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Contents

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Special Editorial

Dear members of the Groupement AMPERE,

We find ourselves navigating through challenging times. When looking through the last editorials of the AMPERE bulletin, we consistently encounter pressing issues such as global supply shortages, health inconveniences, armed conflicts, and alterations in weather patterns. While these concerns may trouble our minds, it is essential that we also celebrate the remarkable advancements and beauty that our science offers.

Innovations that seemed unimaginable just a few years ago are now part of our reality, such as ultrafast and ultrasensitive NMR techniques, access to complex biological systems, advanced diagnostic methodologies, and the development of ultrastrong magnetic fields. We can now predict protein structures and even generate entire editorials at the touch of a button.

How can we contribute to addressing the global challenges mentioned above? While opinions may vary, I am convinced, that as scientists we should do what we do best, finding fundamentally new and creative solutions. Technologies that save resources, contribute to medical advance, and connect people are needed more than ever. We should continue to take risks, and identify technology solutions that make fundamental differences. A strong community, international cooperation and exchange is thereby more important than ever. This year, the AMPERE society witnessed an impressive conference in Bilbao, excellently organized, with large turnout and strong science, sparking hope for a bright future.

As we approach the year‘s end, the AMPERE Bureau wishes you and your loved ones all the best for the holidays.

S. Hiller

Sebastian Hiller
Executive Secretary
Groupement AMPERE

Call for nominations:

AMPERE Prize for Young Investigators 2025

The AMPERE prize is given to a young principle researcher (a “rising star”) for her/his first achievements in her/his independent career. There is no strict age limit but typically researchers below the age of forty are envisioned. The prize is given biannually.

The committee now calls for Nominations for the AMPERE Prize 2025 for a young principal investigator in the field of magnetic resonance. The prize will be presented during EUROMAR Oulu (Finland) 6-10 July 2025. The prize carries a value of € 3000.

You are kindly invited to submit nominations by e-mail to the president of the prize committee:
ampereprize@ampere-society.org

Nominations must be received by 15th February 2025 and should include the following documents:

• Nomination letter
• Curriculum vitae
• List of publications and presentations at conferences

For a list of past AMPERE Prize winners see:
https://www.ampere-society.org/Awards.html

Call for nominations:

Raymond Andrew Prize 2025

In memory of Professor Dr. Raymond Andrew and to honor his pioneering work in the field of magnetic resonance, the AMPERE Group has founded the Raymond Andrew Prize. The prize is awarded to young scientists for an outstanding PhD thesis in magnetic resonance.

For the Raymond Andrew Prize 2025 the AMPERE Prize Committee is seeking your help in searching for qualified candidates who completed their dissertation during the period of 2023/2024. The prize will be presented during EUROMAR Oulu (Finland) 6-10 July 2025.

You are kindly invited to submit nominations by e-mail to:
andrewprize@ampere-society.org

Nominations must be received by 15th February 2025 and should include the following documents:

• Nomination letter
• Curriculum vitae
• List of publications and presentations at conferences
• PhD thesis in PDF

The thesis should be written in English. In exceptional cases, the thesis may also be submitted in triplicate as a hardcopy to the AMPERE Secretariat. Submissions that arrive too late will automatically be transferred to the next year. The prize committee will reconsider excellent contributions for two years in a row.

For a list of past Andrew Prize winners see:
https://www.ampere-society.org/Awards.html

Portrait:

Janez Dolinšek

Why magnetic resonance and why NMR and MRI?

At the University of Ljubljana, where I have studied physics during 1975-1980, one of my professors was Robert Blinc, who was a pioneer of NMR in Slovenia (he was also the president of Groupement AMPERE during 1992-1994). In 1980, he invited me to his laboratory at the Jožef Stefan Institute in Ljubljana for the diploma, where I was "charmed" by this spectroscopy. After diploma, I got employment in that laboratory. In 1980s, the early days of MRI (which we called "Zeugmatography" at that time), it was a matter of prestige that each NMR laboratory has designed and fabricated its own original MRI apparatus. I was involved in that research and we got the first MRI image of an apple on 25th August, 1988.

What is your favorite frequency?

No special favorite frequency. I specialized for the NMR of broad-line solids in metallic materials, like quasicrystals, complex metallic alloys, metallic glasses, high-entropy alloys, metallic magnetic materials,…, where the spectra extend over the interval of many MHz. Special techniques of field-sweep and frequency-sweep, implemented on home-made spectrometers, are needed to record so broad spectra. To date, such spectrometers are still not available commercially (to the best of my knowledge). The height of the frequency (or the magnetic field) is not an issue in such kind of experiments. The first-order quadrupolar broadening of the lines is independent of the magnetic field and the Knight shift is increasing linearly with the field. For metals, high frequencies are sometimes even disadvantageous due to the skin effect, which may reduce the sensitivity.

What do you still not understand?

Many things in solid-state physics, too many to list them here. Even the commonly used basic concepts like the exchange interaction between spins and the Fermi contact interaction between the nucleus and the s-type conduction electrons are still poorly understood (at least for me). Another such issue are quantum fluctuations, associated with the Heisenberg uncertainty principle, which trigger quantum phase transitions between magnetically disordered and ordered phases in solids at absolute zero temperature.

Luckiest experiment you have ever done.

It was the observation of thermal fluctuations of the atomic modulation wave on the sub-nanometer spatial scale in an incommensurate dielectric by 2D exchange difference

NMR spectroscopy, where the slow fluctuation frequencies accidentally matched the frequency observation window of the NMR experiment.

What was the worst mistake you have made during your lab time?

There were many of them, especially during the first years. One has happened during repair of the high-voltage power supply of the NMR spectrometer. With my (insufficient) knowledge of electronics, I tried to measure the electrical resistance of a circuit still under the line voltage, by using an old-fashioned analog voltmeter with a pointer. The pointer jumped to the end of the scale, where it has melted, touched the scale and was attached there. The pointer never moved back to zero. I was afraid that my older colleagues will dismiss me from job, but they have only smiled and told me that this is the way how an experimentalist gains the experience.

Most memorable conference story?

It has happened at the Congress AMPERE 1984 in Zürich. This was during my PhD period and at that time, I was learning NMR theory intensively from two well-known basic text books, one written by Abragam and the other by Slichter. During the coffee break, I was sitting alone at the coffee table and two distinguished gentlemen approached me and asked whether they can join me. Then they introduced themselves – one said "I am Anatole Abragam" and the other said "I am Charlie Slichter".

With whom (historical person) would you like to meet?

In history, many people have significantly and importantly contributed to the development of science and society. It would be my great honor to meet any of them. If I am to pick out one particular name, this is Primož Trubar, a Slovenian protestant reformer of the Lutheran tradition, who in 1550 wrote the first two printed books in Slovenian language (Catechismus and Abecedarium).

When do you get your best ideas?
Usually early in the morning during the weekdays. I am an "early bird" type of a person, waking up soon after 4:00 a.m. Being fresh in mind at such early hours, new ideas sometimes appear.

If you had just one month time for travelling - where would you go to?
No special wishes. I like hiking in the mountains and my domestic Slovenian Alps are just great to do that.

Your idea of happiness?
It is when I know that all my people are healthy and doing well.

Position:
(1) Full professor of physics and the University of Ljubljana, Faculty of Mathematics and Physics;
(2) Scientific councilor at the Jožef Stefan Institute in Ljubljana, head of a research group.

Awards:
- Zois prize 2010 of the Republic Slovenia for outstanding achievements in solid state physics;
- Zois recognition 2001 of the Republic Slovenia for important achievements in solid state physics.

Homepage: http://slo-hea.ijs.si/?page_id=244

Education:
- PhD in Physics (1987), University of Ljubljana, Faculty of Mathematics and Physics (Thesis title: „Substitutionally-disordered incommensurate dielectrics studied by NMR", supervisor Prof. Dr. R Blinc);
- MSc in Physics (1986), University of Ljubljana, Faculty of Mathematics and Physics;
- BSc in Physics (1981), University of Ljubljana, Faculty of Mathematics and Physics.

Interests:
- Condensed Matter Physics & Materials Science (quasicrystals, complex metallic alloys, bulk metallic glasses, high-entropy alloys, nanomaterials, magnetic materials);
- Physical properties of materials (magnetism, electrical resistivity, thermoelectric power, thermal conductivity, Hall effect, specific heat);
- Nuclear Magnetic Resonance, Experimental condensed matter physics.

Report:

16th international Bologna Concerence on Magnetic Resonance in Porous Media (MRPM16)

Conference Co-Chairs: Kate Anderssen (NOFIMA, Tromsø, Norway) and John Seland (University of Bergen, Norway).

