epr newsletter

2021
volume 31 number 3

The Publication of the International
EPR (ESR) Society

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https://ieprs.org/newsletterpage/

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Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

The *EPR newsletter* is published quarterly by the International EPR (ESR) Society and is available in electronic and printed form to all members of the Society. The deadlines for submission of news for upcoming issues: Spring March, 15; Summer June, 15; Fall September, 15; Winter December, 15.

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epr newsletter

The Publication of the International EPR (ESR) Society

volume 31 number 3 2021

The cover picture illustrates aspects of the research carried out by Elena Bagryanskaya, recipient of the IES Silver Medal for Chemistry 2021. It demonstrates the advantages of orthogonal spin labeling using triarymethyl radical (TAM) and nitroxide (NIT) for studying DNA complexes with human apurinic/apyrimidinic endonuclease 1 and possibility to obtain structural insights revealed by pulsed dipolar EPR with orthogonal spin labeling.

IES business

Awards

In memoriam

Editorial

Dear colleagues,

It seems I was a bit too optimistic, in my editorial of the *EPR newsletter* 31/3, claiming that there is a light at the end of the tunnel as regards the coronavirus pandemic. Even though the vaccination rate increased considerably all over the world, the corona waves, which we are experiencing, show that there is still a long way to go. As a result, the coronavirus restrictions remain, and our personal contacts, which we missed so much in 2020, have been extremely rare in 2021.

Even the IES Annual General Meeting 2021 was held on August 24th in the online format at the ISMAR-APNMR 2021 conference (August 22–27, 2021, Osaka, Japan). This meeting was recorded and it can be viewed at https://ieprs.org/on-line-activities. The detailed report of the IES AGM 2021(pp. 3–6) clearly shows that the pandemic could not hamper the diverse activities of our society aimed at increasing its visibility and attraction to the magnetic resonance community. Elena Bagryanskaya gave the IES Silver Medal for Chemistry 2021 lecture online and received the award certificate from Kev Salikhov, who handed it to her in Akademgorodok (Novosibirsk, Russia) on behalf of Songi Han, IES President. In her article (pp. 8–10), Elena presents three examples, which illustrate the possibilities of EPR in detecting physical, chemical and biological processes.

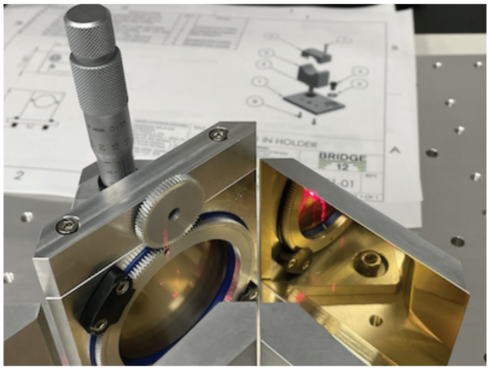
Gabriel Moise (JEOL Prize 2020) and Nino Wili (JEOL Prize 2021) describe their exciting relevant studies (pp. 11–16). It is good to know that Gabriel looks forward to continuing his involvement with the ESR community in the future. Nino was already featured in the newsletter as the initiator of the IES Virtual EPR meetings (30/1-2, pp. 3, 4). Nino recently defended his PhD and has to do some Civil Service now but good news is that he plans to continue with the magnetic resonance research.

The intention to give floor to Luis Fábregas Ibáñez, one of the three IES Best paper Awardees 2020/2021(https://ieprs.org/best-paper-award) revealed a problem. When I asked Stefan Stoll to send me a short write-up on Luis, he reminded me about the recent Luis' contribution to the Software column "DeerLab, new flavor in dipolar EPR data analysis", which was published in the *EPR newsletter* 31/1 (pp. 12–14). Stefan underlined that it was exactly what the IES Best paper was about. This meant that it does not make sense to follow the routine and invite Luis to prepare an article on his research for publication in the newsletter. Instead, I asked him to give an interview and – ta dah! – you are welcome to the first interview of a young researcher to the *EPR newsletter* (pp. 15, 16)!

This interview is not the only novelty in this issue: by the initiative of Songi Han, we introduce a new column, "Meet Our Major Sponsor", and the first contributor to this column is Eric Bryerton, Vice President of Engineering, Virginia Diodes (pp. 6, 7). It is great to add a personal touch and to get an answer to the curiosity about what story lies behind the hardware and software we use in our research.

To end on a sad note, we bid farewell to Jack Peisach, one of magnetic resonance early pioneers and practitioners, the IES Silver Medal in Biology awardee (1999), and caring mentor. John McCracken prepared a comprehensive obituary full of deep feeling (pp. 18–20). We join John in grieving on this loss and send heartfelt condolences to Jack's family, collaborators and friends.

Laila Mosina



IES ANNUAL GENERAL MEETING 2021

Minutes of the Annual General Meeting of the International EPR/ESR Society for 2021 held online at ISMAR-APNMR, 23:05–23:45 (JST) August 24, 2021 (Held via Zoom). AGMs recording can be found in: https://ieprs.org/on-line-activities.

Agenda:

1. Introducing the new Executives (2021-2023) (Songi Han)
2. Announcement of the 2021 IES Awards (Songi Han)
3. Report of IES activities 2021 (Songi Han)
4. Report of the EPR newsletter Editor (Laila Mosina)
5. Report of the Secretary (Aharon Blank)
6. Report of the Treasurer (Peter Qin)
7. Planned Activities for the next year (Songi Han)
8. Questions, Discussion, and Suggestions (Songi Han)

1. Introducing the new Executives (2021-2023) (Songi Han)

Dear Colleagues,

On behalf of the IES Executive Board I wish to welcome all participants of the online IES Annual General Meeting 2021.

IES executives (2021-2023)

President: Songi Han
Vice President Asia Pacific: Yasuhiro Kobori
Vice President Americas: Michael Wasielewski
Vice President Europe: Maxie Roessler
Secretary: Aharon Blank
Treasurer: Peter Qin
Immediate Past President: Thomas Prisner
EPR newsletter Editor: Laila Mosina

2. Announcement of the 2021 IES Awards (Songi Han)

2021 John Weil Young Investigator Award

Thomas Schmidt, Scientist, NIDDK NIH, Clore Lab

Award Lecture delivered at the 2021 Euromar (Virtual) *Accessing Protein Binding Nonequilibrium Kinetics by EPR Dipolar Spectroscopy*

2020 John Weil Young Investigator Award

Sabine Richert, Emmy Noether group leader, Uni Freiburg

Award Lecture was delivered at the 2021 RSC (Virtual) *Exploring photogenerated molecular quartet states as spin qubits*

2021 IES Silver Medal for Chemistry

For significant contributions to EPR including its application, development and improvements in the area of Chemistry.

