

BULLETIN DU GROUPEMENT

d'informations mutuelles



G r o u p e m e n t  
**AMPERE**

SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

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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)

## Editorial



Dear members of the Groupement AMPERE,

seventy years ago, in 1951 during the height of the cold war, the Groupement AMPERE was founded in France to promote better communication between scientists working on radio-frequency spectroscopy all over Europe. One of the main goals was to bring together people from eastern and western Europe for scientific exchange.

While the iron curtain no longer exists, a rise in nationalism observed in recent years all over Europe leading to new closed borders shows that the original goal of AMPERE to bring people from all over Europe together has not become obsolete. I hope that AMPERE can live up to this goal and foster contacts between people working in this field across all borders.

Despite the still ongoing pandemic, planning for conferences has started up again. The AMPERE Biological Solid-State NMR School has already started with an online teaching program which we hope will be complemented by an in-person meeting in Berlin (Germany) in June. The AMPERE NMR School in Zakopane (Poland) is planned for the middle of June as an in-person meeting and can hopefully continue its long tradition of annual meetings. The EUROMAR 2021 is planned as a hybrid meeting in Portoroz (Slovenia) in early July with an exciting program. I hope that at least some of these meetings can happen and as many of you as possible can attend in person. I strongly believe, that personal contacts are very important in science and cannot be replaced by virtual contacts.

I sincerely hope to see some of you again in person at one of our meetings this summer.

Best regards,

Matthias Ernst  
Secretary General, Groupement AMPERE

# 70 years Groupement AMPERE

Seventy years ago, the Groupement AMPERE was founded in France. This is a time to remember and to look forward. With reference to its history as reviewed on the occasion of the Society's 65 anniversary [www.ampere-society.org] a few memories are recalled, and activities of the last years setting the stage for the future are outlined.

The Groupement AMPERE started as an association of scientists engaged in the study of molecules with radio waves. Its mission gave rise to the acronym AMPERE meaning Atomes et Molécules Par Études Radio-Électriques. Five years later the Society was incorporated in Switzerland. Given the complex state of Europe in those days, a key function of the Society was to maintain links between Western and Eastern Europe. In these days without internet the Bulletin du Groupement AMPERE and the main event of the Groupement AMPERE, the Congress AMPERE, were the central communication channels between the different international member laboratories.

The Congress AMPERE, the British Radiofrequency Spectroscopy Group, and the European Experimental NMR Conference merged in 2005 under the umbrella of the Groupement AMPERE to form EUROMAR, the largest of many activities of the Society today. A remarkable Congress AMPERE was the one in September 1961, just a few weeks after the infamous division of EUROPE with the establishment of the iron curtain. It took place in Leipzig, East Germany, with attendees from East and West, proving that science is stronger than politics.

With time, specialized colloquia and schools were organized and new divisions established. The AMPERE homepage [www.ampere-society.org](http://www.ampere-society.org) is an informative source on the Society's activities and history. Landmark discoveries were discussed at these meetings. For example, N. Bloembergen reported on Cross-Relaxation Effects in Magnetic Resonance 1960 in Pisa, A. Abragam on Polarisation dynamiques des noyaux 1961 in Leipzig, E. R. Andrew on Nuclear Magnetic Resonance in Rapidly Rotated Solids, E. L. Hahn on Developments in Nuclear Magnetic Double Resonance, I. Solomon on Magnetic Resonance of Conduction Electrons 1966 in Ljubljana, K. M. Salikhov et al. on Modulation phenomena in Electron Spin-Echo 1968 in Grenoble, R. Blinc on Nuclear Double Resonance Studies of Order-Disorder Ferroelectrics, A. Lösche on Some NMR investigations of Liquid Crystals, and J. S. Waugh, M. G. Gibby, S. Kaplan, A. Pines on Proton-Enhanced NMR of Dilute Spins in Solids 1972 in Turku, P. C. Lauterbur et al. on Magnetic Resonance Zeugmatography and P. Mansfield, P. K. Grannell, A. A. Maudsley on Diffraction Microscopy in Solids and Liquids by NMR 1974 in Nottingham, R. R. Ernst et al. on Application of Two-Dimensional

Spectroscopy to Problems of Physical, Chemical and Biological Relevance 1978 in Tallin, A. Pines on NMR with Lots of Protons and no Magnetic Fields 1986 in Rome, H. W. Spiess on 2D and 3D Solid State NMR of Polymers 1992 in Athens, P. T. Callaghan on Microimaging Studies of Flow and Diffusion 1996 in Canterbury, and A. Schweiger on Dances with Electron and Nuclear Spins 1998 in Berlin. Other key lectures remain in the books of abstracts, including the famous lecture by Jean Jeener proposing 2D NMR spectroscopy at the AMPERE Summer School in Basko Polje, 1971.



Figure 1. The AMPERE tree. The stem and the branches of the crown represent the different activities of the Groupement AMPERE. New branches grown in the last 10 years are marked in green. In 2019, the publication division of the Groupement AMPERE has launched the non-profit, open-access journal 'Magnetic Resonance' (<https://www.magnetic-resonance-ampere.net/>).

Since the fall of the iron curtain and with the formation of a unified Europe, the Groupement AMPERE continues to serve its mission in the spirit of its founders, *Se Connaître, S'Entendre, S'Entraider*, i.e., to get to know each other, to listen to each other, to aid one another. Today it is an umbrella organization for different divisions and a wide range of magnetic resonance activities in Europe. Its function is represented by the AMPERE tree (Fig. 1), a living organism, which keeps on growing. Within the last decade it has grown the new branches of the European School on Biological Solid-State NMR, the Hyperpolarized-Magnetic-Resonance Division, and the Publication Division. The Publication Division has launched the open-access journal 'Magnetic

Resonance' (<https://www.magnetic-resonance-ampere.net/>), which is published non-profit by Copernicus Publications, with the mission to provide affordable open access with high-quality contributions through interactive public peer reviewing. A developing bud of the AMPERE tree is the Alpine Conference on Magnetic Resonance in Solids.

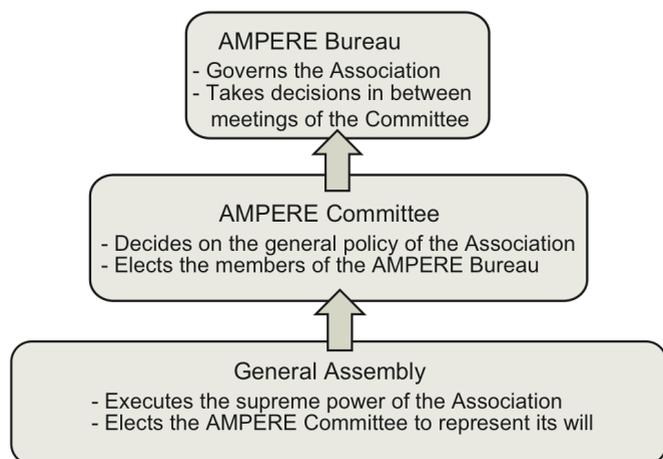


Figure 2. Structure of the Groupement AMPERE.

The Groupement AMPERE maintains and expands its services for the whole community engaged in Magnetic Resonance and Related Phenomena in Europe and worldwide. It aims at accommodating new developments in new areas which are progressively opened by the evolution of science. To maintain the vigor of the Groupement, its statutes, i.e., its constitution, have been revised in 2016. The revision maintains the historical structure of the organization (Fig. 2), where the General Assembly elects the AMPERE Committee to which it delegates most of its power. The committee strives to represent all European countries and magnetic resonance disciplines in a balanced way including attention to gender. The Committee decides on the general policy of the association and elects the members of the Bureau AMPERE to handle the day-to-day business in between its meetings at the EUROMAR conference and in spring each year. In addition to replacing the Congress AMPERE conference by the EUROMAR conference, the major change in the constitution is that the time of service in the AMPERE Committee has been limited to four years with one reelection possible. This assures periodic rejuvenation of the Committee and Bureau members. To enable limited term service of Committee members, many distinguished personalities have gracefully vacated their long-term Committee positions.

Other operational changes were introduced to facilitate the functioning of the Society. One was to increase the visibility of the Groupement AMPERE in an effort to foster its acceptance in the scientific community and better communicate its mission 'to contribute to the progress of Radio Spectroscopy, Magnetic Resonance and Related Phenomena'. The AMPERE tree (Fig. 1), a new AMPERE logo, and posters at AMPERE Conferences explaining the Society and its mission resulted from it. Moreover, the guidelines to organize AMPERE events were updated to assist the members of our Society in organizing conferences and avoiding mistakes as most of us are amateurs in this business. With the registration fee to any AMPERE event, the participant becomes a member of the Groupement AMPERE for one year and as such is eligible for reduced fees at other AMPERE events. Also, each member is entitled to participate and vote in the General Assembly at the annual EUROMAR conference. The budget of the Groupement AMPERE is generated from the membership fees and conference surplus, which is split between the Division treasury and the AMPERE treasury. From the income of the AMPERE umbrella society, its operating costs are covered, awards, and as of recent, also stipends for young scientists to attend AMPERE events. Up to 2016, the distinguished AMPERE Prize was supported by Bruker, when the company decided to diverge the support to the Ernst Prize at the EUROMAR Conference. Since then, the AMPERE Prize for Young Investigators is awarded biannually from the budget of the Groupement AMPERE to an early-stage independent researcher. Since 2002 the Raymond Andrew Prize is awarded by the Groupement AMPERE to a young scientist for an outstanding PhD thesis in magnetic resonance during the opening and prize session of the EUROMAR congress. Its resources are covered by a donation of the Andrew family, which is administered by the Groupement AMPERE.

Several heroes of magnetic resonance have left our community in the last years. Many of them were members or associate members of the Groupement AMPERE. We are commemorating Raymond Andrew (2014), John. S. Waugh (2014), Endel Lippmaa (2015), Erwin Hahn (2016), Peter Mansfield (2017), George Feher (2017), Nicholas Bloembergen (2018), Charles P. Slichter (2018), Zeev Luz (2018), Stefano Caldarelli (2018), Sir Rex Richards (2019), Alfred Redfield (2019), and Yoji Arata (2019). We miss their presence at the AMPERE meetings, but their spirits and their achievements stay with us.

For many years up to 2018, Gunnar Jeschke was the Secretary General of the Society, who carries the major workload. He reformed the AMPERE webpage and converted the Bulletin AMPERE into a more attractive newsletter, which is now disseminated by email. It not only contains the minutes of the meetings of the AMPERE General Assembly, the Committee and the Bureau, but also conference and meeting announcements, reports of recent conferences, award lectures, and a portrait of a distinguished scientist in each of its four annual issues. In 2018 Matthias Ernst

succeeded Gunnar Jeschke and enthusiastically serves the Society as the current Secretary General. As the Covid-19 virus attempts to paralyze our treasured lifestyle and many conferences had to be cancelled in 2020, the Groupement AMPERE is confronting the new challenges. Online platforms and are being explored for common use by all AMPERE Divisions. EUROMAR 2020 has courageously been turned into a very successful online conference by Óscar Millet and his team following a new format with short five-minute talks of young investigators framed by the award lectures for the Richard Ernst Prize, the Raymond Andrew Prize, and the AMPERE Prize for Young Investigators. EUROMAR 2021 is expected to be a hybrid conference with online participation and physical attendance in Portorož following a more established format including vendor interaction. New ideas about how the Groupement AMPERE can better serve the magnetic resonance community are being discussed exploring the wider acceptance of online media. Last but not least it is each of us who defines our Society by her and his interactions and contributions including submissions to the new AMPERE journal Magnetic Resonance.

## **Se Connaitre, S'Entendre, S'Entraider!**

Stay well and let us meet again soon,

Bernhard Blümich  
(President)

## **Preface to Portrait: Prof. Robert Kaptein**

On April 5<sup>th</sup>, 2021 our valued colleague, Prof. Robert Kaptein will celebrate his 80<sup>th</sup> birthday. Prof. Kaptein is prominent NMR scientist, famous for his contributions to spin chemistry, spin hyperpolarization and bio-NMR.