Steering Committee: Yiqiao Song (Chair), Sabina Haber-Pohlmeier (Vice-Chair), Siegfried Stapf (Treasurer), Paola Fantazzini (Ex-Officio), Xueqian Kong (Past Meeting), Ruiliang Bai (Past Meeting), Russ Bowers (Present Meeting), Sergey Vasenkov (Present Meeting) Kate Anderssen (Current Meeting), John Seland (Current Meeting).

Local Organizing Committee: Heidi Katrine Trige, Heidi Nilsen, Frederico Lian.

International Advisory Committee: R. Accosta, M. Appel, K. Anderssen, I. Ardelean, C. Arns, M. Bencsik, B. Blümich, T. Bonagama, V. Bortolotti, R. Bowers, M. Britton, G. Ferrante, P. Galvosas, D. Grebenkov, G. Guthausen, S. Haber-Pohlmeier, M. Johns, M. Komlosh, I. Mastikhin, C. Mattea, N. Nestle, W. Price, J. Seland, J. Seymour, Y. Song, S. Stapf, R. Valliulin, S. Vasenkov, L. Xiao.

The 16th International Bologna Conference on Magnetic Resonance in Porous Media (MRPM16) convened from August 26th-30th, 2024 in Scandic Ishavshotel in the center

of Tromsø, Norway.
120 attendees from 15 countries (Australia, Brazil, Canada, China, Denmark, Finland, France, Germany, Italy, New Zealand, Norway, Poland, Sweden, UK, USA) attended stimulating lectures and engaged in enthusiastic scientific discussions. Session topics included magnetic resonance methodology and hardware development for porous media studies with the following sub-topics: Polymers and Nanoporous systems, Food Science, Biofilms and Biomaterials, Environmental applications, Medical applications, and Petrophysical applications.

The conference was preceded by a one-day Tutorial Workshop. Expert tutorials were presented by Bernhard Blümich (RWTH Aachen University), Siegfried Stapf (TU Ilmenau), Christoph Arns (UNSW Sydney), and Yiqiao Song (Harvard University).

The program opened with plenary lectures by Søren Balling Engelsen (University of Copenhagen) and Daniel Topgaard (Lund University). The first day ended with a Welcome Reception at Polaria Aquarium.

The Giulio Cesare Borgia Prize is awarded to a young researcher at the Bologna MRPM conference. This prize memorializes the contribution made by Dr. Borgia to the development of magnetic resonance in porous media and the attention he always paid to the enthusiasm, passion, and courage of young people who undertook the difficult and adventurous path of scientific investigation in this fascinating area of research. The 2024 Giulio Cesare Borgia Prize went to Teddy Xuke Cai (NIH, USA) for deepening our understanding of exchange processes in biological porous media. Teddy gave a very stimulating talk at the conference with the title “A direct, time domain measurement of the velocity autocorrelation function”.

The Award for the Best Oral Presentation at MRPM16 was given to Tobias Splith (“Soil moisture measurements with compact prepolarization surface NMR sensors”).

The prize committee for the Borgia Prize and the Best Oral Presentation was comprised of Petrik Galvosas, Marc Fleury, John Seland, Yiqiao Song and Siegfried Stapf.

Awards were given to the following top three student posters: Stefan Benders (“The TUHH process imaging system”), Patrick Vogel (“Pore size determination via mobility measurements of magnetic nanoparticles – a proof of concept”), and Matthew Young (“250 and 2 MHz Nuclear Magnetic Resonance Characterization of Water Adsorption in Corn Stover Anatomical Fractions”). The poster prize committee was comprised of John Seland, Joe Seymour, Catherine Kirkland, Nathan Williamson, and Einar Fridjonsson.

After some initial rainy days, the conference attendees enjoyed a sunny afternoon of discovery and sightseeing in the surrounding mountain areas of Tromsø. The conference banquet was held at the Skirri Restaurant located in the harbour area of the city. The conference concluded with a General Assembly.

The MRPM International Advisory Committee met to consider proposals for future venues for MRPM conferences, and it was unanimously agreed that the next MRPM conference (MRPM17 in 2026) will be chaired by Tito Bonagamba (University of Sao Paulo) in the city of Campinas, Brazil. It was also unanimously agreed that the MRPM18 (in 2028) will be chaired by Marc Fleury (IFP Energies nouvelles) in the city of Avignon, France.

Financial support for MRPM16 was provided through the generosity of the following corporate sponsors: Bruker, AnTEK, Resonance Systems, inMR measure, Limecho, NIUMAG, Nofima, MR solutions.

Engaged and happy conference participants at the General Assembly on the final day of MRPM16.

Giulio Cesare Borgia Prize: MRPM16

Teddy Xuke Cai

A direct, time-domain measurement of the velocity autocorrelation function

Teddy Xuke Cai[a], Nathan Hu Williamson[a], Rea Ravina[b], Peter Joel Basser[a]

a: Section on Quantitative Imaging and Tissue Sciences, NICHD, NIH, Bethesda, MD, USA;
b: Celoptics Inc., Rockville, MD, USA

Diffusion microstructural MR aims to reveal features of the tissue microenvironment such as compartment structure size, shape, and permeability. This usually involves fitting diffusion MR data to compartment signal models [1], though such models require assumptions about the number of compartments and their connectivity. A model agnostic approach is to measure the time-dependent diffusion behavior, i.e., fundamental transport quantities such as the velocity autocorrelation function (VACF). In principle, the VACF contains all the information necessary to characterize the microstructure. Conventionally, the VACF is measured via its frequency-domain specturm using oscillating gradient sequences in an approach called temporal diffusion spectroscopy (TDS) [2]. However, the TDS acquisition is limited by gradient hardware and the small range of frequencies one can probe with it [3].

Here, we describe a method that can robustly measure the VACF *in the time domain* across a wide range of timescales. The method is based on taking the ratio of two Diffusion Exchange Spectroscopy (DEXSY) acquisitions, each of which consists of two diffusion encodings separated by a longitudinal mixing time, t_m. In Fig. 1a, we show the DEXSY sequence implemented for static gradients (SG), wherein the timings τ_1 and τ_2 are used to vary the diffusion weighting.

According to Ning *et al.* [4], a diffusion MR experiment can be viewed as a weighting of the instantaneous diffusivity $D_{inst}(t) = \partial_t \langle r^2(t) \rangle /2$, where $\langle r^2(t) \rangle$ is the mean-squared-displacement (MSD), by the cumulative gradient autocorrelation $C(t)$ (valid under stationarity and the Gaussian phase approximation). In Fig. 1b, we show the $C(t)$ curves for two SG-DEXSY acquisitions, one with maximal exchange-weighting achieved via $\tau = \tau_1 = \tau_2$, called S_{mid}, and another with the same diffusion weighting (i.e., $\tau_1^3 + \tau_2^3$ held constant) but little to no exchange weighting ($\tau_2 \approx 0$), called S_{end}. The ratio of these points provides an experimental measurement of $\partial_t D_{inst}(t)$ centered at $2\tau + t_m$ where τ corresponds to S_{mid}. This is equivalently the VACF $= \partial_t^2 \langle r^2(t) \rangle /2$:

$$\partial_t D_{inst}(2\tau + t_m) \approx \frac{9}{4\gamma^2 g^2 \tau^4}\left[\ln\left(\lim_{t_m\to\infty}\frac{S_{mid}(t_m)}{S_{end}(t_m)}\right) - \ln\left(\frac{S_{mid}(t_m)}{S_{end}(t_m)}\right)\right].$$

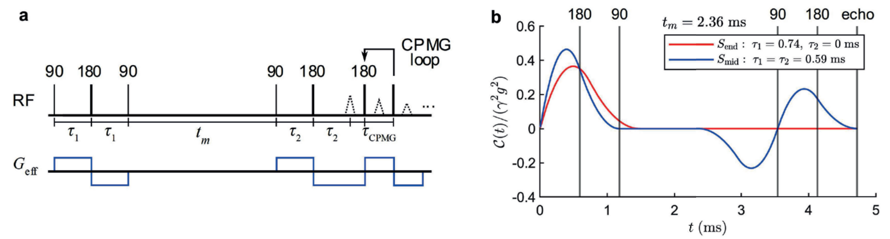

Figure 1 – DEXSY experiment and sampling scheme. (a) SG-DEXSY pulse sequence with a CPMG acquisition. (b) Sampling scheme of S_{mid} and S_{send} with exemplar timing parameters. Note how S_{mid} probes a slope in $D_{inst}(t)$ via the pair of positive and negative lobes. Dividing S_{send} normalizes relaxation effects and roughly cancels the first lobe, leaving an isolated VACF measurement.

