled amorphous films: the singularity of thin films and new opportunities for integrated photonics

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Molecular simulations of clathrate hydrates: An overview

11.30 - A.C.C. Agnissan *(Ifremer, Brest)* 47
Laboratory to field scale characterization of methane hydrate formation in clay-rich sediments using Raman Spectroscopy: study case of the Black Sea natural gas hydrate system

11.45 - End of the session

Session H.2. - Diffraction at ESS

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Using mantid to analyze powder and single crystal data on WISH

9.45 - Invited - S. Heybrock *(ESS, Sweden)* 49
TOF data reduction using Scipp: Fast and flexible handling of event-mode data for time-resolved experiments

10.30 - Coffee break and poster session

10.45 - Invited - I. Kibalin *(LLB, Saclay)* 50
Polarized neutron diffraction data analysis to probe local magnetic anisotropy in single crystals and powders using the CrysPy library

11.30 - Invited - A. Sazonov *(ESS, Sweden)* 51
EasyDiffraction, a new software for neutron diffraction data analysis

12.15 - End of the session

12.15 - Lunch box
End of the JDN2022

LIST OF POSTER CONTRIBUTIONS

MAGNETISM & MATERIALS

SOFT MATTER & BIOLOGY

INSTRUMENTATION

OPTICAL AND NEUTRON SPECTROSCOPY & MOLECULAR MODELING

ESS WORKSHOP

Magnetic fragmentation in pyrochlore iridates and ruthenates

E. Lhotel [1], F. Museur[1,2], E. Lefrançois[1,3], V. Cathelin[1], J. Robert[1], R. Ballou[1], P.C.W. Holdsworth[2] and V. Simonet[1]
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Among the original magnetic states which emerge from frustrated magnetic systems, spin ice has aroused a strong interest because its macroscopically degenerate ground state belongs to the class of Coulomb phases: its organising principle is dictated by a local constraint called the ice-rule, which can be interpreted as a divergence free condition of an emergent gauge field. Magnetic excitations in spin ice, called magnetic monopoles, correspond to a violation of the local ice-rule and introduce a non-zero divergence in the emergent field.

Recently, theoreticians introduced the concept of magnetic moment fragmentation, whereby the local magnetic moment field fragments into the sum of two parts, a divergence full and a divergence free part. A prominent example of fragmentation occurs in spin ice, if the monopoles organise as a crystal of alternating magnetic charges. In that case, the fragmentation leads to the superposition of an ordered configuration and of an emergent Coulomb phase. Experimentally, the fragmentation manifests itself via the superposition of magnetic Bragg peaks, characteristic of the ordered phase, and a pinch point pattern, characteristic of the Coulomb phase.

In this talk, I will show how this magnetic fragmented state can be stabilized in pyrochlore iridates $R_2Ir_2O_7$, with R=Ho, Dy [1,2]. Then I will present a novel type of fragmented state that we recently discovered in in $Ho_2Ru_2O_7$.
Those phases could be identified thanks to powder neutron diffraction as well as thermodynamic measurements (specific heat, magnetization), down to very low temperature (50mK).

[1] E. Lefrançois et al., Nature Commun. 8 (2017), 209.
[2] V. Cathelin et al., Phys. Rev. Research 2 (2020), 032073(R).

Neutron scattering panorama on ensembles of magnetic nanoparticles: magnetic order/disorder and collective excitations

Luis Fernández Barquín[1], Elizabeth M. Jefremovas[1], María de la Fuente[1], David González-Alonso[1,3], Philipp Bender[1], Cristina Echevarria-Bonet[2], Lourdes Marcano[2], Jesús A. Blanco[2], Jose I. Espeso[1], Jesús Rodríguez Fernández[1], Ana García Prieto[4], Javier Alonso[1], Alfredo Garcia-Arribas[5], M. Luisa Fdez-Gubieda[5]

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The activity on magnetic nanoparticles (MNPs) has been at the core of nanoscience since the very beginning, which is typically rooted in a talk by R. P. Feynman in 1959 and (experimentally) the tuning of Scanning Tunneling Microscopes in the 80s [1, 2]. Effectively, already Louis Néel procured us with the basic understanding of the behaviour of what was called fine magnetic particles. In the 70s-80s most of the work was carried out in Fe-oxides (3d, superexchange). The main microscopic technique was then Mössbauer spectroscopy and the best suited groups for the task were those with available temperature variation. Surprisingly, 4f-magnetism was somewhat left behind. Probably, the groups working in magnetic intermetallics evolved more and more to pure Strongly Correlated Electron Systems issues, and the researchers on MNPs were not familiar with RKKY interactions, CEF effects, and the like. Equally, neutron scattering techniques are not within the most popular characterisation routes for MNPs groups. They mostly concentrate now on X-ray, Transmission Electron Microscopy, although groups working in the development of SANSPOL and POLARIS used to employ ultrasoft FINEMET MNPs, among others. In this communication I am reviewing the connection between the macroscopic results and the neutron scattering data to unveil the magnetic order and excitations. This has been performed using RX_2 alloys (R=rare earth, X = nonmagnetic metals [3], and artificial Fe-oxides and natural magnetite magnetosomes from magnetotactic bacteria [4].

I want to acknowledge my fellow partners working in other institutions, some of them belonging to European Large facilities.

[1] R. P. Feynman, “Tiny machines” (https://www.youtube.com/watch?v=-LidL8W7eI4) (2022).
[2] G. Binnig and H. Rohrer, Rev. Mod. Phys. 71 (1999) S324.
[3] E. M. Jefremovas et al., Phys. Rev. B 104, 134404 (2021); E. M. Jefremovas et al., Scientific Reports 12 (2022) 9733.
[4] P. Bender et al., Phys. Rev. B 98, 224420 (2018). L. Marcano et al., Nanoscale 10, 7407 (2018); E. M. Jefremovas et al., Nanoscale Advances 4, 2649 (2022).

Magnetic excitation spectrum of the unconventional superconductor UTe_2

William Knafo[1], Georg Knebel[2], Paul Steffens[3], Koji Kaneko[4], Adrien Rosuel[2], Jean-Pascal Brison[2], Jacques Flouquet[2], Dai Aoki[5] and Stéphane Raymond[6]
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The discovery of the heavy fermion superconductor UTe_2 ($T_{SC} \approx 1.6$ K) has triggered a wealth of research owing to the possible triplet and chiral nature of the superconductivity, the observation of multiple superconducting phases under magnetic field and pressure, as well as the proximity to a magnetic instability. The spin dynamics of UTe_2 was investigated by inelastic neutron scattering on a single crystal sample [1,2]. In the normal state, the presence of incommensurate spin fluctuations peaked at the wave-vector $\mathbf{k_1}$=(0, 0.57, 0) is confirmed. The associated quasielastic response is characterized by a relaxation rate $\Gamma(\mathbf{k_1}) \approx 2.5$ meV. These fluctuations saturate below 15 K in possible relation with anomalies observed in bulk and NMR measurements. The low dimensional nature of the fluctuations is evidenced by the absence of correlations along the c-axis of the orthorhombic structure, where the signal has the characteristic signature of in-phase fluctuations of the two uranium atoms of the primitive unit cell. This peculiarity can be related to the spin ladder structure of UTe_2 with these two uranium atoms forming its rungs. A feedback effect of superconductivity on the magnetic excitation spectrum manifests through the development below T_{SC} of an inelastic mode at $\Omega \approx 1$ meV for the wave-vector $\mathbf{k_1}$. The high ratio $\Omega/k_BT_{SC} \approx 7.2$ and the large damping of this mode contrast with the most common behaviour found for the resonance peak in heavy fermion superconductors. These neutron scattering results are motivating theoretical works on triplet pairing via incommensurate spin fluctuations, with the ferromagnetic coupling in the rungs being a main ingredient.

[1] W. Knafo *et al.*, Phys. Rev. B **104**, L100409 (2021).
[2] S. Raymond et al., J. Phys. Soc. Japan **90**, 113706 (2021).

Study of magnetic epitaxial thin films using neutron diffraction

H. Himanshu [1,2,3], E. Rebolini [1], S. Grenier [4,5], K. Beauvois [1,4], M. B. Lepetit [1,5,] B. Ouladdiaf [1], B. Mercey [6], C. Simon [2,3]
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The field of antiferromagnetic spintronics has been the object of active research over the past decade for the next generation of spin-based devices [1,2]. A particular focus has been on the design of new materials, specifically thin film preparation and detailed understanding of their magnetic properties.

Determination of the magnetic structure of these films is still a challenge and neutron diffraction (ND) technique is a good candidate for such a determination. The D10 instrument at ILL has been increasingly used for measurements on such films [4,5]. This challenging technique is still under development and the future commissioning of D10+ at the ILL will be a very good opportunity.

In this framework, we use ND to solve nuclear and magnetic structure of epitaxial thin films. We are interested in $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) thin films deposited on Si substrate with a $SrTiO_3$ (STO) buffer layer. We have employed SQUID magnetometer, electron diffraction, X-ray diffraction and ab-initio calculations to complement the ND data. Our results show that these films can be treated as single crystals to measure diffraction peaks and determine the nature of magnetic spin configuration in the system.

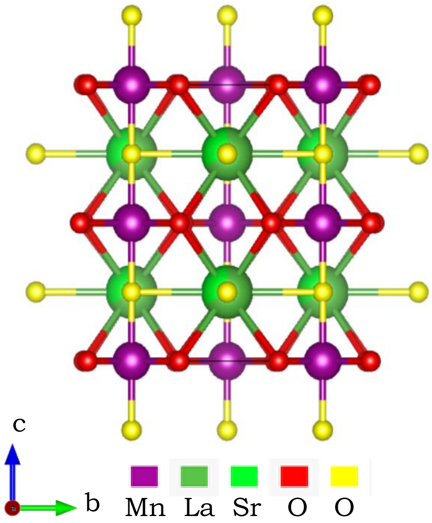

Figure: Schematic of the LSMO film structure deposited with STO buffer layer on Si substrate

In this talk, I will present our most recent results obtained on these manganese oxide thin films.

[1] Jungwirth, T. et al. Antiferromagnetic spintronics. Nature Nanotech 11, 231{241 (2016)
[2] V. Baltz, A. Manchon, M. Tsoi, T. Moriyama, T. Ono, and Y. Tserkovnyak, Rev. Mod.Phys. 90, 015005 (2018)
[3] A Sadoc, B Mercey, C Simon, et al Phys Rev Lett 104 046804 (2010)
[4] R. Ibarra et al, "Noncollinear magnetic order in epitaxial thin films of the centrosymmetric MnPtGa hard magnet", Appl. Phys. Lett. 120, 172403 (2022)
[5] Shimamoto, K., Mukherjee, S., Manz, S. et al. Tuning the multiferroic mechanisms of TbMnO3 by epitaxial strain. Sci Rep 7, 44753 (2017)

Spin dynamics seen by Inelastic Neutrons Scattering in an 1D Fe superconducting compound

A. Roll[1,2], V.Balédent[1] and S.Petit[2]
[1] *Laboratoire Léon Brillouin, CEA Saclay*
[2] *Laboratoire de physique des solides*

Since recent years and the discovery of their high superconducting Tc under high pressure, pnictures have been an intense field of research to understand the necessary ingredients and the origin of pairing mechanism for superconductivity, both experimentally and theoretically. Among universal properties of these system is 2d layers of irons planes and the proximity of vanishing magnetic order, a common feature with the famous cuprates. In this context, we have studied the quasi-1D Fe spin ladder $BaFe_2Se_3$: characterized by a (quasi 1D) “block” magnetic order suggesting frustrated interactions at ambient pressure, different from usual stripe or classical antiferromagnetism, and its quasi-unidimensionality, it becomes superconducting under pressure. This reshape the common usual ingredients for inducing superconductivity in 3d systems: magnetic fluctuations are expected to be responsible of cooper pairs formation [3]. To try out this hypothesis, it is important to determine the magnetic exchange couplings at play, and in turn to estimate the strength of magnetic fluctuations, and the stability of the superconducting phase.

In this context, INS experiments have been carried out [1] to know more about magnetic exchanges in this compound, supported by theoretical studies [2]. However, Ref [1] reports on powder averaged data, casting some doubt on the precise value of the couplings. The model proposed in Ref [1] does not seem physical and is not unique to stabilize the structure. In addition, it suggests many exchanges parameters for fews experimental data (extracted from powder averaged data).

To address this issue and revisit this description of magnetic couplings in $BaFe_2Se_3$, we performed TOF on single crystal; data show nice dispersions and new magnetic modes at low and high energy that could not be resolved previously on powders, suggesting that the actual model is lacking some informations, and is potentially fully antiferromagnetic. We also performed spin wave calculations [4,7] and Monte Carlo simulations to find a model that could support our results, and be compatible with magnetic transition under pressure [6,7]. This presentation will show the first results of this study, and discuss research directions planned for the future.

