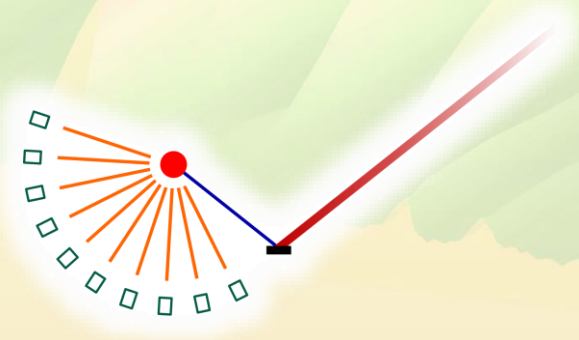
# Neutron Scattering and Complementary Methods in Modern Research

## 27th June – 1st July 2026, Będlewo near Poznań, Poland



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Institute of Molecular Physics, Polish Academy of Sciences
The Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences

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The Foundation for the Development of Poznań University of Technology
Polish Neutron Scattering Society
Faculty of Materials Engineering and Technical Physics, Poznań University of Technology

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**Contact:** neutrons2026@ifj.edu.pl tomasz.tolinski@ifmpan.poznan.pl ewa.juszynska-galazka@ifj.edu.pl

# SCHEDULE

**Saturday 27th June**

**15$^{30}$ – Registration**

**18$^{00}$ – W. Erdmann**, (Not so) Great Old Ones (Popular science lecture)

**19$^{30}$ – Welcome dinner**

**Sunday 28th June**

**8$^{00}$ – Breakfast**

**9$^{00}$ – Registration**

**12$^{00}$ – Conference opening**

***Session A* (12$^{30}$-13$^{30}$)**

**12$^{30}$ – A. J. Jackson**, Proteins in Deep Eutectic Solvents (Opening lecture)

**13$^{30}$ – Lunch break**

***Session B* (14$^{45}$-16$^{30}$)**

**14$^{45}$ – D. Vasiukov**, Magnetism in the homologous series of high-pressure iron oxides (Keynote lecture)

**15$^{45}$ – M. P. Marques**, Novel Cancer Targets Revealed by Neutron Spectroscopy (Invited lecture)

**16$^{30}$ – Coffee break**

***Session C* (17$^{15}$-18$^{55}$)**

**17$^{15}$ – N. K. Chogondahalli Muniraju**, Magnetic structure of murunskite from neutron scattering and other complementary techniques

**17$^{40}$ – M. Orzechowska,** An experimental study on thermal efficiency of $Ga_xFe_{3-x}O_4$ nanoparticles suspended in water

**18$^{05}$ – K. Rećko**, Magnetic behavior of $Fe_3O_4$ substituted with non-magnetic ions

**18$^{30}$ – S. Baran**, Influence of transition metal on magnetic properties of intermetallics – the case of $RE_5T_2In_4$ (RE = Gd-Tm; T = Ni, Rh, Pd, Pt)

**19$^{30}$ – Gala dinner**

**Monday 29th June**

**$8^{00}$ – Breakfast**

***Session A* ($9^{00}$-$10^{45}$)**

**$9^{00}$ – M. Johnson**, Institute Laue-Langevin - instrument and infrastructure upgrades, the science strategy and new research opportunities for Poland (Keynote lecture)

**$10^{00}$ – R. Campbell**, General Physical Description of the Behavior of Spread Polyelectrolyte/Surfactant Films at the Air/Water Interface (Invited lecture)

**$10^{45}$ – Coffee break**

***Session B* ($11^{30}$-$13^{00}$)**

**$11^{30}$ – M. Strobl**, Tackling Societal Challenges with Advanced Neutron Imaging (Invited lecture)

**$12^{15}$ – M. Silarski**, Thermal and epithermal neutrons as probes for hazardous materials detection (Invited lecture)

**$13^{00}$ – Lunch break**

***Session C* ($14^{30}$-$16^{10}$)**

**$14^{30}$ – D. Rusinek**, MNL MARIA Neutron Laboratory, current state, nearest actions and development plans

**$14^{55}$ – R. Przeniosło**, Monoclinic symmetry of the hcp phase of cobalt

**$15^{20}$ – D. Wardecki**, Neutron powder diffraction for probing structure–function relationships in zeolites

**$15^{45}$ – A. Boczkowska**, Neutrons as a study probe in the research of advanced materials

**$16^{10}$ – Coffee break**

**$16^{45}$ – Concert of the Poznan University of Technology Choir „Volantes Soni"**

**$18^{00}$ – Polish Neutron Scattering Society meeting**

**$18^{30}$ – Dinner**

**Tuesday 30th June**

**$8^{00}$ – Breakfast**

**$8^{30}$ – Excursion**

**$13^{00}$ – Lunch break**

***Session A* ($14^{30}$-$16^{30}$)**

**$14^{30}$ – Ch. Balz**, Neutron spectroscopy for quantum materials at the ESS (Invited lecture)

**$15^{15}$ – L. Scheller**, Structural Properties of a Compressible Porous Liquid Based on ZIF-8G Under Hydrostatic Pressure

**$15^{40}$ – A. Deptuch**, Glassforming, structural, and optical properties of two ternary liquid crystalline mixtures

**$16^{05}$ – K. Chat,** From Seconds to Nanoseconds: Equilibration Dynamics of a Polymer under Nanoporer-Confinement Probed by Dielectric and Neutron Spectroscopy

**$16^{30}$ – Coffee break**

**$17^{00}$ – Poster session**

**$18^{30}$ – Dinner**

**Wednesday 1st July**

**$8^{00}$ – Breakfast**

***Session A* ($9^{00}$-$10^{45}$)**

**$9^{00}$ – J. Oberdisse**, Some recent progress on filler structure, polymer conformations, and interfacial layer dynamics of polymer nanocomposites (Keynote lecture)

**$10^{00}$ – P. Horodek**, Defect studies with positron annihilation spectroscopy (Invited lecture)

**$10^{45}$ – Coffee break**

***Session B* ($11^{15}$-$13^{00}$)**

**$11^{15}$ – T. Arnold,** The dynamic behaviour of Styrene Maleic Acid Lipid Particles with and without membrane proteins (Keynote lecture)

**$12^{15}$ – J. Pieper**, Structure and dynamics of the photoactive orange carotenoid protein OCP investigated by neutron scattering with in-situ illumination (Invited lecture)

**$13^{00}$ – Closing**

**$13^{30}$ – Departure lunch**

# (Not so) Great Old Ones

W. Erdmann

Geohazards Research Unit, Institute of Geology, Faculty of Geographical and Geological Sciences, Adam Mickiewicz University, ul. Bogumiła Krygowskiego 12; 61-680 Poznań

Presenting author e-mail: weronika.erdmann@gmail.com

"That is not dead which can eternally lie, …" H.P. Lovecraft wrote in 1926, in one of his most famous stories, describing the ability of his overwhelming monsters, called in his prose "Great Old Ones," to wait for long periods of time, awaiting conditions favorable for their return. However, the father of the Cosmic Horror genre had no idea that just over 150 years earlier, zoologist Johann August Ephraim Goeze [1] had been the first to describe animals that, as we know now, have the ability to survive extremely unfavorable environmental conditions, somewhat similar to Lovecraft's fictional monsters.

The lecture will summarize over 250 years of research on Tardigrades, present the role of Polish research centers in the study of those (Not so) Great Old Ones, and debunk several myths about them [1,2,3].

[1] Schill, R.O. (Ed.), 2018, *Water Bears: The Biology of Tardigrades*. Springer, Cham. https://doi.org/10.1007/978-3-319-95702-9_3
[2] Kaczmarek Ł.. 2009, „Typ: Niesporczaki – Tardigrada” in Zoologia. Bezkręgowce. T. 1. Red. nauk. Czesław Błaszak. S: 694-701 Warszawa: Wydawnictwo Naukowe PWN, 2009, ISBN 978-83-01-16108-8
[3] Degma P.; Bertolani, R.; Guidetti, R., 2026, Actual Checklist of Tardigrada Species. Available online: https://doi.org/10.25431/11380_1178608 (accessed on 29 April 2026)

# Proteins in Deep Eutectic Solvents

A.J. Jackson[1,2]

1. European Spallation Source, Lund, Sweden
2. Department of Chemistry, Lund University, Lund, Sweden

Presenting author e-mail: andrew.jackson@ess.eu

The preservation of biomolecules presents a major challenge, in particular for pharmaceutical applications, and deep eutectic solvents (DESs) have emerged as suitable environments for this purpose [1,2]. DES are solvents obtained through the complexation of organic compounds, where the interaction between the precursors promotes a depression in the melting point that allows the mixture to remain liquid at room temperature. Moreover, through different combinations of precursors the physicochemical properties of the solvent can be tuned for particular applications. One important characteristic of DES is that they can tolerate the presence of relatively high fractions of water before losing the solvent hydrogen bond network. Thus, the degree of hydration is another tunable parameter available for optimization of the system properties [3].

