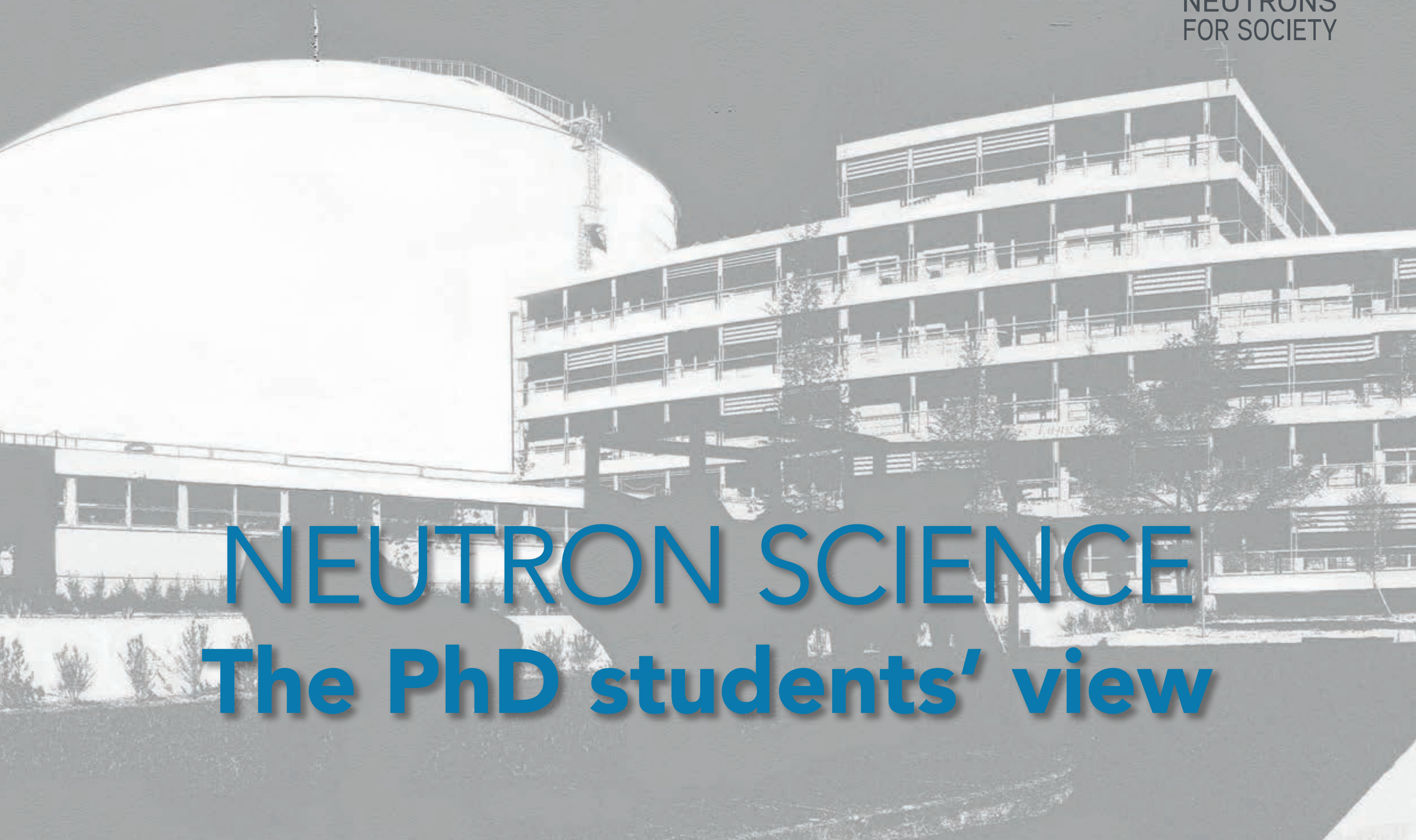
NEUTRONS
FOR SOCIETY



NEUTRON SCIENCE
The PhD students' view

FORWARD

At ILL, we produce a range of documents to communicate the science done with neutrons to different audiences. With this brochure we would like to give a simple snapshot of the whole range of science currently being performed at ILL as represented by the 40-or-so PhD projects running at the present time. The document covers work-in-progress and not necessarily results obtained, particularly for first-year students. We hope this easy-to-read summary of current neutron science is accessible to a very wide audience, including future PhD-students, and that it also communicates the personal stories behind studying at ILL and living in the French Alps.

Science at ILL fits broadly into five areas - biology & health, magnetism, materials science (physics and chemistry), soft matter and nuclear & particle physics - and the contributions have been organised accordingly. They reflect the strengths of the ILL and its users in terms of scientific expertise, instrumentation, sample environment and preparation (e.g. deuteration), software and simulations, etc. It is striking that almost all PhD projects are addressing the major societal challenges, including specific, pressing issues like antibiotic resistance, welds in nuclear power plants and battery materials. In some cases, industry partners are directly or indirectly involved in these projects and, in the future, we intend to enhance these partnerships and therefore the innovation potential of neutron science.

The ILL has always supported PhD students, recognising the need to train, in our facility, future generations of neutron scatterers. This also allows ILL scientists to develop their own projects and techniques, at the same time as fostering strong collaborations with user groups. We fully fund about ten PhD positions each year, with an open call each autumn, which typically results in 13-14 projects being selected with co-funding from user groups. Our PhD programme has been organised for a number of years by the ILL Graduate School, which ensures a strong sense of community among the students, thanks to group activities and well-chosen social events, and also provides various forms of training. And the students perfectly reflect the international character of the ILL. From the 41 entries in the brochure, 18 student nationalities are represented for university affiliations in 11 countries and about two-thirds of students are enrolled in a foreign country.

We hope that you enjoy this brochure and that it will help to attract exciting, new PhD projects as well as talented, motivated PhD-students.

Mark Johnson - Head of the Science Division, UK Associate Director
Henry Fischer - Head of the ILL Graduate School

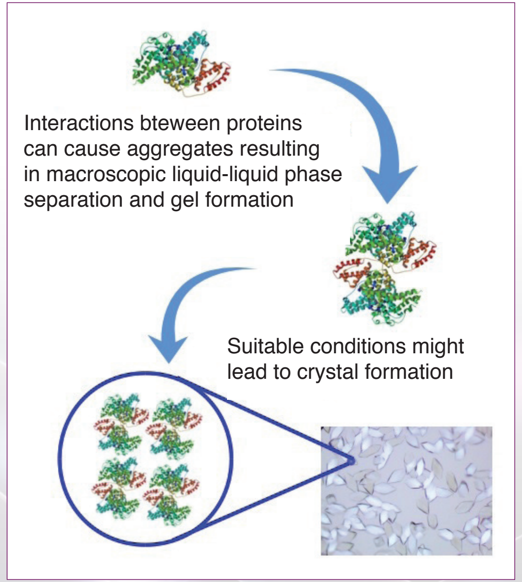
CONTENTS

Nationality: DE
University of Tübingen, DE

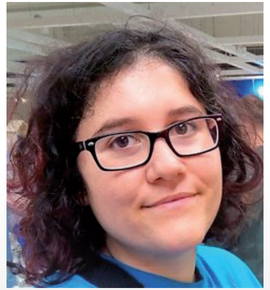
Studying at the ILL offers great possibilities of working in an environment providing unique instrumentation and essential discussions with experts in many fields.

Christian Beck

Diseases such as **Alzheimers, sickel cell anemia or eye cataracts** are induced by **protein aggregates.** To develop new and more efficient drugs against these diseases, it is important to understand the interactions and dynamics of proteins. To probe the dynamics on a length scale commensurate with the protein size and in the short-time limit of diffusion, **quasielastic neutron backscattering** is a very powerful tool. Studying different systems offers insights into the interactions between the proteins inducing cluster formation, liquid-liquid phase separations, crystal growth or the formation of gels. By linking experimental results with **theoretical models** from colloid physics, it is possible to determine quantitative dependencies, which can be used to predict the behavior of systems at a range of conditions.



Cartoon of the process of protein aggregation and crystal growth.



Nationality: IT
Linköping University, SE

I consider studying at ILL a great opportunity and an enriching experience for my professional training. I find it extremely motivating to be in a multicultural environment where high-level facilities are concentrated in one place.

Francesca Caporaletti

The MarR–like proteins are a family of gene regulators which control the expression of **efflux pumps** (Fig 1) - complexes that actively evacuate toxic chemical compounds out of the host cells. Natural selection pressure to acquire **Multi-Drug Resistance** (MDR) mutations leads to the inactivation of the repressors of efflux pump gene expression, resulting in a continuously high production of MarR-like proteins, and thus an increased **survival for the bacteria**.

Analysing the structure–function relationships of MarR family of proteins using **Contrast Matching with SANS** (Small Angle Neutron Scattering) (Fig 2) is fundamental to learn how to overcome MDR in future drug development.

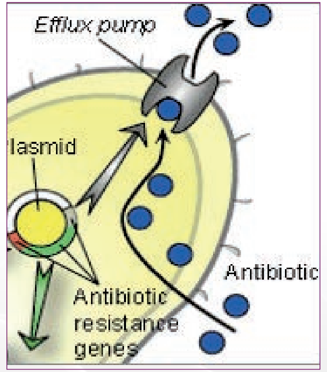


Figure 1. Example of an efflux pump in a Gram-negative bacteria (*P. Aeruginosa*).

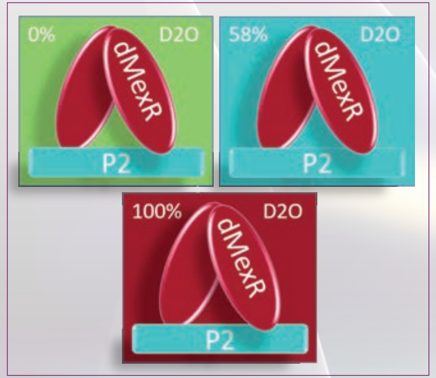


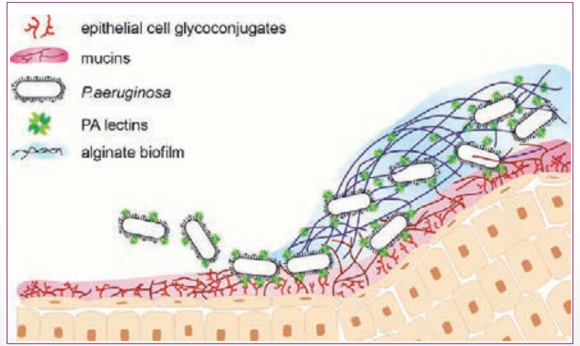
Figure 2. Contrast matching experiment with SANS.

Nationality: SK
Grenoble-Alpes University, FR

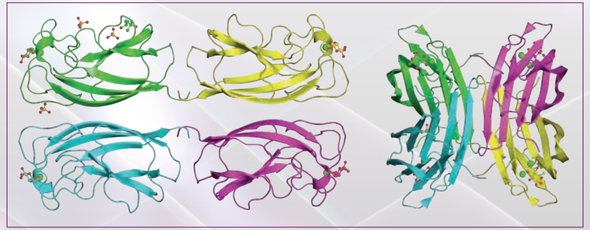
ILL is giving me so much. And with no charge - I Love it!

