Vol. 70, No. 4

ISSN 0432-7136

BULLETIN DU GROUPEMENT

d‘informations mutuelles

Groupement
AMPERE

SE CONNAÎTRE, S‘ENTENDRE, S‘ENTRAIDER

October to December 2021

No. 285

Office: ETH Zürich, Laboratory of Physical Chemistry
8093 Zürich, Switzerland, www.ampere-society.org

Contents

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

Editorial

Dear members of the Groupement AMPERE,

every year the Groupement AMPERE sponsors prizes at the EUROMAR. The **Raymond Andrew Prize** is awarded annually for an outstanding PhD thesis in magnetic resonance. The **AMPERE Prize for Young Investigators** is awarded biannually (odd years, alternating with the Russel Varian Prize) to an early-career independent researcher (less than 10 years after his/her PhD). These prizes are an important part of the opening session of EUROMAR. I would like to encourage you to propose outstanding candidates for these prizes. At EUROMAR 2022 in Utrecht only the Raymond Andrew Prize but at EUROMAR 2023 in Glasgow again both prizes will be awarded. Please help us to find the best candidates for these prizes. The details for submitting proposals can be found on page 4 of this Bulletin or on our website.

As you can see from the reports on various schools and conferences published in this issue, the first in-person AMPERE conference happened this fall. The HYP21 was a big success and I would like to thank all the people involved in the organization. They took a big risk but it paid off judging from the comments I heard from many participants. Let's hope that 2022 will allow us again more in-person conferences.

Best regards and best wishes for the holiday season and for a successful start of the upcoming year 2022,

Matthias Ernst

Matthias Ernst
Secretary General, Groupement AMPERE

Portrait:
Prof. John van Duynhoven

Why magnetic resonance and why NMR and MRI?
The versatility of magnetic resonance in solving problems in chemistry and physics still amazes me. Whether you are dealing with research questions in supramolecular chemistry, biomolecular structures or food science, magnetic resonance always appears to be a powerful tool.

What is your favorite frequency?
Half of my PhD period I was anticipating the arrival of a 600 MHz NMR spectrometer, by then the highest achievable field strength for NMR. Once the spectrometer arrived it was cool to finally see what could not be seen before. After my PhD I learned to appreciate 20 MHz, which is a cool frequency since it can be generated by permanent magnets which allows to bring many practical industrial applications close to non-NMR experts.

What do you still not understand?
How to make use of susceptibility broadening in porous materials.

Luckiest experiment you have ever done.
Without too many expectations we ran some ^{1}H NMR spectra of urine of tea drinkers. It triggered research that culminated in a PNAS paper on tea drinker phenotypes.

What was the worst mistake you have made during your lab time?
As a PhD student I lifted a nitrogen dewar for refilling during a midnight session from a magnetic cart nearby a 500 MHz magnet. I got hold of the dewar but the cart took off, damaged the probehead and then fell down. I missed a few heartbeats and the next morning bravely ran the gauntlet when I went back to the lab.

Most memorable conference story.
At the MRFOOD1998 (Norwich) conference I understood foods are not too complex for NMR, and complex enough to spend a lifetime career

With whom (historical person) would you like to meet?
My father, who died too young.

When do you get your best ideas?
During boring meetings or lectures (boring or not) that are out of my field.

If you had just one month time for travelling - where would you go to?
Revisiting the Surinam jungle. Previous visits with my family were unforgettable.

Your idea of happiness.
Peace, with others and yourself.

Interests:
hiking, history, construction and deconstruction.

Position:
Senior scientist at Unilever, part-time professor at Wageningen University.

Awards:
Company awards, unknown to the public word.

Homepage:
https://www.wur.nl

Education:
PhD in Biophysical Chemistry at Radboud University, Nijmegen, The Netherlands

Call for nominations
Raymond Andrew Prize 2022

In memory of Professor Dr. Raymond Andrew and to honor his pioneering work in the field of magnetic resonance, the AMPERE Group has founded the Raymond Andrew Prize. The prize is awarded to young scientists for an outstanding PhD thesis in magnetic resonance.
For the Raymond Andrew Prize 2022 the AMPERE Prize Committee is seeking your help in searching for qualified candidates who completed their dissertation during the period of 2020/2021.

The prize will be presented during EUROMAR in Utrecht, the Netherlands,
July 10-14, 2022.

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

Nominations must be received by 15th February 2022 and should include the following documents:

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

The thesis should be written in English. In exceptional cases, the thesis may also be submitted in triplicate as a hardcopy to the AMPERE Secretariat.

Submissions that arrive too late will automatically be transferred to the next year. The prize committee will reconsider excellent contributions for two years in a row.

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

Report:
AMPERE NMR School 2021, virtual event

Scientific Committee:
Bernhard Blümich (Aachen), Germany, Janez Dolinšek (Ljubljana), Slovenia, Stefan Jurga (Poznan), Poland, Wiktor Koźmiński (Warszawa), Poland, Danuta Kruk (Olsztyn), Poland, David Lurie (Aberdeen), UK, Alex MacKay (Vancouver), Canada, Beat Meier (Zurich), Switzerland

Organizing Committee:
Stefan Jurga – Chair
Lidia Szutkowska – Executive Secretary, Dorota Flak, Patryk Florczak, Bartosz Grześowiak, Marcin Jarek, Mariusz Jancelewicz, Jacek Jenczyk, Bartosz Kawczyński, Grzegorz Nowaczyk, Roksana Markiewicz, Kosma Szutkowski, Anna Woźniak, Tomasz Zalewski, Karol Załęski.

The AMPERE NMR School was held virtually from June 21-23, 2021.

The School had **250 registered participants from 30 countries:** Argentina, Australia, Brazil, Bulgaria, Canada, Czech Republic,China, Estonia, Finland, France, Germany, India, Israel, Italy, Luxembourg, Mexico, Lithuania, Netherlands, Poland, Portugal, Romania, Russia, Singapore, Slovenia, Spain, Sweden, Switzerland, Saudi Arabia, Turkey, United Kingdom, United States.
The conference was organized by the NanoBioMedical Centre, and the Centre for European Integration of the Adam Mickiewicz University in Poznan, under the auspices of the Groupement AMPERE. It was focused on the basic and advanced NMR techniques and attracted young and experienced scientists from across the world, who had the opportunity to exchange knowledge and ideas on recent NMR and related research, to learn about new techniques and developments in this field and to establish new contacts and collaborations.

