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BULLETIN DU GROUPEMENT

d'informations mutuelles

Groupement
AMPERE

SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

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Contents

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Special Editorial

Groupement AMPERE

Dear members of the Groupement AMPERE, dear colleagues and friends,

first I would like to present you my best wishes for a fortunate 2022, with health, joy and success, even in these difficult and unsettled war-soaked times, and hope that the end of the war in the east of Europe, and also of the pandemic, draw near. Both have had and still have an important impact on science these times, and many efforts are underway in our community to counteract threatening isolation of scientists in different parts of the world, and to support colleagues in difficult situations (see page 4 for the official statement of the Groupement AMPERE).

There is important news from inside AMPERE: two new members joined the AMPERE Bureau to represent the younger generation, including PhD students and early-carrier scientists. The Bureau gives a warm welcome to Guinevere Mathies and Quentin Stern. Also in this issue, you can discover the portrait of Louisa Ciobanu, an MRI specialist from Paris, and the head of the AMPERE Subdivision for Spatially Resolved Magnetic Resonance.
And YES! - we are delighted, there have been MR conferences in the last trimester, some even in presence – as also HYP21 already reported in the previous Bulletin. You can follow in this issue the "Modern Development of Magnetic Resonance" (MDMR2021) conference, where many magnetic resonance specialists gathered around an event not only with a lot of excellent science, but also very celebrational, with awards and birthdays. The conference of the AMPERE subdivision "Applications of Magnetic Resonance in Food Science" (MRFOOD) was held online, in an innovative and interesting format in conjunction with Magnetic Resonance in Chemistry.

With an eye to future events, the Alpine Conference, under the auspices of the AMPERE Society, has published the first announcement for their September meeting – we are looking much forward to meet again in Chamonix. And don't forget, registration for EUROMAR in Utrecht is open.

Sadly, the MR community again mourns the passing of distinguished colleagues, namely Shimon Vega, Chunni Lal Khetrapal, Kenneth Packer, Wes Anderson, Aharon Loewenstein and Girjesh Govil. Certainly, many of you had the privilege of meeting them. Their legacy will continue to inspire.

Anja Böckmann
President, Groupement AMPERE

Portrait:

Prof. Luisa Ciobanu

Why magnetic resonance and why NMR and MRI?
I believe MRI is the MOST versatile technique out there; I cannot think of any other modality with which one can look at rocks, plants and thought formation…

What is your favorite frequency?
730.16 MHz

What do you still not understand?
Why are the MRI scanners so expensive?!

Luckiest experiment you have ever done.
There is no lucky experiment!

What was the worst mistake you have made during your lab time?
During my first week as a postdoc at the University Illinois at Urbana-Champaign I kicked (by mistake ☺) a small metallic ruler and it went into the 14T vertical scanner I was using. Needless to say, in one week everyone found out about the "incident" and I was very "popular" ☹

Most memorable conference story.
My first oral presentation at an ENC conference was in 2002 in Asilomar while I was a graduate student. I presented a sequence we were using to perform high-resolution MR microscopy.
At the end of my short, 10 min talk, I had one question from the "Chapel". I had no idea where to look, where the person asking the question was… The question was: Did you try using XYxxx (I don't remember what) phase cycling?" I just answered "no", but I had no idea what that was about. I thought my adviser (Charles Pennington) would be so upset that I did not know but it turned out he did not know either – or he said he did not to make me feel better ☺ Later I found out the person who asked was Robert Tycko ☹

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

When do you get your best ideas?
When I talk to fellow researchers or when I drive my car to work (one hour drive)

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

Your idea of happiness.
Have a big garden and an MRI scanner in my garage.
(I have none of these two right now ☹)

Position:
Research Director, CEA, NeuroSpin, France
Homepage:
https://www.linkedin.com/in/luisa-ciobanu-1320a66/
Education:
BS Physics, University of Bucharest, PhD Physics, The Ohio State Univeristy, HDR Biology, University Pierre et Marie Curie
Interests:
Besides MRI??? Gardening

Official Statement of the Groupement AMPERE to the Situation in the Ukraine:

The Groupement AMPERE and the magnetic resonance community in Europe have observed with great concern how a war has been started in the center of Europe aimed at destroying the sovereignty and integrity of Ukraine. AMPERE strongly condemns the Russian army‘s invasion of Ukraine, the resulting war and the destruction of human life, society and cities in Ukraine. The Russian invasion is an attack on the elementary values without which scientific freedom and scientific cooperation are difficult. We call on the Russian government to immediately stop all military actions, and our thoughts and solidarity are with all Ukrainian citizens and especially with our colleagues and their families who had to leave their homes to ensure their safety.

The Groupement AMPERE has been working for more than 70 years to promote contacts among scientists working on magnetic resonance and related phenomena throughout Europe. Of importance, though less known, is the role played by the Groupement AMPERE in maintaining effective scientific and human exchanges between Western and Eastern European countries all through the difficulties of the cold war. The motto of AMPERE, se connaître, s‘entendre, s‘entraider, has guided AMPERE since its foundation to help scientists in difficult economic or political situations. Today, more than ever, this motto must guide our thinking.

We remain convinced that research and contacts between researchers can build bridges across national and political borders. Still, as a European institution, we will suspend this year’s provision of auspice for conferences organized in the Russian Federation. Membership to AMPERE will be maintained for all our colleagues, taking into account that Russian scientists who do not support the conflict, are today often unable to voice their opinions without repercussions.

To support efforts to find temporary jobs for displaced researchers from Ukraine, we have also decided to actively sponsor Ukrainian scientists through a donation from AMPERE to cara, a non-governmental organization that provides a lifeline for at-risk academics.

AMPERE News:

Ampere Bureau Young Members

The AMPERE Bureau goes young(er) : the intent was to refresh the Society, to open it up to the younger community, by including representatives of this generation directly in its executive body, the AMPERE Bureau. Following a call for applications published in the AMPERE mailing list and over several online channels, the Groupement received about a dozen of submissions, out of which the AMPERE Prize Committee selected three to be presented to the AMPERE Committee to vote.
The Committee met online, as presented in the Minutes, and the Bureau wishes to welcome Quentin Stern and Guinevere Mathies, who have been elected as student and early-career representatives respectively.

Guinevere Mathies is an Emmy Noether group leader at the University of Konstanz, Germany. She did her PhD in Leiden with Prof. Groenen on high-frequency EPR instrumentation, and joined 2012 the group of Prof. Griffin at MIT to work on MAS NMR and DNP. She currently works on new developments of pulsed DNP methods.

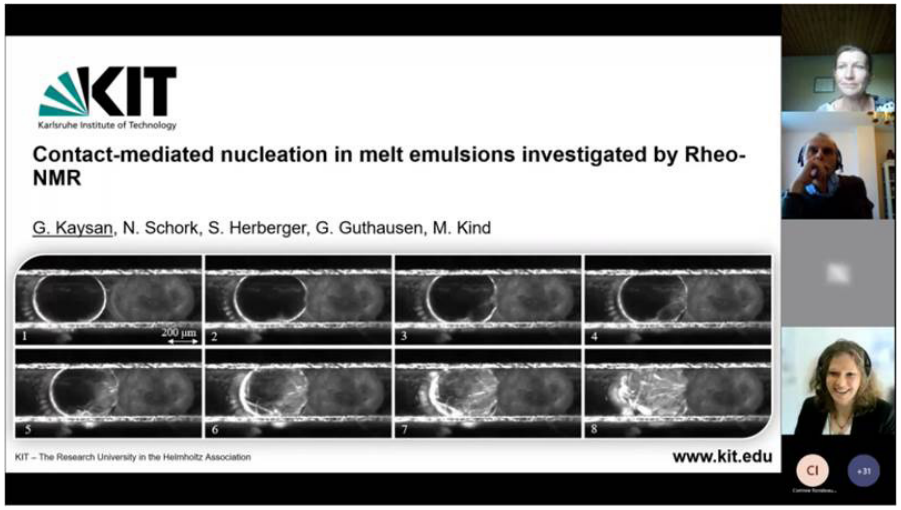
Quentin Stern is a PhD student in the lab of Sami Jannin at the ENS Lyon which he joined after studying at EPFL Lausanne; he works on zero to ultra-low field NMR enhanced by DNP.

The new members are currently presenting the ideas they would like to bring into the community, and they will certainly represent an excellent entry point for members of the young(er) generation who want to get into contact with AMPERE.

Report:

MR FOOD on-line workshop on Multiscale Food Structure and Foodomics

On October 28 and 29 the MRFOOD Division organized an on-line workshop around the theme Multiscale Food Structure and Foodomics.



With the live MRFOOD conference planned in Aarhus for 2020 cancelled due to COVID the MRFOOD community was deprived of scientific interactions and exchange. This in particular affected young scientists and the on-line workshop intended to bridge the gap until next live conference.

In order to stimulate engagement and in depth discussions the workshop was organized in conjunction with a call for papers for a special issue in Magnetic Resonance in Chemistry. These papers had to be submitted three weeks before the workshop in order to give the participants ample time for reading the manuscripts. The papers were made accessible to the participants via a closed repository. The final workshop programme consisted of 11 short presentations, which essentially summarized the papers, followed by ample time for discussions with a prepared audience.