Lukas Gajdos

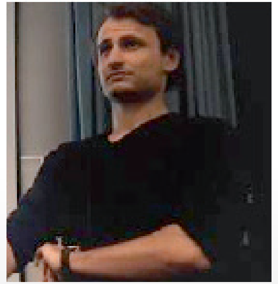
Increasing **antibiotic resistance** among bacteria is currently considered to be one of the most serious threats to global health. For example, ***Pseudomonas aeruginosa*** are multi-drug resistant bacteria that cause fatal infections in immuno-compromised patients. Pseudomonas produce two proteins, called lectins, that play a role in the first steps of infection. Lectins bind carbohydrates presented on the host cell surface, leading to bacterial adhesion and further colonisation. Using **neutron diffraction**, we will be able to explore these interactions and obtain information that will help in the development of new potent drugs with antibacterial properties.



Possible roles of *Pseudomonas aeruginosa* LecA and LecB lectins in host recognition.



X-ray structures of LecA and LecB lectins.



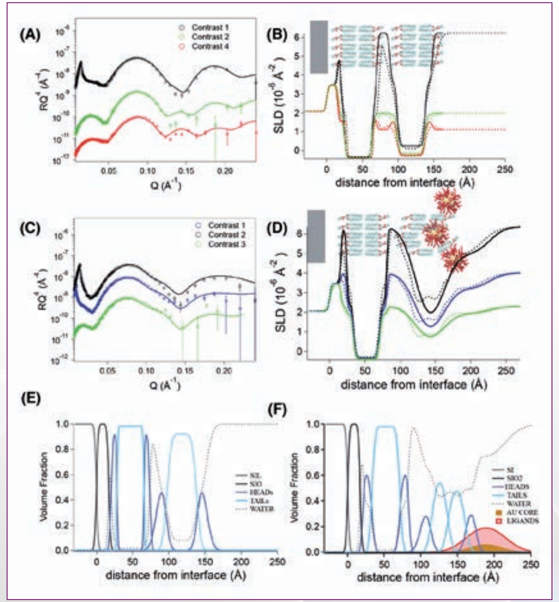
Nationality: FR
University: Politecnico di Milano, IT

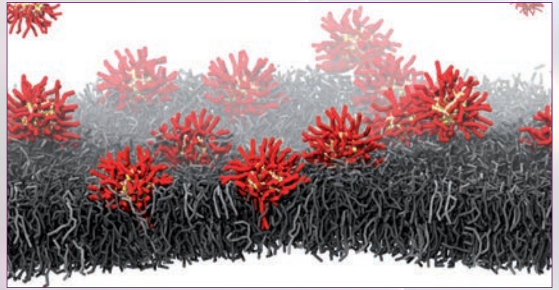
I like studying at ILL in Grenoble because of the great scientific environment.

Loic Joly

The development of **novel nano-engineered materials** poses important questions about their possible adverse **effect on life and the environment.** Understanding how these novel materials interact with living matter will have a great impact on biomedical sciences and provide a controlled interaction with living cells to be exploited in novel drug delivery and biosensing systems.

To address this critical problem, my PhD concerns the study of the interaction between nanoparticles and model lipid membranes using **neutron reflectometry and molecular dynamics simulations.** Combining scattering studies and a computational approach provides a detailed molecular view of the mechanism involved in the incorporation/uptake of nanoparticles into biomimetic membranes and destabilisation processes that can alter the integrity of membranes.





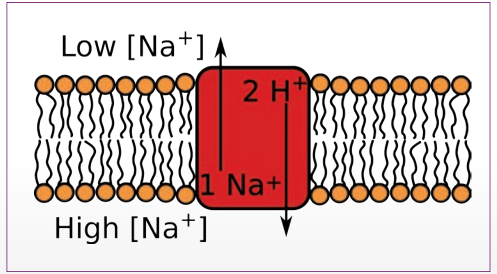
NR data and cartoon from MD simulations of nanoparticles interacting with lipid bilayers.

Nationality: DE
Université de Grenoble, FR

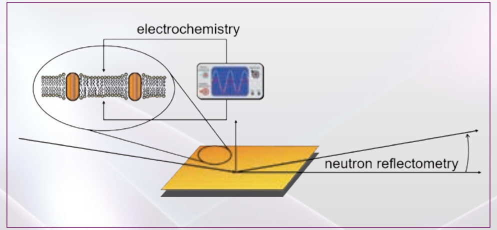
Large scale facilities offer a unique type of work environment. At the ILL, this is combined with a very international atmosphere and the beautiful surrounding mountains, making it the perfect place to work.

Sebastian Koehler

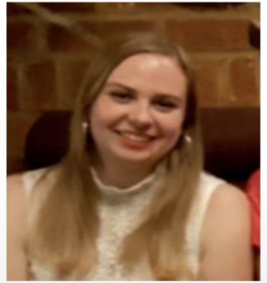
Proteins and membranes are key components of the cells of life. The **function of membrane proteins** depends strongly on the shape of the surrounding environment, especially the structure of the incorporating lipid membrane. However, specific factors behind this influence are still relatively unknown. Using a combination of **neutron reflectometry** to determine the structure of membrane proteins in lipid bilayers and **electrochemical measurements** to characterize its electrophysiology activity, we investigate the relation between protein function and the structure of the membrane environment. In the case of ion-pumping proteins, one potential application is a '**natural battery**' that could be used, for example, to power a heart **pacemaker**.



Concept of an antiporter protein.



Cartoon of the neutron reflectometry experiment and the electrochemistry measurement.



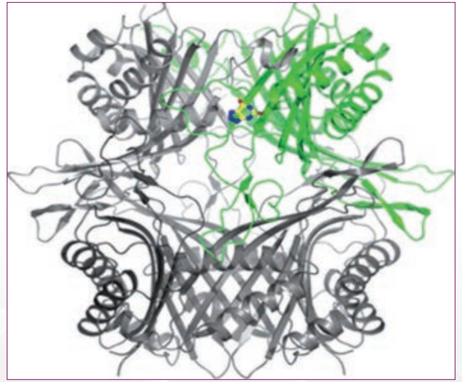
Nationality: UK
King's College London, UK

I like working at the ILL because it has such an international feel to it and there are plenty of opportunities to learn about cutting-edge science in and beyond my field.

Lindsay McGregor

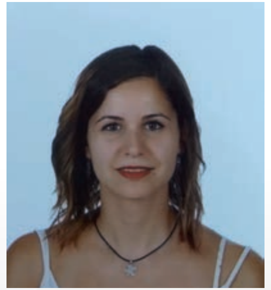
Understanding the structure and **function of enzymes** is a main focus in biology. Hydrogens are essential to biological processes and, by using neutrons, we can reveal their locations, providing information unavailable using other popular techniques.

Urate oxidase (UOX) is a co-factorless enzyme that reacts with oxygen, but the exact mechanism of action is not clear. By studying the **protein structure** using **neutron crystallography**, we hope to decipher the exact mechanism through the role hydrogens play in the catalytic cycle, thus answering a fundamental question in enzymology.



Urate oxidase (UOX) protein structure.

Deuterated crystal of UOX used for neutron diffraction.



Nationality: ES
University of Granada, ES

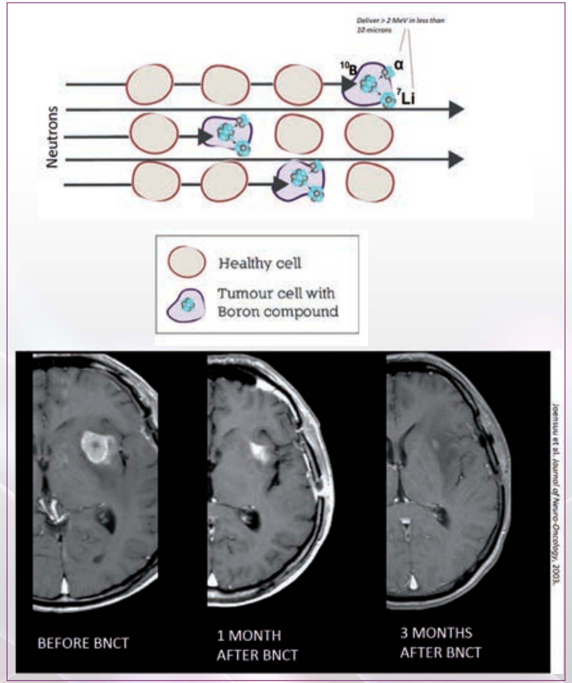
ILL is lots of people from different places working in lots of different fields - I think it's great.

Maria Pedrosa Rivera

The biological effect of neutrons of low and medium energies is not well-known. This data is especially important for **Boron Neutron Capture Therapy** (BNCT) which uses epithermal neutron irradiation plus a boron-10 compound, selectively uptaken by the tumor cells, to **treat** the **cancer.** It is an experimental treatment already used with more than 700 patients with tumors like Glioblastoma or Head and Neck cancer. A better estimation of the biological effect will improve the therapeutic impact.

To study the effect of low energy neutrons, a series of experiment are performed at ILL on the high flux, PF1b beam line to **in vitro samples (mammalian cells)**.

For more information see: : Hopewell *et al.* Applied Radiation and Isotopes, **2011**, 69(12).



Cartoon of how BNCT works and the result in a patient with glioblastoma.

Nationality: FR
Université Grenoble-Alpes, FR

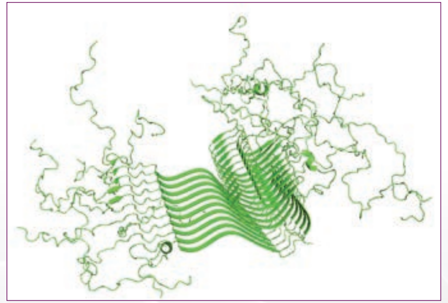
ILL provides a great scientific environment to work, from fundamental physics to Biology.

Kevin Pounot

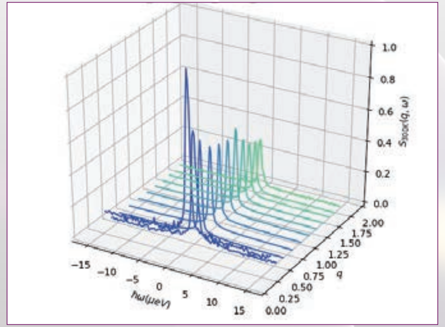
Amyloid proteins are involved in neurodegenerative diseases, such as **Parkinsons and Alzheimers,** when they aggregate and form elongated fibers. Using **protein perdeuteration** and **neutron spectroscopy**, we investigate the physical origin of protein aggregation by studying the protein/water interplay. The effect of metal ions is also investigated. All experimental results are complemented with **molecular dynamics simulations** to build a comprehensive understanding of aggregation.

This knowlodege will be useful for the early detection of neurodegenerative diseases and potential new treatments.

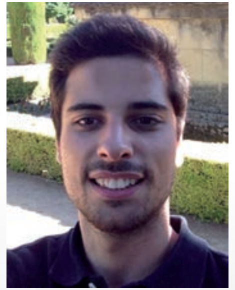
For more information see: Fichou *et al.*, PNAS 2015 112, **20**, 6365-6370.



Fiber of alpha-synuclein (involved in Parkinson).



Experimental data showing the time and length scales of protein dynamics.

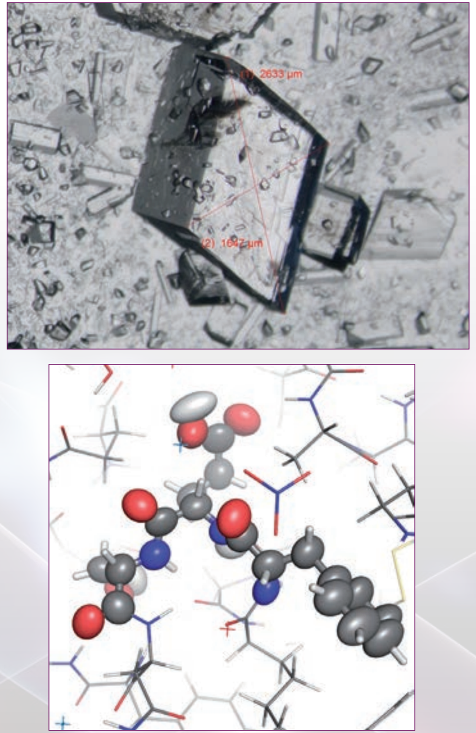


Nationality: PT
University of Copenhagen, DK

There's a fantastic atmospheric surrounding the scientific community at ILL – people from many different nationalities working to push the boundaries of neutron science.

