

Vol. 74, No. 2/3

ISSN 0432-7136

## BULLETIN DU GROUPEMENT

d'informations mutuelles



Groupement  
**AMPERE**

SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

April to September 2025

No. 299 & 300

Office: ETH Zürich, Institute of Molecular Physical Science  
8093 Zürich, Switzerland, [www.ampere-society.org](http://www.ampere-society.org)

## Contents

<b>Special Editorial</b>	1
<b>Portrait</b> Megan Halse	2
<b>Report: AMPERE NMR School 2025</b> Awards	5 8
<b>Report: Euromar 2025</b> AMPERE Prize for Young Investigators Raymond Andrew Prize AMPERE Travel Awards	15 21 23 25
<b>Minutes of the meeting</b> of the AMPERE Bureau of the AMPERE Committee of the AMPERE General Assembly	37 39 41
<b>Finances of the Groupement Ampere and Subdivisions</b>	44
<b>In memory of</b> Jean-Nicolas Dumez (1984 - 2025)	46
Executive Officers and Honorary Members of the Ampere Bureau AMPERE Committee Future conferences and Ampere events	49 51 53

If you would like to become a member of the AMPERE Society, you can register online under: [www.ampere-society.org](http://www.ampere-society.org)

## Special Editorial



Dear members of the Groupement AMPERE,

We live in an era where artificial intelligence (AI) permeates nearly every aspect of life, and NMR spectroscopy is no exception. In fact, the inherent reproducibility of NMR spectra provides the consistent, high-quality datasets that AI algorithms need to learn effectively, validate rigorously, and deliver trustworthy predictions. Already, machine learning models are capable of performing spectral assignment, structural prediction, and dynamic simulations; tasks that once demanded months of human effort. As a result, NMR spectroscopy is evolving to be less about interpreting spectra themselves and more about the scientific questions that can be asked once the spectra cease to be an obstacle.

In my view, the NMR scientist of the future will not be displaced by AI, but rather challenged, inspired, and ultimately liberated to reimagine what it means to do science in a world where machines handle the routine. The inherent versatility of NMR spectroscopy should ensure a harmonious coexistence with AI; one in which we, as humans, are called to strengthen our role and broaden our perspective. The recent conference in Oulu, where outstanding science was seamlessly interwoven with delicate artistic expressions, stands as a perfect example of this vision.

I wish you a pleasant autumn and, for those with teaching duties, a fruitful start to the new term.

Oscar Millet

Vice President  
Groupement AMPERE

## Portrait:

### Meghan Halse

#### Why magnetic resonance and why NMR and MRI?

I was first introduced to magnetic resonance during my undergraduate and masters research projects at the University of New Brunswick in Canada. I can remember a moment during a lecture by my supervisor, Bruce Balcom, on the fundamentals of MRI when for the first time I could see the connection between the quantum mechanics he was describing and the experiments I had been running in the lab. This began my fascination with the way we can use quantum mechanics to understand and predict the outcomes of the NMR measurements that we make in the lab which has continued throughout my career. One of my favourite parts of teaching NMR is inspiring the same fascination students, some of whom I hope will go on to pursue a career in magnetic resonance.

#### What is your favorite frequency?

My favourite frequency is 2600 Hz, which is the  $^1\text{H}$  Larmor frequency in the Earth's magnetic field in Antarctica. At the end of my PhD, I had a once-in-a-lifetime opportunity to spend three weeks doing NMR of sea ice in Antarctica. This amazing experience will always remind me of the joy of doing scientific research essentially just for the fun of it.

#### What do you still not understand?

No matter how well I think I understand NMR, new experiments always throw up new questions that challenge my understanding, particularly on the fundamentals of spin dynamics.

#### Luckiest experiment you have ever done.

After completing my MSc in Canada, I went on holiday to New Zealand for several months. Early in my trip, I stopped in to visit Paul Callaghan's lab at Victoria University of Wellington. During this impromptu visit, Paul offered me a few months of work at his recently founded spin-out company, Magritek, implementing imaging on their Earth's field NMR spectrometer. Our first attempts were very successful and led to the production of the Terranova MRI system, which Magritek subsequently sold as an educational product. These early experiments in low-field instrument design and pulse programming were the luckiest of my career not because of the scientific impact of this work, although I am always pleased when I hear from someone who learned about NMR/MRI using this instrument or the associated YouTube videos that we produced. They were lucky for two more personal reasons. First, because this led directly to my PhD under the supervision of Paul Callaghan, who was a remarkable scientist and mentor

and had a huge impact on my decision to pursue an academic career and how I aspire to lead my own research group. Second, this project introduced me to portable NMR and hyperpolarisation for the first time, two topics that have formed the basis of my independent research career.

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

During my PhD, I was running an experiment on a 400 MHz spectrometer, where we had customized the probe to add an attachment above the coil that made the whole assembly top heavy. I am never at my best first thing in the morning but I had limited magnet time so I started working in the lab first thing to get everything set up. This involved manually tuning the probe on the bench before inserting it into the spectrometer. Unfortunately, as I was crouched down next to the bench I wasn't paying attention properly. The probe overbalanced and came crashing down, bouncing off my head quite painfully on its way to the floor. I don't know how much it cost to have it fixed but I do know that, like most things that involved sending things to and from New Zealand, it was many months before we got it back again!

#### Most memorable conference story?

My most unique conference experience was in 2005, when I attended my first ever ENC. It was during the year I worked for Magritek. The CEO, Andrew Coy, and I had decided to fly over from New Zealand with an Earth's field MRI system in our luggage. Having crossed the dateline enroute, our mid-day flight landed two hours before it took off, leading to possibly the longest day of my life. We drove from San Francisco to Asilomar and immediately set up the Earth's field MRI in our booth. Throughout that evening, we were kept busy chatting to a steady stream of the people who came to try out our live demo, which was a bit of a novelty at that time. It was gone midnight by the time we closed up shop. As a very early career scientist, having the chance to meet and chat to so many scientists of different backgrounds during the conference, in addition to attending the scientific program, was an inspiring and formative experience.

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

I think it would be fascinating to go back and attend the conference where Albert Overhauser presented his first theoretical paper on DNP to hear the debate in the community with the knowledge of what a huge impact this work would go on to have in magnetic resonance.



### When do you get your best ideas?

Whenever I am attending conferences or listening to research seminars I get excited by new ideas and research possibilities. My phone is full of notes taken during talks – every once in a while I go through and find references for interesting papers to read or the start of an idea for a new experiment.

### If you had just one month time for travelling - where would you go to?

Having grown up in Canada, where 100 years is considered a long time, I have always been fascinated by the remnants of ancient civilisations. If I had a month to travel, I would love to go see ancient places like the Great Pyramid of Giza or Machu Picchu in Peru.

### Your idea of happiness?

It makes me happy to experience and be reminded of the beauty that still exists in our world, from a wonderful piece of art to the view from the top of a mountain, particularly if I can experience it with my friends and family.

#### Position:

Senior Lecturer in Chemistry, University of York, UK

#### Awards:

ERC Consolidator Grant (selected by the ERC and funded by UKRI due to Brexit)

#### Homepage:

<https://www.york.ac.uk/chemistry/people/mhalse/>

#### Education:

BSc (2002) & MSc (2004) University of New Brunswick, Canada; PhD (2010) Victoria University of Wellington, NZ; PDRA at the CRMN in Lyon (Emsley Group, 2010-2013)

Interests: Drawing portraits, painting, patchwork quilting, running

## Report:

### AMPERE NMR School 2025

Zakopane, June 8-14, Poland

#### Scientific Committee:

Anja Böckmann (France), Bernhard Blümich (Germany), Janez Dolinšek (Slovenia), Matthias Ernst (Switzerland), Wiktor Koźmiński (Poland), Danuta Kruk, (Poland) David Lurie (UK), Beat Meier (Switzerland), Giacomo Parigi (Italy), Daniel Topgaard (Sweden), Tomasz Zalewski (Poland)

#### Organizing Committee:

Roksana Markiewicz – Chair, Tomasz Zalewski – Co-chair  
Michał Bielejewski, Karolina Dydak, Jakub Jagielski, Jacek Jencyzk  
Administrative support: Alicja Jorasz, Jakub Rybka.

The AMPERE NMR School took place at Zakopane, a small city in the High Tatra Mountains located in the southern Poland, from June 8 to June 14, 2025. It was the 32<sup>nd</sup> meeting of the AMPERE NMR School. The school was organized by Adam Mickiewicz University in Poznan, Poland, and was attended by around 80 researchers from research institutions throughout the world. Like every year, young and experienced scientists from all around the world attended the school, with an emphasis on fundamental and advanced NMR techniques. The attendees got the opportunity to network, exchange information about recent advances in NMR and related fields, discover new partnerships and cooperation, and learn about new development in the area of nuclear magnetic resonance.



The school's program covered the usual topics: NMR relaxometry, NMR diffusometry, solid state NMR, NMR of quadrupolar nuclei, MRI and Field Cycling MRI, application of NMR in the area of biology, medicine, and material science, and technical aspects of NMR. The School is mainly addressed to young scientists and graduate students, or people who start their journey in the field of nuclear magnetic resonance, and aims at acquainting them with theoretical and experimental aspects of various NMR methods applied in nanoscience, materials science and soft materials.

The programme of the School was kept the usual:

**1: Plenary lectures given by world-renowned specialists from the area of nuclear magnetic resonance**

In total, the School consisted of 23 lectures given by:

Bernhard Blümich: Portable MRI for Investigating Cultural Heritage  
Gerd Buntkowsky: Parahydrogen Induced Polarization and Biomolecules  
Daniel Topgaard: Translational motion and magnetic field gradients  
Tomasz Zalewski: Multifunctional nanocarriers investigated by NMR and MRI  
Lionel Broche: Basic of MRI imaging  
Janez Stepišnik: Analysis of Chemical Exchange Processes by NMR  
Anna Zawadzka-Kazimierczuk: High-dimensional NMR experiments for easy resonance assignment of intrinsically disordered proteins  
Fabien Ferrage: Exploring the spectral density function  
Guineivre Matthies: Enhancing the sensitivity of solid-state NMR  
Oscar Millet: Signal assignment of complex mixtures of metabolites assisted by spin dynamics simulations  
Siegfried Stapf: Dynamic Nuclear Polarization (DNP) at room temperature - a closer look on liquids at interfaces  
Greg Stanis: Saturation Transfer MRI - Theory and Practice  
Martin Dracinsky: NMR crystallography of molecular solids  
Matej Pregelj: Muon spin spectroscopy in condensed matter research  
Ilya Kuprov: Machine Learning in Magnetic Resonance: the algebra behind the hype  
Claudia Schmidt: What NMR of probe molecules can tell us about porous materials  
Diana Bernin: Capturing coherent and non-coherent motions in chemical engineering applications with magnetic resonance  
Dietmar Paschek: Computer Simulation of the Frequency Dependent NMR Relaxation in Molecular and Ionic Liquids: Insights, Pitfalls, and Recent Developments  
Camilla Terenzi: Rheo-NMR and MRI velocimetry: principles and applications  
Vyatutas Klimavicius: Solid-state NMR and Functional Materials  
Marta Dudek: Crystal Structure Prediction Calculations in NMR Crystallography Applications  
Giacomo Parigi: Paramagnetic NMR effects for protein structure determination  
Danuta Kruk: Modelling NMR Relaxation Data - from protein solutions to tissues

**2: Young Researchers Forum**, where young scientists had the opportunity to present their findings in the short communications given between the main lectures. 9 short communications were presented with abstracts included in the Book of Abstracts.

**3: Poster session for Young Scientists**, where students, Ph.D. Students, Post-Docs, and any other participants were given the opportunity to share their results.

**4: Workshops/ tutorials about basic and advanced NMR techniques.**

This year, six tutorials about NMR were performed:

a: „NMR diffusometry” – Michał Bielejewski, Joanna Kowalczyk (additional online transmissions from the NMR laboratory of Institute of Molecular Physics, Polish Academy of Sciences, Poznań)

b: “High-dimensional NMR experiments for easy resonance assignment of intrinsically disordered proteins” – Anna Zawadzka-Kazimierczuk

c: “One fit-engine for NMR model fitting and data analysis: Write your interface and automate your processes” – Pedro José Sebastião

d: “The number of NMR relaxation equations is infinite” – Danuta Kruk

e: “D,  $\sigma$  and V . Let's have a look at tensors” – Jacek Jenczyk

f: “Application of High-Resolution NMR Spectroscopy in Polymer Characterization” – Rafał Konefal

The short communications were evaluated by all lecturers and tutors in an unanimous questionnaire, where they were assessed for the topic presented, research performed, and their presentation skills. The poster session was this year evaluated by the Organizing Committee alongside with the tutors of the workshops. All the winners received prizes accompanied by a certificate.

One prize was awarded for the short communication, and three prizes went to the authors of the best posters:

1. The Best Communication Award:

Lennart Kruse for the presentation entitled „Probing Translational Diffusion with FFC NMR: The Role of Heteronuclear Contributions in the Low-Frequency Regime” (additional prize sponsored by Springer)

2. Communications Distinctions:

Karolina Dydak for the presentation “NMR relaxometry of self assembled GMO@DTPA-BSA-Gd nanostructures for biomedical imaging”

Helena Loan for the presentation “Solid-state  $^{119}\text{Sn}$  NMR and DFT Calculations of Large CSAs in  $\text{Sn(II)}$  MOFs”

3. The Best Poster Award:

Laura Iatsin for the poster entitled „ Self-healing under stress: zooming into the response of self-healing materials”

#### 4. Poster distinction:

Wiebke Zielasko for the poster entitled „Multinuclear solid-state NMR Study of the Contrasting Structural Roles of Nb2O5 and La2O3 in silicate glasses”

All abstracts of the oral presentations, tutorials and posters were published as printed proceedings (book of abstracts). The social programme included a welcome reception and Dinner in the Regional Restaurant “Czarci Jar” with the folk music of the Tatras region.

All the additional information about the AMPERE NMR School is presented on the website: school.web.amu.edu.pl and schools’s X account: @AmpereNMR.