[1] M.Mourigal et al., Physical Review L 115, 047401 (2015)
[2] J.Herbrych et al., Nature Communications 9, 3739 (2018)
[3] Mazin, I., *Nature* 464, 183–186 (2010).
[4] S.Petit, Collection SFN (2011)
[5] M. J. Weseloh, V. Balédent et al. Journal of Physics : Condensed Matter 34, 255402 (2022)
[6] W. G. Zheng, V. Balédent et al. Nature Communication Physics (2022)
[7] A. Roll, V. Balédent, S.Petit et al. in preparation (2022)

Small-angle scattering studies of polymer and filler structures

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Laboratoire Charles Coulomb, Montpellier, France

Collective effects in liquids: what scattering methods say and what it does not say

L. Noirez [1], N. Martin[1], P. Baroni[1] and P. Dunne[1]
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The absence of mechanical resistance to a deformation in shear geometry indicates a liquid behavior. In contrast, shear strength indicates a solid response. A solid body deforms under shear while a liquid flows. The dynamic response of liquids to external stimuli such as shear force or shear displacement has recently revealed that at the mesoscopic scale, liquids are endowed with shear elasticity. The mesoscopic shear elasticity is revealed in ordinary liquids both experimentally [1,2] and theoretically by non-extensive models [3]. Its identification is very important because it calls into question that the flow results from the viscous properties. These new properties can be partly apprehended using diffusion methods but not always... We will show what neutron scattering (from wide to small angles) tells about in examples of polymers melts submitted to a steady-state shear flow, small molecules with strong interactions such as ionic room temperature [emim][Tf2N], liquid crystals or nitrate solutions exhibiting paramagnetic properties subjected to a mechanical or magnetic field[4].

[1] "Probing sub-millimeter dynamic to access static shear elasticity from polymer melts to molecular fluids" L. Noirez (2019),Encyclopedia of Polymers and Composites, © Springer-Verlag GmbH Germany, part of Springer Nature 2019, Polymers and Polymeric Composites: A Reference Series, S. Palsule (Editor).

[2] T.D. Li and Elisa Riedo, Nonlinear Viscoelastic Dynamics of Nanoconfined Wetting Liquids, Phys. Rev. Lett. 100 (2008) 106102.

[2] Alessio Zaccone, K. Trachenko, *Explaining the low-frequency shear elasticity of confined liquids*, PNAS 117 (2021) 19653-19655.

[3] Eni Kume, Nicolas Martin, Peter Dunne, Patrick Baroni, Laurence Noirez, *Collective Effects in Ionic Liquid [emim][Tf2N] and Ionic Paramagnetic Nitrate Solutions without Long Range Structure*, submitted 2022.

Controlled synthesis of gold nanoparticles in copolymers nano-molds by x-ray radiolysis: a coupled SANS/laboratory SAXS/synchrotron SAXS study¶

L. Bondaz [1,2,3], P. Fontaine[2], F. Muller3,4, N. Pantoustier[5], P. Perrin[5], I. Morfin[6], M. Goldmann[1,2], F. Cousin[4]

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[2] *Synchrotron SOLEIL, L'Orme des Merisiers, BP 48, Saint-Aubin, 91192 Gif sur Yvette, France*

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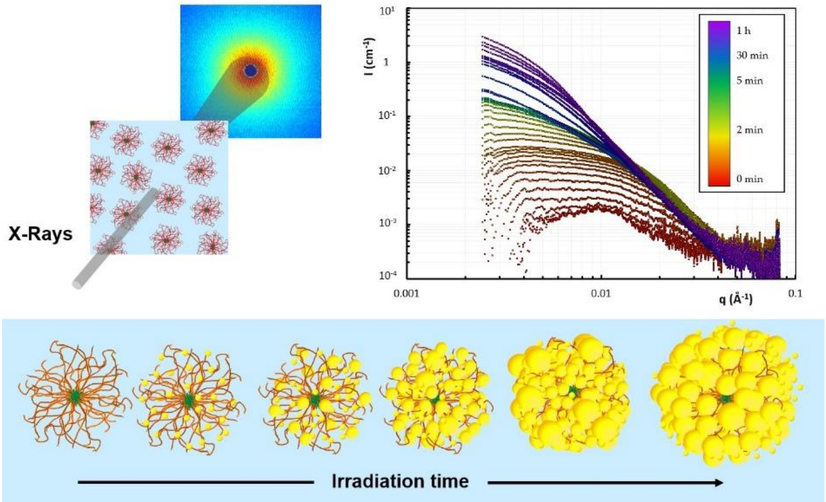
We will show in this lecture how gold nanoparticles with controlled sizes and morphologies can be obtained by the metallic reduction of $AuCl_4^-$ ions trapped in 3D organic molds by x-ray radiolysis [1]. This will exemplify the complementary between SANS, laboratory SAXS and synchrotron SAXS. The molds are spherical frozen micelles of polystyrene-b-poly(dimethylaminoethyl methacrylate) (PS-b-PDMAEMA) block copolymer in acidic aqueous solution with a PS spherical core surrounded by a corona of PDMAEMA chains in good solvent, as demonstrated by SANS with contrast variation where the structure of both the corona and the core of the micelles are determined independently. When $AuCl_4^-$ ions are introduced in the system, they condense on the positively charged DMAEMA moieties without changing the behaviour of the PDMAEMA chains at low $[AuCl_4^-]/[DMAEMA]$ ratio, as shown by SAXS on a laboratory instrument, for which the incident flux is not sufficient to initiate the reduction of the gold salts. When the samples are placed under the intense radiation of an x-ray beam on a small-angle diffractometer in a synchrotron, this allows both the reduction of the gold ions by radiolysis and the monitoring of the evolution of their structure. The radiolysis of the solution produces in a first step gold clusters in the micelle corona, which in a second step merge to form nanoparticles of a similar size to the one of the micelle (figure 1).



[1] L. Bondaz *et al*, Langmuir, 36 (2020), 6132–614

Decorating tunable self-assembled nanostructures with PEG for stealth applications

M. Almeida [1], D. Dudzinski [2], B. Couturaud[1], S. Prevost[3], V. Lütz Bueno[2,4], F. Cousin[2], C. Amiel[1] and C. Le Coeur[1,2]

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In order to reach a specific organ, hydrophobic and hydrophilic drugs have to be carried in nanoparticles such as vesicles. However these nanocarriers are filtered by kidneys and one of the common strategy to enhance their biocompatibility and their stealth relies on their surface functionalization by a corona brush of poly(ethylene glycol) (PEG) chains, the so-called "pegylation" process.

In this lecture, we will present a strategy to obtain various pegylated self-assembled nanostructures based on fatty acids with different morphologies. We use a fatty acid, 12-Hydroxy stearic acid (HSA), obtained from castor oil, that either self-assemble into micrometric multilamellar tubes at low temperature (Figure 1A), or in nanometric micelles at high temperature (Figure 1C) above a given threshold temperature [1]. Such HSA assemblies are then doped by various amount of short PEG chains (5 000 g/mol) that are grafted at each extremity by HSA moieties through a Steglich esterification, so that can insert themselves within the HSA self-assemblies.

The resulting nanostructures of the doped self-assembled were determinated by Small Angle Neutron Scattering. The contrast variation method was used to elucidate either the structure of HSA self-assembly either of the polymer conformation in mixtures at different temperatures from 20°C to 45°C (Figure 1). We demonstrated that our strategy enable us to build a large variety of different thermosensitive pegylated nanocarriers ranging from tubes to vesicles to micelles.

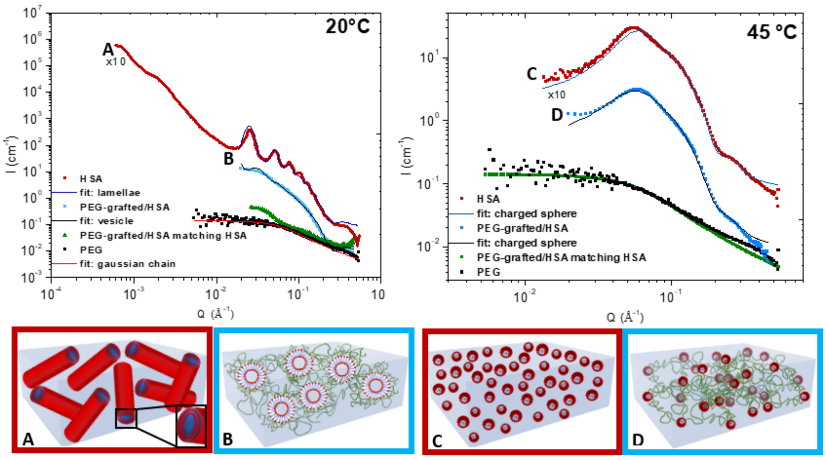

Figure 1 - Left: structure at 20°C. Top panel: SANS intensity profiles for pure HSA solution, PEG-grafted/HSA mixture, PEG-grafted/HSA mixture in the solvent that matches HSA and pure PEG. Bottom panel: sketches of the pure HSA solution (A, not to scale) and mixtures (B, HSA molecules are shown in red and PEG chains in green). Right: Structure at 45°C. SANS intensity profiles for pure HSA solution, PEG-grafted/HSA mixture, PEG-grafted/HSA mixture in a solvent that matches HSA and pure PEG. Bottom panel: sketches of the pure HAS solution – (A) and mixtures (B, HSA molecules are shown in red and PEG chains in green).

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Insights into the microscopic mechanisms responsible for phase separation in a biphasic acidic solution for metallic ion extraction

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Ionic-liquid-based acidic aqueous biphasic solutions (AcABSs) recently offered a breakthrough in the field of metal recycling. The particular mixture of tributyltetradecylphosphonium chloride ([P4,4,4,14]Cl), acid, and water presents the unusual characteristic of a lower solution critical temperature (LCST), leading to phase separation upon a temperature rise of typically a few tens of degrees. Here, we dig into the mechanisms driving the counter intuitive phase separation upon temperature rise observe in this system. Using small angle neutron scattering, we could identify the micellar structure under various conditions of acid and temperature, observing the micelle aggregation eventually leading to the phase separation. Temperature rise and addition of acid both induce the phase separation in an apparently similar mechanism.

Fine titration of the chloride ions present in the solution proved the exothermic adsorption of these ions at the micelle surface, increasing with temperature. Such ionic adsorption, similarly to acid addition, induces a screening of electrostatic interactions between the micelles, indirectly driving the phase separation. Such a mechanism of ionic or molecular adsorption at the micelle surface could be generalised for numbers of molecular systems presenting a Lower Critical Solution Temperature.

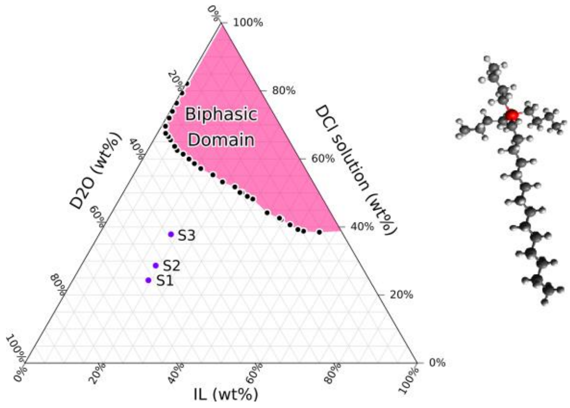

Figure 1 : Ternary phase diagram of the [P4,4,4,14]Cl, water and chlorhydric acid solution, and sketch of the ionic liquid cation. The phase diagram is given for deuterated compounds for the need of neutron scattering. S1, S2 and S3 solutions are the investigated solutions.

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Probing polymers adsorption under highly viscous flows using neutron reflectivity

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Understanding polymer interaction with surfaces is a paramount issue for many applications such as lubrication, enhanced oil recovery, filtration, biological flows and the emergent field of nanofluidics [1-4]. Depending on the chemical properties of the polymer and the surface, polymer chains can either adsorb onto or be repelled from the surface, leading to what is called “adsorption” or “depletion” respectively. When polymer chains are adsorbed onto solid surfaces they can interact with the flow itself and control the rheological properties of the interface, leading to non-linear responses. A good way to probe these chains conformation is to use neutron reflectivity: by looking at the neutrons reflected at the solid/liquid interface and by adjusting the contrast, one can have access to a lot of information on the near-wall chains [5,6].

We have designed a cell which allows us to reach high shear rates and controlled velocity field while doing neutron reflectivity measurements. Using the high-flux D17 reflectometer at ILL, we have managed to probe the interface between a sapphire surface and solutions of polystyrene in a phtalate solvent. Interestingly, we observe a global depletion of polymer chains near the surface but with some slight adsorbed ones, which are insensitive to the flow (see Fig. 1).