Joao Ramos

Protein biological function is intimately related to **dynamical changes in protein structure**. The accurate description of atomic thermal motion in proteins is hampered by limitations inherent to X-ray crystallography. **Neutron diffraction** is an ideal method for obtaining physically meaningful **atomic displacement parameters** (ADPs), routinely in the case of small molecules. Therefore, we will push the boundaries of neutron protein crystallography by determining realistic and unbiased ADPs for a model protein system - partially deuterated and perdeuterated Hen Egg White Lysozyme.



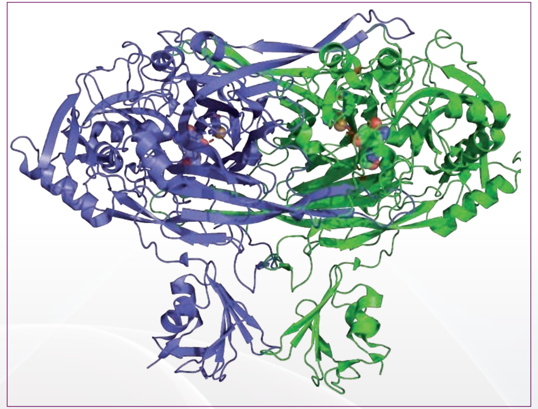
Picture of a Lysozyme crystal for a neutron diffraction experiments (above) and a crystallographic model refined from neutron data showing ADPs (below).

Nationality: IN
University of Hamburg, DE

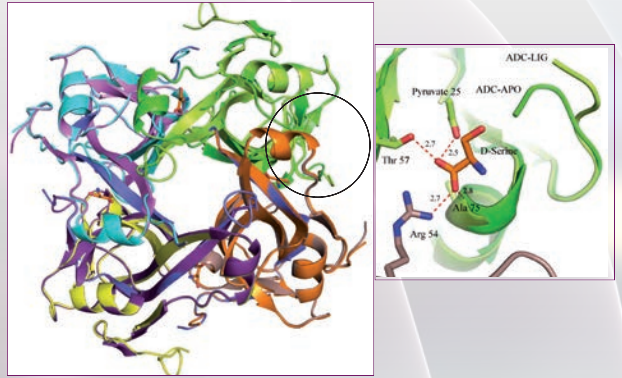
I like working at ILL because of the interdisciplinary environment which will help make me a better scientist.

Tushar Raskar

Unravelling mechanisms underlying the molecular motions in enzymes is extremely important since the catalytic **function of enzymes** depends on their **structure and dynamics**. I work on two enzymes: Aspartate decarboxylase and *E.coli* copper amine oxidase. Both these enzymes are major drug targets. **Quasi-elastic neutron scattering and diffraction** are key experimental techniques to gain insight into the mechanism of enzyme inactivation and structural alteration. This data combined with **molecular dynamics simulations** will help in establishing the structure-dynamics-function relation in these enzymes and in subsequent drug development.



E.coli copper amine oxidase enzyme system.



Loop motion in Aspartate decarboxylase.

Nationality: UK
Malmoe University, SE

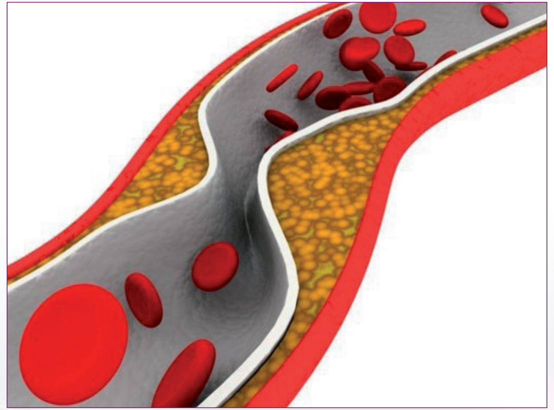
Working at the ILL is a great opportunity to be surrounded by new and exciting science in an ever developing environment!

Sarah Waldie

Atherosclerosis is the largest killer in the West and arises from plaque build up in the arteries causing cardiovascular diseases leading to **heart attacks and strokes.**

'Good' and 'bad' **cholesterol** known as high- and low-density lipoproteins (HDL and LDL) respectively, play a huge role in this process by taking up and depositing lipids from and into the artery wall.

A better understanding of the structure of differing lipoproteins and lipid exchange processes is urgently needed. **Neutron reflectometry and small angle scattering** combined with **deuterium labelling** are the ideal probes to study this.



Plaque build up in the artery wall.

High- and low-density lipoproteins.

Nationality: DE
Université de Grenoble, FR

Friendly atmosphere, diversity in research and internationality are key ingredients of the stimulating working environment at ILL.

Domink Zeller

The structure and **dynamics of a protein** determine its functionality. Elastic Incoherent Neutron Scattering (EINS) enables us to measure these dynamics simply and quickly but data analysis is not straight forward. Consequently, it is crucial to investigate **new approaches and models** to improve the data analysis, leading to a better understanding of both EINS experiments and **molecular dynamics (MD) simulations.**

My study is based on the protein *Alpha-lactalbumin*. I investigate its dynamics on the pico- to nano-second time scale with several spectrometers and MD simulations.

For more information see: Peters and Kneller, JCP **139**, 2013.

Dynamics of *Alpha-Lactalbumin* on the picosecond time scale.

Nationality: IT
University: Warwick, UK

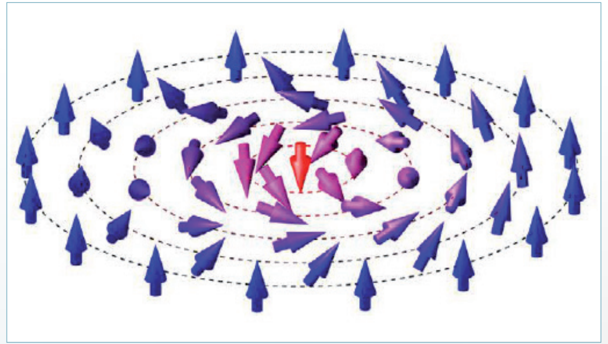
Grenoble was love at first sight.

Marta Crisanti

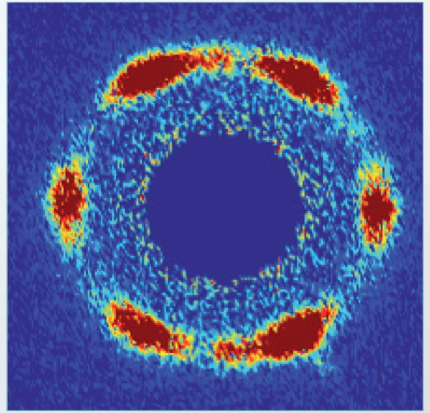
Skyrmions are vortex like arrangements of magnetic moments in matter which constitute a completely new magnetic topology that is currently attracting a lot of interest in the scientific community. Skyrmions are seen as possible new information carriers to be exploited in **future computing devices.**

The complete understanding of skyrmions characteristics is crucial for the delivery of devices.

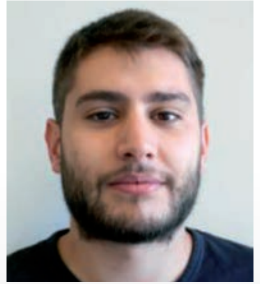
In bulk samples, the characteristic dimension of the skyrmion lattice is in the range of tens of nanometres, which can be perfectly probed via **Small Angle Neutron Scattering**.



Cartoon of a Bloch-type skyrmion.



SANS image of the skyrmion lattice in a single crystal.



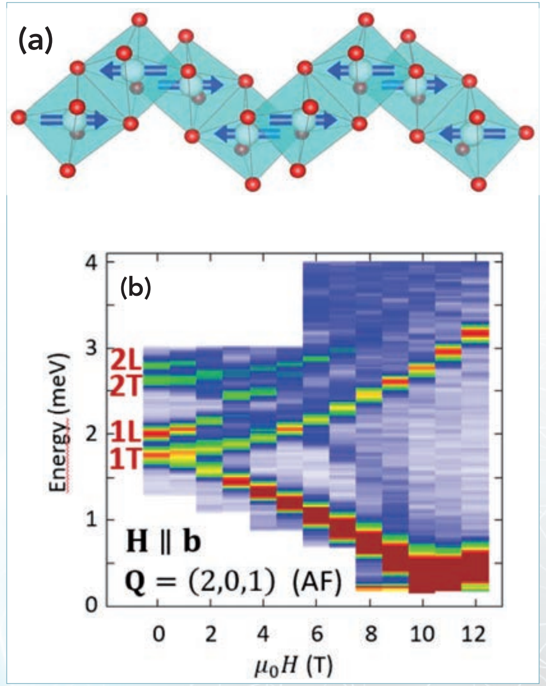
Nationality: FR
Université Grenoble-Alpes, FR

In addition to the facilities being the best in the World, the melting-pot between many nationalities makes the ILL unique and such an interesting place to work.

Quentin Faure

Strongly correlated electron systems are a subject of great interest in Condensed matter physics (and far beyond) as they demonstrate collective phenomena like **high-temperature superperconductivity** or, simply, macroscopic magnetism. In addition, these systems have been challenging theoreticians for more than 40 years. To study the strong interactions, one can focus on systems consisting of chains made of the simplest spin ½ particle. In my PhD I am using neutron scattering, and the fact that neutrons carry a spin ½, in a 'disturb to reveal' strategy. **Neutron diffraction and inelastic scattering** are ideal to probe magnetic structures and excitations of strongly correlated electron systems.

For more information see: Faure *et al.* Nature Physics 2018.



(a): Cartoon of the 1D spin-1/2 Ising-like antiferromagnet $BaCo_2V_2O_8$.
(b): Magnetic field dependence of the excitations of $BaCo_2V_2O_8$ under a transverse magnetic field (perpendicular to the ordered moments at zero-field).

ADVANCED MAGNETIC IONIC LIQUIDS

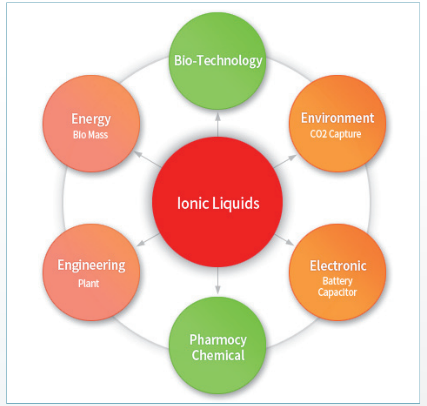
Nationality: ES
University Cantabria, ES

ILL offers a great opportunity to be in contact with other students and groups working in many interesting and different fields, showing the wide range of disciplines that can be studied with neutrons.