**The next edition of the school will be held in Zakopane (Poland) from June 14-20, 2026.**

**Awards: AMPERE NMR School 2025:**  
best communication: Lennart Kruse

#### Probing Translational Diffusion with FFC NMR: The Role of Heteronuclear Contributions in the Low-Frequency Regime

Lennart Kruse<sup>a</sup>, Anne Strate<sup>a</sup>, Angel M. C. Tony<sup>a</sup>, Dietmar Paschek<sup>a</sup> and Ralf Ludwiga<sup>b,c</sup>

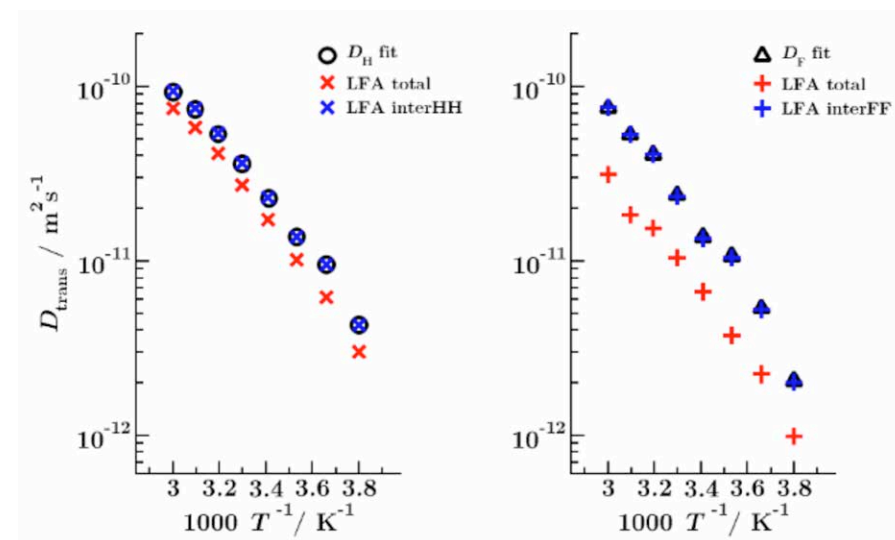
a: Physical and Theoretical Chemistry, University of Rostock, Germany

b: Department LL&M, University of Rostock, Germany

c: Leibniz-Institut für Katalyse, Universität Rostock e.V., Germany

Using fast-field-cycling NMR relaxometry it is possible to measure frequency-dependent relaxation rates of NMR-active nuclei. Fitting of these dispersion profiles provides access to translational and rotational dynamical properties, such as self-diffusion coefficients and rotational correlation times.[1] The fitting procedure becomes increasingly complex as the number of parameters increases with more types of interaction between all the NMR active nuclei in the sample. However, the translational diffusion coefficients can also be extracted directly from the experimentally obtained relaxation data, by using a linear dependence of the relaxation rates at low frequencies. [2] We show, that heteronuclear interactions play a crucial role when applying this so-called low-frequency approach (LFA). Therefore, three different ionic liquids (ILs) have been synthesized. By

selective deuteration of either the cation or the anion, two of the ILs represent a one-spin system with only  $^1\text{H}$ - $^1\text{H}$  interactions on the cation or  $^{19}\text{F}$ - $^{19}\text{F}$  interactions on the anion. In the third IL there are additional  $^1\text{H}$ - $^{19}\text{F}$  interactions between cations and anions. It is an ongoing debate under which circumstances these heteronuclear contributions can be neglected. We can show that the low-frequency approach holds when being applied to the experimentally obtained relaxation data of one-spin systems. In contrast, by neglecting the heteronuclear contribution, the LFA will yield falsified self-diffusion coefficients when being applied to two-spin systems without any further data evaluation. Here, a proper dissection of the total relaxation rates into inter- and intramolecular parts is essential before applying the LFA only to the intermolecular contribution. [3]



**Figures 1.** Self-diffusion coefficients for the ionic liquid [TEA][NTf<sub>2</sub>] obtained by numerical fitting and from the slope of the relaxation rates at low frequencies. Only when the slope of the dissected rates is used the two approaches yield the same self-diffusion coefficients.

#### References:

[1] L. Kruse et al., Phys. Chem. Chem. Phys. 2025, accepted.

[2] D. Kruk et al., Phys. Rev. E 2012, 85, 020201.

[3] L. Kruse et al., J. Phys. Chem. Lett. 2024, 15, 10410.

**Awards: AMPERE NMR School 2025:**  
**communication distinction: Karolina Dydak**

**NMR relaxometry of self assembled GMO@DTPA-BSA-Gd nanostructures for biomedical imaging**

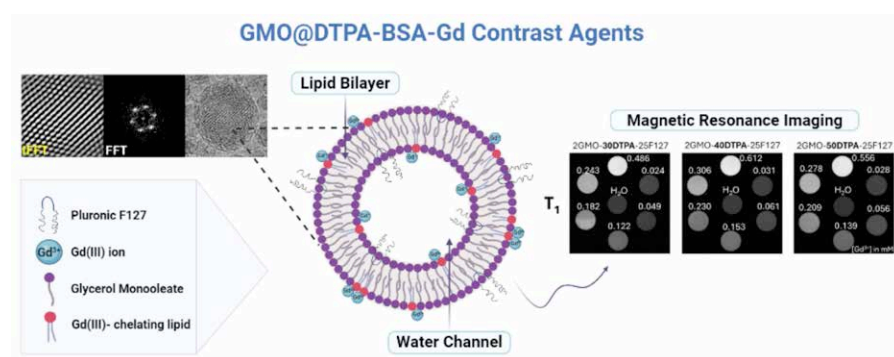
Karolina Dydaka<sup>b</sup>, T. Zalewski<sup>a</sup>, M. Kempka<sup>a,b</sup>, J. Jagielski<sup>a</sup>, G. Nowaczyk<sup>a</sup>, Ł. Przysiecka<sup>a</sup>, P. Florczyk<sup>a</sup>, D. Flak<sup>a</sup>

a: Adam Mickiewicz University, NanoBioMedical Centre, Poznań, Poland

b: Adam Mickiewicz University, Faculty of Physics, Poznań, Poland

Gadolinium-based contrast agents (GBCAs) are crucial for improving organ imaging in MRI due to gadolinium's paramagnetic properties. Despite their widespread use since 1988, concerns remain about the release of toxic Gd<sup>3+</sup> ions. Therefore, researchers aim to develop safer options with higher relaxivity, reduced Gd<sup>3+</sup> release, and improved pharmacokinetics. One promising solution involves embedding Gd-chelating lipids into lipid-based nanocarriers, which lowers the required gadolinium dose while enhancing imaging efficiency.

The studies focused on the glycerol monooleate (GMO)-based nanoassemblies loaded with DTPA-bis(stearylamide) gadolinium salt, stabilized by Pluronic F127. Different concentrations of DTPA-BSA-Gd were tested - low (5% w/w) and high (30-50% w/w) - to optimize relaxivity efficiency. The nanoparticles were analyzed for particle diameter, long-term stability, and structure characteristics. Data obtained showed that low Gd<sup>3+</sup> resulted in internally well-ordered nanoparticles, while higher concentrations disrupted self-assembly, still yielding satisfactory relaxivity.



**Figures 1.** Predicted structure of (GMO)-based lipid nanoparticle modifying Gd(III)-chelating lipid, forming a highly ordered structure.

Relaxometry studies and MRI confirmed that GMO@DTPA-BSA-Gd nanoassemblies achieved higher contrast properties than commercial agents like Magnevist or Gadovist.

The studied lipid-based nanoparticles maintained strong imaging performance, offering a safer and more effective alternative to common GBCAs. The advantages of the prepared GMO@DTPA-BSA-Gd nanoparticles allow us to conclude that they may be considered as a new type of MRI CAs. Furthermore, they hold potential for the development of multifunctional lipid-based systems that integrate both diagnostic and therapeutical properties.

**Acknowledgements:**

The work was financially supported by the research grant Sonata Bis 2016/22/E/ST3/00458 from the National Science Centre, Poland

**References:**

[1] Dydak, K. et al. J. Mater. Chem. B, 2024, 12, 12017-12029

[2] Wahsner, J. et al. Chemical reviews, 2019, 119, 957-1057

**Awards: AMPERE NMR School 2025:**  
**communication distinction: Helena Loan**

**Solid-state <sup>119</sup>Sn NMR and DFT Calculations of Large CSAs in Sn(II) MOFs**

Helena Loan, Caitlyn Walton, Ryan Bragg, Richard Walton and Michael Hope

Department of Chemistry, University of Warwick, Coventry, CV4 7AL

Metal-organic frameworks (MOFs) are promising materials for multiple applications, such as gas separation, energy storage, or catalysis.<sup>1-3</sup> These materials consist of metal cation nodes connected via organic linker molecules to form 2D or 3D structures. The metal and organic molecules can be varied allowing the material to be optimised towards its desired function. Recently, Sn(II) MOFs have been successfully synthesised under hydrothermal conditions,<sup>4</sup> yielding strong metal-ligand bonds that are also stable in water, a limitation for many other Sn(II) MOFs.<sup>5</sup> One such material, Sn2(DOBDC), is able to store lithium as part of lithium-ion batteries, where the MOF acts as a host for the lithium due to the reversible formation of coordination bonds.<sup>6</sup> The reversibility of bond coordination allows the Li ions to be accommodated within the structure without mechanical fracture, thereby enhancing cycling stability.

To explore the Sn coordination environment of Sn(II) MOFs, we used solid-state NMR in combination with density functional theory (DFT) calculations to establish correlations across the different structures. The Sn(II) nucleus exhibits high chemical shift anisotropy (CSA) due to its lone pair, which is very sensitive to the local coordination environment and the presence of any adsorbed species within the structure. However, the large

CSAs are also challenging to measure, requiring a combination of variable MAS and static ultrawide line BRAIN-CP-WCPMG experiments. We measured the CSA of 6 Sn (II) MOFs, between 1 and 3 distinct Sn sites per structure. The CSA of each site varies depending on the environment, with certain MOFs exhibiting very high CSAs, giving wide spectra with spans from -100 ppm up to -1500 ppm. Comparing the experimental NMR tensors with those calculated from GIPAW DFT, we find good agreement with the isotropic shift. However, although there is a positive correlation between the experimental and calculated CSAs, they remain difficult to accurately calculate.

#### References

- [1] Liu, J.; Chen, L.; Cui, H.; Zhang, J.; Zhang, L.; Su, C. Y. Chem. Soc. Rev. 2014, 43 (16), 6011-6061.
- [2] Baumann, A. E.; Burns, D. A.; Liu, B.; Thoi, V. S. Communications Chemistry 2019, 2 (1).
- [3] Yan, J.; Wang, X.; Ning, F.; Yi, J.; Liu, Y.; Wu, K. Dalton Trans. 2023, 52 (34), 11904- 11912.
- [4] Ramana, A. K.; Tidey, J. P.; de Lima, G. M.; Walton, R. I. Small Methods 2025, 9 (2). (5) Ding, M.; Cai, X.; Jiang, H. L. Chem. Sci. 2019, 10 (44), 10209-10230.
- (6) Liu, J.; Xie, D.; Xu, X.; Jiang, L.; Si, R.; Shi, W.; Cheng, P. Nat. Commun. 2021, 12 (1), 3131.

### **Awards: AMPERE NMR School 2025:**

**best poster: Laura Iatsin**

### **Self-healing under stress: zooming into the response of self-healing materials**

Laura Iatsin

Laboratory of Biophysics, Wageningen University and Research, Wageningen, The Netherlands

Inspired by the remarkable efficiency of natural self-healing processes, researchers have developed synthetic materials that mimic self-healing by incorporating dynamic chemical bonds, such as hydrogen bonds (HBs), that enable reversible interactions. Tracking how HBs rebuild a damaged polymer network demands MRI techniques that capture both chain-scale and bulk mechanics. We therefore integrate tensile-MRI and micro-magnetic-resonance- elastography ( $\mu$ MRE) to obtain NMR relaxation-time and viscoelastic stiffness maps that showcase crack propagation and viscoelastic recovery in self-healing supramolecular hydrogels.

Preliminary tensile-MRI tests on model gelatin samples were conducted on a 7T wide bore vertical magnet using an in-house built setup consisting of a 10-mm NMR glass tube with inner coaxial silicone tube containing the sample, and coupled to a syringe pump. Multi-echo spin-echo (TE = 10 ms, TR = 9000 ms, pixel size = 0.16 mm) and gradient echo (TE = 10 ms, TR = 9000 ms, pixel size = 0.16 mm) sequences were

used to monitor longitudinal ( $T_1$ ) and transverse relaxation parameters ( $T_2$ ,  $T_2^*$ ) at rest and under tensile stress. Concurrently, an algorithm based on using multifrequency wave data to solve the inversion of viscoelasticity reconstruction problem was built to determine mechanical properties of self-healing polymers under stress and during self-healing [1].

Preliminary tensile-MRI studies on model gelatin samples stretched up to 140% engineering strain show that  $T_1$  is insensitive to polymer chain rearrangements induced by increased tensile stress. Alternatively,  $T_2$  decreases as a function of tensile stress, indicating possible HBs-mediated alignment, tighter polymer network packing, and possible HBs fracture [2]. A similar behavior is observed for  $T_2^*$ .

By unifying spatially- resolved relaxation-parameter maps ( $T_1$ ,  $T_2$ ,  $T_2^*$ ) and shear modulus maps obtained via  $\mu$ MRE, this project will make the first step in delivering an operando road map to self-healing in HBs supramolecular networks.

#### References

- [1] K. J. Streitberger et al., 'High-Resolution Mechanical Imaging of Glioblastoma by Multifrequency Magnetic Resonance Elastography', PLoS One, vol. 9, no. 10, p. e110588, Oct. 2014, doi: 10.1371/JOURNAL.PONE.0110588.
- [2] P. T. Callaghan and A. M. Gil, '1H NMR spectroscopy of polymers under shear and extensional flow', AcRhe, vol. 38, no. 6, pp. 528-536, 1999, doi: 10.1007/S003970050205.

### **Awards: AMPERE NMR School 2025:**

**poster distinction: Wiebke Zielasko**

### **Multinuclear solid-state NMR Study of the Contrasting Structural Roles of Nb<sub>2</sub>O<sub>5</sub> and La<sub>2</sub>O<sub>3</sub> in silicate glasses**

Wiebke Zielasko<sup>a</sup>, Rafael Bonacin de Oliveira<sup>b</sup>, Edgar Dutra Zanotto<sup>b</sup>, Michael Ryan Hansen<sup>a</sup>, Hellmut Eckert<sup>c</sup> and Henrik Bradtmüller<sup>b,c</sup>

a: Institute of Physical Chemistry, University of Münster, Germany

b: Department of Materials Engineering, Vitreous Materials Laboratory, Federal University of São Carlos, Brazil

c: São Carlos Institute of Physics, University of São Paulo, São Carlos, Brazil

Glass is an important technological material with a broad range of chemical and physical properties. One key application is in the field optics, where glasses are used for displays and lenses. An important property of an optical glass is its high refractive index. To replace the toxic PbO that was used in the past, alternative metal oxides such as Nb<sub>2</sub>O<sub>5</sub> and La<sub>2</sub>O<sub>3</sub> are now being used more frequently.[1]

As the properties of glass depend on its composition and the manufacturing conditions, designing new glass formulations is highly complex, and machine learning (ML) techniques are now frequently used to address this instead of the conventional trial-and-error-procedure.[2] However, improving the ML predictions requires detailed knowledge of the structure-property relationships in glasses.

Due to the amorphous nature of glass, nuclear magnetic resonance (NMR) is one of the most suitable quantitative and element-selective measurement techniques for characterizing the structure of glass. NMR can be used to determine the degree of polymerization of glass and the effective distance between two nuclei.[3]

In this contribution, we have investigated the structural roles of  $\text{Nb}^{2}\text{O}^5$  and  $\text{La}^{2}\text{O}^3$  in optical glasses. The base composition was designed using the ML GlassPy [4] to achieve a high refractive index. The content of  $\text{Nb}^{2}\text{O}^5$  and  $\text{La}^{2}\text{O}^3$  (0–10 mol%) were systematically added to the base glass, and the resulting structural changes were analyzed using multinuclear solid-state NMR. Specifically, we used  $^7\text{Li}$ ,  $^{23}\text{Na}$ ,  $^{29}\text{Si}$ ,  $^{93}\text{Nb}$ , and  $^{139}\text{La}$  NMR, as well as  $^7\text{Li}\{^{93}\text{Nb}\}$  W- RESPDOR experiments, to characterize the effects of the additions on the glass structure.