Elena Bagryanskaya, Novosibirsk Institute of Organic Chemistry

Delivered @ ISMAR-APNMR Award Session

2021 IES Silver Medal for Instrumentation and Methods

For significant contributions to EPR including its development and improvements in the area of Instrumentation and Methods

Stefan Stoll, University of Washington, Seattle

Award Lecture to be delivered at the 2022 Royal Society Conference – EPR (University of St. Andrews, in Person)

2021 IES Fellow

Fellowship is conferred on individuals who have made influential and distinguished contributions to the practice of EPR Spectroscopy and its welfare over a long period

Klaus-Peter Dinse, Freie Universitaet Berlin

Award and Award Lecture to be delivered in person (TBD)

2021 Best Poster Prizes (to date)

RSC ESR Spectroscopy Group

Fabian Hecker, MPI Biophysical Chemistry: "^{17}O ENDOR detection of water molecules on the radical transfer pathway of ribonucleotide reductase"

Luis Fábregas Ibáñez, ETZ Zurich: "DeerLab and new aspects in dipolar EPR spectroscopy analysis"

EUROMAR2021 Conference

Annemarie Kehl, MPI Biophysical Chemistry: "Resolution of Chemical Shift Anisotropy in ^{19}F ENDOR Spectroscopy at 263 GHz/9.4 Tesla"

Matthias Bretschneider, Uni Frankfurt: "Multiquantum Counting on Trityl Radicals"

More Best Poster Prizes to come at ISMAR-APNMR and MDMR2021.

2021 Best Paper Awards

Luis Fábregas Ibáñez (ETH Zuerich): *DeerLab: a comprehensive software package for analyzing dipolar electron paramagnetic resonance spectroscopy data*, J. Magn. Reson. 1, 2020 (DOI: 10.5194/mr-1-209-2020)

Michal Kern (University of Stuttgart): *Hybrid Spintronic Materials from Conducting Polymers with Molecular Quantum Bits*, Adv. Funct. Mater. 31, 2020 (DOI: 10.1002/adfm.202006882)

Nandita Abhankar (University of Maryland, NIST): *Scalable microresonators for room-temperature detection of electron spin resonance from dilute, sub-nanoliter volume solids*, Science Advances 6, 2020 (DOI: 10.1126/sciadv.abb0620)

3. Report of IES activities 2021 (Songi Han)

Short Report of the previous Minutes of the Annual General Meeting of the International EPR/ESR Society for 2020 held online on November 4 and 5, 2020 (Held via Zoom). Two AGMs recording can be found in: https://ieprs.org/on-line-activities. See EPR newsletter 30/4 (2020) pp. 4–6.

IES Virtual EPR Meeting (IVEM)

https://ieprs.org/on-line-activities.

Run and organized by students and young researchers

March 2020 – July 2021

Committee EU/West Coast Edition

Nino Willi, ETG Zuerich
Annalisa Pierro, BIP Marseille
Dennis Buecker, University of Konstanz
Shreya Ghosh, University of Pittsburgh
Sonia Chabbra, MPI for Chemical Energy Conversion
Lizzy Canarie, University of Washington
Jason Sidabaras, MCW

Committee Asia Pacific Edition

Hiroki Nagashima, Saitama University
Fei Kong, University of Science and Technology of China
Martyna Judd, Australian National University in Canberra
Julien Langley, Australian National University in Canberra

August 2021 – present

IVEM Committee

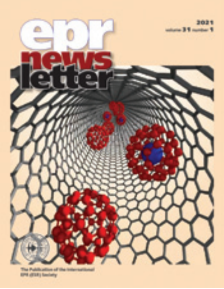
Zhongyu Yang, North Dakota State University, USA
Thomas Schmidt, NIH, USA

Annalisa Pierro, Centre National de la Recherche Scientifique (CNRS), France
Zhijie Li, University of Science and Technology of China
Jana Eisermann, Imperial College London, UK
Jaideep Singh, University of Southern California, USA
Jing Jin, Boston College, USA
Julien Langley, Australian National University, Australia
Li Feng Li, Australian National University, Australia
Nir Dayan, Technion - Israel Institute of Technology

IES Virtual EPR Meetings (IVEM) are broadcasted via Twitter and Emails
IES Twitter (https://twitter.com/EPR_ESR)
681 Followers, 91 Following
NEW Online Activity Manager: Zhongyu Yang (NDSU)
Together with Aharon Blank and Songi Han are tweeting from @EPR_ESR
Critical medium to reach young scientists and a broader audience
EPR_ESR tweets are embedded on several webpages (ieprs, RSC EPR group, etc)
Join and follow us @EPR_ESR
Encourage your students to follow @EPR_ESR and stay active
The IES:
Tweets about EPR Job Postings, EPR Conferences, Tweets about EPR Publications
We will find your paper, but you can request a tweet from the IES (via its webpage)

4. Report of the EPR newsletter Editor (Laila Mosina)

Since the previous online AGM of the IES in November 2020, we published 30/3, 30/4, 31/1 and just finished 31/2. We hope you had a look at 30/3, 30/4, 31/1 and 31/2 on the IES website and got color copies 30/3, 30/4 and 31/1.



EPR newsletter covers all aspects of the life of the EPR community.

Now we finalized 31/2 and work on the forthcoming issue 31/3. To remind you, we present the columns of the newsletter:
– Editorial
– IES business
– Awards
– IES Young Investigator Award Revisited
– Another Passion
– Anniversaries
– EPR newsletter Anecdotes
– In Memoriam
– Present Meets Future
– Software
– Tips and Techniques
– Notices of Meetings
– Conference Reports
– New EPR Faculty
– New Books and Journals (including EPR Hot Science)
– Market Place
– Reader's Corner
– Guest of the Issue

Please feel free to submit YOUR material, dear colleagues! You produce the news, and we present it in the EPR newsletter.

On behalf of the Editorial Board, I thank most heartily all contributors to the EPR newsletter with special thanks going to the CEOs of the IES and editors of the columns in the EPR newsletter: John Pilbrow, Candice Klug, Wolfgang Lubitz, Stefan Stoll, Keith Earle, Sabine Van Doorslaer, and Sergei Akhmin, our Technical Editor.

I gratefully acknowledge collaboration with Associate Editors Candice Klug, Hitoshi Ohta and Sabine Van Doorslaer.

5. Report of the Secretary (Aharon Blank)

The Secretary is responsible for the day-to-day operations of the Society, and ensures efficient functioning of the Society, e.g.:

1. The Secretary shall maintain all the records of the Society, shall keep the minutes of Society meetings, and be responsible for the distribution of all essential information to members.
2. Sending out invoices to the sponsors (in consultation with the Treasurer).
3. Informing members (and sponsors) of the various items of interest, e.g., announcements of conferences, workshops, publication of new issues of EPR newsletter.
4. Organization of material for awards given by the IES: medals, certificates and citations.
5. Overlooking financial status and membership of the Society (in consultation with the Treasurer).
6. Website: maintenance and upgrades, ads and positions. We are looking for interesting photos, papers, links (see next) – please send them out.
7. Answering any enquiries.
8. Organizing AGM.
9. Liaisons with the President, Treasurer, Editor of the EPR newsletter, and the members of the IES Executive.