During his PhD research at the Chemistry Department at the University of Leiden, Prof. Kaptein has made a key contribution in understanding the effect of magnetic fields and magnetic interactions on chemical reactions. Trying to explain the puzzling observation of Chemically Induced Dynamic Nuclear Polarization (CIDNP) he proposed the radical pair mechanism for the observed polarization.<sup>1</sup> This attempt turned out to be very successful, allowing to formulate the famous Kaptein rules,<sup>2</sup> which describe the sign of the CIDNP signals. This proposal of the radical pair mechanism can be considered as the birth of a new branch of chemistry, which we now call "Spin Chemistry". Prof. Kaptein has made a strong contribution to applications of CIDNP-derived spin hyperpolarization to study fast reactions. Furthermore, amino acid residues endowed with photo-CIDNP can be used to probe protein surface and protein interactions in solution.<sup>3</sup>

Prof. Kaptein is one of the pioneers of biomolecular NMR, with a strong focus on determining the structure and dynamics of gene regulatory proteins and protein-DNA complexes. His laboratory developed among others non-selective homonuclear 3D NMR,<sup>4</sup> restrained molecular dynamics<sup>5, 6</sup> and methods for relaxation matrix calculations<sup>7</sup> and for protein structure validation<sup>8</sup>. The structure of Lac headpiece in 1985 was one of the first protein structures solved by NMR<sup>6</sup>. This was followed by studies on the structure and dynamics of other gene regulatory proteins and protein-DNA complexes such as the glucocorticoid receptor,<sup>9</sup> the Arc repressor<sup>10</sup> and the POU domain of the transcription factor Oct1.<sup>11</sup> Central throughout his research were the studies on the DNA complexes of the Lac repressor; that not only deepened our understanding on protein-DNA recognition<sup>12</sup> but also provided a model for protein sliding along the DNA.<sup>12,13</sup> These studies have been of prime importance in establishing NMR as key method for studies on structure and dynamics of proteins and protein complexes and an important stimulus in developing high-field NMR instrumentation and establishing national and international Research Infrastructures. Also beyond his research Prof. Robert Kaptein made excellent contributions to science. He established a world-class biomolecular NMR lab in Utrecht, which has become one of the key players in a cluster of European NMR facilities open to researchers in Europe and world-wide. Over many years, Prof. Kaptein has been and he still is associate editor of the Journal of Biomolecular NMR. He also initiated the EMBO course for Multidimensional NMR in Structural Biology and organized it for many years. For several years, he has been the Director of the Bijvoet Center for Biomolecular Research and Secretary General of the Royal Dutch Academy of

Sciences (KNAW).

A special issue of *Magnetic Resonance*, a new journal established by Groupement AMPERE, will appear which will be dedicated to the 80th birthday of Prof. Robert Kaptein, the "Robert Kaptein Festschrift". This issue contains a series of papers from his colleagues, all in the fields of research, to which Prof. Kaptein immensely contributed – spin chemistry, spin hyperpolarization and biomolecular NMR. This issue reflects the broad scientific interests and inspirations Robert Kaptein has given to generations of magnetic resonance scientists.

Rolf Boelens, Konstantin Ivanov and Jörg Matysik

#### References:

1. R. Kaptein, PhD thesis (University of Leiden, 1971).
2. R. Kaptein, *Journal of the Chemical Society D: Chemical Communications* (1971) 732.
3. R. Kaptein, K. Dijkstra, and K. Nicolay, *Nature* 274 (1978) 293.
4. G. W. Vuister, R. Boelens, and R. Kaptein, *Journal of Magnetic Resonance* 80 (1988) 176.
5. W. F. van Gunsteren, R. Kaptein, and E. R. P. Zuiderweg, in „Nucleic Acid Conformation and Dynamics“ (W. K. Olson, ed.). Report of the NATO/CECAM Workshop, Orsay, 1983.
6. R. Kaptein, E.R.P. Zuiderweg, R.M. Scheek, R. Boelens and W.F. van Gunsteren, *J. Mol. Biol.* 182 (1985) 179.
7. R. Boelens, T. M. G. Koning, and R. Kaptein, *J. Mol. Struct.* 173 (1988) 299.
8. R. A. Laskowski, J. A. C. Rullmann, M. W. MacArthur, R. Kaptein, and J. M. Thornton, *J. Biomol. NMR* 8 (1996) 477.
9. T. Hard, E. Kellenbach, R. Boelens, B. A. Maler, K. Dahlman, L. P. Freedman, J. Carlstedtduke, K. R. Yamamoto, J. A. Gustafsson, and R. Kaptein, *Science* 249 (1990) 157.
10. J. N. Breg, J. H. J. Vanopheusden, M. J. M. Burgering, R. Boelens, and R. Kaptein, *Nature* 346 (1990) 586.
11. N. Dekker, M. Cox, R. Boelens, C. P. Verrijzer, P. C. Vandervliet, and R. Kaptein, *Nature* 362 (1993) 852.
12. C. G. Kalodimos, R. Boelens, and R. Kaptein, *Chem. Rev.* 104 (2004) 3567.
13. C.G. Kalodimos, N. Biris, A.M.J.J. Bonvin, M.M. Levandoski, M.Guennuegues, R. Boelens, and R. Kaptein, *Science* 305 (2004), 386

## Portrait: Prof. Robert Kaptein

- why magnetic resonance and why NMR?

When I started my master study at Leiden University in 1962 there was an opening in the NMR group to work with the new Varian A60. Although I only had a vague notion about NMR, I accepted it and had never any regrets.

- as a PhD student how did you come across CIDNP and discovered the Radical Pair Mechanism (RPM)?

In 1965 I started as a PhD student. My supervisor Prof. L.J. Oosterhoff suggested me to work on NMR of stable free radicals, an area that was started by Hausser and Stehlik a bit earlier. After about two years I had some results, but I was not very happy with the topic. I should note that in those days the PhD students had a lot of freedom and no time pressure. After a few years they would even get a decent salary. So when I read the papers by Bargon & Fischer and Ward & Lawler in '67 on the discovery of CIDNP, I found this a much more challenging subject. The DNP mechanism that Bargon & Fischer had proposed (based on an earlier idea by Rex Richards) looked perfectly reasonable, except that the W&L paper showed a strange "multiplet effect" (both positive and negative polarization in the split lines of a single nucleus). Thus, with the consent of Oosterhoff I started my work on CIDNP. I tackled the problem both experimentally and theoretically, which in hindsight turned out to be essential (see next question).

- luckiest experiment you have ever done?

I had a good training in organic chemistry, so I started by synthesizing some peroxides as free radical precursors. My luckiest experiment was the thermal decomposition of acetyl peroxide (AP) in the NMR tube (don't do this experiment, in pure form AP is extremely explosive!). The NMR spectrum (see Fig.) showed opposite polarization for radical recombination products (ethane and methyl acetate) vs. "escape" or scavenging products (methyl chloride). This was clearly inconsistent with a DNP-like mechanism and put me on the right track to consider the role of radical pairs rather than single radicals. It still took me some time to work out a proper theory for the radical pair mechanism (RPM), which was published in '69, at about the same time that Gerhard Closs in Chicago published essentially the same idea.



- what do you still not understand?

At my age one starts wondering how the brain works and how one could avoid memory loss and worse.

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

It was not really a mistake, but the worst incident was the suicide of one of our PhD students in '95. His thesis was finished, and it happened one week before the thesis defense and ceremony. For a long time I wondered what I could have done to help him and avoid this tragedy.

- most memorable conference story?

This happened on one of the Banff conferences in the Canadian Rockies. On the last day there was an enormous rainfall. The torrent of water in the river had destroyed the bridge and thereby blocked the only road to Calgary for our flight home. So we were stuck there for a couple of days. Actually this was not so bad, because there was enough food and drinks in the hotel, and we could share our misery with the other participants.

- with whom (historical person) would you like to meet?

I would like to ask Goudsmit and Uhlenbeck how they discovered the concept of nuclear and electron spin, that played such a big role in my scientific life.

- when do you get your best ideas?

After thinking intensely about a problem and then relax for a while, you may suddenly have these flashes of insight that can help you further.

- your idea of happiness?

In science it is in the eureka moments as I mentioned above, but these are very rare. Otherwise in connecting with family and friends, but these moments are now also rare in this corona time.

Position: Emeritus Professor of Chemistry at Utrecht University, since 2006.

Education: PhD at Leiden University, 1965-1971

Main Awards: 1971 Golden Medal of the Royal Dutch Chemical Society, 1985 Holleman Award of the Royal Dutch Academy of Arts and Sciences, 2006 Royal decoration: Knight of the Order of the Dutch Lion, 2012 Voevodsky Award, Russian Academy of Science.

Interests: Playing chess, history of science, traveling (but not now, unfortunately).

## First announcement:



Dear NMR Community,

On behalf of the Organizing Committee it's my great pleasure to announce that the AMPERE NMR School 2021, an annual event organized since earlier 90<sup>th</sup> under auspices of the Groupment AMPERE, due to COVID-19 epidemic, will take place in the hybrid form (in person/virtually) in June 21-23, 2021.

Lectures, poster presentations, and discussions will be carried out virtually.

The topics of the School will be the following:

- Solid-state and soft matter NMR
- NMR diffusometry and relaxometry
- Magnetic Resonance Imaging
- NMR and quantum information
- Dynamic Nuclear Polarization
- NMR methodology and techniques
- Application of NMR in biology and medicine

The School is addressed to PhD students of various fields of physics, chemistry, biology, materials science, medical sciences, and is focused on theoretical and experimental aspects of NMR.

More detailed information you will find on the conference website.

[www.school.home.amu.edu.pl](http://www.school.home.amu.edu.pl)

We will be updating you regularly on the nature of the virtual conference with updates and announcements.

With my best wishes,  
Stefan Jurga

Director  
NanoBioMedical Centre  
Adam Mickiewicz University in Poznan

[www.cnbm.amu.edu.pl](http://www.cnbm.amu.edu.pl)

## Second announcement:



The 17<sup>th</sup> EUROMAR 2021 conference will take place in Portorož, Slovenia between July 4 and 8, 2021, as an innovative hybrid event combining face-to-face interactions in a wonderful scenic environment with the best possible experience for virtual participation for those that may not be able to attend in person.

EUROMAR 2021 will transfer the live experience in a virtual form to you, our dear participants, enabling you to experience the conference virtually and be able to interact with all other participants including vendors, and access all the content and make important contacts that are intertwined through the social program of the conference.