#### Acknowledgements:

This work was supported by the São Paulo Research Foundation (FAPESP) under grant no. 2013/07793-6 (CEPID program) and the Companhia Brasileira de Metalurgia e Mineração (CBMM) (UFSCar-ProEx n° 019876/2020-10 - Desenvolvimento de vidros Nb-cristal guiado por inteligência artificial).

#### References:

- [1] R.O. Alekseev, et al., *J. Alloys Compd.* 2025, 1014, 178622. [2] D. R. Cassar, et al. *Ceram. Int.* 2021, 47, 10555–10564.
- [3] H. Eckert, *Int. J. Appl. Glass Sci.* 2018, 9, 167–187.
- [4] D. R. Cassar, *Ceram. Int.* 2023, 49, 36013–36024.

## Report:

### Euromar 2025

Oulu, July 6-10, Finland

The 21<sup>st</sup> EUROMAR conference took place in Oulu, in northern Finland, only 200 km South from the Arctic Circle. The conference began on Sunday July 6 and finished on Thursday July 10. Most of the activities took place in the Music Center. The Madetoja hall, the home of Oulu Symphony, served as a venue for the opening and closing ceremonies as well as plenary and parallel sessions. The second parallel session venue was the adjacent Tulindberg chamber music hall. The sponsor exhibition areas were around the Madetoja and Tulindberg halls. The third parallel session hall as well as poster sessions were located in the adjacent Pohjankartano multipurpose building.



### Committees

The international Scientific Committee was composed by Ville-Veikko Telkki (Chair, University of Oulu), Juha Vaara (University of Oulu), Patrick Giraudeau (University of Nantes), Isabella Felli (University of Florence), Camilla Terenzi (Wageningen University & Research), Marilena Di Valentin (University of Padova), Anne Lesage (CNRS), Claudia Avalos (New York University), Marcel Utz (Karlsruhe Institute of Technology), Alexander Barnes (ETH Zürich), Rina Rosenzweig (Weizmann Institute of Science), Chantal Tax (UMC Utrecht), and Olav Schiemann (University of Bonn).

The members of the Local Organizing Committee were Ville-Veikko Telkki (Chair, University of Oulu), Anu Kantola (Vice Chair, University of Oulu), Juha Vaara (University of Oulu), Perttu Lantto (Sustainability, University of Oulu), Vladimir Zhivonitko (University of Oulu), Anne Selent (Visual Design, University of Oulu), Otto Mankinen (University of Oulu), Miika Nieminen (University of Oulu), Elina Sievänen (University of Jyväskylä), Perttu Permi (University of Jyväskylä), Mikko Kettunen (University of Eastern Finland), Olli Gröhn (University of Eastern Finland), and Pasi Soininen (Nightingale Health).

## Promotion and Communication

The conference website ([www.euromar2025.org/](http://www.euromar2025.org/)) was launched just before the previous EUROMAR in Bilbao. In addition, the conference was advertised and information spread by frequent e-mails to the AMPERE mailing list as well as the people registered in the mailing list of EUROMAR 2025. Social media channels included Twitter and Facebook



## EUROMAR 2025 in Figures

Regardless of the northern location as well as many cancellations due to war in the Middle East, visa issues in the USA and flight strikes, the number of participants was rather high, 640. Altogether 36 countries were represented. The conference program comprised 180 scientific oral presentations, from which 75 was given by female speakers. The oral presentations included 13 (45 min) invited plenary, 2 (60 min) invited tutorial, 41 (30 min) invited parallel, 44 (20 min) contributed and 80 (5 min) flash talks. Topics covered BioNMR, Materials, Solid-state methods, Liquid-state methods, Benchtop and low field, Small molecules and pharmaceutical, Metabolomics, MRI, EPR, Hyperpolarization, Theory and computation, Hardware, Paramagnetic NMR, and Single-molecule/NV. The tutorials given by Profs. Mei Hong and Daniel Topgaard focused on biomolecular solid-state NMR techniques as well as multidimensional diffusion-relaxation correlation NMR and MRI. In addition, 339 posters were presented in dedicated poster sessions on three consecutive days.

## Prizes

Three major prizes were given in the opening ceremony. The 2025 Richard R. Ernst award was given to Prof. Thomas Prisner for his significant contributions to the development and application of new methods in EPR and DNP. The Chair of the Prize Committee Lucio Frydman could not attend the conference. Therefore, the prize was introduced by the Member of the Prize Committee Ville-Veikko Telkki and given by the President of the Bruker BioSpin Group Falco Busse. The AMPERE Prize for Young Investigators was given to Prof. Tuo Wang in recognition of his outstanding contributions to solid-state NMR spectroscopy in heterogeneous biomaterials expanding the frontiers of biomolecular NMR and DNP. The Raymond Andrew Prize was given to Dr. Nergiz Şahin Solmaz for her doctoral thesis titled "Single Chip Dynamic Nuclear Polarization Microsystems". The two latter prizes were introduced and given by the President of AMPERE Prize Committee Bernhard Blümich.



Several other prizes were given at the closing ceremony. JMR/JMRO Young Scientist Awards were given to Ana Paula Aguilar Alva (École Normale Supérieure), Claire Ollier (CRMN), Hugo Karas (ETH Zürich), and Marvin Lenjer (MPI for Multidisciplinary Sciences) by the Editor-in-Chief Tatyana Polenova. Shimon Vega Travel Award was given to Yao Fu (University of Cambridge) by Prof. Ilya Kuprov. MRC Awards were given to Kawarpal Singh (University of Cambridge) and Pia S. Mayer (University of Copenhagen) by the Deputy Editor Patrick Giraudeau. IES Poster Awards were given to Julian Stropp (ETH Zurich) and Sudipta Khamrui (Tel Aviv University) by Prof. Marilena Di Valentin. Chemistry Europe awards were given to Nouran Hamed (University of Manchester), Johannes Denninger (RWTH Aachen University), and Gabriel Balavoine (CRMN) by Prof. Olav Schiemann.



## Sponsors

We are deeply grateful to sponsors for their generous support for EUROMAR 2025 – without their support the conference would not have been possible. We had altogether 36 sponsors, including 1 platinum (Bruker), 1 gold (JEOL), 1 silver (Magritek), 2 bronze (Merck and CIQTEK), 25 supporter and 6 brand partner sponsors. The sponsor exhibition areas were centrally located at the Music Center around main lecture halls and lunch/coffee service points.

## Sustainability

About 95% of the CO<sub>2</sub> emissions of international conferences arise from air travel. Consequently, the participants were instructed to consider more sustainable travel options, which were described on the conference website. For example, we offered a guided (by Daniel Topgaard) train-boat-train trip from Copenhagen to Oulu and back. More than 20 people joined the guided trip and enjoyed at the same time entertaining preconference meetings. In addition, we invested 12.6 € per participant in Hiilipörssi to restore dried Finnish marshland. This will turn the bog from CO<sub>2</sub> emitter (+5.5 tCO<sub>2</sub>e/y/ha) to carbon sink (-1.0 tCO<sub>2</sub>e/y/ha). With 8078.55 € we bought 164 tons of CO<sub>2</sub>e compensation. This corresponds to about 760 000 km (1200 km/person) of flying.

## Social Activities

In addition to the outstanding scientific content, EUROMAR 2025 included a diverse social program.

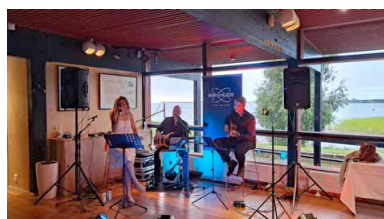
The opening and closing ceremonies began with the first and last movement of Einojuhani Rautavaara's Cantus Arcticus – Concerto for Birds and Orchestra. Cantus Arcticus is an internationally well-known composition, which was ordered by the University of Oulu for its first Doctoral Conferment Ceremony in 1972. Rautavaara recorded most

of the bird sounds at the Liminganlahti bay next to Oulu. Prof. emeritus Erkki Alasaarela and his brother Matti Alasaarela prepared multimedia presentations of Cantus Arcticus for EUROMAR 2025, combining the music with impressive bird photos and videos.

The opening ceremony included also many live performances of Finnish classical music. At the end of his opening speech, the Chair of the Conference Ville-Veikko Telkki sang a lullaby Heijaa composed by Leevi Madetoja, who was born in Oulu and after whom the plenary hall is named. In addition, opera singer Anna-Maria Jurvelin-Pesola and pianist Markus Vaara performed songs of the most famous Finnish composer Jean Sibelius as well as Oskar Merikanto and Ilmari Hannikainen.



The opening ceremony was followed by the Welcome Night, including buffet dinner and live jazz music, hosted by the City of Oulu. The Chairman of the City Board Lauri Nikula highlighted Oulu's status as the European Capital of Culture in 2026 and the Silicon Valley of the North.



The Bruker night on Monday evening was in Restaurant Nallikari next to the beautiful Nallikari beach as well as the iconic Nallikari Lighthouse. The atmosphere was warm regardless of a bit chilly and windy evening.



The JEOL music night on Tuesday evening began with wonderful piano, cello, guitar and singing performances by the participants of the conference – researchers in the field of magnetic resonance are really musical! At the end, the Oulu University Chamber Orchestra played a string quartet of Erik Tulindberg, who is another composer from Oulu and after whom the second lecture hall is named.



Wednesday evening offered us refreshing sports exercises and best parts of Oulu city in the form of guided group walks and runs.

The conference culminated in the dinner at the Hotel Radisson Blu on Thursday night. We had the pleasure of enjoying the energetic music of the band Shut the Funk Up as well as beautiful midnight sun on the terrace of the restaurant next to Oulu river delta.

### Bird side theme

In the conference advertisements, we raised a mystery: what this bird is and how it relates to EUROMAR 2025? In the opening ceremony, the secret was revealed: it is a shore lark, which is the soloist of the second movement, Melancholy, of Rautavaara's Cantus Arcticus. The shore lark lives mostly in the Arctics, and it is very rare in Finland. However, recently it visited in Oulu: this photo was taken by Erkki Alasaarela from Hailuoto island in spring 2024. Similarly, EUROMAR is very rare in Oulu, but not completely unique: in 1994, the predecessor of EUROMAR, EENC, was organized in Oulu. Many of the participants of EUROMAR 2025 were also in EENC 1994 in Oulu.



Birds were a side theme of the conference. Prof. Peter Hore gave scientifically, pedagogically and visually outstanding presentation entitled "Animal Detected Magnetic Resonance" about bird's ability to detect Earth's magnetic field. We encouraged all participants to make a connection between research and birds in their presentation. It was absolutely fantastic to see how well the participants responded to our wish – birds appeared in nearly every presentation in extremely creative ways.

At the closing ceremony, we awarded a humorous „Beak Performance“ prize to Prof. Sami Jannin for his highly amusing, creative, and psychologically nuanced incorporation

of the bird theme in his plenary lecture. It featured a bit of a beak-to-beak showdown between the speaker and an angry turkey. In the end, the turkey ended up as a roast.

### Conclusions

We are deeply grateful to AMPERE and EUROMAR for trusting us and giving us a chance to organize EUROMAR 2025. We are also really thankful to all participants for accepting our invitation to attend the conference. It was amazing, like a dream, to see so many of our dear magnetic resonance friends from all around the world in our distant small city in the North. Everything worked surprisingly well, thanks to the excellent work of the local organizing committee, scientific committee, professional conference organiser Talo Events, staff of the venue, congress technique and catering, as well as all the members of the NMR Research Unit at the University of Oulu. It was a perfect team for organizing a conference. The feedback was very positive. We are especially grateful that many people felt the atmosphere of the conference warm, inclusive, constructive and relaxed. The participants were very satisfied with the scientific program, and 96% of the responders of the feedback survey would like to see student flash talks highlighting their posters also in future EUROMAR conferences. Several responders criticized that some of the flash talks were only after poster sessions. This criticism was delivered to organizers of the next EUROMAR – one simple potential solution is to move the Monday poster session to Thursday.



Organizing EUROMAR 2025 was a huge amount of work. It started already in autumn 2022 with the preparation of the proposal for EUROMAR Board of Trustees Meeting in EUROMAR 2023 in Glasgow. Frequent Local Organizing Committee meetings started immediately after the Glasgow EUROMAR. The workload increased gradually, and it was practically full day

job for the key organizers in the last months before the conference. However, it was also highly rewarding. It was enjoyable to work together with very pleasant, highly motivated and skilful people. The common effort glued people together. Thorough preparations were rewarded with a highly successful event. It was a unique experience, which remains in our memories and hearts for rest of our lives.

## Awards Euromar 2025:

### AMPERE Prize for Young Investigators

Dr. Tuo Wang

Dr. Tuo Wang has received the AMPERE prize for Young Investigator during EUROMAR 2025. The prize was given in recognition of his achievements in solid-state NMR spectroscopy in heterogeneous biomaterials.

Tuo Wang received his Ph.D. in Physical Chemistry under the supervision of Dr. Mei Hong in 2016, where he was trained in solid-state NMR spectroscopy, with applications to membrane proteins, plant primary cell walls, and amyloid fibrils. After a brief postdoctoral appointment in the research group, Tuo joined the faculty at Louisiana State University as an Assistant Professor in 2017 and was promoted to Associate Professor in 2021. The following year, he was appointed the Carl H. Brubaker Associate Professor of Chemistry at Michigan State University and, in 2025, promoted to the Carl H. Brubaker Professor.

Tuo's independent research program focuses on advancing our understanding of the structure–function relationships of complex carbohydrates in diverse organisms and heterogeneous biomaterials, primarily through solid-state NMR and DNP techniques [1]. His work began with investigations of plant lignocellulosic biomass [2,3] and has since expanded to fungal pathogens [4-11] and algal cells [12,13]—systems that are central to both biomedical and bio-renewable research—and, more recently, to explorations of wetland plants and soils [14], which are profoundly influenced by global climate change. By integrating a range of NMR methods, including  $^{13}\text{C}$ ,  $^{15}\text{N}$ , and  $^1\text{H}$  solid-state NMR, spectral editing techniques, as well as DNP [14,15], he has been able to obtain molecular-level insights into the biological and structural roles of carbohydrate polymers within their native cellular environments. His lab also developed a carbohydrate solid-state NMR database ([www.ccmrd.org](http://www.ccmrd.org)), which prepared us to rapidly assess carbohydrates from various heterogeneous sources.

During his presentation at EUROMAR 2025, titled “High-Resolution Analysis of Carbohydrate-Rich Heterogeneous Biomaterials: Exploring the Wild with Solid-State NMR and DNP,” Dr. Wang highlighted key advances in understanding the structure of plant lignocellulose. He outlined current capabilities for characterizing both  $^{13}\text{C}$ -labeled biomass and unlabeled samples, the latter made possible by natural-abundance DNP methods. He then posed an important question: “Can DNP tackle real-world samples?” This led to his study of native wetland soil, endangered by rapid wetland loss due to erosion, where all samples are unlabeled and exceptionally complex. Dr.

Wang demonstrated that DNP enables a molecular-level view of plant decomposition into soil over millennia. He concluded his talk with a summary of recent progress in high-resolution solid-state NMR, particularly the integration of <sup>1</sup>H-detection approaches with DNP. These methods provide new insights into fungal cell wall architecture and reveal correlations between peak multiplicity, structural polymorphism, and the biological functions of cellular carbohydrates.