In Figs. 2a and b, we apply Eq. (1) to estimate the VACF using data from Monte Carlo simulations in a grid of permeable, monodisperse spheres (radius = 0.95 μm) and from measurements of viable, *ex vivo* neonatal mouse spinal cord using the PM- 10 (Magritek, Aachen, Germany) permanent magnet ($g \approx 15.3$ T/m, $B_0 \approx 0.3$ T), respectively. The VACF curves reproduce the expected behavior of a negative tail (due to reflection) that asymptotically approaches 0 as the system loses its memory. The VACF is seen to be highly sensitive to exchange – the pore residence time, measured in a similar manner [5], is marked in the log-log insets as τ_k. To our knowledge, this is the only method capable of directly measuring the VACF in the time domain and does so across orders of magnitude in time. The method paves the way for future studies of these fundamental transport quantities.

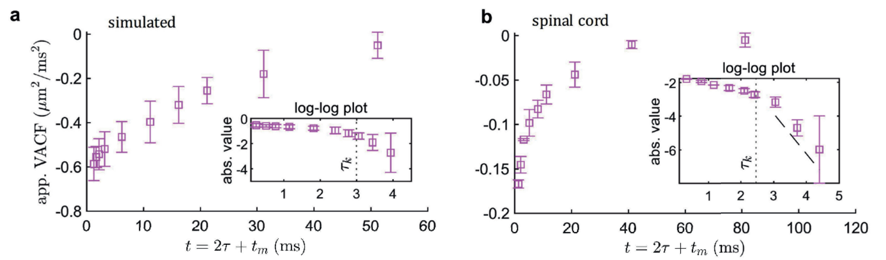

Figure 2 – Apparent VACF curves from (a) simulations in monodisperse spheres of radius 0.95 μm and (b) viable spinal cord. Insets show a log-log plot. Note the accelerated approach to 0 as $t > \tau_k$, suggestive of exchange having a significant effect on the VACF. In spinal cord, a long-time power law with $\sim t^{2.4}$ is plotted (dashed line), which is roughly consistent with disordered domains in 3-D [6].

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Best oral presentation: MRPM16

Tobias Splith

Soil moisture measurements with compact prepolarization surface NMR sensors

Tobias Splith[a], Thomas Hiller[b], Stephan Costabel[c], Mike Müller-Petke[a]

a: LIAG Institute for Applied Geophysics, Hannover, Germany
b: Federal Institute for Geosciences and Natural Resources, Cottbus, Germany
c: Federal Institute for Geosciences and Natural Resources, Berlin, Germany

Understanding the temporal dynamics and spatial distribution of soil moisture is essential for numerous bio-geochemical processes. In recent years efforts have been made to use prepolarization surface nuclear magnetic resonance (PP SNMR) for non-destructive soil moisture investigations [1, 2]. PP SNMR layouts can be designed relatively compact (coil diameters in the range of meters) compared to classical SNMR layouts (coil diameters from 10 to 150 meters). Therefore, it can be used for mobile measurements schemes, i.e. mapping of soil moisture. Nonetheless, the short NMR pulses, which are necessary because of the short relaxation times expected in the unsaturated soils, and the prepolarization, which is needed to boost the received signals, introduce some significant extension to the general SNMR forward description. Because of the short pulses of high intensity, the Bloch-Siegert effect needs to be considered [3, 4]. Additionally, the prepolarization field switch-off is never completely adiabatic for all practical applications, i.e. the macroscopic magnetization before the pulse will not be aligned with the direction of Earth's magnetic field $\boldsymbol{B}_0$ in significant parts of the subsurface [5]. The combination of both effects strongly influences the received signal and introduces a dependence on the excitation pulse phase and the timing of the pulse sequence, which needs to be considered in order to model the experiments, understand the measured data, and obtain correct soil moisture distributions by inversion.

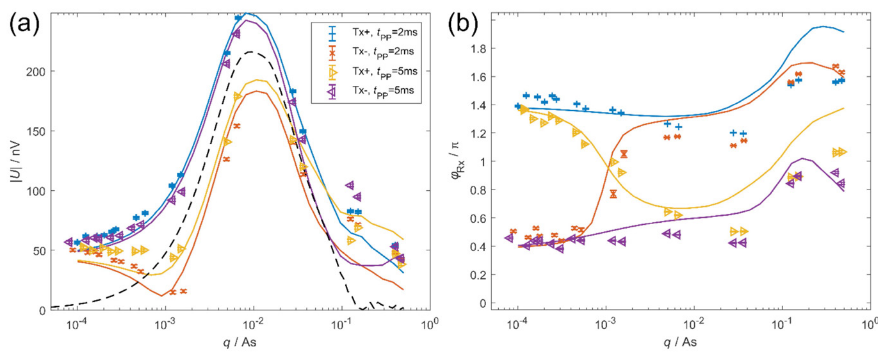

Figure 1: Signal amplitude (a) and phase (b) of SNMR measurements performed on top of water containers as a function of the pulse moment q. The measurements were performed with a pulse duration of τ_{Tx} = 1.89 ms (four periods at the local Larmor frequency of f_L = 2113 Hz), two delay times t_{PP} between prepolarization and pulse, and at both transmitter phases. The straight lines represent models considering the Bloch-Siegert effect and the non-adiabatic PP switch-off. If these two effects are neclected, the signal amplitude (black dashed line in (a)) is independent of both the transmitter phases and the delay time, while the signal phase remains constant.

In order to evaluate the theoretical considerations, measurements were performed on water containers. Figure 1 presents the signal amplitude (a) and the signal phase (b) obtained in these measurements for different transmitter phases and prepolarization delays t_{PP}. For models that neglect both, the Bloch-Siegert effect and the non-adiabatic prepolarization switch-off, the signal is independent of the transmitter phase and the prepolarization delays t_{PP}, i.e. all models yield the same signal amplitude (dashed line in Fig.1a), and a constant phase (not shown), which fails to describe the measured data. On the other hand, the models considering both effects (continous lines) are in good agreement with the respective data for a large range of pulse moments q. The remaining deviation between models and measurments at higher pulse moments might be attributed to imperfect (non- sinusoidal) pulse shapes and transients at pulse switch-off.

To demonstrate the practical applicability of the PP SNMR technique to soil moisture investigations, we performed additional measurements in the Gnarrenburger Moor peatland area. The refined modelling is used to describe and invert the measured data. We are able to obtain the soil moisture distribution and detect the upper boundary of the fully saturated peat body with the PP SNMR technique.

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Poster Prize: MRPM16

Stefan Benders

The TUHH process imaging system

Stefan Benders[a], Hannah Rennebaum[a], Alexander Penn[a]

a: Hamburg University of Technology, Insitute of Process Imaging, Hamburg, Germany

Chemical engineering is a crucial field in the production of many essential goods, with its processes undergoing major changes in the transition to a less fossil-dependent product chain. Yet, understanding these processes is often based on modeling and measurements with integral or local invasive sensors. Tomographic techniques such as magnetic resonance imaging (MRI) can overcome these limitations and provide essential information. However, MRI systems are typically not constructed with the needs of (bio) chemical reactors in mind. Most vertical MRI systems feature probe diameters of below 8 cm and maximum sample heights of below 1 meter. On the other end, clinical MRI systems are usually built horizontally and feature bore sizes of bigger than 30 cm and maximum sample lengths of a few meters. However, due to their orientation, processes based on gravity have to conform to the bore size and are therefore limited.

The TUHH system combines the advantages of both systems. It is a vertical bore magnet with a 40 cm bore diameter. Sitting on legs at 4 m height, samples of up to 3 meters can be measured. This is especially relevant for reactors based on gravity such as fluidized beds or bubble columns. The magnet itself is a cryogen-free magnet with a field strength of 3 T. The clinical backend of the system enables to exploitation of the benefits of MRI techniques developed for the medical field as well as the use of modern techniques such as parallel imaging. The RF body coil is driven by a 2×17 kW amplifier and the gradients are capable of producing up to 125 mT/m with a slew rate of 330 T/m/s. Up to 32 channel receive arrays can be connected to enable high SENSE acceleration factors.