## Preliminary programme of the conference:

Time	Sunday, July 4	Monday, July 5	Tuesday, July 6	Wednesday, July 7	Thursday, July 8	Friday, July 9
9 a.m.	User meetings	Plenary 1, 2	Plenary 5, 6	Plenary 8, 9	Plenary 12, 13	Transfers
		Break	Break	Break	Break	
		Session 1   Session 2	Session 5   Session 6	Session 11   Session 12	Session 15   Session 16	
12 a.m.	Lunch	Lunch	Lunch	Lunch		
13 p.m.	Tutorial lectures	Posters session	Posters session	Posters session	Session 17   Session 18	
15 p.m.		Plenary 3,4	Plenary 10, 11	Plenary 7	Break	
		Break	Break	Session 7   Session 8	Session 19   Session 20	
	Prize session	Session 3   Session 4	Session 13   Session 14	Break	Plenary 14, 15	
19 p.m.			Posters session	Session 9   Session 10		
20 p.m.	Welcome reception	Bruker night	Vendor's night, cheese and wine party	Hospitality	Gala dinner	

## The scientific program of EUROMAR 2021 consists of 16 different topics:

- o Solution and solid-state biomolecular NMR
- o Biomolecular dynamics
- o Integrated Structural biology: NMR in hand with complementary methods
- o NMR in combat against COVID-19
- o Small molecules
- o Metabolomics
- o Field-cycling NMR relaxometry
- o NMR of quantum materials
- o Frontiers in magnetic resonance
- o MRI in material science and biomedical applications
- o Solids: From energy storage and conversion to organic and composite solids
- o Hyperpolarization
- o EPR in biomolecular and material science
- o In-cell magnetic resonance
- o Drug design
- o Methods Development
- o Benchtop and low-field

## We are honoured to announce plenary speakers:

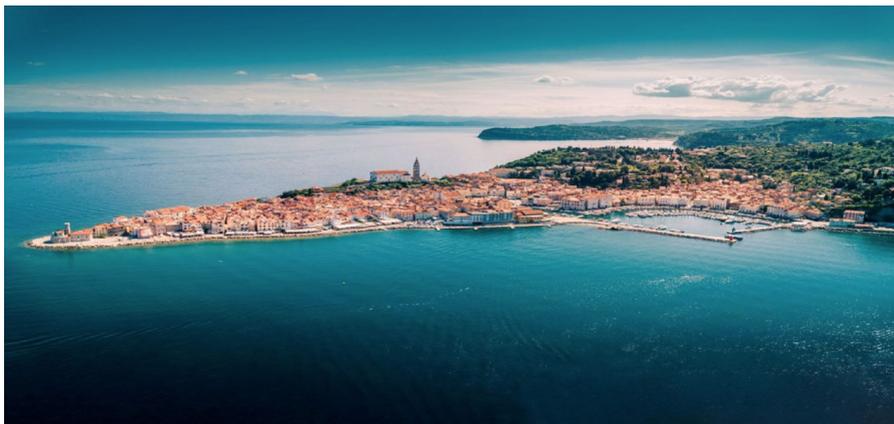
- o Enrica Bordignon, Ruhr University Bochum, Germany
- o Craig Butts, University of Bristol, United Kingdom
- o Teresa Carlomagno, Leibniz University Hannover, Germany
- o Eugenio Coronado, University of Valencia, Spain
- o Lyndon Emsley, EPFL, the Swiss Federal Institute of Technology in Lausanne, Switzerland
- o Fabien Ferrage, École normalesupérieure, Sorbonne Université, France
- o Lucio Frydman, Weizmann Institute, Israel
- o Ana Gil, University of Aveiro, Portugal
- o Arno P.M. Kentgens, Radboud University, The Netherlands
- o Philippe Mendels, Université Paris-Saclay, France
- o Gary J. Pielak, The University of North Carolina at Chapel Hill, United States
- o Roberta Pierattelli, University of Florence, Italy
- o Guido Pintacuda, University of Lyon, France
- o Noam Shemesh, Champalimad Centre for the Unknown, Portugal
- o Sabine Van Doorslaer, University of Antwerp, Belgium

You are cordially invited to attend EUROMAR 2021 conference with its exciting scientific programme and excellent speakers, and in this way help a wider magnetic resonance community to stay connected.

For more information visit our website

[www.euromar2021.org](http://www.euromar2021.org)

Let's spin into the future in Portorož together.



## **Report: Modern Development in Magnetic Resonance**

**September 28. to October 2. 2020, Kazan, Russia**

The annual International Conference “Modern Development of Magnetic Resonance” was held from September 28 to October 2, 2020 in Kazan. The conference was organized by the Kazan Zavoisky Physical-Technical Institute of the Federal Research Center “Kazan Scientific Center Russian Academy of Sciences” and the Kazan Federal University under the auspices of the AMPERE Society. The conference also included the ceremony of the International Zavoisky Award 2020 and the Workshop “Diamond-Based Quantum Systems for Sensing and Quantum Information”. All events were organized in a mixed format: actual participation of scientists from Russia and online participation of scientists of other countries.

The conference topics were extremely diverse and included reports in the following fields:

- Chemical and Biological Systems
- Low-dimensional, Nanosized and Strongly Correlated Electronic Systems;
- Magnetic Resonance Instrumentation
- Electron Spin-Based Methods for Electronic and Spatial Structure Determination in Physics, Chemistry and Biology.
- Modern Methods of Magnetic Resonance
- Molecular Magnets and Liquid Crystals
- Other Applications of Magnetic Resonance and Related Phenomena.

The participants of the conference were leading scientists and experts in the field of magnetic resonance from Australia, China, Germany, Italy, Japan, Moldova, Russia, Scotland, Sweden, and USA. The total number of participants was 178, who presented 130 reports (12 plenary lectures, 62 oral talks, and 64 posters). The program of the conference and abstracts can be found at <http://www.kfti.knc.ru/mdmr/2020/MDMR.2020.program.pdf> and <http://www.kfti.knc.ru/mdmr/2020/MDMR.2020.abstract.pdf>, respectively.

The opening ceremony and the first scientific session of the conference took place on September 28, 2020 and were chaired by Alexey Kalachev, Deputy Director of the Federal Research Center. Kev Salikhov, Chairman of the International Zavoisky Award Selection Committee, announced the name of the Zavoisky Awardee 2020: Professor Klaus-Peter Dinse (Free University of Berlin, Berlin, Germany). He was distinguished for his contributions to EPR spectroscopy of organic supramolecular systems and novel catalytic complexes. Leila Fazleeva, Deputy Prime Minister of the Republic of Tatarstan, and Oleg Sinyashin, Director of the Federal Research Center, congratulated heartily Klaus-Peter Dinse on his highly deserved award. Klaus-Peter

Dinse also received congratulations from Thomas Prisner, IES President, Bernhard Blümich, President of the AMPERE Society, Robert Tycko, ISMAR President, and Christian Caron, Executive Publishing Editor, Springer-Verlag.



From left to right: Kev Salikhov demonstrates the Zavoisky Award medal, and Alexey Kalachev holds the Zavoisky Award 2020 Diploma.

The first plenary session included the following plenary lectures: From High Power to Low Power – Recipes for a Successful Scientific Life! by Klaus-Peter Dinse, DNP Enhanced Solid-State NMR Spectroscopy of Functional Materials by Gerd Buntkowsky (Technical University Darmstadt, Darmstadt, Germany) and New Paradigm of Spin Exchange by Kev Salikhov (Zavoisky Physical-Technical Institute, Kazan, Russia).

A number of topical fundamental problems were discussed at the conference. These include:

search for the element base of quantum computing and quantum informatics; synthesis and study of the properties of new materials with specified functional properties; problems of magnetism in solids; a new paradigm of spin exchange in dilute solutions of paramagnetic particles and its manifestation in EPR spectroscopy; etc.

New possibilities of NMR were featured in invited talks Picoliter NMR Spectroscopy with Diamond NV Centers by Victor Acosta (University of New Mexico, USA) and Optically Hyperpolarized Nanodiamonds: Applications in Accelerated NMR and Sensing by Ashok Ajoy (UC Berkeley, Berkeley, USA), which were presented at the Workshop “Diamond-Based Quantum Systems for Sensing and Quantum Information”.

Two IES Student Poster Awards were granted at the MDMR2020. The IES Student Poster Award Selection Committee consisted of Kev Salikhov (Chairman) and members: Roman Babunts (Ioffe Physical-Technical Institute, St. Petersburg), Elena Bagryanskaya (Novosibirsk Institute of Organic Chemistry, Novosibirsk), Murat Tagirov (Kazan Federal University, Kazan) and Valery Tarasov (Zavoisky Physical-Technical Institute, Kazan). George Andreev and Andrey Petrov (both Kazan Federal University, Kazan) were chosen as the awardees.



From left to right: Kev Salikhov, and IES Student Poster Awardees at MDMR2020: George Andreev and Andrey Petrov.

The conference favored the exchange of ideas and recent achievements and its participants received a good impetus for their further research, which was especially important in the pandemic we all live through.

The organizers of the conference are sincerely grateful to the Government of the Republic of Tatarstan, Federal Research Center “Kazan Scientific Center of the Russian Academy of Sciences”, and the Russian Foundation for Basic Research for the financial support.

Kev Salikhov  
Chairman of the Organizing Committee MDMR2020  
Violeta Voronkova  
Scientific Secretary MDMR2020

## Posterprize MDMR:

Andrey Petrov

### Ultrafast Magnetization Dynamics in Thin Films of L1<sub>0</sub>-Ordered FePt and FePd Compounds

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Intermetallic compounds and heterostructures based on elements of the platinum group are the basis of modern media for super-dense magnetic recording of information. The choice is determined by the unique magnetic properties of such compounds and long-term stability, as well as the insensitivity of their magnetic properties to the corrosive effects of oxygen and air humidity. [1]

Thin films of FePd and FePt compounds 10 nm thick were grown by molecular beam epitaxy (MBE) on MgO (001) substrates at room temperature in an ultrahigh-vacuum chamber on a 3 nm thick chromium (Cr) seed layer deposited at a substrate temperature of 600 °C. To transfer the equimolar systems FePd and FePt to the ordered tetragonal phase L1<sub>0</sub>, the film was annealed for 30 minutes at a temperature of 650 °C.

The crystal structure and epitaxiality of the grown FePd and FePt films were studied by low-energy electron diffraction (LEED) methods directly in the ultrahigh-vacuum chamber and X-ray diffraction (XRD) analysis. The contrasting patterns of the LEED maxima indicate the single-crystal nature of the films and their coherent growth on substrates, that is, cube by cube type epitaxy. The observation of the (001) maximum along with (002) in the X-ray diffractogram indicates the tetragonal symmetry of the crystal lattice of the films, which, in turn, indicates their successful synthesis in the desired ordered L1<sub>0</sub> phase.

Using femtosecond optical and magneto-optical spectroscopy, it was shown that thin films of the L1<sub>0</sub> phases of FePd and FePt compounds are characterized by different times of photoinduced demagnetization. Such a difference is a prerequisite for the creation of artificial multilayer ferrimagnetic structures of the F1/N/F2 type, where F1 and F2 are ferromagnetic layers, the nature of the interaction between which is determined by the thickness of the separator made of normal metal N. The difference in the demagnetization rates is a necessary condition for ultrafast photoinduced handling magnetization.

In the future, the synthesis of three-layer structures based on L1<sub>0</sub>-FePd and L1<sub>0</sub>-FePt is supposed. The latter are isostructural and have very close lattice constants, both with respect to each other and to the Fe<sub>0.08</sub>Pd<sub>0.92</sub> system. This makes it possible to create perfect heteroepitaxial structures based on them.

This work was supported by the RSF project No. 18-12-00459. Synthesis and analysis of the films were carried out at the PCR Federal Center of Shared Facilities of KFU.

1. Iihama S. et al.: Applied Physics Letters 14, 105 (2014)

## Posterprize MDMR:

George Andreev

### Abnormal Magnetism of Nano- and Microscaled Tetrafluorites LiTbF<sub>4</sub> and LiDyF<sub>4</sub>

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Rare earth tetrafluorides LiReF<sub>4</sub>, Re = La—Lu, are a promising material for laser technology [1, 2], medicine and biotechnology[3]. LiTbF<sub>4</sub> is an Ising dipolar uniaxial ferromagnet; T<sub>C</sub> = 2.8741(16) K [5]. LiDyF<sub>4</sub> is a layered antiferromagnet; T<sub>N</sub> = 0.610(15) K [5].

Nanosized powders of LiTbF<sub>4</sub> were synthesized using hydrothermal method[6]. Microsized LiTbF<sub>4</sub> and LiDyF<sub>4</sub> powders were baked at 650. XRD patterns, TEM HR and optical microscope were used for characterization. Temperature and field dependencies of magnetization were measured at the vibrational magnetometer. LiTbF<sub>4</sub> nanopowder at B = 10 mT showed reduction of Curie temperature compared with monocrystal. Field dependence of LiDyF<sub>4</sub> micropowder's magnetization at temperatures below 7 K takes the form of antiferroelectric hysteresis. Temperature dependence of loops' area is measured. Also, this sample's magnetisation does not set instantly when the external field is set, but follows exponential law exp(-t/τ). Values of τ are different for magnetization and demagnetization of LiDyF<sub>4</sub> micropowder. The financial support of the Russian Foundation for Basic Research and the Government of the Republic of Tatarstan (project 18-42-160012 p\_a) is gratefully acknowledged.