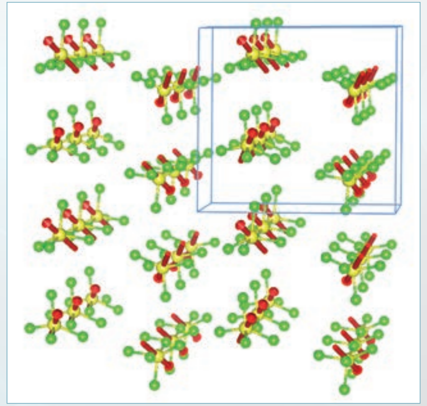
Palmerina Gonzalez Izquierdo

Magnetic Ionic Liquids (MILs) are a class of molten salts composed of organic and inorganic ions with a paramagnetic component in their structure. MILs possess a range of interesting physicochemical properties and present a strong response to magnetic fields. They are being applied in different fields, like **electrochemistry, catalysis, organic synthesis or analytical chemistry**. We are investigating a family of imidazolium-based MILs with tetrahaloferrate anion. **Neutron diffraction** is indispensable to obtain their magnetic structure and understand the origin of their properties.

For more information see: Gonzalez-Izquierdo *et al.* Inorganic Chemistry 2018 57 1787-1795.

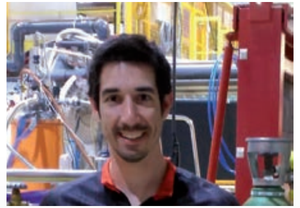


http://www.c-tri.co.kr/english/rnd/chemistry.asp



Magnetic structure of the magnetic ionic liquid 1,2,3-trimethylimidazolium tetrahalferrate (organic molecules omitted for the sake of clarity).

MAGNETIC SHAPE MEMORY ALLOYS FOR MAGNETIC REFRIGERATION



Nationality: ES
Public University of Navarra, ES

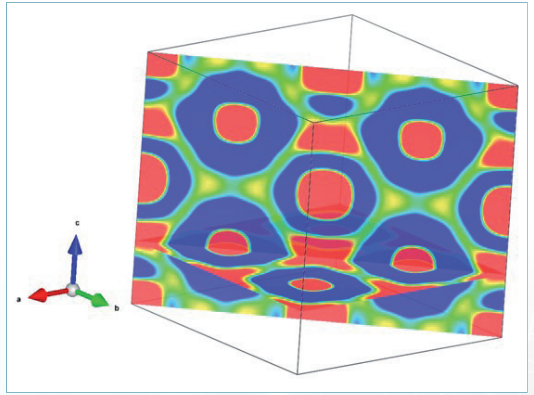
I like studying at ILL because of the diversity of the students and also because of the mountains which are great to ride by bike.

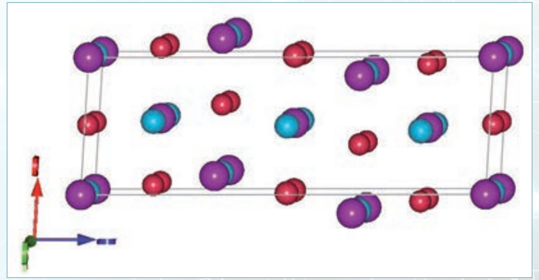
Javier Lopez-Garcia

As multifunctional materials, **magnetic shape memory alloys** are promising for many applications, like **sensing and magnetic refrigeration**, due respectively to their giant magnetoresistance and magnetocaloric effect, associated with the structural transformation that they present between two magnetic states.

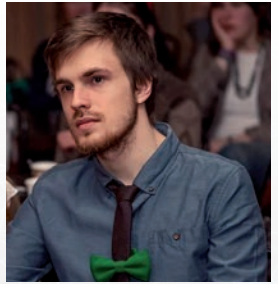
Neutron diffraction is an essential tool to analyze the magnetic coupling and the microstructure (long range atomic order, grain size, defects...) induced by different thermal treatments or mechanically milling the alloy to control particle size, in order to improve their properties for their potential applications.

For more information see: Appl. Phys. Lett., vol. 110, no. 18, p. 181908, 2017 Intermetallics, vol. 94, pp. 133–137, 2018.





Magnetic structure and interactions in austenitic and martensitic structures of $Ni_{45}Co_{5}Mn_{37}In_{13}$.



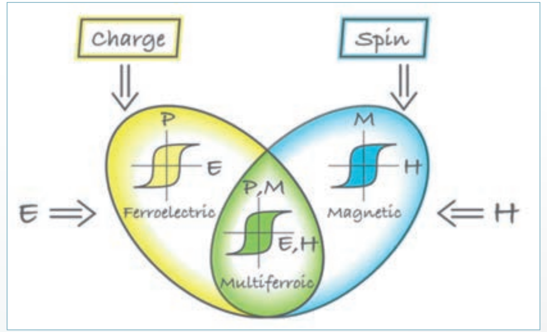
Nationality: RU
University of Caen Normandy, FR

ILL provides a fantastic possibility to work on cutting-edge topics in modern science with the help of the most prominent researchers of our time. I feel how this place helps me to grow professionally and personally each day.

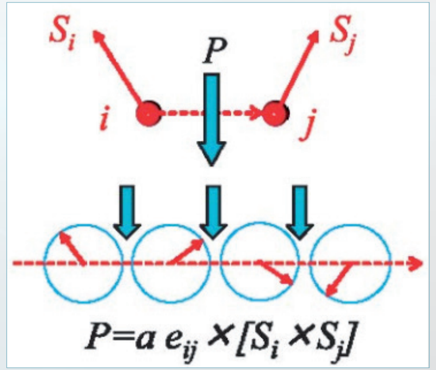
Stanislav Podchertsev

Multiferroic materials have huge potential for a numerous technological applications: **magnetic field sensors, magnetic storage and spintronic devices**. Compounds with chemical formula AB_2O_4, so-called spinels, in turn are great place to look for novel multiferroic type-II materials which possess a stronger magnetoelectric coupling.

Multiferroic type-II compounds have complicated spiral or conical magnetic spin ordering which results in electrical polarization. **Neutron diffraction** is the only experimental technique to get complete information on spin arrangements in magnets and thus the ideal method to study mechanisms of formation of multiferroic type-II states.



Multiferroics combine spin and charge subsystems, allowing to change electrical polarization by applying a magnetic field and magnetization with an electric field.



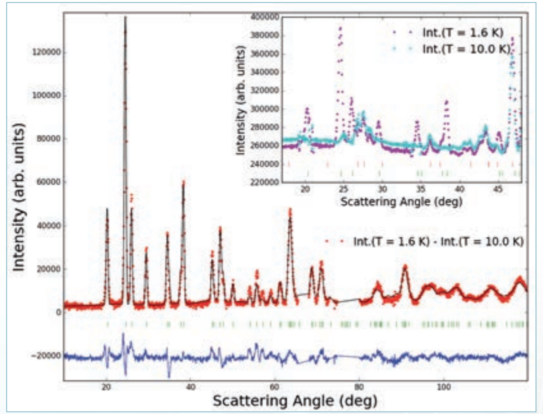
Mechanism of electronic polarization formation is spiral magnets.

Nationality: FR
University: Warwick, UK

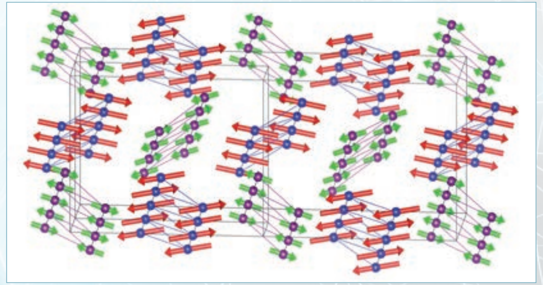
ILL offers me state-of-the-art techniques to investigate some of the most complex types of magnetic order.

Simon Riberolles

$SrLn_2O_4$materials host lanthanides (Ln^{3+}) magnetic ions in a triangular configuration placing their strong antiferromagnetic interactions in a competing environment. This phenomenon of **magnetic competition** is referred to as **frustration** and often results in the stabilisation of complex magnetic phases at temperatures approaching absolute zero. More generally, these systems are known to exhibit a variety of interesting physics and **novel properties** of great scientific interest. In my project I am using **neutron diffraction** to investigate the nature of magnetic order stabilised by the different members of the $SrLn_2O_4$crystalline family.



Magnetic neutron scattering pattern measured on a polycrystalline sample of $SrNd_2O_4$. The appearance of new peaks at low temperature (see inset) reveals the temperature stabilisation of a magnetic order in the system.



Magnetic structure of $SrNd_2O_4$ obtained from Rietveld analysis of the neutron diffraction pattern.

Nationality: RU
University: EPFL, CH

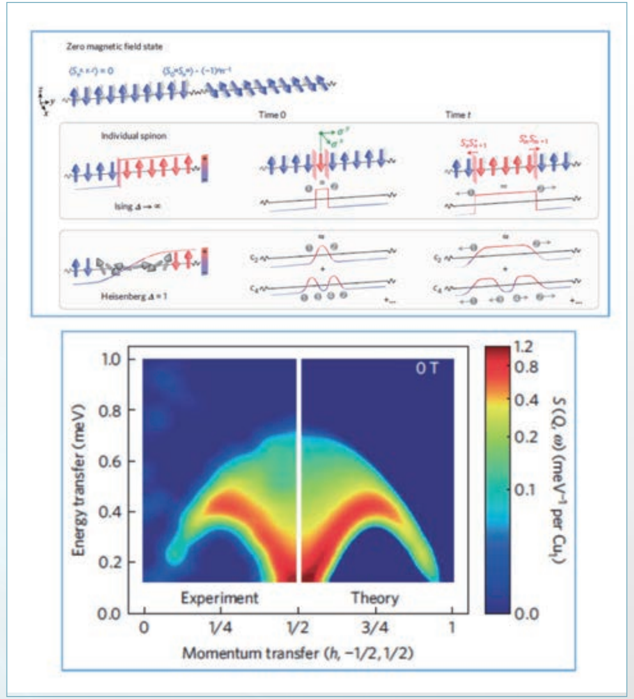
Neutrons are everywhere, but mainly in Grenoble.

Irina Safiulina

Quantum magnetism is one of the most active research areas in condensed matter physics. There is a significant interest in low-dimensional quantum spin systems.

The **quantum spin liquids** (QSL), in theory, represent a new state of matter. They occur in a variety of contexts ranging from the quantum Hall effect and high temperature superconductivity to confined ultracold gases and carbon nanotubes. Materials supporting QSL states may have applications in **data storage and memory**.
The nature of such magnetism can be studied by **inelastic neutron scattering**.

For more information see: M. Mourigal *et al.* Nature Physics 2013 **9(7)** 435.



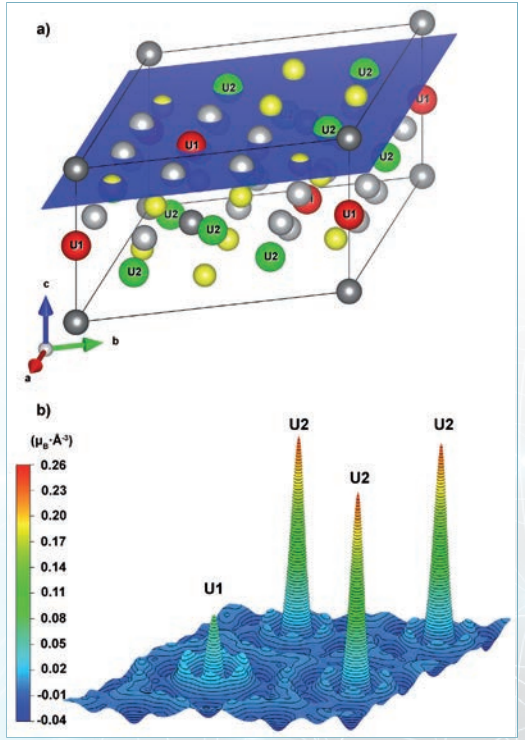
Schematic representation of the magnetic excitations in a spin-1/2 antiferromagnetic chain and (below) neutron scattering results for $CuSO_4{\cdot}5D_2O$.