This resulted in active in depth discussions, and provided take out for presenters to further improve their papers which were mostly still under review.

Besides the 12 presenters also 32 participants engaged in the discussions, mostly their direct colleagues. The recordings of the presentations and discussions will be posted on Zenodo, a EU-funded public repository for scientific publications and data.

The presenters will be stimulated to enclose the doi's of their presentations as references in their papers. As an experiment to keep the debate alive in the MRFOOD community the organizers consider the workshop a success. The chosen format stimulated engagement and in-depth discussion during the workshop, and will also promote the quality of the papers submitted to the special issue of Magnetic Resonance in Chemistry.

Report:

International Conference "Modern Development of Magnetic Resonance" (MDMR2021)

The annual International Conference "Modern Development of Magnetic Resonance" was held from 1 November till 5 November 2021 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 2021 and the celebration of the 85th birthday of Prof. Kev M. Salikhov. All events were organized in a mixed format: face-to-face and online participation.

The conference topics were extremely diverse and included reports in the following fields:
- Perspectives of magnetic resonance in science and spin technology
- 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.
- New trends in spin chemistry

The participants of the conference were leading scientists and experts in the field of magnetic resonance from Australia, Belgium, Canada, Czech Republic, Germany, Israel, Italy, Japan, Moldova, Poland, Russia, Sweden, Switzerland, Tajikistan, Turkey, United Kingdom and USA. The total number of participants was 181, who presented 146 reports (7 plenary lectures, 79 invited and oral talks, and 67 posters). The abstracts can be found at: https://ampere-society.org/Conferences.html

Leila Fazleeva presents the Zavoisky Award diploma to Sergei Demishev (from left to right: Leila Fazleeva, Sergei Demishev, Kev Salikhov).

The opening ceremony and the first scientific session of the conference took place on November 1. 2021 and were chaired by Alexey Kalachev, Director of the Federal Research Center. The Zavoisky Prize ceremony was held before the opening of the conference. Kev Salikhov, Chairman of the International Zavoisky Award Selection Committee, announced the names of the Zavoisky Awardees 2021: Professor Sergei Demishev (Prokhorov General Physics Institute of Russian Academy of Sciences, Russia) and Jörg Wrachtrup (University of Stuttgart, 3rd Institute of Physics and Center for Applied Quantum Technology, Stuttgart, Germany). Sergei Demishev was distinguished for his achievements in the field of application of EPR methods to the study of quantum materials including strongly correlated metals and quantum critical systems. Jörg Wrachtrup was distinguished for his achievements in the field of application of EPR methods to the study of quantum materials including single-spin systems and materials for spin technology.
Leila Fazleeva, Deputy Prime Minister of the Republic of Tatarstan, Myakzyum Salakhov, President of the Tatarstan Academy of Sciences, Dmitry Tayursky, Deputy Rector of the Kazan Federal University congratulated heartily Sergei Demishev and Jörg Wrachtrup on their highly deserved awards. The laureates also received congratulations from Songi Han, IES President, Anja Böckmann, President of the AMPERE Society, Robert Tycko, ISMAR President, and Akash Chakraborty, Publishing Editor, Springer-Verlag.

Traditionally, the laureates gave Zavoisky Award lectures: Magnetic Resonance One Spin at a Time (Jörg Wrachtrup) and EPR Adventures in the Strongly Correlated World: Quantum Materials and Quantum Critical System (Sergei Demishev).

The first plenary session included the following plenary lectures: Adventures and Advances with Compact Magnetic Resonance by Bernhard Blümich (ITMC, RWTH Aachen University, Aachen, Germany) and CW and Pulsed EPR of Radicals in Solutions Undergoing Exchange by Michael Bowman (Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia; Chemistry & Biochemistry Dept., University of Alabama, Tuscaloosa, USA).

A number of topical fundamental problems were discussed at the conference. These included: search for promising applications of magnetic resonance in science and spin technology; the recent development of magnetic resonance method, study of the properties of new materials with specified functional properties; a new trends in spin chemistry; recent developments in the application of solid-state NMR of quadrupolar nuclei to understand inorganic materials; etc.

On November 3, the celebration of Kev Salikhov's 85th birthday was held, when the hero of the day presented a report on his ambitious scientific plans. Kev Salikhov was congratulated by leaders of the Republic of Tatarstan, the city of Kazan, the Academy of Sciences of the Republic of Tatarstan, Federal Research Center «Kazan Scientific Center of Russian Academy», Kazan Federal University, colleagues and friends.

Farid Mukhametshin (left) presents the Order of Friendship of the People of the Republic of Tatarstan to Kev Salikhov (right).

Farid Mukhametshin, Chairman of the State Council of the Republic of Tatarstan, awarded Kev Salikhov the Order of Friendship of the People of the Republic of Tatarstan. Ilsur Khadiullin, Minister of Education of the Republic of Tatarstan, presented him Insignia „Honorary mentor".

Many congratulations were received online, including those from the Physics Department of the Russian Academy of Sciences and Songi Han, IES President.

Two IES Student Poster Awards were granted at the MDMR2021. The IES Student

Poster Award Selection Committee consisted of Kev Salikhov (Chairman, Zavoisky Physical-Technical Institute, Kazan, Russia) and members: Michael Bowman (Chemistry & Biochemistry Dept., University of Alabama, Tuscaloosa, USA), Sergei Demishev (Prokhorov General Physics Institute of RAS, Moscow, Russia), Marat Gafurov (Kazan Federal University, Kazan, Russia) and Dmitri Stass (Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia).

Kev Salikhov presents the IES Student Poster Award diploma to Arina Tarasova (right).

Arina Tarasova (Moscow State University, Moscow, Russia) and Bogdan Rodin (International Tomography Center SB RAS, Novosibirsk, Russia, PSL University, Sorbonne Université, Paris, France) were chosen as the awardees.

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 Science Foundation for the financial support.

Kev Salikhov
Chairman of the Organizing Committee MDMR2021
Violeta Voronkova
Scientific Secretary MDMR2021

Posterprize MDMR 2021

Ariana Tarasova, Moscow State University, Russia

Fluorine and Sodium MRI on 0.5 T Clinical Scanner

A. A. Tarasova[1], N. V. Anisimov[2], O. S. Pavlova[1,2], M. V. Gulyaev[2], I. A. Usanov[1], Yu. A. Pirogov[1]
[1]Faculty of Physics, Lomonosov Moscow State University, Moscow 119991, Russian Federation; arina.tarasova99@mail.ru
[2]Faculty of Fundamental Medicine, Lomonosov Moscow State University, Moscow 119991, Russian Federation

Typical MR scanners are focused on the detection of proton (^{1}H). Detection of other nuclei provides additional diagnostic information – about the state of tissues, cellular processes, etc. Sodium is of considerable interest – the natural abundance of the ^{23}Na isotope is 100%, and the gyromagnetic ratio is 3.8 times lower than of proton. However, the sodium content in living tissues is 2-3 orders of magnitude lower than that of hydrogen, which determines the low sensitivity of the method. The detection of fluorine signals is also of interest in MRI. The ^{19}F isotope has 100% natural abundance and its gyromagnetic ratio is only 6% less than of proton. So, ^{1}H and ^{19}F MRI are comparable in sensitivity. The content of fluorine in living tissues is extremely low, therefore, it is very productive to detect signals from fluorine-containing substance injected into the body, for example, a drug, as well as from gases in the lungs, since there is no background from normal tissues in the images. The use of strong fields – from 3 T and more increases the sensitivity of multinuclear methods. However, such fields are unattainable with open-type magnets and compact portable MRI systems. Therefore, it is of interest to evaluate the productivity of multinuclear research on low-field equipment. We carried out these studies on a 0.5T clinical scanner Bruker Tomikon S50 (^{1}H NMR frequency is 21.1 MHz). The technical rework concerned only the coils, which were used as modified proprietary prototypes, originally intended for the detection of protons [1, 2].

In experiments on ^{19}F MRI (19.8 MHz) of human lungs, we used octafluorocyclobutane gas C_4F_8 [1]. The patient inhaled a gas mixture (80% C_4F_8 + 20% O_2) and during the breath holding, scanning was performed. Since this gas has T_1 ~50ms,we use FSE method (TE_{min} = 8 ms, ETL = 4).There were 2D FSE in 3 projections (TR = 69 ms, NA = 30, in-plane resolution of 1×1 cm^2, no slice selection, scan time of one projection of 20s), SNR up to 43) and 3D FSE (TR = 42 ms, NA = 4, voxel size = 1×1×1 cm^3, scan time = 33 s, SNR up to 11). Measurements were carried out on 6 volunteers: females – 23 and 27 y.o. and males – 23, 23, 40 and 71 y.o. The 3D scan data were used to calculate the volumes of lung lobes and their volumetric reconstructions. Real-time studies of lung filling during inhalation and exhalation have also been conducted. For this, 2D scans (TR = 45 ms) were carried out 16÷30 times every 5÷7 seconds, NA = 16÷20. 2D scan data was used also to create maps of T1, ventilation and perfusion.

^{23}Na MRI (5.6 MHz) was done using 3D GRE technique (TR/TE = 44.7/12 ms, FA = 45°, NA = 1, voxel size = 6×6×6 mm^3, scan time = 24.5 min) [2, 3].