The programme of the School covered the following 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 t4echnical aspects of NMR. In total it consisted of **24 lectures**, given by:

Esteban Anoardo National University of Cordoba, Argentina
Field-Cycling MRI relaxometry

Bernhard Blümich RWTH Aachen University, Aachen, Germany
Molecular Dynamics in NMR for Materials Testing: Relaxation, Exchange and MRI

Michał Bielejewski Polish Academy of Sciences, Poznań, Poland
The kinetics of proton transport and thermal processes in anhydrous nanocomposite ptoton conductor based on cellulose

Anja Böckmann Institute of Biology and Chemistry of Proteins, IBCP, Lyon, France
Protein structure determination

Vladimir Chizhik Saint Petersburg State University
Conformational and aggregation behavior of some surfactants in aqueous solutions by 1H and 13C NMR

Anton Duchowny RWTH Aachen University
NMR Studies of Complex Samples Using Compact Instruments

Janez Dolinšek Jožef Stefan Institute, University of Ljubljana, Slovenia
High-entropy alloys

Matthias Ernst ETH Zürich, Switzerland
Residual Line Width in MAS Solid-State NMR

Fabien Ferrage CNRS and Ecole Normale Supérieure, PSL University, Paris, France
Exploring scalar couplings and chemical exchange from low to ultra-high fields

Wiktor Koźmiński University of Warsaw, Warsaw, Poland
High dimensionality and high resolution NMR experiments for biomolecules

Julia Krug Laboratory of BioNanoTechnology and Biophysics, Nijmegen, Nederland
The higher, the better?! The promises and perks of ultra-high field MRI at 22.3 T

Danuta Kruk University of Warmia & Mazury, Olsztyn, Poland
Molecular dynamics by means of NMR relaxometry

Ilya Kuprov University of Southampton, Southampton, United Kingdom
Why are some nuclei non-spherical and what does that have to do with spin?

Olivier Lafon ENSCL University of Lille, France
Solid-state NMR of quadrupolar nuclei and their neighbors

David Lurie University of Aberdeen, Scotland, United Kingdom
Basic Physics of MRI and Research on Fast Field-Cycling MRI

Alex MacKay University of British Columbia, Vancouver, Canada
Are Relaxation Times Useful in Medicine?

Beat Meier ETH Zürich, Switzerland
Fast MAS and Biomolecules

Kay Saalwaechter Institute of Physics, Faculty of Natural Sciences II, Halle/Saale,
Proton low-field NMR for the study of (bio)macromolecular dynamics or: understanding 1H T2

Claudia Schmidt Department Chemie, Universität Paderborn, Germany
NMR studies of polymer gel electrolytes

Siegfried Stapf Technische Universitat Ilmenau, Germany
What can go wrong with relaxation experiments ?

Janez Stepišnik University of Ljubljana, Slovenia
Insight into the details of molecular translation dynamics in liquids by NMR gradient spin echo meth

Ville-Veikko Telkki University of Oulu, Oulu, Finland
Ultrafast multidimensional relaxation and diffusion measurements

Daniel Topgaard Lund University, Lund, Sweden
Diffusion-relaxation correlation MRI

Jadwiga Tritt-Goc Polish Academy of Sciences, Poznań, Poland
NMR studies of solid cellulose-based proton conductors

All participants were given the opportunity to present their research in a poster session (virtual meeting through Zoom) which consisted of 49 presentations. The prizes were awarded to the authors of the **three best posters:**

First place:
Rita Alves
Champalimaud Centre for the Unknown, Lisbon, PT for the poster entitled:
Unraveling the Underlying Sources of Diffusion Kurtosis in Focal Ischemia by Correlation Tensor MRI

Second place:
Marzola Coronel MB
Laboratorio de Relaxometría y Técnicas Especiales (LaRTE) FaMAF, Universidad Nacional de Córdoba, Argentina for the poster entitled:

Characterization of Dynamic Regimes and Membrane Elasticitiy of Flexible Liopsomes using Fast-Fieldcycling.

Third place:
Jing Li
Fibre and Particle Engineering Research Unit, Faculty of Technology, bNMR Research Unit, Faculty of Science, University of Oulu, Finland, for the poster entitled:
Pore Structures and Connectivity of Metakaolin-Based Geopoymers Detected by ^{129}Xe NMR Methods.

A "Special Award" for exceptional activity during this year's conference for:
Anton Duchowny
Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, Germany, the author of 3 posters and one oral presentation.

The posters were evaluated by the members of the Poster Committee. All the winners received prizes (partial conference fee waiver in 2022).

The winner of a special award is to deliver an oral presentation at the next School as an invited speaker.

All abstracts of the oral presentations, tutorials and posters were published as printed proceedings (book of abstracts).
All the additional information about the AMPERE NMR School are presented at the website: school.amu.edu.pl or Twitter account: @AmpereNMR.

The next edition of the School will be held in Zakopane (Poland) from June 19-25, 2022.

First Poster Prize, AMPERE NMR School 2021
Rita Alves

Unraveling the Underlying Sources of Diffusion Kurtosis in Focal Ischemia by Correlation Tensor MRI.

Rita Alves[a], Rafael Neto Henriques[a], Leevi Kerkelä[b], Cristina Chavarrías[a], Sune Nørhøj Jespersen[c,] Noam Shemesh[a]
a: Champalimaud Research, Champalimaud Centre for the Unknown, Lisbon, PT.
b: UCL Great Ormond Street Institute of Child Health, University College London, London, UK.
c: Center of Functionally Integrative Neuroscience and MINDLab, Clinical Institute, Aarhus University, Aarhus, DK.
d: Department of Physics and Astronomy, Aarhus University, Aarhus, DK.

Stroke is a leading cause of long-term disability and death worldwide [1]. Resolving infarct core from penumbra with specificity and assessing or predicting functional recovery are important goals for contemporary neuroimaging. Here, we harness Correlation tensor MRI (CTI) [2] – a method capable of resolving the sources of non-Gaussian diffusion (kurtosis) by extraction of unique tensors arising from the cumulant expansion of double diffusion encoding (DDE) signals – to enhance specificity and improve acute ischemic lesions characterization.

A photothrombotic stroke was induced in mice, followed by brain extraction after 3h. A sham group underwent identical procedures except for the lesion-inducing illumination. Diffusion MRI data were acquired on a 16.4 T Bruker Aeon (*ex-vivo*) and on a 9.4 T Bruker Biospec (*in-vivo*). DDE experiments were repeated for different gradient magnitude and direction combinations following the CTI methodology described by Henriques et al. [3], which enables breaking down the total excess kurtosis to its underlying sources.