Major tasks over the last year:

1. Continued updating of IES webpage
2. Recruit speakers to present EPR tutorials at Bruker Webinars
3. Handling of Awards, fellowships and the "Best paper Award" new initiative
4. Updating of the IES twitter page (with Songi Han, Thomas Casey, and now led by Zhongyu Yang)
5. Printing and distribution of EPR Newsletter (with Secretary's kids)
6. Adding new sponsors

6. Report of the Treasurer (Peter Qin)

2020 Financial Report ($)

Balance on January 1, 2020	**51,499.61**
Deposits:	
Membership	2,658.00
Sponsor Contributions	27,000.00
TOTAL deposits:	29,658.00
Expenditures:	
Internet Commerce & Merchant Services, Banking	666.20
IES Community Support (Conferences, Training, Poster Awards)	3,229.98
IES Operation (Web, Printing, Editorial)	21,030.73
Misc (Registration, Postage, etc.)	75.00
TOTAL expenditures:	25,001.91
Balance as on 12/31/2020	**56,155.70**

▶

2021 January-June Financial Report ($)

Balance on January 1, 2021	**56,155.70**
Deposits:	
Membership	2,690.12
Sponsorship	4,350.00
TOTAL deposits:	7,040.12
Expenditures:	
Financial Service Fees (Merchant Services, Banking)	435.28
IES Community Support (Virtual Gp Mtg)	2,610.00
IES Operation (Web, Printing, Editorial)	18,686.50
Misc (Registration)	75.00
Total expenditures:	21,806.78
Balance on June 30, 2021	**41,389.04**

John Weil Fund

Established in 2010 in memory of Prof. John Weil by family, friends, and colleagues to support John Weil Young Investigator Award.

Starting Balance on 01/01/2020:	**$ 22,625.82**
Interest Income:	$ 332.76
Distributions for 2020 YIA:	$ 1,045.00
Ending Balance on 12/31/2020:	**$ 21,913.58**

7. Planned Activities for the next year (Songi Han)

Best Poster Prizes in 2022

RSC (Royal Society Conference) EPR Group in St. Andrews, Scottland
RMC (Rocky Mountain Conference) EPR in Denver, USA
Euromar of the Groupment Ampere in Utrecht, The Netherlands
MDMR (Modern Development of Magnetic Resonance) in Kazan, Russia

Silver Medal for Physics/Material

Fellows of IES

John Weil Young Investigator Award

Deadline for Nominations December 1st 2021

Nominations by active IES members; 100–150 word citation; CV; Publication List

IES Best Paper Award (for young scientists) – Deadline for nominations March 2022

Self nomination; First author with support letter from corresponding author/ supervisor which explains the contribution of first author

2022 IES AGM at the 17th Spin Chemistry at Northwestern University, Chicago

Local Organizer: Michael Wasielewski (IES Vice President Americas)

IES Membership Drive: WE NEED YOU!

$6/year for students, $12/year for emeritus and post-doctoral fellows, $36/year for full members.

1. Lowered barrier for becoming first time members
   Immediate email confirmation is sent
   Accepts credit card, Paypal, Alipay (there are some problems)
2. Automated renewal system
   Email reminder is being sent
   Automatic subscription is possible (could an email be sent confirming this annually?)
3. Collection hub for membership fee
   Russian EPR society offers a model
   IES designated conferences, such as the ISMAR-APNMR
4. Group subscription options NEW $50 for 6 members

8. Questions, Discussion, and Suggestions (Songi Han)

Suggestion to amend IES bylaws

– IES best paper Award has been “running”on “pilot”mode for the last 3 years.

– IES proposes to formalize this procedure by setting it up in the IES bylaws.

IES Best paper Award

The IES will acknowledge each year up 2 publications as “best papers” in the field of EPR. The first author is recognized with this award. The expectation is that the first author is a young scientist. Nomination can be made by any active IES member. If self-nomination is made, it can be made only by the first author or the corresponding author. Any nomination should be accompanied by letter from the PI and/or advisor explaining the role of the nominee.

The application material should include the following items:

a. Cover letter not exceeding 1 page with your name, role and affiliation, full citation of the paper and explanation as to why this paper represents an exciting advance and breakthrough development in the broad area of EPR and ESR.
b. PDF of the nominated publication.
c. Letter from the PI and/or advisor, not exceeding 1 page, explaining the role of the nominee.

Create more visibility of the Society – also for **young researchers!**

– Invite young scientists (YIA/Poster Prize winners) to the IES Board Meeting – **at real meetings** ...

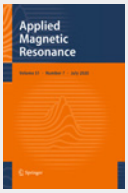
– Create an interactive Communication Platform on our Webpage

– **Twitter** ...

– Put links to tutorials, special articles on our new Webpage

– Create a directory of EPR groups

Host EPR database – first for Dipolar EPR Data base



Thanks

The IES thanks the following Corporate Sponsors for their contributions in 2021:

- Applied Magnetic Resonance (Springer) – Major sponsor
- Bridge 12 – Major sponsor
- Bruker BioSpin Corp. – Patron
- GMW Associates – Supporter
- JEOL Resonance Inc. – Major sponsor
- L & M EPR Supplies – Contributor
- LOGS – Major sponsor
- Rotunda – Sponsor
- Virginia Diodes, Inc. – Major sponsor

Special thanks go to all paid up IES members and the Zavoisky Physical-Technical Institute, Kazan for supporting the EPR newsletter.

The meeting was attended by all ISMAR-APNMR participants from the field of EPR.

Meet Our Major Sponsor

Virginia Diodes

Mission. To make the terahertz region of the electromagnetic spectrum as useful for scientific, military and commercial applications as the microwave and infrared bands are today.

Products. VDI manufactures state-of-the-art test and measurement equipment for mm-wave and THz applications. These products include Vector Network Analyzer, Spectrum Analyzer and Signal Generator Extension Modules that extend the capability of high performance microwave measurement tools to higher frequencies. VDI's component products include detectors, mixers, frequency multipliers and custom systems for reliable operation at frequencies between 50 GHz and 2 THz. All VDI components include in-house fabricated GaAs Schottky diodes and microelectronic filter structures.