This talk will discuss deep eutectic solvents in general, the tunability of the solvents, the behaviour of proteins in these solvents, and the effect of hydration on the folding and stability of proteins. It will conclude with a forward looking view of work to be done and the role that a large scale facility such as the European Spallation Source can play in understanding protein structure and structural changes in solution.

[1] A. Sanchez-Fernandez, K. J. Edler, T. Arnold, D. A. Venero and A. J. Jackson, *Phys. Chem. Chem. Phys.*, **19** (2017) 8667-8670
[2] A. Sanchez-Fernandez and A. J. Jackson, in *Advances in Botanical Research*, Elsevier, **97** (2021) 69-94
[3] A. Sanchez-Fernandez, M. Basic, J. Xiang, S. Prevost, A. J. Jackson and C. Dicko, *J. Am. Chem. Soc.*, **144** (2022) 23657-23667

# Magnetism in the homologous series of high-pressure iron oxides

D.M. Vasiukov[1,2]

1. European Spallation Source ERIC, 221 00 Lund, Sweden
2. Division of Synchrotron Radiation Research, Lund University, 221 00 Lund, Sweden

denis.vasiukov@ess.eu

Iron oxides are normally Mott insulators with the only notable exception of magnetite ($Fe_3O_4$), which has good electrical conductivity due to the itinerant mixed-valence state of iron. During the last decade of high- pressure research a whole new series of iron oxides with the same quality was discovered, like $Fe_4O_5$, $Fe_5O_6$, $Fe_7O_9$ etc. [1], featuring closely related structures with arrays of one-dimensional (1D) chains of trigonal prisms embedded between slabs of octahedra. Here, we present a unified approach to the series based on a specific crystallographic generation mechanism which predicts the structures of these oxides and naturally classifies them in terms of the slab cycle [2]. When including magnetic interactions, we conjecture a generic magnetic structure featuring the 1D chains symmetry protected against magnetic perturbations from the iron ions in the slabs [2]. The slab size determines the type of magnetic order, which alternates between ferromagnetic and antiferromagnetic depending on the slab width. This magnetic conjecture was tested using numerical simulations [3,4] as well as in the recent neutron powder diffraction experiment at WISH instrument of the ISIS facility.

[1] E. Bykova *et al., Nat. Commun.,* **7**(1) (2016) 10661
[2] D. M. Vasiukov *et al., arXiv preprint,* (2022) *arXiv:2207.14111*
[3] V. S. Zhandun *et al., Dalton Transactions*, **53**(5) (2024) 2242-2251
[4] V. S. Zhandun *et al., JETP Letters*, **119**(4) (2024) 294-298

# Novel Cancer Targets Revealed by Neutron Spectroscopy

M.P.M. Marques

Univ. Coimbra, Molecular Physical-Chemistry, LAQV/Requimte, Portugal

Presenting author e-mail: pmc@ci.uc.pt

This is a pioneer study on the impact of metallodrugs on vital cellular components, providing key insights into the molecular basis of their cytotoxicity. Pt-, Pd- and Ni-complexes with more than one metal centre, extensively studied by the authors in the last decade, trigger a selective DNA damage *via* metal coordination to the purine bases or electrostatic interaction with the phosphate groups. Additionally, the design of improved anticancer drugs relies on a thorough understanding of the processes underlying normal-to-cancer transition (NTC), which is still an ill-understood process.

Inelastic and quasi-elastic neutron scattering (INS and QENS), combined with Raman and Fourier Transform Infrared (FTIR, including with synchrotron radiation) spectroscopies, were applied to deliver a comprehensive set of conformational and dynamic data, on: (i) NTC transformation; (ii) activity of newly developed Pt-, Pd- and Ni-based anticancer agents (on DNA, glutathione, proteins, cellular metabolism and intracellular water).

Variations in the dynamical profile of intracellular water (plasticity) were evidenced by QENS for malignant cells/tissues compared to healthy counterparts. Moreover, the metal-based agents were shown to exert distinct effects on cancer cells, differentially impacting on cytoplasmic and hydration water, as well as displaying specific interactions with biomolecules. Intracellular water is therefore emerging as a potential secondary therapeutic target in cancer treatment. These findings are expected to foster the design of more specific and effective anticancer drugs, ultimately improving cancer patient outcomes.

FCT-Portugal: UID/50006/2025 and COMPETE2030-FEDER-00672800.

# Magnetic structure of murunskite from neutron scattering and other complementary techniques

Naveen Kumar Chogondahalli Muniraju[1]

1. Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

e-mail: naveen.chogondahalli@ifj.edu.pl

Murunskite ($K_2FeCu_3S_4$) is a quasi-two-dimensional semiconductor that structurally and electronically bridges the cuprate and iron-pnictide families of high-temperature superconductors. Magnetic Fe ions are randomly distributed over only one-quarter of the metal sites within the layers, the remaining sites being occupied by non-magnetic $Cu^+$, so that the compound behaves as a high-entropy magnetic alloy. Despite this real-space disorder, it develops an antiferromagnetic-like ordered phase below 97 K. The magnetic ground state was investigated by neutron powder diffraction (D20, ILL) and single-crystal neutron diffraction (ZEBRA, PSI), complemented by $^{57}$Fe Mössbauer spectroscopy, XPS and DFT. Short-range correlations set in near 150 K as a broad diffuse peak, followed by long-range order below 100 K that saturates around 40 K. The order is nearly commensurate, described by two close quarter-zone propagation vectors $k_1$ = (0.266, 0.266, 0) and $k_2$ = (0.24, 0.76, 0). Rietveld refinement with Mag2Pol, using a two-domain single-$k$ model, yields predominantly in-plane Fe moments of about 3.0 $\mu_B$. Mössbauer spectra reveal two paramagnetic Fe sites that merge into a single magnetic site on cooling, indicating an accompanying orbital transition. Mean-field simulations reproduce the data and show that the positional disorder is absorbed into the widths of the reciprocal-space peaks, the magnetic analogue of a disordered alloy. Murunskite thus displays emergent long-range magnetic order in a structurally disordered lattice, challenging the assumed direct link between crystal structure and the location of magnetic moments [1].

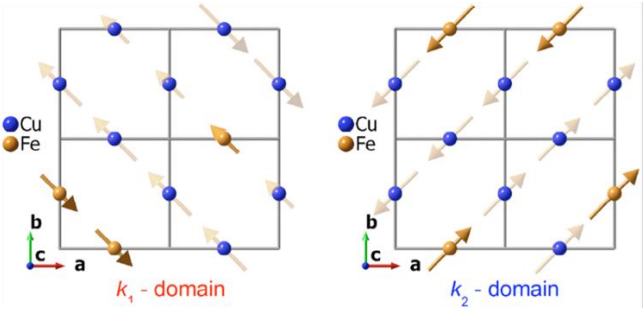


*Figure 1: In-plane Fe magnetic structure for the $k_1$ (left) and $k_2$ (right) quarter-zone domains from Rietveld refinement of the neutron data.*

## References

[1] D. Tolj *et al.*, *Adv. Funct. Mater.* **35** (2025) 2500099.

# An experimental study on thermal efficiency of $Ga_xFe_{3-x}O_4$ nanoparticles suspended in water

M. Orzechowska[1], K. Rećko[1], U. Klekotka[2], B. Kalska - Szostko[2], D. Soloviov[3] and A. Miaskowski[4]

1. Faculty of Physics, University of Białystok, Poland (m.orzechowska@uwb.edu.pl, k.recko@uwb.edu.pl)
2. Faculty of Chemistry, University of Białystok, Poland (u.klekotka@uwb.edu.pl, kalska@uwb.edu.pl)
3. European Molecular Biology Laboratory (EMBL), Hamburg, Germany (dmytro.soloviov@embl-hamburg.de)
4. Faculty of Electrical Engineering and Computer Science, Lublin University of Technology, Lublin, Poland (a.miaskowski@pollub.pl)

Presenting author e-mail: m.orzechowska@uwb.edu.pl

Gallium ferrite nanoparticles ($Ga_xFe_{3-x}O_4$) are promising materials for magnetically induced heating due to their tunable composition and favorable magnetic properties [1]. In this work, the thermal efficiency of their aqueous suspensions was investigated with particular emphasis on the relationship between crystal structure, aggregation and heating performance [2].

Nanoparticles were synthesized by a co-precipitation method [3]. X-ray diffraction confirmed the formation of a single-phase cubic spinel structure within the studied compositional range ($0 \leq x \leq 1$). Small-angle X-ray scattering and small-angle neutron scattering provided insight into the internal organization of the suspensions, revealing significant polydispersity and aggregated structures with mass fractals characteristics. These results were consistent with electron microscopy observations indicating irregular particle morphology and a broad size distribution.

Thermal efficiency was evaluated by calorimetric measurements in an alternating magnetic field and expressed as the specific absorption rate (SAR). All samples exhibited efficient heat generation, with SAR generally increasing with gallium content. The highest SAR value, 83.4 ± 2.2 W/g, was obtained for $Ga_{0.73}Fe_{2.27}O_4$ at a concentration of 2.8 mg/mL under f = 532 kHz and H = 15.3 kA/m. For this composition, SAR increased as nanoparticle concentration decreased [4].

