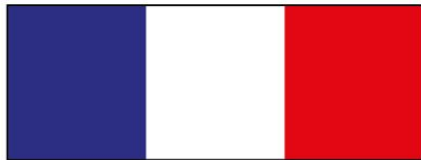


# LLB / MLZ Workshop 2024 in Herrsching



## Report of Contributions

Contribution ID: 26

Type: **Invited Talk**

# New Perspectives for Neutron Imaging and Diffraction through Advanced Event-Mode Data Acquisition

*Monday, May 27, 2024 9:25 AM (25 minutes)*

Recently developed event-driven detectors are capable of registering spots of light induced by neutron interactions in scintillators. Reconstructing the center-of-mass of the individual interactions, it is possible to significantly enhance the spatiotemporal resolution of recorded radiographs. Utilizing this principle, we present a novel detector concept capable of Time-of-Flight imaging with adjustable field-of-view including n/g discrimination via analysis of the event shape in space and time.

**Primary author:** LOSKO, Adrian (Technische Universität München, Forschungs-Neutronenquelle MLZ (FRMII))

**Co-authors:** WOLFERTZ, Alexander (TUM FRM2); SCHULZ, Michael

**Presenter:** LOSKO, Adrian (Technische Universität München, Forschungs-Neutronenquelle MLZ (FRMII))

**Session Classification:** Presentations

Contribution ID: 27

Type: **Invited Talk**

# Neutron Imaging of Ammonia Carriers for Energy Storage

*Monday, May 27, 2024 9:50 AM (25 minutes)*

Ammonia is among the largest produced chemicals in the world and finds significant application as a fertilizer. It is also seen as an alternative for high density hydrogen storage. Chemicals that absorb ammonia are seen as promising options for energy storage.

In this talk manganese chloride–silica gel composite and additively manufactured Strontium chloride–Na Bentonite ammonia sorbent materials studied using in situ neutron radiography and neutron CT will be discussed.

**Primary authors:** KUMAR, Richi; KARABANOVA, Anastasiia (Technical University of Denmark); AKHTAR, Farid (LTU)

**Presenter:** KUMAR, Richi

**Session Classification:** Presentations

Contribution ID: 28

Type: **Invited Talk**

## **Robotics –Application for Stress Analysis using Neutron Diffraction**

*Monday, May 27, 2024 4:55 PM (25 minutes)*

The original robot setup at the neutron diffractometer STRESS-SPEC has been upgraded to a high accuracy positioning/metrology system. I will give a short introduction on the complete measurement process chain for the new robot environment. To achieve a spatial accuracy of 50  $\mu\text{m}$  or better during measurement of the strain tensor, the sample position is tracked by a camera system and actively corrected. A brief overview of additional sample environment for the robot will also be given.

**Primary author:** HOFMANN, Michael

**Co-authors:** WANG, Lijiu; Mr LANDESBERGER, Martin (TUM); KEDILIOGLU, Oguz (Friedrich-Alexander Universität Erlangen); Dr GAN, Weimin (Helmholtz-Zentrum Hereon)

**Presenter:** HOFMANN, Michael

**Session Classification:** Presentations

Contribution ID: 29

Type: **Invited Talk**

## **KWS-X: A Powerfull SAXS/WAXS Beamline at MLZ**

*Monday, May 27, 2024 2:25 PM (25 minutes)*

The customized SAXS/WAXS instrument commenced user operation in April 2023. As a young member of our small-angle scattering instrument family, which utilizes X-rays as the primary beam, the new instrument is equipped with a high-flux Metal-Jet source and a movable Eiger 2R 4M SAXS detector. Additionally, it features a 4-axis motorized WAXS detector and a Bonse-Hart USAXS, enabling a wide range of scattering vector  $q$ , covering values from  $0.0002$  to  $7 \text{ \AA}^{-1}$ .