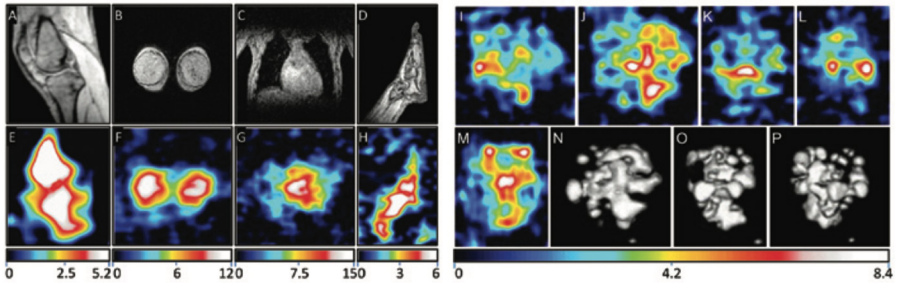


Fig. 1. MR images of different human organs: ^{1}H (A-D) and ^{23}Na (E-O).

To increase the SNR by an order of magnitude, the k-space data were exponentially apodized. To eliminate external RF interference, scans were performed at specific times of the day, and pulse noise bursts detected in k-space were edited [4]. Fig.1 shows examples of MRI of different human organs. Images A,E, I-M were obtained using a saddle coil and B-D, F-H using a solenoid coil. These coils are optimized for extremities and breast studies, respectively. For assignment of anatomical structures on ^{23}Na images E (knee, sagittal), F (breast, coronal), G (heart, coronal), H (foot, sagittal), corresponding ^{1}H images are shown: A-D. The right panel shows MRI of the head – separate slices: I,J (sagittal), K,L (coronal), M (axial), as well as 3D reconstruction – rendering at different azimuthal angles: –90°(N), 0°(O), 10°(P). The brightness scale corresponds to the SNR values. Optimization of the transceiver path can increase the SNR by more than 2 times [3].
^{19}F MRI on a 0.5 T clinical scanner is easy to implement. ^{23}Na MRI on it is also possible, but it is necessary to pay attention to the design of the coils and setting up the transceiver path.

The presented research was supported by the Russian Foundation for Basic Research (grants 19-29-10015, 20-52-10004) and by the Interdisciplinary Scientific and Educational School of Moscow State University “Photonic and Quantum Technologies. Digital Medicine”.

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Posterprize MDMR 2021

Bogdan Rodin, Novosibirsk State University, Russian Federation, Sorbonne Université, France

General Adiabatic Pulses for Transferring Singlet Order to Heteronuclear Magnetization: Application to Fumarate Hyperpolarized with Parahydrogen

B. A. Rodin[1,2,3], V. P. Kozinenko[1,2], J. Eills[4], K. Ivanov[1,2], A. Yurkovskaya[1,2]
1 International Tomography Center SB RAS, Novosibirsk 630090, Russian Federation
2 Novosibirsk State University, Novosibirsk 630090, Russian Federation
3 Laboratoire des biomolécules, LBM, Département de chimie, École normale supérieure, PSL University, Sorbonne Université, CNRS, Paris 75005, France
4 Helmholtz Institute Mainz, Johannes Gutenberg University, Mainz 55099, Germany

Singlet order can be defined for a coupled spin pair as the difference between the singlet state population and the mean population of triplet states. Singlet order often relaxes much slower than magnetization, i.e., it is often long-lived, which allows one studying various slow processes and preserving hyperpolarized spin order in the singlet state. A particularly interesting and relevant problem in this area is given by transfer of the singlet order of two protons to polarization of a neighboring heteronucleus. Several methods were proposed achieve such a transfer, including techniques using adiabatic adiabatic rf-pulses or B_0-field pulses. Here we propose a significant improvement of such adiabatic methods by using “constant-adiabaticity” temporal profiles of the pulses* which were originally proposed to generate singlet order in a spin pair. All constant-adiabaticity methods were implemented for the important metabolite [1-13C]fumarate, representing an AA’X-type spin system.

First of all, we have generalized and improved the procedure to evaluate constant-adiabaticity ramps by using a pertinent restriction of the space of spin states. With this method, we have introduced constant-adiabaticity rf-field ramps to manipulate spin order in high-field experiments, allowing us to reach an excellent efficiency of 96.2% for singlet order to heteronuclear polarization transfer. In experiments with parahydrogen, such rf-pulses allowed us to obtain 6.8% 13C polarization. Last but not least, the same optimization method has been utilized in ultralow-field experiments, using field cycling (FC) and field sweeping (FS) to convert the proton spin order into the 13C polarization. The constant adiabaticity profiles have demonstrated a much better performance in comparison with their linear analogues used before: one can achieve efficient polarization transfer in much shorter times, getting around the problem of relaxation losses of spin order during the field pulse.

The highly efficient polarization transfer techniques used here are of a more general scope and can be exploited to generate heteronuclear spin hyperpolarization in various molecules, notably, in metabolites.

This research was supported by Russian Foundation for Basic Research (Grant No. 20-53-15004).

* B.A. Rodin, K.F. Sheberstov, A.S. Kiryutin, J.T. Hill-Cousins, L.J. Brown, R.C.D. Brown, B. Jamain, H. Zimmermann, R.Z. Sagdeev, A.V. Yurkovskaya, K.L. Ivanov: Constant-adiabaticity RF-pulses for generating long-lived singlet spin states in NMR, J. Chem. Phys. 150, 064201 (2019)
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First announcement

Alpine Conference on Magnetic Resonance in Solids

4-8 September 2022 Chamonix-Mont-Blanc, France

Dear Colleagues,

We cordially invite you to participate and contribute to the Alpine "Chamonix" Conference on Magnetic Resonance in Solids, that will take place in Chamonix Mont-Blanc, France, on 4-8 September 2022.

Aims and scope of the meeting

The Alpine conference is a high-level international forum for the discussion of recent developments and applications in the field of magnetic resonance in solids. The conference focuses on novel concepts, methods and instrumentation, as well as applications in fields including physics, chemistry, biology and materials science.
Beyond its original and still core focus on solid-state NMR, the Alpine Conference welcomes contributions from EPR and MRI in solids.

Program

The program of the conference will consist of plenary lectures, contributed oral communications, and roundtable sessions. Round table sessions will provide opportunities for discussions in small groups following a short pitch talk on contributed work. A perspective session will provide personal views on selected topics and questions of the field.

The following speakers will give plenary lectures:
Alexander Barnes (ETH),
Marina Bennati (U. of Göttingen, Max-Planck Institute for Biophysical Chemistry),
Christian Degen (ETH),
Lyndon Emsley (EPFL),
Mei Hong (MIT),
Michal Leskes (Weizmann Institute of Science),
Rachel Martin (U. of California, Irvine),
Tatyana Polenova (U. of Delaware),
Kâmil Uğurbil (U. of Minnesota)

Registration

Registration will open in March 2022 and the deadline for registration is May 31st, 2022. Registration will be limited to around 200 participants. A number of student grants will be available.

Venue and Accommodation

The conference takes place at the Le Majestic, a beautiful and welcoming Belle Epoque palace, in Chamonix at the feet of Mont-Blanc. Three lunches (Mon – Wed) and two dinners (Sun and Tue) will also be served at le Majestic.

Chamonix Mont-Blanc is a charming lively town at the heart of breathtaking Alps, about 1 hour drive from Geneva Airport and about 2 hours drive from Lyon. Chamonix caters both to mountain enthusiasts who are into pushing their physical limits and being one with nature, and city dwellers whose idea of fun is more about enjoying a glass of wine and a spectacular view without breaking a sweat.

A number of hotels with different range of comfort and affordability will be bookable at the registration at prices negotiated with Office du Tourisme de Chamonix. All of the hotels are within maximum 15 minutes walking distance from the conference center, Le Majestic.

Looking forward to seeing you in Chamonix!

Scientific Committee

Anja Böckmann (MMSB Lyon), Alexej Jerschow (New York University) Anne Lesage (CRMN Lyon)

Organizing Committee

Jean-Nicolas Dumez (CEISAM Nantes) Daniel Lee (University of Manchester) Michal Leskes (Weizmann Institute)
Józef Lewandowski (University of Warwick)
Charlotte Martineau-Corcos (CortecNet),
Paul Schanda (IST Austria)

Contact: Email: contact@alpine-conference.org | Web: www.alpine-conference.org
Facebook: www.facebook.com/alpine.conference | Twitter: @alpineconferen1

Under the auspices of the Groupement Ampere and the International Society of Magnetic Resonance

First announcement

EURO MAR 2022 JULY 10-14 UTRECHT THE NETHERLANDS

On behalf of the Scientific Committees of the EUROMAR and AMPERE organisations, we are delighted to welcome you to EUROMAR 2022 in Utrecht, The Netherlands!