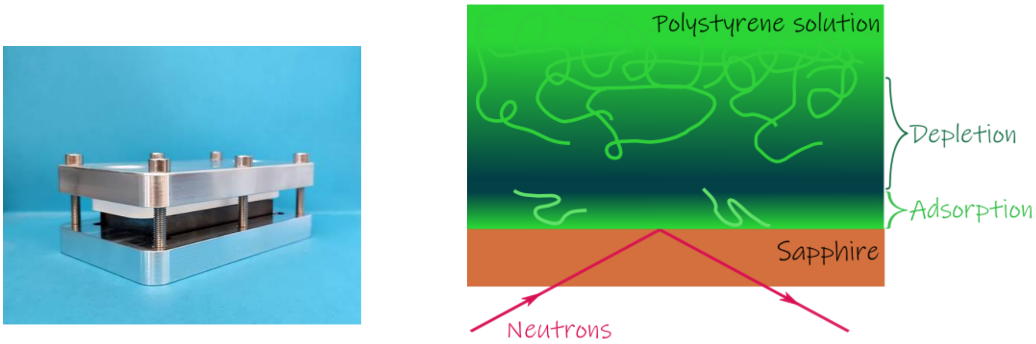

Figure 1 – Left: measuring cell. Right: Adsorption/Depletion cartoon.

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Dynamically disordered solids across physical and chemical space

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This talk provides an overview of our current efforts to explore, understand, and ultimately control dynamical disorder in the solid state. This programme of work is driven by the increasing number of families of materials of technological relevance whose ultimate performance is predicated upon its emergence and prevalence, well before entering a fully fledged fluid phase. From a conceptual viewpoint, such a task requires a stark departure from commonly accepted (textbook) notions of what a solid is, including how its behaviour evolves as a function of external stimuli like temperature or pressure, as well as chemical doping. Likewise, they place state-the-art neutron-scattering techniques at the center stage of contemporary materials discovery, given their superb and unique ability to probe structure and motion simultaneously at atomic and molecular scales. Hybrid organic-inorganic perovskites constitute a timely and important case-in-point to illustrate all of the above, and this talk will place a special focus on what we have learnt so far about this fascinating class of hybrid materials. Regarded as mere academic curiosities until about a decade ago because of their exotic 'ionic plastic-crystal' character, they have become the most promising platform for the development and subsequent deployment of next-generation photovoltaic and photonic technologies. The main hurdle at present relates to their poor physico-chemical stability, a challenge that requires taking a much-closer look at their thermophysical behaviour in both stable and metastable phases, not only in the laboratory but also on a computer. The ubiquity and importance of dynamical disorder in the solid state is further illustrated in other classes of technological and sustainable materials, including those based on fullerene adducts or room-temperature ionic-liquid systems. All throughout, we make an effort to relate our findings to recent and ongoing developments in neutron science, particularly those in the inelastic-scattering realm heavily supported by the quantitative prediction of experimental observables using first-principles computational modelling.

Batteries and fuel cells

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Self-Organised Vortex Structures under the Influence of Current in Superconducting Niobium

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We are familiar with the concept that an electrical current, in the presence of a magnetic field, experiences a force orthogonal to both. This is the basis of how electric motors work. The inverse situation of a field of current creating a force on a 'wire' of magnetic flux can also occur. Superconductors have the remarkable property that 'wires' of magnetic field are quantised and sustained by a small vortex of current. In the presence of an electric current each vortex also feels a force and whether it moves or not determines if the superconductor is useless or useful. All applications of superconductors like levitating trains or MRI machines rely on the property of zero electrical resistance and a finite resistance always occurs when vortices move under the influence of a current. In a conventional type II superconductor, vortices exist all through the bulk and move collectively once a critical current has been exceeded. There is a special case with Niobium where vortices are restricted to a certain volume fraction of the material with a fixed local density.

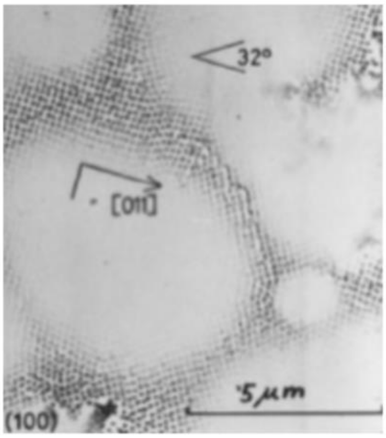

Figure 1: Magnetic decoration image of Nb (taken from [1]). Here, the darker areas contain the vortices and only in these regions can current flow.

The question was, given current can only flow in regions where there are vortices, how does the system arrange itself given this current also exerts a force on the vortex rich regions it travels through? Small angle neutron scattering is the perfect technique to study such a system as we can analyse Bragg peaks from the local vortex lattice and in parallel the very small angle scattering from the larger micron scale structure of domains. We found [2] there is a self-organised structure of stripes of vortices parallel to the direction of vortex flow. We present the results from these experiments that have answered many questions but as is often the case, have also posed more. Not least the seemingly paradoxical situation where the current flows across the sample but the regions where the current can flow are broken into domains perpendicular to the current.

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Thermal conductivity of spinons in the 1D spin ½ cuprate SrCuO2

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$SrCuO_2$ is a 1D magnetic compound that exhibits a remarkably large and anisotropic thermal conductivity. Measurements have shown that its ability to transport heat along spin chains is close to 800 $W.m^{-1}.K^{-1}$, comparable to that of Copper [1]. While phonons are the main heat carriers in insulators, spinons, unconventional magnetic excitations typical of 1D magnets, strikingly participate to these very peculiar thermal properties in $SrCuO_2$ [2]. Understanding these thermal properties may unravel new aspects of the ground states of such spin ½ chains [2].
The aim of this work was to estimate the contribution of the spinons to the thermal conductivity $\kappa(T)$ of $SrCuO_2$ using a different method than the one described in [1]. Two types of quasiparticles have to be considered to characterize heat transport $\kappa(T)$ in this compound, phonons and spinons, with $\kappa(T) = \kappa_{Phonons}(T) + \kappa_{Spinons}(T)$. First, we focused on the estimation of heat transport by phonons, $\kappa_{Phonons}(T)$ [3]. Theoretical calculations based on DFT force constants were performed initially to obtain the phonon dispersion in $SrCuO_2$, which was subsequently compared with inelastic neutron scattering measurements. Our calculations were found to be in good agreement with experimental data, thus validating the approach. From the phonon dispersion spectra, we then computed $\kappa_{Phonons}(T)$. Strikingly, it was found to be very anisotropic, being much larger in the $\vec{c}$ direction parallel to the spin chains. By subtracting the calculated $\kappa_{Phonons}(T)$ to the experimental $\kappa(T)$ along $\vec{c}$, we were then able to estimate the contribution of spinons to the thermal conductivity along $\vec{c}$, $\kappa_{Spinons}(T)$. Our results suggest that the spinons mean free path is much shorter than the phonons' at low temperature , and drops sharply above 40 K, down to a few dozen ångströms only.

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Seeing the Chemistry in Biology

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

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The understanding of protein crystallization is of great interest for many areas of biological research. Examples include drug delivery of crystalline substrates and structural biology, which relies on diffraction-quality crystals. Some crystallization pathways are characterized by a one-step process and can be described by classical nucleation theory (CNT). However, for different systems, several steps are visible in the crystallization process resulting in an insufficient description of the crystallization process by CNT. These cases require a more detailed investigation to obtain a comprehensive picture of the underlying mechanisms.

Bovine β-lactoglobulin (BLG) in the presence of the divalent salt $CdCl_2$ is characterized by a rich phase diagram. The protein solutions become turbid after crossing a first threshold salt concentration c* upon further increasing the salt concentration, the solutions become less turbid but not completely clear again (pseudo-c**). Near pseudo-c**, crystallization follows a nonclassical process with a metastable intermediate phase (MIP). Here we explore the MIP in detail with a focus on the structural evolution and the growth kinetics of the MIP prior to crystal nucleation [1].

We present a systematic study using real-time SANS, optical microscopy [1] and neutron backscattering (NBS) [2] to study the protein crystallization process in the presence of a MIP.

Real-time SANS measurements on D11 show that a correlation peak develops inside the MIP, and its peak position shifts to higher q-values with time, finally stabilizing at a characteristic length scale of $d_{MIP} \approx 84$ Å. The area of this peak (proportional to the amount of MIP in the sample) first increases with time, reaches a maximum, and then decreases quickly upon crystallization due to consumption by crystal growth. The evolution of the correlation peak indicates a "preordering" nature of the MIP as precursors of crystal nucleation, which lowers the nucleation barrier for subsequent crystallization. These results on structural evolution and the role of MIPs during a nonclassical crystallization process may be relevant for other fields ranging from structural biology to pharmacology.

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Monitoring digestion of protein gels: Neutron Small Angle Scattering and Dark Field Imaging completed with SAXS

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Abstract for oral presentation

Proteins are crucial macronutrients, but also structure elements of ingested food. They form structures at multiple spatial scales, in particular in gels. We study gastro-intestinal digestion of plant proteins from canola seed (cruciferin and napin), after heat-set gelation of their solutions prepared at pH 8 and pH 11.

Small-Angle Scattering techniques (SANS, SAXS) coupled with Neutron imaging (ICON, PSI) allows obtaining multi-length structural information about digested proteins: on nanometer scale (proteins and aggregates) for SAS and on micron scale (large aggregates) for neutron imaging.

For SANS and Neutron Imaging, ∅10 mm samples (mimicking in-vivo food particles) were pre-infused with inactivated enzymes for further homogenous digestion and measured after different digestion time steps. Conversely, for SAXS we monitored digestion in-situ, as a function of time *t* and height *z*, by vertical scanning of gels in ∅ 0.15µm capillaries, submitted to enzymatic diffusion from the top of the gels downwards the capillaries. We will compare information from each method.

SANS showed (i) destruction of protein aggregates and (ii) conformational changes of proteins, different for gastric phase (unfolding/local aggregation) and intestinal phase (compaction). **SAXS** enabled more accurate monitoring of the conformational behavior, through many (*z, t*) pairs, obtained over long digestion times, revealing complex paths of proteins under digestion (with back and forth variations in sizes and shapes). **Neutron imaging** showed a rather fast deconstruction of micron scale aggregates under digestion. Coupling these methods enabled also to tackle the problem of the intrinsic heterogeneity of samples during digestion: (i) prevented by inactive enzyme imbibition for big samples for SANS and Neutron imaging, (ii) observed directly by SAXS (spatial scans).

Differences in initial gel structures (compact or unfolded proteins, induced by preparation pH) influenced their evolutions under digestion. The feasibility of linking the behaviors at lower scale with the larger ones can be extended to different proteins, but also other, e.g. multi-ingredients foods, possible to study by the use of neutron contrast matching.

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Using polarisation analysis to compare the dynamics of protonated and per-deuterated samples of proteins.

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Neutron scattering data collected from biological systems are mostly analysed with classical approaches; however, it has already been proven for instance that purely quantum-based effects such as tunnel effects can explain the enhancement of information rates in enzyme catalysis [1]. Our approach is to study both a per-deuterated sample of the green fluorescent protein ($dGFP$) and a fully protonated sample ($pGFP$) hydrated in D_2O, in order to evidence signature of quantum effects thanks to the difference of mass of the two isotopes of hydrogen nuclei combined to supposedly equivalent dynamics. However, it quickly raised more fundamental questions about how careful one has to be when analyzing per-deuterated samples, as already highlighted in [2].

We performed QENS experiments on the TOF spectrometer IN5 at ILL. We describe the subdiffusive motion of hydrogen atoms in the protein with fractional Brownian dynamics, using a Mittag-Leffler function as relaxation function ([3]). It yields a 3-parameter model for dGFP dynamics that catches the importance of the dynamics of water through a heterogeneity parameter (α, see figure 1, a), the impact of water within the time window with the relaxation time parameter (τ) and the impact of coherent scattering from both water and the protein through the shape of the Elastic Coherent Scattering Factor obtained with the pseudo-EISF parameter ($EISF$). This corroborates with static studies combined with polarized neutrons carried out on the diffuse diffractometer D7 at ILL (figure 1, b). Therefore, in order to correctly compare the dynamics of deuterium to the dynamics of hydrogen it is paramount to access only the incoherent contribution of scattering for our dynamic studies using QENS combined to polarization analysis.