1. Zhai X., Lei P., Zhang P. et al.: Biomaterials 65, 115–123 (2015)

2. Castellano-Hernández E., Kalusniak S., Metz P.W., Kränkel C.: Laser & Photonics Reviews 14, no. 2, 1900229 (2020)

3. Zelmon D.E., Erdman E.C., Stevens K.T. et al.: Applied Optics 55, 834–837 (2016)

4. Als-Nielsen J., Holmes L.M., Krebs Larsen F., Guggenheim H.J.: Phys. Rev. B 12, 191–197 (1975)

5. Mennenga G., de Jongh L.J., Huiskamp W.J.: Journal of Magnetism and Magnetic Materials 44, 48–58 (1984)

6. Zhang Q., Yan B.: Inorganic Chemistry 49, no. 15, 6834–6839 (2010)

## Report: Euromar 2020



BILBAO, SPAIN | 5 - 9 JULY 2020

EUROISMAR 2020 was supposed to be held in the Palacio Euskalduna (Bilbao) between the 5 and the 9 of July of 2020. It finally took the shape of an on-line meeting, during the 7 and 8 of December of 2020. The meeting allowed celebrating the award ceremonies and it was complemented by a plethora of flash presentations selected from the many abstracts submitted and where the young scientist's participation was promoted. Their participation was instrumental for the success of the on-line meeting.

### Committees:

International Scientific Committee:

Inés Garcia Rubio (ICMA, Zaragoza, Spain), Ana M. Gil (University of Aveiro, Aveiro, Portugal), Jesús Jiménez-Barbero (CIC bioGUNE, Derio, Spain), Arno Kentgens (Radboud University, Nijmegen, Netherlands), Antoine Loquet (IECB, Bordeaux, France), Oscar Millet (Chair, CIC bioGUNE, Derio, Spain), Miquel Pons (Universitat de Barcelona, Barcelona, Spain), Thomas Prisner (University of Frankfurt, Frankfurt, Germany), Christina Redfield (University of Oxford, Oxford, UK), Cristina M Thiele (Technische Universität Darmstadt, Darmstadt, Germany), Thomas Vosegaard (Aarhus University, Aarhus, Denmark), Andrew G. Webb (Leiden University, Leiden, Netherlands).

Local Organizing Committee:

Ignacio Alfonso (IQAC), Ana Ardá (CIC bioGUNE), Tammo Diercks (CIC bioGUNE), Nieves Embade (CIC bioGUNE), Marga Gairí (Universitat de Barcelona), M. Angeles Jiménez (IQFR), Jesús Jiménez-Barbero (CIC bioGUNE), Óscar Millet (Chair, CIC bioGUNE), Ana Poveda (CIC bioGUNE).

### EUROMAR2020 and COVID-19

COVID-19 has resulted in a worldwide first order catastrophe that has affected the very fabric of our daily life, forcing us to constantly adapt to everchanging situations. As a result, EUROMAR 2020 was severely affected by the evolution of the COVID-19

pandemia. In an optimistic attempt of overcoming COVID-19 and after the first wave of the infection, it was decided to postpone the meeting from the original dates (5-9 July 2020) to the first week of December of the same year. I wanted to emphasize that the speakers were contacted and asked to reschedule, and the response was extremely positive and cooperative. Yet, in spite of the COVID-19 summer break, it was soon clear enough that a physical meeting at the end of the year would also be unrealistic. After careful deliberation between the committees and the organizing institutions it was finally decided to cancel the meeting as it was normally understood. Instead, we offered a minimalistic version of EUROMAR to render tribute to the prize awardees and also to allow the young scientist to actively participate in the format of poster submissions and flash presentations.

### Promotion & Communication

Leading up to the EUROISMAR 2020 the conference website, <https://www.euromar2020.org>, was launched in October 2019, right after the Berlin EUROISMAR conference. Yet, the most effective communication channel was the tweeter account. With a weekly periodicity, a tweet was sent to introduce a speaker or to distribute relevant information. In the end the effort paid off and the EUROMAR tweeter account increased the number of followers during the year in about four hundred.

### The online conference Structure

Based on the COVID-19 pandemic escalation, EUROMAR 2020 Organising Committee proposed to celebrate an on-line meeting version to cover the following goals: awarding ceremony of the prizes and short talks selected from the abstracts submitted by early-stage researchers. The platform chosen was zoom. In addition, the same zoom platform was also used to organize the customary meetings for the different committees in charge of the governance of EUROMAR and ISMAR. The conference was distributed in two days and arranged in a time-zone that favoured the attendance worldwide. The award lectures and introductions were held in Room 1 for all the attendees, while two parallel sessions (Room 1 and Room2) hosted the flash presentations from the selected abstracts. The topics for the parallel sessions were: Biomolecular NMR, Computation, EPR /ESR, Hyperpolarization, Instrumentation /hardware, In cell NMR, Materials, Metabolomics, MRI / In vivo, Small molecules & drug design, Solid state NMR – methods, Solid state NMR – applications and Solution NMR -methods.

The attendance was free of charge but required previous registration. The sessions were recorded and a youtube channel was created to host all the lectures that were accepted to be made public. The links to the lecture channels are:

(7 Dec) <https://drive.google.com/drive/folders/1ldOfzailKB15Z2ED1sqyA3pkazYCo-Wn?usp=sharing>

(8 Dec) <https://drive.google.com/drive/folders/1MMbzN9KhTRsGzVZmxccIXioprbageWNn?usp=sharing>

A PDF with all the abstracts and the CV of the awardees was distributed among all the registered users.

### Facts and Figures

4 Prize award conferences. 44 Poster presentations (5 min each). 170 Posters presented. 7 Best poster awards. 760 Unique e-mail addresses that participated. 1090 Registered e-mail addresses. 565 joint participants at the peak of the meeting.

### Prizes

The prestigious Richard R. Ernst Prize to recognize recent beneficial applications of Magnetic Resonance was sponsored by Bruker. It was rightfully granted to honour the work of Clare Grey who currently is full Professor at the Department of Chemistry from Cambridge University.

The Raymond Andrew Prize is awarded to a young scientist for his/her outstanding PhD thesis in magnetic resonance. In this occasion Christian Bengs got the award. Christian did his Ph. D. Thesis in the group of Prof. Malcolm Levitt at the University of Southampton.

The also renowned AMPERE Prize was given to Thomas Theis who currently is Assistant Professor at the Department of Chemistry of the North Carolina State University. Finally, Paul Schanda was awarded with the Varian Young Investigator Award. Paul will become Full Professor at the Institute of Science and Technology in Austria as of 2021.

On the other hand, the Journal of Magnetic Resonance, Elsevier, awarded 4 prizes to early-stage investigators in recognition of their excellent work. The „Magnetic Resonance in Chemistry Awards“ were awarded to Dr. Kathrin Aebischer (ETH, Zurich), Lauriane Lecoq (University of Lyon), María Pía Lenza (CIC bioGUNE, Bilbao), Julien Manon (IIB, Gif-sur-Yvette). The awards were selected from the flash presentations by the Scientific Committee. Finally, the EPR society also gave award to the lecturers: Arnau Bertran (Oxford University), Yuri Kutin (Technical University Darmstadt) and Andreas Meyer (MPI Biophysics, Göttingen).

Óscar Millet  
January 2021

### Ampere Prize for young investigators:

Prof. Dr. Thomas Theis

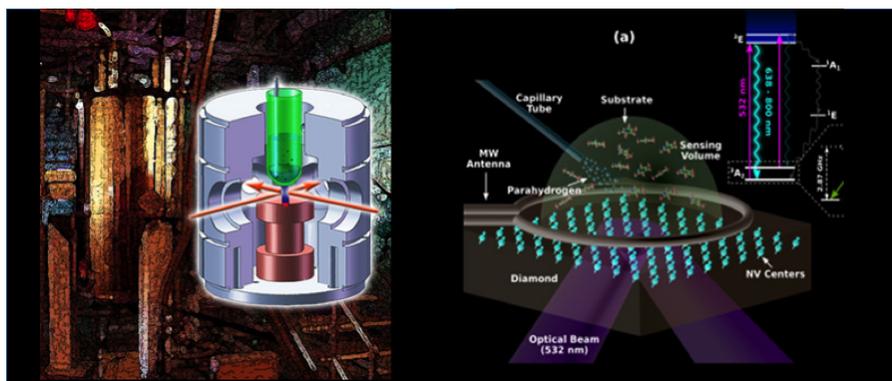
The AMPERE prize for young investigators was awarded to Prof. Dr. Thomas Theis at the virtual EUROMAR conference (Bilbao, Spain) on December 8<sup>th</sup> 2020. The prize was awarded in recognition of his achievements in hyperpolarization and long-lived states.

Dr. Theis established a nuclear spin hyperpolarization technique that enhances NMR and MRI signals on heteronuclei (e.g. <sup>15</sup>N, <sup>13</sup>C, <sup>19</sup>F etc.) by several orders of magnitude.<sup>1-4</sup> His technique, dubbed SABRE-SHEATH (for Signal Amplification By Reversible Exchange in Shield Enables Alignment Transfer to Heteronuclei), is a parahydrogen based hyperpolarization technique that works directly in room temperature solutions to hyperpolarize small molecules including vitamins, drugs and metabolites.<sup>4</sup> SABRE-SHEATH breaks the sensitivity limitations of NMR and MRI, and opens new windows of opportunity for magnetic resonance techniques.

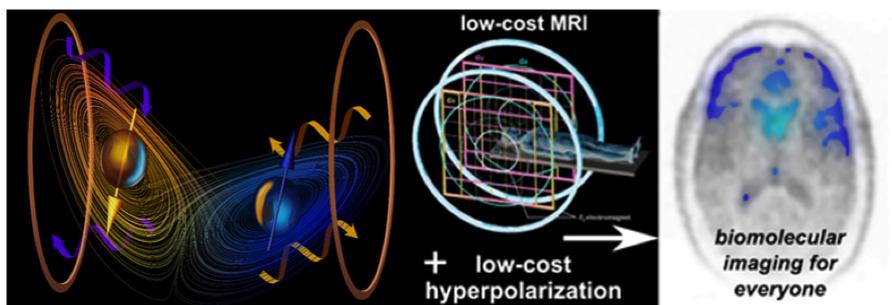
By studying the detailed chemical mechanisms and nuclear spin dynamics controlling hyperpolarization transfer, Dr. Theis was able to maximize hyperpolarization on many substrates and to store hyperpolarization in long-lived quantum states.<sup>5-7</sup> His lab continues to work on parahydrogen and ventures into new hyperpolarization strategies. For example, he now devises optically induced hyperpolarization in room temperature solutions by exploiting optically excited states, spin selective photo-physics and Overhauser dynamic nuclear polarization. His lab explores new applications enabled by his breakthroughs in hyperpolarization chemistry illustrated in Figure 1.

in Fig. 1a shows, Dr. Theis' developments of portable NMR for *“chemical analysis on your cell phone”* by combining hyperpolarization technology with highly sensitive Rubidium vapor magnetometers.<sup>8-10</sup> NMR signals are detected from the hyperpolarized molecules with Faraday rotation of polarized light as it traverses the Rubidium vapor. All components, including hyperpolarization unit, spectrometer, optical detector, electric amplification circuits can be miniaturized to obtain well resolved, information rich NMR spectra.

Fig. 1b illustrates the development of *“NMR microscopes”* by exploiting nitrogen-vacancies in diamond as optical quantum sensors of hyperpolarized NMR signals.<sup>11</sup> Here the power of optical microscopy is expanded by the chemical dimension, because we will be able to acquire NMR spectra of every pixel in optical images. Hyperpolarized tracers can be fed to cells on the surfaces quantum sensing chips that are imaged with microscopic resolution to monitor metabolic turnover in cells.



a) optically detected NMR      b) NMR with solid state quantum sensor



c) RASER      d) Hyperpolarized imaging with long-lived states

As shown in Fig. 1c, Dr. Theis establishes “*decoherence-free quantum sensors*” by generating large negative nuclear spin polarization in highly resonant RF circuits. This results in a RASER, which in analogy to a LASER, also emits highly coherent waves, except the RASER waves are in the kHz to MHz regime and reports directly on chemical structure through chemical shifts and  $J$ -couplings.<sup>12,13</sup> With a RASER one can achieve arbitrarily narrow NMR lines to obtain precision measurements of NMR parameters.