The results show that both gallium substitution and aggregation strongly affect the thermal efficiency of $Ga_xFe_{3-x}O_4$ suspensions. The role of experimental parameters in optimizing SAR will be discussed.

[1] Y. Chen *et al., Bioact. Mater.*, **53** (2025) 591-629
[2] M. Orzechowska *et al., Int. J. Mol. Sci.*, **24** (2023) 14184
[3] R. Massart, *IEEE Trans. Magn.*, **17** (1981) 1247-1248
[4] M. Orzechowska *et al., Molecules*, **31** (2026) 177

# Magnetic behavior of $Fe_3O_4$ substituted with non-magnetic ions

K. Rećko[1], M. Orzechowska[1], K.A. Szarkowska[2], V. Nassif[3], W. Olszewski[1]
M. Biernacka[1], U. Klekotka[4], B. Kalska-Szostko[4]

1. Faculty of Physics, University of Białystok, Poland (k.recko@uwb.edu.pl, m.orzechowska@uwb.edu.pl, w.olszewski@uwb.edu.pl, m.biernacka@uwb.edu.pl)
2. Doctoral School, University of Białystok, Poland (k.szarkowska@uwb.edu.pl)
3. French National Centre for Scientific Research, Paris, France (nassif@ext.ill.fr)
4. Faculty of Chemistry, University of Białystok, Poland (u.klekotka@uwb.edu.pl, kalska@uwb.edu.pl)

Presenting author e-mail: k.recko@uwb.edu.pl

The magnetism of the $M^{3+}Fe_5O_8$ cubic system ($Fd\bar{3}m$, no. 227) where $M^{3+}$ denotes a non-magnetic $Fe^{3+}$ substituent ($Ga^{3+}$ or $La^{3+}$) is highly sensitive to the preparation method [1,2]. X-ray and neutron diffraction methods, as well as Mössbauer spectroscopy, were used to determine the location of cations in the analyzed tetroxides. Neutron studies were carried out at different temperature points (see *Figure*). The studies focused on compositions with ionic ratios of 1:5:8. In the gallium ferrite, iron magnetic moments $\mu_{Fe(8a)}$ and $\mu_{Fe(16d)}$ (blue and red arrows in the inset) form a collinear axial ferrimagnet up to 300 K, with the 3.57(7) $\mu_B$ and -3.01(5) $\mu_B$, achieved per iron ion. Despite the presence of impurity, an agreement of $I_{440}^{exp} \cong I_{440}^{theor}$ fundamental reflection guarantees the preservation of the nominal stoichiometry of the system.

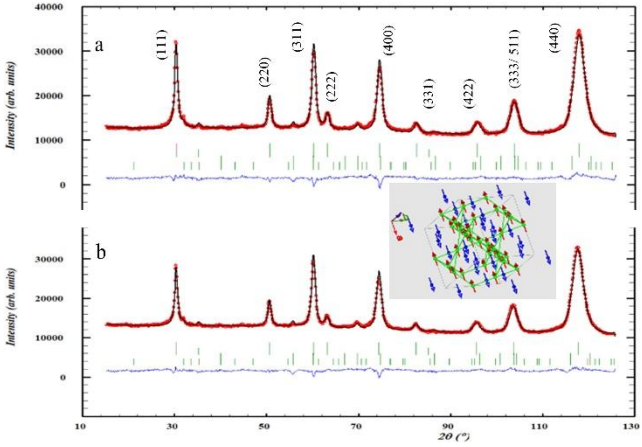


*Figure. Rietveld refinement of neutron diffraction patterns collected at temperatures of 2 K (a) and 300 K (b) with an inset showing the magnetic structure. Red dots refer to the experimental pattern. The black line represents the calculated pattern. A series of green vertical lines illustrates the Bragg peak positions of the nuclear and magnetic phases of $GaFe_5O_8$ with blue difference diagrams.*

**Acknowledgements** The authors K. R., M. O., and K.A. S. acknowledge the Polish Ministry of Education and Science decision nr 2023/WK/08 to fund the scientific membership of Poland at the ILL, which made this research possible.

[1] M. Orzechowska *et al.*, *Int. J. Mol. Sci.*, **24** (2023) 14184
[2] M. Orzechowska *et al.*, *Molecules*, **31** (2026) 177

# Influence of transition metal on magnetic properties of intermetallics – the case of $RE_5T_2In_4$ (RE = Gd-Tm; T = Ni, Rh, Pd, Pt)

S. Baran[1]

1. Jagiellonian University, Faculty of Physics, Astronomy and Applied Computer Science, M. Smoluchowski Institute of Physics, Prof. Stanisława Łojasiewicza 11, PL-30-348 Kraków, Poland

Presenting author e-mail: stanislaw.baran@uj.edu.pl

The $RE_5T_2In_4$ (RE = Gd-Tm; T = Ni, Rh, Pd, Pt) intermetallics crystallize with the orthorhombic $Lu_5Ni_2In_4$ -type structure (space group Pbam, No. 55). Their crystal structure parameters can be found in [1-4] for T = Ni, Rh, Pd and Pt, respectively. The structure is a layered one with layers formed by the rare earth atoms separated by the layers formed by the two remaining elements. The magnetic properties of $RE_5T_2In_4$, including magnetocaloric performance and/or magnetic structures for selected compounds, have been reported in a number of papers ([5-8] for T = Ni, Rh, Pd and Pt, respectively). In the $Lu_5Ni_2In_4$-type crystal structure, the rare earth atoms occupy three non-equivalent Wyckoff sites. Such a distribution of the magnetic atoms leads to competition of different magnetic interactions, resulting in appearance of complex magnetic properties, like: coexistence of ferro- and antiferromagnetic components of the magnetic structure, diferent propagations vectors describing magnetic order in different magnetic sublattices, temperature- and/or magnetic field-induced magnetic transitions of the order-order type, individual critical temperatures of magnetic ordering for individual magnetic sublattices. Interestingly, for a fixed T-element, the critical temperatures of magnetic ordering are significantly lower for the Rh-based compounds when compared to those of the Ni-, Pd- and Pt-related ones, indicating an important role of number of the d-electrons of the transition metal in formation of magnetic order. This feature makes possible construction of hybrid functional materials showing good magnetocaloric performance over wide temperature interval.

**Acknowledgments**: This research was supported by the Excellence Initiative - Research University Program at the Jagiellonian University in Kraków.

**References**

[1] V.I. Zaremba *et al.*, *Kristallografiya*, **36** (1991) 1415-1418
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[5] Z. Zhang *et al.*, *Intermetallics*, **100** (2018) 136-141, and references therein
[6] A.R. Hayyu *et al.*, *arXiv*:2505.14831 [cond-mat.mtrl-sci]
[7] A.R. Hayyu *et al.*, *Phys. B: Condens. Matter*, **710** (2025) 417184, and references therein
[8] A.R. Hayyu *et al.*, *J. Alloys Compd.*, **1001** (2024) 175054, and references therein

# Institute Laue-Langevin - instrument and infrastructure upgrades, the science strategy and new research opportunities for Poland

Mark Johnson[1]

[1] Institut Laue Langevin, Grenoble, France

Presenting author email: johnson@ill.eu

The comprehensive Endurance upgrade programme was completed in 2024. With a budget of 50+ M€, about 30 projects have been delivered, including neutron guide systems, new and upgraded instruments, sample environment and data and software services. More intense neutron beams combined with more efficient detector systems provide major new capability for measuring ever smaller samples, including in extreme sample environments, and weaker signals. In addition, significantly shorter measuring times facilitate parametric studies and increase throughput and, therefore, overall capacity. Thus the upgrade programme as a whole, supported by ongoing and new projects, ensures that research capability at the ILL will continue to be world leading for the next decade, offering new opportunities for cutting-edge science. In this context, the ILL has elaborated a science strategy to optimise the use of its state-of-the-art scientific infrastructure over the next decade and enhance the delivery of societal impact with neutrons.

The Endurance programme, ongoing and new projects, and the science strategy will be presented, including recent science highlights, and set in the context of future reactor operation to 2033 and beyond...

# General Physical Description of the Behavior of Spread Polyelectrolyte/Surfactant Films at the Air/Water Interface

Javier Carrascosa-Tejedor,[1,2] Andrea Tummino,[2,3] Philipp Gutfreund,[2]
M. Jayne Lawrence,[1] Imre Varga[3] and Richard A. Campbell[1]

1. Division of Pharmacy and Optometry, Faculty of Biology, Medicine and Health, University of Manchester, Oxford Road, Manchester M13 9PT, United Kingdom.
2. Institut Laue-Langevin, 71 Avenue des Martyrs, CS20156, 38042 Grenoble, France.
3. Institute of Chemistry, Eötvös Loránd University, 112, Budapest H-1518, Hungary.