#### References

- [1] Ghassemi...Wang, Solid-state NMR investigations of extracellular matrices and cell walls of algae, bacteria, fungi, and plants. *Chem Rev.* 122, 10036-10086 (2022).
- [2] Kang...Wang, Lignin-polysaccharide interactions in plant secondary cell walls revealed by solid-state NMR. *Nat. Commun.* 10, 347 (2019).
- [3] Kirui...Wang, Carbohydrate-aromatic interface and molecular architecture of lignocellulose. *Nat. Commun.* 13, 538 (2022).
- [4] Widanage...Wang. Distinct Echinocandin Responses of *Candida albicans* and *Candida auris* Cell Walls Revealed by Solid-State NMR. *Nat. Commun.* 16, 6295 (2025).
- [5] Dickwella...Wang, Adaptive survival of *Aspergillus fumigatus* to echinocandins arises from cell wall remodeling beyond  $\beta$ -1,3-glucan synthesis inhibition. *Nat. Commun.* 15, 6382 (2024).
- [6] Cheng...Wang, Molecular architecture of chitin and chitosan-dominated cell walls in zygomycetous fungal pathogens by solid-state NMR. *Nat. Commun.* 15, 8295 (2024).
- [7] Fernando...Wang, Structural adaptation of fungal cell wall in hypersaline environment. *Nat. Commun.* 14, 7082 (2023).
- [8] Chakraborty...Wang, A molecular vision of fungal cell wall organization by functional genomics and solid-state NMR. *Nat. Commun.* 12, 6346 (2021).
- [9] Kang...Wang, Molecular architecture of fungal cell walls revealed by solid-state NMR. *Nat. Commun.* 9, 2747 (2018).
- [10] Ankur...Wang, Polymorphic  $\alpha$ -glucans as structural scaffolds in *Cryptococcus* cell walls for chitin, capsule, and melanin: Insights from <sup>13</sup>C and <sup>1</sup>H solid-state NMR. *Angew. Chem. Int. Ed.* e202510409 (2025).
- [11] Solid-state NMR analysis of *Schizosaccharomyces pombe* reveals role of  $\alpha$ -amylase family enzymes in cell wall structure and function. Jacob...Wang\*, KL Gould\*. *Proc Natl Acad Sci USA* (2025).
- [12] Poulhazan ... Wang, Identification and quantification of glycans in whole cells: architecture of microalgal polysaccharides described by solid-state NMR. *J. Am. Chem. Soc.* 143, 46, 19374-388 (2021).
- [13] Molecular-level architecture of *Chlamydomonas reinhardtii*'s glycoprotein-rich cell wall. A Poulhazan... Wang\*, Warschawski\* and Marcotte\*. *Nat. Commun.* 15, 986 (2024).
- [14] Zhao...Wang, Enriched molecular view of saline wetland soil carbon by sensitivity-enhanced solid-state NMR. *J. Am. Chem. Soc.* 147, 519-531 (2025).
- [15] Proton-detected solid-state NMR for deciphering structural polymorphism and dynamic heterogeneity of cellular carbohydrates in pathogenic fungi. Yarava...Wang. *J. Am. Chem. Soc.* 147, 17416-17432 (2025).

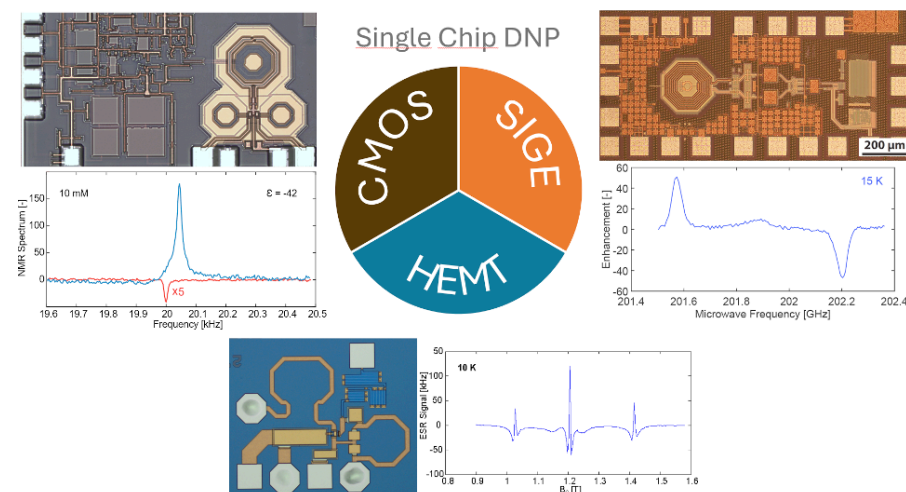
## Awards Euromar 2025:

### Raymond Andrew Prize

Dr. Nergiz Sahin Solmaz

#### Single Chip Dynamic Nuclear Polarization Microsystems

Nuclear magnetic resonance (NMR) methods are powerful tools employed in many fields, including physics, chemistry, material science, biology, and medicine. The use of NMR methodologies in an even wider range of applications is often hindered by the relatively large number of resonating spins needed to achieve a sufficiently large signal-to-noise ratio (SNR) in the available experimental time. An efficient approach to increase the SNR is hyperpolarization where the nuclear spin polarization is increased, e.g., by microwave, optical, and chemistry-based methodologies. Dynamic nuclear polarization (DNP) is one of the most versatile hyperpolarization methods. Microwave DNP employs a microwave magnetic field to excite the unpaired electrons in the sample under investigation into electron spin resonance (ESR). A major drawback of DNP is the cost and complexity of the required microwave hardware, especially at high magnetic fields and low temperatures. To overcome this drawback and with the focus on the study of nanoliter and subnanoliter samples, this thesis demonstrates single chip DNP microsystems where the microwave excitation and detection are performed locally on a chip without the need of external microwave generators and transmission lines.



During the last two decades, the separate integration on a single chip of the front-end electronics of NMR and ESR spectrometers has been demonstrated. In this thesis, the co-integration on a single chip of the front-end electronics of NMR and ESR detectors is presented for the first time. This combination of sensors allows to perform DNP

experiments using a single chip having an area of about 2 mm<sup>2</sup>.

Firstly, a DNP microsystem operating at 10.7 GHz (ESR)/16 MHz (NMR) is integrated into a single CMOS chip. The ESR detector is an oscillator that generates microwave magnetic fields  $B_{1e}$  up to 70  $\mu$ T. The NMR detector is a broadband transceiver operating up to 1 GHz. <sup>1</sup>H DNP-enhanced NMR experiments on liquid and solid samples having a volume of about 1 nL are performed. Overhauser enhancements up to 50 are achieved on TEMPOL/H<sub>2</sub>O solutions and solid effect enhancements up to 20 are achieved on BDPA:SEBS at room temperature.

Secondly, a DNP microsystem operating at 200 GHz (ESR)/300 MHz (NMR) is integrated into a single SiGe:BiCMOS chip. The ESR detector is a voltage controlled oscillator (VCO) operating at 200 GHz with a tuning range of 8 GHz which generates a  $B_{1e}$  of about 10 G. The NMR detector is a broadband receiver operating up to 1 GHz. <sup>1</sup>H DNP experiments on BDPA:PS samples having a volume of 2 nL and 125 pL show solid effect enhancements up to 50 and 10 at 15 K and 100 K, respectively. A single chip DNP array is also demonstrated. The array has four frequency locked 200 GHz VCOs which interrogates a sample volume an order of magnitude larger compared to the single VCO. Measurements on BDPA:PS samples having a volume of 1 nL show solid effect enhancements up to 20 at 200 K.

Finally, an In<sub>0.7</sub>Ga<sub>0.3</sub>As high electron mobility transistor (HEMT) technology is investigated for the possible integration of low power single chip DNP microsystems that might be able to operate down to 1 K and below. HEMT transistors and ultra low power oscillators operating at 11 GHz and 35 GHz are investigated down to 1.4 K.

This thesis demonstrates the realization of single chip ESR and DNP microsystems operating up to 200 GHz and down to 15 K. By suppressing the need for external microwave sources and connections, the single chip approach proposed in this thesis reduce drastically the cost and the complexity of the DNP instrumentation and, hence, should allow for more widespread use and study of DNP methodologies, particularly for nanoliter and subnanoliter samples.

## AMPERE Travel Awards Euromar 2025:

Durga Prasad

### Structural and Dynamic Insights into the Loss of Activity of Tolaasin I, an antimicrobial cyclic lipopeptide.

Durga Prasad<sup>1</sup>, Benjamin Kovacs<sup>1</sup>, Niels Geudens<sup>1</sup>, Monic Hofte<sup>2</sup> and Jose C. Martins

<sup>1</sup> NMR & Structure Analysis Unit, Dept. of Organic and Macromolecular Chemistry, Ghent University, Ghent, Belgium

<sup>2</sup> Laboratory of Phytopathology, Department of Plants and Crops, Ghent University, Coupure Links 653, B-9000 Gent, Belgium

Cyclic lipopeptides (CLiPs) are secondary metabolites characterized by a peptide moiety with an N-terminal lipid tail and a macrocycle formed via a depsi bond. Produced by various bacteria like *Pseudomonas* and *Bacillus*, CLiPs have diverse biological functions, including enhancing bacterial motility and exhibiting antibacterial and antifungal activities.[1] Tolaasin, a CLiP from *Pseudomonas tolaasii*, is responsible for brown blotch disease in mushrooms and shows inhibitory effects against fungi and Gram-positive bacteria. A natural defense mechanism, where tolaasin's antagonistic properties are neutralized by hydrolysis of the depsi bond, involves an enzyme from a cohabiting bacterium.[2] Understanding how structural changes impact membrane interactions is vital for developing new therapeutics and biocontrol agents.

In this study, we use NMR spectroscopy to investigate conformational changes and membrane interactions of both native and hydrolyzed tolaasin in SDS micelles. To enable multidimensional NMR analysis, <sup>13</sup>C- and <sup>15</sup>N-labeled tolaasin and its hydrolyzed form are produced by growing the bacterium on minimal medium. Followed by full resonance assignments and <sup>15</sup>N relaxation experiments provide insights into peptide backbone dynamics, with order parameters (S<sup>2</sup>) shedding light on molecular motions on the ns-ps timescale. 3D-HNHA experiments were conducted to access backbone conformation dependant <sup>3</sup>J<sub>H<sub>N</sub>H<sub>α</sub></sub> scalar couplings. Long-range HNCO measurements identify long-lived hydrogen bonds through <sup>3</sup>J<sub>N-C'</sub> scalar couplings. Additionally, <sup>1</sup>H R<sub>1</sub> rates, recorded with and without a paramagnetic agent, map the paramagnetic relaxation enhancement (PRE) wave of tolaasin, allowing to determine helix orientation.

Our findings suggest that opening the macrocycle leads to partial loss of peptide backbone rigidity, resulting in conformational changes in exocyclic residues. These insights are crucial for the design of biocontrol agents and novel therapeutics.

#### References

[1] Geudens, N. and J.C. Martins, Front. Microbiol. 9, 1867, (2018)

[2] Hermenau, R., et al., Proc. Natl. Acad. Sci. U.S.A. 117(38), 23802-23806, (2020)

## AMPERE Travel Awards Euromar 2025:

Domenico Gioffrè

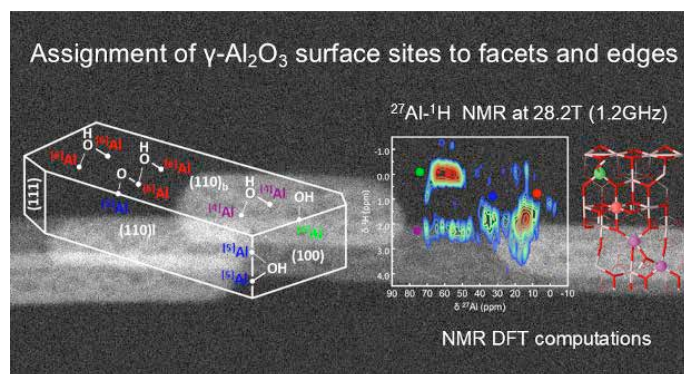
### Classification and Identification of Facet and Edge Specific $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Surface Sites from 1H/27Al NMR Cross-Signatures and DFT Modelling

Domenico Gioffrè,<sup>a</sup> Pierre Florian,<sup>a,b</sup> Thomas Pigeon,<sup>c</sup> Pascal Raybaud,<sup>c</sup> Céline Chizallet,<sup>c</sup> Christophe Copéret,<sup>a</sup>

<sup>a</sup> Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich CH-8093, Switzerland

<sup>b</sup> CNRS, CEMHTI UPR3079, Univ. Orléans, Orléans F45071, France

<sup>c</sup> IFP Energies nouvelles, Solaize BP 3, 69360, France



$\gamma$ -Al<sub>2</sub>O<sub>3</sub> finds applications in industry as catalyst or support for catalytic active phases. The properties of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> have been ascribed to surface sites with varying Al coordination number, acidity and basicity. The presence of specific <sup>IV</sup>Al( $\mu$ -OH) has been proposed to be associated with certain facets or edges.[1] In recent years, solid-state NMR (ssNMR) has emerged as a powerful tool because of its high sensitivity to the chemical environment and its potential to resolve the various <sup>1</sup>H, <sup>27</sup>Al and <sup>17</sup>O surface sites. [2,3] Furthermore, two-dimensional ssNMR correlations helped gaining a better understanding of the connectivity of surface species. However, Al surface sites are experimentally challenging to detect on de-hydroxylated surfaces, central to catalytic processes, due to expected large C<sub>Q</sub> values, typically >15 MHz. Here, we combine surface-specific D-HMQC <sup>27</sup>Al{<sup>1</sup>H} ssNMR at high field (28.2T) at fast MAS (50kHz) to observe four main distinct families of surface Al-OH sites, including an <sup>IV</sup>Al-OH site with an unprecedented CQ approaching 18MHz.[4] We applied this methodology to two  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> samples, dehydroxylated at 500° (2.8 OH/nm<sup>2</sup>), an edge-rich needles shaped  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, and the commercially available SBA200. All resulting <sup>27</sup>Al-O<sup>1</sup>H environments are fitted with pairs of (<sup>27</sup>Al, <sup>1</sup>H) lines allowing us to recover coupled NMR parameters. Comparing the measured NMR signatures (<sup>27</sup>Al  $\delta_{iso}$ , C<sub>Q</sub> and <sup>1</sup>H  $\delta_{iso}$ ) to computed values from a large range of structural DFT models allowed the identification of facet- and

edge-specific Al-OH surface sites in  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>. The assignments revealed different edge/facet ratio in the studied samples, consistent with their different morphologies. Our findings enabled the derivation of 3D model of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> surface and can serve as a tool to advance the synthesis of materials with specific surface features. This knowledge can be applied to understand the interactions of molecules with  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> surface, and to develop more accurate surface models.

#### REFERENCE LIST:

- (1) Busca, G. Structural, Surface, and Catalytic Properties of Aluminas. In *Advances in Catalysis*; Jentoft, F. C., Ed.; Academic Press, 2014; Vol. 57, pp 319–404.
- (2) Batista, A. T. F.; Wisser, D.; Pigeon, T.; Gajan, D.; Diehl, F.; Rivallan, M.; Catita, L.; Gay, A.-S.; Lesage, A.; Chizallet, C.; Raybaud, P. Beyond  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Crystallite Surfaces: The Hidden Features of Edges Revealed by Solid-State <sup>1</sup>H NMR and DFT Calculations. *J. Catal.* 2019, 378, 140–143.
- (3) Wischert, R.; Florian, P.; Copéret, C.; Massiot, D.; Sautet, P. Visibility of Al Surface Sites of  $\gamma$ -Alumina: A Combined Computational and Experimental Point of View. *J. Phys. Chem. C* 2014, 118 (28), 15292–15299.
- (4) Gioffrè, D.; Florian, P.; Pigeon, T.; Raybaud, P.; Chizallet, C.; Copéret, C. Classification and Identification of Facet- and Edge-Specific  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Surface Sites from 1H/27Al NMR Cross-Signatures and DFT Modeling. *J. Am. Chem. Soc.* 2025, 147 (8), 6934–6941.