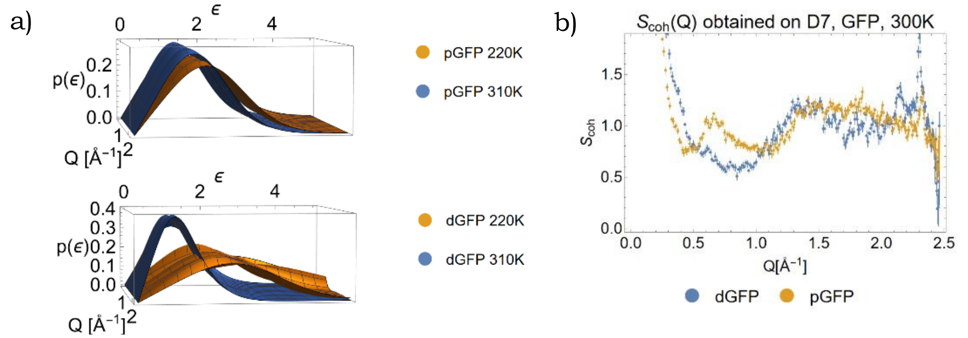

Figure 1 a) Distribution $p(\epsilon)$ of the dimensionless energy barriers ($\epsilon = \frac{\Delta E}{kbT}$, ϵ is a function of α) seen by hydrogen nuclei in a rough harmonic potential. Fractional Brownian model applied to IN5 data. b) Coherent contribution to the static structure factor S(Q) compared for both proteins.

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MIRACLES, the time-of-flight backscattering spectrometer at the European Spallation Source

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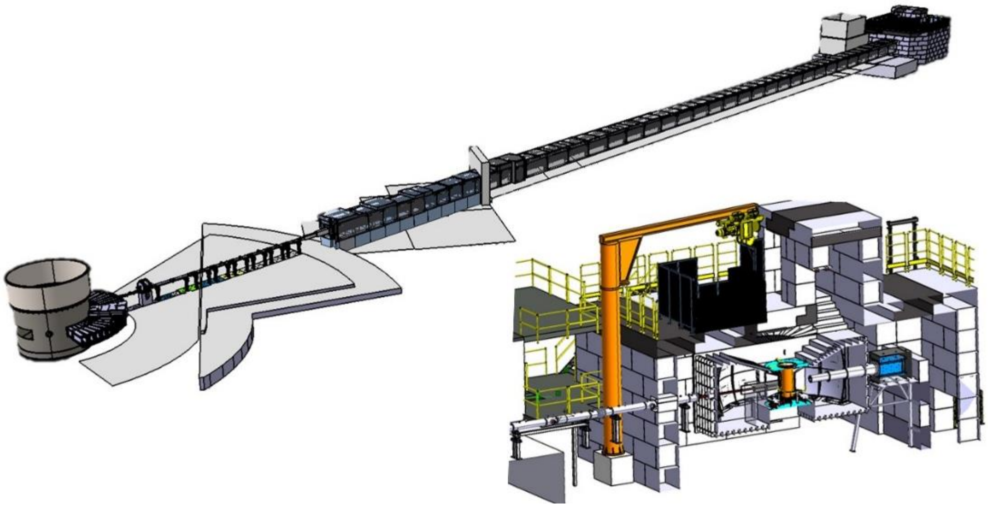
MIRACLES is the time-of-flight backscattering instrument at the European Spallation Source (ESS).[1] This high-resolution spectrometer will display a wide energy transfer (bandwidth ~1.1 meV) and a tunable energy resolution for quasielastic neutron scattering (QENS) measurements between 2 and 50 μeV, enabling the observation of a broad range of dynamics timescales, ranging from the nanosecond to the picosecond. Moreover, the flexibility to select the incident energy within a wide range will allow to carry out inelastic neutron scattering (INS) spectra of about 20 meV.

The science case of MIRACLES is primarily focused on soft matter and molecular dynamics (protein dynamics, drug delivery, water dynamics, polymers...), also covering condensed matter topics (catalysis, magnetism). After the optimization of the chopper cascade,[3] the guide [4] and the final setup of the scattering system [5], MIRACLES is its detailed design phase, with some components already in the manufacturing period. It is envisioned that these design solutions will contribute to an outstanding performance of MIRACLES that will unfold new opportunities in neutron spectroscopy.



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Wide Angle Polarization Analysis and first results with PASTIS-3 for IN20

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XYZ polarization analysis for inelastic neutron scattering is a powerful method for the separation of magnetic, nuclear coherent and incoherent scattering. However, in the thermal neutron range, these experiments have typically been carried out using the conventional triple-axis technique with a single analyzer and detector, where polarized cross sections are measured point by point. We will here present the results of the third generation PASTIS device for XYZ wide-angle polarization analysis [1]. The PASTIS-3 device uses two independent polarized ^{3}He neutron spin filters for polarizing and analyzing the neutron spins. The incident neutron beam polarization can be inverted by reversing the spin state of the polarizing entrance cell and the ^{3}He analyzer cell provides a continuous 102-degree coverage of scattering angle. To obtain a high spatial homogeneity of the magnetic field in any field direction, a new coil design has been developed using sets of tilted coils. The setup has been tested on the thermal triple-axis instrument IN20 together with the multi-angle analyzer Flatcone. Finally, we will discuss the future possibilities for wide-angle polarization analysis on direct-geometry TOF-spectrometers such as PANTHER at the ILL.

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SAM, your future SANS instrument at the Institut Laue Langevin

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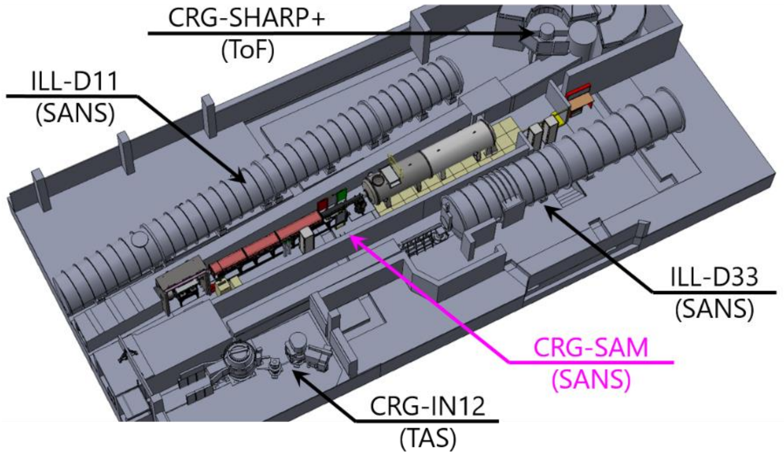
SANS is a ubiquitous technique in condensed-matter physics with applications spanning a broad number of scientific areas. It is therefore imperative to maintain an access to efficient beamlines in order to satisfy its large user base. This is particularly true to the French community, which has been greatly impacted by the shutdown of the Orphée reactor in October 2019.

The SAM project was proposed in the frame of the "*Endurance 2*" rejuvenation program of the Institut Laue Langevin (ILL) and officially kicked-off in February 2020 as a response to this situation. It involves a collaborating work by a team of technicians, engineers and scientists from the Laboratoire Léon Brillouin (LLB, Saclay) and the ILL. The installation of SAM on the fully renovated H15 guide shall take place in the course of 2023 and should lead to a commissioning in April 2024.

We will first discuss SAM's main features and timeline *[1]*. Given its dimensions and the emphasis put on polarized neutrons, SAM will be particularly adapted to the study of magnetic meso-structures. In a second part, we will thus review potential applications in this field, besides the more traditional studies in soft-matter, biophysics and material science.



Layout of the SAM instrument in the ILL7 guide hall.

[1] A functional description of SAM can be found on the LLB website: https://tinyurl.com/z9r57ssk

IN13+: current status and perspectives

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IN13 is a backscattering spectrometer working with thermal neutrons with wavelength 2.23 Å corresponding to energy of 16.45 meV. The energy resolution is of the order of 8 μeV and the energy window is ± 100 μeV. In addition the value of the incident energy gives the availability of high momentum transfers ($Q < 4.9$ Å^{-1}), much larger than obtainable with currently worldwide available spectrometers. The instrument fills the energy gap between IN6-SHARP or IN16B and IN5 at ILL, IRIS and OSIRIS at the Rutherford-Appleton laboratory (RAL) in United-Kingdom, BASIS at ORNL or HFBS-NCNR at NIST in the US, and DNA at J-Parc in Japan.
The major drawback of IN13 is the low neutron flux on the sample, implying long acquisition times that put limits on the experimental data obtainable and requires important sample masses. That is why the instrument is currently under a major upgrade, including guide refurbishment, the design of a new monochromator, a new deflector recently installed and further additional minor improvements.
The instrument has been dismounted in late 2021 and it is now in the reconstruction phase.
I will report here the status of the upgrade and the perspectives in terms of increase in flux expected and opening to a wider range of scientific applications.

Towards a new neutron source in France for materials science and industry.

F. Ott, B. Annighöfer, J. Darpentigny, J.-L. Meuriot, X. Guillou, O. Tessier, A. Menelle
IRAMIS/Laboratoire Léon Brillouin CEA/CNRS, CEA Saclay 91191 Gif sur Yvette.

The European landscape of neutron facilities is evolving quickly with the closure of a number of aging research reactors: for example the reactor Orphée in France, BER in Berlin and Kjeller in Norway closed in 2019. While the European Spallation Source (ESS) should start later in this decade, its capacity will not be sufficient to replace the closed facilities. Hence, the Laboratoire Léon Brillouin (LLB), operated by the CEA and the CNRS in France, is developing the technologies necessary to build a new type of neutron source using low energy proton accelerators: *High Current Compact Accelerator driven neutron sources* (HiCANS).

We will describe the ideas driving the design of HiCANS and present the potential capabilities of such sources. Since 2018, the CEA has been engaged in an experimental research program around the IPHI accelerator and has demonstrated a number of technologies on the IPHI – Neutrons platform [1]. We will report on the recent progress in the field of neutron producing targets, the first diffraction measurements on the DIoGENE instrument and the developments around cold moderators.

The neutron scattering instrument DIoGENE around the IPHI – Neutrons source.

[1] The IPHI – Neutron project is supported by the region Ile-de-France. For more information, see the SONATE and IPHI – Neutron Project website.

Resonant Inelastic X-rays Scattering: an emergent technique to probe spin-dynamics (and beyond) in quantum materials.

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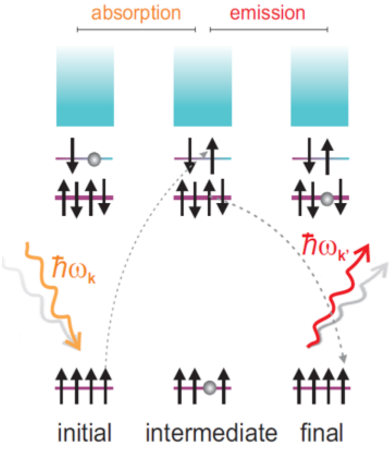
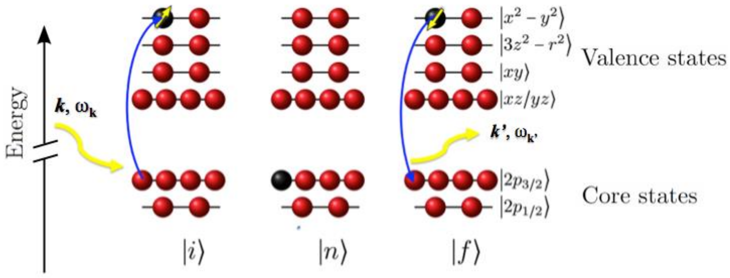
Resonant Inelastic X-rays Scattering is an emergent spectroscopy technique that has rapidly become an essential tool over the last decade to probe electronic excitations in quantum materials, hence being complementary to neutron scattering [1]. Indeed, due to recent advances in optics and the rapid development of high-brilliance synchrotron x-ray radiation sources, this photon-in/photon-out technique which was firstly restricted to probe electronic structures due to poor energy resolution (~1 eV 10 years ago to ~20 meV nowadays) is now able to probe energy and momentum dependence of a multitude of collective excitations such as phonons, magnons or crystal-field excitations [1]. In this oral presentation, I will briefly introduce the history behind this technique and the concept of RIXS: the photon-in/photon-out process, the meaning of the term “Resonant”, the Kramers-Heisenberg equation describing the RIXS cross-section and few scientific highlights of the past 10 years, e.g. spinons and orbitons excitations in cuprates [2] or the study of collective excitations in thin films [3]. Finally, to give a detail example of what RIXS can do, I will expose some recent results obtained on the pyrochlore iridate $Tb_2Ir_2O_7$ on ID20 at ESRF [4] where both orbital (so called *d-d*) and magnon dynamics were probed.





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The SIESTA method as a tool in materials science: latest developments and some applications

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Low-frequency lattice dynamics in lead halide hybrid perovskites

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The low-frequency lattice vibrations and relaxations are investigated in single crystals of the four 3D hybrid organolead perovskites, MAPbBr3, FAPbBr3, MAPbI3, and α-FAPbI3, using Brillouin, Raman, and inelastic neutron scattering [1].