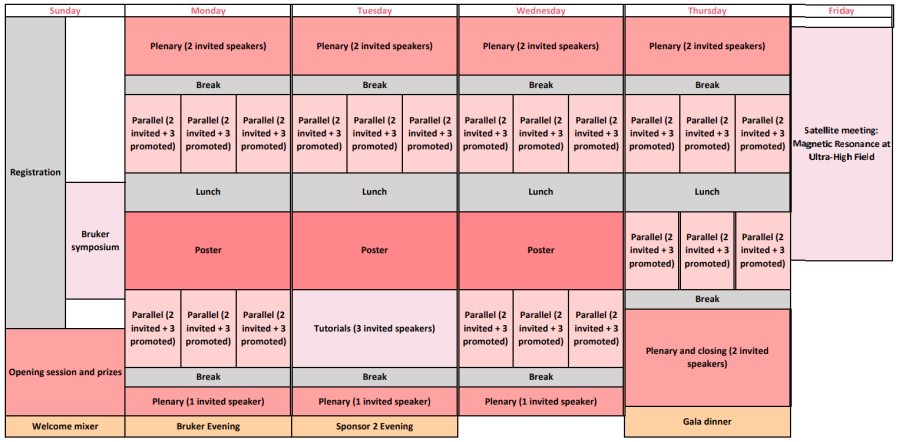
Our meeting will take place from 10-14 July 2022 followed by a satellite meeting on Magnetic Resonance at Ultra-High Field on 15 July.

Together with our partners, we will provide a stimulating forum to exchange on the most recent breakthroughs in magnetic resonance and to showcase the latest developments of our industrial sponsors. After two virtual meetings, our mission is to organize a fully live event but our preparations also include backup options (online or hybrid).

Abstract submission is now open at:
https://cbd.eventsair.com/euromar-2022/euromar2022abstractportal - Stay tuned to our website www.euromar2022.org for the latest information.

The local organizers:
Marc Baldus, Alexandre Bonvin, Markus Weingarth, Hugo van Ingen, Andrei Gurinov, Geeske Badart

Program outline:
The program will consist of both plenary and parallel sessions with multiple time intervals allowing direct interactions between participants and sponsors.



The following topics will be covered:

Bio NMR Computation EPR / ESR Hyperpolarization Hardware	Materials Metabolomics MRI -in vivo Small mol. / Drug discovery Solid-state NMR - Methods & Applications	Solution NMR - Methods & Applications Benchtop / Low field Single molecule detection / NV centers Tutorial session on MRI

We are honoured to announce the following speakers:
Plenary:
Anja Bockmann (France),
Christian Griesinger (Germany),
Robert G . Griffin (USA),
Songi Han (USA),
Mutusko Hatano (Japan),
Sophia Hayes (USA),
Kresten Lindorff-Larsen (Denmark),
Claudio Luchinat (Italy),
Tatyana Polenova (USA),
Gregg Siegal (The Netherlands),
Stefan Stoll (USA),
Andrew Webb (The Netherlands),
Carel Windt (Germany)

See you all in Utrecht in July 2022!

Minutes of the meeting of the AMPERE Committee

online, on January 12, 2022

Members present (34):
A. Böckmann, B. Blümich, H. Oschkinat, T. Prisner, A. Gil, A. Pastore, B.H. Meier, C. Thiele, D. Topgaard, E. Bordignon, G. Bodenhausen, G. Parigi, G. Mollica, I. Reile, I. Felli, J. Tritt-Goc, J. Dolinšek, J. Plavec, J. van Duynhoven, J. Matysik, K. Jaudzems, K. Köver, L. Ciobanu, M. Sardo, P. Giraudeau, P. Schanda, P. Vasos, R. Boelens, S. Ashbrook, S. Jurga, V.-V. Telkki, W. Kozminski, M. Ernst, S. Hiller

Agenda:
1. Approval of the agenda.
2. Approval of the minutes of the AMPERE Committee meeting online on June 28, 2021
3. Report on the state of the AMPERE Society (A. Böckmann)
4. Discussion and Vote on the AMPERE Young Member Representative (B. Blümich)
5. Varia

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

Ad 1.
The agenda was approved as is.

Ad 2.
The minutes of the AMPERE Committee were approved.

Ad 3.
A. Böckmann reported on the state of the society. She welcomed the newly elected committee members. The past year was still governed by the corona virus. Nonetheless, she mentions the meetings that were held, some online, some hybrid. The AMPERE prize 2021 for young investigators was given to Antoine Loquet and the Andrew prize to Reid Alderson. For 2022, most conferences will be in-person or hybrid, with the Euromar 2022 being hopefully in real life. Other activities are the AMPERE visual encyclopedia, as well as personal interviews with selected researchers in the bulletin. Last year, 4 such “portraits” were made, with G. Bodenhausen, J. van Duynhoven, C. Thiele and R. Kaptein. A. Böckmann memorates four community members who passed away recently, Shimon Vega from Weizman Institute, Prof. Khetrapal from Indian Institute of Science, Kenneth Packer, and Girjesh Govil.

Ad 4.
B. Blümich reported on the application procedure for bureau young member(s), which was handled by the prize committee. 11 applications were received. In a pre-vote, the committee members selected 3 top candidates for further discussion. These are Dennis Kurzbach, associate Prof. at Uni Vienna, AUT, working on dissolution DNP methods. Guinevere Mathies, University of Konstanz, DE, she is an Emmy Noether Group leader, working on DNP and EPR methods. Quentin Stern, PhD student in group of Sami Jannin at University of Lyon, FR, working on low field NMR and DNP.

The present members discussed the three candidates. Different aspects were raised in favor of the individual candidates. The suggestion was made to elect two young members. A majority voted for the option that two members be elected rather than one. A majority voted for Mathies and Stern, while highlighting that Kurzbach due to his position as associate Prof. is an excellent candidate who would perfectly fit being a regular committee member. The committee also decided that in the two young members should in the future ideally be one person at PhD level and one person at junior PI level, just as represented by the pair Stern / Mathies.

Ad 5.
G. Bodenhausen announces that the new journal Magnetic Resonance has been running for around two years and all associated procedures work now very well. Presumably, Web of Science and Pubmed indexing will start very soon, this is a highly protected privilege and Magnetic Resonance fulfills all criteria necessary for it. The next committee meeting will take place on the occasion of the EUROMAR 2022.

The meeting closed at 15:03.

Basel / the internet, 12 Januar 2022
Minutes: Sebastian Hiller

In memoriam

Remembering Shimon Vega, November 14, 1943-November 16, 2021
(November 14, 1943-November 16, 2021)

Shimon Vega was born in Amstel, Holland, on November 14, 1943. During the war period he was protected by a Dutch family, from the age of six weeks, until the end of the second world war. He, thus, survived the Holocaust along with his whole immediate family which included his sister Bea and his brother and fellow NMR scientist Alex Vega. Shimon would later say that "this was not a good time and place for a Jewish child to be born, and led to what perhaps was the most interesting part of my life". Shimon did his school education in the Elementary School Ouderkerk, Amstel, during 1950-56, and later in the Maimonides High School, Amsterdam, during 1951-1961. He did his university education in the University of Amsterdam with Physics as the main subject. He was, however, already aligned to magnetic resonance due to the influence from his brother Alex who was already pursuing a PhD in NMR with Daniel Fiat in the Weizmann Institute of Science (WIS), Israel. Shimon finished the final exams in the University on October 8, 1969. He was associated with a number of extra-curricular activities, prominent being the member and group leader of the Bnei Akiva movement, chairman of the Jewish Students' organisation, and member of the general students' organisation.

Shimon joined the Feinberg graduate school of the WIS on November 1, 1969. His PhD supervisor was Zeev Luz, however, his publications during the PhD were mostly authored only by Shimon. The thesis was on NQR and dealt with topics such as, relaxation, Overhauser effect, and tensor properties of quadrupole spins. The papers provided, as was going to be the case throughout Shimon's career, comprehensive mathematical derivations supporting the conclusions. Shimon would never run away from equations, a trait that he kept up with all along his life; more importantly, he had the unique ability to make others understand them as well. He believed in completeness and rigour. For him it was simply clear that excellence is not negotiable.

Following his PhD Shimon joined Alex Pines at the University of Berkeley, CA, USA, as his first postdoctoral fellow. Pines was already warned by Zeev that Shimon is a brilliant student, but older than Pines, and that he should listen to Shimon. In Pines's opinion, Shimon was one person who was able to understand the entire essence of the ideas he presented him with, and execute them well. These included multiple-quantum excitation and subsequent line-narrowing experiments in solid-state NMR, deuterium spectroscopy, and operator formalism for double-quantum NMR. It was during this period that Shimon began to develop one of the versions of the fictitious spin-1/2 operator formalism, which has henceforth proved to be vital in the understanding and development of many experiments in solid- and solution-state NMR and later in EPR and even in quantum optics. Shimon was clearly ahead of others in the field and had planted his imprint on the magnetic resonance scenario at that young age itself.

Shimon joined the WIS as a faculty in 1976. He concentrated on the study of half-integer spin quadrupolar nuclei, a passion that he held on to till the last months. Shimon was as eager as ever to discuss with us some of our recent attempts to spin lock such quadrupole spins and we had three rounds of Zoom meetings in March 2021 the last of which was probably a couple of days before he was hospitalised. It was in the same week that Shimon also shared with us his sadness in losing Kostya (Konstantin Ivanov who succumbed to Covid19 on March 5, 2021) who was a great friend and colleague of both of us.