## AMPERE Travel Awards Euromar 2025:

Ummugulsum Gunes

### <sup>1</sup>H-<sup>87</sup>Rb Double Resonance NMR to Detect the Incorporation of Formamidinium into Rb-based Non-perovskite Phases

Ummugulsum Gunes<sup>1</sup>, Michael A. Hope<sup>1,2</sup>, Yuxuan Zhang<sup>1</sup>, Likai Zheng<sup>1</sup>, Lukas Pfeifer<sup>1</sup>, Michael Grätzel<sup>1</sup>, Lyndon Emsley<sup>1</sup>

<sup>1</sup> Ecole Polytechnique Fédérale de Lausanne, Lausanne 1015, Switzerland

<sup>2</sup> Department of Chemistry, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK

Hybrid organic-inorganic perovskite materials, such as formamidinium lead iodide (FAPbI<sub>3</sub>), are promising candidates for next-generation photovoltaic materials. However, the utilization of FAPbI<sub>3</sub> perovskite in commercial solar cells is hindered due to its the spontaneous phase transition (from the photoactive perovskite phase to a photoinactive non-perovskite phase). This phase transformation issue can be solved by including alkali metal cations such as Cs<sup>+</sup> and Rb<sup>+</sup> in the perovskite synthesis. It has been demonstrated by solid-state NMR spectroscopy that the Rb<sup>+</sup> cation cannot incorporate into the hybrid perovskite lattice in single and double halide systems but instead forms a non-perovskite Rb-based phase. However, the mechanism by which Rb causes improved stability is still unclear.

Here, <sup>1</sup>H-<sup>87</sup>Rb double resonance experiments are carried out to show that instead of

Rb<sup>+</sup> cations being incorporated in the perovskite lattice, FA<sup>+</sup> cations incorporate into the Rb-based non-perovskite phases (FA<sub>x</sub>Rb<sub>1-x</sub>Pb<sub>2</sub>Br<sub>5</sub> and δ-FA<sub>x</sub>Rb<sub>1-x</sub>PbI<sub>3</sub>) for both bromide and iodide perovskites. This is shown by <sup>1</sup>H and <sup>87</sup>Rb chemical shifts changes, <sup>1</sup>H–<sup>87</sup>Rb heteronuclear correlation (HETCOR) experiments, and complete dephasing in the <sup>87</sup>Rb{<sup>1</sup>H} REDOR spectra.

Finally, REDOR dephasing curves are simulated to determine the amount of FA<sup>+</sup> incorporated into the Rb-based non-perovskite phase. Our findings show that up to ~60% FA<sup>+</sup> can incorporate for the bromide system and ~15% for the iodide system. We propose that the improved stability imparted by Rb salts in the synthesis of FA-based perovskites can be attributed to the segregation of excess FA<sup>+</sup> cations.

## AMPERE Travel Awards Euromar 2025:

Urvashi D. Heramun

### Double-Quantum Excitation in Systems at Near-Equivalence

Urvashi D. Heramun, Mohamed Sabba, Gamal Moustafa, and Malcolm H. Levitt

School of Chemistry, University of Southampton, SO17 1BJ, United Kingdom

Double-quantum coherence excitation via standard methods such as INADEQUATE<sup>1</sup> is inefficient in the near-equivalence limit, where the chemical shift difference between two spins is much smaller compared to the respective scalar coupling. This results in extensive signal losses due to T<sub>2</sub> relaxation.

A recently devised<sup>2</sup> double-quantum excitation method, GEODQ, exploits the Aharonov-Anandan geometric phase, and has shown to be more efficient than conventional INADEQUATE, leading to stronger signals.

Pulse sequences such as SLIC<sup>3</sup> and PulsePol<sup>4</sup> have been used to access nuclear singlet order in the past. We adapt both methods, now SLIC DQ, and PulsePol DQ, to excite double-quantum coherences within an AB type chemically inequivalent two-spin system. In addition, we plan to explore the case of an AA'MM'XX' type six-spin system where the spins are chemically equivalent, but magnetically inequivalent.

We show that the GEODQ, SLIC DQ, and PulsePol DQ pulse sequences can be employed for efficient double-quantum excitation in the near-equivalence limit. Possible applications<sup>5,6</sup> include selectively observing double-quantum filtered signals from metabolites, providing scope for in vivo experiments, as well as for new contrast agents.

#### References

1. A. Bax, R. Freeman, T. A. Frenkiel and M. H. Levitt, J. Magn. Reson., 1981, 43, 478–483.
2. C. Bengs, M. Sabba and M. H. Levitt, J. Chem. Phys., 2023, 158, 124204.
3. S. J. DeVience, R. L. Walsworth and M. S. Rosen, Phys. Rev. Lett., 2013, 111, 173002.

4. M. Sabba, N. Wili, C. Bengs, J. W. Whipham, L. J. Brown and M. H. Levitt, J. Chem. Phys., 2022, 157, 134302.
5. S. Mamone, N. Rezaei-Ghaleh, F. Opazo, C. Griesinger and S. Glöggler, Science Advances, 2020, 6, eaaz1955.
6. S. Mamone, A. B. Schmidt, N. Schwaderlapp, T. Lange, D. von Elverfeldt, J. Hennig and S. Glöggler, NMR in Biomedicine, 2021, 34, e4400.

## AMPERE Travel Awards Euromar 2025:

Johannes Schmoll

### Water-detected NMR allows dynamic observations of repeat-expansion RNA condensates

Johannes Schmoll<sup>#</sup>, Mihajlo Novakovic<sup>#</sup> & Frédéric H.-T. Allain

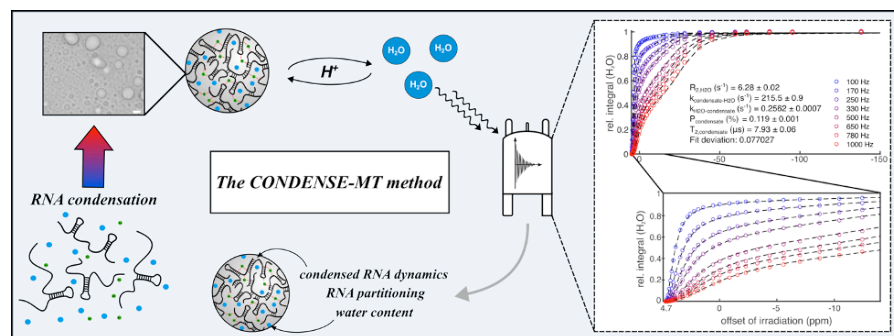
Department of Biology, Institute of Biochemistry, ETH Zurich, Zurich, Switzerland

<sup>#</sup>These authors contributed equally

#### Abstract

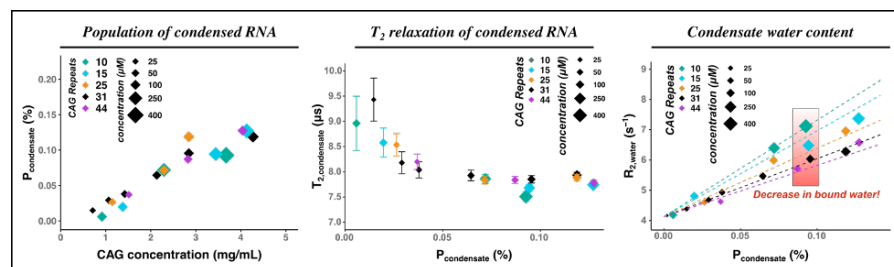
RNA condensation is implicated in the formation of toxic RNA foci in cells affected by genomic expansions of trinucleotide repeats.<sup>1</sup> The physical properties of such condensates are, however, poorly understood due to the limited number of available methods for their characterization. Using CAG repeat-expansion RNA as a model system, we show that these condensates are broadened beyond detection via liquid-state NMR spectroscopy. However, selective saturation of condensate resonances can be relayed to H<sub>2</sub>O via fast through-space dipolar transfer in rigid materials, allowing information about condensed RNA to be encoded in solvent water. Based on this, we developed a method, termed *CONDensate DETection by SEMI-solid Magnetization Transfer* (CONDENSE-MT), for characterization of NMR-invisible biological condensates (Fig. 1).<sup>2</sup> CONDENSE-MT is based on semi-solid magnetization transfer<sup>3</sup> and exploits multiple exchange processes to water during prolonged saturation. The resulting 150-fold signal amplification enabled detection of condensates at RNA levels as low as 1 mg/mL (Fig. 2, *panel 1*). CONDENSE-MT revealed a 1000-fold decrease in molecular tumbling of RNA upon condensation, leading to T<sub>2</sub> relaxation constants below 8 μs and suggesting semi-solid material properties of these condensates (Fig. 2, *panel 2*). We show that, upon condensation, RNA partitioning depends on the MgCl<sub>2</sub> concentration, implying that this process is driven by heterotypic interactions between RNA and Mg<sup>2+</sup>. Further, we detected a dramatic reduction of condensate-bound water when increasing the number of CAG repeats per RNA oligomer (Fig. 2, *panel 3*). Given the crucial role of the number of CAG repeats for disease progression, our work provides new mechanistic insights into RNA condensate formation and yielded a broadly applicable NMR method

for characterization of disease-associated biological semi-solids. The findings of this work are currently being published in the journal *Nature Chemistry*.<sup>2</sup>



**Figure 1: Characterization of NMR-unobservable RNA condensates by water detection**

The physical properties of NMR-unobservable RNA condensates (scale bar: 2  $\mu\text{m}$ ) are relayed to solvent water by proton exchange. The properties of condensed RNA can then be extracted by solvent water resonance attenuation as a function of off-resonance irradiation at multiple irradiation strengths via multi-parameter global fitting (right panel).



**Figure 2: Characterization of CAG RNA condensates**

Quantification of CAG repeat-expansion RNA condensates, consisting of a variable number of CAG trinucleotide repeats, using CONDENSE-MT. Number of CAG repeats per oligomer is given by color, molar concentration of the respective RNA oligomer is indicated by marker size.  $P_{\text{condensate}}$ : Fraction of protons in solution contributing to the semi-solid RNA pool.  $R_{2,\text{water}}$ : Apparent  $R_2$  rate of overall water in the presence of RNA condensates (shown in panel 3 as a function of the respective  $P_{\text{condensate}}$ ), indicating the presence of slow-tumbling water molecules in the RNA condensates.

#### References

- Jain, A. & Vale, R. D. RNA phase transitions in repeat expansion disorders. *Nature* 546, 243–247 (2017).
- Schmoll, J., Novakovic, M. & Allain, F. H.-T. Water-detected NMR allows dynamic observations of repeat-expansion RNA condensates. *Nature Chemistry* - in press (2025).
- Henkelman, R. M. et al. Quantitative interpretation of magnetization transfer. *Magn Reson Med* 29, 759–766 (1993).

## AMPERE Travel Awards Euromar 2025:

Leonardo Levorin

### Isoleucine Side Chains as Reporters of Conformational Freedom in Protein Folding Studied by DNP-Enhanced NMR

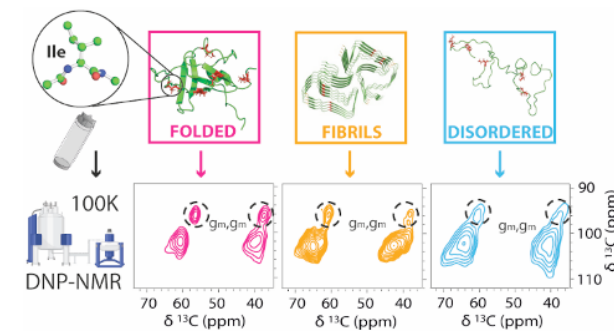
L. Levorin<sup>1,2</sup>, N. Becker<sup>1,2</sup>, B. Uluca-Yazgi<sup>1,2</sup>, L. Gardon<sup>1,2</sup>, M. Kraus<sup>1,2</sup>, P. Neudecker<sup>1,2</sup>, L. Gremer<sup>1,2</sup>, H. Heise<sup>1,2</sup>

<sup>1</sup> Institute of Physical Biology, Heinrich-Heine-Universität Düsseldorf, Germany

<sup>2</sup> Institute of Biological Information Processing, Forschungszentrum Jülich, Germany

Understanding the dynamic conformations of protein side-chains is essential for deciphering protein function. We employed DNP-enhanced solid-state NMR (ssNMR) at cryogenic temperatures to dissect isoleucine (Ile) side-chain dynamics across diverse protein states. We examined three Ile labeled proteins, representing key biological states: intrinsically disordered ( $\alpha$ -synuclein), well-folded (GABARAP), and the whole folding/unfolding/misfolding transition (PI3K SH3).

By analyzing  $^{13}\text{C}$  chemical shifts, which reflect Ile side-chain angles, and performing line-shape analysis of 2D spectra, we obtained comprehensive information about secondary structure and protein mobility. Furthermore, through peak volume integrations, we could quantify the prevalence of specific conformations.



Our results revealed that in well-folded proteins, Ile residues exhibit well-resolved chemical shifts, reflecting structural rigidity. Here, residue-specific conformations could be identified and quantified. In contrast, unfolded and intrinsically disordered proteins displayed significant line broadening, as consequence of higher conformational freedom. We demonstrated that solvent conditions profoundly influence conformational ensembles, distinguishing different unfolded states of PI3K SH3. In amyloid fibrils,  $\beta$ -sheet-like chemical shifts dominated, indicating restricted conformations. Concurrently,

broad signals were observed, reflecting the residual disorder of Ile within the fuzzy coat surrounding the fibril core.

Our research demonstrates the capability of DNP-enhanced ssNMR to overcome limitations in studying (partially) disordered biomolecules. Freeze-trapping physiological exchange provides a precise ensemble snapshot, representing each conformation's probability, offering a more accurate representation than time-averaged data. This approach is a significant advancement in structural biology.