The temperature dependence of the PbX6 lattice modes in the four compounds can be renormalized into universal curves, highlighting a common vibrational dynamics at the cubic to tetragonal transition. In particular, no soft vibration is observed in Raman and neutron scattering excluding a displacive-like transitional dynamics.

The reorientational motions of the molecular cations exhibit a seemingly order-disorder character recalling that of plastic crystals, but they do not necessarily drive the phase transitions.

At ultralow frequency, a quasielastic component evidenced by Brillouin scattering and associated to the unresolved central peak observed in neutron scattering, is attributed to translational-like modes of the molecular cations in the perovskite cavities. Its partially unexpressed critical behavior at the transition might point toward the general importance of defects in HOPs preventing the net divergence of order parameter correlations at the critical temperatures.

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Atomistic simulation of disordered carbons: from structure to properties

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Atomistic simulation techniques have become extremely valuable tools for the elucidation of the structure of disordered or partially ordered materials. Largely overpassing early handmade drawings, these techniques, that can make use of experimental data (diffraction, microscopy, NMR, etc.) as simulation constraints or for validation purposes, currently allow for the production of large-scale three-dimensional representations of the materials. These structural models can thus be used to predict most of their properties, and even in some cases, to assess their formation mechanisms. Disordered or partially ordered carbon materials represent the perfect playground for such structural investigations, owing to the wide varieties of structure and texture they can exhibit, with materials such as amorphous carbon, carbon fibres and composites, nuclear grade graphite, soot and carbon blacks, coal, kerogen, etc. In this talk I will present some recent work where such simulations techniques have been used to characterize (i) dense anisotropic carbons like pyrolytic carbons and nuclear grade graphite, and their mechanical behaviour prior and after irradiation [1-3]; and (ii) natural porous carbons (kerogen), following their behaviours with respect to gas adsorption and diffusion along their geological carbonization pathway [4-7].

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Endofullerenes: Dynamics in Confinement - $CH_4@C_{60}$ Study

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Endofullerenes are substances in which small molecules or atoms are encapsulated in highly symmetrical cages of carbon atoms. Each encapsulated atom or molecule behaves as a textbook example of a quantized particle-in-a-box. The newest and largest member of the endofullerene family tree, namely $CH_4@C_{60}$, is the first organic molecule trapped inside the cage and the main interest of this abstract. The use of various spectrometers at ILL, namely PANTHER, IN5 and IN1-LAGRANGE, have allowed us to probe a large energy window up from 1 to 100 meV. The goal from these experiments was to probe the rotational and translational states of the confined CH_4 molecule, and observe the coupling between said states due to the confinement. A novel result that we have observed in this endofullerene, was the effect of the I_h symmetry of the C_{60} on the rotational states of the CH_4 using inelastic neutron scattering, an effect that was absent in previous endofullerene studies. We have also performed QENS measurements, using PANTHER, that have allowed us to observe slight differences in the rotational dynamics of both the C_{60} and CH_4, confirming the stronger guest-host coupling that we observed in our INS measurements.

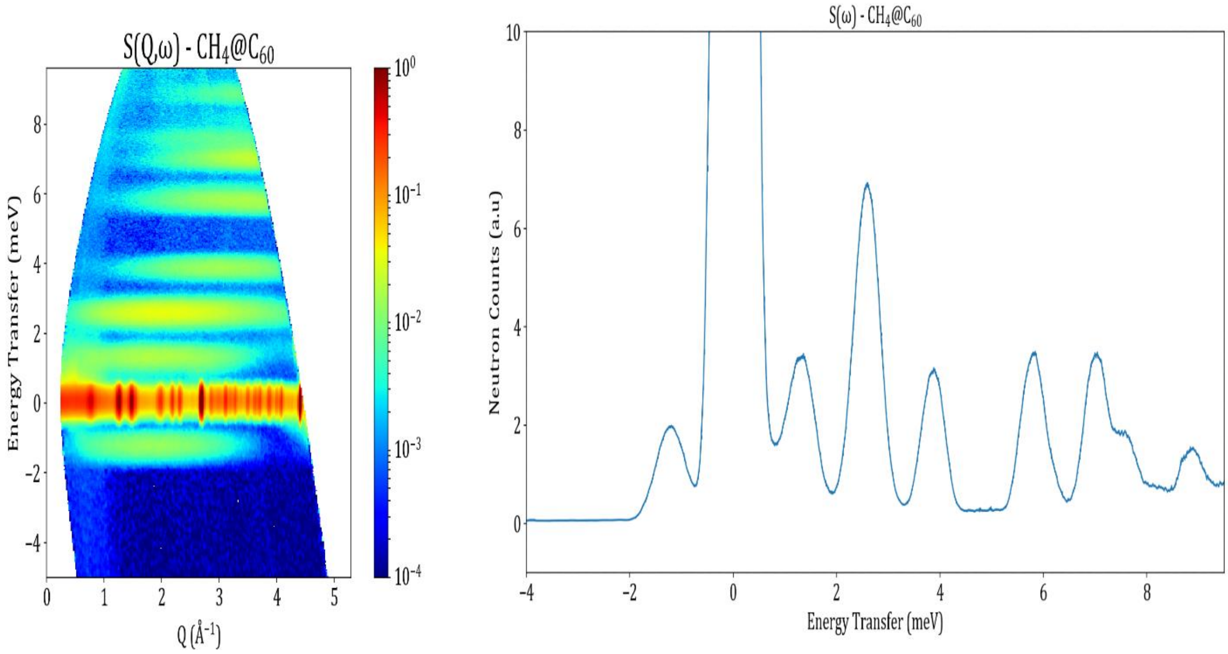

Figure 1: Inelastic neutron scattering results from the $CH_4@C_{60}$ measurements

Hydrogen Storage and Dynamics in Clay Materials

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Hydrogen storage technologies play an important and crucial role in the so-called “hydrogen economy”. However, clay minerals have poorly been studied for this purpose, while they possess valuable properties (stability, low cost, green material) to be exploited in this domain

We have recently studied H_2 adsorption on a synthetic clay, laponite and on gel-laponite, obtained at an intermediate step of the synthesis; nickel ions are inserted into the structure (Fig.1(a)). Obtained X-ray scattering (Fig. 1(b)), the local structure of the gel-laponite sample, noted gel-Ni-laponite, is shown to be similar to that of Ni-laponite, while long-distance order is significantly reduced. The adsorption isotherms (Fig.1(c)) reveal a higher sorption of gel-laponite than that of laponite.

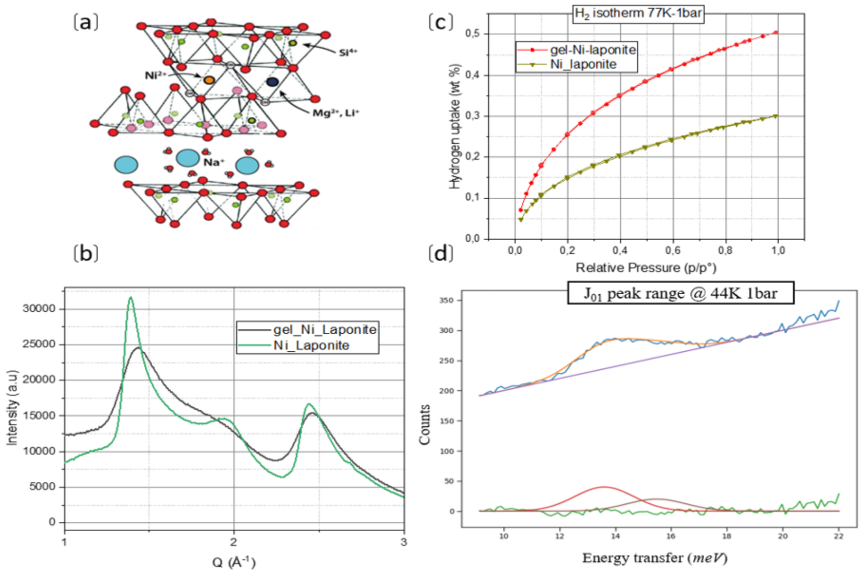

Figure 1. (a) Atomic structure of Ni_Laponite, (b) X-ray scattering of Ni_Laponite & gel_Ni_Laponite, (c) Hydrogen adsorption isotherm, (d) INS spectra in the region of the J_{01} transition (blue: data, orange: fit results, green: difference between data and fit, red & brown: splitted components, violet: slopping background)

Inelastic neutron scattering (INS) is extremely useful at probing locally the direct vicinity of adsorbed molecular H2. The INS spectrum of a free H2 molecule is characterized at low temperature by a sharp and well-defined rotational feature at an energy of 14.7 meV corresponding to the transition of H2 from a para- (molecular spin S = 0, angular momentum J = 0) state to an ortho- (S = 1, J = 1) state. The para-to-ortho transition line J01 has a three-fold degeneracy which is lifted as a function of the local symmetry of the adsorption site, with line-shifts that are dependent on the interaction between the H2 molecule and the host surface. We will present here the results obtained on gel-laponite using the spectrometer PANTHER at the ILL (fig. 1(d)). At 41K, well above the solidification temperature of bulk H2, the J01 peak exhibits a fine structure which can be can fitted by two gaussian lines with an intensity ratio of 2:1 (low energy component: high energy component, fig. 1(d)). The splitting is in line with 1D hindering (H2 axis lying parallel to a surface) and attractive potential wall equal to ~ 27 K. The evolution of the J01 fine structure down to 5K will be discussed.

TOF powder neutron diffraction through the lens of quantum materials

A. Gibbs, Inst. Scientist, HRPD @ ISIS

In this talk I will outline the key concepts and advantages of TOF powder neutron diffraction and its complementarity to constant wavelength techniques. The current state-of-the-art in powder neutron diffraction instrumentation and capabilities, illustrated using examples from the field of quantum materials, will be introduced. Although quantum materials form the basis for these examples, these experiments are equally appropriate to many other science areas including e.g. catalysis, battery research and ferroics and these will also be touched on.

Single crystal neutron diffraction in time-of-flight

Silvia Capelli, Inst. Scientist HRPD @ ISIS

Single crystal neutron diffraction at pulsed sources is meant to take advantage of both the polychromatic radiation and the time structure that the source provide. The Laue technique allows to exploit the multi-wavelength beam while the time-of-flight allows to separate harmonics of Bragg reflections that would otherwise fall at the same spatial position on a PSD detector. The talk will illustrate the principles of the time-of-flight Laue method used on the single crystal neutron diffractometer SXD at the ISIS Neutron and Muon Source and show examples of experiments in chemical and physical crystallography.

Overview of Neutron Diffraction Instruments at ESS

A. Jackson, ESS, Lund, Sweden

The European Spallation Source (ESS) is a multi-disciplinary research facility based on the world’s most powerful neutron source with a vision to enable scientific breakthroughs in research related to materials, energy, health and the environment, and address some of the most important societal challenges of our time. The initial suite of neutron instruments will consist of 15 instruments, 5 of which are dedicated to neutron diffraction measurements. In this talk, I will cover the science case and design features of BEER, DREAM, MAGIC, NMX and HEIMDAL diffractometers. Each of the instruments has a unique design and targets specific scientific user communities around the world. Taking advantage of the unprecedent brightness of the ESS source, and the use of cold and thermal neutron moderators, these instruments will open new frontiers in time-of-flight neutron powder diffraction, engineering diffraction, single-crystal diffraction with polarized neutrons, and macromolecular crystallography. I will outline specific advances in neutron detection technology, fast choppers design, and bi-spectral neutron extraction that underlie the novel capabilities of the neutron diffraction instruments at ESS.

DREAM: Neutron powder diffraction at the ESS

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The "Diffraction Resolved by Energy and Angle Measurements" (DREAM)[1] diffractometer is one of the first instruments to be constructed at European Spallation Source (ESS). The DREAM instrument is built in a collaboration of the Laboratoire Léon Brillouin (France) and Forschungszentrum Jülich (Germany). The concept of the instrument utilizes the long pulse and unpreceded peak brightness of the ESS source by pulse shaping choppers and by viewing both thermal and cold moderators. As a result, a particularly flexible choice between high resolution and high intensity modes can be offered to the users. 2D position-sensitive ^{10}B-detector technology will be capable for high position-sensitive resolution and also for expected high count rates. It is also possible to install a complex sample environment with a relatively open access to the sample position. Powder diffraction, pair-distribution function and low-angle neutron scattering measurements with polarized neutrons will be possible at DREAM. A full potential of DREAM will be realized through a new approach to the data analysis, which is based on 2D Rietveld refinements of the angular- and wavelength-dispersive diffraction data[2]. The DREAM instrument will outreach the large scientific communities in material science, solid state physics, chemistry, magnetism and nanoscience. The installation of the instrument is currently under way at the ESS.