Our CTI experiments (Fig.1) revealed that microscopic kurtosis (μK) substantially contributes to the total kurtosis excess (K_T), and that anisotropic kurtosis (K_{aniso}) decreases substantially, consistent with predictions for neurite beading [5,6]. Edema was relatively small as evidenced by isotropic kurtosis (K_{iso}). CTI also enhanced the sensitivity towards stroke detection: when comparing the post-stroke and control groups: K_T and μK revealed mean values for both GM and WM with significant differences; Kiso presented significant differences within WM regions; Kaniso differences were shown to be significant between GM regions (p-value < 0.05) (Fig.2). μK was found to be the most sensitive source to ischemic tissue.

We demonstrated CTI's ability to resolve non-Gaussian diffusion sources without prior microstructural assumptions. Such characterizations are pivotal in resolving the long-standing debate on the origins of diffusion sensitivity to acute stroke lesions [4-5]. Future studies will aim to resolve the ischemic core and penumbra using CTI metrics. The CTI-driven local changes in anisotropy [2], diffusivity distributions, and increases in structural disorder and restriction (or exchange) are promising for enhancing microstructural specificity post-ischemia, which bodes well for novel characterizations and treatment efficacy.

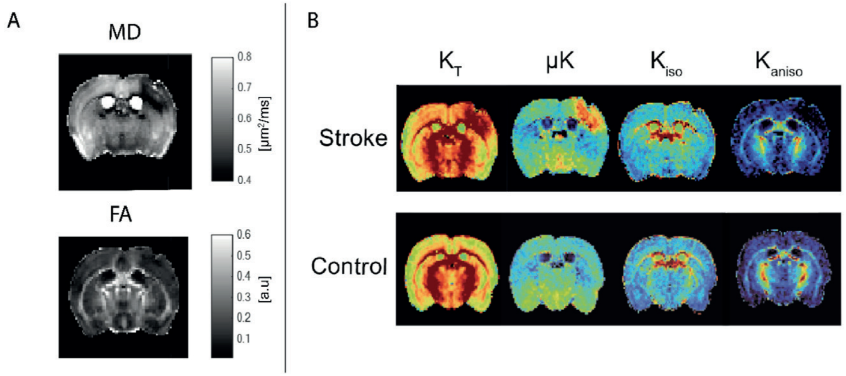


Figure 1. *ex-vivo* (A) conventional Mean Diffusivity (MD), Fractional Anisotropy (FA) and (**B**) CTI kurtosis measures for a representative slice of brain specimens from the 3h post-stroke and control animal groups. Panels show the total kurtosis (K_T), microscopic kurtosis (µK), isotropic kurtosis (K_{iso}) and anisotropic kurtosis (K_{aniso}). In the ischemic group, the ipsilesional hemisphere shows higher K_T intensity values in gray matter (GM) and a clear distinction between hemispheres is observed in µK values, showing greater intensities in both white matter (WM) and GM. K_{aniso} presents lower values in WM and GM within the ipsilesional hemisphere when compared to the contralesional hemisphere.

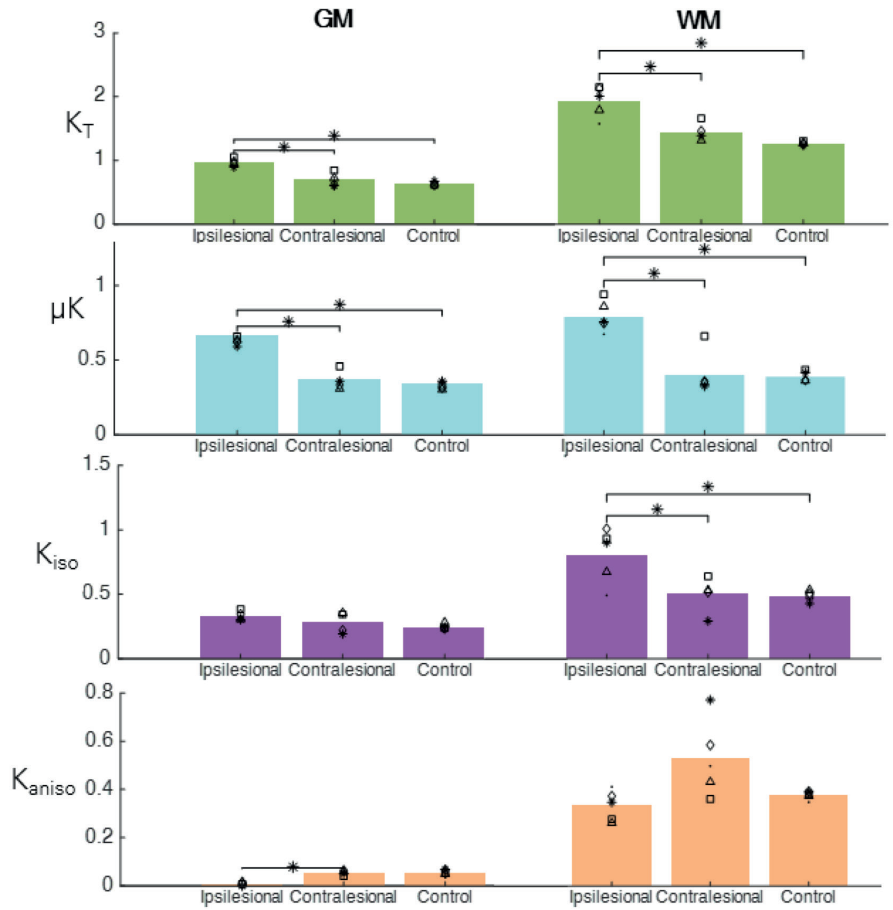


Figure 2. Specificity analysis after ANOVA (multiple comparisons) across different regions of interest (GM and WM). Different kurtosis sources are plotted along rows and each plot contains the respective kurtosis source measure for the ipsilesional hemisphere, contralesional hemisphere and counter control animal group ipsilateral hemisphere, consecutively. Each column refers to only GM and only WM, respectively ($p < 0.05$).