#### References:

Uluca B., Viennet T., Petrovic D., Shaykhalishahi H., Weirich F., Gönülalan A., Strodel B., Eitzkorn M., Hoyer W., Heise H., *Biophys. J.* 2018, 114, 7, 1614-1623  
Siemons L., Uluca-Yazgi B., Pritchard R.B., McCarthy S., Heise H., Hansen D.F.; *Chem Commun.* 2019, 55, 14107-10  
Leverin L., Becker N., Uluca-Yazgi B., Gardon L., Kraus M., Sevenich M., Apostolidis A., Schmitz K., Rüter N., Apanasenko I., Willbold D., Hoyer W., Neudecker P., Gremer L., Heise H.; *J. Am. Chem. Soc.* 2025, 147, 18, 15867–15879

## **AMPERE Travel Awards Euromar 2025:**

**Udina Guillerm**

### **Combined solution- and MAS NMR reveal a locally unfolded state of the bacteriophage tail tube that prevents premature assembly**

Undina Guillerm,<sup>a</sup> Yong Wang,<sup>b</sup> Charles-Adrien Arnaud,<sup>c</sup> Claudine Darnault,<sup>c</sup> Kresten Lindorff-Larsen,<sup>d</sup> Cécile Breyton,<sup>c</sup> Paul Schanda,<sup>a,c,d</sup>

<sup>a</sup> Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria;

<sup>b</sup> College of Life Sciences, Zhejiang University, China;

<sup>c</sup> Institut de Biologie Structurale, Univ. Grenoble Alpes-CEA, CNRS, IBS, Grenoble, France,

<sup>d</sup> Linderstrøm-Lang Centre for Protein Science, Department of Biology, University of Copenhagen, Denmark

The assembly of large functional protein assemblies, such as virus capsids or phage tail tubes must be a well-orchestrated process, ending at a well-defined and highly complex supramolecular structure. NMR spectroscopy is an excellent tool for studying proteins in solution – but only as long as they are small. MAS NMR, on the other hand, is a versatile tool to probe the how the major protein of the bacteriophage tail assembles from monomers to large tube-like architectures. In particular, we interrogated why in the cell the tube forms only when the rest of the bacteriophage is “ready” to be assembled. What keeps the protein from assembling?

With the 50 kDa large tail-tube protein from bacteriophage T5 – which represents a challenge for any NMR study – we thus addressed the dynamics and structure both in

the monomeric state (pre-assembly) and the assembled tube state, using both solution- and MAS NMR.

Interestingly, an extensive set of dynamics experiments revealed that the monomeric protein exists in a dynamic equilibrium of a partially unfolded state (the major form) and the folded state. CPMG relaxation dispersion experiments quantified the thermodynamics and kinetics of the process. MAS NMR, including dynamics measurements, revealed that upon assembly the protein adopts a rigid structure.

Using molecular-dynamics simulations we gained more detailed insights into the partially folded state. Importantly, guided by these data, we were able to identify mutations which shift the equilibrium from the predominantly partially-unfolded state to a fully folded state. This mutant protein has dramatically altered self-assembly, which allowed us to identify the mechanism by the protein is protected from premature assembly: the folding-unfolding equilibrium keeps the protein primarily in a state that cannot assemble, until the rest of the phage is in place.

Collectively, our study highlights the power of combining solution- and MAS-NMR techniques to address complex biological questions of self-assembly.

## **AMPERE Travel Awards Euromar 2025:**

**Elisa Villani**

### **NMR Approaches in Waterlogged Archaeological Wood Conservation**

Elisa Villani<sup>1</sup>, Valeria Stagno<sup>1,3</sup>, Otto Mankinen<sup>2</sup>, Ville-Veikko Tellki<sup>2</sup> and Silvia Capuani<sup>3</sup>

<sup>1</sup> Department of Earth Sciences, Sapienza University of Rome, Italy

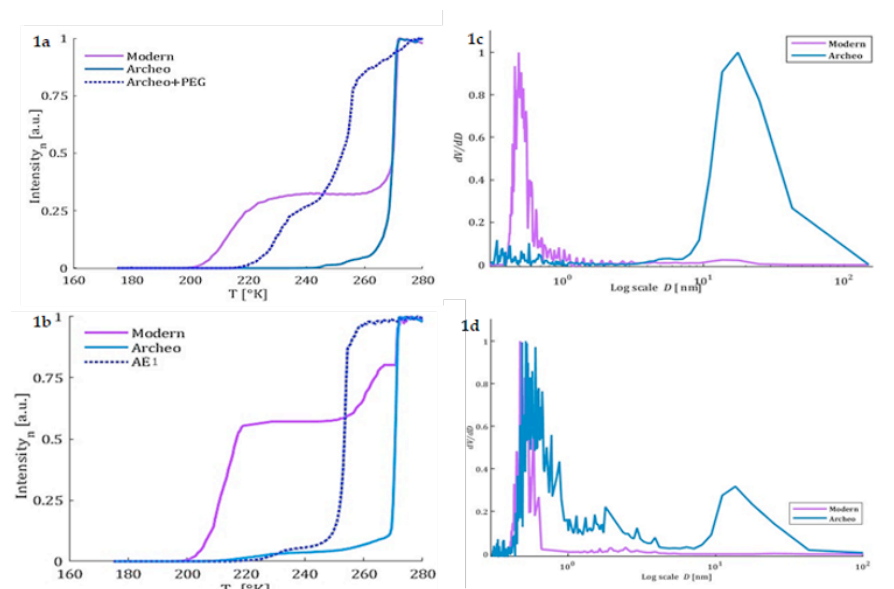
<sup>2</sup> NMR Research Unit, University of Oulu, Finland

<sup>3</sup> National Research Council, Sapienza University of Rome, Italy

Wood plays a crucial role in cultural heritage, as wooden artifacts preserve records of our past. The anoxic conditions of submerged environments can protect wood for millennia but degradation still occurs. Once excavated, waterlogged wood (WW) rapidly deteriorates, losing mechanical strength unless kept submerged.<sup>1</sup> However, this makes it ideal for NMR analysis. Recently, interest in non-destructive NMR studies on fragile heritage has increased, although some possibilities remain unexplored.<sup>2,3</sup> From a conservation perspective, WW requires stabilization and when in-situ conservation is unfeasible, consolidation becomes essential to replace water within the wood tissue while reinforcing its structure. Treatment effectiveness depends on consolidants' penetration and distribution, influenced by their properties and the wood's porous structure.<sup>4</sup> This study combines a multimodal approach using high- and low-field techniques to assess wood degradation and monitor conservation treatments. While MRI and diffusion NMR offer structural and dynamic insights, they lack the resolution to examine the cell wall

at the nanometer scale, achievable with NMR cryoporometry.<sup>5,6</sup> With these methods, we conducted a comprehensive study of wood from the Neolithic submerged village of La Marmotta, assessing degradation after millennia of submersion. Moreover, we explored portable NMR's potential for monitoring the consolidation of WW from the 10<sup>th</sup> century.<sup>7</sup> Samples were treated with polyethylene glycol (PEG) solutions at varying concentrations and weights, following standard practices. PEG's use as a consolidant is well-supported, making it ideal for heavily degraded wood.

### NMR Cryoporometry Highlights: Pore Size Distribution in Modern and Archaeological wood

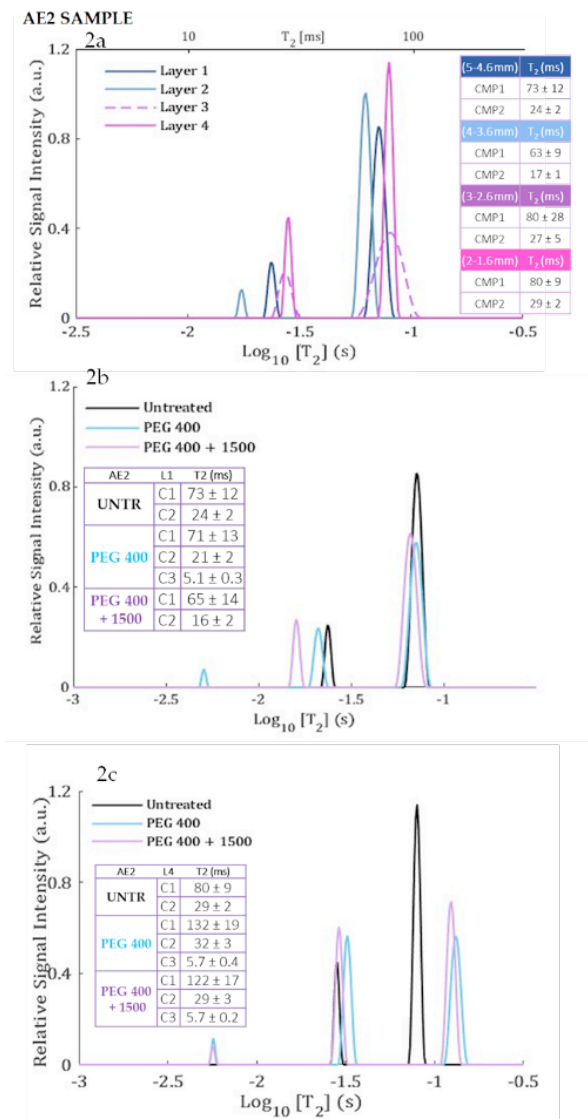


**Figures 1c–d** show pore size distributions derived from the Gibbs–Thomson equation. In archaeological beech (c), pores range from 10 to 80 nm, whereas the modern sample is mostly confined to sizes below 5 nm. A similar trend is observed in elm wood (d): both modern and archaeological samples fall within comparable ranges to beech, although the archaeological elm also shows additional contributions from smaller pores.

### References

- Villani E, et al. *Forests* 16,1(2025)
- Stagno V, et al. *MagnRes Imag* 102,164(2023)
- Stagno V, et al. *MagnRes Imag* 83,139(2021)
- Cavallaro G, et al. *J ThermAnalCalor* 111,1449(2013)
- Stagno V, et al. *PhysChemChemPhys* 26,27189(2024)
- Kekkonen P.M, et al. *J PhysChemC* 118,2146(2014)
- Blümich B, et al. *MagnRes* 2,149(2021)

### Low-Field NMR Highlights: Evolution of T<sub>2</sub> Components in Treated Wood Layers



**Figures 2a–c** show T<sub>2</sub> components obtained from 1D profile experiments. In the untreated sample (2a), all layers display two main components, likely associated with larger vessels in both EW and LW. Figures 2b–c illustrate the evolution of these components in Layer 1 (deepest, 2b) and Layer 4 (superficial, 2c) after treatment. In Layer 1 the central peak shifts to lower T<sub>2</sub> values, with an additional signal probably related to water confined in smaller environments due to PEG 400. In Layer 4, both main components shift toward higher T<sub>2</sub>, and a third peak emerges, possibly associated to water confinement in the presence of PEG.

## AMPERE Travel Awards Euromar 2025:

Yufei Wu

### The role of formate mobility for adaptive hydrogenation catalysts probed by solid-state NMR spectroscopy

Yufei Wu<sup>1,2</sup>, Yuyan Zhang<sup>1</sup>, Julius Schlüter<sup>2</sup>, Henrik Walschus<sup>1</sup>, Walter Leitner<sup>1,2</sup>, Alexis Bordet<sup>1</sup>, Thomas Wiegand<sup>1,2</sup>

<sup>1</sup> Max Planck Institute for Chemical Energy Conversion, Mülheim (Ruhr), Germany

<sup>2</sup> Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Aachen, Germany

Ruthenium nanoparticles (Ru NPs) immobilized on supported ionic liquid phases (SILPs) show adaptive catalytic properties in hydrogenation reactions of ketones in response to adding CO<sub>2</sub> to the feed gas. Using SILPs as silica surface modifiers increases the equilibrium concentration of formate species at the catalytically-active centres, which affects the selectivity of hydrogenation reactions [1]. In this study, we apply solid-state Nuclear Magnetic Resonance (NMR) spectroscopy to investigate molecular interactions between formate and the SILPs to unravel the principles responsible for the increased formate equilibrium concentrations on Ru@SILP catalysts.

We investigate the mobility of formate on SILP surfaces using relaxation properties and polarization efficiencies as sensitive probes. Faster <sup>1</sup>H transverse relaxation times and changes of <sup>1</sup>H-<sup>13</sup>C polarization transfer efficiencies in Cross-Polarization (CP) and Inensitive Nuclei Enhanced by Polarization Transfer (INEPT) experiments point to reduced molecular mobility of formate in case of certain SILPs. Deshielding of formate <sup>1</sup>H and <sup>13</sup>C chemical-shift values in this case points to an increase in local pH, which underpins the role of the IL head groups as Brønsted bases causing deprotonation of formic acid. The resulting molecular interactions between the IL and formate are responsible for improved adsorption of formate on the surface, leading thus to higher equilibrium concentrations during the hydrogenation reaction.

In addition, we carry out <sup>31</sup>P-<sup>31</sup>P and <sup>31</sup>P-<sup>29</sup>Si homo- and heteronuclear distance measurements to probe conformations and ordering phenomena of the ILs on the surface. With the aid of Molecular Dynamics (MD) simulations, we are in the process of deriving a structural model using NMR-based distance restraints.

Reference:

[1] Zhang, Y.; Levin, N.; Kang, L.; Müller, F.; Zobel, M.; DeBeer, S.; Leitner, W.; Bordet, A., J. Am. Chem. Soc., 2024, 146, 30057-30067.

## Minutes of the meeting of the Ampere Bureau

Oulu, on July 8, 2025

### Members present (14):

A. Böckmann, M. Ernst, S. Hiller, G. Jeschke, V.-V.-Telkki, J. Martins, P. Giraudeau, B.H. Meier, G. Bodenhausen, A. Lesage, O. Millet, R. Markiewicz, T. Zalewski, B. Blümich

### Excused:

L. Ciobanu, Y.-Q. Song, G. Otting, H. Oschkinat, G. Mathies, J. Dolinšek, J.-M. Bonny, M. Baldus, D. Savchenko

### Agenda:

1. Approval of the agenda.
2. Approval of the minutes of the AMPERE Bureau meeting online March 12, 2025
3. Report on the state of the AMPERE Society (A. Böckmann)
4. Financial Report (M. Ernst)
5. Report on the state of EUROMAR 2025 and 2026 (A. Lesage)
6. Preparation of AMPERE Bureau elections (A. Böckmann)
7. Preparation of AMPERE Committee elections (M. Ernst/A. Böckmann)
8. AMPERE/Dror NMR mailing list (M. Ernst/A. Böckmann)
9. Varia: Proposal for GA: Monday, September 1<sup>st</sup>, 2025 (M. Ernst)

At 13:05 hours, Matthias Ernst opened the meeting.

Ad 1. The agenda was approved as is.

Ad 2. The minutes of the AMPERE Bureau were approved unanimously.

Ad 3. The president A. Böckmann introduced the state and the structure of the AMPERE society. A. Böckmann commemorated the colleagues that passed away since the last meeting and acknowledged their contributions to NMR science. The society mourns the passing of Anil Kumar, Sir George Charles Radda, Alexander Pines, Klaus Möbius, Ray Dupree, Sunney I. Chan, Arnaud Bondon, and Alexander S. Arseniev. They will be kept in the memory of the society members.

A. Böckmann then reports on various aspects of the society. AMPERE Bureau young member G. Mathies is resigning from her role. The AMPERE café organized by her has been an extremely successful endeavor that was well attended. Young member D. Savchenko has created a job announcement platform which is going well. The society journal *Magnetic Resonance* works generally well, however, it has seen this year a decline in submissions. The journal is on PubMed and Scopus. The sustainability committee has forwarded the discussions to propose measures for CO<sub>2</sub> reduction and published a discussion paper in *Magnetic Resonance*. A. Böckmann briefly reports on the previous conferences of the society and holds an outlook to the future conferences.

Ad 4. M. Ernst presented the financial report. Finances are developing in a positive manner. The society has currently increased expenses on conferences, while income in form of membership fees remains stable. The available finances have thus slightly increased. Finances of the subdivisions also continue to be stable. Finances will be up for approval by the general assembly later in the year.