Figure 1: The TUHH process imaging system

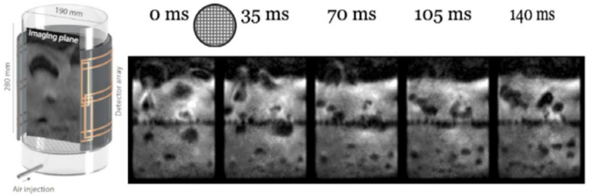

Figure 1: A fluidized bed with a grid baffle insert at 1.2 U_{mf} [1,2]

The system is freshly commissioned in 2024 and is planned to be used in various projects. In particular, the work of Alexander Penn in ultrafast imaging will be continued and extended in scope[1,2]. A main focus here are fluidized beds and liquid-gas reactors, which can be investigated with temporal resolutions below 30 ms. Furthermore, techniques such as thermometry and chemically resolved imaging will be employed to reveal the processes inside important reactor systems.

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Poster Prize: MRPM16

Patrick Vogel

Pore size determination via mobility measurements of magnetic nanoparticles – a proof of concept

J. Günther[a], T. Reichl[a], T. Driessle[b], M.A. Rückert[a], T. Kampf[a,c], V.C. Behr[a], P. Vogel[a,b]

a: Department of Experimental Physics 5 (Biophysics), University of Würzburg, Germany
b: Pure Devices GmbH, Rimpar, Germany
c:Department of Diagnostic and Interventional Neuroradiology, University Hospital of Würzburg, Germany.

Porous materials are found throughout nature and are important for a multitude of industrial, medical, and natural processes. For instance, the pores within catalysts increase the surface available for reactions to occur, reactants and products are directed to and from active sites through the porous structure and the size of the pores present in pharmaceutical tablets directly relates to their dissolution rate. Pores are the openings in solid surfaces which gases, liquids, or even foreign microscopic particles can occupy. When considering pore size, a set of standards approved by IUPAC has defined pore size ranges based on different size widths [1]. Pores are also defined by their accessibility to the surface of the material (blind pores, through pores, and closed pores). Multiple methods for studying pore size distribution and pore connectivity have been introduced in the past. For example, methods such as gas adsorption, mercury intrusion, capillary flow porometry and NMR are widely used today.

A novel approach measuring the mobility of magnetic nanoparticles (MNPs) [2] is the **C**ritical **O**ffset **M**agnetic **PA**rticle **S**pectro**S**copy (COMPASS). This technique uses a combination of dynamic (AC) and static (DC) magnetic fields in the range up to 50 mT and frequencies up to 25 kHz to measure slight changes in the mobility of MNPs [2]. MNPs come in many different variations of iron-core diameters, hydrodynamic diameters, causing a unique measurement signal in a COMPASS measurement. Extending such a measurement to a range of different field strengths a fingerprint-like pattern (Fig. 1 left) occurs for each particle system influenced by the MNPs' surrounding. Furthermore, MNPs often show a high wetting ability, making them an interesting candidate for investigating porous media.

In this abstract we demonstrate a proof-of-concept experiment using the magnetic nanoparticle-based COMPASS method to investigate the influence of the pore-sizes

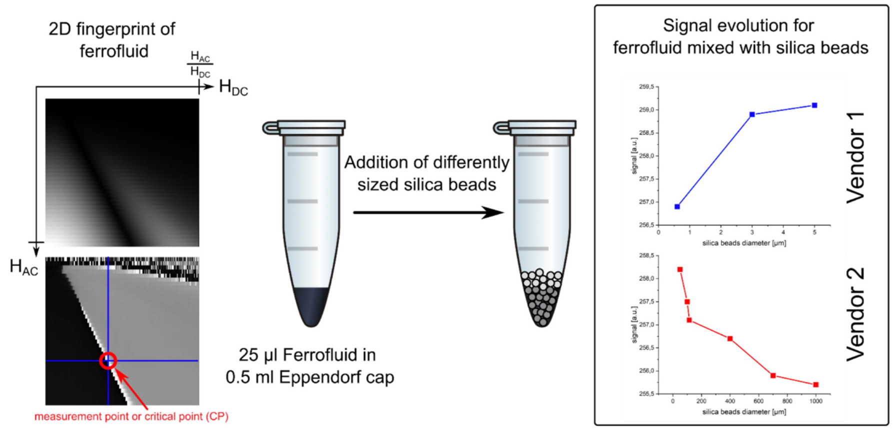

Figure 1: Left: Example of unique fingerprint of MNPs (Ferrofluid) showing the abs value (top) and phase (bottom) of the 3rd higher harmonic. At specific AC/DC ratios, critical points (CPs) occur, providing high sensitivity to MNP mobility. **Center:** Preparation of the silica- bead samples: in a first step, the Eppendorf caps were filled with 25 µl of common Ferrofluid (average iron-core diameter of 3-7 nm). After that, silica-beads with different diameters were added to guarantee a full coverage of the surface of all silica-beads with the MNPs. **Right:** For two different vendors of silica-beads with different diameter ranges, differences in the critical point (CP) position with changing silica-bead diameters size are visible.

between silica-beads with different diameters. Silica-beads with different diameters from two vendors (Vendor 1 & Vendor 2) have been prepared in an Eppendorf cap and tested as described in Figure 1 center. Studying the 1st critical-point position (AC/DC ratio) of the 3rd higher harmonic of the COMPASS signal, two different behaviors can be detected as depicted in Figure 1 right. In both cases, the signal clearly shows difference in the signal for different diameters of the silica-beads.

Initial results presented in this abstract indicate the ability to differentiate silica-bead sizes using COMPASS. This is a first step in investigating its potential as a highly portable and robust method for studying porous media.

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Poster Prize: MRPM16

Matthew C. Young

250 and 2 MHz Nuclear Magnetic Resonance Characterization of Water Adsorption in Corn Stover Anatomical Fractions

Matthew C. Young[a], Sarah L. Codd[b], Evan R. McCarney[c], David B. Hodge[a] and Joseph D. Seymour[a]

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b: Montana State University, Department of Mechanical and Industrial Engineering, Bozeman, MT 59717, USA
c: Korimako Chemical Ltd., Wellington, New Zealand

Fossil feedstocks are finite natural resources frequently used to produce high value goods including fuels and chemicals, despite their contribution to global CO_2 emissions. Recent emphasis has been placed on the deconstruction and conversion of agricultural residues, such as corn stover, as a fossil feedstock alternative. The cell walls of agricultural residues are predominantly made of cellulose, a dense polysaccharide which can be hydrolyzed to glucose monosaccharides. As lignocellulosic biomass, these cell walls also contain lignin and hemicellulose, which limit enzymatic accessibility to cellulose and make the cell wall recalcitrant. A pretreatment step improves cellulose accessibility by disrupting the cell wall matrix. Optimized pretreatment improves scalability of deconstruction processes but requires rapid characterization techniques and strong predictors of enzymatic hydrolysis yield.

Since water facilitates enzyme delivery within biomass, the distribution of water is a proxy for enzyme accessibility. 250 MHz nuclear magnetic resonance (NMR) relaxometry is applied to corn stover to improve understanding of enzyme accessibility within these systems [1]. These techniques directly measure water adsorption in anatomical fractions of corn stover. NMR transverse T_2 relaxation time distribution measurements indicate multiple water populations, which vary with anatomical fraction and water adsorption. Measured T_2 data are used to calculate thermodynamic properties of Brunauer-Emmet-Teller (BET) adsorption theory using a model to estimate mono and bilayer relaxation [1, 2]. T_2 data are used to determine rotational diffusion correlation times indicating adsorption interaction strength. T_1-T_2 longitudinal-transverse relaxation time correlation measurements quantify differences in the molecular level structural order of the adsorbate surface water as a function of water activity, i.e. relative humidity or water vapor partial pressure. The T_1 /T_2 ratio provides a measure of the surface energy related to the adsorption strength and surface diffusive mobility of the water adsorbate, and differentiates the anatomical fractions [1, 3].

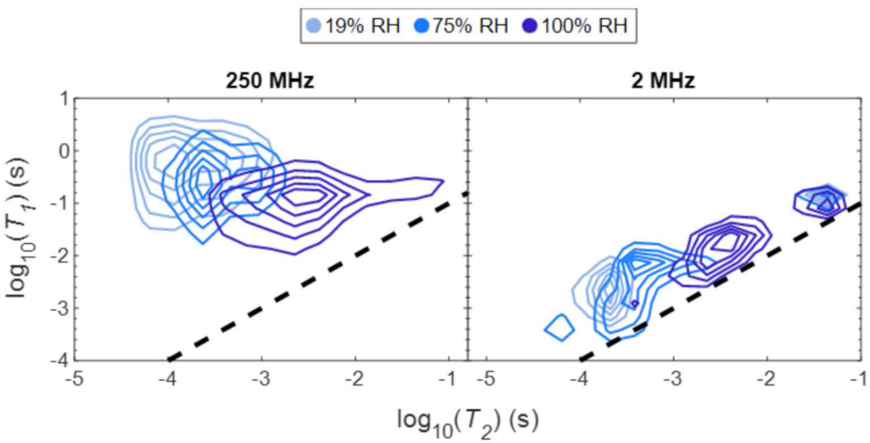

Figure 1: NMR T_1-T_2 correlations of corn stalk leaf at 19, 75 and 100% relative humidity (RH). 250 MHz data, on left, was acquired with 12 μs τ_2 and 2 MHz data, on right, was acquired with 50 μs τ_2. The dashed line is the T_1=T_2 parity line.