Finally, depicted in Fig. 1d is another major thrust in the Theis lab geared towards “*affordable molecular imaging*” by hyperpolarized MRI. The Theis lab created a cryogen-free MRI system featuring magnetic fields between 5 mT and 3 T. His lab is showing that with hyperpolarized MRI there is no longer a need for magnetic fields of large superconducting magnets for high quality molecular imaging. With these tools, the Theis lab can track the metabolic turnover of individual metabolites directly in animals and patients,<sup>14</sup> setting the stage for affordable MRI.

In summary, Dr. Theis is emerging as a leader in hyperpolarization chemistry and its applications to quantum sensing and molecular imaging. The Theis lab fosters deep knowledge of chemical kinetics and spin evolution to continually innovate spin technologies and molecular imaging modalities.

Figure 1. Achievements in the Theis hyperpolarization lab.

- a) Rubidium vapor magnetometer for miniaturizable NMR (see refs. 8-10)
- b) NV-diamond detected NMR (see ref. 11)
- c) Radiofrequency amplification by stimulated emission of radiation (see refs. 11,13)
- d) Molecular imaging with long-lived hyperpolarization (see refs. 1-7)

#### References:

- (1) Theis, T.; Truong, M. L.; Coffey, A. M.; Shchepin, R. V.; Waddell, K. W.; Shi, F.; Goodson, B. M.; Warren, W. S.; Chekmenev, E. Y. Microtesla SABRE Enables 10% Nitrogen-15 Nuclear Spin Polarization. *J. Am. Chem. Soc.* 2015, 137 (4), 1404–1407. <https://doi.org/10.1021/ja512242d>.
- (2) Truong, M. L.; Theis, T.; Coffey, A. M.; Shchepin, R. V.; Waddell, K. W.; Shi, F.; Goodson, B. M.; Warren, W. S.; Chekmenev, E. Y. 15N Hyperpolarization by Reversible Exchange Using SABRE-SHEATH. *J. Phys. Chem. C* 2015, 119 (16), 8786–8797. <https://doi.org/10.1021/acs.jpcc.5b01799>.
- (3) Shchepin, R. V.; Truong, M. L.; Theis, T.; Coffey, A. M.; Shi, F.; Waddell, K. W.; Warren, W. S.; Goodson, B. M.; Chekmenev, E. Y. Hyperpolarization of “Neat” Liquids by NMR Signal Amplification by Reversible Exchange. *J. Chem. Phys. Lett.* 2015, 6 (10), 1961–1967. <https://doi.org/10.1021/acs.jpcllett.5b00782>.
- (4) Colell, J. F. P.; Logan, A. W. J.; Zhou, Z.; Shchepin, R. V.; Barskiy, D. A.; Ortiz, G. X.; Wang, Q.; Malcolmson, S. J.; Chekmenev, E. Y.; Warren, W. S.; Theis, T. Generalizing, Extending, and Maximizing Nitrogen-15 Hyperpolarization Induced by Parahydrogen in Reversible Exchange. *J. Chem. Phys. C* 2017, 121 (12), 6626. <https://doi.org/10.1021/acs.jpcc.6b12097>.
- (5) Theis, T.; Feng, Y.; Wu, T.; Warren, W. S. Composite and Shaped Pulses for Efficient and Robust Pumping of Disconnected Eigenstates in Magnetic Resonance. *J. Chem. Phys.* 2014, 140 (1), 014201. <https://doi.org/10.1063/1.4851337>.
- (6) Theis, T.; Ortiz, G. X.; Logan, A. W. J.; Claytor, K. E.; Feng, Y.; Huhn, W. P.; Blum, V.; Malcolmson, S. J.; Chekmenev, E. Y.; Wang, Q.; Warren, W. S. Direct and Cost-Efficient Hyperpolarization of Long-Lived Nuclear Spin States on Universal 15N2-Diazirine Molecular Tags. *Sci. Adv.* 2016, 2 (3), e1501438. <https://doi.org/10.1126/sciadv.1501438>.
- (7) Zhou, Z.; Yu, J.; Colell, J. F. P.; Laasner, R.; Logan, A.; Barskiy, D. A.; Shchepin, R. V.; Chekmenev, E. Y.; Blum, V.; Warren, W. S.; Theis, T. Long-Lived 13C Nuclear Spin States Hyperpolarized by Parahydrogen in Reversible Exchange at Microtesla Fields. *J. Phys. Chem. Lett.* 2017, 8 (13), 3008–3014. <https://doi.org/10.1021/acs.jpcllett.7b00987>.
- (8) Theis, T.; Ganssle, P.; Kervern, G.; Knappe, S.; Kitching, J.; Ledbetter, M. P.; Budker, D.; Pines, A. Parahydrogen-Enhanced Zero-Field Nuclear Magnetic Resonance. *Nat. Phys.* 2011, 7 (7), 571–575.
- (9) Tayler, M. C. D.; Theis, T.; Sjolander, T. F.; Blanchard, J. W.; Kentner, A.; Pustelny, S.; Pines, A.; Budker, D. Invited Review Article: Instrumentation for Nuclear Magnetic Resonance in Zero and Ultralow Magnetic Field. *Rev. Sci. Instrum.* 2017, 88 (9), 91101. <https://doi.org/10.1063/1.5003347>.
- (10) Theis, T.; Ledbetter, M. P.; Kervern, G.; Blanchard, J. W.; Ganssle, P. J.; Butler, M. C.; Shin, H. D.; Budker, D.; Pines, A. Zero-Field NMR Enhanced by Parahydrogen in Reversible Exchange. *J. Am. Chem. Soc.* 2012, 134 (9), 3987–3990. <https://doi.org/10.1021/ja2112405>.
- (11) Arunkumar, N.; Bucher, D. B.; Turner, M. J.; TomHon, P.; Glenn, D.; Lehmkuhl, S.; Lukin, M. D.; Park, H.; Rosen, M. S.; Theis, T.; Walsworth, R. L. Micron-Scale NV-NMR Spectroscopy with Signal Amplification by Reversible Exchange. *PRX Quantum* 2021, 2 (1), 10305. <https://doi.org/10.1103/prxquantum.2.010305>.

(12) Appelt, S.; Lehmkuhl, S.; Fleischer, S.; Joalland, B.; Ariyasingha, N. M.; Chekmenev, E. Y.; Theis, T. SABRE and PHIP Pumped RASER and the Route to Chaos. *J. Magn. Reson.* 2021, 322, 106815. <https://doi.org/10.1016/j.jmr.2020.106815>.

(13) Joalland, B.; Ariyasingha, N. M.; Lehmkuhl, S.; Theis, T.; Appelt, S.; Chekmenev, E. Y. Parahydrogen-Induced Radio Amplification by Stimulated Emission of Radiation. *Angew. Chemie Int. Ed.* 2020, 59 (22), 8654–8660. <https://doi.org/10.1002/anie.201916597>.

(14) Nelson, S. J.; Kurhanewicz, J.; Vigneron, D. B.; Larson, P. E. Z.; Harzstark, A. L.; Ferrone, M.; van Criekinge, M.; Chang, J. W.; Bok, R.; Park, I.; Reed, G.; Carvajal, L.; Small, E. J.; Munster, P.; Weinberg, V. K.; Ardenkjaer-Larsen, J. H.; Chen, A. P.; Hurd, R. E.; Odegardstuen, L.-I.; Robb, F. J.; Tropp, J.; Murray, J. A. Metabolic Imaging of Patients with Prostate Cancer Using Hyperpolarized [1-13C]-Pyruvate. *Sci. Transl. Med.* 2013, 5 (198), 198ra108. <https://doi.org/10.1126/scitranslmed.3006070>.

## Raymond Andrew Prize:

Dr. Christian Bengs

## Non-Equilibrium Nuclear Spin States

### Abstract

Any physical quantum system is in thermal contact with its environment and if left undisturbed, will always come to thermal equilibrium with its surroundings. Nuclear magnetic resonance techniques however displace the system from its thermal equilibrium position. The amount of time a system may be displaced from its thermal equilibrium position is inherently time limited due to constant information exchange between the system and the environment. This fundamental process is known as quantum relaxation or quantum decoherence.

In this thesis we focus our attention on the relaxation dynamics of nuclear spin ensembles. Particular spin configurations may display surprisingly long relaxation time constants and surprising dynamical behaviour as the system deviates further from its thermal equilibrium position. A simple framework for the description of nuclear spin systems far from thermal equilibrium is described and its necessity is experimentally demonstrated by consideration of simple model systems. The presented framework aims to advance recent developments in the storage of hyperpolarised materials, which ideally possess exceptionally long relaxation times and highly ordered spin configurations.

### Introduction

The humble beginnings of Nuclear Magnetic Resonance (NMR) can be tracked back all the way to the 1940s. Following Rabi's description of the magnetic resonance effect Purcell, Torrey, Pound and Bloch, Hansen, Packard almost simultaneously (24th of December, 1945 and 29th of January, 1946) reported the observation of nuclear induction for the first time /

Since then, it is probably fair to say that NMR has grown into something much bigger than the founding fathers could have hoped for. The applicability of NMR is seemingly endless and ranges from elementary physics to quantum computation, material science, organic chemistry, medical science, biology and many other fields of active research. Major landmarks in the field of NMR include the development of magnetic resonance imaging, two-dimensional NMR and its extension to protein structure elucidation. For obvious reasons these developments continue to influence our every day life by guiding biomedical and pharmaceutical research.

Nowadays NMR is considered a standard tool in many areas of active research. Nonetheless, it seems that whenever the community is convinced to have reached the stories end, a new idea magically appears and opens up a new chapter. In recent years, this has certainly been the development of hyperpolarisation techniques.

Despite a great number of benefits, NMR suffers from a weak magnetic response of the sample. Hyperpolarisation techniques try to address this problem by displacing the system from its equilibrium position to a highly non-equilibrium state. The non-equilibrium state often displays a much stronger magnetic response than the thermal state under identical conditions. In practical applications this leads to a tremendous reduction in experimental time.

It will be the aim of this thesis to explore some properties of equilibrium and non-equilibrium systems with focus on their theoretical description. Surprisingly, the standard description of NMR experiments can lead to non-physical predictions in the case of strongly perturbed spin systems. A new approach for the treatment of highly non-equilibrium systems will be discussed in order to clarify and remedy the situation.

The complete thesis can be found at:

<https://ampere-society.org/index.php?page=andrewprize>

## PosterPrize Euromar 2020:

Kathrin Aebischer

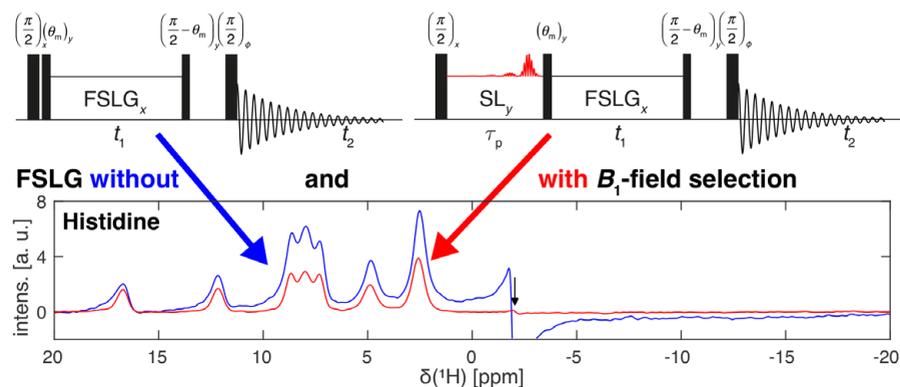
### Using $B_1$ -field selective pulses to improve FLSG-decoupled spectra.

Kathrin Aebischer<sup>1</sup>, Nino Wili<sup>1</sup>, Zdeněk Tošner<sup>2</sup>, Matthias Ernst<sup>1</sup>.

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The inhomogeneity of the radio-frequency (rf) field is a prevalent problem in solid-state NMR and one of the major contributions to the residual linewidth achieved with homonuclear decoupling sequences under magic-angle spinning (MAS)<sup>1</sup>. Experimentally, the detrimental effects of the rf inhomogeneity can be reduced by physically restricting the sample to the central part of the coil. Alternatively, sample restriction can be achieved using radio-frequency selective pulses. Such  $B_1$ -field selective pulses have been demonstrated some years ago, however, the numerically optimized rf selective pulses proposed showed many sidebands<sup>2</sup>.