History. VDI was founded in 1996 by Dr. Thomas W. Crowe, VDI CEO & President. From 1996 to 2001 VDI sold only Schottky Diodes for scientific applications including radio astronomy and high frequency radar. During this period, VDI operated as a University of Virginia (UVa) spin-off and utilized the facilities at the University. Around 2001 VDI expanded to include offices in downtown Charlottesville, VA and started selling complete mixer, detector and multiplier products for 50–1000 GHz operation. By 2004 VDI started selling subsystems such as THz Transmitter & Receiver modules. Also in 2004 all VDI operations moved to the 979 Second Street location in Charlottesville and VDI stopped utilizing UVa facilities. Since then VDI continued to grow the number of product offerings and employees needed to satisfy a broad range of terahertz and millimeter wave customers. Today, VDI employs over approximately 100 engineers, technicians and administrative staff working in a high tech 20,000 sq. ft. facility.

Interview with Dr. Eric W. Bryerton, Vice President of Engineering, Virginia Diodes, Inc.

EPR newsletter: *Dear Dr. Bryerton, the IES greatly appreciates the support of Virgina Diodes, which contributes to the EPR community by generating products of importance to our community. We are most appreciative that you agreed to answer the questions of this interview. What is your educational and/or research background?*

After receiving my PhD in electrical engineering from the University of Colorado, I wanted to work in a scientific environment. The development of the Atacama Large Millimeter Array (ALMA) was just beginning and it looked like a fascinating international project with quite esoteric technology, especially at that time (1999). I did not have any experience yet working above 10 GHz, but the challenges of millimeter-waves fascinated me, being at the cross-over of electronics and optics. After completion of this immense project, in 2013, I was looking for a different type of work environment, but I wanted to stay in millimeter-wave and THz development. As an engineer at NRAO, I had been a customer of Virginia Diodes for many years, as they provided the critical frequency multipliers for all the receivers on ALMA. From this long interaction, I really respected the company, so it was a perfect fit. It also meant that I could continue to support the scientific community, not only in radio astronomy, but also in many other disciplines where millimeter-wave technology was required, such as EPR and DNP.

How was the idea conceived to found a company? What were the stages of the formation and development of your company?

I have been with VDI since 2013, but the company was founded in 1996 by Dr. Thomas Crowe, then a Professor of Electrical Engineering at the University of Virginia (UVa). Even before this, the UVa semiconductor device lab was providing Schottky diodes for radio astronomy applications since the 1970s. In the early years, it was just Tom and one other person in the UVa cleanroom producing Schottky diodes for highly specialized scientific applications. Then in 2001, two more principals were added, including Dr. Jeffrey Hesler, the current CTO. Responding to the needs of the community, VDI began to offer packaged waveguide mixers and multipliers, in addition to bare diodes. A few years later, these waveguide components were integrated together with other components to form complete sub-systems, again responding to calls from our customers to produce complete turnkey solutions. Then in 2008, we developed frequency extension modules, a more standardized version of the sub-systems we had already been producing. This was in response to the need from the general test and measurement community for easier measurements at these high frequencies, similar to what they were accustomed to at microwave and RF. The development of the company has followed this path of increased integration and functionality, though it should be noted that we do still sell bare diodes for those who wish to build their own components.

What specific challenges have you had as a company? How were these obstacles overcome?

The challenge in our field is there are many niche applications for our products, but none of them on their own is a particularly large market. So we are a "low-volume, high-mix" manufacturer. We have many many products, each one operating at or near the state-of-the-art. This requires the ability to fabricate many different variations of diodes with many different assembly techniques tested to many different requirements. It requires us to be extremely agile and to be highly responsive to the needs of our wide and diverse customer base. As a design and development engineer, you need to learn a little about a lot of different topics… I need to know enough about astronomy, chemistry, magnetic resonance, communication, etc. to be able to understand the customer's requirements and offer a solution. It's tremendously challenging, but also extremely fun as you are continuously learning.

Where are most of your customers located?

Serving the scientific and research community as we do, we have customers all over the world. Roughly one-third of our business is in the US, one-third is in Europe, and one-third in East Asia. As with the low-volume, high-mix concept, this requires a lot of agility. Dealing with customers from many different regions and cultures is sometimes challenging, but it is a fun challenge if you enjoy travel and learning about different parts of the world. We have terrific distributors in many of these locations, including France, Germany, Italy, Scandinavia, Japan, and China.

What is your idea about the secrets of business success?

I'm not sure there is any "secret". I think you need to have a product that people want, and you have to listen to the customer to be responsive to their needs… Most of all, you should be having fun!

What is your message to the magnetic resonance community?

Please let us know how we can help! We love to develop new hardware with new capabilities. ●

IES Silver Medal for Chemistry 2021

Nitroxides and trytils for biophysics and material science

Elena Bagryanskaya

Elena Bagryanskaya and Kev Salikhov, who handed the IES Silver Medal for Chemistry 2021 certificate to her on behalf of Songi Han, President of the IES

It is a great honor for me to receive the 2021 Silver Medal for Chemistry from the International EPR Society. I see this medal as an award to many talented young scientists with whom I was lucky to work and to the Novosibirsk scientific school I was raised in. I am very thankful to the stimulating interdisciplinary environment in Akademgorodok, which shaped me as scientist and to the broad international network of collaborators and friends with whom I share my main scientific passion – interest to radicals and magnetic resonance effects. Already in my diploma thesis at the Institute of Chemical Kinetics and Combustion SB RAS I was fascinated by rich information, which magnetic resonance provide about radical intermediates of chemical reactions, particles – which live so short, that they could not be detected directly. This fascination helped me to build up my own group in International Tomography Center SB RAS in very difficult times just after the break down of Soviet Union, with low budget available for science. Now, after more than forty years of working in the field, I am excited by broad applications of radicals in physics, chemistry and biology. In my position and as a leader of the Novosibirsk Institute of Organic Chemistry I see this field expanding faster than ever.

In this paper I am happy to share with you three scientific examples illustrating the power of electron paramagnetic resonance to detect physical, chemical and biological processes.

EPR of breathing crystals

This story started in 2006 in collaboration with Victor Ovcharenko. He and his team designed the synthesis of novel compounds that held promise as the basis for various molecular-spin and magnetomechanical devices. These compounds of the Cu(hfac)$_2$LR family (where R is a nitronyl nitroxide) are called “breathing crystals”, because with temperature changes, they undergo reversible structural rearrangements accompanied by alterations of their magnetic moment. With a decreasing temperature, distances between unpaired electrons – located on two oxygen atoms of the nitroxides and one copper atom – decrease, leading to strong enhancement of the exchange interaction. As a result, the magnetic moment of this three-spin unit changes, reflecting the coupling of two electrons of the three. The reversible change of the unit cell volume during the rearrangements (“breathing”) reaches ca. 13% in some crystals of Cu(hfac)$_2$LR and is accompanied by a ~30% change in the magnetic moment. We found that the EPR analysis of these compounds is informative, even though in these systems, the exchange interaction is several orders of magnitude greater than the Zeeman interaction. EPR can detect only transitions between triplet states, and temperature significantly affects the population of states with spins of 1/2 and 3/2, which strongly influence the observed EPR spectrum. At low temperatures, only some EPR lines are present in the spectrum. Later, we noticed that a change in the magnetic moment can also be achieved by irradiation with light. Therefore “breathing crystals” can be used as magnetomechanical nano-switches operated by means of temperature or light. Using the EPR at different microwave frequencies (9, 35 GHz, and higher), we characterized the magnetic properties of breathing crystals and their alterations under the influence of temperature changes or light, thereby obtaining the information necessary for subsequent synthetic research on the pathway to molecule-based magnetic devices. The main results of this research are summarized in [1, 2]. To study these systems, we needed high-field EPR spectrometers, while in my lab, we had only X- and Q-band pulse EPR instruments. These investigations were only possible to be done in collaboration with well-known prominent scientists laboratories Arthur Schweiger and Gunnar Jeschke, Wolfgang Lubitz, Daniella Gorlfarb, Seigo Yamauchi.