Presenting author e-mail: richard.campbell@manchester.ac.uk

Polyelectrolyte/surfactant mixtures have been studied extensively because of their use in everyday products as well as drug delivery and biomedical applications [1, 2]. A few years ago, we invented a methodology to create spread films by dispensing aliquots of nanostructured aggregates on the surface of pure water [3]. The films are more substantial than layers formed from adsorption, and there is no requirement for use of organic carrier solvent, which hint at economic and environmental benefits for applications.

Work on the poly(sodium styrene sulfonate)/dodecyltrimethylammonium bromide (PSS/DTAB) system showed that films exhibit transient 3D structures upon compression only when prepared from aggregates with excess surfactant [4]. Work on the poly(ethylene imine/sodium dodecyl sulfate (PEI/SDS) system showed that a compact conformation is adopted in rigid films only at low subphase pH [5]. Work on the poly-l-lysine (PLL)/SDS system showed that we can precisely control stable 3D structures during compression of films, with the structure comprising a surfactant monolayer, bound polypeptide, and then one or two layers of mixed micelles [6, 7].

Surface pressure-area isotherms, ellipsometry and Brewster angle microscopy were essential complementary techniques to key data provided by compositional and structural applications of neutron reflectometry. The basis of the less common compositional analysis application will be described [8]. Data on the spread film properties of four systems will then be reviewed to extract key insight into their behavior. Notably, 3D structure formation and film stability will be contextualized in terms of the polyelectrolyte characteristics, polyelectrolyte/surfactant interactions, and presence of macroscopic aggregates embedded in the films.

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[2] M. Gradzielski et al. *Langmuir* **38** (2022) 13330-13343.
[3] R. A. Campbell et al. *Soft Matter* **12** (2016) 5304-5312.
[4] A. Tummino et al. *Langmuir* **34** (2018) 2312-2323.
[5] J. Carrascosa Tejedor et al. *Langmuir* **39** (2023) 14869-14879.
[6] J. Carrascosa Tejedor et al. *Chem. Commun.* **58** (2022) 10687.
[7] J. Carrascosa Tejedor et al. *Nanoscale* **15** (2023) 11141-11154.
[8] R. A. Campbell *Curr. Opin. Colloid Interface Sci.* **37** (2018) 49-60.

# Tackling Societal Challenges with Advanced Neutron Imaging

M. Strobl[1,2,3,4]

1. Institute Laue Langevin (ILL), 71 Avenue des Martyrs, F-38042 Grenoble, France
2. Paul Scherrer Institu, Forschungsstrasse 111, 5232 Villigen Switzerland
3. University of Copenhagen (KU), 2100 Copenhagen, Denmark
4. Technical University of Denmark (DTU) 2800 Kongens Lyngby, Denmark

Presenting author e-mail: markus.strobl@psi.ch

Benefitting from the unique capabilities of neutrons as a probe neutron imaging is a research tool that allows observations throughout the volume of large and heterogeneous sample systems in order to assess the local interplay of various material phases on multiple length and time scales [1]. Neutrons penetrate many structural materials of devices better than other radiation while they provide at the same time high contrast for many key elements enabling quantitative observations of critical internal processes. Key examples concern the roles of Li and hydrogen, which neutrons in contrast to x-rays are highly sensitive to, in today's energy research. State-of-the-art observations utilize attenuation, elastic and inelastic scattering, diffraction and polarisation to map density, crystallographic features, nanostructure, magnetic fields, temperature, isotope distribution, diffusion, chemical compounds and phase composition. Applications today contribute to the development of emerging technologies in the context of societal challenges such as industry 4.0, power-to-X, circular economy and the Green Deal.

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# Thermal and epithermal neutrons as probes for hazardous materials detection

M. Silarski[1] , K. Dziedzic-Kocurek[1], K. Drużbicki[2], and M. Krzystyniak[3]

1. Faculty of Physics, Astronomy and Applied Computer Science, M. Smoluchowski Institute of Physics, Jagiellonian University, 30-348, Kraków, Poland
2. Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza, 112, 90-363, Lodz, Poland
3. STFC Rutherford Appleton Laboratory, ISIS Neutron and Muon Source, Chilton, OX11 0QX, UK

Presenting author e-mail: michal.silarski@uj.edu.pl

The increasing severity of damage that can result from a single terrorist attack highlights the need for more effective hazardous-material detection technologies. This challenge is particularly acute in maritime environments, where reliable methods for monitoring threats to offshore infrastructure and port facilities remain limited. Current state-of-the-art detection techniques can accurately determine the density distribution and geometry of inspected objects; however, their ability to identify specific substances is limited. A promising alternative or supplementary method employs neutron activation, which enables non-invasive determination of the stoichiometry of an unknown object. Its sensitivity may be further enhanced through the use of complementary neutron techniques, such as neutron transmission and neutron Compton scattering.

In this contribution the feasibility of using several analytical techniques available at the thermal-to-epithermal neutron beamline VESUVIO at the ISIS Neutron and Muon Source (UK) for hazardous-material detection. A series of experiments was conducted using simultaneous neutron transmission and Compton scattering measurements on boric acid and melamine, a widely used surrogate for explosive materials[2,3]. The objective was to characterize the material's response signatures and to evaluate the corresponding limits of detection and quantification, thereby assessing the potential of these methods for substance identification in security-screening applications.

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# MNL MARIA Neutron Laboratory, current state, nearest actions and development plans

D. Rusinek[1]

1. National Centre for Nuclear Research (Dariusz.Rusinek@ncbj.gov.pl)

Presenting author e-mail: Dariusz.Rusinek@ncbj.gov.pl

The construction of the MNL Laboratory has been successfully completed. The physical hall has been modernized, and all utilities required for experimental work have been installed, including electrical power, helium recovery infrastructure, and gaseous helium and nitrogen systems. Laboratory spaces dedicated to MNL operations, researchers, and technical staff have also been upgraded.

New equipment has been procured, such as a helium recovery and liquefaction station, liquid helium and nitrogen dewars, a dosimetry gate, radiation detectors, as well as computers and servers. The missing shielding components have been made. The neutron radiography station has been upgraded, and a 3D tomographic reconstruction system has been added.

We are currently commissioning, calibrating, and testing the laboratory systems and instrumentation. We invite collaborators to participate in initial test measurements. We aim to expand our scientific community by providing new capabilities for advanced neutron measurements.

# Monoclinic symmetry of the hcp phase of cobalt

Radosław Przeniosło[1],* Piotr Fabrykiewicz[2], Izabela Sosnowska[1], Paweł Kozłowski[1]
François Fauth[3], Anatoliy Senyshyn[4], Emmanuelle Suard[5] and Dariusz Oleszak[6]

1. Faculty of Physics, University of Warsaw, Pasteura 5, PL-02-093 Warsaw, Poland
2. Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich, Lichtenbergstraße 1, D-85747 Garching, Germany
3. CELLS-ALBA, Carrer de la Llum 2-26, ES-08290 Cerdanyola del Vallés, Barcelona, Spain
4. Heinz Maier-Leibnitz Zentrum, Technical University of Munich, Lichtenbergstraße 1, D-85747 Garching, Germany
5. Institut Laue-Langevin, 71 Av. des Martyrs, F-38000 Grenoble, France
6. Faculty of Materials Science and Engineering, Warsaw University of Technology, Wołoska 141, PL-02-507 Warsaw

Presenting author e-mail: radek@fuw.edu.pl

The gradual ferromagnetic spin reorientation in hexagonal close packed cobalt (hcp-Co) phase between 230°C and 330°C reported for a Co single crystal [1] suggests that this phase could not have a hexagonal symmetry [2]. This hypothesis is verified positively by synchrotron radiation diffraction and neutron diffraction on polycrystalline powder cobalt samples [2]. The analysis of diffraction data has been done by using a specific set of Bragg peaks, which are not sensitive to the stacking faults present in abundance in hcp-Co. The crystal structure of the hcp-type ordered areas of cobalt is described by the monoclinic symmetry with the magnetic space group C2'/m'.

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# Neutron powder diffraction for probing structure–function relationships in zeolites

D. Wardecki[1], K. Mlekodaj[2], E. Tabor[2], J. Wieser[3], T.C. Hansen[4] and P. Rzepka[2]

1. Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland
2. J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague 8, 182 23, Czech Republic
3. Department of Chemistry and Applied Biosciences, Institute for Chemical and Bioengineering, ETH Zurich, 8093 Zürich, Switzerland
4. Institut Laue-Langevin, 71 Avenue des Martyrs, Grenoble 38000, France

Presenting author e-mail: dward@fuw.edu.pl

Zeolites are porous aluminoslicates widely used in catalysis and gas adsorption. Their performance is governed by the location of extra-framework cations and their dynamic behaviour under operando conditions. Neutron powder diffraction (NPD) offers unique capabilities for investigating these systems, offering sensitivity to light elements (C, O, H) and enabling discrimination between cations with similar X-ray scattering factors. The experiments reported here were conducted on the high-intensity D1B diffractometer at the Institute Laue-Langevin (ILL), Grenoble, France.