**Primary author:** Dr WU, Baohu (JCNS-MLZ, FZ Juelich)

**Presenter:** Dr WU, Baohu (JCNS-MLZ, FZ Juelich)

**Session Classification:** Presentations

Contribution ID: 30

Type: **Invited Talk**

## Sustainable Food Colloids

*Tuesday, May 28, 2024 9:10 AM (25 minutes)*

Food colloids are part of everyone's life: milk, yogurt or cheese. Socio-economical trends demand for more sustainable, plant-based food formulations, but represent a scientific challenge. Colloidal systems have been studied, but not fully understood. Xray and neutron scattering techniques deliver the nanoscale mechanisms. We commenced with traditional food colloids stabilized by beta lactoglobulin and phospholipids studied by SANS and NSE. These findings are linked to the viscoelastic behavior.

**Primary authors:** FRIELINGHAUS, Henrich (JCNS); HEIDEN-HECHT, Theresia (JCNS-4); HOLDERER, Olaf (Forschungszentrum Jülich GmbH, JCNS at MLZ)

**Presenter:** FRIELINGHAUS, Henrich (JCNS)

**Session Classification:** Presentations

Contribution ID: 31

Type: **Invited Talk**

## Perspectives on Fractal dimensions: Rheology and Neutron scattering studies on Dairy gels

*Tuesday, May 28, 2024 9:35 AM (25 minutes)*

The Fractal dimension ( $D_f$ ) is a key structural parameter of the networks formed by several food systems. In the present work, dairy gels from skim milk at different concentrations are formed via two different mechanisms: acidification, and enzymic (rennet)-induction. Oscillatory rheology, and ultra-small-angle neutron scattering (USANS) studies are performed to characterize their structural evolution. The perspectives on  $D_f$  thus obtained will be discussed to understand the inherent physics.

**Primary author:** KODUVAYUR ANANTHANARAYANAN, Ramya (GNeuS research fellow, TUM Garching)

**Co-authors:** GARVEY, Christopher J. (MLZ); Dr BOUÉ, François (Laboratoire Léon Brillouin, CEA Saclay, Gif-sur-Yvette Cedex, France); Dr DE CAMPO, Liliana (Australian Centre for Neutron Scattering, Australia Nuclear Science and Technology Organisation, Lucas Heights, Australia); Dr STROBL, Markos (Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Villigen, Switzerland.)

**Presenter:** KODUVAYUR ANANTHANARAYANAN, Ramya (GNeuS research fellow, TUM Garching)

**Session Classification:** Presentations

Contribution ID: 32

Type: **Invited Talk**

## **POWTEX –Angular- and Wavelength Dispersive High-Intensity Neutron TOF Diffractometer**

POWTEX, a future TOF neutron powder diffractometer @MLZ is funded by BMBF (05K22PA2) and built by RWTH Aachen and Forschungszentrum Jülich. The innovative design resulted in advance components, i.e. the 10B jalousie volume detector with large coverage. POWTEX is designed for short measurement times, allowing in situ chemical experiments and texture analysis with reduced sample rotations. Developed multidimensional algorithms allowed first refinement of angular- and wavelength-dispersive data.

**Primary author:** Dr HOUBEN, Andreas (RWTH Aachen University, Institute of Inorganic Chemistry)

**Co-authors:** MEINERZHAGEN, Yannick; Mr NACHTIGALL, Noah (RWTH Aachen University, Institute of Inorganic Chemistry); SCHWEIKA, Werner (European Spallation Source, Forschungszentrum Jülich); DRONSKOWSKI, Richard (RWTH Aachen University)

**Presenter:** Dr HOUBEN, Andreas (RWTH Aachen University, Institute of Inorganic Chemistry)

**Session Classification:** Presentations



Contribution ID: 33

Type: **Invited Talk**

## High-efficiency diffractometer ERWIN

*Monday, May 27, 2024 5:20 PM (20 minutes)*

The instrument ERWIN, currently being assembled at MLZ, is a high-efficiency powder diffractometer designed for rapid data collection, time-resolved measurements, parametric studies and investigations on small samples. This contribution will provide an overview on applications, specifications and the current status of the instrument.