The development of novel spin labels based on sterically hindered nitroxides, hydrophilic trityl radicals, photoactive spin labels and new conjugation chemistries and their application to biomolecules

During last decade we closely collaborate with chemists of NIOCh SB RAS: especially with Igor Kirilyuk, who is absolutely unmatched in the synthesis of diverse stable nitroxides, and Victor Tormyshev, a top expert in the synthesis of triarylmethyl radicals (TAMs). The result of this collaboration was the development of novel spin labels and spin probes [3]. We researched their magnetic-resonance properties and applied them to the investigation of biomolecules and materials science. For applications to biomolecules we were aimed to develop spin labels with high resistance to reduction in reducing media in order to study

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biomolecules in mammalian cells and to devise spin labels for distance measurements in biomolecules at room temperature.

Nitroxides with bulky substituents at positions close to the NO group possess the highest stability and are the most promising as pH-sensitive spin probes and sensors for oxygen in EPR tomography and as spin labels for biomolecules in mammalian cells. A large series of high stable spin labels and spin probes based on nitroxides were designed in group of Kirilyuk and we studied their oxidant properties to understand the main parameters of their stability. These data implied that the key point is following: bulky substituents can stabilize a nitroxide and/or destabilize a hydroxylamine.

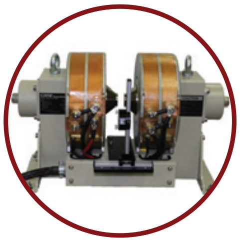
The long relaxation of TAMs at room temperature in liquid solutions makes them a promising alternative to traditional nitroxides. Victor Tormyshev and his team have synthesized a series of TAMs including a perdeuterated Finland trityl (D_{36} form); mono-, di-, and triester derivatives of the Finland-D_{36} trityl; a deuterated form of OX063; the dodeca-*n*-butyl homolog of the Finland trityl; and triamide derivatives of the Finland trityl with primary and secondary amines attached while we have studied room temperature electron spin relaxation properties of these TAMs and made conclusions concerning the most promising spin labels [4].

Pulse electron double resonance (PELDOR) spectroscopy allowing measurements of nanometer distances was proposed more than 30 years ago in Novosibirsk [5] and nowadays is widely used in biophysics and materials science. Until recently, these experiments have been limited to cryogenic temperatures (<80 K). It was very challenging to perform EPR distance measurements at room temperatures. The requirements for such experiments are long electron spin relaxation time and immobilization of biomolecules to prevent averaging of dipole-dipole interaction. We were lucky to perform the first distance measurement in a nucleic acid at a physiological temperature. A model 10-mer DNA duplex was labeled with reactive forms of a TAM, immobilized on a sorbent in an aqueous solution, and investigated by double quantum coherence (DQC) EPR [6]. Our later study revealed that saccharides, and especially trehalose, can efficiently serve as immobilizers of nucleic acids while mimicking their natural environment and allowing for a wide range of structural EPR studies at room temperature [7]. We also demonstrated that room temperature distance measurements can be performed not only using DQC by using other approaches DEER and RIDME.

It was important to develop a new versatile strategy for TAM attachment at arbitrary sites of nucleic acids, utilizing an achiral non-nucleoside phosphoramidite monomer for automated solid-phase synthesis of oligonucleotides, which were then postsynthetically functionalized with a TAM [8]. FTAM is rather lipophilic and susceptible to self-aggregation, to noncovalent binding with lipophilic sites in proteins, and to noncovalent docking at the termini of duplex DNA. Thus, in our recent paper, the highly hydrophilic OX063 TAM, which has low toxicity and negligible propensity for aggregation, was employed as the basis for a spin label [8]. Specific features of pulse dipolar (PD) EPR at ambient temperatures, in particular, requirements on electron spin phase memory time, ways to immobilize biomolecules, the influence of a linker between the spin probes and a biomolecule, and future opportunities, are reviewed in detail in [9].

Another type of spin label is photoexcited triplet molecules [10]. We proposed and validated the use of photoexcited fullerenes as spin labels for distance measurements by PD EPR. The hyperpolarization and narrower spectrum of fullerenes as compared to other triplets (e.g., porphyrins) boost the sensitivity and offer superior relaxation properties allowing PD EPR measurements almost at room temperature. This approach was demonstrated by means of fullerene-nitroxide and fullerene-triarylmethyl pairs as well as a supramolecular complex of a fullerene with a nitroxide-labeled protein [11].

In collaboration with Galina Karpova (Institute of Biochemistry and Fundamental Medicine SB RAS) we started to study of structural and functional organization of human ribosomal translational complexes. At the time, site-directed spin labeling (SDSL) of long RNA sequences remained a challenging task. We proposed a novel SDSL approach potentially suitable for long natural RNAs and based on the attachment of a linker containing an aliphatic amino group to a target nucleotide residue followed by selective coupling of a spin label with this amino group. Such a linker can be attached to an RNA residue of interest via a sequence-specific reaction with derivatives of oligodeoxyribonucleotides. We demonstrated that a novel complementarily targeted SDSL approach enables efficient spin labeling and subsequent structural EPR analyses of long RNAs, spin-labeling a hepatitis C virus RNA internal ribosome entry site consisting of ~330 nucleotides and having complicated spatial structure [12]. Recently we applied DEER/PELDOR spectroscopy to investigate model complexes mimicking different states of the human 80S ribosome during elongation and termination of translation [13, 14] using the following approach. The conformation of mRNA in the region of the human 80S ribosome decoding site was monitored using 11-mer mRNA analogues that bore nitroxide spin labels attached to the terminal nucleotide bases. Lately, we use TAM spin labels to study complexes of damaged DNA with apurinic/apyrimidinic (AP) endonuclease 1 (APE1). The use of orthogonal spin labels in the enzyme and in the DNA substrate has a crucial advantage: it permits detailed investigation of local damage and conformational changes in AP site-containing DNA alone or in its complex with APE1 [15].