The results indicate that direct measurement of NMR relaxation times can be used to characterize corn stover biomass water adsorption, which are data relevant to biomass processing and handling. This approach to characterize water adsorption in corn stover was repeated with 2 MHz NMR [4]. The 125 times decrease in field strength forces measurements into the transition and fast motion, or motionally narrowed, regimes. Comparison of slow motion, or motionally broadened, data at 250 MHz and motionally narrowed 2 MHz data demonstrates motional regime dependent behavior. 2 MHz NMR data transitions through the T_1 minimum with hydration, and the corresponding T_1 / T_2 does not directly track with moisture as at 250 MHz. Hardware limited 50 μs τ at 2 MHz versus 12 μs at 250 MHz, manifests in low field data through enhanced molecular exchange averaging between sites of different molecular restriction. Resulting from these compounding effects, 2 MHz relaxometry directly indicates the hydration level at which significant water mobility changes and exchange between high and low mobility domains occur.

This is a clear signature of biomass microstructural changes due to saturation of sorption and solvation sites. These procedures may be extended to pretreated lignocellulosic biomass to study how morphological changes impact adsorption, and applied to monitor enzymatic hydrolysis progress *in situ*.

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Report:

XII^th Conference of the European Federation of EPR groups (EFEPR 2024)

September 8-12 2023, Marseille, France

https://efepr2024.sciencesconf.org/

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The 2024 edition of the EFEPR conference happened 5 years after the previous one hosted in Bratislava, due to the COVID outbreak. It gathered, in Marseille a total of 128 participants from Belgium, Canada, Switzerland, Germany, Denmark, Spain, France, UK, Greece, Croatia, Israel, Iceland, Italy, Lithuania, the Netherlands, Slovakia, and the United States of America and was organized by the CNRS and Aix-Marseille University. It coincided as well with the 20th anniversary of ARPE, the French EPR Association.

The scientific program consisted of 7 plenary lectures, 9 keynotes, 28 oral communications and 55 posters and covered a broad range of EPR applications throughout the fields of physics, chemistry and life sciences. In addition, 3 sponsor communications were given by Bruker Biospin, Cryogenic and Jeol.

Plenary lectures were given by:
Sharon Ruthstein, Bar-Ilan University (IL) *The copper cellular transfer mechanism in eukaryotic and prokaryotic systems*
Patrice Bertet, CEA Saclay (FR) *Single-spin spectroscopy using microwave photon counting*
Sabine Richert, University of Freiburg (DE) *Exploring the properties of photogenerated molecular multi-spin systems*
Daniella Goldfarb, Weizmann Institute of Science (IL) *Distance measurements in proteins in solution and cells by ^{19}F ENDOR*

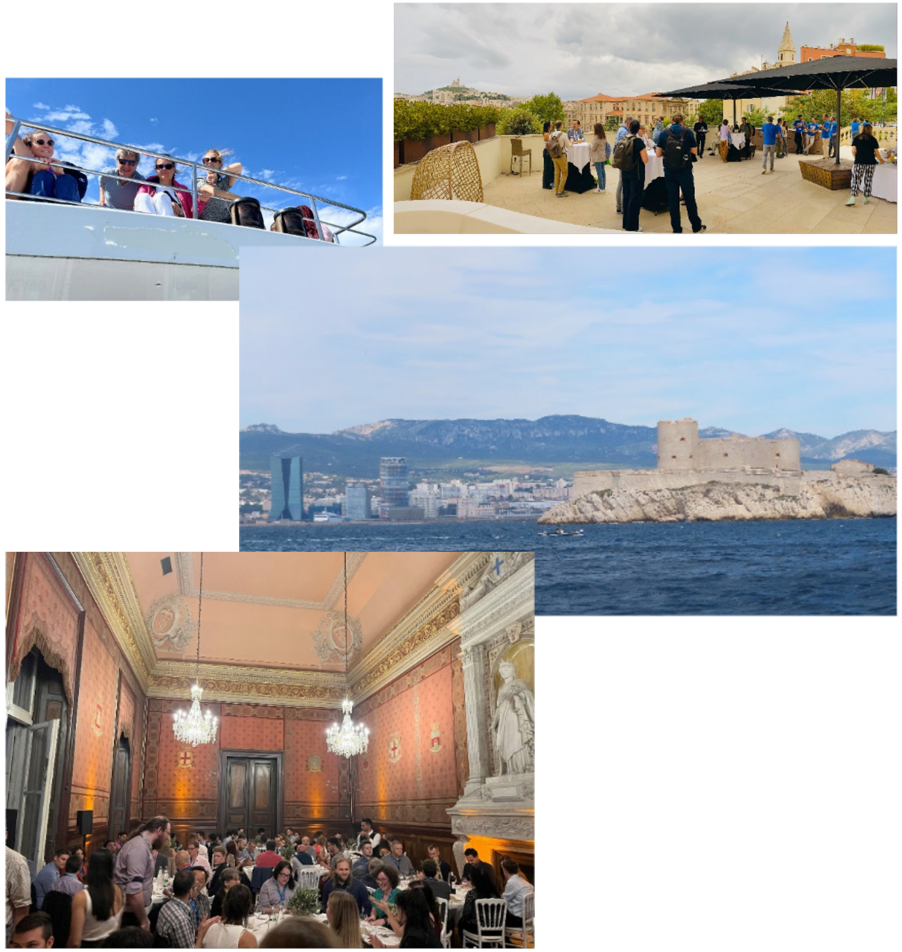
José Vidal Gancedo, Barcelona Institute of Materials Science (ES) *EPR in the characterization of radical dendrimers*
Enrica Bordignon, University of Geneva (CH) *Pros and Cons of probing dynamic proteins interactions in liquid droplets and membrane bilayers with EPR*
Eric McInnes, The University of Manchester (UK) *Magnetic resonance studies of supramolecular chemistry based on heterometallic rings*

Keynote lectures were given by:
Daniel Klose, ETH Zurich (CH) *Intertwined instrumentation and method developments for multifrequency EPR hyperfine spectroscopy*
Mantas Šimėnas, Vilnius University (LT) *Towards the sensitivity limit of EPR cryoprobes*
Valérie Belle, Aix-Marseille University (FR) *Site directed spin labeling-EPR spectroscopy in all its facets*
Claudia Tait, University of Oxford (UK) *Characterisation of photoinduced spin states in organic photovoltaics by transient and pulse EPR*
Emma Richards, Cardiff University (UK) *Long-lived, ambient Cr(III)-based near-IR emission, and donor-acceptor dyads for upconversion technologies*
Maria Fittipaldi, University of Florence (IT) *Spin-electric effects on magnetic molecules revealed by electric-field-modulated EPR spectroscopy*
Jan Behrends, Freie Universität Berlin (DE) *Electron spins at work in organic radical batteries*
Andreas Pöppl, Leipzig University (DE) *An EPR study of hydrogen molecule adsorption on nanoporous materials*
Bela Bode, University of St Andrews (UK) *Pulse dipolar EPR spectroscopy in the age of computational structure prediction - new structures and functions of proteins*

Posters were displayed throughout the conference and two poster sessions were more specifically planned on the evenings of Monday 9th and Tuesday 10th September. Two poster prizes were awarded by the International EPR Society (IES) to Zichen Wang (University of Cambridge, UK) and Dr Ilenia Serra (Aix-Marseille University, France). The IUPAB awarded an oral communication prize to Marvin Lenjer (Max Planck Institute Göttingen, DE).

The EFEPR general assembly was held before the second poster session on Tuesday and was also hosted online so that EFEPR members who could not be present at the conference would be able to attend as well. Information was given on EFEPR as a Groupement AMPERE subgroup. Next events were discussed: the 10th EFEPR Summer School will be held in Manchester from August 31st till September 6th 2025. Proposals for the future schools in Spain (Barcelona/Zaragoza) in 2027 and Italy (Caorle/Padova) in 2029 were presented by Inés García Rubio and Marilena Di Valentin. Proposal for the next conference in Brno in 2026 was presented by Petr Neugebauer. These proposals were accepted unanimously. Information were then given on the EFEPR website (www.efepr.org) and the mailing list. Finally, a proposal was made for the composition and term duration of the EFEPR board: the board is composed of a president, 2 vice-presidents (ideally the former president and the designated future president to ensure continuity) and a secretary general. Elections would happen at the general assembly held at the EFEPR conferences. After the elections, the composition of the EFEPR board is: President Gunnar Jeschke; Vice-Presidents Inés García Rubio and Pierre Dorlet, Secretary General Daniel Klose.