Nationality: CZ
Charles University, CZ

Excellent science in a beautiful place.

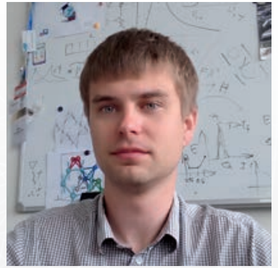
Michal Valiska

The search for entirely new compounds that exhibit unusual physical properties is one of the main goals of **fundamental research**. Uranium-based compounds, due to the special nature of the 5f-electrons, show variety of magnetic and superconducting states and phases that can even coexist together. Structural and dynamical properties of these unique systems can be very efficiently studied by **neutron diffraction and inelastic scattering methods** and add microscopic information to the **bulk measurements.** Confrontation of the experimental results with theoretical models drives progress in the field.



Two different densities of magnetic moments in $U_4Ru_7Ge_6$ – determined by neutrons.

WHEN MAGNETISM MEETS GEOMETRY



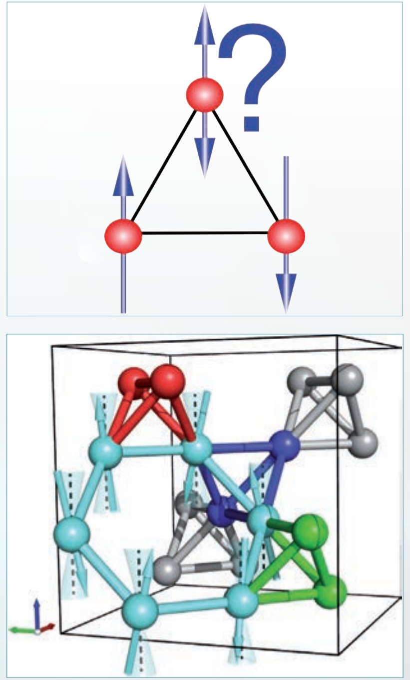
Nationality: PL
University: Basel, CH

Grenoble through a combination of world leading scientific institutions and surrounding mountains makes perfect place for exciting work and active leisure.

Rafal Wawrzynczak

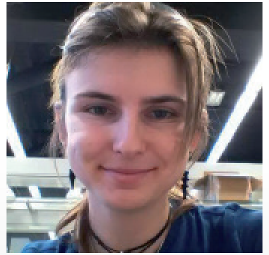
Thanks to deep insight into purely quantum phenomenon in **magnetism**, some subtle traits found applications in down-to-earth areas e.g. **computer memory**. Coexistence of specific atomic structures and magnetic interactions (e.g. triangular motifs with opposing polarizations) leads to appearance of **magnetic frustration**, resulting in numerous exotic features and opens new, exciting opportunities for application in **quantum computing** and **spintronics**. **Neutron scattering** techniques have always been employed in cutting-edge investigations of magnetic systems and our work aims at a full understanding of these fascinating effects with this well-suited toolbox.

For more information see: Wawrzynczak *et al.* Phys. Rev. Lett. 119 087201 (2017).



Top: Frustration in triangular arrangement of magnetic ions preferring mutually opposite polarisation of magnetic moments (pictured with arrows). Bottom: Precessive modes observed in a highly frustrated breathing, pyrochlore lattice.

MORPHOLOGY OF MAGNETIC NANOPARTICLES

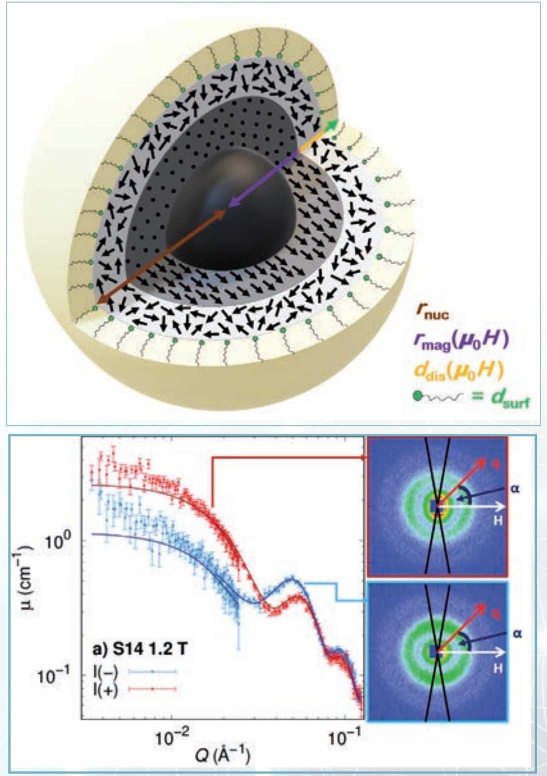


Nationality: SK
University: Köln, DE

The ILL is a great place to acquire unique scientific experience and it is surrounded by the scenic beauty of the Alps.

Dominika Zakutna

Magnetic nanoparticles hold great potential in **biomedicine applications** like cancer treatment by magnetic hyperthermia, magnetic resonance imaging, biosensing as well as magnetic drug targeting. The magnetic behaviour of the nanoparticles is defined by the intended use, demanding a full understand of the chemical structure and magnetic properties of the nanoparticles at the microscopic level. **Polarized Small-Angle Neutron Scattering** (SANS) is a versatile characterization tool, which allows us to study in detail the chemical morphology and structural properties, such as size and shape, and simultaneously gives us access to the spatially resolved magnetization distribution in magnetic nanoparticles.



Polarised SANS of spherical $CoFe_2O_4$ with 14 nm diameter at a magnetic field of 1.2 T. Lines indicate fits to the model depicted at the top. Right insets: 20° vertical sectors used for integrating the spin-dependent, two-dimensional (2D) scattering cross-sections I(+) and I(–).

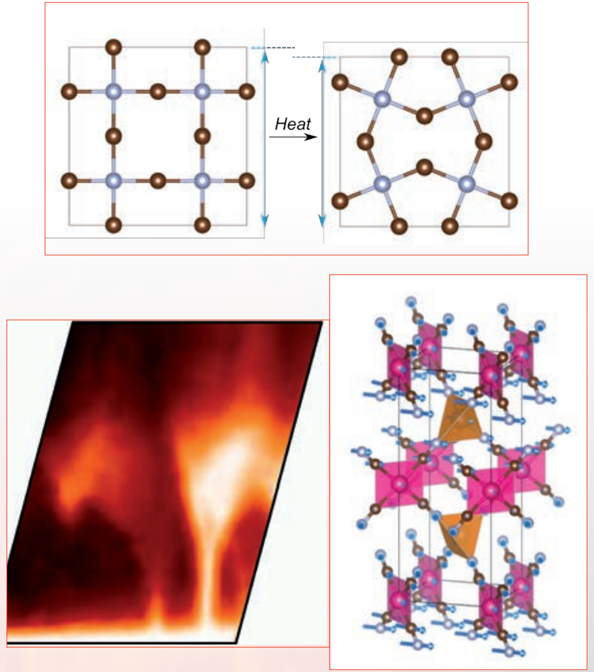
Nationality: UK
University of Reading, UK

Studying at the ILL in Grenoble is a unique opportunity to work with neutrons at an international scientific research facility whilst living in a beautiful landscape.

Stella d'Ambrumenil

Negative thermal expansion (NTE), whereby a compound shrinks when it is heated, has many potential uses in materials with a targeted thermal response or in composite materials with zero overall thermal expansion. The possibility of **tuning the effect** by changing the material's composition is of great interest.

To understand the phenomenon, knowledge of the compound's **structure** and dynamics is required. **Neutron scattering** provides the perfect tool with which to probe these at the atomistic level. Comparison of measurements with **atomistic simulations** validates a proposed model. Once the NTE mechanism is established, work towards its **control for a targeted practical use** can begin.



Top: Illustration of how atomic motions can result in structural contraction when an NTE material is heated up.
Bottom: Neutron scattering measurements (left) together with atomistic simulations, reveal the atomic motions (right) responsible for a compound's NTE.

MATERIALS SCIENCE

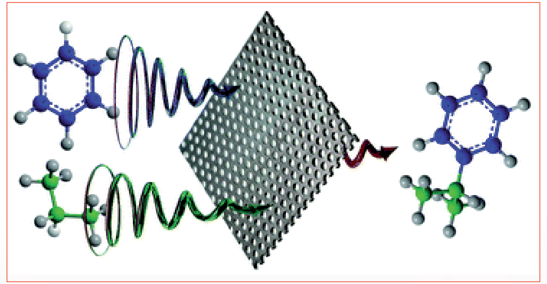
Nationality: UA
Universitat Politècnica de València, ES

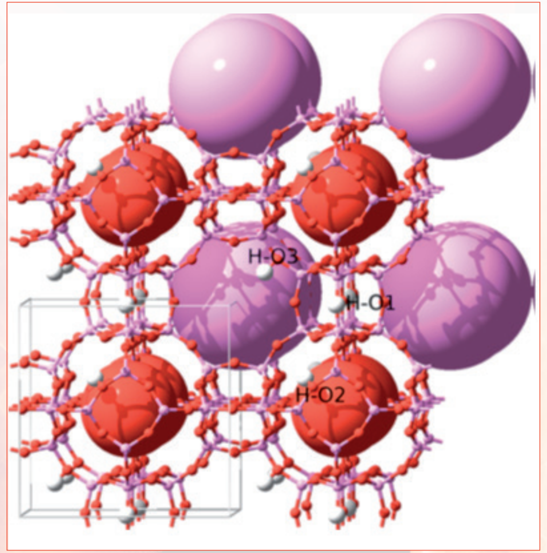
ILL gives access to advanced techniques that allow excellent results to be obtained.

Tetiana Lemishko

Zeolites are minerals, widely used as cheap solid acid catalysts in a number of important **industrial processes.** Catalytic properties of zeolites depend on their acidity and one of the main factors that influences this is the location of Brönsted acid sites. We have developed a new approach that combines **Inelastic Neutron Scattering, Computational Modeling and NMR** techniques in order to fully detemine the location of acid sites in two zeolites: LTA-40 with small number of acid sites and LTA-5 with high number of acid sites per unit cell.

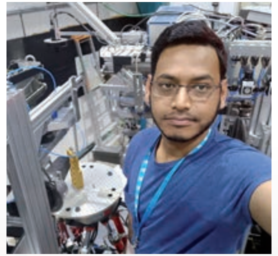
For more information see: Lemishko *et al.* J.Phys.Chem.C2016, 120, 24904 –24909 and J.Phys.Chem.C 2018, 122, 11450–11454.





LTA showing acid sites in different possible positions.

MATERIALS SCIENCE



Nationality: BD
Open University, UK

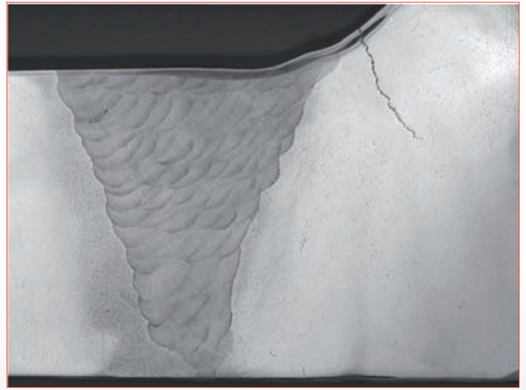
The ILL studentship has given me the opportunity to learn and develop skills through hands-on experience supported by the leading experts in my research field.