In situ NPD studies of $CO_2$ adsorption in zeolite NaK-A revealed three crystallographically distinct adsorption sites within the α-cavities, enabling the derivation of site-specific Langmuir isotherms and direct identification of chemisorbed carbonate-like species near the 8-ring windows [1]. In Cu-exchanged zeolite omega, NPD combined with anomalous X-ray diffraction showed that hydration-driven migration of Cu cations between active 8-membered ring positions and inactive 6-ring sites governs methane-to-methanol conversion activity [2]. In Fe-containing ferrierite, NPD identified reversible displacement of Fe(II) species from the 6-membered ring plane upon $CO_2$ interactions, consistent with the formation of hydrocarbonate intermediates supported by complementary operando FTIR/MS, Mössbauer spectroscopy and DFT calculations [3].

These studies demonstrate the power of NPD to resolve structure-function relationships in zeolites under working conditions, providing insights that support the rational design of advanced materials for energy and environmental applications.

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# Neutrons as a study probe in the research of advanced materials

A. Boczkowska

Warsaw University of Technology, Faculty of Materials Science and Engineering, Wołoska 141, 02-507 Warsaw

Presenting author e-mail: anna.boczkowska@pw.edu.pl

Neutrons are powerful probes for advanced materials due to their unique properties such as deep penetration, sensitivity to light elements and magnetic sensitivity. Neutrons can easily penetrate bulky components, enabling their non-destructive testing. They also interact strongly with light elements like hydrogen, lithium, and oxygen. Because neutrons have a magnetic moment, they can directly probe magnetic structures.

Scientific research conducted at the Faculty of Materials Science and Engineering of Warsaw University of Technology relates to the main issues of modern materials science and materials engineering. The main scope of research includes: nanocrystalline and amorphous materials, biomaterials, intelligent and functional materials, modern ceramic and polymer materials, materials for power engineering, surface engineering, materials degradation processes and characterization of materials.

Warsaw University of Technology researchers are seeking neutron probes to support investigation of:

- functional materials - investigating atomic occupancies and magnetic site densities in magnetic shape memory alloys (MSMAs) for smart sensors and actuators.
- energy systems - studying light-element dynamics in materials for next-generation hydrogen storage, batteries, and fusion power.
- structural materials - analyzing residual stresses, microstructural changes, and phase evolution in 3-D printed scaffolds, metal components or Nd-Fe-B alloys processed by Laser Powder Bed Fusion method.

An example of successfully conducted studies proves possibility of measurements of residual stresses in ceramic-elastomer composites using diffuse scattering instrument [1]. On the other hand, small angle neutron scattering was applied to investigation of reversible and irreversible effects of magnetic field upon hard-segment domains in magnetorheological elastomers [2].

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# Neutron spectroscopy for quantum materials at the ESS

Christian Balz[1] and Pascale Deen[1,2]

1. European Spallation Source ESS ERIC, Box 176, 221 00 Lund, Sweden
2. Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen Ø, Denmark

Presenting author email: christian.balz@ess.eu

Inelastic neutron scattering (INS) is a cornerstone technique for probing the dynamic properties of quantum materials. By measuring the exchange of energy and momentum between neutrons and the sample, INS reveals collective excitations such as phonons, magnons, and other quasiparticles that underpin superconductivity, magnetism and topological phenomena. Traditionally, neutron spectroscopy is used to study phonon and magnon dispersion curves as well as crystal field excitations thus enabling the determination of strengths of chemical bonds, magnetic exchange couplings, and crystal field level schemes.

The past decades have seen a shift in attention toward studies of exotic low-energy excitations in quantum materials, e.g., low-dimensional [1] and/or frustrated quantum magnets [2], as well as strongly correlated electron materials, including heavy fermion metals [3], cuprate- [4], and iron-based high-$T_c$ superconductors [5], as well as phonon dispersions in energy materials. Here, the spectral signatures of scientific interest are inherently weak and broad in energy and momentum transfer, requiring the coverage of large regions of momentum and energy space for satisfactory comparisons between experiment and theory. INS on modern time-of-flight spectrometers enables the measurement of collective coherent spin and lattice dynamics with high resolutions and large coverage in both energy transfer and wavevector transfer. At the ESS, 3 spectrometers for quantum materials CSPEC [6], BIFROST [7], and T-REX are currently being build. With those we will address emergent behaviour in quantum spin liquids, unconventional superconductors, and low-dimensional magnets.

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# Structural Properties of a Compressible Porous Liquid Based on ZIF-8G Under Hydrostatic Pressure

L. Scheller[1], P. Zajdel[1], D. Caporale[2], V. Cristiglio[3]

1. Instytut Fizyki im. Augusta Chełkowskiego Uniwersytetu Śląskiego w Katowicach, ul. 75 Pułku Piechoty 1, 41-500 Chorzów
2. CIC energiGUNE, Parque Tecnológico de Álava, Albert Einstein Kalea, 48, 01510 Vitoria-Gasteiz, Álava, Spain
3. Institut Laue-Langevin (ILL), 71 Av. des Martyrs, 38000 Grenoble, France

Presenting author e-mail: lukasz.scheller@us.edu.pl

Type-III porous liquids based on metal-organic frameworks represent a novel class of functional materials that combine the structural flexibility of crystalline porous solids with macroscopic fluidity. ZIF-8, a hydrophobic zeolitic imidazolate framework, is a well-established molecular spring capable of storing mechanical energy via pressure-induced water intrusion into its cages. To extend this concept to porous liquids, ZIF-8 nanoparticles were functionalized with mPEG-epoxide (ZIF-8G), enabling stable colloidal dispersion in $D_2O$ and compensation of negative buoyancy. We report a neutron diffraction study of ZIF-8G under hydrostatic pressure performed on the D16 diffractometer (ILL, $\lambda = 4.477$ Å) in WANS configuration.

The evolution of the cubic lattice parameter, tracked via the (330)/(411) and (110) Bragg reflections over a full intrusion/extrusion pressure cycle, reveals three distinct regimes: an initial linear contraction (negative compressibility), a pronounced expansion linked to $D_2O$ intrusion into the framework cages, and a pressure-independent plateau after full filling. A moderate hysteresis between intrusion and extrusion confirms that confinement effects persist in the porous-liquid form. Comparison with bulk ZIF-8 and mixed-linker ZIF-7-8 shows that mPEG-epoxide functionalization moderates the lattice expansion and shifts the intrusion/extrusion pressure range, while the molecular-spring behavior is preserved. No material instability or phase separation was observed during the in-situ experiment, demonstrating the robustness of the colloidal system. SANS measurements are to reveal the core-shell nanoparticle architecture of ZIF-8G, probe the response of the mPEG-epoxide shell to applied pressure, and independently track the intrusion/extrusion process via scattering contrast changes between empty and $D_2O$-filled cages, potentially elucidating the molecular origin of the observed hysteresis.

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# Glassforming, structural, and optical properties of two ternary liquid crystalline mixtures

A. Deptuch[1], Z. Zając[2], M. Piwowarczyk[1], A. Drzewicz[1], M. Kozieł[3], M. Urbańska[4], and E. Juszyńska-Gałązka[1,5]

1. Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31342 Kraków, Poland
2. Faculty of Materials Science and Ceramics, AGH University of Cracow, Mickiewicza 30, 30059 Kraków, Poland
3. Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30387, Kraków, Poland
4. Institute of Chemistry, Military University of Technology, Kaliskiego 2, 00908 Warsaw, Poland
5. Research Center for Thermal and Entropic Science, Graduate School of Science, Osaka University, 560-0043 Osaka, Japan

Presenting author e-mail: aleksandra.deptuch@ifj.edu.pl

Fluorinated liquid crystals with acronyms 3FmHPhF6 and 3FmHPhH6 (m = 5, 6) are mixed with a non-fluorinated MHPOBC liquid crystal. MIXmHFHH6 mixture with the molar ratio of MHPOBC : 3FmHPhF6 : 3FmHPhH6 equal to 0.5 : 0.25 : 0.25 is obtained for each m. Both mixtures show the smectic A*, C*, and $C_A$* phases. An increasing smectic layer spacing in supercooled $SmC_A$* suggests an approaching transition to the hexatic smectic $X_A$* phase, but it does not occur, stopped by the glass transition of $SmC_A$* at 220-240 K. Both MIXmHFHH6 reflect green or red light in SmC*. MIX5HFHH6 shows a strong thermochromic effect (change of color with temperature) in 270-310 K in $SmC_A$*, and weak reflection of blue light in the $SmC_A$* glass. MIX6HFHH6 reflects presumably in the infra-red range in $SmC_A$* and its glass. The temperature dependence of the α-relaxation process in $SmC_A$* reveals a decrease of the dynamic fragility index in both mixtures compared to pure glassforming components. Detailed description is available in a preprint [1]. It is a part of a wider, systematic study of glassforming smectic liquid crystals and their mixtures [2-5].