In 1982, during a sabbatical Robert Griffin at MIT, MA, USA, Shimon worked on the theory of magic-angle spinning (MAS) in solid-state NMR and MAS sidebands. This is also when he first introduced Floquet theory to MAS experiments to explain the origin of rotor-frequency lines in the spectra of rotating solids, and continued with line shape analysis for 2-site exchange processes and homonuclear dipolar interactions. Later he worked on recoupling methods in the group of Jacob Schaefer, where he also spent a 1990/1991 sabbatical which led to TEDOR and SEDRA. It was these research programmes that highlighted the complex time dependencies in MAS which were further complicated in the presence of radiofrequency fields, as in the case of decoupling or recoupling. Shimon was quick to realise that the popular average Hamiltonian theory based on Magnus expansion was not enough to treat solid-state NMR experiments with such complex and simultaneous time-dependent perturbations. This resulted in the adaptation of single-mode and later multi-mode Floquet theory. The Floquet approach, once simplified Hamiltonians could be derived, was most insightful, as it allowed to actually see the origin of various conditions, for e.g. energy level anti-crossings and the resulting resonance conditions. However, getting there often had a high „activation barrier" which made its progress slow among the community. It was later realised that indeed Floquet theory is the way to treat processes that involve multiple time dependencies which could be simultaneous and non-commensurate. During the last two decades Floquet theory has become the tool to handle complex

pulse schemes in solid-state NMR and pulse sequences have been predicted as well for specific purposes. The theory is also gaining importance and application in DNP as well. Again Shimon was ahead of his time!

Additional path breaking research of Shimon included the development and understanding of heteronuclear spin decoupling pulse methods, design of homo- and hetero-nuclear recoupling methods, such as, RFDR and REAPDOR, high-resolution proton NMR with phase-modulated Lee-Goldburg (PMLG) scheme, fast-amplitude-modulated pulse methods (FAM) for sensitivity enhancement of the spectra of half-integer quadrupole spins, and deuterium spectroscopy and associated dynamics. Many of these methods have found applications in both materials science NMR and biomolecular NMR. During the last decade he became increasingly involved in a collaboration with his long-term colleagues Daniella Goldfarb and Akiva Feintuch, in dynamic nuclear polarisation (DNP)–particularly in understanding the mechanism of DNP at high magnetic fields and under MAS. He was instrumental in introducing quantum mechanical models to explain DNP with a direct correlation to experiments. He was deeply involved with various facets of DNP and occasionally, solid-state NMR, till the day he was hospitalised and also in the last days whilst he was in the hospital.

Shimon was an exceptionally great scientist and person, who was deeply caring as well. He was a patient and constructive listener and had the ability to get to the root of the issues with minimal fuss. At the same time, he was detached enough to give the entire credit to his co-workers. With his infectious enthusiasm and boundless energy, it was always engaging and a pleasure to discuss science and even other matters with him at length. His idea of understanding was not a superficial one, but rigorous and total. He had equations, matrices, Hamiltonians, and all such things right in his heart and always on the top of his head. Not only that he never ran away from difficult equations, but he had that impeccable quality to make his co-workers understand them as well. As a mentor, Shimon was always there irrespective of his other busy schedules and administrative commitments. He made sure that each one of his students developed their personality and scientific temperament in an unblemished way. The scientific rigour and comprehension were of paramount importance, not the publications and the associated paraphernalia. It is, hence, no wonder that most of Shimon's graduate students and post-doctoral fellows are all well placed in academia. In fact, Shimon had this to say in December 2018, "An important person is not made by other persons. They are special in their own ways and when they get basis, they stand out. I don't believe I created scientists, I was lucky that they were good scientists and we did it together. It turned out that they did good jobs. I give credits only to others. That's how I look at it." This is quintessential Shimon with an unadulterated, unabashed, and non-negotiable honesty, sincerity, and empathy with legendary generosity and selflessness.

Shimon had a special flair for teaching, whether basic or advanced. He was one of the most sought after teachers in the WIS and he used to give tutorial kind of lectures in conferences, which were all unscheduled, to packed audiences. Such was his aura and wisdom that these talks were deeply appreciated by all in the magnetic resonance community. Seldom did Shimon realise that he was indeed a rock star in the field of magnetic resonance.

Shimon served twice as the department head, first in 1986-89 when it was the Department of Isotope Research and again in 2005-11 after it was renamed as Department of Chemical Physics. His scientific achievements were recognised by many prizes that include the Kolthoff, ISMAR, the 2003 ICS (Israel Chemical Society) prize for the Outstanding Scientist, and the 2018 ICS Gold Medal.

The magnetic resonance community will miss Shimon dearly. This is a hole with which we have to live from now on. However, thank you Shimon for all the wonderful and elegant contributions that you made to our field, enhancing our knowledge, and making our life easier. Our heartfelt condolences to his wife Margriet, and daughters Yocheved, Batia, and Irit.

P. K. Madhu, Tata Institute of Fundamental Research, Hyderabad 500 046, India
Asher Schmidt, Technion-Israel Institute of Technology, Haifa 32000, Israel

Shimon Vega in the eyes of his students and postdocs

Remembering Shimon Vega, November 14, 1943-November 16, 2021
(November 14, 1943-November 16, 2021)

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Introduction

Professor Shimon Vega (1943–2021) of the Weizmann Institute of Science passed away on the 14th of November. Shimon Vega established theoretical frameworks to develop and explain solid-state nuclear magnetic resonance (NMR) and dynamic nuclear polarization (DNP) techniques and methodologies. His departure left a profound mark on his many students, postdocs, and colleagues. Shortly after his passing away, we all assembled spontaneously for an international online meeting to share our reflections and memories of our experiences in Shimon's lab and how they affected us deeply during that period of time, and throughout our scientific careers. These thoughts and feelings are put here in writing.

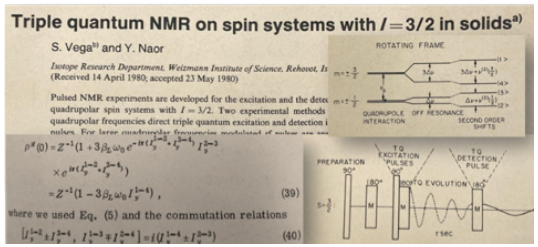
Amir Goldbourt

When I was a PhD student with Shimon, Cohen-Tannoudji visited the Weizmann Institute. Perhaps his most memorable advice was how to pick your supervisor. He said – "find a person that you like and the science will be great." I thought how lucky I was to choose the right supervisor. I was learning from an amazing scientist but moreover, a unique human being that always gave you the feeling that you are the most important person in his life at that moment and those that follow. The years 1996–2003 will always be engraved in my memory.

I joined Shimon's lab as I wanted to see in my own eyes how quantum mechanics comes to life in experiments, and magnetic resonance was the right choice for that. Shimon made quantum mechanics real and beautiful. For that reason, although Shimon suggested that I work on 2H NMR (which I did at the beginning), I was asking for more energy levels. Thus my PhD studies focused on half-integer spin quadrupolar nuclei. From Shimon's perspective that only meant that the math is more fun, because he could now diagonalize 4x4 and 6x6 matrices, and he could do it in ease by scratching transformation operators on the blackboard. But Shimon would make you do it yourself with his endless patience. You would stand in his famous room at the end of the corridor, stand by near the blackboard, and try with all your effort to diagonalize Hamiltonians. While you are mixing up Hamiltonians with density matrices, Shimon would work on his computer and occasionally throw insightful remarks, and you would realize that while working on his own affairs, he would still be one-hundred percent focused on your endless struggle and lead you to the correct solution. The greatness of Shimon as a PhD mentor was his ability to make you learn in a gentle and elegant way by guiding you without explicitly solving anything directly. Somehow, he would cause your mind to arrive at the correct answers.

Shimon wrote many seminal papers when I was still at elementary school, many of them on multiple-quantum NMR using fictitious spin operators. The most influential paper that goes with me everywhere (I still have the yellowish hard-copy, as authors used to get them by mail from the journal) was on triple-quantum excitation of quadrupolar nuclei[1]. I still think and feel fictitious spin-half operators, and use these tools to understand problems we encounter in our lab. I feel obliged and enthusiastic to always pursue better ways to perform quadrupolar NMR spectroscopy.

I try to take from Shimon the patience, the quest for every detail, the devotion to scientific truth and integrity, and the devotion to be there for any eager student, be it your own, or of other.


Triple quantum NMR on spin systems with $I=3/2$ in solids[a)]

S. Vega[b)] and Y. Naor

Isotope Research Department, Weizmann Institute of Science, Rehovot, Is
(Received 14 April 1980; accepted 23 May 1980)

Pulsed NMR experiments are developed for the excitation and the detec
quadrupolar spin systems with $I=3/2$. Two experimental methods
quadrupolar frequencies direct triple quantum excitation and detection i

$$\rho^{M}(0)=Z^{-1}(1+3\beta_L\omega_0 e^{-i\pi(I_y^{3-2}+I_y^{3-4})}I_y^{3-3}\times e^{i\pi(I_y^{3-2}+I_y^{3-4})})=Z^{-1}(1-3\beta_L\omega_0 I_y^{3-4}), \quad (39)$$

where we used Eq. (5) and the commutation relations

$$[I_x^{3-2}\pm I_x^{3-4},\ I_x^{3-3}\mp I_x^{3-4}]=i(I_z^{3-4}\pm I_z^{3-3}) \quad (40)$$

Like all great artists, Shimon's scientific song and spin art will always be with us.