Ad 5. A. Lesage reports on the EUROMAR. The current EUROMAR 2025 in Oulu goes very well in terms of participant and sponsors. The next EUROMAR will be in Gothenburg in 2026. The planning is well on the way, location is booked, and organization is rolling. G. Bodenhausen mentions that Copernicus, the publishing house of *Magnetic Resonance*, has a division that organizes conferences, and this could be used for future EUROMARs. Copernicus will be invited to one of the next EUROMARs to present their business model. The EUROMAR 2027 will be joint with ISMAR in Lyon. Five proposals have been received for future EUROMARs. After Lyon, EUROMAR will be organized in Vienna and then Porto. The EUROMAR board is evaluating whether the conference will continue to take place every year or every second year. This depends also on consultation with the ENC executive committee.

Ad 6. Several elections of Bureau members are scheduled for the upcoming committee meeting. The president, both vice presidents, the two young members and the president of the prize committee are up for election. A. Böckmann will run for a second term as president, there are no other nominations. P. Giraudeau will run for a second term as vice president. J. Dolinsek has completed the second term as vice president and is no longer eligible. Nominees for his succession are Oscar Millet and G. Mathies. For the prize committee, B. Blümich agrees to extend his presidency by one year.

Ad 7. Fourteen members of the AMPERE Committee will end their term in 2025. Three of these members resign or are no longer eligible. These are E. Bordignon CH, she could be replaced by M. Kowalska; G. Spyroulias GR could be replaced by E. Mikros; D. Topgaard SE could be replaced by D. Bernin. The other 11 members can be re-elected. The Bureau proposes these names for consideration by the AMPERE Committee for eventual re-election by the general assembly.

Ad 8. The Bureau then discusses whether the AMPERE society should continue its association with the NMR mailing list run by Dror Warschawski. The reason for this discussion was that, due to the escalation of the conflict between Israel and Gaza, DW considers it unacceptable to provide economic support to Israel and has therefore rejected job listings from there. After being approached by groups from the Weizmann Institute, the AMPERE Bureau opted to discontinue the association following a vote that resulted in 11 to 3. The Bureau thanks Dror Warschawski for his many years of continued efforts and service to the community.

Ad 9. The general assembly will be held online on Monday, September 1 at 2 pm CEST on zoom.

The meeting closed at 14:10.

Oulu, 8 July 25  
Minutes: Sebastian Hiller

## **Minutes of the meeting of the Ampere Committee Oulu, on July 9, 2025**

### **Members present (27):**

B.H. Meier, M. Ernst, A. Zawadzka-Kazimierczuk, A. Lesage, M. Sardo, K. Houben, A. Kantola, V.-V. Telkki, P. Novak, G. Mollica, P. Vasos, P. Giraudeau, D. Kurzbach, A. Böckmann, D. Topgaard, G. Bodenhausen, G. Karlsson, B. Blümich, I. Reile, R. Pieratelli, J. Martins, E. Bordignon, G. Jeschke, T. Zalewski, R. Markiewicz, O. Millet, S. Hiller

### **Excused:**

L. Ciobanu, P. Crowley, A. Gil, K. Jaudzems, I. Komarov, H. Oschkinat, G. Otting, A. Pastore, F. Rise, S. Ruthstein, P. Schanda, Y.-Q. Song, G. Spyroulias, J. Tritt-Goc, P. van der Wel, A. Kentgens, M. Baldus, M. Halse, V. Klimavičius, G. Parigi, G. Mathies, J. Dolinšek, J. Matysik, T. Vosegaard, L. Trantírek, D. Savchenko, J.-N. Dumez, M. Britton, J.-M. Bonny, J. Plavec, A.-C. Pöppler

### **Agenda:**

1. Approval of the agenda.
2. Approval of the minutes of the AMPERE Committee meeting Bilbao July 4, 2024
3. Report on the state of the AMPERE Society (A. Böckmann)
4. Financial report to be presented at the General Assembly (M. Ernst)
5. AMPERE Bureau elections (M. Ernst)
6. Publication Division: Magnetic Resonance (G. Bodenhausen)
7. Preparation of Committee Elections at GA (M. Ernst, A. Böckmann)
8. Varia

At 12:54 hours, Matthias Ernst opened the meeting.

Ad 1. The agenda was approved as is.

Ad 2. The minutes of the previous AMPERE Bureau meeting were approved unanimously.

Ad 3. The president A. Böckmann introduced the state and the structure of the AMPERE society. A. Böckmann commemorated the colleagues that passed away since the last meeting and acknowledged their contributions to NMR science. The society mourns the

passing of Anil Kumar, Sir George Charles Radda, Alexander Pines, Klaus Möbius, Ray Dupree, Sunney I. Chan, Arnaud Bondon, and Alexander S. Arseniev. They will be kept in the memory of the society members.

A. Böckmann then reports on various aspects of the society. AMPERE Bureau young member G. Mathies is resigning from her role. The AMPERE café organized by her has been an extremely successful endeavor that was well attended. Young member D. Savchenko has created a job announcement platform which is going well. The society journal *Magnetic Resonance* works generally well, however, it has seen this year a decline in submissions. The journal is on PubMed and Scopus. The sustainability committee has forwarded the discussions to propose measures for CO<sub>2</sub> reduction and mentions that a discussion paper has been submitted to *Magnetic Resonance*. A. Böckmann briefly reports on the previous conferences of the society, the MRPM16 in August 2024 in Norway, the EFEPR 2024 in Marseille, the AMPERE school in Zakopane June 2025. She holds an outlook to the future conferences, such as the ICMRM in Würzburg (August 2025), EFEPR Summer School in Manchester (September 2025), the Alpine Conference in Chamonix (September 2025), the Biological Solid-State NMR School in Munich (October 2025). Details can be found on the homepage of the Groupement AMPERE.

Ad 4. M. Ernst presented the financial report. Finances are developing positively. The society has slightly increased expenses for conferences, whereas the overall income is continuing to be large due to the attractivity and attendance of the EUROMAR conference. Plans are to further increase conference support to move towards a net zero growth. Finances of the subdivisions also continue to be stable, some of which are very well funded. Finances will be up for approval by the general assembly later in the year.

Ad 5. A. Böckmann was elected unanimously for a second term as president. P. Giraudeau was elected unanimously for a second term as vice president. As the second vice president, Oscar Millet was elected (Millet 15: Mathies 10: abstain 1). D. Savchenko was unanimously elected for a second term as a young member. For the succession of G. Mathies, five candidates were running as young member: Sara Andres (Madrid), Shira Haber (Bar-Ilan), Yuliia Horbenko (Nantes), Hilla Perttu (Oulu), and Marco Schiavina (Florence). After some discussion, the committee elected all five to form a young member group that sends one delegate to the Bureau besides D. Shevchenko. P. Giraudeau will coordinate the activities of the young member group and invite them for an on-line discussion round.

Ad 6. G. Bodenhausen mentions that the quality of the *Magnetic Resonance* journal is very high. Unfortunately, it is not yet accepted by Web of Science from Clarivate and hence has no impact factor. The journal has reduced the number of board members and encourages submissions.

Ad 7. 14 members of the AMPERE Committee will end their term in 2025. Some can and some cannot be re-elected. E. Bordignon resigns, a nomination for her replacement

is M. Kowalska (CERN, Uni Geneva). D. Topgaard SE will be replaced by nomination D. Bernin. G. Spyroulias GR will be replaced by E. Mikros. The 11 others can be re-elected and are willing to do so. The Bureau proposes these names for election by the general assembly.

The Committee then discussed the election of Russian scientists into the Committee. Some members believed representatives of Russia should be excluded due to the ongoing Russia-Ukraine war, others were in favor of including a representative for Russia in the AMPERE Committee. Some members were unsure if and how scientists active in Russia would at all be able to participate. To decide on the issue, a secret vote was held. With a vote of 23 Yes, 3 No, 1 abstention, the Committee then decided to postpone a possible election of a Russian member and to continue the discussion of the topic in the future.

Ad 8. O. Millet was nominated as a Bureau representative to the EUROMAR division. The General Assembly will be held on September 1st, 2025, at 2pm (CEST, Zurich time) on Zoom. Invitations will be sent to all members of the Groupement AMPERE. G Karlson distributed posters for EUROMAR 2026.

The meeting closed at 14:17.

Oulu, 9 July 2024

Minutes: Sebastian Hiller

## **Minutes of the meeting of the Ampere General Assembly online, on Monday, September 1, 2025**

### **Members present (47):**

J. Dolinšek, M. Ernst, A. Gil, V. Denysenkov, G. Mollica, M. Sardo, D. Bernin, G. Bodenhausen, M. Vasilescu, P. van der Wel, G. Parigi, G. Jeschke, O. Millet, V. Klimavicius, W. Kozminski, B. Reif, M. Bennati, T. Vosegard, M. Britton, G. Buntkowsky, D. Savchenko, I. Koptuyug, I. Geru, P. Giraudeau, W.Y. Chow, P. Vasos, M. Levitt, A. Böckmann, A. Sadet, M. Wenka, V. Smrecki, A.C. Pöppler, J. Matysik, V.V. Telkki, K. Takeda, Y. Horbenk, I. Marin, A. Simion, A. Zawadska-Kazimierczuk, K.T. Movellan, A. Kantola, D. Suter, S. Grimaldi, D. Sakellariou, G. Stevanato, H. Heise

Agenda:

1. Approval of the agenda
2. Approval of the minutes of the AMPERE General Assembly online September 2, 2024
3. Report on the state of the AMPERE Society (A. Böckmann)
4. Financial report and approval (M. Ernst)

5. Report on AMPERE Bureau elections (A. Böckmann)
6. AMPERE Committee elections (M. Ernst)
7. Varia (M. Ernst)
8. Closing remarks (A. Böckmann)

At 14:00 hours, Matthias Ernst opened the meeting.

Ad 1. The agenda was approved as is.

Ad 2. The minutes of the previous AMPERE General Assembly were approved unanimously.

Ad 3. At first A. Böckmann reminded us of the colleagues that passed away during the past year: Anil Kumar, George Rada, Alexander Pines, Klaus Möbius, Ray Dupree, Sunney Chan, Alexander Arseniev, Edwin Becker, Arnaud Bondan, and Jean-Nicolas Dumez.

She then gave an overview on the activities of the society. The portraits in the Bulletin are a special way to learn more about people involved in AMPERE. The Visual Encyclopedia tries to collect short educational videos about magnetic resonance topics. New contributions are very welcome. The AMPERE Cafe organized by G. Mathis was a big success with a wide range of topics and formats. Due to too many other obligations, she resigned from the AMPERE Bureau as a young member. D. Savchenko organizes the job advertisements and other information pages on the AMPERE web site. Since this year, we have a young AMPERE division with six members. We welcome their new ideas and are looking forward to working with them.

Since 1998 Dror Warschawski has been running the NMR mailing list. In 2007 AMPERE endorsed the mailing list which since then had a footer with advertisement for AMPERE. Due to the ongoing war in Gaza, Dror decided to no longer publish job advertisements for groups from Israel. The AMPERE Bureau decided that this is not in line with AMPERE's values and decided to end the endorsement.

She also reminded us of the prizes and conferences that AMPERE organizes. A list of the past and present meetings can be found on the AMPERE web site and reports about the meetings can be found in the AMPERE Bulletin. In this context she thanked B. Blümich for his work as president of the prize committee during the past years. She mentioned also Magnetic Resonance (MR) a community driven journal that AMPERE initiated. It is not for profit, open access but economic and open peer review. Please consider MR for your publications. As a final activity she mentioned the sustainability initiative where Paul Schanda has analyzed the carbon footprint of conference travel. A report on this can be found as a preprint on the website of MR.

Ad 4. M. Ernst presented the financial report of the past year and discussed key aspects. Finances of the society developed positively and the financial situation of all subdivisions remains stable and partially very positive. The society is financially in a very healthy state.

the main expenses are support for conferences which we will try to increase further. The main income is from membership fees collected at AMPERE conferences. The financial report was unanimously approved by the members present.

Ad 5. M. Ernst reported that A. Böckmann (president) and P. Giraudeau (vice president) have both been reelected for a second term. He thanked J. Dolinšek for his long service in the AMPERE Bureau who has already finished his second term as vice president. The AMPERE Committee elected O. Millet as the new vice president. D. Savchenko was reelected as a young member for a second term. In addition, Sara Andres (Madrid), Shira Haber (Bar-Ilan), Yuliia Horbenko (Nantes), Hilla Perttu (Oulu), and Marco Schiavina (Florence) were elected to the young AMPERE division.

Ad 6. M. Ernst explained the current composition of the AMPERE committee and the nominees for additions. Enrica Bordignon (CH) resigns from the AMPERE Committee due to too many other obligations. George Spyroulias GR and Daniel Topgaard SE have already served two terms and cannot be reelected. The AMPERE Committee proposes reelection of the following members for a second four-year term: Klaartje Houben NL, Vytautas Klimavičius LT, Jose Martins BE, Jörg Matysik DE, Giulia Mollica FR, Giacomo Parigi IT, Annalisa Pastore UK/FR, Mariana Isabel Coutinho Sardo PT, Paul Schanda AT, Lukáš Trantírek CZ, Jadwiga Tritt-Goc PL The AMPERE Committee proposes election of the following new members for a four-year term: Magdalena Kowalska (CH), Emmanuel Mikros (GR), Diana Bernin (SE). There was a discussion that with the resignation of Enrica Bordignon, EPR would no longer be represented in the AMPERE Committee. This is actually only partly true since Sharon Ruthstein works on EPR and Gunnar Jeschke is a member of the AMPERE Bureau and, therefore, also of the AMPERE Committee. It was agreed that we try to balance different fields of magnetic resonance better in the upcoming elections for the AMPERE Committee. The proposed candidates were unanimously approved by the members present.

Ad 7. G. Bodenhausen reminded people to consider the journal Magnetic Resonance for their publications. AMPERE has given money to pay for the open-access fees in case they are not covered by institutional agreements

M. Levitt raised again the topic of the NMR mailing list and AMPERE's decision to withdraw its association with it due to the topics discussed by A. Böckmann. He argued that AMPERE should take a stand against the inhumanity of this war.

Ad 8. A. Böckmann thanked everyone for the participation in the meeting. The meeting closed at 15:15.

Grenoble / the internet, 1 September 2025  
Minutes: Matthias Ernst

## Finances of the Groupement AMPERE and Subdivisions

Period from June 1. 2024 to May 31. 2025

	Balance on June 1. 2024	Membership Fees / Registration Payments	Donations/ Conference support, Copernicus Licence Fee, Seedfunding paid back	Travelgrants/ Prizes, Publishing Agreement	Conference Sponsoring/ Copernicus support	Conference Surplus / Licence fees Copernicus & reimb. taxes	Administrati on, Web Bureau Meetings / domains, credit card	Bank Charges / Depot Charges/ losses on Depot	Account Closing / Account carry over, withholding tax	Bank Interests Account carry over, Dividends	Gains on Value Paper withholding taxes	Balance on May 31. 2025
<b>Groupement Ampere</b>												
Ampere (CHF)	20'138.50	5'759.20					992.75	93.50	464.53	2'299.98		26'646.90
Ampere (Euro)	62'037.82	23'949.56		10'057.50	5'000.00		50.00	96.59	3'000.00	1'070.64		68'853.93
Andrew (CHF)	19'748.28			1'690.96				544.30			1'036.92	18'549.94
Andrew Depot (CHF)	92'614.48										445.42	93'059.90
<b>Subdivisions</b>												
Biol. Solid State (Euro)	13'621.10						161.10	89.98				13'370.02
EPR (CHF)	7'434.15			2'875.70			20.00			50.55		4'589.00
Food NMR (CHF)	7'201.49			2'883.50						47.05		4'365.04
MRPM (CHF)	29'683.50			8'955.23						204.95		20'933.22
SMRM (CHF)	61'983.44						37.28	26.00	133.60	381.75	243.85	62'412.16
Hyp (CHF)	4'147.50									29.55		4'177.05
Publication Div. (Euro)	4'815.14		735.53					96.59				5'454.08
<b>Euromar</b>												
Euromar (Euro)	143'716.83		15'000.00	15'580.00		34'316.88	7'080.95	96.59				170'276.17

## In memory of Jean-Nicolas Dumez (1984-2025)



© Amélie Dumez

Jean-Nicolas Dumez was one of those scientists who shone in so many ways. As a student at the Ecole Normale Supérieure in Lyon, and holder of the Agrégation in physics and chemistry (the most difficult competitive examination for teachers in France), he discovered a passion for NMR at an early age. His Ph.D. thesis, entitled «Many body dynamics in nuclear spin diffusion», supervised by Lyndon Emsley at the CRMN (Very high field NMR center) in Lyon, was brilliantly defended on July 4<sup>th</sup> 2011, in front of a world-class jury of NMR spectroscopists (Malcolm Levitt, Dominique Massiot, Beat Meier, Dieter Suter). In his thesis, Jean-Nicolas tackled very complex spin physics problems, and he managed to provide a quantitative description of the spin diffusion phenomenon from first principles. This early work would have major impact later on in the simulation of DNP phenomena.