The development of new approaches to living polymerization reactions using nitroxide radicals on the basis of our studies of DNP and free-radical reactions

Nitroxide-mediated polymerization (NMP) is a controlled/living radical polymerization technique that enables the design of well-defined, functional, and complex macromolecular architectures. The main parameters which determine the process of NMP are recombination rate constants of nitroxides with alkyl radicals and decomposition rate constants of correspondent alkoxymines. We applied EPR and original technique developed in my group: switched external magnetic field Chemically Induced DNP to study the mechanism of NMP [16, 17]. Later, we successfully employed nitroxides synthesized at NIOCh as mediators of methyl methacrylate polymerization [18]. EPR and NMR are helpful for elucidating the mechanisms of NMR, and eventually, we proposed various new approaches to the activation of smart alkoxyamines by pH changes, metal complexation, and 1,3-cycloaddition, which can be used for NMP and theranostics [19].

I am very lucky to work and collaborate with many scientists worldwide and would like to express my deep gratitude to all my former PhD students and postdocs, colleagues and coauthors: it's been a great pleasure to work with all of you, and I hope our collaboration will continue.

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JEOL Prize 2020

Gabriel Moise:

The Royal Society of Chemistry ESR conference is a major focal point in the calendar of many doctoral students in the field of ESR spectroscopy, both in the UK and internationally. I first became acquainted with the RSC ESR community in 2017, as a first-year doctoral student in the group of Prof. Christiane R. Timmel at the University of Oxford. I have since become very fond of the RSC ESR conference and benefited greatly from the power of this event to initiate interesting discussions and collaborations in the world of ESR.

It was thus upsetting when the cancellation of the 2020 edition, due to be hosted at The University of Manchester, was announced. Fortunately, one of the main attractions of the conference, the Annual JEOL Prize Talk Competition, was able to go ahead in an online format. I had the honour of participating in this competition as part of a cohort of seven excellent candidates, two of whom were awarded the runner-up: Kaltum Abdiaziz with a talk entitled '*Film electrochemical EPR spectroscopy as a new technique to investigate redox-based reactions*', and Janne Soetbeer with a talk entitled '*Noise spectroscopy – a quantitative relaxation descriptor and predictor*'.

I am thankful to the ESR Group Committee and JEOL for selecting my talk '*Spin delocalisation and fine-structure mysteries of the photoexcited triplet state of metalloporphyrins*' as the winning contribution in 2020. I am both honoured and humbled, particularly so considering the outstanding calibre of the presentations and research of the other contestants.

The work showcased in my talk is underpinned by the idea of designing molecular wires, nonlinear optical materials, and spintronic devices using porphyrins as fundamental building blocks [1]. Porphyrins are a class of π-conjugated macrocyclic molecules which play a central role in many fundamental biological processes such as photosynthesis and oxygen transport [2]. This is a result of both their remarkable charge transport ability and diverse redox chemistry, as well as their varied photophysical and magnetic properties. Furthermore, the porphyrin macrocycle is able chelate a multitude of metals from across the periodic table, thus resulting in a vast array of different electronic structures and applications thereof. It is the union of these properties which inspires the use of porphyrins in manufacturing nano-scale devices.

A functional oligoporphyrin based spintronic device relies on the ability to control and exploit the electron spin density and spin polarisation of the system by tuning the properties and structures of its constituent monomers [3]. Hence, ESR spectroscopy is instrumental in characterising the ability of porphyrins to act as building blocks for such devices because it probes these key properties directly. I have explored a variety of spin states and porphyrin systems using ESR in my doctoral work [4, 5]. In particular, my talk was focused on the characterisation of the spin density, its symmetry, extent of delocalisation, and spin polarisation in the photo-excited triplet state of a series of metalloporphyrin monomers, homodimers, and heterodimers. These properties were measured by a combination of transient continuous wave ESR, magneto-photo-selection, and pulse ENDOR techniques. The first of these techniques formed the basis of the data presented in the talk, whereas the latter two were indispensable in the interpretation of the data.

The parameters of interest were the magnitude and sign of the zero-field splitting D-value, and the pattern of spin polarisation, all of which dominate the ESR signatures of these triplet states. The D-value relates to the extent of spin delocalisation and the symmetry of the spin density, whereas the spin polarisation reflects the non-Boltzmann triplet sub-level populations arising from the cascade of intersystem crossing (ISC) events initiated by laser excitation.

The relatively recent work of Claudia Tait and Sabine Richert, former members of the Timmel group, has established an invaluable framework for the measurement and analysis of the D-value and spin polarisation pattern in porphyrin triplets [6, 7]. My work relied heavily on their results, and in particular, on the following observations regarding free-base and Zn^{2+} porphyrin monomers and homodimers: (1) both monomers have a positive D-value, reflective of an oblate (pancake-like) spin density, (2) both dimers have a negative D-value, reflective of a prolate (cigar-like) spin density, (3) the triplet Z sub-level is preferentially populated in the presence of Zn^{2+} by means of a direct spin-orbit mediated intersystem crossing mechanism, and (4) the free-base systems achieve their in-plane (XY triplet sub-levels) spin polarisation by means of a vibronic spin-orbit mechanism.

Equipped with the clarity of the results mentioned above for free-base and Zn^{2+} porphyrins, we were then faced with an exciting 'mystery': when the Zn^{2+} is replaced by Pd^{2+}, the magnitude of the D-value almost doubles, its sign becomes negative (from experiment) in both monomers and dimers, and the spin polarisation is maintained exclusively out-of-plane. However, when the heterodimer between free-base and Pd^{2+} was measured, the D-value was unchanged in sign and magnitude compared to the pure free-base system, and yet, the transient ESR spectrum was 'upside-down', suggesting that the spin polarisation was no longer in-plane!

The solution to the problem came from a combination of group theoretical considerations and electronic structure calculations. The fundamental difference with the Pd^{2+} systems is that the greater radial extent of the d-orbitals facilitates the overlap with the porphyrin SOMO and LUMO molecular orbitals. Hence, these triplet wavefunctions have a small, but important, contribution from the Pd^{2+} orbitals. A similar, yet weaker, contribution is found in the Zn^{2+} systems. The net result is that both metal systems exhibit out-of-plane ISC characteristics via a direct spin-orbit mechanism. These direct spin-orbit driven ISC events manifest strongly in all our metalloporphyrin systems (monomers, dimers, heterodimers) because they are a first-order perturbation, and hence do not depend on energy differences. By contrast, the second-order contributions of the spin-orbit coupling to the D-value will have a pronounced effect only for the palladium monomers and homodimers. The Pd^{2+} doped heterodimers exhibit a (first-order) spin-spin-only D-value because the triplet wavefunction is 'pushed' away from the heavy metal towards

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either the free-base or Zn^{2+} moiety (both of which have a lower energy).