Gil Goobes

As an undergraduate student, I had a sense that nuclear magnetic resonance is an exciting field, and probably what I will want to carry out my research on. Professor Gil Navon taught a course on magnetic resonance spectroscopy at that time and was running in parallel a graduate level course on the subject – which I, naturally, joined. Before moving to the Weizmann Institute for my graduate degrees, determined to continue with NMR, I asked the teaching assistance in the graduate course, Itamar Ronen, now Professor at the Leiden University Medical center, who should be contacted in case I am interested in NMR theory, and his immediate response was Shimon Vega! So, this has paved the way to carrying out both my MSc and PhD research with Shimon and turned out to be a judicious and gratifying experience. One aspect of working with

Shimon on NMR problem solving is the perpetual test of the depth of dive into the theory that one was willing and capable of taking. You can imagine climbing a winding road to a high snowy peak with a cheerful clear-eyed guide always showing up in front of you, restless, at each curve and turn, never tired and always leaping forward two steps ahead, effortlessly. Mind you, you still had to climb up yourself, whether it was writing down the correction terms for finite-pulse XY-8 REDOR using Floquet theory or working out the analytical expressions for matrix diagonalization of homonuclear-coupled spin Hamiltonians.

One quality of Shimon which may not strike immediately as typical of him is his openness to new ideas and initiatives. We were allowed the time to program a Matlab code for the REDOR transform (which was already proposed by Karl Mueller at the time) and amused ourselves with possible core functions suitable for the other anisotropic interactions. We discussed ways of polarization enhancement and delved into fundamental reasons why an equivalent of stimulated emission population inversion in a MASER in the microwave region was not possible in the radiofrequency region for NMR. However, large out-of-course excursions were gently and cleverly discouraged as Shimon was too knowledgeable to allow a complete waste of time. One of the projects, in which I felt that Shimon was caught slightly surprised with an unanticipated result, was flipping individual proton lines while applying a phase modulated Lee Goldberg (PMLG) decoupling field, which we were running together with Elena. We tested the crystalline hydrate of histidine*H_2O with its 10-proton spin system and were trying to record the magnetization transfer between protons after such DANTE-PMLG flip, only to discover that the protons would diffuse fast! too fast when the strengths of all contributing interactions were accounted for. It dawned on us, then, that the sample we used was uniformly ^{13}C labeled and that the homonuclear carbon-carbon couplings would serve as a spin bath

that would cause the extra leakage of spin magnetization through the non-negligible ^{1}H-^{13}C couplings. By including CW decoupling on the ^{13}C through the sequence and verifying with a natural abundance histidine sample we could confirm that this was the reason for the faster spin diffusion.

Shimon, it is the outstanding combination of your true caring mentorship and a sweeping endeavor of solving fundamental research challenges that has made the experience of spending time under your tutorship unforgettable, thank you.

Yonatan Hovav

I have been a student of Prof. Shimon Vega during my masters and PhD, as well as during a short postdoctoral period, with most of our period together devoted to the study of static solid state DNP. There are many praises to give Shimon as a teacher, a mentor, a scientist, and a person. Below are some glimpses into who he was to me, and I believe to his other students and co-workers as well.

I joined Shimon's Group after taking his NMR primer. Something in his enthusiasm and friendliness drew me to him. I did not have a quantum mechanical background, but was

fascinated by it, and hoped Shimon would help me understand it better. To join the lab, you had to go through Shimon's fire test (I believe most, if not all, of his students passed it): "Why would you come to my lab?" he would ask, "you will need to work much harder to get the same results as in other labs". And he was right – my MSc period left me confused and with little results, at least in my mind, and yet I stayed for a PhD. It was there that all the hours spent with Shimon and his students sank in, and suddenly things made sense. I ended up spending most of my time writing and playing with quantum mechanical simulations, trying to understand the basic mechanisms of DNP.

Shimon would often say that our task in science is to transfer the knowledge from one generation to the next – starting from the giants of old and building the generation to come – and in his knowledgeable and patient way he acted on it. His door was always open to us, and we could come and ask any question. The main obstacle was finding a time where there wasn't another student in the room already, being one of his own students or not. Going into his office with a question, he would often take me back several steps to the basics, making sure I built a solid foundation in his patient way. I would then solve my question with him on the board or at the office armed with the new understanding he gave me. He had a way of simplifying the physics – one day he took me on a gedanken bus ride to explain perturbation theory. But as time went on, we talked more and more in matrices and Hamiltonians, creating a Vega group shorthand DNP convention. When a hard question came, we would often work on it in parallel.

Shimon would take research to heart, as well as his student's wellbeing. He would come to see how an experiment was going (spinning on the lab chair in his energetic way), coming to the student's office to hear the latest experiment or simulation results, or calling you to his office and saying he didn't sleep at night thinking about the problem at hand. He would help out when needed, learn about what we discovered, and give direction in his gentle way: "if I were you I would do this and that next" he would say. His reactions were often an inverse reflection of my own feelings: when I was excited about some new result, he would cool me down, talking about possible problems or the next steps; and when I was down – he would try to pick me up, pointing to past successes. Shimon would always have something good to say about everyone. If he disagreed with the theory, he would point out to the experiment, and while he worried that a competitor would publish something before us – it always felt we belonged to the same group. While he believed in his way of thought – he tried to connect it to that of others. Before anything else, he would view you as a person, and as such would treat you in his friendly and polite way.

I feel fortunate, thankful, and privileged to have had Shimon as my mentor, and to have taken part in his group.

Ilia Kaminker

As perhaps all the others who have passed through Shimon's research group, I share the same experience of having to convince him to take me in. I spent six years, during my PhD with Daniella Goldfarb, sitting in the student room two doors from Shimon's

office. By the time I was looking for a postdoctoral position, we knew each other. I took Shimon‘s NMR primer, he helped us with theory on one of my papers with Daniella, and I heard him present many times in various magnetic resonance conferences. Still, when I asked him if I could join his group, he tried, as was his custom, to talk me out of it. Fortunately, I was persistent enough and had the honor and privilege to work with Shimon for two years (2012–2014).

During that time, we worked closely with Shimon‘s PhD students Daphna and Yonatan with constant support from Akiva Feintuch. When I joined the group, the three of us were working on separate projects, all having to do with understanding of DNP. Somehow, after a few months, all the projects had merged, and we realized that we are actually all working together on different aspects of one bigger problem. The combined effort during the remaining year and a half remains a unique scientific experience with the three of us under constant guidance from Shimon tackling, revealing and slowly understanding a complicated phenomenon.

Another profound influence of Shimon on me was the realization that there are different levels of understanding. All of us sometimes say to ourselves „now I understand it“. Shimon had very strict requirements as to what „understanding“ means. Understanding for him had to do with rigorous derivation; it had to be firmly based on the very basics of magnetic resonance and quantum mechanics. He did not believe in hand waving arguments – they never convinced him. It took me quite some time to adapt myself to Shimon‘s requirement of „understanding“ and I am very grateful to him for this. It has undoubtedly made me a better scientist.

I greatly miss Shimon. After returning to Israel I had many ideas that I was hoping to discuss with him. I wanted to invite him to see my lab – something that, now, will never happen. Rest in peace Shimon.

Vladimir Ladizhansky

I joined Shimon’s group as an MSc student in 1993 on the advice of Professor Yehiam Prior, and had the privilege of spending the next six years in his lab and continuing to learn from him for much longer. My MSc and PhD theses were at the interface of chemistry and physics, focusing on the analysis of II-VI diluted magnetic semiconductors and semiconductor nanoparticles. As Shimon’s main interest was in the fundamentals of NMR spectroscopy, most other graduate students and postdocs in the lab worked on various spectroscopic problems (e.g., RFDR, NMR of quadrupolar nuclei, proton spectroscopy). Early in my PhD, I became somewhat dissatisfied with my “outcast” status and asked Shimon to involve me in the spectroscopy projects. At the time, he was working on the theory of cross polarization (CP) and offered me the opportunity to join these efforts. My first assignment was to read and understand an article that Shimon had just published along with another PhD student, David Marks, in which they established a unified view of static and magic-angle spinning CP experiments.[2] The CP paper was one of my first encounters with complex NMR spectroscopy, and it served as an entry to my scientific career. I struggled with that paper back then (and still do now!) as it is

quite mathematically intense, but after numerous hours of discussions, working through our disagreements together, and getting through the equations with his guidance, a consistent picture of one of the most important solid-state NMR experiments began to emerge. The CP paper shaped my understanding of dipolar recoupling experiments, and specifically those that involve strongly coupled systems.

Shimon had an amazingly clear and at the same time constantly evolving picture of magnetic resonance and the ability to bring physics to life. His door was always open to students, and interacting with them and mentoring them were among his greatest joys. He valued our opinions and ideas even if they were nonsensical. In many ways, his influence, which was not limited just to science, had a profound impact on my life and future career. We have lost a true scientist and scholar. He will be missed dearly.

Michal Leskes

I got to join Shimon’s group pretty randomly. I was a Chemistry undergraduate in my second year at Tel Aviv University, looking for something to do in the summer. I came across the summer program at Weizmann and thought I’d try. I quickly realized I had no idea how to choose a lab for the summer and going through the webpages of researchers at Weizmann didn’t help at all, since nothing made sense. I knew I liked spectroscopy, but beyond that I decided to choose based on who was smiling in their photo – and that is how I got to Shimon Vega’s group. This was probably the best career move I made… joining Shimon’s group for that summer completely determined what kind of research I would do in the next few years and what kind of scientist I aspire to be.