Eager to discover the many facets of magnetic resonance, Jean-Nicolas Dumez then joined two major international groups for his post-doctoral studies. With Lucio Frydman at the Weizmann Institute, he brought a major contribution to the development of 2D MRI pulses that led to various applications. Then he worked for a few months with Malcolm Levitt in Southampton, where he worked on the theory of long-lived nuclear spin states in methyl groups.

With such a great and diverse knowledge and expertise, Jean-Nicolas had already acquired a very broad vision of magnetic resonance at a very young age, and it not surprising that he was recruited as a «Chargé de Recherche» by the French CNRS in 2013, through an extremely competitive hiring process. He then joined the «Institut de Chimie des Substances Naturelles» in Gif-sur-Yvette, where he was asked to develop a small molecule NMR activity together with Stefano Caldarelli and Carine van Heijenoort. Jean-Nicolas supervised several Ph.D. and post-doctoral students there, and he started to make groundbreaking contributions to the field of complex mixture analysis by NMR. Early work in Gif-sur-Yvette included the development of multiple quantum ultrafast 2D NMR experiments and spatially-encoded DOSY methods. He also wrote a single-author seminal paper in *Prog. Nucl. Magn. Reson. Spectrosc.* That provided a unified description of spatially encoded NMR experiments.

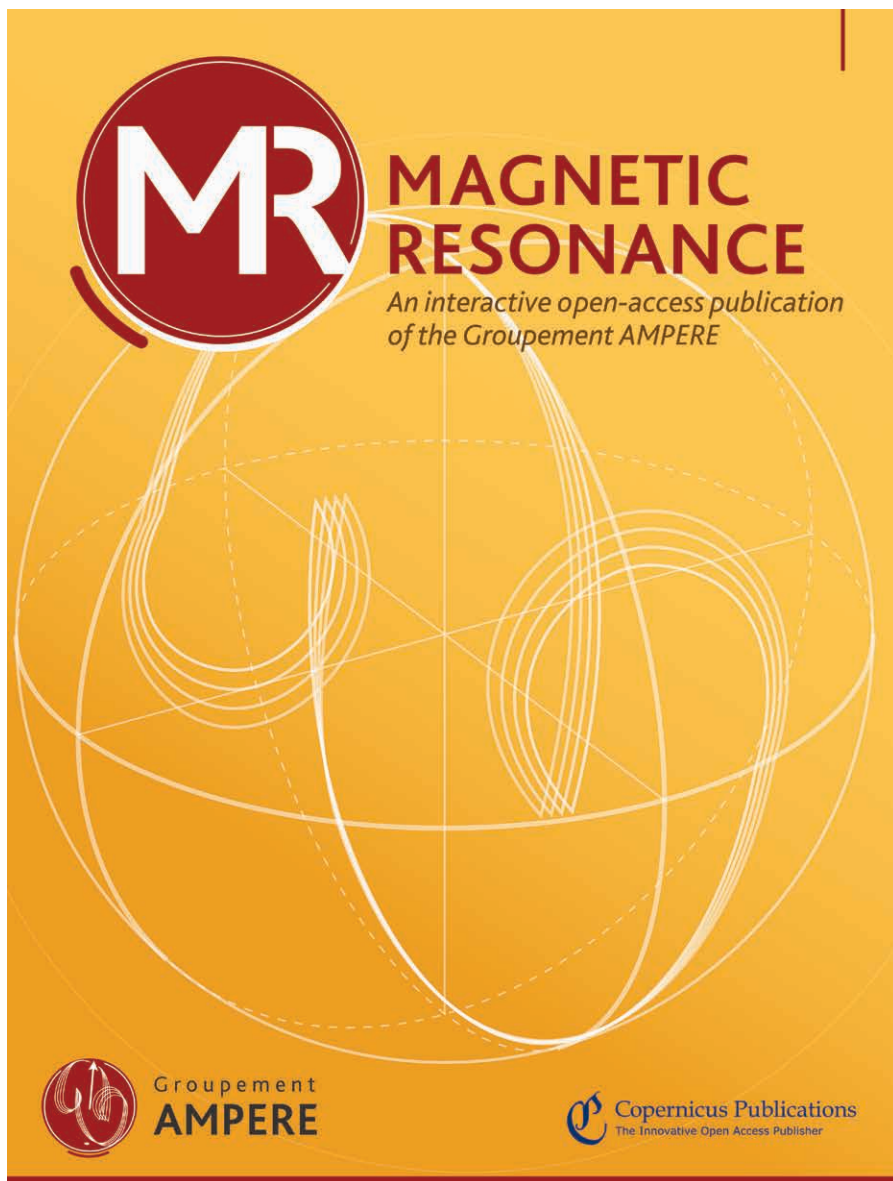
In 2018, Jean-Nicolas Dumez joined the CEISAM (Chemistry and Interdisciplinarity: Synthesis, Analysis, Modelling) institute in Nantes, where he teamed up with Patrick Giraudeau, a long-term collaborator. He obtained an ERC starting grant on the real-time NMR analysis of mixtures. In this project, he was the first to develop spatially-encoded experiments immune to the flow, making it possible to record in real-time ultrafast 2D NMR spectra of reacting mixtures. Jean-Nicolas benefited from the stimulating environment of CEISAM, collaborating with experts in organic chemistry to apply his new methods to online flow monitoring, but also to in-line flow chemistry experiments. Jean-Nicolas also developed an impressive network of national and international collaborations. Beyond his core project, his contributions include the development of 2D NMR pulse sequences for the analysis of hyperpolarized mixtures (through para-hydrogen, dissolution DNP and more), and more recently, the design of highly sensitive ultrasensitive experiments. Jean-Nicolas Dumez was promoted to «Directeur de Recherche» position in 2023, and in 2024 he was awarded an ERC consolidator grant that had just started in 2025, on the development of unmixing methods for flow NMR. His many projects included the development of innovative pulse sequences and processing methods and their application to a variety of chemistry problems.

Jean-Nicolas was a great mentor, who was very much appreciated by the students and young colleagues he supervised. He was also a great team member, and was involved in many collective activities. At the international level, these included the organization of conferences (in particular the Alpine conference where he was very active as an organizing committee member from 2019 to 2023). He was a member of the Ampere Committee, and an associate editor for NMR journals, including *Magnetic Resonance* and *MRC*. At the local level, Jean-Nicolas was very much involved in the CEISAM's life, as a European correspondent as well as for gender equality in science, and as the Deputy Director of the CEISAM NMR facility.

Jean-Nicolas left us far too early, on August 18<sup>th</sup> 2025. While he was a bright scientist, Jean-Nicolas was ill, suffering from a mental disease that led him to take his own life. He left loving and being loved, but he felt like he had no other choice. We generally see only the sunny side of science, but being successful does not prevent us from suffering, and this tragic event reminds us to show kindness and help each other.

He leaves an immeasurable void in the international NMR community, and his contributions will undoubtedly inspire several generations of spectroscopists.

Patrick Giraudeau  
Nantes, September 16<sup>th</sup> 2025



<https://www.magnetic-resonance-ampere.net>

## Executive Officers and Honorary Members of the AMPERE Bureau

The AMPERE BUREAU includes the executive officers (which take the responsibility and the representation of the Groupement between the meeting of the committee), the honorary members of the Bureau and the organizers of forthcoming meetings.

### President

Anja Böckmann, CNRS/University of Lyon, France  
anja.bockmann@ibcp.fr

### Vice President

Óscar Millet, CIC bioGune  
omillet@cicbiogune.es

### Vice President

Patrick Giraudeau, Université de Nantes  
patrick.giraudeau@univ-nantes.fr

### Secretary General

Matthias Ernst, ETH Zurich, Switzerland,  
maer@nmr.phys.chem.ethz.ch

### Executive Secretary

Sebastian Hiller, University of Basel, Switzerland  
sebastian.hiller@unibas.ch

### Young Members

Darya Svachenko, Institute of Physics of the CAS, Czech Republic, dariyasvachenko@gmail.com  
Sara N. Andres, McMaster University, Canada, andressn@mcmaster.ca  
Shira Haber, Ben-Gurion University, Israel, habersh@post.bgu.ac.il  
Perttu Hilla, University of Oulu, Finland, perttu.hilla@oulu.fi  
Yuliia Horbenko, University of Nantes, France, yuliia.horbenko@univ-nantes.fr  
Marco Schiavina, University of Florence, Italy, marco.schiavina@unifi.it

### EF-EPR

Gunnar Jeschke, ETH Zurich, Switzerland  
gieschke@ethz.ch

### SRMR

Luisa Ciobanu, CEA/Neurospin, France  
luisa.ciobanu@gmail.com

### MRPM

Yi-Qiao Song, Schlumberger-Doll Research, USA  
ysong@slb.com

### **MR-Food**

Jean-Marie Bonny, French National Institute for Agriculture, Food, and Environment, France  
jean-marie.bonny@inra.fr

### **Hyperpolarisation**

Geoffrey Bodenhausen, ENS, France,  
geoffrey.bodenhausen@ens.fr

### **Publication Division**

Gottfried Otting, Australian National University, Australia  
gottfried.otting@anu.edu.au

### **Biological Solid State NMR**

Hartmut Oschkinat, Leibniz Forschungsinstitut für Molekulare Pharmakologie, Germany  
oschkinat@fmp-berlin.de

### **AMPERE NMR School**

Roksana Markiewicz, Adam Mickiewicz University, Poland

### **Euromar**

Anne Lesage, Centre National de la Recherche Scientifique (CNRS), France  
anne.lesage@ens-lyon.fr

### **Euromar Treasurer**

Marc Baldus, Utrecht University, The Netherlands  
m.baldus@uu.nl

### **Past President**

Bernhard Blümich, RWTH Aachen University, Germany  
bluemich@itmc.rwth-aachen.de

### **Honorary member**

Beat Meier, ETH Zürich, Switzerland  
beme@nmr.phys.chem.ethz.ch

## **AMPERE Committee**

**Diana Bernin** (2025-2029) Chalmers University of Technology, Sweden

**Melanie Britton** (2024-2028) University of Birmingham, United Kingdom

**Peter Crowley** (2018-2026) National University of Ireland, Ireland

**Ana Maria Pissarra Coelho Gil** (2018-2026) University of Aveiro, Portugal

**Meghan Halse** (2022-2026) University of York, United Kingdom

**Klaartje Houben** (2021-2025) DSM, Delft, The Netherlands

**Kristaps Jaudzems** (2019-2027) University of Latvia, Latvia

**Anu Kantola** (2024-2028) University of Oulu, Finland

**Vytautas Klimavičius** (2021-2025) Vilnius University, Lithuania

**Igor Komarov** (2022-2026) Taras Shevchenko National University of Kyiv, Ukraine

**Magdalena Kowalska** (2025-2029) CERN, University of Geneva, Switzerland

**Dennis Kurzbach** (2022-2026) University of Vienna, Austria

**Jose Martins** (2021-2025) Ghent University, Belgium

**Jörg Matysik** (2021 - 2025) University Leipzig, Germany

**Emmanuel Mikros** (2025-2029) University of Athens, Greece

**Óscar Millet** (2024-2028) CIC bioGUNE, Spain

**Giulia Mollica** (2021-2025) ICR, Aix Marseille University, France

**Predag Novak** (2019-2027) University of Zagreb, Croatia

**Giacomo Parigi** (2021-2025) University of Florence, Italy

**Annalisa Pastore** (2021-2025) King's College London, England

**Roberta Pieratelli** (2024-2028) University of Florence, Italy

**Janez Plavec** (2024-2028) Slovenian NMR Centre, Slovenia

**Ann-Christin Pöpller** (2024-2028) University of Würzburg, Germany

**Indrek Reile** (2019-2027) National Institute of Chemical Physics and Biophysics, Estonia

**Frode Rise** (2018-2026) University of Oslo, Norway

**Sharon Ruthstein** (2018-2026) Bar-Ilan University, Israel

**Mariana Isabel Coutinho Sardo** (2021-2025) University of Aveiro, Portugal

**Paul Schanda** (2021-2025) The Institute of Science and Technology, Austria

**Lukáš Trantířek** (2021-2025) CEITEC - Central European Institute of Technology, Czech Republic

**Patrick van der Wel** (2022-2026) University of Groningen, The Netherlands

**Paul Vasos** (2019-2027) Horia Hulubei Institute for Nuclear Physics (IFIN-HH), Romania

**Thomas Vosegaard** (2022-2026) Aarhus University, Denmark

**Anna Zawadzka-Kazimierzczuk** (2024-2028) University of Warsaw, Poland

## Honorary members

**Hans Wolfgang Spiess**, Max Planck Institute for Polymer Research, Germany

**Kurt Wüthrich**, ETH Zürich, Switzerland

## Prize Committee

**President: Bernhard Blümich**, RWTH Aachen University, Germany

### Members:

**Mark E. Smith**, University of Southampton, England

**Annalisa Pastore**, King's College London, England

**Alexej Jerschow**, New York University, USA

**Enrica Bordignon**, University of Geneva, Switzerland

**Hartmut Oschkinat**, FMP Berlin, Germany

## Future conferences

### Ampere Event 2025

Alpine Conference on Magnetic Resonance in Solids	Chamonix, France	September 14-18
Biological Solid-State NMR School	Munich, Germany	October 19-24

### Other Events 2025

46 <sup>th</sup> FGMR Annual Discussion Meeting	Bonn, Germany	September 15-18
-------------------------------------------------	---------------	-----------------

### Ampere Event 2026

MRFOOD 2026	Milano, Italy	June 9-12
AMPERE NMR School 2026	Zakopane, Poland	June 14-20
Euromar 2026	Gothenburg, Sweden	June 28 to July 2
XIII EFEPR Conference	Brno, Czech Republic	Aug. 29 to Sept. 3
HYP 26	Göttingen, Germany	September 6-10

### Other Events 2026

FGMR Annual Discussion Meeting	Mainz, Germany	September 13-17
--------------------------------	----------------	-----------------



Groupement  
**AMPERE**

[www.ampere-society.org](http://www.ampere-society.org)