Mushfiqur Rahman

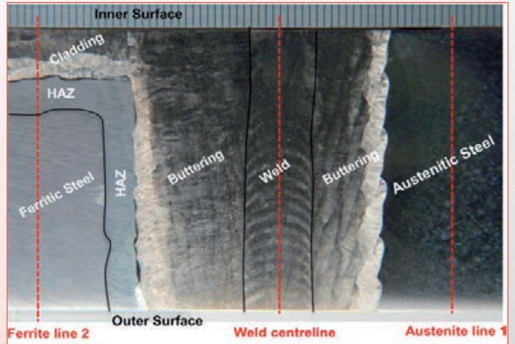
Residual stresses are locked-in stresses induced by the fabrication processes of engineering components such as welding used in **nuclear industry.** Accurate characterization of residual stresses is critical for assessing the **structural integrity** of components. **Neutron diffraction** is an ideal technique for characterizing residual stress **non-destructively** deep inside a real component. This is done by capturing the change in the separation of atomic planes due to stress.

The challenges faced by this technique in characterizing dissimilar metal welds, is addressed and will facilitate improved prediction of the lifetime of complex and **safety-critical** engineering structures.

For more information see: Kerr *et al.* Pressure Vessel Tech. 2013 **135** 1205.



Crack formed in a nuclear pressure vessel.



40 mm thick DMW manufactured by AREVA
Traore, Y. et al. (2014)

Complex dissimilar weld pipe used in a nuclear reactor.

Nationality: IT
University: EPFL, CH

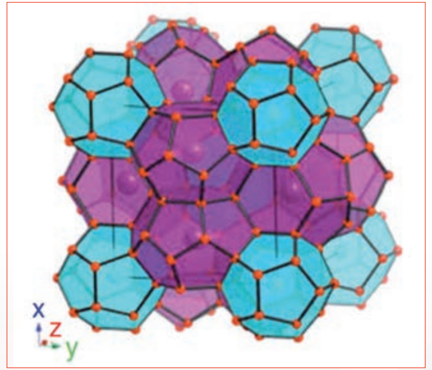
I like studying at ILL in Grenoble and collaborating with people of different nationalities and cultural backgrounds

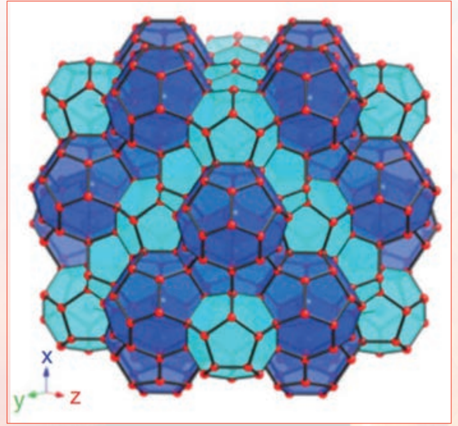
Umbertoluca Ranieri

Gas hydrates are ice-like solids, in which guest molecules are 'trapped' inside a crystalline host framework of water molecules that is typically made of polyhedral cages (see figures).

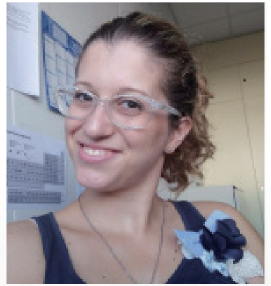
Occurring on the sea floor, they are a **potential energy source** as well as a source of **greenhouse gases** and they can form in e.g. oil drilling pipework. In these systems small guest molecules such as CH_4 or H_2 are able to perform many different **dynamical processes**: diffusive or quantized intra-cage jump motion, rotation, cage-to-cage hopping, and translational diffusion at the interface of domains. Investigating these processes is a very interesting topic from a fundamental point of view and highly relevant to the potential technological applications of gas hydrates. **Inelastic and quasi-elastic neutron scattering** are the ideal probes for our investigations.

For more information see: U. Ranieri *et al.* Nature Comm. 2017 **8** 1076.





Unit cell of two common gas (clathrate) hydrate structures.



Nationality: IT
Université de Bordeaux, FR

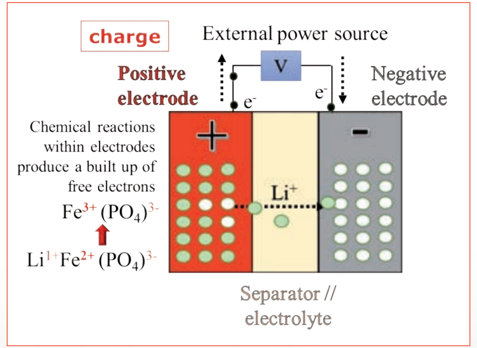
At ILL I found a stimulating and challenging work environment that gave me an invaluable opportunity for professional and personal growth. It also gave me the opportunity to meet scientists from all around the world.

Tatiana Renzi

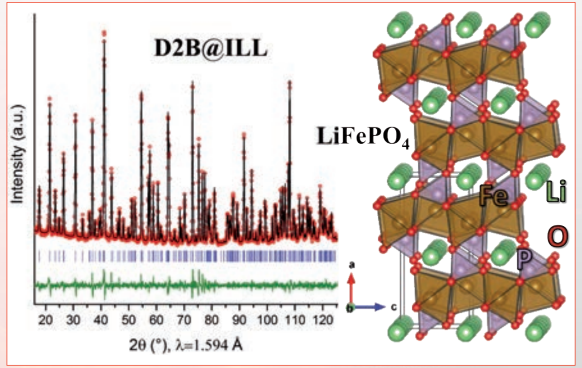
Li-ion batteries are the technology of choice for portable electronics. A Li-ion rechageable battery stores electrical energy in the form of chemical energy. During charging, Li+ ions flow from a positive electrode towards a negative one, through an electrolyte and a separator, while electrons pass through an external circuit. The process is reversed when a device is connected.

Neutron diffraction is an ideal technique to localise O and Li atoms and discriminate between transition metal elements. Developing electrochemical cells to perform **in-situ operando** experiments is fundamental to achieve a better understanding of mechanisms taking place inside electrode materials. Proposing **new battery solutions** (improved in cost, energy, safety and power capability), powering sustainable vehicles and integrating renewable energy in smart grid systems are the next challenges.

For more information see: M. Bianchini *et al.*, J. Electrochem. Soc., 2013, 160(11): A2176-A2183.



Schematic of a Li-ion secondary battery while charging.



On the left, neutron powder diffraction pattern (red points) of $LiFePO_4$ and fit of the data (black line). Data allow to refine the structure of $LiFePO_4$, shown on the right side.

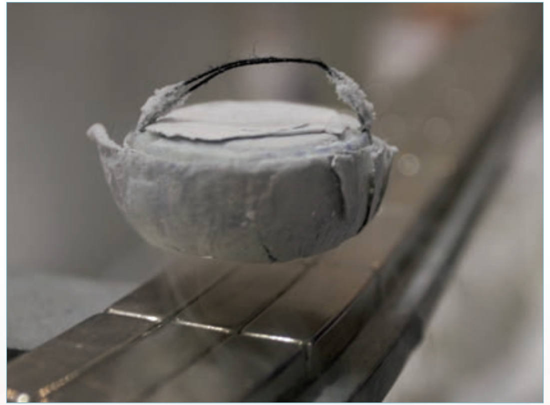
MATERIALS SCIENCE

Nationality: DK
University of Copenhagen, DK

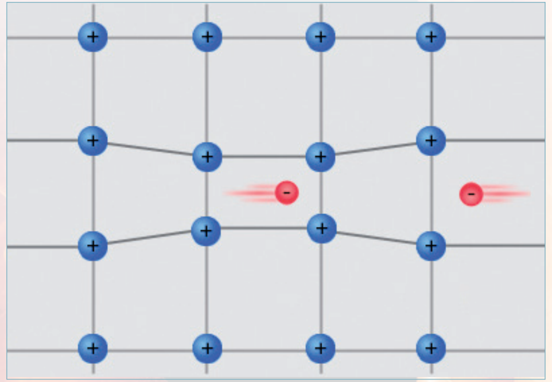
Studying at ILL is a unique experience where you get to interact with scientists and students from a variety of fields and nationalities.

Tim Tejsner

At the heart of condensed matter physics is a desire to understand the quantum-mechanical building blocks responsible for macroscopic material properties. A deeper understanding of these fundamental properties will eventually give us greater control when **designing new materials**.
One of the major unsolved mysteries in physics is the emergence of **unconventional superconductivity** from subtle atomic-scale changes to ceramic, insulating materials. We know that electrons in superconductors pair up in order to propagate through the material without resistance. **Inelastic Neutron Scattering** is the primary experimental technique used in the search for the “glue” that binds the electrons together.



A superconductor levitating above a magnet.



Cooper pair. The “glue” in conventional superconductors.

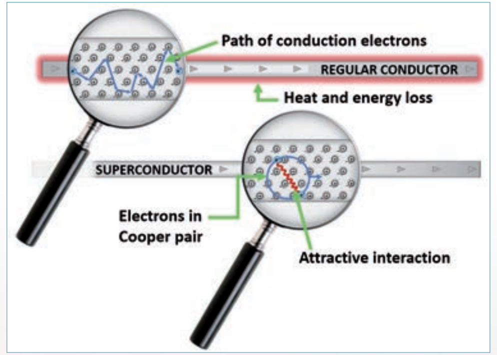
MATERIALS SCIENCE

Nationality: RO
University of Copenhagen, DK

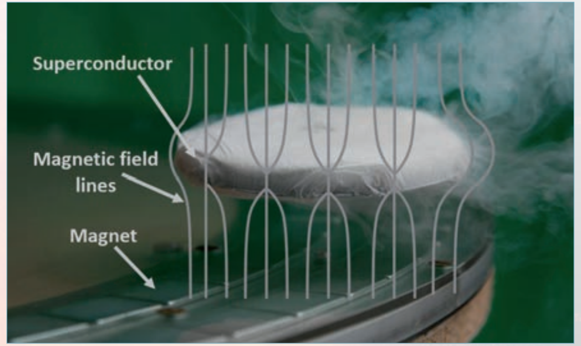
Studying at ILL means having access to a vast pool of expertise and instruments. This not only enriches the quality of the research but also adds an experimental component to ones education as user of large scale facilities.

Ana Tutueanu

Superconductors are extraordinary materials which are able to conduct electricity with zero resistance and expel magnetic fields. The phenomena are well understood in conventional superconductors where electrons move freely in pairs formed through their interaction with the crystal lattice. However, the origin of this attractive interaction in high-temperature superconductors remains one of the **major unsolved problems** in physics. There is ample evidence that the complex magnetism found in these materials is strongly connected to superconductivity. **Inelastic neutron scattering** is one of the few techniques that allows us to probe the magnetic structure in our quest to understand the role of magnetism in the emergence of superconductivity.



Cartoon of electrons carrying current along a regular and a super - conductor.



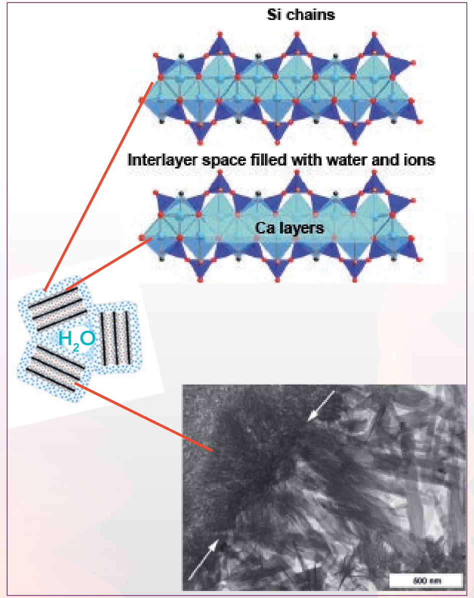
Quantum levitation of a superconductor above a magnet.