References
[1] Thrift et al, Global stroke statistics. Int. J. Stroke,12 (2017), 13–32/1;
[2] Henriques et al, Neuroimage, 211 (2020),116605;
[3] Henriques et al, Magnetic Resonance in Medicine, 00 (2021), 1–20;
[4] Moseley et al, Magnetic Resonance in Medicine, 14 (1990), 330–346/2;
[5] Budde et al, PNAS, 107 (2010), pp. 14472–14477/32
[6] Skinner et al, NMR in Biomedicine, 28 (2015), 1489–1506;

Acknowledgments
This study was funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Starting Grant, agreement No. 679058). We acknowledge the vivarium of the Champalimaud Centre for the Unknown, a facility of CONGENTO financed by Lisboa Regional Operational Programme (Lisboa 2020), project LISBOA01-0145-FEDER-022170.

Second Poster Prize, AMPERE NMR School 2021

Marzola Coronel MB

Characterization of Dynamic Regimes and Membrane Elasticitiy of Flexible Liopsomes using Fast-Fieldcycling.

Marzola Coronel MB[a], Fraenza CC[b] and Anoardo Ea[b].
a: Laboratorio de Relaxometría y Técnicas Especiales (LaRTE).
FaMAF, Universidad Nacional de Córdoba, Ciudad Universitaria X5000HUA, Córdoba, Argentina.
b: IFEG – CONICET, Ciudad Universitaria X5000HUA, Córdoba, Argentina.

At present, the development of nanometric vesicles for drug delivery in the human body by different routes has become of great interest for academic and industrial research groups. Flexible liposomes have proved to be useful for transdermal transport, therefore it is important to understand the underplaying mechanisms associated to the molecular dynamics, that influence the membrane elasticity.

In previous works [1-5], a model was presented to interpret the spin-lattice relaxation rate dispersion of protons, obtained with the fast field cycling nuclear magnetic relaxometry technique (FFC), for unilamellar liposomes (Fig. 1). In addition to providing general information on the lipid dynamics, this model allows us to infer about the elastic properties of the liposomes by means of the elastic constant κ, which is one of the physical parameters involved in the model. This model has been validated from measurements of κ for cholesterol doped vesicles and for surfactant doped vesicles, in order to increase or decrease the value of the constant respectively.

In order to study the influence of the temperature and the surfactant's characteristics in the behavior of the molecular parameters in flexible liposomes, experiments using elastic vesicles were performed in this work. Specifically, we analyzed experimental relaxation dispersions obtained at four different temperatures (291-328K) for liposomes of radius of 50nm, composed of SPC (soy phosphatidylcholine) with four different detergents added to modulate the membrane flexibility, at concentrations up to 20%mol.

For the lowest temperature the elastic modulus of the membrane decreases with the addition of surfactant, as expected. Also, after a correlation analysis, a great influence of some properties of the surfactant on specific physical parameters of the system was found. In addition comparing with previous works [4; 5], a different dynamical properties a molecular level have been observed depending on the purity of the used lipids. Finally, a deeper analysis about how the relationship between the elastic constant and the diffusion constant of the membrane can describe changes in the deformability performance of a liposome formulation was made (Fig. 2).

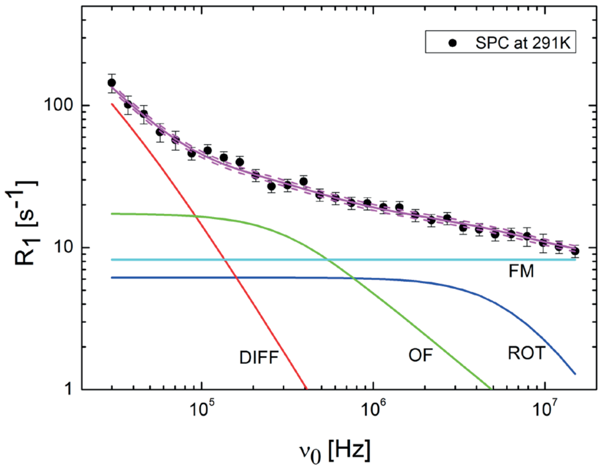


Figure 1:
Relaxation rate dispersion of SP C liposomes with average radius of 50nm, recorded at 291K. Experimental points (•) are compared with the optimal model curve (magenta solid line). Contributions from each type of motion are included: traslational diffusion (red solid line), order fluctuations (green solid line), molecular rotations (blue solid line), and fast motions (cian solid line).

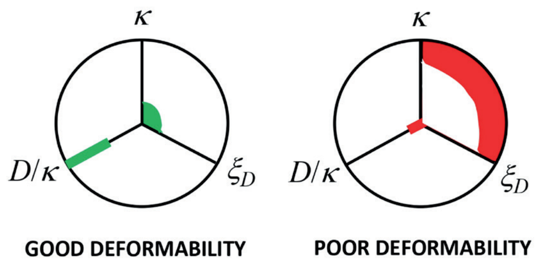


Figure 2: Deformability performance maps for a formulation according to the values of the involved relevant physical quantities. Values increase outward from the center of the circle.

References
[1] C. J. Meledandri, J. Perlo, E. Farrher, D. F. Brougham, E. Anoardo. J. Phys. Chem. B 113: 15532-15540, 2009.
[2] J. Perlo, C. J. Meledandri, E. Anoardo, D. F. Brougham. J. Phys. Chem. B 115: 3444-3451, 2011.
[3] C. C. Fraenza, C. J. Meledandri, E. Anoardo, D. F. Brougham. ChemPhysChem 15: 425-435, 2014.
[4] G. A. Domingez, J. Perlo, C. C. Fraenza and E. Anoardo. Chem. Phys. Lipids 201: 21-27, 2016.

Third Poster Prize, AMPERE NMR School 2021
Jing Li

Pore Structures and Connectivity of Metakaolin-Based Geopoymers Detected by ^{129}Xe NMR Methods.