Comparison of experimental FLSG decoupled proton spectra of histidine with and without  $B_1$ -field selection at a static field of 11.7 T recorded using a 1.9 mm Bruker MAS probe spinning at 14 kHz. The spectral improvements are evident. The zero-frequency peak is eliminated and narrower lines with reduced feet on the high-frequency side are obtained.

Here we present the implementation of band-selective pulses in the spin-lock frame by using a modulation of the pulses that is resonant with the spin-lock field. Thus, arbitrary nutation-frequency selective pulses can be applied to spins experiencing selected parts of the rf-field distribution. In our measurements the family of I-BURP<sup>3</sup> pulses was chosen, but in principle any band-selective pulses can be used. The implementation of these pulses is straightforward and presents a simpler and more effective alternative to spatial sample restriction. Using such  $B_1$ -field selective pulses, significant improvements in homonuclear decoupled proton spectra under MAS

using frequency-switched Lee-Goldburg decoupling were achieved. The otherwise prominent zero-frequency artefact is almost eliminated, and substantially narrower lines are obtained due to the reduction of the rf-field distribution. These spectral improvements coincide with a loss in signal intensity and a compromise between resolution and sensitivity must be found.

#### References:

- 1 J. Hellwagner, L. Grunwald, M. Ochsner, D. Zindel, B. H. Meier, M. Ernst, Origin of the residual line width under frequency-switched Lee-Goldburg decoupling in MAS solid-state NMR. *Magnetic Resonance* 1, 13-25 (2020).
- 2 P. Charmont, D. Sakellariou, L. Emsley, Sample restriction using radiofrequency field selective pulses in high-resolution solid-state NMR. *Journal of Magnetic Resonance* 154, 136-142 (2002).
- 3 H. Geen, R. Freeman, Band-selective radiofrequency pulses. *Journal of Magnetic Resonance* 93, 93-141 (1991).
- 4 K. Aebischer, N. Wili, Z. Tošner, M. Ernst, Using nutation-frequency-selective pulses to reduce radio-frequency field inhomogeneity in solid-state NMR. *Magnetic Resonance* 1, 187-195 (2020).

## PosterPrize Euromar 2020:

Arnau Bertran

### Light-induced triplet-triplet electron resonance spectroscopy.

Arnau Bertran,<sup>1</sup> Kevin B. Henbest,<sup>1</sup> Marta De Zotti,<sup>2</sup> Marina Gobbo,<sup>2</sup> Christiane R. Timmel,<sup>1</sup> Marilena Di Valentin<sup>\*2</sup> and Alice M. Bowen<sup>\*3</sup>

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The suitability of the porphyrin photoexcited triplet state for nanometre distance measurements by ESR Pulsed Dipolar Spectroscopy was demonstrated in combination with nitroxide radicals.<sup>1</sup> Thanks to its non-Boltzmann population, the photoexcited triplet enhanced signal intensity when used as detection spin in PELDOR<sup>2</sup> and improved modulation depth when used as pump spin in LaserIMD.<sup>3</sup> Here we present the new technique of Light-Induced Triplet-Triplet Electron Resonance spectroscopy (LITTER),<sup>4</sup> which uses photoexcited triplet states as both detection and pump spins (Fig. (a)), enabling both the distance and angular distributions between the two triplet moieties to be determined on a nanometre scale. This is demonstrated for a model bis-porphyrin peptide (Fig (b) inset) which renders dipolar traces with strong orientation selection effects (Fig. (c)). Using simulations and DFT calculations, we extract distance distributions (Fig. (c) inset) and relative orientations of the

porphyrin moieties, allowing the dominant conformation of the peptide in frozen solution to be identified. LITTER removes the requirement of current light-induced ESR Pulsed Dipolar Spectroscopy techniques to have a permanent paramagnetic moiety, becoming more suitable for in-cell applications and potentially giving access to distance determination in unmodified macromolecular systems containing photoexcitable moieties. LITTER also has the potential to enable direct comparison with FRET and combination with microscopy inside cells.

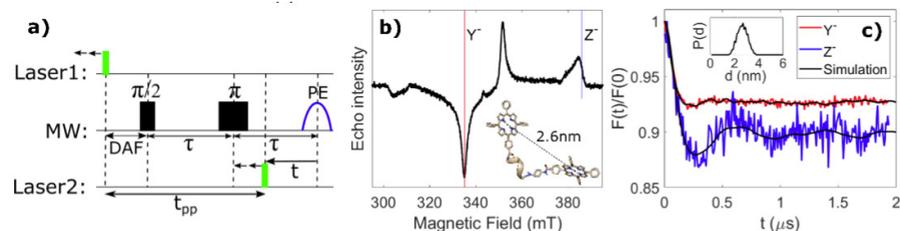


Figure. (a) Pulse sequence for LITTER. (b) Echo-detected ESR spectrum of the bis-porphyrin peptide (inset) after photoexcitation, showing the two field positions used for LITTER. (c) Background-corrected LITTER traces (red and blue) and fits (black) leading to the distance distribution (inset).

#### References:

1. M. G. Dal Farra, S. Ciuti, M. Gobbo, D. Carbonera, M. Di Valentin, Triplet-state spin labels for highly sensitive pulsed dipolar spectroscopy. *Mol. Phys.*, 117, 2673-2687 (2019).
2. M. Di Valentin, M. Albertini, E. Zurlo, M. Gobbo, D. Carbonera, Porphyrin triplet state as a potential Spin label for nanometer distance measurements by PELDOR spectroscopy. *J. Am. Chem. Soc.*, 136, 6582-6585 (2014).
3. C. Hintze, D. Bückler, S. Domingo Köhler, G. Jeschke, M. Drescher, Laser-Induced Magnetic Dipole Spectroscopy. *J. Phys. Chem. Lett.*, 7, 2204-2209 (2016).
4. A. Bertran, K. B. Henbest, M. De Zotti, M. Gobbo, C. R. Timmel, M. Di Valentin, A. M. Bowen, Light-Induced Triplet-Triplet Electron Resonance Spectroscopy. *J. Phys. Chem. Lett.* (2020) (in press).

## PosterPrize Euromar 2020:

Yuri Kutin

### Duplex-bridged unimolecular DNA G-quadruplexes: an EPR investigation.

Yury Kutin<sup>1</sup>, Lukas M. Stratmann<sup>1</sup>, Guido H. Clever<sup>1</sup>, Müge Kasanmascheff<sup>1</sup>

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G-quadruplexes (GQs) are DNA secondary structures formed by self-assembly of guanine-rich sequences via Hoogsteen base pairing stabilized by central cations. GQs form in vivo in oncogene regulatory regions and within telomeres, which makes them an interesting target for cancer research<sup>1</sup>. Various GQ species are known to assemble higher-order structures, which are believed to affect their biological activity. Thus, understanding these structures and their formation is an important goal, where the EPR spectroscopy (DEER/RIDME techniques) can make a substantial contribution.

Recently, we used rigid square planar  $\text{Cu}^{\text{II}}(\text{pyridine})_4$  complexes covalently incorporated into tetramolecular GQs as spin labels to gain insight into the GQ dimerization *via*  $\pi$ -stacking of terminal G-tetrads.<sup>2</sup> Detection of the dipole-dipole interaction between two  $\text{Cu}^{\text{II}}$  ions each residing in a GQ monomer demonstrated the dimer formation and intercalation of small molecules via an exceptionally precise measurement of Cu-Cu distances.

Oligonucleotides adopting mixed duplex/quadruplex conformations have recently gained a lot of attention<sup>3,4</sup>. In the present work we extend the EPR-based approach to novel structures representing two unimolecular GQs connected via a duplex bridge (Figure A). Two oligonucleotides were synthesized by solid-phase DNA synthesis, each containing the GQ-forming sequence AGGLTTALGGTTAGGLTTALGG with pyridine-modified nucleotides (L) capable of binding  $\text{Cu}^{\text{II}}$ . Separated by a single nucleotide spacer A, complementary single-stranded overhangs TACAGCTTAT and ATAAGCTGTA were attached to the 3' ends:

AGGLTTALGGTTAGGLTTALGGATAAGCTTAT (Oligo1),  
AGGLTTALGGTTAGGLTTALGGAATAAGCTGTA (Oligo2).

The design allowed the linking of two spin-labeled unimolecular GQs by a duplex bridge containing 10 base pairs, as evidenced by DEER (Figure B-E). The time traces yielded clear dipolar modulations. The mean Cu-Cu distance of 6.3 nm showed good agreement with the MD simulations. Our results demonstrate that the  $\text{Cu}^{\text{II}}(\text{pyridine})_4$  spin labels can be successfully applied to complex DNA structures, containing biologically relevant duplex/quadruplex junctions.

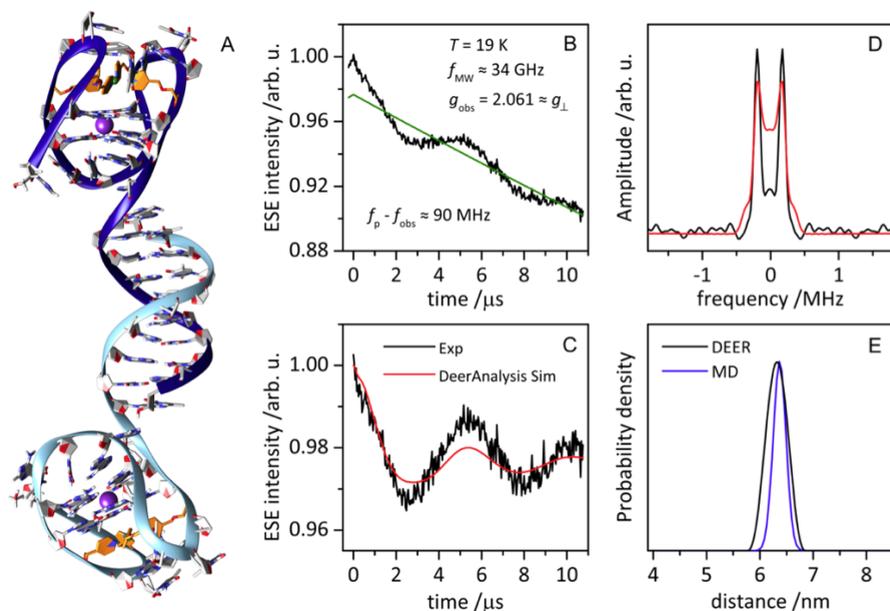


Figure. (A) MD-derived model of two duplex-bridged spin-labeled GQs; Oligos 1 and 2 are shown as the light and dark blue ribbons; K<sup>+</sup> and Cu<sup>2+</sup> ions: violet and green spheres, respectively; pyridine ligand modification: orange; (B) primary DEER trace with background; (C) form-factor and simulation; (D) dipolar spectrum; (E) DeerAnalysis-derived Cu-Cu distance distribution with the MD simulations result.

#### References:

1. D. Rhodes and H. J. Lipps, G-quadruplexes and their regulatory roles in biology. *Nucleic Acids Res.* 43, 8627–8637 (2015).
2. L. M. Stratmann et al., Precise Distance Measurements in DNA G-Quadruplex Dimers and Sandwich Complexes by Pulsed Dipolar EPR Spectroscopy. *Angew. Chem. Int. Ed.* doi.org/10.1002/anie.202008618.
3. B. Gatto et al., Nucleic Acid Aptamers Based on the G-Quadruplex Structure: Therapeutic and Diagnostic Potential. *Curr. Med. Chem.* 16, 1248–1265 (2009).
4. I. Russo Krauss et al., Different duplex/quadruplex junctions determine the properties of anti-thrombin aptamers with mixed folding. *Nucleic Acids Res.* 44, 983–991 (2016).