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MAGiC: a polarized diffractometer at ESS

Xavier Fabrèges[1], Sergey Klimko[1], Thomas Robillard[1], Werner Schweika[2,3], Peter Harbott[3], Christine Klauser[4]

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The European Spallation Source is now well advanced in its construction phase, with the first neutrons expected on the instruments in 2025. On the instrumentation side, the first 8 instruments, covering most of the needs of the scientific community (imaging, SANS, inelastic neutron scattering, diffraction, reflectometry), will be opened to international users along 2026 and 2027.

Among those, MAGiC is a polarized diffractometer designed to serve the broad scientific case of magnetism. The instrument will allow the refinement of magnetic properties (structure, local susceptibility, magnetic diffuse scattering, spin density) on sub-mm3 and thin-film samples on a daily basis. The scientific case covers systems with strong potential applications such as multifunctional materials, molecular magnets and superconductors as well as fundamental materials such as quantum spin liquids, skyrmions and strong spin-orbit coupling materials.

To do so, MAGiC will make full use of the ESS high brilliance on the thermal and cold spectra, both permanently polarized thanks to the use of FeSi coated super-mirrors. Two detectors will ensure high-efficiency data collection with a 0.8 sr area detector for flipping ratios experiments and a 120°x10° detector for polarization analysis experiments on the cold spectrum. The polarization analyzer will be based on Si blades coated with FeSi and accompanied by a XYZ setup ensuring data collection on all available channels.

Simulations of the MAGiC performance, with the help of the McStas software package, on single crystals and powder samples show an expected gain compared to state of the art polarized diffractometer of 1 to 2 orders of magnitude.

The instrument is now in its manufacturing phase with a start of installation on-site scheduled for early 2023, a hot commissioning in 2026 and an opening to users in 2027.

Study of IR and UV photochemistries of intra and intermolecularly H-bonded molecules and aggregates trapped in cryogenic matrices

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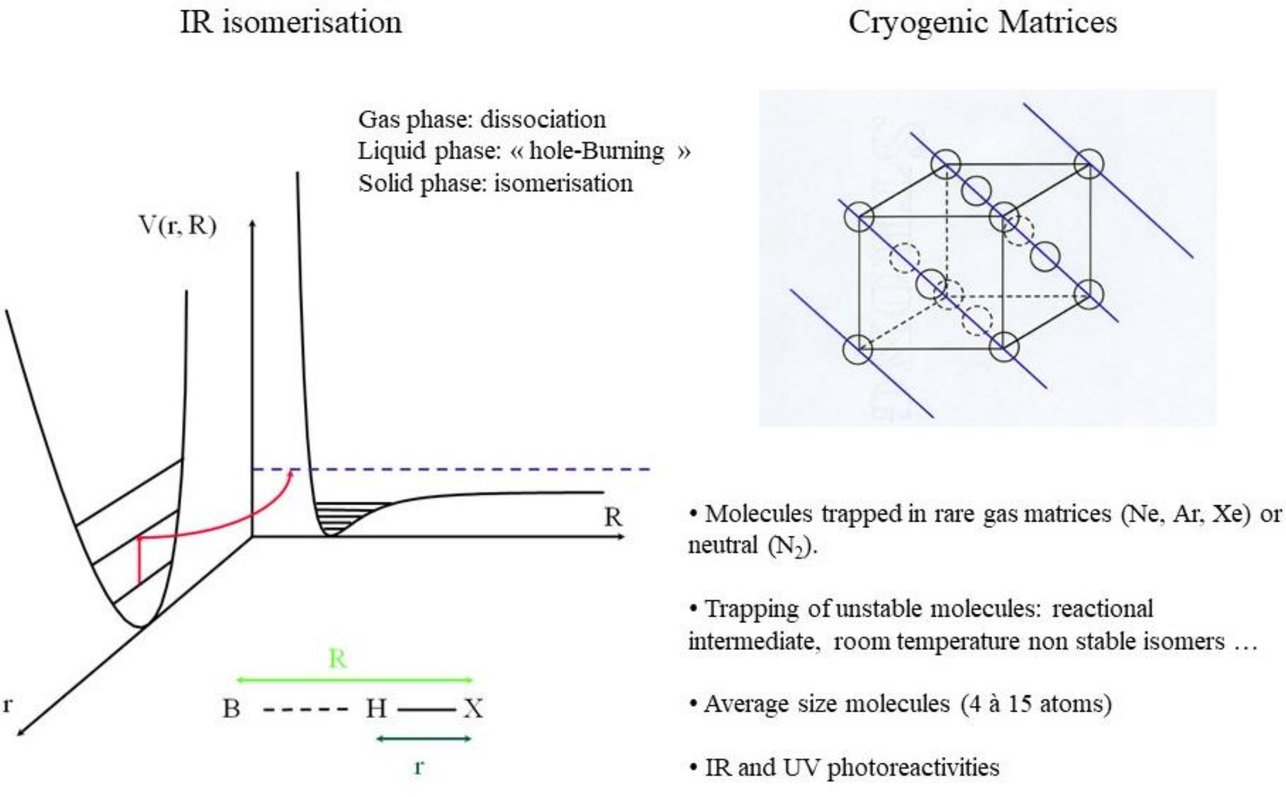
The cryogenic matrix technique associated with FTIR and UV-Visible spectroscopies has proven since 1954, its efficiency in the study of molecules and aggregates with intra and intermolecular hydrogen bonds. These studies concern as much the elucidation of the structures of these systems, as their IR and UV-Visible photoreactivities. These systems are of interest for fundamental research as well as for fields with a strong societal impact. Through some examples I will illustrate the power of this technique which unfortunately tends to disappear from the sciences of molecular physics.



IR isomerisation

Gas phase: dissociation
Liquid phase: « hole-Burning »
Solid phase: isomerisation

Cryogenic Matrices

- Molecules trapped in rare gas matrices (Ne, Ar, Xe) or neutral (N_2).
- Trapping of unstable molecules: reactional intermediate, room temperature non stable isomers …
- Average size molecules (4 à 15 atoms)
- IR and UV photoreactivities

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

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

The archetypal case of this family is the ternary mixture of water, ethanol and octanol. Its phase diagram presents a biphasic region with a critical point (Upper Solution Critical Temperature) close to which a strong nanostructuration of the liquid can be observed. In the biphasic region, this emulsion was termed Ouzo effect, following the dilution of the greek beverage. In the monophasic state, a « pre-Ouzo » region has also been evidenced [1], extending between identified frontiers around the critical point (see Fig. 1, [2]). Scattering of light (DLS) or neurons/X-rays (SANS/SAXS) enables to identify aggregates of about 100 molecules similar to a micro-emulsion formed by a water-poor mixture of octanol and ethanol and water, surrounded by a surface excess of ethanol that is immersed in a water-ethanol solution saturated with a low quantity of octanol.

In this system, we investigated, using Quasi-Elastic Neutron Scattering and various isotopic mixtures, the relaxation dynamic of each component along different composition lines crossing the phase diagram. The evolution of the diffusion coefficient is measured over distances bridging characteristic droplet size to molecular distances, i.e. from collective to individual dynamics. We will show how the dynamics also reflect the (nano)structural organization.

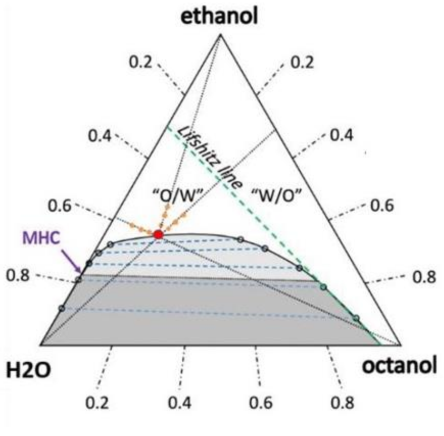

Fig. 1 : phase diagram (wt.%) of the ternary mixture octanol/ethanol/water. The binary region is colored in grey ; the Widom line starts from the critical point (red dot) and crosses the monophasic region toward the ethanol-water binary line ; the Lifshitz line delimitates the onset of structural organization ; the minimum hydrotrope concentration (MHC) indicates the minimum quantity of ethanol required to form a monophasic solution as soon as octanol is added to water ; the dynamics was investigated along the blue dotted line.

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Second order optical response in poled amorphous films: the singularity of thin films and new opportunities for integrated photonics

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The design of active optical devices integrating second-order nonlinear (SONL) optical responses typically relies on the use of dielectric crystalline materials such as lithium niobate (LN) or semiconductors such as GaAs. Despite high SONL susceptibilities, these materials present important geometry constrains inherent to their crystalline nature limiting the complexity of the designed photonic systems.

Conversely, amorphous materials are versatile optical media compatible with broad platform designs possessing a wide range of optical properties attributable to their composition flexibility. Here, we demonstrate for the first time in an amorphous inorganic material, a magnitude of SONL optical susceptibility ($\chi^{(2)}$ = 29 pm/V at 1.06 µm) comparable to that of LN single crystal is reported. It constitutes an improvement of at least one order of magnitude compared with other poled amorphous inorganic materials.

By using a thermo-electrical imprinting process, fine control of the induced uniaxial anisotropy is demonstrated at the micrometer scale. Furthermore, by probing the geometry and the magnitude of the second-order nonlinear (SONL) optical response at different scales, a key aspect of thin film's poling mechanisms compared with bulk glasses is evidenced. It lies in the appearance of a charge accumulation at the film/substrate interface and is described by the Maxwell–Wagner effect.

This work paves the way for the future design of integrated nonlinear photonic circuits based on amorphous inorganic materials enabled by the spatially selective and high SONL optical susceptibility of these promising and novel optical materials.

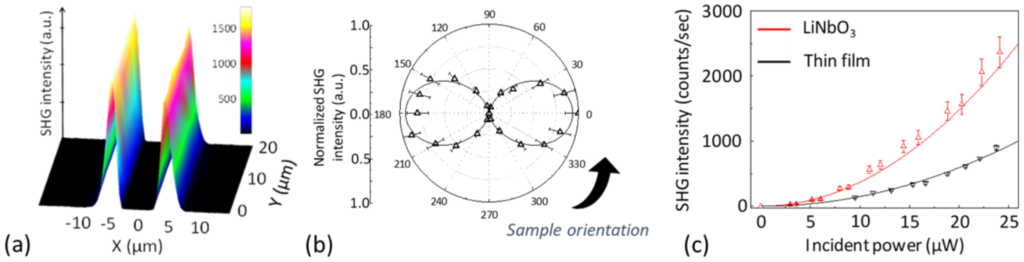

Figure 1: (a) Localization, (b) geometry and (c) magnitude of the SONL response. [1]

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Abstract title : Molecular simulations of clathrate hydrates: An overview

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Clathrate, or gas, hydrates are inclusion compounds made of hydrogen-bonded water molecules forming a network of cages stabilized by encapsulated gaseous molecules [1]. These crystalline solids have first drawn a lot of attention in the oil industry when it was understood that they could dramatically form plugs in pipelines, where hydrocarbons and water meet in the right thermodynamic conditions. Later, naturally occurring gas hydrates, mainly trapping methane, were evidenced, and they are now thought to be ubiquitous on Earth, especially on the ocean floor. The amount of gas stored in those clathrates is significant enough to be viewed as a potential energy resource [2]. Moreover, with the current environmental concerns in mind, gas hydrates are also considered to be used as storage devices for CO_2 [3], but also H_2 [4]. Beyond our own planet, gas hydrates are also conjectured to be stable in various astrophysical environments, e.g. planets, satellites, comets across the Solar System [5]. Their structural properties and trapping capabilities have now been invoked in many planetology models.

The study of those water-based structures is a vibrant and promising area of scientific research, significantly growing for the past three decades [6]. Helped by a computing power on an exponential rise during the same time period, molecular simulations now constitute a decisive tool to complement already well established experiments and thermodynamic modelling in all fields of applications related to gas hydrates [7]. Their phase equilibria, their composition, their structural, mechanical, thermal, and transport properties, in various kinds of environments, have been studied using almost the whole range of molecular simulation techniques available, from cage-focused high precision quantum calculations, to huge (spatial and time) scale classical molecular dynamics, with statistically biased Monte Carlo simulation methods in between.

In this talk, a quick general overview of molecular simulations involving clathrate hydrates will be presented, before diving, with more details, into several past and current computational investigations from our consortium, focusing on structures, selective sequestration, and diffusion within gas hydrates.

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Laboratory to field scale characterization of methane hydrate formation in clay-rich sediments using Raman Spectroscopy: study case of the Black Sea natural gas hydrate system

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The Black Sea, considered as one of the most isolated and methane-rich water body in the world[1], has been the object of scientific campaigns for several decades and host important accumulations of gas hydrates[2-4]. These hydrates accumulate in clay-rich sediments (~60% clay) of various types and depth-variable proportion [5-7], which have a significant impact on their formation mechanisms. During the scientific cruise Ghass2 (2021), natural hydrate specimens have been sampled in the Romanian sector of the Black Sea. In order to better understand the formation process of these hydrates, in particular the role of the sediment mineralogy, laboratory experiments on methane hydrate formation in different mixtures of sand, illite and montmorillonite have been performed, coupled with in-depth micro-scale characterization of natural hydrate samples. Raman micro-spectroscopy was achieved to describe in details the hydrates distribution and to study their cage occupancy in relation with the sediment. This work presents the macro and microscale differences and similarities between natural and synthetic specimens to get insights into the process governing the accumulation of hydrates within the Black Sea sediment and their gas storage capacity.