In addition of all the discussions and exchanges that occurred during the conference held on the CNRS Campus Joseph Aiguier in Marseille, the social program enriched the friendly atmosphere and good spirit of the event. During the Wednesday afternoon, people could choose between a boat trip to the Calanques, a visit to the Museum of the History of Marseille or to the replica of the Cosquer cave, before heading to the Gala Dinner which was held in the Salon d'Honneur of the Stock Exchange Palace on the famous Canebière Avenue.



Poster Prize: EFEPR 2024

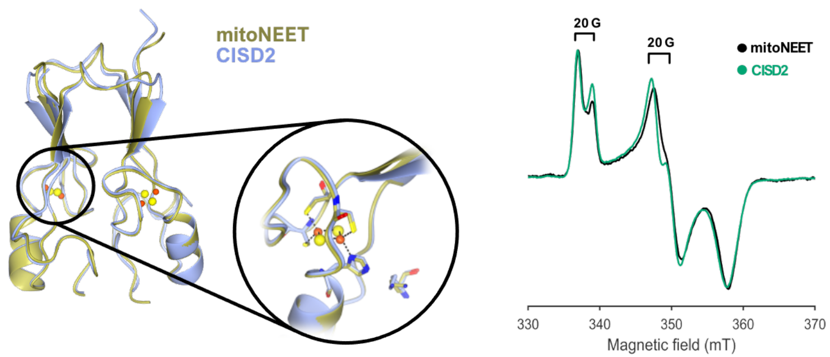
Ilenia Serra

Insights into the [2Fe-2S] cluster of human mitoNEET and CISD2: Fe-S cluster stability investigated by EPR spectroscopy

Ilenia Serra,[1] Guillaume Gerbaud,[1] Marie-Pierre Golinelli,[2] Bénédicte Burlat[1]

1 Laboratory of Bioenergetics and Protein Engineering, CNRS/AMU, Marseille, France
2 Institut de Chimie des Substances Naturelles, CNRS-Université Paris-Saclay, Gif-sur-Yvette, France

NEET proteins are recently discovered iron-sulfur (Fe-S) cluster-containing proteins that are distributed across all kingdoms of life and are involved in a variety of biological functions, including ageing, ROS homeostasis and iron metabolism, to cite a few[1].
In addition, pathological overexpression or depletion of NEET proteins have been associated to the development of different types of cancer[2]. Human mitoNEET and CISD2 are dimeric proteins in which each monomer coordinates a [2Fe-2S] cluster through an unusual 3Cys–1His motif. MitoNEET and CISD2 are anchored to the mitochondrial and endoplasmic reticulum membranes, respectively, and their cytosolic domains, which bind the [2Fe-2S] cluster, share high sequence and structure similarities[3].
While the redox-active cluster of mitoNEET has been extensively investigated from



Left: Wild-type human mitoNEET and CISD2 bind a [2Fe2S] cluster per monomer, with an uncommon $(Cys)_3(His)_1$ coordination geometry (PDB codes: 2QH7, 4OO7). Right: X-band CW-EPR of mitoNEET and CISD2 showing the dipolar splitting due to the close distance between the $[2Fe2S]^{1+}$ (S = ½) centers (~ 16 Å).

a biochemical and spectroscopic[4] point of view, the CISD2 protein remains less characterized. Human mitoNEET is able to donate its cluster to different acceptor partners, in a pH- and oxidation state-dependent manner; on the other hand, CISD2 has been shown to be a much worse cluster donor[3]. In this study, we aim at elucidating the

structural determinants of the FeS cluster stability in different NEET proteins, including wild-type human mitoNEET, its variants K55A and H87C - where important residues in the proximity of the cluster have been modified - and CISD2. Insights from X-band and Q-band continuous-wave EPR, as well as HYSCORE spectroscopies will be presented.

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Poster Prize: EFEPR 2024

Zichen Wang

Continuous-wave electrically detected magnetic resonance unveils structural features of trap states in disordered organic semiconductors

Zichen Wang,[1] Ilia Kulikov,[2] Jan Behrends,[2] Henning Sirringhaus[1]

1 Optoelectronics Group, Cavendish Laboratory, University of Cambridge, UK;
2 Berlin Joint EPR Lab, Freie Universität Berlin, Fachbereich Physik, Germany Other affiliation

Study of organic semiconductors have gained significant attention over decades, showing some killer applications in optoelectronic and flexible electronic devices with simple device fabrication steps and mild conditions [1]. Trapped charges play important role in electrical transport properties of organic semiconductors, where hopping through percolation pathways is the main contribution for charge transport in these disordered material systems [2,3]. However, the study of the trapped charges is usually focused on material morphology or energy level distributions, the link to their electrical transport properties remains vague. Here we present by first time a continuous-wave electrical-detected magnetic resonance (cw-EDMR) measurement to organic field-effect transistors (OFET) based on solution-processed conjugated polymers and observed current peaks at magnetic resonance caused by trapped charges.
We first observed the EDMR peak in poly[2,5-(2-octyldodecyl)-3,6-diketopyrrolopyrrole-alt-5,5-(2,5-di(thien-2-yl)thieno [3,2b] thiophene)] (DPP-DTT) polymer OFET under both positive and negative gating (corresponds to electrons and holes as conducting carriers) [4]. Then we compared the EDMR signal intensity in a wide range of FET biasing conditions, and confirmed the origin of the signal is from the interaction between the trapped charges and mobile charges with well-defined spin states, namely spin blockade effect, apart from the well-recognized contribution from electron-hole recombination [5].

Various polymer systems under different treatment conditions are examined, unveiling how the changes electrical properties correspond to the changes in the trap states. We also performed an in-situ measurement on FETs with applied stress and observed the evolution of trapped states during the stress progression. Our finding suggests the cw-EDMR is a sensitive technique for the direct observation of structure-property relationship in disordered materials, providing information on the evolution of trap filling processes during the device operations.

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Best oral presentation: EFEPR 2024

Marvin Lenjer

Electron spin dynamics during MW pulses
studied by 94 GHz chirp and phase-modulated EPR experiments

Marvin Lenjer,[1] Nino Wili,[2] Fabian Hecker,[1,3] Marina Bennati,[1,4]

1 RG EPR Spectroscopy, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany
2 Interdisciplinary Nanoscience Center, Aarhus University, Aarhus C, Denmark
3 Center for Hyperpolarization in Magnetic Resonance, Danish Technical University, Lyngby, Denmark
4 Department of Physical Chemistry, Georg August University Göttingen, Göttingen, Germany

Over the last decade, shaped microwave (MW) pulses have evolved into valuable tools for EPR spectroscopy. They have been used to improve existing experiments by providing tunable broadband or band-selective frequency profiles as well as to design new experimental approaches [1-3]. However, most applications were done at low fields (X- or Q-band) where high MW powers are available. Recently, application of broadband chirp echoes at W-band was demonstrated using the non-resonant HiPER spectrometer [4].
Here, we show the implementation of chirped and phase modulated pulses at a commercial Bruker E680 W-band (94 GHz) EPR spectrometer using a SpinJet arbitrary waveform generator. We apply these experimental tools to the analysis of spin dynamics during long MW spin lock pulses. As frequently used building blocks in EPR and

hyperfine spectroscopy experiments like ELDOR detected NMR or cross-polarization ENDOR, improved understanding of these pulses is important for future experimental design. In particular, we measure inversion profiles in the intermediate regime between Rabi oscillations and saturation pulses via chirp echo EPR spectroscopy [2] and analyze spin-spin relaxation during spin locking (i.e. $T_{2\rho}$) via phase modulation echoes during spin lock [3]. Combination with density matrix simulations allows us to better understand electron spin evolution during long periods of MW irradiation. Altogether, these results promise future advances in design and ap- plicability of hyperfine spectroscopy at high fields by use of spin locks and shaped pulses.