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# From Seconds to Nanoseconds: Equilibration Dynamics of a Polymer under Nanopore-Confinement Probed by Dielectric and Neutron Spectroscopy

K Chat[1], Markus Appel[2] and K Adrjanowicz[3]

1. Institute of Nuclear Physics, Polish Academy of Sciences, PL-31-342 Kraków, Poland
2. Institut Laue-Langevin, Avenue des Martyrs 71, Cedex 9 Grenoble, 38042, France
2. Institute of Physics, University of Silesia, 75 Pułku Piechoty 1, 41-500 Chorzów, Poland

Presenting author e-mail: katarzyna.chat@ifj.edu.pl

The dynamics of glass-forming polymers confined in nanoporous materials are strongly affected by non-equilibrium phenomena. Although confinement initially accelerates molecular mobility, prolonged annealing gradually restores bulk-like behavior. Recent dielectric studies have shown that this equilibration process can be described within the material-time concept, suggesting that the evolution of the confined system is governed by a single internal clock despite the complexity of nanoconfinement.[1–3] Whether this description also applies to fast molecular motions remains an open question. In this presentation, we investigate the equilibration dynamics of poly(phenylmethyl siloxane) (PMPS) confined in anodic aluminum oxide (AAO) nanopores using simultaneous broadband dielectric spectroscopy and neutron backscattering spectroscopy. This approach enables direct observation of molecular motions spanning from nanoseconds to seconds under identical thermal conditions. Dielectric measurements reveal accelerated segmental α-relaxation in confinement and its gradual recovery toward bulk behavior during annealing following temperature jumps. Simultaneously collected neutron data show corresponding changes in elastic and inelastic fixed-window scans as well as in the mean-square displacement. Studies performed for PMPS confined in 200 nm pores demonstrate consistent equilibration time scales obtained from both techniques, indicating that fast nanosecond-scale dynamics evolve together with slow segmental relaxation. These findings provide new insight into the coupling of fast and slow dynamics in nanoconfined polymers. The observed consistency between equilibration time scales obtained from dielectric and neutron measurements suggests that molecular motions spanning many orders of magnitude in time may be governed by a common material-time framework. Such a description would offer a unified view of equilibration processes in confined glass-forming systems.

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# Some recent progress on filler structure, polymer conformations, and interfacial layer dynamics of polymer nanocomposites

A.C. Genix and J. Oberdisse

Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS, F-34095 Montpellier, FRANCE

Presenting author e-mail: julian.oberdisse@umontpellier.fr

The macroscopic properties of polymer nanocomposites (PNCs) depend in a crucial way on the microscopic state of the filler nanoparticles (NPs) and the polymer. In particular mechanical properties are strongly affected by percolation of hard phases, which may be NP networks, or dynamically modified (i.e. hardened) polymer regions, or combinations of both. In this talk, we will review some recent progress in small-angle scattering associated with simulations to study particle dispersions, and broadband dielectric spectroscopy (BDS) to investigate polymer dynamics at the NP interface.

Nanoparticles used in industrial applications may be very polydisperse, and form agglomerates of complex geometry. The conceptual difficulty of their analysis goes hand in hand with their superior performances. We will present one of the first self-consistent models of their structure based on a combination of electron microscopy with scattering [1]. We did not realize it back then, but this approach was the first based on a correlation hole analysis [2], which is a measure of the strength of interaction between particles or small aggregates, and thus the local concentration. In collaboration with Vera Bocharova and Alexei Sokolov [3,4], we then moved to an in-depth characterization of the dynamic state of the polymer using BDS in strongly attractive model systems. Here the combination of structural analysis based on scattering, with a careful look on interparticle distances, with BDS turned out to allow for a better quantitative determination of the thickness of the interfacial layer. The experimental system under scrutiny is a silane surface-modified PNC, where the NP structure and the interfacial layer dynamics can be followed simultaneously as a function of grafting density and particle content. The strongest dynamical slow-down in the polymer is found for unmodified NPs, while grafting weakens this effect progressively. The combination of all three techniques enables a unique measurement of the true thickness of the interfacial layer, which is ca. 5 nm.

If time allows, we will discuss recent results on a porous nanocomposite system, where the quantitative comparison of SANS and SAXS data gives insights into the dispersion and (tunable) conformation of polymer molecules [5].

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# Defect studies with positron annihilation spectroscopy

P. Horodek[1]

1. Institute of Nuclear Physics of the Polish Academy of Sciences, 152 Radzikowskiego Str., 31-342 Kraków, Poland

Presenting author e-mail: pawel.horodek@ifj.edu.pl

Modern materials characterization increasingly emphasizes the importance of studying structural defects alongside conventional analyses of phase composition, morphology, and crystallographic structure. Since defects strongly affect the physical, mechanical, and functional properties of materials, their investigation is essential for a complete understanding of material behavior. In this context, positron annihilation spectroscopy (PAS) constitutes a highly sensitive method for the detection of structural defects, such as vacancies, their cluster, voids, etc. PAS can provide unique information inaccessible to conventional characterization methods such as neutron techniques, X-ray diffraction (XRD), electron microscopy, or spectroscopic analyses.

In the frame of the presentation, the basics of PAS, experimental procedure, data analysis and interpretation as well as examples of application in various fields will be discussed.

# The dynamic behaviour of Styrene Maleic Acid Lipid Particles with and without membrane proteins

Stephen Hall[1], Tom Arnold[2], Karen Edler[3], Ellen Wilson[1,3], Glenn Coope[3], Hanna Wacklin-Knecht[1,2], Timothy Dafforn[4], Richard A. Campbell[5]

1 European Spallation Source ERIC, Lund, Sweden
2 ISIS Neutron and Muon Source, STFC, Harwell, UK
3 University of Lund, Lund, Sweden
4 University of Birmingham, Birmingham, UK
5 University of Manchester, Manchester, UK

Presenting author e-mail: tom.arnold@ess.eu

In recent years, there has been a rapid development of membrane-mimetic systems to encapsulate and stabilize planar segments of phospholipid bilayers in solution. One such system has been the use of amphipathic copolymers to solubilize lipid bilayers into nanodiscs. The attractiveness of this system, in part, stems from the capability of these polymers to solubilize membrane proteins directly from the host cell membrane. The assumption has been that the native lipid annulus remains intact, with nanodiscs providing a snapshot of the lipid environment. However recent studies have shown that lipids in such particles are able to rapidly exchange between both nanodiscs in solution and external sources of lipids e.g. [1]. These observations draw into doubt some of the received wisdoms about these systems. Over the last 10 years, we have investigated the fundamental properties of nanodiscs and their formation, including the influence of membrane charge on free polymer interaction, and the impact of polymer chemistry on the propensity of nanodiscs undergo lipid exchange [2]. These studies include various implementations of neutron reflectometry (NR) and have also shown that both free polymer and SMALPs are surface active and disassemble when adsorbed to a clean air-water interface and that nanodiscs stabilised by three different polymers will exchange both lipids and polymer with a monolayer and a silicon supported bilayer. In one case, depending on the polymer used, we have also adsorbed nanodiscs to a bilayer interface. We have now extended these studies to include Styrene Maleic Acid Lipid Particles (SMALPs) containing membrane proteins and recent results demonstrate similar behaviour in these systems. Together these results demonstrate the dynamic nature of nanodiscs, even those containing integral membrane proteins, that interact with the local environment and are likely to deposit both lipids and polymer at all stages of use. I will conclude with an outlook on how NR studies like these will soon be able to take advantage of new reflectometers at ESS.

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# Structure and dynamics of the photoactive orange carotenoid protein OCP investigated by neutron scattering with in-situ illumination

J. Pieper[1]

1. University of Tartu, Institute of Physics, W. Ostwald str. 1, 50411 Tartu, Estonia.

Presenting author e-mail: pieper@ut.ee

Efficient harvesting of solar radiation is essential for photosynthesis, a fundamental physiological process that has generated our oxygen-containing atmosphere and provides storable chemical energy as the basis for all life on earth. Excess light intensity, however, may damage the photosynthetic apparatus of bacteria and plants so that protective mechanisms are required. In cyanobacteria, the orange carotenoid protein (OCP) acts as a high-light sensor and dissipates excess energy as heat to prevent photodamage. OCP is a photoactive protein that undergoes a drastic structural change from a compact dark-adapted state to a very flexible active state upon illumination with blue light.

We have investigated the solution structures and dynamics of both OCP states using neutron scattering methods combined with molecular dynamics simulations. According to small angle neutron scattering (SANS) data, the active state structure of OCP is largely elongated with well separated protein domains [1]. In solution, the N-terminal domains of OCP are clearly detached and reoriented by about 90° relative to the C- terminal domains compared with the OCP high-resolution structure. This apparent structural difference implies the need for a previously unknown structural rearrangement [2]. A rarely considered aspect is the internal protein dynamics facilitating the OCP structural transitions. Therefore, we directly probed protein dynamics in a wide observation time range in the dark and under illumination using quasielastic neutron scattering (QENS). After photoactivation to the active state, the internal dynamics is enhanced, while the global diffusion is slowed down [2,3]. A residue-resolved molecular dynamics simulation [2] indicates that the interdomain linker becomes more flexible and may mediate the structural adaptation to the phycobilisome binding site. In turn, the β-sheet structures remain the most rigid part of the active state structure, which is essential for protein dimerization.