Only in retrospect I can appreciate the dedication of Shimon. I was only a second-year undergraduate student, yet Shimon spent a few hours every day with me, teaching me the basics of NMR in solids. We would talk during the day, and he would give me questions to think about and get back to him for the next day. Taking the train from Tel Aviv to Rehovot and back every day gave me time to process these lessons. After a month Shimon said I was ready to run the first NMR experiment of 1H-29Si CP on mesoporous silica (of course with guidance from Shifi Kababya). By the end of the summer I was running variable temperature ^{13}C-{^{17}O} REAPDOR experiments that in addition to generating useful dephasing curves also caused a mini flood in the NMR room. This was a great summer and I summarized it in a poem to Shimon – ‘A fun summer it’s been, with magnetic resonance and O seventeen. But after all of the time you’ve put in, I still don’t know what is spin!’

Without saying

I really did not fully appreciate this period in real time, but when I came back to Weizmann as a graduate student I realized what a unique person and teacher Shimon was and chose to join his group for my PhD. With Shimon, and a yearly visit from Madhu, we were working on homonuclear and heteronuclear decoupling using Floquet theory to understand our results. Life was a constant debate between theory and experiment and a feeling of uncertainty and confusion. But what kept me going and kept it all fun was

a kind of safety net Shimon provided – I felt that Shimon had it all figured out. That in fact he had this master plan of what we were doing, and perhaps we're missing a minus sign here or factor of two there, but overall he already knows what we will get because he solved it all late at night. I was never alone, any doubt or panic about some basic or complex concept that suddenly did not make any sense could be resolved after talking to Shimon (or after an email from him written at 4 am!). It was also great fun to argue with him about results and to be joyful together when theory perfectly matched the experiment.

Towards the end of my PhD, during my postdoc and then after joining the Weizmann Institute as faculty, I learned that Shimon was also the kindest, most patient listener. It never mattered what he was in the middle of or how stressed he was, he was always happy to take a break and talk about whatever was on my mind, be it the next scientific or personal challenge. It was such a privilege to have my office two floors above his and my NMR lab two floors below his office, making it my first stop coming up from the lab whenever we got a new scientific success or failure. It will take me some time before I don't pause on the second floor of the Perlman building. Shimon, I miss you. Thank you for all that I know and all that I don't know… and now have no one to ask.

Fred Mentink-Vigier

"If you join us, then what will you do after your post-doc?" Shimon started my interview with this question. To be honest, I think the question made me join Daniella Goldfarb and Shimon Vega back in 2012. The question revealed how much he cared about the people he worked with, and this is probably the reason why, up to his illness, we have remained close.

The two years I spent at the Weizmann were very stimulating. From the very first days I was exposed to the group discussions about Liouville space, relaxation, and DNP. I was fascinated by the discussion between Akiva Feintuch, Yonatan Hovav, and Shimon but barely understood them.

Shimon's office door was always open, and we could come in anytime to bring up a question or discuss the experimental results. Shimon was a fantastic teacher for whom no question is stupid. Instead, he would not only explain in detail, but would reformulate until we really understood. The open door-policy had additional perks. During the discussion someone would come in and contribute or bring another question, expanding the scope of my initial visit.

As a postdoc, Shimon and Akiva gave me the MAS-DNP project due to my coding skills but I barely understood the theory when I started it (of course, Shimon made me familiar with it). One day, I wanted to check the cross-effect simulations and ran them in absence of microwave irradiation. The result was "weird": the nuclear polarization at steady state deviated from thermal equilibrium. I did not believe it and was sure that something was wrong with the code. Shimon had a different stance and we spent four days discussing and running simulations until we understood it. The effect was real. Shimon's attitude taught me to welcome any result that would change my view of the problem.

After two years at the Weizmann Institute, the MAS-DNP simulations officially became my project, one that I still work on. I was afraid I would lose contact with him and felt rejoice when my (French) phone plan included unlimited calls to Israel: I could continue talking with Shimon while riding my bike in the morning.

We officially continued to work together until 2017 and we last were in touch for science on a daily basis during spring 2020, when I was deriving the "Landau/Zener" cross-effect evolution operator for strongly coupled electron spins.

Shimon was always modest in his presentations, and clearly was driven by the genuine interest of "understanding" any experimental observations. However, I would dare say that for him, personal relations were the most important aspect in his life. I witnessed it firsthand from his lifelong friendship with Daniella Goldfarb, Lucio Frydman, Zeev Luz and many others. As one may expect, after nine years, our relationship expanded well beyond the professional sphere. We would always begin our discussions with "How is life treating you?" or "How are the kids?" We last met at Euromar 2019 and it's hard to express how much I'll be missing him. Shimon has done his best to promote my work and help me integrate in the NMR community. He made me meet people and talk at conferences, and in that sense, he went beyond the question he asked during my interview: he helped me build my career.

He was conscious of the role of mentor, and I owe Shimon so many things that I hope the reader can measure the respect I and others have for him.

PK Madhu

Shimon Vega was an exceptionally kind and compassionate person and a scientist par excellence. My own association with Shimon as a post-doctoral fellow was from November 9, 1997, till May 9, 1999. However, our collaboration continued strongly with our joint last paper on heteronuclear spin decoupling that came out in 2017. We had very regular discussions on NMR and related science, life in general, a bit on politics, culture, and history all along till March 10, 2021, before he was admitted to a hospital. Our last discussion was on the possibilities of locking half-integer quadrupole spins, one of his favorite topics which he shared with his brother Lex. In our conversations in the second week of March 2021, Shimon also shared his pain in losing Kostya (who succumbed to Covid19 on March 5, 2021), a common friend and colleague of both of us.

Shimon, noted for some of the most insightful research in the area of magnetic resonance, both electron and nuclear magnetic resonance, has influenced professionally and to some extent personally the lives of many of us who have come in contact with him. This could be in the form of graduate students, post-doctoral fellows, colleagues, course students, or listeners to one of his great talks packed with science, wit, and active involvement. His enthusiasm has been often contagious and his understanding deep enough to compel chairmen of his talk sessions to give him enough time after regular sessions to explain to the particular conference audience nuances of his theoretical

ideas. These were always done with a deep flair to packed audiences. Shimon was indeed one of those rare combinations of openness to new ideas with deep-rooted knowledge on sound, pen-and-paper principles, rather than pursuing transient fashions. He belonged to that genre with a great willingness to share his knowledge with others and was a restless researcher ready to question the so-called established paradigms. His inquisitiveness had always motivated his colleagues, taking the respective research to even higher levels. Of the many contributions Shimon had made, some to highlight are in the magic-angle spinning experiments in solid-state NMR, breaking the barrier into understanding quadrupole spins, introducing Floquet theory to understanding and developing various experiments and improving resolution and sensitivity of solid-state NMR experiments, and in the last few years providing insights into the important field of DNP in NMR.

Shimon had fun doing science and was never shy of sharing his ideas and thoughts at any stage of a concept, whether published or not. For him, understanding an idea was important and the only key issue. The rest were all details for the sake of others. He was a great, active, and patient listener who put all at ease and treated others with a child-like innocence and unbridled laughter. I remember various conferences, including the Indian Magnetic Resonance Society meetings for which he came a few times, schools and workshops, and other gatherings where his infectious enthusiasm would be influencing positively the students and others and even the on-lookers. He did not know that he was a rock star, but he was indeed one in the field of NMR and in science.

The NMR community and I will definitely miss Shimon. It was indeed a privilege to have worked with him, known him a bit, and travelled and interacted with him. The dimensions of the matrices he worked with are most often boundless, and his memories with us also will remain so.

Silvia Pizzanelli

I joined Shimon's lab in 2002–2003 as a postdoc with a fellowship funded by the Center of Excellence on "the origin of ordering and functionality in meso-structured hybrid materials" of the Israel Science Foundation and the Italian National Research Council. During my PhD in Chemistry at Pisa University under the supervision of Carlo Alberto Veracini I had studied liquid crystals using 2H NMR and often had come across papers by Zeev Luz and Shimon Vega. As I wished to further specialize in solid state NMR, my obvious choice was Shimon's lab. I simply wrote him an e-mail, and he simply answered inviting me to the Weizmann Institute for a first meeting.

My project dealt with the adsorption-desorption kinetics of tetra-alanine at the surface of the pores of an MCM-41 mesoporous material. I spent the first months in the preparation of the sample. Since an aqueous solution of the peptide was to be inserted in the pores of MCM-41, I could not use the capillary condensation method, usually employed for the insertion of pure liquids. Therefore, I just added MCM-41 to the solution, but this method was fraught with potential problems, like incomplete filling, location of the solution in the extra-porous space, or instability of the MCM-41 structure. In this process, Shimon

was a continuous source of critical questions and pertinent suggestions, constantly challenging the interpretation of a phenomenon through the experimental evidence. But Shimon was also a man of great humanity. When Saddam Hussein was captured during the second Gulf War, I have a vivid memory of his sense of discomfort as he could not rejoice over the misfortune of any person. Sometimes he shared with me his genuine interest on the people around us, referring either to science or to human relationships. In these small talks, he was sharp and direct, and my personal views were usually in consonance with his, which created a positive and friendly atmosphere. His humbleness still echoes in my mind in the words "there is a whole world out there" that he used to say when he came across some robust and comprehensive study of a subject he had only marginally touched.