## PosterPrize Euromar 2020:

Lauriane Lecoq

### Solution and solid-state NMR to study viral assemblies in hepatitis B and Dengue viruses.

Lauriane Lecoq<sup>1</sup>; Marie Dujardin<sup>1</sup>; Shishan Wang<sup>1</sup>; Maarten Schledorn<sup>2</sup>; Marie Bartenschlager<sup>3</sup>; Karen Cobas<sup>4</sup>; Marie-Laure Fogeron<sup>1</sup>; Thomas Wiegand<sup>2</sup>; Gerardo Guillen<sup>4</sup>; Ralf Bartenschlager<sup>3</sup>; Lázaro Gil González<sup>4</sup>; Michael Nassal<sup>5</sup>; Beat H. Meier<sup>2</sup>; Anja Böckmann<sup>1</sup>

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We present NMR studies of two different viral ribonucleoprotein complexes, one yielding highly symmetric objects, and the other aggregates devoid of visible symmetry. We investigated the Dengue virus (DENV) and the hepatitis B virus (HBV), which both represent a threat to human lives with several hundreds of millions of new infections each year. While the nucleocapsid of HBV is formed by 240 copies of core proteins which assemble into stable and well-ordered icosahedral capsids<sup>1</sup> with the packaged genome inside, DENV (and flaviviruses in general) form less ordered ribonucleoproteins, presenting a yet unknown organization with respect to the icosahedral envelope<sup>2</sup>.

We characterized the dimeric and capsid conformational states of the two core proteins; for this we compared carbon and proton-detection solid-state NMR to solution NMR spectra. We observed that the spectra show subtle differences between isolated dimers and assembled capsids, and also that for the HBV capsid, the different asymmetric subunits can be distinguished<sup>3,4</sup>. For the DENV ribonucleoprotein, the aggregates consistently observed under the microscope in a large screen of assembly conditions surprisingly resulted in highly resolved NMR spectra indicative for a structured protein. Comparison with the <sup>13</sup>C solution-NMR chemical shifts of the DENV core protein dimers reveals the regions involved in ribonucleoprotein assembly. For both capsids, <sup>31</sup>P NMR experiments allowed to observe the respective viral RNAs.

Our work demonstrates that viral capsids can be studied by NMR whether or not they form regular-shaped objects under the electron microscope<sup>5</sup> (see Figure). When large enough quantities are available, they can be investigated with both <sup>1</sup>H- and <sup>13</sup>C-detected NMR, and <sup>13</sup>C chemical shifts are best used to compare isolated core protein and capsid conformations, since they are less sensitive to unavoidable temperature and pH variations between the samples.

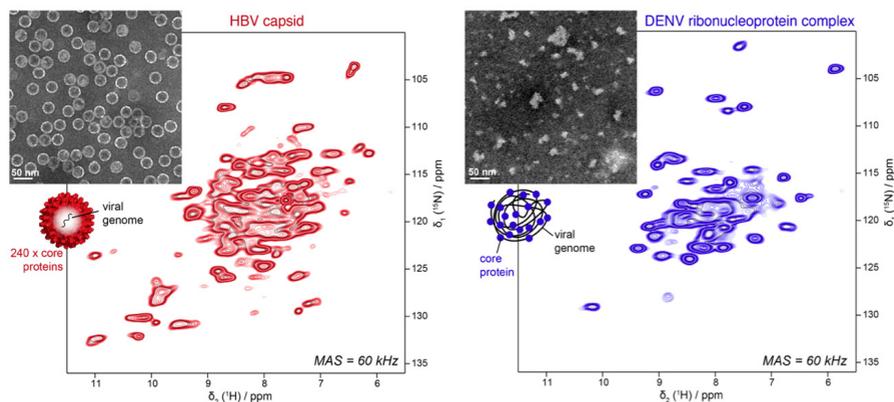


Figure: Negative-staining EM pictures of HBV capsid (left) and DENV ribonucleoprotein complex (right) and their corresponding 2D hNH spectra recorded at a MAS frequency of 60 kHz and a magnetic field of 800 MHz.

#### References:

- Wynne, S. A., Crowther, R. A., and Leslie, A. G. The crystal structure of the human hepatitis B virus capsid. *Mol. Cell* 3, 771–780 (1999).
- Kuhn, R. J., Zhang, W., Rossmann, M. G., Pletnev, S. V., Corver, J., Lenches, E., Jones, C. T., Mukhopadhyay, S., Chipman, P. R., Strauss, E. G., Baker, T. S., and Strauss, J. H. Structure of dengue virus: implications for flavivirus organization, maturation, and fusion. *Cell* 108, 717–725 (2002).
- Lecoq, L., Wang, S., Wiegand, T., Bressanelli, S., Nassal, M., Meier, B. H., and Böckmann, A. Localizing Conformational Hinges by NMR: Where Do Hepatitis B Virus Core Proteins Adapt for Capsid Assembly? *ChemPhysChem* 19, 1336–1340 (2018).
- Lecoq, L., Schledorn, M., Wang, S., Smith-Penzel, S., Malär, A. A., Callon, M., Nassal, M., Meier, B. H., and Böckmann, A. 100 kHz MAS Proton-Detected NMR Spectroscopy of Hepatitis B Virus Capsids. *Front. Mol. Biosci.* 6 (2019).
- Lecoq, L., Fogeron, M.-L., Meier, B. H., Nassal, M., and Böckmann, A. Solid-State NMR for Studying the Structure and Dynamics of Viral Assemblies. *Viruses* 12, 1069 (2020).

## PosterPrize Euromar 2020:

Maria Pia Lenza

### NMR structural characterization of the N-linked glycans in the receptor binding domain of the SARS-CoV-2 spike protein and their interactions with human lectins.

Maria Pia Lenza<sup>1</sup>; Iker Oyenarte<sup>1</sup>; Tammo Diercks<sup>1</sup>; Jon Imanol Quintana<sup>1</sup>; Ana Gimeno<sup>1</sup>; Helena Coelho<sup>2</sup>; Ana Diniz<sup>2</sup>; Francesca Peccati<sup>1</sup>; Sandra Delgado<sup>1</sup>; Oscar Millet<sup>1</sup>; Filipa Marcelo<sup>1</sup>; Gonzalo Jiménez-Osés<sup>1</sup>; Jesús Jiménez-Barbero<sup>1</sup>; June Ereño-Orbea<sup>1</sup>; Ana Arda<sup>1</sup>

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Many viral proteins are found to be glycosylated, which have important implications in viral pathology.<sup>1</sup> These N- and O-linked sugars have been shown, among others, to participate in viral attachment and to modulate immune responses. The spike protein (S) of SARS-CoV-2 contains 22 N-glycosylation sites per monomer, two of them located in the Receptor Binding Domain (RBD).<sup>2</sup>

Herein, we have produced the RBD fragment of SARS-CoV-2 in a human cell culture (HEK293F) achieving <sup>13</sup>C-labeling on the N-glycans.<sup>3</sup> This has allowed an unprecedented detailed characterization of the specific glycan structures. Additionally, <sup>1</sup>H-<sup>13</sup>C HSQC spectroscopy on the RBD was exploited as fingerprint in order to dissect the interaction of this glycosylated domain with a variety of human lectins, which are expressed in different organs and tissues that may be affected during the infection, revealing the specific glycan-epitopes responsible for each interaction.<sup>4</sup>

#### References:

- Y. Watanabe, T. A. Bowden, I. A. Wilson, M. Crispin Exploitation of glycosylation in enveloped virus pathobiology. *Biochim. Biophys. Acta - Gen. Subj.* 1863, 1480–1497 (2019).
- (a) A. Shajahan, N. T. Supekar, A. S. Gleinich, P. Azadi Deducing the N- and O- glycosylation profile of the spike protein of novel coronavirus SARS-CoV-2, *Glycobiology*, 1-20 (2020). (b) Y. Watanabe, J. D. Allen, D. Wrapp, J. S. McLellan, M. Crispin Site-specific glycan analysis of the SARS-CoV-2 spike, *Science*, 369, 330–333 (2020).
- A.W. Barb, D. J. Falconer, G. P. Subedi, *Methods in Enzymology*, Academic Press, New York, 2019, 239–261.
- Lenza, M.P., Oyenarte, I., Diercks, T., Quintana, J.I., Gimeno, A., Coelho, H., Diniz, A., Peccati, F., Delgado, S., Bosch, A., Valle, M., Millet, O., Abrescia, N.G.A., Palazón, A., Marcelo, F., Jiménez-Osés, G., Jiménez-Barbero, J., Ardá, A. and Ereño-Orbea, J. Structural Characterization of N-Linked Glycans in the Receptor Binding Domain of the SARS-CoV-2 Spike Protein and their Interactions with Human Lectins, *Angew. Chem. Int. Ed.* (2020) doi:10.1002/anie.202011015.

## PosterPrize Euromar 2020:

Manon Julien

### Monitoring phosphorylations in the disordered region of BRCA2 and identifying their impact on binding to partners.

Manon Julien<sup>1,3</sup>; Simona Miron<sup>1,3</sup>; Asa Elhen<sup>2,3</sup>; Aura Carreira<sup>2,3</sup>; François-Xavier Theillet<sup>1,3</sup>;

Sophie Zinn-Justin<sup>1,3</sup>

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3. Paris Sud University, Paris-Saclay University, France

BRCA2 is an oncoprotein frequently mutated in hereditary breast cancers. BRCA2 is involved in genomic stability pathways such as DNA repair and chromosome segregation. A dysfunction of this protein increases the cancer risk. To improve the diagnosis of these cancers, several molecular studies identified key positions and associated mutations causing a loss of function of BRCA2. However, these studies mainly focused on the C-terminal globular domain of BRCA2.

Here, we characterized the N-terminal region of BRCA2 from aa 48 to aa 284 (BRCA2<sub>48-284</sub>). This well-conserved region from mammals to fishes is disordered, i.e. it lacks stable secondary structure<sup>1</sup>. It is also highly phosphorylated by the kinase Plk1 at the entry into mitosis. However, previous studies using mass spectrometry didn't allow to precisely identify all the phosphorylation sites.

We established real-time NMR protocols to monitor *in vitro* phosphorylation of BRCA2<sub>48-284</sub><sup>2,3</sup>. We identified that Plk1 phosphorylates BRCA2 at 4 positions, including the 2 highly conserved S193 and T207. From this result, we searched for the functions of phosphorylated S193 (pS193) and T207 (pT207) in mitosis.

First, we identified that pT207 creates a docking site for Plk1 on BRCA2. In collaboration with the group of Dr. Aura Carreira, we showed that this interaction triggers the assembly of a quaternary complex involving BRCA2, Plk1, BubR1 and PP2A at the kinetochore, and contributes to the alignment of chromosomes at the metaphase plate<sup>4</sup>. We also demonstrated that breast cancer variants impact the phosphorylation of BRCA2 and the formation of the complex.

Second, we initiated proteomics experiments to identify new partners specific to phospho- BRCA2<sub>48-284</sub> and found Plk1 as well as other proteins involved in mitosis.

#### References:

1 Julien M, Miron S, Carreira A, Theillet FX, Zinn-Justin S. 1H, 13C and 15N backbone resonance assignment of the human BRCA2 N-terminal region. *Biomol NMR Assign.* 2020 Apr;14(1):79-85.

2 Julien M, Bouguechtouli C, Alik A, Ghouil R, Zinn-Justin S, Theillet FX. Multiple Site-Specific Phosphorylation of IDPs Monitored by NMR. *Methods Mol Biol.* 2020;2141:793-817.

3 Alik A\*, Bouguechtouli C\*, Julien M\*, Bermel W, Ghouil R, Zinn-Justin S, Theillet FX. Sensitivity-Enhanced 13 C-NMR Spectroscopy for Monitoring Multisite Phosphorylation at Physiological Temperature and pH. *Angew Chem Int Ed Engl.* 2020 Jun 22;59(26):10411-10415.

4 Ehlen A, Martin C\*, Miron S\*, Julien M\*, Theillet FX, Ropars V, Sessa G, Beaupere R, Boucherit V, Duchambon P, El Marjou A, Zinn-Justin S, Carreira A. Proper chromosome alignment depends on BRCA2 phosphorylation by PLK1. *Nat Commun.* 2020 Apr 14;11(1):1819.