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# Inelastic neutron scattering, magnetic properties and crystal field for non-isoelectronic substitutions in the antiferromagnet $CeCoGe_3$

P. Skokowski, K. Synoradzki, and T. Toliński

Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179, Poznań, Poland

Presenting author e-mail: tomtol@ifmpan.edu.pl

The compounds $CeCoGe_3$, $PrCoGe_3$ and $CeFeGe_3$ are three isostructural (space group *I*4*mm*), but not isoelectronic, systems with well-defined ground states (antiferromagnetic, paramagnetic, and paramagnetic heavy fermion, respectively) [1,2]. Therefore, transitions between these parent compositions can lead to the formation of peculiar intermediate states, e.g., non-Fermi liquid (NFL) state in the neighborhood of quantum critical point when Fe replaces about half of the Co atoms (Fig. 1). Based on the inelastic neutron scattering, magnetic susceptibility and specific heat measurements, we also observed a pronounced decay of the crystal electric field excitations. Our studies indicate a strong evolution of physical properties with non-isoelectronic substitutions due to the rearrangement of the electronic structure, the important role of disorder, and sensitivity of the d-f hybridization.

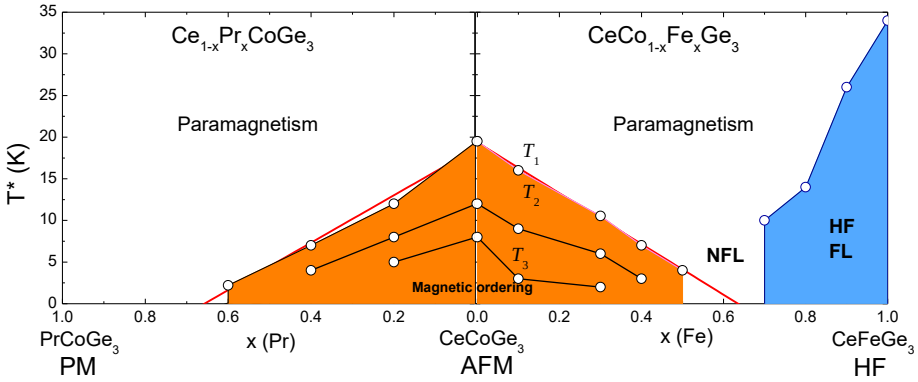


*Figure 1. Magnetic phase diagram for Pr-Ce and Co-Fe substitutions in the parent antiferromagnetic (AFM) $CeCoGe_3$ compound. PM – paramagnetic, HF – heavy fermion system, $T_1$, $T_2$, $T_3$ – different AFM phase transitions.*

[1] P. Skokowski, *et al.*, *Intermetallics*, **153** (2023) 107776
[2] P. Skokowski, *et al.*, *Phys. Rev. B*, **102** (2020) 245127

# Magnetic properties and magnetocaloric effects in antiferromagnetic $TiFe_2$ Laves phase

V. Anière[1], T. Toliński[1], and K. Synoradzki[1]

1. Institute of Molecular Physics, Polish Academy of Sciences, ul. Smoluchowskiego 17, 60-172 Poznań, Poland

Presenting author e-mail: karol.synoradzki@ifmapan.edu.pl

Thanks to their rich magnetic behavior, Laves phase intermetallics are highly relevant for magnetic cooling applications. This study examines the magnetocaloric effect (MCE) in the C14 hexagonal $TiFe_2$ alloy (space group $P6_3/mmc$). Arc-melted polycrystalline samples display an antiferromagnetic phase transition at a Néel temperature ($T_N$) of 278(1) K. Analysis of the isothermal magnetization reveals a dual nature, where normal and inverse MCE coexist. Subjected to a 5 T field change, the inverse MCE yields a peak entropy change ($|\Delta S_m|$) of 130(1) mJ $kg^{-1}K^{-1}$ at 270(1) K, outperforming the normal MCE peak of 72(1) mJ kg−1K−1 at 297(1) K. Paradoxically, the normal MCE exhibits a much larger relative cooling power (RCP ≈ 8 J $kg^{-1}$) than the inverse effect (≈ 4 J $kg^{-1}$). Despite the relatively low magnitude of the MCE, the near-room-temperature transition makes $TiFe_2$ an excellent base system for tuning magnetocaloric properties through elemental substitution.

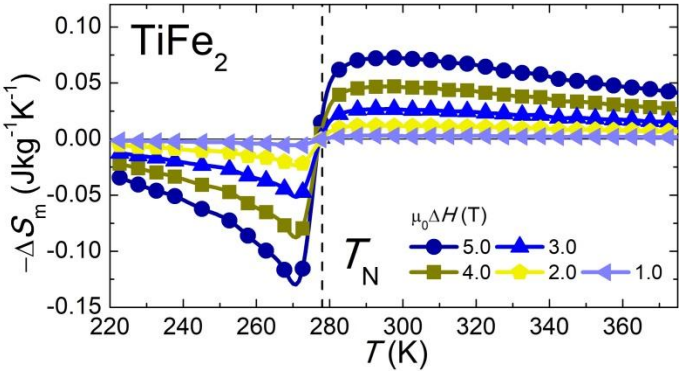


*Figure 1. Isothermal entropy change $\Delta S_m$ for $TiFe_2$ Laves compound near antiferromagnetic phase transition $T_N$ for different values of magnetic field change $\mu_0\Delta H$.*

**Acknowledgments** This study was supported by the National Science Centre (Poland) under grant 2023/51/I/ST11/02562.

# The Impact of Confinement on LC Binary Mixtures: A Comparative Study of Bulk, Electrospun Fibers, and Membranes Using Multi-Scale Techniques

M. Piwowarczyk[1], A. Deptuch[1], A. Drzewicz[1], O. Tomchuk[2], P. Jeleń[3], M. Gałązka[1], Z. Galewski[4] and E. Juszyńska-Gałązka[1,5]

1. The Henryk Niewodniczański Institute of Nuclear Physics Polish Academy of Sciences, Kraków (PL)
2. ISIS Neutron and Muon Source, Rutheford Appleton Laboratory, Didcot (UK)
3. Faculty of Materials Science and Ceramics, AGH University of Kraków, Kraków (PL)
4. Faculty of Chemistry, University of Wrocław, Wrocław (PL)
5. Research Center for Thermal and Entropic Science, Graduate School of Science, Osaka University, Osaka (JPN)

Presenting author e-mail: marcin.piwowarczyk@ifj.edu.pl

Multicomponent mesogenic systems are of particular interest due to their potential for tailoring the physicochemical properties of liquid-crystalline (LC) materials. Understanding phase behaviour in bulk and under spatial confinement is crucial for specific applications such as LC thermography. Spatial confinement, such as electrospun fibres or nanoporous membranes, restricts molecular mobility and can strongly influence mesophase formation, vitrification, and crystallization processes.

A series of binary LC mixtures with varying molar compositions was prepared. The first component was a mesogenic azo compound from the (E)-4-((4-alkyloxyphenyl)diazenyl)phenyl alkanoates group (*n*OABOOC*m*, for n = 3, 5, 7, 8, 10, and m = 1 19) [1-3], while the second component was a chiral LC, cholesteryl pelargonate (PC). Selected mixtures containing PC exhibit glassy SmA* or crystalline phases. The influence of mixture composition on glass-forming ability, thermal stability, and phase formation is discussed.

Mesomorphic behaviour, thermal properties, dynamic processes, and structural organization were studied using Polarized Optical Microscopy, Differential Scanning Calorimetry, Broadband Dielectric Spectroscopy, and X-ray Diffraction. The observed phenomena include SmA* and crystalline glass formation, melt and cold crystallization, and double-step cold crystallization. Bulk studies were extended to spatially confined systems, including electrospun fibres and nanoporous membranes, using the same techniques complemented by Small-Angle Neutron Scattering and Fourier-transform Infrared spectroscopy. The results demonstrate that confinement significantly modifies mesophase behaviour and glass formation.

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[1] M. Piwowarczyk, *et al.*, *Thermochim. Acta*, **731** (2024) 179649
[2] M. Piwowarczyk, *et al.*, *Phase Trans.*, **92** (2019) 1066
[3] M. Piwowarczyk, *et al.*, *Liq. Cryst.*, **51** (2024) 2104-2116

# Structural and magnetic characterization of REE-doped magnetite nanoparticles for wastewater treatment (REE = La, Pr, Tb, Gd)

K. A. Szarkowska[1], W. Olszewski[2], U. Klekotka[3], M. Biernacka[2] and K. Rećko[2]

1. Doctoral School, University of Białystok, Poland (k.szarkowska@uwb.edu.pl)
2. Faculty of Physics, University of Białystok, Poland (w.olszewski@uwb.edu.pl, m.biernacka@uwb.edu.pl, k.recko@uwb.edu.pl)
3. Faculty of Chemistry, University of Białystok, Poland (u.klekotka@uwb.edu.pl)

Presenting author e-mail: k.szarkowska@uwb.edu.pl

This study investigates the structural and magnetic properties of rare-earth doped $Fe_3O_4$ nanoparticles. X-ray powder diffraction (XRPD) analysis confirmed that all synthesized samples are single-phase with a cubic inverse spinel structure ($Fd\bar{3}m$, no. 227), similarly to [1]. Mössbauer spectroscopy (MS) showed that REE dopants preferentially occupy both sites with preference to tetrahedral (A) positions. These findings require neutron studies to determine the stable magnetic state, considering the location and individual magnetic moments of cations. Due to their crucial and easily tunable magnetic properties, these materials represent promising candidates for effective eco-filters for the treatment of industrial wastewater and soils, as mentioned in [2–4].