Jing Li[b], Sarah Mailhiot[b], Harisankar Sreenivasan[a], Anu M. Kantola[b], Ville- Veikko Telkki[b] and Paivo Kinnunen[a].
a: Fibre and Particle Engineering Research Unit, Faculty of Technology, P.O.Box 4300, FIN- 90014, University of Oulu, Oulu, Finland
b: NMR Research Unit, Faculty of Science, P.O.Box 3000. FIN-90014, University of Oulu, Oulu, Finland

Geopolymer is a inorganic adsorbent and catalyst with disordered three-dimentional framework, which is also regared as amorphous zeolite. The unstanding of its pore structure is important for its development as adsorbent and catalyst [1]. Here, six metakaolin-based geopolymers with different water-to-solid *(w/s)* ratios were prepared and their pore structures and connectivity were studied by ^{129}Xe NMR methods, which has been proved to be a good method to study the pore structure in various porous systems [2]. The ^{129}Xe NMR spectra were acquired to detect pores with different sizes (Fig. 1a) and the averaged pore diameters as well as heats of adsorption were acquired by fitting the ^{129}Xe spectra as a function of temperature (Fig. 1b and c). The connectivity of pores were studied by quantifying the exchange rates of Xe in different environments with performing selective IR experiments (Fig. 1d and e). The G0.75 was found to have one less pore type, higher averaged pore diameter, heat adsorption and exchange rates than the four samples with medium water contents (G0.66-0.50), while the G0.42 did not form a good pore strcutre as the theoretical lowest *w/s* ratios was used.

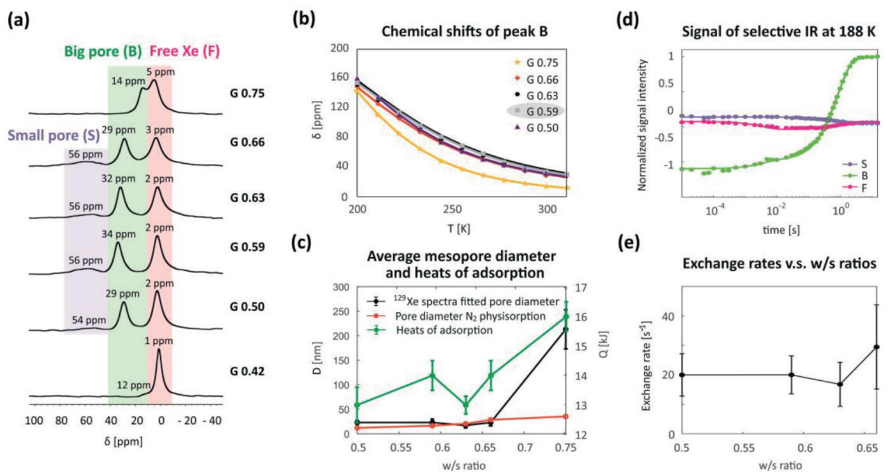


Figure 1. (a) The ^{129}Xe NMR spectra of six metakaolin-based geopolymers with variable *w/s* ratios at room temperature. (b) The ^{129}Xe chemical shifts as a function of temperature. (c) The average mesopore diameter
and heats of adsorption fitted from ^{129}Xe spectra. (d) The signal of selective IR of G0.59 at 188 K. (e) The fitted exchange rates from selective IR data as a function of w/s ratios at 188 K.

References
[1] Rolison, D. R. Catalytic Nanoarchitectures--the Importance of Nothing and the Unimportance of Periodicity. Science 2003, 299 (5613), 1698–1701.
[2] Weiland, E.; Springuel-Huet, M.-A.; Nossov, A.; Gédéon, A. 129Xenon NMR: Review of Recent Insights into Porous Materials. Microporous Mesoporous Mater. 2016, 225, 41–65.

Acknowledgements
Funding of this research is provided by the University of Oulu Kvantum Institute under Emerging projects – program (Zero-CO2 cement concept via phase-seperated nano-glass).

Special Award, AMPERE NMR School 2021
Anton Duchowny

NMR Studies of Complex Samples using Compact Instruments.

Anton Duchowny, Bernhard Blümich, Alina Adams
Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, 52074 Aachen, Germany

The usage of compact NMR instruments has steadily increased in the last decade. This is unsurprising given that capital and operational expenditures are about one order of magnitude lower than conventional high-field spectrometers, and specialized personnel is not required for operation in many cases. In addition, the field strength and performance of compact spectrometers are continuously improving. However, benchtop NMR spectrometers are still inferior to their conventional high-field counterparts in signal-to-noise ratio and spectral dispersion. Compared to high-field NMR spectra, low-field spectra appear crowded with overlapping peaks, which challenges the analysis of complex molecules and mixtures.

At the AMPERE NMR Summer School 2021, three scenarios were reported where complex samples were analyzed with benchtop NMR spectrometers. First, it was shown that the large plasticizer molecules found in polyvinyl chloride (PVC) could be identified and quantified by low-field ^{1}H NMR spectroscopy (Fig. 1). The chosen approach is rapid and simple, abolishing long measurement times and deuterated solvents while maintaining a low concentration limit of quantification. A limit of quantification of 2.49 wt% plasticizer in a PVC product was achieved within just 1 minute measuring time. This limit is only three times higher than that achieved with conventional high-field NMR spectroscopy at 400 MHz [1]. The reported workflow provides a rapid tool for identifying and quantifying plasticizers in PVC, even for untrained NMR users [2].

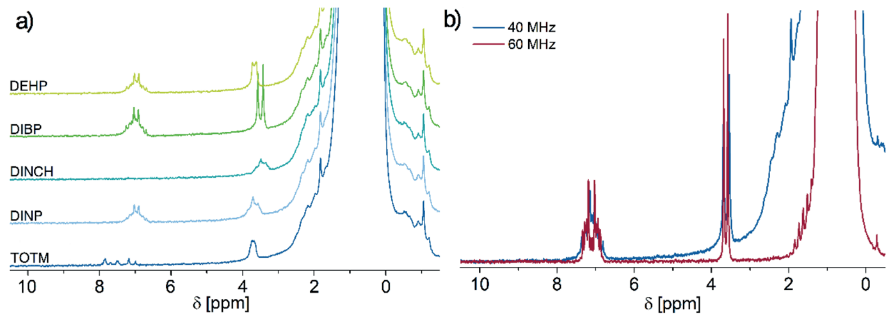


Figure 1. Comparison of ^{1}H spectra acquired with 4 scans. a) Five plasticizers dissolved in non-deuterated n-hexane (1 vol%) acquired on a 40 MHz benchtop spectrometer. b) Diisobutyl phthalate dissolved in non-deuterated n-hexane (16.17 mg mL^{-1}) acquired at 40 (blue) and 60 (red) MHz.

Second, different petrol- and bio-based fuels were examined in view of aging products formed during extended real-world applications that can damage hardware components. These substances occur in mixtures of fuels, which themselves are complex mixtures of natural products. We found that mono- and di-substituted esters of glycerol, which are residual intermediates from the biofuel production, accumulate and precipitate at 8 °C and can clog up filters while dissolving again at room temperature. Additionally, brown and tacky deposits could be extracted from a self-built test rig simulating a real-world system. These deposits are insoluble in oil, require extreme temperatures and oxygen to degrade, and comprise oxidized biofuel species. In this research, benchtop NMR spectroscopy proved to be a valuable source of information, alongside other techniques [3].