**Primary author:** HOELZEL, Markus

**Presenter:** HOELZEL, Markus

**Session Classification:** Presentations

Contribution ID: 34

Type: **Invited Talk**

## Capabilities, applications and status update of ODIN, the imaging instrument at ESS

*Tuesday, May 28, 2024 11:20 AM (20 minutes)*

ODIN is ESS state-of-the-art multipurpose Neutron Imaging Instrument, designed and being built by TUM and PSI. Using wavelength-resolved imaging with tuneable medium to high wavelength resolution, will provide significantly increased chemical and structural sensitivity compared to other neutron imaging instruments, with fixed (or absent) wavelength resolutions. We present some of the design highlights, instrument capabilities, possible applications and the present status of the installation.

**Primary author:** TARTAGLIONE, Aureliano (Technische Universität München, MLZ (FRM2))

**Co-authors:** Mr GONCALVES GERK, Alexandre (ESS); Mr CALZADA, Elbio (TUM - FRM II); Mr HOVIND, Jan (PSI); MORGANO, Manuel (ESS); STROBL, Markus (PSI); SCHULZ, Michael; Mrs MARTINEZ, Virginia (TUM FRM II)

**Presenter:** TARTAGLIONE, Aureliano (Technische Universität München, MLZ (FRM2))

**Session Classification:** Presentations

Contribution ID: 35

Type: **Invited Talk**

## Temperature dependent crystal structure of Ethylene Carbonate

*Monday, May 27, 2024 4:05 PM (25 minutes)*

Neutron and synchrotron radiation diffraction studies are often conducted to investigate the structure of batteries and their components. While most of the research in this field has focused on the electrode materials, there have been fewer studies on the electrolytes that mediate charge transfer. This work presents a systematic approach to determining the structure of ethylene carbonate, which is a solvent commonly used in the liquid electrolytes of state-of-the-art Li-ion batteries.

**Primary author:** WESTPHAL, Lea (TUM/MLZ)

**Co-authors:** SENYSHYN, Anatoliy; PORCHER, Florence (LLB, CEA/Saclay (France)); AVDEEV, Max (Australian Nuclear Science and Technology Organisation); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Dr BARAN, Volodymyr (DESY, FS-PE-TRA-D, P02.1)

**Presenter:** WESTPHAL, Lea (TUM/MLZ)

**Session Classification:** Presentations

Contribution ID: 36

Type: **Invited Talk**

## Hydrogen mobility in an amide-based hydrogen storage system

*Monday, May 27, 2024 11:30 AM (25 minutes)*

The hydrogen storage performance of a reactive hydride composite,  $\text{Mg}(\text{NH}_2)_2 + 2\text{LiH}$ , can be significantly improved by the addition of  $\text{Li}(\text{BH}_4)$  and the subsequent formation of an amide-borohydride compound  $\text{Li}_4(\text{BH}_4)(\text{NH}_2)_3$  during hydrogen release. This improvement has been attributed to the enhanced hydrogen mobility in the latter compound, due to which the reaction becomes diffusion-controlled. We studied the hydrogen mobility in this system by neutron scattering.