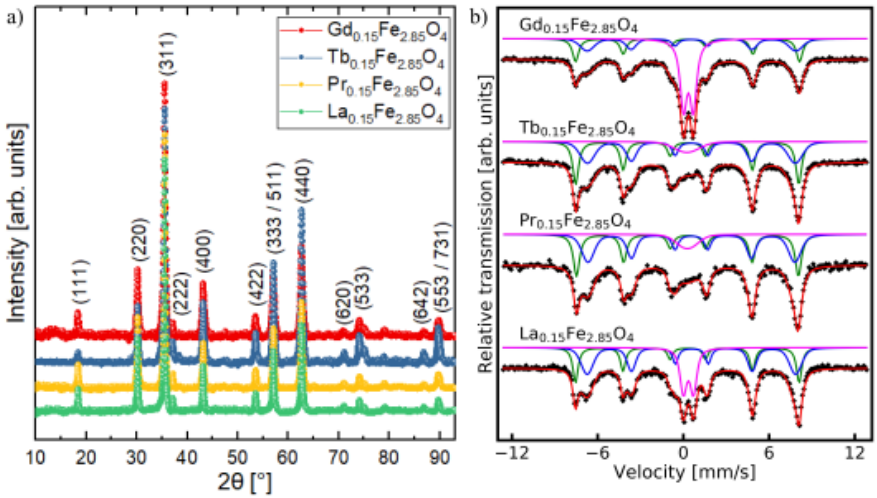


Figure 1. a) XRPD diagrams of doped magnetite samples.
b) MS spectra of $REE_{0.15}Fe_{2.85}O_4$ ($^{57}Co$ isotope, $Rh$ matrix).

[1] A.V. Rutkauskas *et al., J. Nanopart. Res.*, **27** (2025) 1-15
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[3] D. L. Hutchins *et al., Sep. Sci. Technol.*, **55** (2019) 2822-2829
[4] S. Daffalla, *Int. J. Mol. Sci.*, **26** (2025) 8499

# Multiscale Characterization of AZ31 Deformation Using Neutron and X-ray Diffraction Methods

A. Ludwik[1], M. Wronski[1], P. Kot[2], A. Baczmanski[1], S. Wronski[1], K. Wierzbanowski[1],

G. Farkas[3], K. Máthis[4], G. Garcés[5], E. Oñorbe[6], G. Bruno[7]

1. AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland
2. National Centre of Nuclear Research, A. Sołtana 7, 05-400 Otwock-Świerk, Poland
3. Nuclear Physical Institute, ASCR, Hlavní 130 25068, Rež, Czech Republic
4. Department of Physics of Materials, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3 12116, Prague, Czech Republic
5. National Center for Metallurgical Research (CENIM-CSIC), Madrid, Spain
6. CIEMAT, Division of Energy Interest Materials, Av. Complutense, 40, 28040 Madrid, Spain
7. Physikalisch-Technische Bundesanstalt (PTB), Abbestr.2-12, 10587 Berlin, Germany

Presenting author e-mail: aludwik@agh.edu.pl

AZ31 magnesium alloy, a representative hexagonal close-packed material, exhibits pronounced plastic anisotropy governed by crystallographic slip and twinning. This work presents a comparative analysis of complementary diffraction-based experimental methodologies for investigating these deformation mechanisms.

In-situ neutron diffraction combined with the crystallite group method (CGM) enables direct determination of resolved shear stress (RSS) and critical resolved shear stress (CRSS) for individual deformation systems by analysing lattice strains in selected grain families. Its main advantage lies in statistical representativeness and identification of active mechanisms under loading paths.[1]

In contrast, energy-dispersive synchrotron X-ray diffraction (ED-XRD) provides high angular resolution and simultaneous acquisition of multiple reflections, allowing detailed tracking of lattice strain evolution. When coupled with the q-parameter method, it enables separation of macroscopic and intergranular stresses, offering insight into stress partitioning and strain incompatibilities.

The comparison demonstrates strong complementarity of both techniques, integrated approach provides a robust experimental framework for validation of crystal plasticity models and improved understanding of anisotropic behaviour in magnesium alloys.

This work was founded by the National Science Centre, Poland (NCN), under grant no. UMO - 2023/49/B/ST11/00774.

[1] A. Ludwik, M. Wroński, P. Kot, A. Baczmański, S. Wroński, K. Wierzbanowski, G. Farkas, K. Máthis, *Journal of Magnesium and Alloys*, **14** (2026), 101872

# Magnetization behavior and Magnetocaloric Effect in the Laves phase compound $Sc_{0.2}Ti_{0.85}Fe_{1.95}$

V. Anière,[1] T.J. Bednarchuk,[2] and K. Synoradzki[1]

1. Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
2. Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland

Correspondence to: valentin.aniere@ifmpan.edu.pl

As it shows a distinctive, highly stoichiometry-dependent magnetic behavior [1], the pseudo-binary intermetallic Laves phases system $Sc_{1-x}Ti_xFe_2$ is of important interest in studying systems showing high values of magnetic entropy change $\Delta S_M$ at room temperature for use in solid-state cooling devices based on the Magnetocaloric Effect (MCE). Presented here are the magnetic properties and the MCE in a polycrystalline sample of $Sc_{0.2}Ti_{0.85}Fe_{1.95}$ in low temperatures ($T$ = 2-380 K) and in fields up to 9 T. This compound crystallizes in the hexagonal $MgZn_2$-type structure $C_{14}$ (space group $P6_3/mmc$). It exhibits a complex magnetic structure, with two close yet distinct transitions for $H \leq 0.1$ T around $T_{C1}$ = 256 K and $T_{C2}$ = 225 K; and, for fields $H \geq 0.5$ T, a further increase in magnetization around $T_{C3}$ = 72 K. The magnetization of the sample (showing a soft ferromagnetic behavior, with $H_C$ = 2.2(5) mT) saturates at 5 K with a value of 0.51815(3) $\mu_B$.Fe$^{-1}$ at 9 T, but still increases for $T \geq 200$ K, reaching at 200 K a value of 0.53187(5) $\mu_B$.Fe$^{-1}$ at 9 T. For a magnetic field change $\mu_0\Delta H$ = 5 T, a peak value of magnetic entropy change $\Delta S_M$ is found around $T_{C1}$ with $|\Delta S_M|$ = 1.262(3) J kg$^{-1}$ K$^{-1}$. Furthermore, for a magnetic field change lower than 1 T, an additional peak is found close to $T_{C2}$, yielding $|\Delta S_M|_{C1}$ = 0.17(1) J kg$^{-1}$ K$^{-1}$ and $|\Delta S_M|_{C2}$ = 0.18(1) J kg$^{-1}$ K$^{-1}$ given a magnetic field change of 0.5 T. This work contributes to further mapping the magnetic properties of $Sc_{1-x}Ti_xFe_2$ around the alloying composition $x$ = 0.8, where the compound shows a very composition-sensitive interplay between magnetic structure and values of lattice parameters.

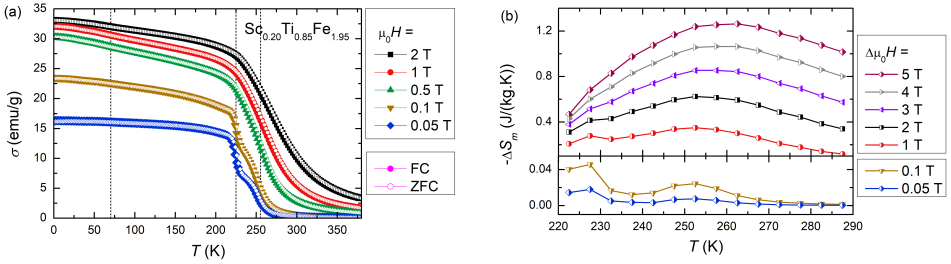


*Figure: (a) Temperature-dependent magnetization curves of $Sc_{0.2}Ti_{0.85}Fe_{1.95}$ at 0.05, 0.1, 0.5, 1 and 2 T in the range 2-380 K; and (b) magnetic entropy change as a function of temperature for 0.05, 0.1, and 1-5 T values of magnetic field change and in the range 220-290 K.*

*Funded by the National Science Centre, Poland under the OPUS call in the Weave programme 2023/51/I/ST11/02562.*

[1] Y. Nishihara and Y. Yamaguchi, *Journal of the Physical Society of Japan,* **54** (1985) 1122-1130