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Using mantid to analyze powder and single crystal data on WISH

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WISH has been operational on the Second Target Station at ISIS for ~10 years and has undergone a few instrumentation upgrades since then. Software-wise, it was one of the very first instruments to adopt the mantid framework. Initially, the science output was focused on powders but eventually moved onto single crystals (diffuse scattering and then quantitative magnetic structure determination) and thin films. This expansion required new algorithms and tools in Mantid to be developed. I will present how mantid is currently used for all aspects of data reduction on WISH and possible future extensions.

TOF data reduction using Scipp: Fast and flexible handling of event-mode data for time-resolved experiments

Simon Heybrock, Software scientist, ESS

Scipp is the result of a long evolution of packages for scientific computing in Python. NumPy, the fundamental package for scientific computing in Python providing a multi-dimensional array object, sits at the core of this evolution. On top of this, libraries such as SciPy, Pandas, and Xarray provide more advanced functionality and user convenience.

Scipp's central ambition is to make scientific data analysis safer and intuitive. Safety, i.e., avoidance, detection, and prevention of mistakes, is crucial given the rapidly growing complexity of scientific data and data analysis. At the same time it has to be ensured that scientific results are reproducible. For reproducible results, open data must be complemented by open and non-cryptic analysis scripts. This enables the user, the referee, or other scientists to re-run the analysis or to inspect and understand each processing step.

Scipp aims to achieve its ambition in multiple ways:

- A concise and intuitive “language” (programming interface) allows the user to clearly express their intent and makes this intent apparent to future readers of the code. For example, named dimensions remove the need for cryptic axis indices or explicit array transposition and broadcasting.
- Coordinate arrays associated with an array of data ensure that no incompatible data is combined and allow for direct creation of meaningful plots with labeled axes.
- Physical units associated with all arrays as well as their coordinate arrays eliminate a whole set of potential errors. This includes the risk of combining data with different units (such as adding “meters” and “seconds”) or unit scales (such as adding “meters” and “millimeters”).
- Binned data provides an efficient and powerful multi-dimensional view of tabular data. This unifies the flexibility of working with such record-based data with the same concise, intuitive, and safe interface that Scipp provides for dense arrays.
- Features targeting Jupyter, such as rich HTML visualizations of data, give the user the tools to understand their data at every step and share their work with collaborators.

Scipp comes with multi-threading enabled by default, providing good out-of-the-box performance for many applications.

POLARIZED NEUTRON DIFFRACTION DATA ANALYSIS TO PROBE LOCAL MAGNETIC ANISOTROPY IN SINGLE CRYSTALS AND POWDERS USING THE CRYSPY LIBRARY

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Magnetic anisotropy is an essential property of primary importance in areas ranging from molecular magnetism and magneto-optics to magnetoelectric transport. It is an inherent characteristic of magnetic materials that describes the response of the magnetization to a magnetic field. Several techniques are currently used to extract information about the bulk magnetic anisotropy; the most well-known are single crystal and torque magnetometry and ESR. However, all these techniques provide information about the bulk anisotropy of material [1].

A powerful alternative method for characterizing magnetic anisotropy is single-crystal polarized neutron diffraction (PND). In this approach, measured flipping ratios are used to fit the atomic magnetic susceptibility tensors for each of the magnetic atoms in the asymmetric unit, which allows one to quantify the magnetic anisotropy at the local level [2]. It is becoming a reference in mapping the magnetic anisotropy at the atomic scale in molecular magnets. However, PND can't be applied to many highly interesting topics due to the difficulties encountered in growing sufficiently large single crystals. Thus, the step forward from performing experiments on single crystals is extending this approach to powder samples.

Developed by LLB the crystallographic library CrysPy characterizes local magnetic anisotropy based on PND measurements [3, 4]. Application of CrysPy to a range of PND measurements carried out on single crystals and powders will be presented in the report [5-7]. The issue of comparing the local magnetic anisotropy with the bulk magnetic anisotropy will be discussed in the report.

Studies of local anisotropy will certainly receive a massive boost when the European Spallation Source (ESS) becomes operational in the near future. For example, the novel high-performing time-of-flight (TOF) diffractometer MAGiC, which is being developed by LLB, will combine the Laue technique with the exceptional brilliance of the ESS thermal and cold moderators, to yield gains of about two orders of magnitude or more compared to currently existing instruments. However, TOF diffractometers generate rather complex three-dimensional angular- and wavelength-dispersive data that cannot be routinely treated using the standard software packages. The latest release of CrysPy includes a 1D refinement procedure of TOF-PND data by the Rietveld method, which is a necessary step for the development of appropriate software.

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EasyDiffraction, a new software for neutron diffraction data analysis

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Diffraction is a key tool for structure analysis. However, currently available software for modelling and analysis of diffraction data may be, on the one hand, difficult for new users looking to apply diffraction to their field of expertise and, on the other hand, not flexible enough for domain experts.

EasyDiffraction [1] aims to lower the barrier of entry to diffraction data analysis by providing an intuitive and user-friendly graphical interface allowing for the simulation of diffraction patterns based on structural models and refinement against experimental data. It is distributed as an all-in-one package that includes all dependencies and can be installed with just a few clicks on different operating systems. For more complex problems and increased flexibility the Python library behind EasyDiffraction can be used through Jupyter notebooks and scripting.

Simple interface of EasyDiffraction can help improve the user experience and thereby make it easier to train users and students, as well as be better prepared for experiments. We plan to integrate EasyDiffraction into the full data processing workflow to increase experiment automation and make better use of beam time.

EasyDiffraction is built on the EasyScience framework [2], a platform aimed at unifying neutron scattering analysis software. In addition to diffraction, this framework has been successfully applied to reflectometry. Quasielastic neutron scattering will also be targeted in the future.

EasyDiffraction relies on existing crystallographic libraries as calculation engines to cover the necessary functionality. It is still in beta and has only some basic features of the CrysPy [3] and CrysFML [4] libraries, such as support for one-dimensional constant wavelength and time-of-flight powder neutron diffraction data. We are collaborating with LLB and ILL regarding the CrysPy and CrysFML, respectively, and more functionality will become available as the project matures.

EasyDiffraction is being developed free and open source and we hope to attract interested people to jointly contribute to this project and help us, for the benefit of everyone, in making diffraction data analysis and modelling easier.

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Characterization of different fabrication configurations of magnetostrictive Fe-Ga thin films

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Fe-Ga alloys (Galfenol) have recently received intense interest due to their giant magnetostriction in low saturation magnetic fields, with possible applications in many industries. These include automotive, biomedical [1], defence and aerospace. In addition, the emergence of compact cavity-based strain sensors has seen a renewal of interest in magnetostrictive thin films [2]. While the influence of the composition of Fe-Ga on its magnetostriction is well-studied for the bulk material [3], for thin films, the final crystallographic structures and the potential additional induced stresses are still new topics of research [4] with many points still to be understood.

Here we report on different experimental characterisation techniques for magnetostrictive Fe-Ga thin films deposited on geometrically distinct substrates (flat wafers and optical fibres) which were either lying at the bottom of the deposition chamber or continuously rotated below the sputtering target. Additional deformations were also applied to some substrates during deposition to evaluate the stress effects on film properties. The crystal structures were characterised using Scanning Electron Microscope (SEM) (Fig. 1a, b), Energy Dispersive x-ray Spectroscopy, and X-ray diffraction (lab and synchrotron Fig. 1c). Investigations of the magnetic properties used a Vibrating Sample Magnetometer to obtain magnetic hysteresis loops (Fig. 1d), enabling first order reversal curve (FORC) analysis.

Our aim was to determine the optimal deposition settings in order to later investigate the magnetostrictive properties with neutron scattering.

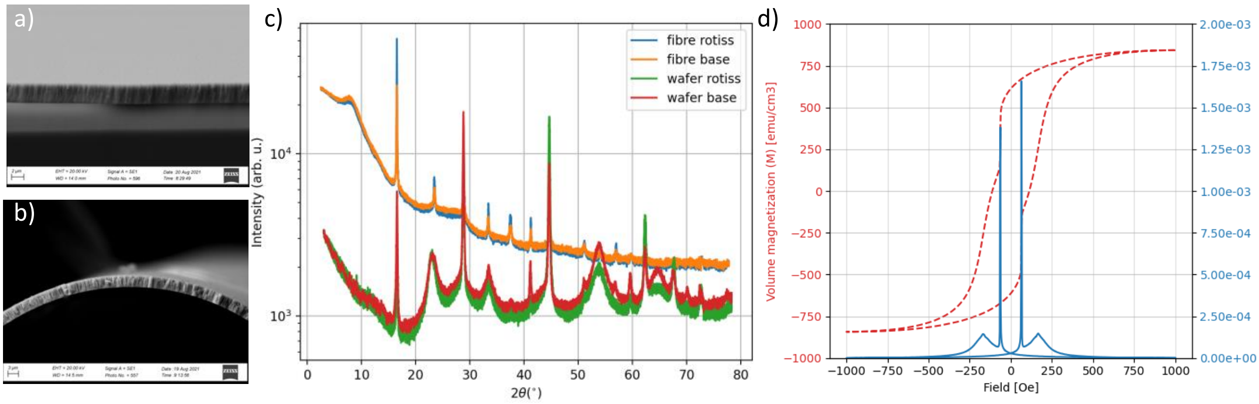

Figure 1: *SEM image of film deposited a) Si wafer, and b) optical fibre, c) films XRD spectra collected at synchrotron in Melbourne, and d) magnetic hysteresis loop for thin films deposited on Silicon wafer.*

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Computing low-energy excitations in strongly-correlated systems: RelaxSE

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Determining the magnetic order from neutron diffraction or finding the low energy magnetic Hamiltonian and its parameters from inelastic neutron spectroscopy is a delicate task. The accurate evaluation of the magnetic interactions by ab-initio calculations could be of tremendous help to refine the parameters of the model Hamiltonian.

Strongly-correlated systems are characterized by the fact that their low-energy properties are not driven by the delocalization resulting from their kinetic energy, but by the effect of Coulomb repulsion between electrons. As a result, they cannot be described, even in a qualitative way, by a single determinant wave-function. Methods based on such a representation (HF, DFT) thus encounter difficulties to correctly describe both their ground state and their low energy excited states.

In these systems, low-lying excitations often corresponds to magnetic excitations, as they cannot be qualitatively described as charge transfers or electronic density changes, but rather as spin state changes (spin orders between magnetic atoms) on a given charge density.

The accurate calculation of this type of excitations requires specific ab-initio methods. Over the years, the CAS+DDCI [1,2,3] method have proved its efficiency, but due to its computational cost, its use is restricted to systems with few magnetic orbitals per magnetic atom. When the number of magnetic orbitals per atoms increases, it becomes compulsory to rely on the SAS+S [4] method developed in our group.

After introducing the different effects that should be considered for an accurate treatment of the magnetic excitations, we will present our new code RelaxSE [5], recently developed to describe this type of excitations, and its applications to magnetic exchange calculations.

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Bulk and interfacial structure of polymerized ionic liquids.

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Poly(Ionic Liquid) (PIL) refer to a special type of polyelectrolyte in which each monomer unit is composed of an ionic liquid (IL). They have recently drawn significant attention since they present a unique combination of the properties of ILs with those of polymers. Among the former is their particular nanostructure arising from local interactions and segregation of the alkyl moiety which confers the bulk IL with either a globular or a sponge-like structure depending on the alkyl chain length [1]. To understand the influence of this nanostructure on the macromolecular conformation of PIL chains, we measured for the first time the form factor of poly(1-vinyl-3-alkylimidazolium) (PC_nVIm) PILs with varying side-chain length n and counter-anions by an extensive use of Small Angle Neutron Scattering (SANS). By probing structural features of PILs chains at length scales ranging from the radius of gyration to the chain diameter and the correlation length between neighbouring chains, we unveiled a surprising non-monotonic evolution of the radius of gyration with *n* in bulk (Figure 1-a), originating from varying flexibility of the main chain and potential modulated electrostatic repulsions, as well as interdigitation of the side chains [2].