Nationality: KZ
Université Grenoble-Alpes, FR

I like working at ILL because of the opportunity to learn from and exchange ideas in a unique international scientific community.

Zhanar Zhakiyeva

Cement is the single **most manufactured material** globally, and the second individually **most consumed one after water,** with an average annual production of 3 tons per person. The cement industry is also one of the primary producers of CO_2. Water organization in a hydrated cement is important not only for the setting behaviour, but also for cement dissolution-recrystallization and carbonation processes. Understanding better these processes will improve the mechanical properties of cement and reduce its greenhouse gas impact. **Neutron Diffraction** and **Inelastic Incoherent Scattering** experiments, with **Isotopic Substitution**, are powerful tools which give key insight into the structure and dynamics of water in cement.



Atomistic (top), meso (middle) and micro structures (bottom) of the main hydrated phase in cement.

Nationality: IT
Imperial College London, UK

I like studying at ILL because of its international environment.

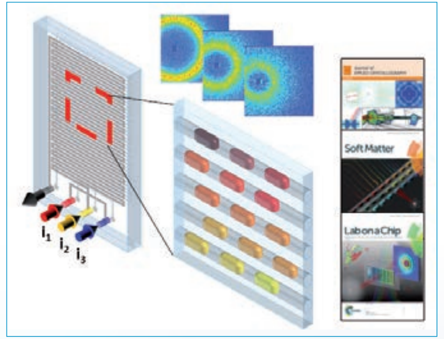
Marco Adamo

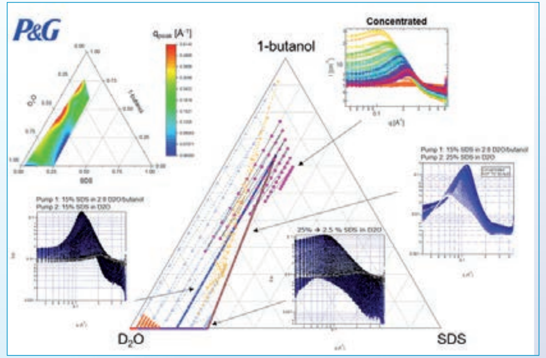
Complex fluids and formulations are generally multicomponent fluids, characterised by non-Newtonian rheology and complex phase behaviour and (meta)-stability.

Microfluidics provides an exceptionally well controlled environment for the handling of fluids, subjected to various flow types and magnitudes, as well as undergoing precise changes including mixing, dilution and flow or thermally induced transitions. Small Angle Neutron Scattering (SANS) is a unique experimental probe for matter at the molecular to mesoscopic lengthscales.

My project couples microfluidics with **SANS** to autonomously explore phase diagrams with adaptive resolution and evaluate their response to flow.

Adamo et *al.*, Lab on Chip, 2017, **9**, 1559-1569
Adamo et *al.*, Soft Matter, 2018, **14**, 1759-1770
Lopez et *al.* J. Appl. Cryst, 2018, **51**, 570-583.





Top: Microdroplet SANS setup. Bottom: Scanning of the ternary phase diagram SDS/1-butanol/D_2O.

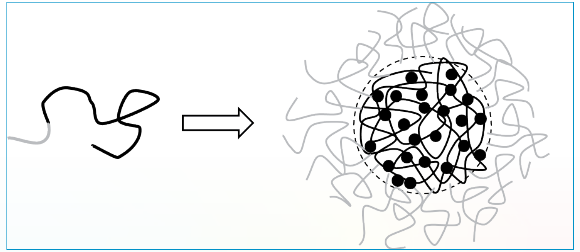
Nationality: DE
University: Paderborn, DE

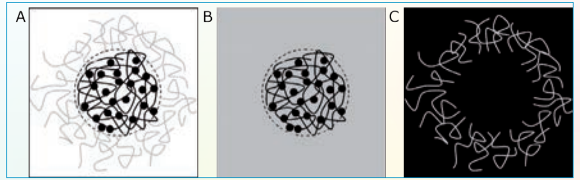
ILL is a unique facility: high neutron flux, excellent performance of the instruments, a variety of complementary techniques, a synchrotron next door and everything surrounded by mountains. For me it is the perfect place to do a PhD.

Nico Carl

Polyelectrolytes are polymers carrying charges along the chain. They are for example widely used for **waste-water treatment**, to prevent the built up of lime-scale, or as **rheology modifier in cement**. The basis of many of these applications is the interaction with oppositely charged species such as ions or surfactants.

I study the self-assembly of anionic polyelectrolytes and cations into structures such as micelles using **neutron small angle scattering**. In particular, **isotope labelling**, gives unique structural information that no other technique can provide. My work contributes to the fundamental understanding of interactions within this type of polymer and the development of new functional materials.





Top: Formation of a spherical micelle from a block copolymer. Bottom: Sketch of a contrast variation experiment: (A) Full contrast (B) core contrast (C) corona contrast.

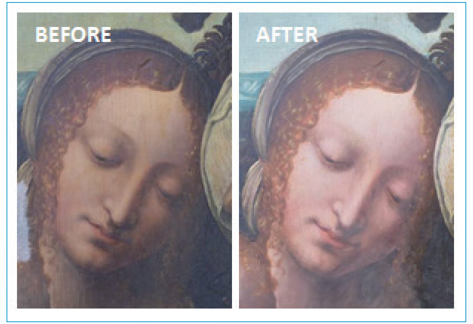
Nationality: FR
Université UGA Grenoble, FR

The ILL is synonym of passionate scientists, diversity of projects and multiculturalism.

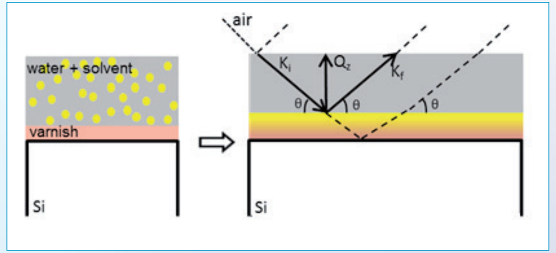
Amélie Castel

According to Cicero 'To know nothing of what happened before you, is to forever remain a child.' **Preserving Cultural Heritage** is therefore essential for our cultural, educational, aesthetic, inspirational and economic legacies. **Art works**, which are subject to natural or non-natural degradation of the constituent materials, must be **restored** and **preserved**.

In the case of easel paintings, removal of the old and yellowing varnish layers is one of the treatments which presents the highest risk of deterioration of the pictorial layer. Restorers use strong solvents, that can penetrate into the deeper layers and weaken the structure of the pictorial layer. In order to propose **new solutions** to this destructive treatment and eventually develop an automatic and well-controlled restoration process, I use **neutron reflectometry**, which is a non-destructive method to understand the nanoscopic structure of materials in situ. The composition of thin films at liquid interfaces can be determined with a resolution of a few Å.



Detail painting after (left) and before (right) removal the varnish layer.



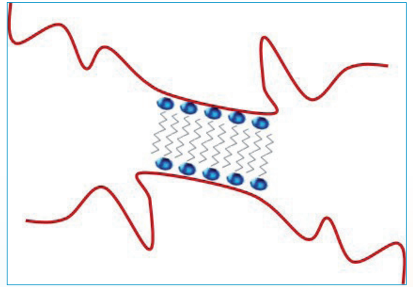
Neutron Reflectometry characterizes the varnish layers during the transfer of the solvent from water to the varnish layer.

Nationality: IT
University of Potsdam, DE

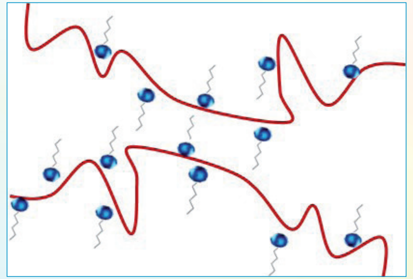
ILL, an international environment where you can improve your skills by being part of the scientific ecosystem. I really enjoy it!

Giuseppe Rosario Del Sorbo

Systems composed of oppositely charged **polyelectrolytes** (PEs) and **surfactants** show a rich and complex self-aggregation behaviour. The structures formed vary over a large size range and they have many applications, e.g., in **cosmetics, detergency, drug delivery.** The rheology of these mixtures depends strongly on the mixing ratio between the two components and on the polyelectrolyte and surfactant characteristics. Changing the length of the surfactant tail, can modify the interconnection between PE chains resulting in a different **viscosity behaviour**. Longer tails form more viscous systems (Fig.1). **Neutron small angle scattering** is ideal to understand the structure of PE-surfactant complexes and to explain their viscosity changes.



PE chains interconnected by long (C_{14}) rodlike surfactants --> viscous system.



PE chains interconnected by short (C_8) surfactant molecules --> low viscosity system.

3D STRUCTURE OF BURIED SOFT INTERFACES WITH OFF-SPECULAR REFLECTIVITY

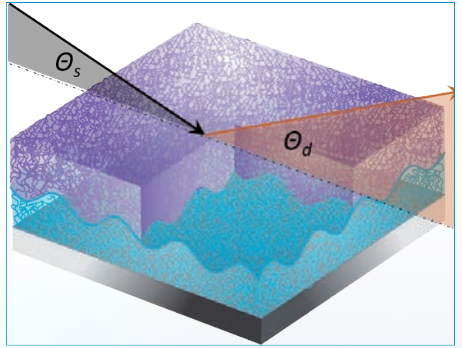
Nationality: SI
University ULB, Brussel, BE

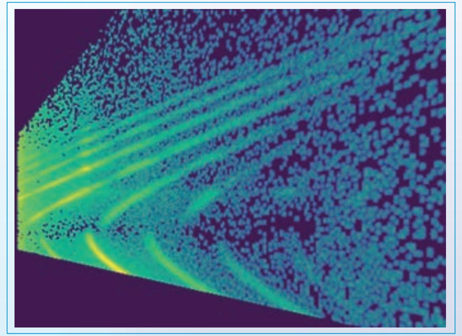
International environment and beautiful nature.

Aljosa Hafner

Thin **polymer films** are an ideal model system for the investigation of the effects of long-range van der Waals forces which is responsible for many phenomena found in soft matter. Their understanding is of significant fundamental importance and fundamental to the fields of **organic semiconductors (LEDs, sensors), lithography or coatings.**

Since most of the phenomena happen at a buried interface, they cannot be studied in-situ with real space techniques. Combined with isotopic labelling, **specular and off-specular neutron reflectometry** are ideal techniques for establishing the 3D morphology of such systems.





Top: off-specular reflectometry geometry.
Bottom: specular and off-specular reflection from a grating.

THE ORIGINS OF LIFE

Nationality: IT
Université Grenoble-Alpes, FR

I first came to Grenoble for a summer school after my undergraduate degree.
I then visited the ILL for my first experiment - I fell in love with it and kept coming back (Erasmus-Internships-PhD)! Working here I can use world class instruments, collaborate with expert scientists in my field and meet new people from all over the world.