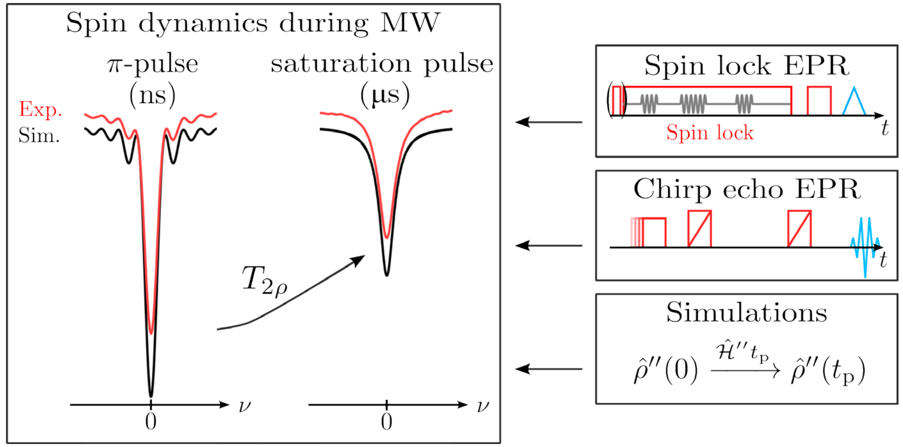

Figure 1: Methods for the analysis of spin dynamics during MW spin locking, including shaped pulse experiments

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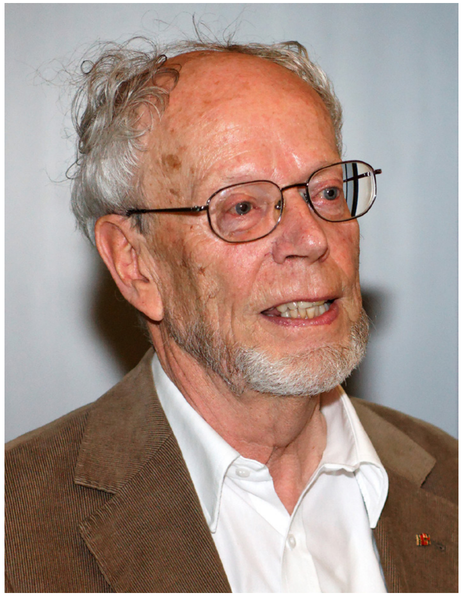
In Memoriam

Prof. Klaus Möbius

(4.6.1936 - 18.10.2024)



We are mourning the passing of Klaus Möbius who died on October 18, 2024, at the age of 88 in Berlin.

Klaus Möbius was a pioneer of modern advanced EPR spectroscopy, including electron-nuclear double resonance (ENDOR), cw and pulse high field EPR, and various applications to pertinent questions in chemistry and the life sciences (1).

He was born June 4, 1936 in Berlin and studied physics at the Freie Universität Berlin (FUB), where he also received his doctoral degree (1965). After his habilitation in Experimental Physics 1969 at FUB he spent a postdoctoral year with his family at UC Riverside in California. Back in Berlin he received a professor position at the Physics Department of the FUB in 1971. In the following years Klaus Möbius and his group built up a variety of multiple magnetic resonance methods including local and distant ENDOR and TRIPLE resonance, optically detected magnetic resonance (ODMR) and nuclear quadrupole resonance and studied organic and organometallic molecules in various matrices in their singlet and doublet ground and excited triplet states.

Within one decade his laboratory became one of the leading places for magnetic resonance, attracting many international guests and collaborators.

A highlight during these years was the application to the light-induced processes in photosynthetic reaction centers of bacteria and plants, and related model systems. This seminal work has substantially contributed to an understanding of the initial charge separation and subsequent electron transfer processes in photosynthesis.

Initiated by earlier work of Yakov Lebedev (Moscow) Klaus Möbius also engaged in the development of High Field EPR and published details of a cw HF-EPR instrument at 95 GHz in the mid-eighties, which was later extended to time resolved (transient) and pulse work, including ESEEM/HYSCORE, DEER/PELDOR, ELDOR-detected NMR (EDNMR) and pulse ENDOR. This opened many interesting applications across the sciences (2). The field was boosted - in Germany and worldwide - by the DFG Priority Program “High Field EPR in Biology, Chemistry and Physics” that was co-initiated and coordinated by Klaus Möbius (1998-2004).

Klaus, stayed in Berlin during his entire career. His dedication to his home city, the great scientific surrounding, and the excellent funding situation contributed to this decision. This enabled a continuity of his research that could hardly be matched anywhere else. At FUB – and other schools – he engaged in teaching the next generation of scientists. He gave truly excellent lectures.

After his formal retirement at the FUB (2001) he successfully continued his work as permanent guest scientist at the Max Planck Institute for Chemical Energy Conversion in Mülheim/Ruhr. Klaus published over 100 scientific papers and wrote 3 books after his retirement. An overview of his scientific publications and his impressive list of awards and honors can be found in (3).

Klaus was a great supporter of the Groupement AMPERE. I vividly remember how he explained to me how important the work of this society was during the Cold War for holding contacts to scientists in Eastern Europe, especially in the Soviet Union, the motherland of EPR. He was regularly invited to speak at AMPERE meetings; in 1998 he obtained the AMPERE Prize. Klaus was also one of the founding fathers of the European Foundation of EPR societies (EFEPR), now a subdivision of AMPERE, and its first president (1991-1994). During his entire career he was establishing and maintaining sustainable international cooperations worldwide, e.g. with Russia, Israel, Japan, Italy and many other nations, which particularly benefited the next generation of young scientists. For these activities he was awarded the German “Federal Cross of Merit, First Class” in 2006.

Klaus Möbius has worked his whole life for international understanding, for peace and actively against war - against the use of weapons, especially nuclear weapons. Also nuclear power plants were taboo for him. The deterioration of international scientific relations in recent years due to the military conflicts in Ukraine and the Middle East was terrible for him.

He was also concerned about the massive use of fossil fuels leading to global warming and engaged in search for alternative, sustainable energy sources. His great interest and work in natural and artificial photosynthesis was directly related to this problem.

His fascination of photosynthesis is documented by the play „Life on Earth through Photosynthesis“, which he wrote together with Giovanni Giacometti (Padua), published in 2016.

His interests and knowledge far beyond the natural sciences is documented in a beautiful way by his last book the “Möbius Strip Topology”, a comprehensive work with excursions into science history, chemistry, nanotechnology, material science, architecture, art and music (4).

Klaus was convinced that good science and cooperations should be built upon personal relations and friendships. He deeply respected other scientific disciplines, from which he obtained important impulses for his research. His students and postdocs appreciated his interdisciplinary scientific approach, it often laid the foundation for their later work. I personally couldn‘t have wished for a better scientific teacher, mentor and advisor for my professional career.

With Klaus Möbius we are losing an excellent scientist, a strong advocate for magnetic resonance and for science in general, a great human being and for many of us a good friend.

Our condolences go to his family and friends. We will preserve his memory and continue his work.

Wolfgang Lubitz
Mülheim an der Ruhr, November 2024

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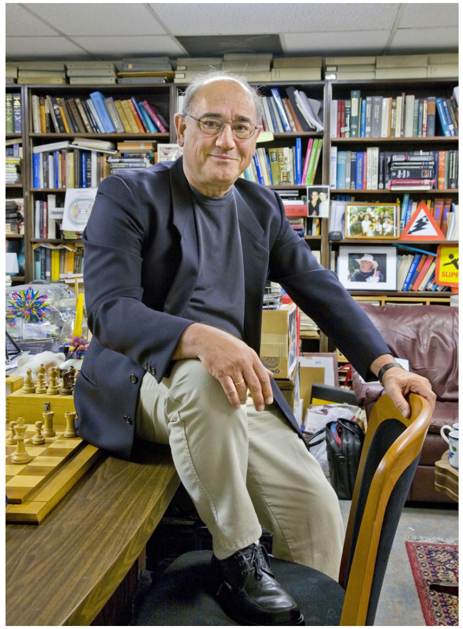
Prof. Alexander Pines

(22.6.1945 - 1.11.2024)



Our cherished colleague Alexander Pines, the Glenn Seaborg Professor of Chemistry Emeritus at the University of California Berkeley, passed away on November 1.

From his time as a student with John Waugh at MIT until just days before his passing, Alex was an irresistible *force* in magnetic resonance, perhaps most broadly recognized by his receipt of the Wolf Prize in chemistry in 1991.