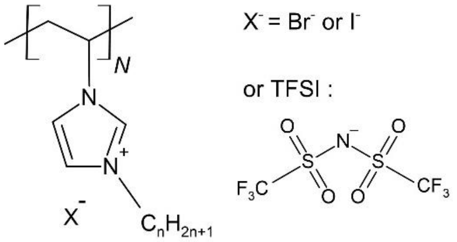

Figure 1: Chemical structure of poly(1-vinyl-3-alkylimidazolium) (PC_nVIm) PILs

We also investigated the structure of PILs at interfaces by combining Grazing Incident Wide Angle X Ray Scattering (GiWAXS) and specular X-Ray reflectivity measurements on PIL thin films which allowed to probe respectively the in plane and out of plane structure. We showed that the in-plane distance between neighbouring chains is modulated by confinement (*i.e.* the thickness of the thin film) possibly due to the preferential orientation of imidazolium groups limiting the number of accessible configurations. Additionally, and similarly to the layered structure of alternating cationic and anionic layers reported for ILs at interfaces [3], early signs of a layered structure were unveiled by X Ray reflectivity on PIL thin films. All these features are precious insights into understanding the behaviour and viscoelastic properties of these attracting materials in bulk and at interfaces.

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Towards the ESS User Programme: Tracking Scientific Key Performance Indicators and Providing User Support for Deuteration and Macromolecular Crystallisation

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Though not yet in operation, we are systematically tracking the published scientific output from ESS. By the end of 2021 this dataset included nearly 1000 publications which form the basis of 2500 citations in 2021. These scientific key performance indicators (KPIs) are a testament to the work being carried out every day, our large collaboration sphere around the globe as well as the multitude of research and development areas covered.

For many neutron scattering experiments, using deuterated samples has numerous benefits. The molecules that are of most interest include proteins, lipids, fatty acids, small organic molecules, surfactants, and membranes. Deuteration is used to (i) enable contrast variation, allowing scientist to selectively “match out” components of complexes and / or (ii) to boost weak signal-to-noise ratios, reduce the incoherent background due to hydrogen, improve neutron scattering length maps, and enable direct visualization of hydrogen bonds and solvent networks. ESS has established a deuteration and macromolecular crystallization support laboratory, which will be available to all users of ESS instruments and includes chemical deuteration, biological deuteration and large protein crystal growth.

As ESS does not provide neutron scattering possibilities at this point in time, since 2019 we have supported science using neutrons at other facilities by providing deuteration and macromolecular crystallisation support. We offer service for specific classes of deuterated inorganic or organic small molecules (e.g. pyruvate, trehalose, lactic acid), deuterated biomass/crude lipids/proteins, and access to our crystallization labs for large crystal growth. Access to support is managed through a peer-reviewed, proposal-based system and is currently free of charge to user upon acceptance. For more details or information, researchers can contact us at demax@ess.eu. We have successfully executed small, pilot calls for proposals for deuterated materials which also enabled us to test the proposal management part of the User Office Software (UOS) and it is useful to review the calls to gain insight to our user community. Up to now, this activity has led to 26 publications supporting more than 55 unique users.

Elucidating the structure of MAPbI3 using neutron spectroscopy, first-principles calculations and thermophysical properties – A first peek at high-pressures

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Hybrid Organic-Inorganic Perovskites (HOIPs) have recently emerged as a promising class of materials for photovoltaic and lasing applications due to their exceptional optoelectronic properties [1]. Several lead halides within this family of materials continue to attract considerable interest, methylammonium lead iodide ($MAPbI_3$) representing the prime example. Notwithstanding the above, $MAPbI_3$ exhibits three phases at different temperatures (and ambient pressure) whose atomic structure and stabilization mechanisms remain elusive and require further investigation [2,3]. On these grounds, we have recently developed a model-selection protocol for HOIPs combining inelastic-neutron scattering (INS), first-principles calculations and thermophysical data [4]. This protocol has been implemented with success for $MAPbI_3$, indicating that the local structure around the organic moiety is distinctly different and more intricate relative to that inferred from previous crystallographic studies. In support of the above, we also present new results of first-principles molecular dynamics (MD) simulations for MAPbI3 across its temperature-pressure phase diagram. The pressing need to extend the study of HOIPs to higher pressures comes from the very limited number of available works on the subject. These MD simulations pave the way to achieving a deeper understanding of the available experimental data for MAPbI3, obtained with radiation-scattering techniques.

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Raman spectroscopy of strong acid hydrate: towards new proton conducting electrolyte.

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Designing new devices dedicated to energy storage and production is at the center of nowadays concerns. In this area, the development of new electrolytes is of prime importance. Clathrate hydrates systems represent an opportunity as a new electrolyte for fuel cells, for which fundamental questions are opened. Clathrate hydrates [1] possess interesting properties depending on the nature of the invited molecules, due to their nanostructuration and their specific physical-chemistry properties [2]. When acidic species are encapsulated, clathrate hydrates are classified as super-protonic conductors, due to the encapsulation of anionic species generating delocalized protons into the cationic cage network [3]. To better understand the conductivity mechanism, experimental and theoretical approach are combined in the cases of $HClO_4$ and HPF_6 hydrates – both systems being among the best conductors [4][5].

Two issues are addressed: the role played by the ionic defects in terms of concentration and of localization in the clathrate structure. It is possible to prepare mixed hydrates (i.e. encapsulating two guest species) by co-including HClO4 acid and tetrahydrofuran (THF) molecules. By varying the ratio of THF to HClO4, such mixed hydrates offer the opportunity to tune the concentration of the acidic defects in the clathrate structure [6]. By means of impedance measurements, it is shown that the protonic conductivity is controlled by the ionic defect concentration, but also by the formed clathrate structure as revealed by X-ray diffraction analysis and Raman imaging. Regarding the ionic localization, HPF6 hydrates exhibit molecular defects, due to the existence of impurities (e.g. H3PO4) associated with the high reactivity of the anions [4]. Locating these defects at a molecular scale and understanding their effect is a fundamental question for improving the electrolytic properties of the strong acid hydrates. Quantum mechanics calculations have been employed to investigate such properties in the Density Functional Theory (DFT) approximation.

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Aging of atmospheric particles using acoustic levitation coupled with Raman spectroscopy

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Atmospheric aerosols are well known to impact both air quality and climate change. Once generated, they may further react through complex multiphasic processes so-called aging process of aerosols. These physical and chemical transformations may affect both chemical composition and physical properties of aerosols in the atmosphere and thus influence their impacts. The interactions between atmospheric water vapour and aerosols play a key role in determining the observed microphysics properties of aerosols in the atmosphere. Indeed, particles' hygroscopicity, ability to act as Cloud Condensation Nuclei (CCN) and cloud–aerosol interactions remain a major obstacle to understanding climate and severe weather [1]. Hygroscopicity can be defined as the ability of particles to capture water molecules inducing reversible solid-liquid transitions. Raman spectroscopy is helpful to probe liquid – solid transition as a shift on Raman spectrum may be observed with in situ and on line conditions [2,3]. In this work, we have optimized a coupling between Raman microspectrometry and acoustic levitation device to analyze the chemical composition and the mixing states of the particulate phase during hydration and dehydration of model particles. We are able to determined deliquescent and efflorescent values for particles with various compositions. In particular, we investigated hygroscopicity properties of organic/salt mixture particles which are models of sea salts and organic aerosols mixture. We have demonstrated that mixture induce modifications in deliquescence behavior of particles and that organics react with during hydration and dehydration cycles [4]. These results show that chemical complexity of aerosols may contribute indirectly to the global climate change.

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Development of a Raman Setup for combined Raman and neutron measurements.

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We have developed a Raman spectrometer for measurements on samples placed in standard Orange Cryostat available at neutron large scale facilities. An original optical head plugged to a dedicated can has been designed allowing to work at high pressures and low temperatures. Thanks to this instrumental development, we can perform Raman measurements (vibrational spectroscopy) coupled with neutron diffraction/spectroscopy in situ measurements on metastable or transitioning samples (eg IN6-SHARP, D1B, etc.). This correlative setup is automated and remotely control to meet the requirements of neutron large scale facilities. It uses several excitation wavelengths (lasers at 532 and 785 nm) for measurements adapted to various samples and minimize any fluorescence contribution.

Clathrate hydrates FTIR spectroscopy to understand cometary ices

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Jupiter Family Comets (JFCs) have been widely studied as the most pristine remnants of the solar system formation (e.g. the ESA/Rosetta mission). The direct detection of various species of highly volatile material [1] is the figurehead of evidence suggesting that JFCs have not been modified since their formation. However, recent studies [2] have shown that the dynamical cascade that brings JFC nuclei, from the outer solar system reservoirs to the orbit on which we observe them, entails some significant thermal processing. In short, hypervolatiles should be lost, unless they can be trapped and stored during JFCs' chaotic orbital journey, when heated subsurface layers consist in a gas phase in contact with an icy matrix.

Gas hydrates could be key in this context: they constitute a class of solids in which the guest molecules occupy cages in a host structure made of H-bonded water molecules. They only form and remain stable in specific temperature and pressure regimes that depend on the nature of the guest molecules. In the context of JFCs, we need to study the formation and stability of hydrates in extreme conditions, i.e. temperatures under 50K and pressure around 10^{-7}mbar to represent conditions in the Kuiper Belt, between 80 and 200 K with pressures below 1 mbar to represent comets' active phase. Theoretical phase diagram of clathrate hydrates shows that it would be possible to form clathrates at these conditions [3], but no experimental data currently support these models.

In an effort to assess whether hydrates may play a role in maintaining volatile species in cometary material, characterisation of water-gas samples in conditions relevant to cometary nuclei was explored using FT-IR spectroscopy. Experimental results of the spectroscopic identification of water-CO_2 and water-CH_4 samples at 10 K and 10^{-7} mbar [4], suggesting that gas hydrates have been formed under cometary conditions, will be presented. In order to fully characterisation, a cryogenic cell for both structural and spectroscopic characterisation have been developed. Recent Raman microspectroscopy experiments of water-gas mixtures using this device, with various deposition processes and temperature/pressure regimes, will be unveiled.

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Diffraction data processing at the European Spallation Source

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The European Spallation Source (ESS) will operate a suite of diffractometers, with the DREAM diffractometer [1] among the first instruments to be commissioned with neutrons. In order to take full advantage of this powerful source and to ensure that even first-time users can easily process their data, the ESS Data Management and Software Centre is developing an integrated data pipeline linking all the steps from data acquisition to data analysis. The software used in the data pipeline should be efficient enough to deal with large amounts of data and respond to requirements from the scientific community while providing an intuitive workflow at the same time.

To test this pipeline during the construction phase of ESS and of its instruments, we use instrument simulations with McStas [2], which has to be combined with GEANT4 [3] due to the complex three-dimensional geometry of the new ^{10}B detectors of the ESS diffractometers.

Here we report on preliminary tests of parts of the data pipeline using McStas and GEANT4 simulations of the DREAM instrument focussing on the treatment of powder diffraction data (see Figure 1).

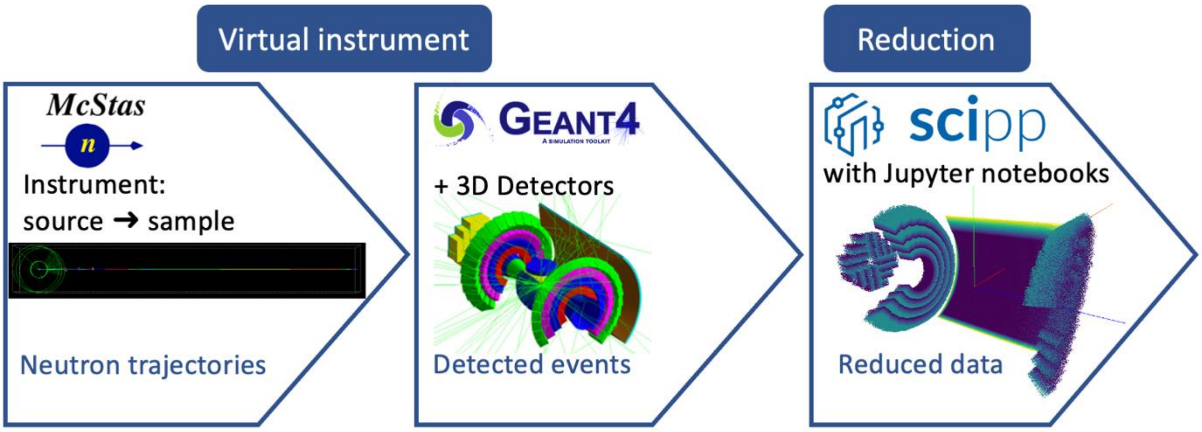

Figure 1: Part of the data pipeline for a virtual DREAM experiment. *McStas simulations record neutron trajectories from the source to the powder sample. Then GEANT4 simulations give the events recorded by the 3D detectors. These raw event files are reduced in scipp [4] using Jupyter notebooks. Note that the text in blue marks the output generated at the end of the corresponding stage.*

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