After 2003 I chose to go back to Italy and life brought me far from the adsorption project started with Shimon. On the contrary, he went on for another ten years investigating different peptides and porous materials. Today my only regret is that I did not continue collaborating with him, although he gave me the chance to do it by giving me samples and a program for simulating MAS spectra in the presence of a two-site motion.

Ingolf Sack

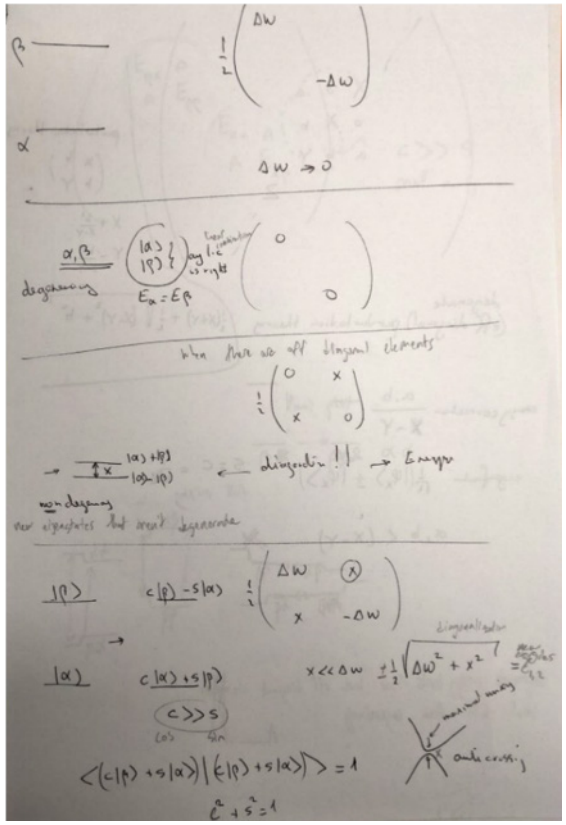
Shimon was an extraordinary person and outstanding teacher. Perhaps he was the most important teacher for me, with whom I was fortunate to spend a certain period of my life in Israel, at the Weizmann Institute. Shimon had the ability to explain things that loomed only hazily on the horizon of my experimental work in solid-state NMR. This allowed him to predict early on how we would need to design the experiments to accurately determine ^{2}H-^{13}C distances with maximum signal yield. Whether it was the analytic derivation of the Hamiltonian in this specific spin-1 spin-1/2 quantum system, or tensor diagonalization in general, Shimon did this with an ease as if it were small talk. Indeed, working with Shimon had the joy, inspiration and ease of a long conversation among friends in which one learns much about the essentials of science and the meaning of life. I am forever grateful to Shimon for the time I was privileged to spend with him, which had a lasting impact on me beyond the realm of science.

Daphna Shimon

I'm honored to be Prof. Vega's last PhD student. When I joined his group in 2008, the interest in DNP was seeing resurgence, and I had the great privilege of learning NMR and DNP from Shimon, while also learning DNP together. We spent many hours sitting together trying to understand the experimental data I had accumulated, and to figure out how to model the spin physics of DNP when we could only simulate at most 5–6 spins. There were many days when he would come in the morning and tell me that overnight he had thought of another way we can try and simulate the thing we were looking for. This persistence is something that I always associate with Shimon. He would never give up on trying to understand even the smallest experimental feature. The things I will most remember about Shimon are probably the things many others will remember

too: how kind he was, how humble, how good a teacher, and how he always knew how to adapt his explanation of a topic to the person he was talking to. At the very beginning of my masters, I was starting to write simulations of DNP, but I did not fully understand what I was doing. One day, I was simulating a small spin system, and he had me look at the energy levels as a function of the off-resonance. He had me zoom all the way in, and then asked me what I saw. He used this exercise to explain anti-crossings and state mixing. That was the day I finally understood the simulations. I kept the paper, which he wrote upside down so I could read it while he was writing, and I still have it to this day. It's a joy to look back and realize how clearly he could explain complicated topics. Part of this paper is shown here.

Jayanthi Sunderasan



I was fortunate to be associated with Shimon during my graduate studies at the Indian Institute of Science (IISc) in Bangalore. Thanks are due to Madhu for introducing me to Shimon in 2004. While at the IISc, I had frequent email conversations about NMR with Shimon, and most of the time he responded within 24 hours. He had invested time and patience in answering my NMR-related queries, and those discussions were very helpful for me in my early research and also throughout my career.

Subsequently, I joined Shimon at the Weizmann Institute as a postdoctoral student in 2010–2013. I was his last postdoctoral student who worked on a solid state NMR project. During that time, we worked closely with Asher Schmidt and Shifi Kababya, which involved multiple train journeys to Haifa, starting early morning, utilizing the time during our journey to discuss Floquet theory and deuterium dynamics. The eight-hour computational time for a Floquet Matlab simulation was addressed in one of those train journeys with a lot of equations, and in the following

week, we could reduce the computational time to a few minutes. Whenever I was stuck with the underlying theory of deuterium dynamics and adsorption-desorption kinetics of small molecules in mesopores, he reassured me that „we are together in this project, we will understand it soon". That was more than an assurance and I realized only later, when I started my career, that the knowledge I acquired when I was with him was abundant and priceless. Whenever I reached out, he continued his support by all possible means, with no hesitation and no delay, but each time with more energy, enthusiasm and joy. He helped me tremendously in every aspect of my life, be it NMR, career, or personal life.

Shimon was such a wonderful person, a "spring of wisdom" as Asher would say, a humble human being and a great scientist. His passing away has left a void impossible to fill. Yet I consider myself privileged and fortunate to have known him. The amount of cheerfulness, knowledge, care, concern, friendliness, and comfort that he has given each one around him, I hope will lead me ahead in my journey. The contagious energy and enthusiasm when he was around is what I would like to carry in his absence. By behaving the ‚Shimon way', he taught me how to treat others, how to be humble yet competitive, ambitious but aware of our own limitations, and finally to respect everyone for what they are. I will be missing Shimon, yet Shimon will always be around.

Elena Vinogradov

When I was accepted to the PhD program at the Weizmann Institute I was elated and somewhat surprised. I was not sure what I would study, but I was quite sure it would not be NMR. In fact, during the admission interview I was asked about NMR and I told them, honestly: "I don't know much about it, I am not interested in it and I prefer not to answer any questions about it". Despite my hutzpah, I was accepted. And then, I had to take a quantum mechanics course. And I was privileged to meet the best Teacher I had ever met and one of the best people I was fortunate to encounter. Shimon's approach to teaching stunned me. He rarely gave a straight answer. He was always asking what we thought. He was actually making sure that we understood. He was always saying that he does not know/remember or only recently understood the answer. It was always "answering a question with a question", but taken to unbelievable levels of scientific curiosity. I was hooked on the discussion. On the opportunity to think. I thought to myself that it would be interesting to do a rotation in his lab. The rest "is history".

My first project was under the supervision of him and Professor Zeev Luz (another giant of NMR). The project failed, but the remnants of the simulation code came useful in the next steps. I was lucky to join Madhu and work on the PMLG experiment. The most challenging and rewarding part was the derivation of the bimodal Floquet theory and its application to describe the combined effects of MAS and periodic RF. We spent countless hours going over the equations, of course with me trying mostly to catch up with what Shimon had already understood. Many times Shimon would come in the morning and say something like "I was thinking about it…" which would start derivations and discussions that ensued for several days. The whiteboard would be covered with formulas, and signs of "do not erase" would be written. Floquet theory described all the

experiments beautifully. Not only were we able to explain experimental observations (broadenings at specific spinning frequencies) but also to predict experimental features, such as the position of the rotary lines. Moving on to less steps and expanding to a windowed version, the scaling factors, the deterioration of efficiency, everything was explained there, by the Floquet theory. To have a theory that correctly predicts experimental outcomes and to be able to confirm it by doing the actual experiment is exactly what science is about.

Shimon was always respectful of others. He was humble and always knew something wise to say (or not to say) in challenging situations. I left solid state NMR and moved to imaging. During all the years after my PhD I would call Shimon often to talk about science and life. He was always interested, even in the projects that had little to do with his own research. When DNP reached in vivo imaging we had several interesting discussions about its applications and the future of the technology. After these conversations I always felt enlightened and optimistic about science and life in general.

Without Shimon, the world is darker. Shimon, you are greatly missed.

Edited by Dr Yuval Elias, Bar-Ilan University, Israel

On January 18th, 2022, Massachusetts Institute of Technology held an online tribute symposium “Remembering Shimon Vega” organized by his long-time friends and colleagues Robert Griffin, Kong Ooi Tan, Daniella Goldfarb and Lucio Frydman. This seminar is available online[3].

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Magnetic Resonance in Porous Media	Hangzhou (China)	August 21-26
Alpine Conference on Magnetic Resonance in Solids	Chamonix (France)	September 4-8

Ampere Event 2023

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