Professor Pines emerged in the magnetic resonance community at a time just after the physics community established “nuclear Zeeman spectroscopy” as NMR and the fundamentals were ripe for transitioning to other disciplines. Alex began thinking about spins as an undergraduate at The Hebrew University, publishing a JACS article on hindered rotation in small molecule liquids NMR. A gifted pianist, Alex could have pursued music as profession, yet instead decided to pursue a Ph.D. in chemistry. During his thesis years at MIT, however, Alex spanned the world of quantum and statistical physics where he, along with W-Q. Rhim, reversed the dynamics of a system on interacting particles (Phys Rev Lett, 1970); this in turn opened the way for observation of chemical shifts, such as ^{19}F, in solids (JCP, 1971). He revealed the chemical shift anisotropy in carbon-13 as a tool for *chemistry* (also JCP, 1971); chemical applications of chemical shifts in solids was in turn was advanced by his demonstration of cross-polarization of dilute spines (*Jour. Chem Phys*, 1973). This paper has been cited over four thousand times.

Professor Pines began his independent academic career at the University of California Berkeley in 1972 as an assistant professor in chemistry: no postdoc necessary – such was the impact of his intellect on his new colleagues. For the next fifty years Professor Pines was the mentor to an astonishing collection of emerging scholars, publishing works spanning multiple-quantum spectroscopy, zero-field NMR, broadband and adiabatic sech/tanh pulses for MRI, double rotation and dynamic-angle spinning of quadrupolar nuclei, and iterative maps for quantum control, optical pumping of xenon and diamond systems for spin polarization, *ex situ* and mobile NMR and MRI, targeted NMR sensors for molecular imaging, ultralow and zero-field NMR and MRI, detection of magnetic resonance amplified by means of laser magnetometers, miniaturization of NMR, including its combination with microfluidic ("lab on a chip") technologies – just to name a few of his outstanding published works. Professor Pines was recognized for these works by being named a member of the National Academy of Sciences and the Royal Society; holding honorary degrees from the Universities of Rome, Paris, Marseilles, Amritsar, and the Weizmann Institute of Science; and many awards included the Wolf Prize in Chemistry. In his honor, the Pines Magnetic Resonance Center (PMRC) at Berkeley was launched on November 28, 2023, at a gathering for the annual UC Berkeley *Alexander Pines Endowed Lecture in Physical Chemistry.*

As impressive as these works and recognitions are, perhaps most impactful are the *Pinenuts*, alumni of his laboratory whose names are recognizable to anyone in the magnetic resonance community. The Pinenuts are founders of companies, national lab researchers, imminent scholars, and members of their communities that seek to emulate the generosity, magnanimity, and personal engagement of Professor Pines. Long before the word *underrepresented* became important, Professor Pines was the cherished mentor for many female doctoral students, postdocs, and visitors, furthering their representation throughout education and industry,

Professor Pines was not only a pillar of our resonance community, but he also dedicated himself to teaching chemistry to thousands of Berkeley undergraduates, with particular attention to the introductory course for non-majors. Professor Pines won every teaching award given by the Berkeley campus, spending hundreds of hours preparing, then delivering, lectures on chemistry that were illustrated with demonstrations, group discussions, and novel assessment schemes that worked for a course with an enrollment of over one thousand per term. His keen insight into the visual display of information led to legendary (and sometimes controversial) talks, such as those employing road signs that poignantly highlighted popular culture as well as group theory. For those of us fortunate enough to have met Professor Pines, we recall his charisma and enthusiasm for art, music, and all fields of science were infectious.

Jeffrey Reimer
UC Berkeley, December 2024

Prof. Anil Kumar

(25.6.1941 - 9.11.2024)

The international NMR community has received the sad news that our colleague Anil Kumar passed away on the 9th of November, 2024.

Anil was an extraordinary scientist and person. His influence on our field deserves to be widely known. During a few years, between 1974 and 1980, during two visits to ETH-Zürich, he made decisive contributions to at least three central themes of modern NMR: Fourier transform MRI, two-dimensional nuclear Overhauser spectroscopy (NOESY), and the estimation of dipole-dipole couplings by solid-state NMR. His contributions led directly to the Nobel prizes of both Ernst and Wüthrich. In his later career, he made important contributions to NMR relaxation theory and the applications of NMR to quantum information processing, and established India as one of the centres of modern NMR.

Two giants of NMR: Anil Kumar and Erwin Hahn. Photo: Sankeerth Hebbar.

The first of his major contributions was the observation of transient oscillations in cross-polarization experiments in solids, published in 1974 in Phys. Rev. Letters.[1] The transfer of spin polarization between species in solids had been pioneered by Hartmann and Hahn in the 1960's[2], and exploited as a method for facilitating the solid-state NMR of dilute nuclei by Pines, Waugh and co-workers[3]. However, the polarisation transfer itself was believed to follow a rather uninformative monotonic trajectory. After joining Ernst's lab, Anil helped a new graduate student, Luciano Müller, to implement this technique, using a large single crystal of ferrocene which had been grown by Luciano (I recall this crystal well, since when I joined Ernst's lab much later, I also used this crystal to learn about cross-polarisation and also discovered some interesting effects using it[4]). Anil once told me that Luciano complained that the experiment was not working properly since the cross-polarised 13C signal was observed to vary in amplitude in an unpredictable way. Anil and Luciano worked together to show that the apparent variations were due to regular oscillations in the cross-polarisation trajectory – an entirely unexpected effect at the time. The oscillations were identified as a signature of the heteronuclear dipole-dipole coupling between 1H and 13C nuclei[1]. This experiment established the possibility of measuring internuclear dipole-dipole couplings, and hence internuclear distances, by solid-state NMR. Viewed in retrospect, this experiment underpins many of the applications of solid-state NMR to structural biology and materials science.

Anil was then involved in one of the earliest, and most important, applications of the newly invented technique of two-dimensional Fourier NMR. The basic idea of two-dimensional Fourier NMR was advanced by Jeener in 1971, at a famously obscure summer school5. Ernst saw the enormous possibilities, but Jeener was not publishing anything, and Ernst was reluctant to press ahead. However, soon afterwards, the first report of NMR imaging appeared[6]. Ernst immediately saw the way to put these two new techniques together, with major advantages in simplicity and signal-to-noise, and without infringing too much on Jeener's publication rights. Anil realised this new experiment with the help of Dieter Welti, leading to the seminal 1975 paper on two-dimensional Fourier MRI (mercifully, the name "zeugmatography" is no longer used)[7].

The third major contribution, and the one which may be most clearly attributed to Anil, is the first demonstration of two-dimensional nuclear Overhauser spectroscopy in a biomolecule (NOESY), first published in 1980[8]. The story of this experiment has been given by Anil himself[9,10]. These articles make clear how much determination, innovation, and clarity of thought was needed at the time to push through an experiment which is nowadays routine. NOESY is one of the few experiments that works much better for large molecules than for small molecules. This is because small molecules in solution tend to have correlation times close to the "crossing point", where the cross-relaxation rate constants change sign. Hence the NOESY peaks are often very weak for small molecules, while they are usually consistently large for large molecules in solution. However, at the time, the poor results for experiments of this kind, for small molecules, had convinced almost everyone that such an experiment would be a waste of time on a protein. This perception made it difficult for Anil to secure the machine time needed for such an obviously pointless experiment. Anil's case was not helped by the first results, which were negative due to instrumental or software issues[9,10]. Fortunately, the resistance was eventually broken down, the results on a small protein were immediately spectacular[8], and this experiment underpins much of NMR in structural biology.

On return to India, Anil established an NMR centre at the Indian Institute of Science in Bangalore, which became a training ground for many of India's leading NMR scientists, a legacy that continues into the future. Anil's own research interests included cross-correlation effects in NMR relaxation[11], and especially the implementation of quantum computing concepts and algorithms in NMR spectroscopy. Here, Anil combined his expertise in advanced NMR methodology and his deep understanding of quantum mechanics to demonstrate quantum information technologies by room-temperature NMR experiments. A particular speciality of Anil was using quadrupolar nuclei in the context of NMR quantum computation[12–17].

Apart from his scientific qualities, Anil was a wonderful person with a warm and cheerful personality. Famously, his neighbours once sent the Swiss police to his Zürich apartment to ask him to stop laughing so much – an anecdote that says as much about Zürich at that time as it does about Anil. My family and I were fortunate to enjoy the matchless hospitality of Anil, his wonderful wife Padma, and his lovely children Ankur and Pankaja, during our stay in Bangalore in 1999. The warmth of their hospitality, Padma's delicious dinners (often at midnight or later), and the opportunity for delightful tea-break discussions with Anil contributed greatly to my abillity to write the first draft of my book Spin Dynamics. Anil would chuckle and laugh about anything, and if there was really nothing to chuckle about, Anil would chuckle anyway – and his chuckle was so infectious that so would everyone else. He is greatly missed.

Malcolm Levitt
Southampton, December 2024

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