Third and last, a high-pressure setup was presented, with which samples can be investigated with benchtop NMR spectroscopy at pressures between 0 and 200 bar [4]. The setup is simple in design, easy to operate, small in size, yet still highly versatile. It was used to study gas mixtures, gas-solid interactions, and gas-liquid interactions. For instance, a three-component mixture containing methane, ethane, and hydrogen gas was mixed inside a reservoir and analyzed *in situ* with ^{1}H NMR spectroscopy at 60 MHz. The component concentrations quantified with NMR spectroscopy are in excellent agreement with those determined by gas chromatography. Furthermore, CO_2 was used as a non-wetting solvent for solid PVC resulting in pressure-dependent improvement of line-width and integral. Also, the solubility of methane in benzene between 1-200 bar could be quantified within minutes, matching literature data.

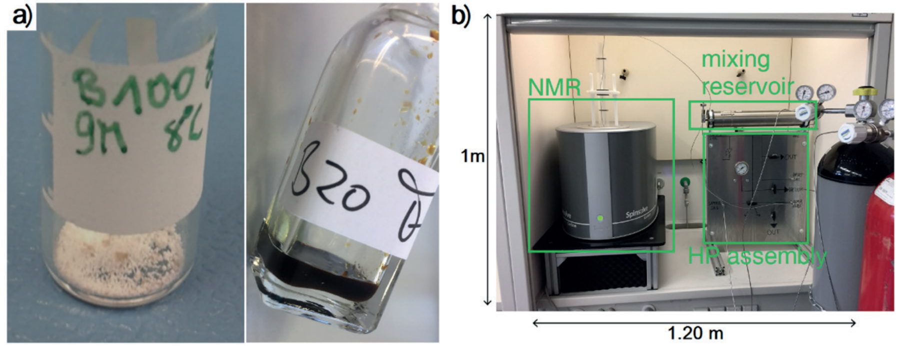


Figure 2. a) Left: precipitate found during storage at 8 °C. Right: deposits found in the self-built test rig. b) Self-built high-pressure apparatus for compact NMR spectroscopy.

These three scenarios illustrate new opportunities for analyzing complex samples with compact NMR spectrometers, be it by simplifying an analytical procedure for an untrained user, concentrating on peak clusters rather than the spectral fine-structure, or employing benchtop spectrometers on grounds forbidden to high-field magnets. There are many niches and potential applications for compact NMR instruments.

References
[1] Genay, S. et al. Anal. Bioanal. Chem. 2017, 409, 1271–1280
[2] Duchowny, A.; Adams, A. Molecules 2021, 26(5), 1221
[3] Duchowny, A.; Brendel, B.; Blümich, B.; Adams, A. (to be submitted)
[4] A. Duchowny, et al., Journal of Magnetic Resonance, 329, 2021,107025

Acknowledgments
Financial and technical support from Equinor, Gassco and Baker Hughes is gratefully acknowledged. The fuel study was part of the IGF Project number 18951 N/1, supported by DGMK under number 778 via AiF within the program for promoting the Industrial Collective Research (IGF) of the German Ministry of Economic Affairs and Energy (BMWi), based on a resolution of the German Parliament.

Anton Duchowny expresses his gratitude to the organization committee for allowing him to present his research at the AMPERE Summer School 2021.

Report:

The HYP21 international conference on nuclear hyperpolarization was held in person from the 5th to the 9th September 2021 in Lyon France, with 145 attendees on site.

This conference follows a series of symposia on Dynamic Nuclear Polarization, which were held in Nottingham, UK (2007), Königstein, Germany (2009), Lausanne, Switzerland (2011), Copenhagen, Denmark (2013), Egmond aan Zee, The Netherlands (2015) and Southampton, UK (2018). The HYP21 meeting had a broad scope, covering a range of hyperpolarization methodologies including optical pumping and parahydrogen, as well as dissolution and MAS DNP. A representative set of applications of hyperpolarization, ranging from clinical medicine to materials science and structural biology were also covered. The HYP21 meeting was an activity of the Hyperpolarization subdivision of AMPERE.

The conference was chaireed by Anne Lesage and Sami Jannin from the High Field NMR Center (CRMN Lyon), a research institute of the University of Lyon.

The scientific committee was composed of the following members:
Marina Bennati (Göttingen)
Konstantin Ivanov* (Novosibirsk)
Sami Jannin (Lyon), chair
Mathilde Lerche (Lyngby)
Anne Lesage (Lyon), chair
Malcolm Levitt (Southampton)
Harmut Oschkinat (Berlin)
Thomas Theis (North Carolina)

* Kostya has largely contributed to the definition of the scientific program together with the other committee members. We profoundly missed him. A dedicated tribune has been organized during the conference to honor his memory.

Despite the difficult health situation and travel restrictions still going on for some countries due to the COVID-19 crisis, the meeting attracted 145 attendees from the following countries: Austria, Belgium, Denmark, Estonia, Finland, France, Germany, Israel, Italy,

Poland, Sweden, Switzerland, The Netherlands, United Kingdom, United States.

The following topics were covered during 4 plenary lectures, 8 invited talks, 21 promoted talks, and 53 round tables:
- Pulsed DNP, from new pulse sequences to instrumentation.
- DNP for in vivo Imaging and metabolic contrast agents
- Applications of SABRE
- Theory of DNP MAS NMR
- DNP in the liquid state
- Parahydrogen induced polarization
- Dissolution DNP, from instrumental and methodological developments to applications in biology and health
- Dynamic Nuclear Polarization from Paramagnetic Metal Ion Dopants
- DNP MAS NMR of surfaces, organic solids and biomolecules

Plenary Speakers
Jan Henrik Ardenkjær-Larsen (Technical University of Denmark, Lyngby, Denmark)
Song i Han (University of California, Santa Barbara, USA)
Bob Griffin (MIT, Boston, USA)
Matthew Rosen (Center for Biomedical Imaging, Harvard Medical School, Charlestown MA, USA)