**Primary author:** BUSCH, Sebastian (GEMS at MLZ, Helmholtz-Zentrum Hereon, Germany)

**Co-authors:** ASLAN, Neslihan (HZG, GEMS at MLZ); MAJUMDAR, Arnab (Helmholtz Zentrum hereon); THASE, Anastasiia (GEMS at MLZ, Helmholtz-Zentrum Hereon); GIZER, Gökhan (Helmholtz-Zentrum Hereon); PISTIDDA, Claudio (Helmholtz-Zentrum Hereon); DORNHEIM, Martin (University of Nottingham); LOHSTROH, Wiebke; Prof. MÜLLER, Martin (Helmholtz-Zentrum hereon GmbH)

**Presenter:** BUSCH, Sebastian (GEMS at MLZ, Helmholtz-Zentrum Hereon, Germany)

**Session Classification:** Presentations

Contribution ID: 37

Type: **Invited Talk**

## **SAPHiR: Neutron diffraction and radiography under extreme pressure and temperature conditions**

*Monday, May 27, 2024 10:15 AM (20 minutes)*

The new instrument SAPHiR is dedicated to time-of-flight neutron diffraction and radiography of powder samples, fluids, and melts at pressures up to 15 GPa and temperatures between 86–2300 K. Future applications include in-situ crystallography and phase relations of light-element-bearing phases, equations of state, reaction kinetics, and radiography for the Earth and materials sciences. Currently, SAPHiR is used offline for conducting deformation experiments to investigate planetary formation.

**Primary author:** WALTE, Nicolas

**Co-author:** KEPPLER, Hans

**Presenter:** WALTE, Nicolas

**Session Classification:** Presentations

Contribution ID: 38

Type: **Invited Talk**

## **SAM (Small-Angle Modular) the new Small-Angle instrument at the Institut Laue Langevin**

*Monday, May 27, 2024 3:15 PM (20 minutes)*

SAM, a medium size small-angle neutron scattering (SANS) instrument developed by the Laboratoire Léon Brillouin and the Institut Laue Langevin (ILL), is part of the ILL “Endurance II” rejuvenation programme. This SANS instrument with a polarised beam option will be also equipped with a “MIEZE” option, for high-resolution spectroscopy with sub- $\mu\text{eV}$  resolution. Following current friendly user experiments, the beam time will be divided equally between ILL and French community user programmes.

**Primary author:** Dr BRULET, Annie (Laboratoire Léon Brillouin)

**Presenter:** Dr BRULET, Annie (Laboratoire Léon Brillouin)

**Session Classification:** Presentations

Contribution ID: 39

Type: **Invited Talk**

## CSPEC - the cold chopper spectrometer for the ESS

*Tuesday, May 28, 2024 12:00 PM (20 minutes)*

The cold chopper spectrometer CSPEC at the ESS is a joint project from the Technische Universität München (TUM), Germany, and the Laboratoire Léon Brillouin (LLB), Saclay, France. CSPEC will benefit from the high brilliance of the ESS spallation in addition to the cumulative flux provided by repetition rate multiplication (RRM) that results in large flux gains. CSPEC is in the construction phase and the current status and expected performance will be presented.

**Primary author:** LOHSTROH, Wiebke

**Co-authors:** NOFERINI, Daria; MOREIRA, Fernando (ESS); DEEN, Pascale (ESS); LONGEVILLE, Stephane (LLB)

**Presenter:** LOHSTROH, Wiebke

**Session Classification:** Presentations

Contribution ID: 40

Type: **Invited Talk**

## Tracking the solution structures of membrane proteins by scattering and modeling

*Monday, May 27, 2024 2:00 PM (25 minutes)*

SAXS and SANS combined with modeling have proved to be essential techniques in structural biology when the classical high-resolution methods are not appropriate. The “contrast matching” method in SANS is particularly suitable to specifically probe membrane proteins by contrast-matching their amphiphilic environment. I will illustrate this feature with TSPO translocator protein, a ubiquitous and functionally important membrane protein used as a pharmacological marker in neuroimaging.