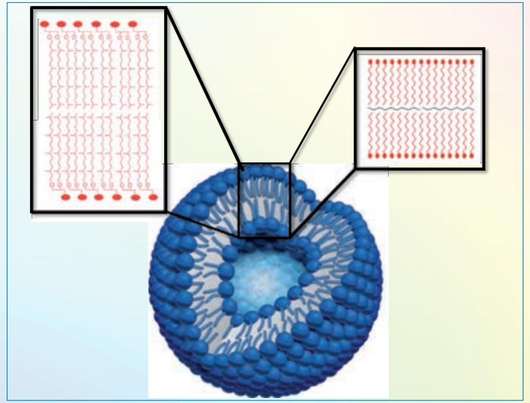
Loreto Misuraca

How did **life** form on our planet? Neutrons can help us solving some of the related, yet unsolved, issues. For instance, it is unknown how the first simple proto-cells could have survived in a very hostile young Earth with hot oceans and other extreme conditions.

A **new model membrane barrier,** similar to those of modern cells, could give a possible answer. The proto-membrane would have additional molecular components lying between the lipid layers as a protection against the external harsh environment.

Neutron diffraction is a unique tool to determine the structural model at the molecular level. **Inelastic neutron scattering** can then explore the dynamics of the proto-cells to determine whether they adapt and enable the cells to survive.

The extreme environment of deep undersea volcanoes.



Model membrane for a modern cell (left) and a protocell (right).

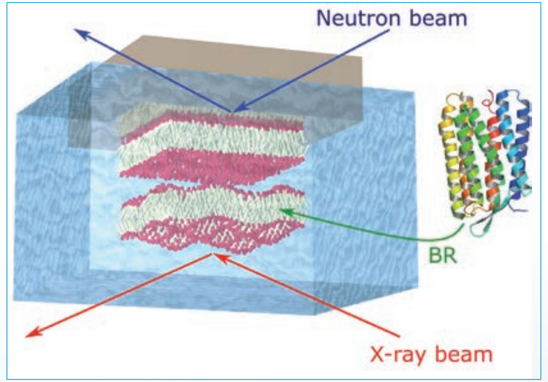
Nationality: UA
Université de Strasbourg, FR

ILL! it's not about place, it's about the extraordinary people, who are working here and putting all their efforts and skills into performing excellent science and making the ILL a world leading neutron facility. It's an honour to have the opportunity to work here.

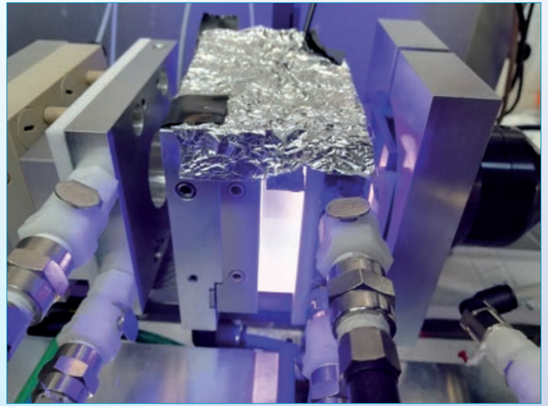
Tetiana Mukhina

Lipid bilayers have a very complex and diverse composition and play a pivotal role in a large number of cellular processes. Serving as a natural boundary in living cells, lipid bilayers maintain cell homeostasis and allow the transfer of substances, ions and energy in and out of cells.

Neutron reflectometry (NR) is a non-destructive technique which is ideal to reveal the structural features of thin biofilms in the Ångstrom to nanometre range. In my work, NR serves as an ideal probe to investigate the internal structure of biomembranes and the modifications induced by membrane – protein interactions. The figures show the case of the Bacteriorhodopsin, **light-harvesting, proton-pumping protein,** which I have studied.



Sketch of a floating lipid bilayer and structure of Bacteriorhodopsin protein.



The new setup for sample illumination on the D17 reflectometer.

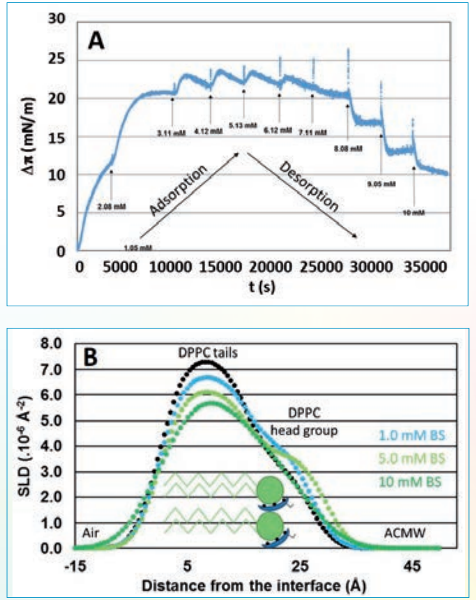
Nationality: FR
King's College London, UK

Neutron scattering is a technique that requires a very specific expertise, which I have acquired during my PhD thanks to ILL scientists.

Olivia Pabois

Bile salts (BS) are biosurfactants released into the small intestine, which play key roles in promoting lipid (fat) digestion and absorption. Understanding the mechanisms governing BS functionality during lipolysis will thus help develop **therapeutic strategies** aiming to control fat uptake and go some way to addressing the severe health problems associated with **obesity**.

Neutron reflectometry and **small-angle neutron scattering** are powerful techniques that can, respectively, provide a detailed molecular picture of the BS/ lipids interface and resolve what is happening in the bulk, thus mimicking lipid digestion.



Effect of successive BS injections below a lipid monolayer on A. the adsorption/desorption behaviour of BS at the air/water interface (Langmuir trough), B. the interfacial lipid film structure (neutron reflectometry).

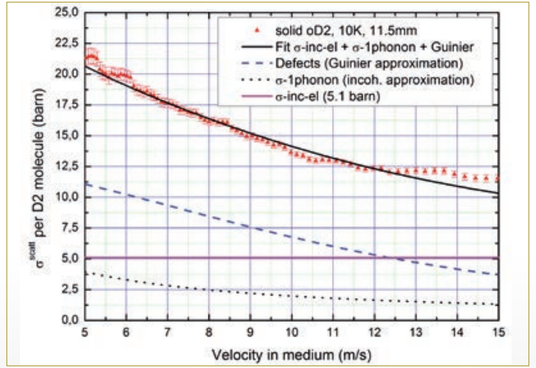
Nationality: DE
TU Munich, DE
UGA Grenoble, FR

I really enjoy the fruitful discussions with international researchers and the interdisciplinary atmosphere at ILL. Skiing and hiking in the mountains around Grenoble provides a great counterbalance to the work of the mind.

Stefan Doegé

Ultracold neutrons (UCNs) are used for a variety of fundamental physics experiments, such as the determination of the free **neutron lifetime** and the search for the **electric dipole moment** of the neutron. UCN sources based **on solid deuterium** have not yet been able to deliver significantly higher UCN densities than older designs. My PhD work helps understand how UCNs interact with deuterium crystals, liquid deuterium, rough metal surfaces and neutron guides. This knowledge is pivotal to the **advancement of UCN sources** and has the potential to significantly improve the statistics of fundamental physics experiments.

Stefan Döge (Doege) and Jürgen Hingerl, Rev. Sci. Instrum. 89, 033 903 (2018).
Stefan Döge (Doege) *et al.*, Phys. Rev. B 91, 214309 (2015).



Fit to the data with 1-phonon cross section and Guinier two-phase model. The radius of defects R = 88 Å and the concentration of defects c = 8.2 × 10E−11 can be extracted from the fit.

Transparent sample cell for UCN transmission experiments developed as part of my PhD work.

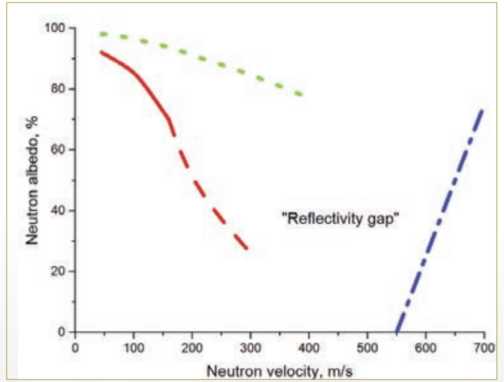
Nationality: RU
University of Moscow, RU

The most unique people I know all over the world study and work at ILL.

Aleksander Nezvanov

Diamond nanopowders providing a huge albedo for the reflection of slow neutrons (E<3meV), bridging the so-called **reflectivity gap** in the neutron spectrum. We have created a model of neutron interactions with nanopowders and implemented it in a **software package** that helps us to optimize the properties of a new generation of nanostructured reflector. Our software also describes and predicts experimental measurements of neutron reflection, direction, storage, and transportation using nanopowders.

For more information see: Nesvizhevsky *et al.* Phys. Rev. A 2018 **97** 023629.



Top - Graph of neutron reflectivity from reflectors of different types. Bottom - Example of a reflector with a nanostructured surface.

Nationality: ES
Universidad Complutense de Madrid, ES

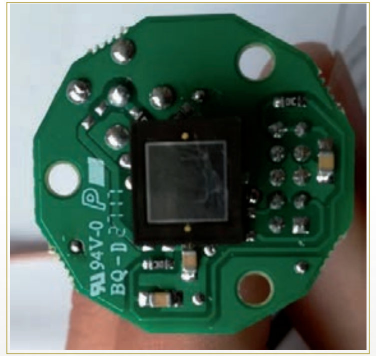
Studying at ILL is a great opportunity to work with all kinds of scientists in one of the top research facilities in the world.

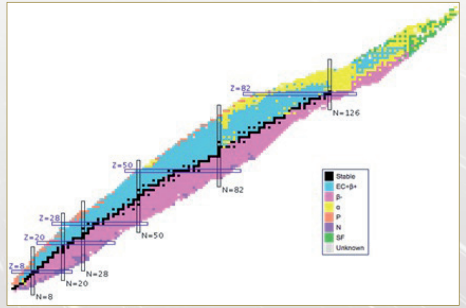
Javier Rodriguez-Murias

Nuclear Shell evolution far from the β stability line is one of the great challenges of the past two decades, especially for very **neutron-rich** nuclei close to a magic number. Life-time study is key to **nuclear spectroscopy** and fast scintillators give the chance of measuring them.

The presence of magnetic fields suggests that coupling SiPM sensors to scintillators will be a great alternative to PMT.

For more information see: L. M. Fraile, J. Phys. G: Nucl. Part. Phys. 44 (2017) 094004(24pp).





SiPM (up) and nuclide chart (bottom).

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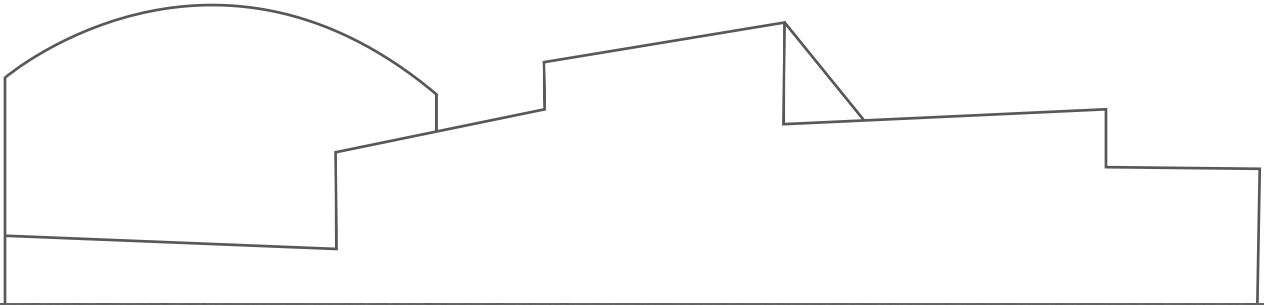

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