The main conclusion of my talk was that Pd^{2+} can be integrated into oligo-porphyrin molecular wires as a way of controlling the spin polarisation without compromising the delocalisation length of the spin density. For example, the free-base and Pd^{2+} heterodimer exhibits an almost pure free-base spin density (confirmed by transient ESR, density functional theory, and ENDOR) whilst being spin polarised out-of-plane by the heavy metal.

The work outlined in my presentation was made possible by the Centre for Advanced Electron Spin Resonance at the University of Oxford where all the EPR measurements were done, and I am also thankful for the synthesis of the porphyrins which was done by the group of Prof. Harry L. Anderson. I am eternally grateful to my mentor Christiane Timmel for all her guidance and support.

Since finishing my doctorate in November 2020, I have been lecturing Physical Chemistry at several colleges at the University of Oxford and have recently also taken up a PDRA position in the group of Prof. Arzhang Ardavan in the Clarendon Laboratory. My current research is aimed at achieving coherent control of electronic and nuclear spins in graphene-inspired spintronic devices. I look forward to continuing my involvement with the ESR community in the future.

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Christiane Timmel:

In September 2015, with outstanding references and results from his undergraduate degree, Gabriel joined my research group first as a Master of Chemistry (MChem) and then a doctorate (DPhil) student.

I was one lucky supervisor.

Gabriel proved himself a truly outstanding graduate student, full of refreshing, genuine enthusiasm for all he did, even in the face of adversity keeping up his spirits and drive, without fail hard-working and mathematically extremely talented. As his supervisor, I always seemed to be two steps behind him in understanding either theory or experiment. Impressively, his hands-on experimental capabilities matched his remarkable mathematical and computational skills. In short, his research progress and outputs are truly due to him: his theoretical and experimental skills, patience and above all, determination to get things done.

Gabriel's doctorate work, as he so clearly explains in his article, was primarily focussed on the elucidation by means of ESR spectroscopy of the molecular and electronic structure of porphyrin-based molecular wires in both their cationic and excited triplet states, employing both experimental strategies and theoretical tools. He skilfully used a powerful combination of transient continuous wave ESR, magneto-photo-selection, and pulse ENDOR techniques, but above all he excelled in the theoretical modelling of the obtained results. He established robust recipes for the interpretation of spin delocalisation patterns in supramolecular complexes and through skilful symbiosis of group theoretical considerations and electronic structure calculations succeeded to gain unprecedented insights into the interplay of spin-orbit coupling and spin-spin contributions to the zero-field splitting, especially in the discussion of Pd vs Zn metalloporphyrin structures. It is the latter work he presented in his JEOL prize talk.

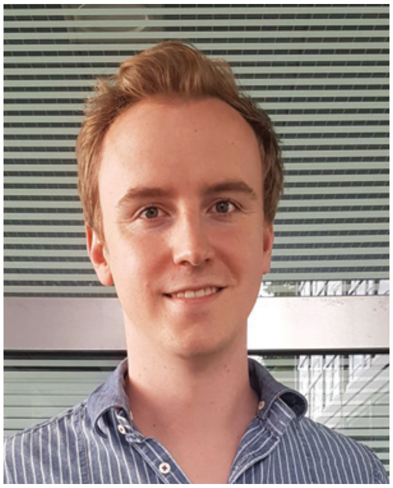
But Gabriel impressed not only through his depth of understanding and application; he showed a natural curiosity for all things scientific. It is hence no surprise that he quickly added to his portfolio of interests and publication list the field of avian magnetoreception. This work resulted in his authorship of a front cover of Nature in 2021 for his work on the ESR of cryptochromes.

I cannot finish this reference without also mentioning Gabriel's exemplary attitude towards those junior to him: he was a true inspiration to all incoming group members, providing gentle, daily guidance. One fact to illustrate his impact on the group shall suffice here. Each of the three students Gabriel took under his wing during his doctorate won the highly competitive MChem (Masters) thesis prize of our department, a pattern certainly recognised widely in our institution.

Gabriel is now a postdoctoral researcher in the group of Professor Arzhang Ardavan in the Physics Department in Oxford and I am watching his progress, proudly, from afar.

To finish how I started: I was one lucky supervisor and I wish Gabriel all the best for his future. I am sure that whatever he touches will become a success. And whoever works with him – well, will be one lucky colleague!

JEOL Prize 2021



Nino Wili:

I feel very honoured to have been awarded the JEOL Prize at the RSC ESR conference 2021 “in” Cardiff. In hindsight, I was quite lucky, because I handed in nearly the same abstract in 2021 as in 2020, but a year earlier I did not consider applying for a JEOL lecture.

I presented work on so called “Dressed Spin Resonance”, and its application to distance measurements between trityl radicals. I am only touching the scientific part here briefly and refer the more interested readers to the peer-reviewed publication [1]. Rather I will focus on how the ideas were generated, and what twists and turns the project took.

Dressed spin resonance refers to the following idea: In “normal” magnetic resonance, there is a large static field in the z-direction, and irradiation is applied with a frequency that matches the Zeeman frequency of the spins. The magnetic component of the irradiation must be perpendicular to the external field, sometimes also called the quantisation field. Now imagine the situation of a spinlock. In this case, the quantisation axis in the rotating frame is given by the spinlock field. The magnitude of this field is the nutation/Rabi frequency. The direction of the spinlock field in the rotating frame is determined by the phase of the irradiation.

What if, in the rotating frame, you could generate a perpendicular, oscillating field component? If this field oscillates with the Rabi frequency, you will generate a “pulse” on the spins in the rotating frame, the microwave-dressed spins, just as we usually use pulses to act on “bare” spins.

To me, this first sounded like a cute, but also rather esoteric idea. So let me tell you how I first heard about it.

In fall 2018, Gunnar (Jeschke), my PhD supervisor, offered a project on dressed spin resonance to an undergraduate student at ETH, Lukas Schreder. The last time Gunnar worked on this idea was about 20 years earlier, and even this was serendipity. Back in his PhD time, Gunnar worked on hyperfine-decoupled ENDOR. In this technique, nuclear transitions are irradiated *during* a spinlock pulse. Under strong enough irradiation, this leads to ENDOR spectra without any hyperfine coupling, which is sometimes helpful. However, he always observed a peak that was independent of any nucleus, and he quickly realised that the rf-frequency of this peak was determined by the nutation frequency of the spinlock pulse he used. The figure caption of the original publication that shows this peak comments on it: “The peak designated with an asterisk is due to the excitation of electron spin transitions” [2]. Which is true, but how on earth should an rf-irradiation of <50 MHz act on electron spins with a Zeeman frequency of 9.5 GHz?