Invited Speakers
Alexander Barnes (Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland)
Danila Barskiy (University of California, Berkeley, USA)
Gerd Buntkowsky (Technische Universität Darmstadt, Germany)
Eleonora Cavallari (Dept. of Molecular Biotechnology and Health Science, University of Torino, Italy)
Christian Hilty (Department of Chemistry, Texas A&M University, College Station, USA)
Michal Leskes (Weizmann Institute of Science, Revohot, Israël)

Thomas Meersman (Sir Peter Mansfield Imaging Centre, University of Nottingham, Nottingham, UK)
Tomas Orlando (Max Planck Institute for Biophysical Chemistry, Göttingen, Germany)

Promoted speakers

Karel Kouril (Karlsruher Institut für Technologie, Germany)
Raphael Kircher (Laboratory of Engineering Thermodynamics, TU Kaiserslautern, Germany)
Pascal Wodtke (Technical University of Munich, Germany)
Ilya Kuprov (University of Southampton, UK)
Andrea Capozzi (Department of Physics, EPFL, Switzerland)
Jean-Nicolas Dumez (CEISAM – CNRS – Univ. Nantes, France)
Théo El Darai (Centre de Resonance Magnetique Nucleaire, Villeurbanne, France)
Quentin Stern (Centre de Resonance Magnetique Nucleaire, Villeurbanne, France)
Xizhou Zhang (Max Planck Institute for Biophysical Chemsitry,Göttingen, Germany)
Meike Emondts (Leibniz Insitute for Interactive Materials, Aachen, Germany
James Eills (Johannes Gutenberg University, D-55090 Mainz, Germany)
Sylwia Ostrowska (School of Chemistry, University of Southampton, UK)
Laurynas Dagys (School of Chemistry, University of Southampton, UK)
Pernille Rose Jensen (HYPERMAG, Technical University of Denmark)
Marie Juramy (Aix Marseille Univ, CNRS, ICR, Marseille, France)
Konstantin Tamarov (Department of Applied Physics, University of Eastern Finland, 70210 Kuopio, Finland)
Arnab Dey (Université de Nantes, CNRS, CEISAM UMR 6230, F-44000 Nantes, France)
Sabine Hediger (Univ. Grenoble Alpes, Grenoble, France)
Guinevere Mathies (University of Konstanz, Switzerland)
Ilai Schwartz (NVision Imaging Technologies, Germany)
Seyma Alcicek (Institute of Physics Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Krakow, Poland)

The conference included an evening dinner as well as a free afternoon where guided tours of Lyon were organized.

First Announcement

Saint Petersburg State University
19th International School-Conference
Spinus 2022
«Magnetic resonance and its applications»

28 March - 1 April, 2022
Online, Saint Petersburg, Russia

http://spinus.spb.ru

Invitation

Welcome to the 19th International School-Conference "Spinus. Magnetic Resonance and its Applications" organized by the Saint Petersburg State University from March 28 to April 1, 2022. This time the conference will be held online format (will be up dated) due to limitations of the COVID-19 pandemic.

The goal of "Spinus" is to provide to young scientists a platform for discussion of the use of all aspects of magnetic resonance methods and techniques, as well as computational and theoretical approaches, for the solving of fundamental and applied problems in physics, chemistry, medicine and biology.
The official language of the "Spinus" is English.

Scope

The scope of the "Spinus" Conference includes the following topics:
- Modern trends in NMR, ESR and NQR
- Magnetic resonance for fundamental science
- Magnetic resonance imaging
- Computer Modeling
- NMR in the Earth magnetic field
- Magnetic resonance for industry
- Related phenomena

Extended abstracts will be published in the Book of Proceedings.
Selected papers of participants will be published in a journal which is indexed by Web of Science and Scopus.

Application to SPINUS 2022

The application for "Spinus 2022" is now available on the website spinus.spb.ru.
If you were registered for Spinus 2018-2021, your account is valid and in this case you

can just create an application for Spinus-2022 in your profile.

Conference Fee

The conference fee is 2000 ₽ (≈ 25 €) for a participant. Conference fees include organization costs and conference materials.

Proceedings and abstract submission

Abstracts up to 3 pages (including tables and figures) in the MS Word format, according to the conference template, should be uploaded to the Spinus website until **March 1st, 2022**.

The abstract template is available at the Spinus website spinus.spb.ru.

All accepted abstracts will be placed in Russian Science Citation Index and be available on the resource www.elibrary.ru and Google scholar.

In 2022 selected papers of the participants will be published in a special issue of a journal which is indexed by Web of Science and Scopus.

Awards

The organizing committee continues the tradition of rewarding young participants for the best oral and poster presentation.

Organizing Committee
Chairman: Prof. Denis Markelov,
Vice-chairman: M. Sc. Alexandr Ievlev,
Committee members:
Prof. Marina Shelyapina
Dr. Andrey Egorov
Dr. Andrey Komolkin
Dr. Pavel Kupriyanov
Dr. KonstantinTyutyukin
M. Sc. Timofey Popov

Scientific adviser of the School-Conference “Spinus”
Professor Vladimir Chizhik

Advisory Board

Chairman
V.I. Chizhik, Professor, Saint-Petersburg State University, St. Petersburg, Russia

Scientific Advisory Board Members

V. Balevicius, Professor, Vilnius University Vilnius, Lithuania

C. Cabal, Professor, Havana University, Cuba.
S.V. Dvinskikh, Professor, Royal Institute of Technology, Stockholm, Sweden
J. Fraissard, Professor, University Pierre and Marie Curie, Paris, France
L.Yu. Grunin, Associate Professor, CEO, Resonance Systems, Germany
E. Lahderanta, Professor, Lappeentanta Technical University, Finland
B. Rameev, Professor, Gebze Technical University, Turkey
N.R. Skrynnikov, Professor, St. Petersburg University , Russia
M.S. Tagirov, Professor, Kazan Federal University, Russia
L.M. Varela, Professor, University Santiago de Compostela, Spain
S. Vasiliev, Professor, University of Turku, Finland

Contacts

Prof. Denis Markelov,
Alexandr Ievlev
1, Ulyanovskaya st., Peterhof, 198504, Saint Petersburg, Russia,
Dept. Nuclear-Physics Research Methods
St. Petersburg State University,
Tel.: +7-981-1226846
(Alexandr Ievlev)

e-mail: spinus@spinus.spb.ru
URL: http://spinus.spb.ru
Facebook: https://www.facebook.com/groups/SPINUS/
Vkontakte: https://vk.com/spinus_iys

Enable Education Everywhere…

…with *EquipSent!*

Initial Situation

In high-income countries, scientific equipment is often stored unused after its usage time in research laboratories. Older devices are eventually discarded, even though they are still functional.