\* co-authors

## PosterPrize Euromar 2020:

Andreas Meyer

### High field <sup>19</sup>F-ENDOR for distance measurements in the angstrom to nanometer regime in structural biology.

Andreas Meyer<sup>1</sup>; Annemarie Kehl<sup>1</sup>; and Marina Bennati<sup>1,2</sup>.

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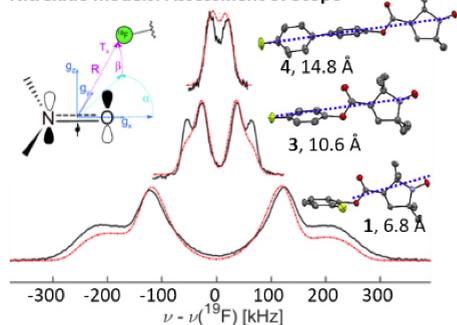
EPR spectroscopy is a powerful method for structural investigations in biomolecular systems that contain unpaired electron spins. The interaction of these unpaired spins with other electron spins can be probed selectively using pulsed dipolar spectroscopy (PELDOR, DQC, etc...) for inter-spin distances of 15 – 100 Å,<sup>1</sup> whereas hyperfine spectroscopy (ENDOR, ESEEM, etc...) addresses electron-nuclear spin interactions at distances usually  $\leq 5 - 7$  Å.<sup>2</sup> This restriction to relatively low distances in hyperfine spectroscopy is caused by the low gyromagnetic ratio  $\gamma$  of nuclear spins (<sup>2</sup>H, <sup>13</sup>C, <sup>14</sup>N, ...) or by spectral crowding in the case of <sup>1</sup>H nuclei, which are ubiquitous in biosystems.

This work presents pulsed W-band (94 GHz/3.4 T) <sup>19</sup>F-ENDOR as a tool for structural biology. The method benefits from the high gyromagnetic ratio of <sup>19</sup>F, which is only ~6% lower than that of protons. This property allows the <sup>19</sup>F resonances to be addressed selectively and with high sensitivity at distance ranges clearly exceeding 5 Å. Since fluorine labeling strategies have already been established in other areas of research,<sup>3</sup> W-band <sup>19</sup>F-ENDOR has great potential for application in biochemical contexts.

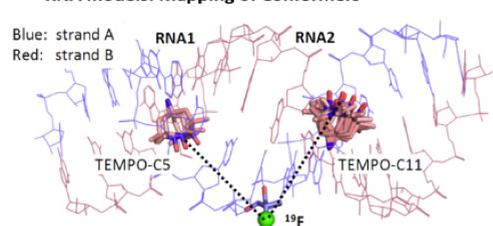
Using a series of small nitroxide model compounds we found that information about the <sup>19</sup>F – electron spin distance at atomic resolution can be obtained up to 15 Å.<sup>4</sup>

To demonstrate the applicability of the method in a biochemical context, we investigated <sup>19</sup>F- and nitroxide-labelled RNA molecules using <sup>19</sup>F-ENDOR<sup>4</sup> and were able to refine a previous structural model.<sup>5</sup> As another biochemical example, preliminary results on the <sup>19</sup>F-labelled protein ribonucleotide reductase are presented, where the method enables investigating the proton coupled electron transfer in a natural radical transfer chain. Finally, opportunities of employing higher magnetic fields (9.5 T) are discussed.

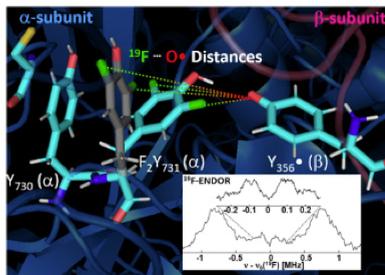
### Nitroxide models: Assessment of Scope



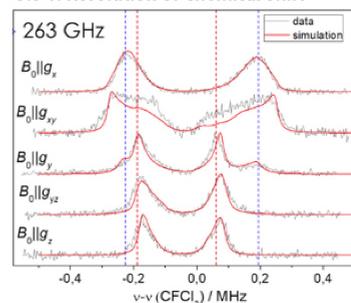
### RNA models: Mapping of Conformers



### Ribonucleotide Reductase: Radical Transfer



### 9.5 T: Resolution of Chemical Shift



### References:

1. G. Jeschke, The Contribution of Modern EPR to Structural Biology. *Emerg. Top. Life Sci.* 2, 9–18 (2018).
2. G. E. Cutsail III, J. Telser, B. M. Hoffman, Advanced Paramagnetic Resonance Spectroscopies of Iron-Sulfur Proteins: Electron Nuclear Double Resonance (ENDOR) and Electron Spin Echo Envelope Modulation (ESEEM). *Biochim. Biophys. Acta BBA-Mol. Cell Res.* 1853, 1370–1394 (2015).
3. H. Chen, S. Viel, F. Ziarelli, L. Peng,  $^{19}\text{F}$  NMR: A Valuable Tool for Studying Biological Events. *Chem. Soc. Rev.* 42, 7971–7982 (2013).
4. A. Meyer, S. Dechert, S. Dey, C. Höbartner, M. Bennati, Measurement of Angstrom to Nanometer Molecular Distances with  $^{19}\text{F}$  Nuclear Spins by EPR/ENDOR Spectroscopy. *Angew. Chem. Int. Ed.* 59, 373–379 (2020).
5. K. Halbmaier, J. Seikowski, I. Tkach, C. Höbartner, D. Sezer, M. Bennati, High-Resolution Measurement of Long-Range Distances in RNA: Pulse EPR Spectroscopy with TEMPO-Labeled Nucleotides. *Chem. Sci.* 7, 3172–3180 (2016).

## Obituary:

### Professor Dieter Michel (1940 – 2020)



It is with great sadness that the AMPERE community received a message that Professor Dieter Michel from University of Leipzig had died unexpectedly on December 28, 2020. He was an eminent German physicist and widely recognized colleague in the international NMR scientific community and also, a very dear friend of the AMPERE Groupement Society.

Dieter Michel was born on March 17, 1940. He studied Physics at the University of Leipzig. His academic career was associated with this University. His research was mainly conducted in the Department of Physics led by two outstanding German physicists, namely Professor Artur Loesche and Professor Harry Pfeiffer. Under the supervision of Professor Pfeiffer, Dieter Michel received a diploma in Physics in 1964, and four years later in 1968, a doctorate in Physics in the area of NMR. He is known for having developed the systematic NMR relaxation analysis method to study the molecular dynamics of adsorbed molecules. In 1973, while working with Professor Pfeiffer's group, he received a habilitation in experimental physics. Together with Dieter Geschke, he applied high-resolution  $^{13}\text{C}$  nuclear magnetic resonance spectroscopy to adsorbed molecules for the first time. Most of his papers in the mid 1980's were related to studies of adsorbed molecules on surfaces using NMR. He applied NMR relaxation in studies of ionic solutions and molecules adsorbed on surfaces of highly porous solid materials, particularly zeolites. He was also very active in Professor Pfeiffer's Group in dealing with NMR multiple-pulse techniques in solids, with high-resolution solid-state NMR spectroscopy, and with NMR self-diffusion studies. Later on, his research was focused on the investigations of phase transitions in solids by NMR, ESR, dielectric and related methods, including the issues of critical phenomena at phase transitions of systems with incommensurable phases. This research has been successfully conducted in collaboration with Jörg Petersson from Saarland University.

It is worth mentioning a book published by Dieter Michel on Basics and Methods of NMR in 1981 ("Grundlagen und Methoden der kernmagnetischen Resonanz", Wissenschaftliche Taschenbücher, 1981) - "a small red book" - as international students used to call it due to its red cover. The book was very clearly written and widely used by many students and colleagues as a reference when presenting the background of high-resolution NMR in solids.

After the reunification of Germany in 1990, Dieter Michel was appointed in 1992 full professor for experimental physics at the University of Leipzig, serving also to his University in various positions, including the functions of deputy director for research in the physics section, deputy head of the department of physics, Dean and Vice -Dean of the Faculty of Physics and Earth Sciences, and until his retirement in 2005 he worked as the head of the Physics of Dielectric Solids Department at the current Felix Bloch Institute for Solid State Physics. In 1997, Dieter Michel was elected full member of the Saxon Academy of Sciences in Leipzig and worked there as deputy secretary and secretary of the mathematics and natural sciences class. The State University of St. Petersburg awarded him the title of honorary professor in 2001. Dieter Michel was very much involved in the Groupement AMPERE activities, as a member of the AMPERE Committee and as a lecturer at various AMPERE meetings, including RAMIS Conferences in Poznań organized by Jan Stankowski, NMR Summer Schools in Zakopane managed from 90th to 2005 by Jerzy Blicharski and since 2006 by myself, SPINUS NMR Conferences in Sankt Petersburg organized by Vladimir Chizhik. From the mid-1990's until 2019 he was a permanent lecturer of the Zakopane NMR Schools. His lectures attracted large groups of students, doctoral candidates and colleagues. He always answered questions and remarks with patience, personal culture and with great respect to his interlocutors. During the Zakopane Schools, he also gave organ concerts for participants, guests and residents of Zakopane in the local church. It has always been a great artistic event for attendees of the School and we looked forward to it every year. We will miss his lectures and concerts very much.

He made a significant contribution to building mental, cultural and scientific bridges between earlier divided Western and Eastern Europe. He was not only an outstanding physicist but also a scientist who did a lot for the German-Polish reconciliation. He understood the political division in Europe after the end of World War II. As a Protestant Christian, he was able to build trust and understanding between Poles and Germans. The Polish NMR community is very grateful to him for his friendly relations with our nation.

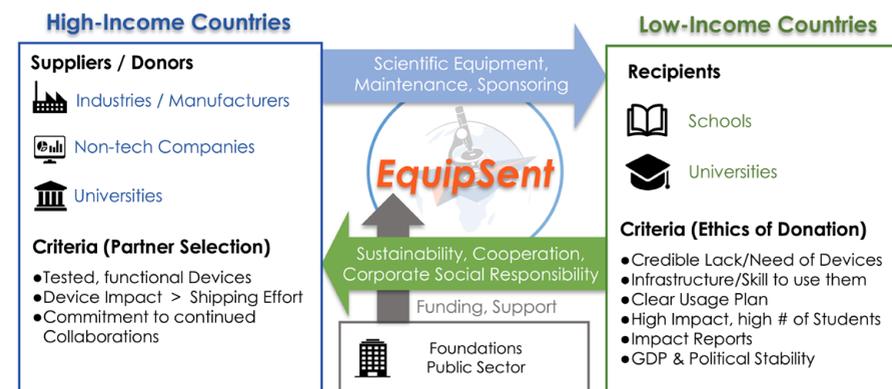
We say goodbye to an outstanding scientist, our dear friend, whose great personality radiated internationally, a man full of simplicity, warmth and hospitality, a man who set an example of being a good man, a good scientist and artist, a man of great culture and dignity. RIP.

Stefan Jurga

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## Future conferences

### Ampere Event 2021

Ampere Biological Solid-State NMR School	Part 1, online	January 14 to May 7
18 <sup>th</sup> International Youth School-Conference „Magnetic resonance and its applications - Spinus-2021“	online St. Petersburg (Russia)	March 29 to April 2
Ampere Biological Solid-State NMR School	Part 2, Berlin (Germany)	June 14-18
Ampere NMR School 2021	Poznań (Poland)	June 20-26
Euromar 2021	Protorož (Slovenia)	July 4-8
16 <sup>th</sup> ICMRM	Malmö (Sweden)	August 1-5
HYP20 + Dissolution and MAS DNP hands-on training at CMRN	Lyon (France)	September 5-9
Alpine Conference on Magnetic Resonance in Solids	Chamonix (France)	September 12-16

### Non Ampere Event 2021

V International School for Young Scientists, Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics	Roshchino, St. Petersburg (Russia)	Fall 2021
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### Ampere Event 2022

MR FOOD 2022	Aarhus (Denmark)	June
Euromar 2022	Utrecht (Netherlands)	July 3-7
Magnetic Resonance in Porous Media	Hangzhou (China)	August

### Ampere Event 2024

HYP24	Leipzig (Germany)	September
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# 70 years



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