**Primary author:** COMBET, Sophie (LLB)

**Co-authors:** Dr KOUTSIOUMPAS, Alexandros; SAADE, Christelle; EXIL, Gaston; WIMALAN, Krushika

**Presenter:** COMBET, Sophie (LLB)

**Session Classification:** Presentations



Contribution ID: 41

Type: **Invited Talk**

## The HBS neutron source project and the associated instrumentation

*Tuesday, May 28, 2024 10:25 AM (25 minutes)*

The HBS („High Brilliance neutron Source”) is an ambitious HiCANS project being developed by the Jülich Centre for Neutron Science (JCNS). The technical design report [1] for the facility has been published in 2023 featuring the accelerator (protons, 70 MeV, 100 mA), three individual target-moderator-reflector stations and the associated instrumentation, which will allow scientific applications on the level of today’s well-established research reactor neutron sources.

In addition to ...

**Primary authors:** LIEUTENANT, Klaus (FZJ); RÜCKER, Ulrich (JCNS, Forschungszentrum Jülich)

**Presenters:** LIEUTENANT, Klaus (FZJ); RÜCKER, Ulrich (JCNS, Forschungszentrum Jülich)

**Session Classification:** Presentations

Contribution ID: 42

Type: **Invited Talk**

## The ICONE project: towards a new French neutron scattering facility.

*Tuesday, May 28, 2024 10:00 AM (25 minutes)*

The Laboratoire Léon Brillouin 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).

The long-term goal is to eventually build a new user facility, ICONE, which would offer a suite of 10 neutron scattering instruments to the French community. We aim at achieving performances comparable to the instruments which were operated around the Orphée reactor.

**Primary authors:** OTT, Frédéric (Laboratoire Léon Brillouin CEA/CNRS, Univ. Paris Saclay); Dr FABRÈGES, Xavier (Laboratoire Léon Brillouin CEA-CNRS)

**Presenter:** OTT, Frédéric (Laboratoire Léon Brillouin CEA/CNRS, Univ. Paris Saclay)

**Session Classification:** Presentations

Contribution ID: 43

Type: **Invited Talk**

## **MLZ Introduction**

*Monday, May 27, 2024 9:00 AM (5 minutes)*

**Presenter:** PFLEIDERER, Christian (TUM FRM II)

**Session Classification:** Presentations

Contribution ID: 44

Type: **not specified**

## **LLB Introduction**

*Monday, May 27, 2024 9:05 AM (5 minutes)*

**Presenter:** DESMEDT, Arnaud (CNRS - ISM Univ. Bordeaux)

**Session Classification:** Presentations

Contribution ID: 45

Type: **not specified**

## **Presentation of the IRP: past, present, future**

*Monday, May 27, 2024 9:10 AM (15 minutes)*

**Presenter:** CHABOUSSANT, Grégory (LLB (CNRS-CEA))

**Session Classification:** Presentations

Contribution ID: 46

Type: **not specified**

## Final Discussion & Conclusive Remarks

*Tuesday, May 28, 2024 12:20 PM (20 minutes)*

**Presenters:** DESMEDT, Arnaud (CNRS - ISM Univ. Bordeaux); PFLEIDERER, Christian (TUM FRM II)

Contribution ID: 47

Type: **Invited Talk**

## **Presentation of 2FDN**

*Monday, May 27, 2024 5:40 PM (15 minutes)*

**Presenter:** PLAZANET, Marie (LIPhy)

**Session Classification:** Presentations

Contribution ID: 48

Type: **Invited Talk**

## **DREAM: The future neutron diffractometer for crystallography at the ESS**

*Tuesday, May 28, 2024 11:40 AM (20 minutes)*

The European neutron source (ESS) in Lund in Sweden should see its first neutrons in 2025 and welcome its first users in early 2027. One of the first operational instruments will be DREAM, a diffractometer developed and built for ESS by the consortium (Forschungszentrum Jülich (Germany) / Laboratoire Léon Brillouin (France)).

I will present the DREAM project and its current status.