In low-income countries, schools and universities are lacking the funds to acquire even the most basic devices for adequate training of talented students. The resulting ‚brain-drain' to other countries hinders the self-development in such regions.

Our Solution

EquipSent seeks to connect these two worlds by directly matching donors of scientific equipment with those in need. As an intermediary between both parties, we reduce administrative efforts and help organizing the shipping, installation and legal contracting. Expenses are shared between the recipient and the industrial sponsors in return for CSR, new markets and advertisement.

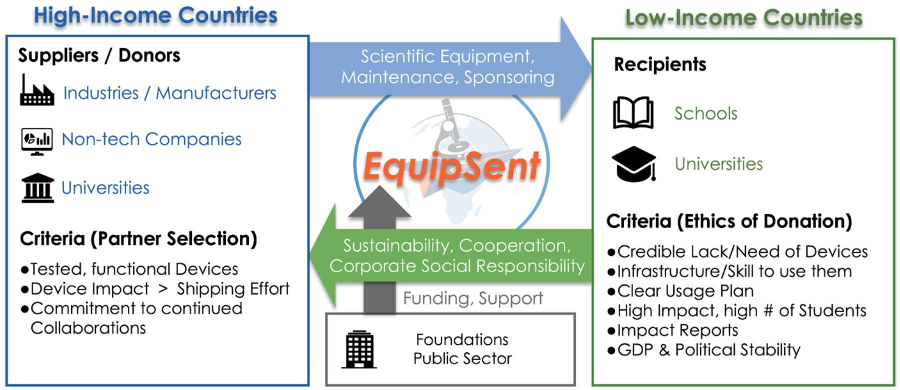
Target Impact

• Access to Education. Students around the world will be granted access to hands-on training and education, rather than theory only.

• Collaboration and Development. The matched donor, sponsor and recipient of equipment are encouraged to collaborate on a long-term basis, which offers learning opportunities on all sides.

• Resource Efficiency & Waste Minimization. The equipment donor profits by reducing costs for space, waste and personnel, while benefitting from a positive image generated through sustainable use.

Founded by a group of ETH students, EquipSent is giving a second life to devices, promotes sustainable use and offers access to education and research to more people.



Do you know about no longer used, but functional scientific equipment in your research group or do you know of a university in need?

Do you want to learn more about what we do?

Check out our website EquipSent.org and get in touch with us!

our Partners:

CGI U COMMITMENT-MAKER 2016 AVETH Projecttogether STUDENT PROJECT HOUSE

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
Janez Dolinšek, Jožef Stefan Institute, Slovenia
jani.dolinsek@ijs.si

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

EF-EPR
Sabine van Doorslaer, University of Antwerp, Belgium
sabine.vandoorslaer@uantwerpen.be

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

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

MR-Food
John van Duynhoven, Wageningen University & Research, The Netherlands
john-van.duynhoven@unilever.com

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

Euromar
Thomas Prisner, Goethe University Frankfurt, Germany
prisner@chemie.uni-frankfurt.de

Euromar Treasurer
Arno Kentgens, Radboud University, The Netherland
a.kentgens@nmr.ru.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

Honorary member
Stefan Jurga, Adam Mickiewicz University, Poland
stjurga@main.amu.edu.pl

AMPERE Committee

Sharon Elizabeth Marie Ashbrook (2016-2024) University of St. Andrews, United-Kingdom

Rolf Boelens (2016-2024) Utrecht University, The Netherlands

Enrica Bordignon (2021-2025) Ruhr University, Germany

Vladimir Chizhik (2016-2024) University of St. Petersburg, Russia

Peter Crowley (2018-2022) National University of Ireland, Ireland

Janez Dolinšek (2016-2024) Institute Jozef Stefan, Slovenia

Isabella Caterina Felli (2016-2024) CERM, University of Florence, Italy

Ana Maria Pissarra Coelho Gil (2018-2022) University of Aveiro, Portugal

Patrick Giraudeau (2016-2024) Université de Nantes, France

Klaartje Houben (2021-2025) DSM, Den Haag, Nederland

Kristaps Jaudzems (2019-2023) University of Latavia, Latvija

Vytautas Klimavičius (2021-2025) Tecnical University Darmstadt, Germany

Katalin Köver (2021-2025) Universtiy of Debrecen, Hungary

Wiktor Kozminski (2016 - 2024) University of Warsaw, Poland

Birthe Brandt Kragelund (2018-2022) University of Copenhagen, Denmark

Jose Martins (2021-2025) Ghent University, Belgium

Jörg Matysik (2021 - 2025) University Leipzig, Germany

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

Predag Novak (2019-2023) University of Zagreb, Croatia

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

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

Miquel Pons (2016-2024) University of Barcelona, Spain

Indrek Reile (2019-2023) National Institute of Chemical Physics and Biophysics, Estonia

Frode Rise (2018-2022) University of Oslo, Norway

Sharon Ruthstein (2018-2022) 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

George Spyroulias (2017-2025) University of Patras, Greece

Ville-Veikko Telkki (2016-2024) University of Oulu, Finland

Christina Thiele (2016-2024) Technische Universität Darmstadt, Germany

Daniel Topgaard (2017-2025) Lund University, Sweden

Lukàš Trantírek (2021-2025) CEITEC - Central European Institute of Technology, Czech Republic

Jadwiga Tritt-Goc (2021-2025) Polish Academy of Sciences, Poland

Paul Vasos (2019-2023) Horia Hulubei Institute for Nuclear Physics (IFIN-HH), Romania

Honorary members

Jean Jeener
Université Libre, Belgium

Karl Alexander Müller
IBM Zurich Research Laboratory, Switzerland

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, Ruhr University, Germany

Future conferences

Ampere Event 2022

19th International School-Conference on Magnetic Resonance and it's applications, Spinus 2022	online, St. Petersburg (Russia)	March 28 to April 1
MR FOOD 2022	Aarhus (Denmark)	June
Euromar 2022	Utrecht (Netherlands)	July 10-14
Magnetic Resonance in Porous Media	Hangzhou (China)	August
Alpine Conference on Magnetic Resonance in Solids	Chamonix (France)	September

Ampere Event 2023

Euromar 2023	Glasgow (United Kingdom)	July 9-13
HYP23	Leipzig (Germany)	September 24-28

Groupement
AMPERE

www.ampere-society.org