**Primary author:** PORCHER, Florence (ESS, Lund (sweden) & LLB, CEA/Saclay (France))

**Co-author:** FEYGENSON, Mikhail (European Spallation Source ERIC)

**Presenter:** PORCHER, Florence (ESS, Lund (sweden) & LLB, CEA/Saclay (France))

**Session Classification:** Presentations



Contribution ID: 49

Type: **Invited Talk**

## **Ionic liquids in bulk and under 1D CNT nanometric confinement. A multiscale study.**

*Monday, May 27, 2024 11:05 AM (25 minutes)*

We address the physics of Ionic Liquids charged with lithium salts under confinement in a carbon nanotube (CNT) based membrane. In bulk, we combine QENS, PFG-NMR and rheology to highlight a one order of magnitude difference of the transport quantities, depending whether they are inferred at the molecular or at the micrometric scale. We probe the same IL confined in the CNT membranes. Compared to the bulk situation, we show a conductivity gain as high as one order of magnitude. A patent is filed.

**Primary author:** ZANOTTI, Jean-Marc (Laboratoire Léon Brillouin CEA-CNRS)

**Presenter:** ZANOTTI, Jean-Marc (Laboratoire Léon Brillouin CEA-CNRS)

**Session Classification:** Presentations

Contribution ID: 50

Type: **Invited Talk**

## From IN6 to SHARP then SHARPER

*Monday, May 27, 2024 11:55 AM (20 minutes)*

Starting in 2017, IN6 has been operated by a LLB as a CRG and the design of a brand new IN6 secondary spectrometer. This was the SHARP (Spectromètre Hybride Alpe Région Parisienne) project. On March 2021, the first neutrons have enlightened the brand-new instrument. From 2021 to 2024, the primary spectrometer has been fully redesigned and built and the instrument is now SHARPER (SHARP Etendu en Résolution). We introduce this new spectrometer to come online in June 2024.

**Primary author:** ZANOTTI, Jean-Marc (Laboratoire Léon Brillouin CEA-CNRS)

**Presenter:** ZANOTTI, Jean-Marc (Laboratoire Léon Brillouin CEA-CNRS)

**Session Classification:** Presentations

Contribution ID: 51

Type: **Invited Talk**

## Canola protein digestion studied by SAS and Neutron Imaging

*Tuesday, May 28, 2024 8:45 AM (25 minutes)*

Proteins, as elements of the ingested food, can form structures at multiple spatial scales. We studied digestion of canola protein heat-set gels and monitored their structure by SANS (LLB), SAXS (Synchrotron Soleil) and Neutron Imaging (PSI). SANS coupled with Neutron imaging provided information about digested “real-like” foods on nm (local protein re-arrangements) and  $\mu\text{m}$  scale (large aggregates destruction), while in-situ capillary SAXS complemented SANS, showing complexity of protein digestion

**Primary author:** Ms NAPIERAJ, Maja (CNRS)

**Co-authors:** BRULET, Annie (Laboratoire Léon Brillouin UMR12 CEA CNRS); GARVEY, Christopher (FRM II, Technical University Munich); LUTTON, Evelyne (MIA, INRAE-AgroParisTEch-UPsay, Paris); Prof. BOUÉ, François (LLB-CNRS-CEA\_UPSaclay France); PEREZ, Javier (Synchrotron SOLEIL, UPSay, Gif-sur-Yvette); STROBL, Markus (PSI)

**Presenter:** Ms NAPIERAJ, Maja (CNRS)

**Session Classification:** Presentations

Contribution ID: 52

Type: **Invited Talk**

## Polymers

*Monday, May 27, 2024 2:50 PM (25 minutes)*

Polymers

**Primary author:** DUDZINSKI, David

**Presenter:** DUDZINSKI, David

**Session Classification:** Presentations

Contribution ID: 53

Type: **Invited Talk**

## Catalysis / Mesoporous

*Monday, May 27, 2024 4:30 PM (25 minutes)*

Catalysis / Mesoporous

**Primary author:** ALBA-SIMIONESCO, Christiane

**Presenter:** ALBA-SIMIONESCO, Christiane

**Session Classification:** Presentations