The answer is exactly the dressed spin resonance effect. It turns out it is basically impossible to position an ENDOR probe head perfectly inside a magnet. There is always a tiny component of the rf-field that is parallel to the external field. For normal ENDOR experiments, this does not matter, because the transition moments are small anyway. But in the case of dressed electron spin resonance, the transition moment in the rotating frame is governed by the electron gyromagnetic ratio, which is roughly three orders of magnitude larger than the nuclear transition moment. Even a tiny parallel rf-component with the right frequency then leads to a significant reduction in electron spin echo intensity. This hypothesis could be tested very easily. In case of an X-band ENDOR probe head, you can simply turn it 90 degrees around its long axis in the cryostat. The microwave field is then still perpendicular to the static field, but the rf-field of the ENDOR coil is parallel. Indeed, the dressed spin resonance becomes even more intense in this case, and the ENDOR effect vanishes.

Back to the student project in 2018. From time to time, Gunnar supervises an undergraduate by himself, and in this case, this was also the original plan. But in August 2018, Gunnar became head of the Department of Chemistry and Applied Biosciences at ETH Zurich. It quickly became clear that it was impossible for him to supervise Lukas appropriately. He asked me if I could do it, and I said yes without thinking too much. I neither knew what the project was really about, nor how to use the spectrometer to do the experiment – so far in my PhD, I was mostly working with our home-built AWG spectrometer, and only seldomly with a Bruker one, and I have not done any ENDOR before at that point.

Around Christmas, the student project was finished, Lukas and I learned a lot about spectrometers and spin dynamics, but there was no obvious use for dressed ESR. Nevertheless, I was wondering if there was another way of doing the experiments, without the use of a longitudinal ENDOR coil. If you think about a z-field modulation, it is basically the same as a frequency-modulation. And a frequency-modulation can easily be implemented on an

AWG spectrometer. I tested the hypothesis, and indeed one could do dressed spin experiments on our home-built spectrometer, and many of the signals were cleaner and easier to set up (also because the software is very versatile). No ENDOR capabilities were needed anymore.

I presented these results during an internal seminar in spring 2019, and found it very neat, but not much more. There was another interesting finding, though. Because all these experiments involved spin locked echoes, I always saw that the relaxation under the spinlock was slowed down compared to Hahn echo decays. This was not a new finding, but I was wondering whether I could make use of this.

From my lectures in solid-state NMR, I remembered that there is a "magic echo" in NMR. Basically, the sign of the homonuclear dipolar coupling is inverted and scaled by –1/2 during a strong spinlock. Refocusing the dipolar coupling – this is exactly what is needed for distance measurements. And slower relaxation means longer accessible distances. I did not have a real idea how I could make use of this, but it was always at the back of my head.

Around the same time, another PhD student at ETH, Agathe Vanas, was presenting work that involved new trityl model compounds, synthesized by Henrik Hintz in the group of Adelheid Godt in Bielefeld. I knew that trityls have narrow EPR lines, but the SIFTER data really sparked my curiosity – I had to try to somehow measure the dipolar coupling with spinlocks.

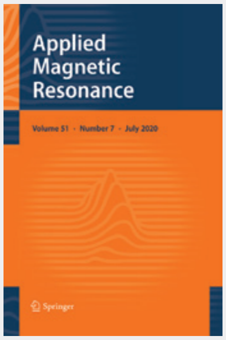
With many group members on holiday or at conferences over the summer, I had 2-3 weeks of spectrometer time, with no teaching, no seminars whatsoever. I asked Agathe if I could use one of the model compounds, and started to play around. There are many possibilities how one could use spinlocks to measure dipolar couplings. When I tried a dressed spin echo sequence, the results were just beautiful. I still remember how I felt, when I told Gunnar on a Friday afternoon.

The rest was just systematically investigating different parameters and working out the exact theory. After some input from Michael Garwood (member of the JMR editorial board), I also found a literature rabbit hole. The whole concept of dressed spin resonance, and using pulse sequences in the rotating frame, was already introduced by Hoult in 1979. The idea of using phase/frequency modulation instead of field modulation was used by Grzesiek and Bax in 1995. Even Gunnar was unaware of these works. Judging from the citations of the respective papers, also many scientists working with dressed spins in quantum information processing are unaware of the work in magnetic resonance decades earlier. In defence, I have to point out that neither the titles nor the abstracts make it obvious that "dressed spins" are involved in the old papers. Different terminologies in different fields – unfortunate for students doing literature reviews.

The pulse sequence does not solve every problem there is in pulsed dipolar spectroscopy, not at all. But it shows new possibilities that we could exploit as a community to overcome the distance range limitations. It was important to me to point out the limitations of my approach in the presentation, and I am very glad that this was considered something positive by the price committee.

Again, I would like to thank JEOL for sponsoring this price, and the organising committee for giving me the opportunity to take part in the competition. I want to thank Gunnar Jeschke for giving me time and resources to play around and encouraging me to follow my intuition. And without the great collaboration with the Bielefeld group, developing these sequences would be impossible.

▶



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Gunnar Jeschke:

Laila Mosina asked me to write a few hundred words about Nino (Wili). I could now tell you the usual stuff that one also finds in reference letters, but this would only bore you out. Instead, let me tell you what I learned from Nino. He joined my group first time for his Bachelor thesis in Interdisciplinary Sciences. Already then, I was properly impressed by Nino and I learned from him about the German stand-up comedian (in the best sense) and writer Marc-Uwe Kling. I am still reading books by Marc-Uwe Kling. Also already then, I heard that Nino played music in a band, which reminded me of a famous quote by Georg Christoph Lichtenberg (1742–1799): "Whoever understands only chemistry, does not understand it either." Nino did his Master thesis with Matthias Ernst. This equipped him with a far better solid-state NMR education than my rusty one from decades ago (and reading his manuscripts, I secretly brushed up a bit). He made very good use of this education in the second half of his thesis work, when I did not actually supervise him anymore, but served only as a testbed for his ideas. Nino writes in his piece that I was Head of Department during some of his thesis work. For part of this time, Nino was one of the two presidents of the union that defends interests of doctoral students in our Department. Let me tell you a secret: Nino is a talented politician – and I mean this in a good sense. He also convinced me, patiently and bit by bit, of new ways to Open Data and Open Access publications. I was (and am) skeptical about making a zealous religion out of this. However, with Nino I learned faster than I would have otherwise that, in general, this is a necessity. When Covid-19 and the political response to the virus struck, Nino organized on-line life of our group in an eyeblink – and then went on to start an international on-line seminar for young scientists. What else did I want to say? Nino is a very good teacher. But I guess, I had already told you that.

●

Interview with Mr. Luis Fábregas-Ibáñez on the Occasion of His IES Best Paper Award 2020/2021

EPR newsletter: *Dear Mr. Fábregas-Ibáñez, on behalf of the readers of the EPR newsletter we congratulate you on your IES Best paper Award 202/2021. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I have always been a very curious person and found an elegant simplicity in numbers. I picked a particular interest in chemistry in high school, but I was very dedicated to the study and practice of classical guitar. At time when I had to choose a direction I was torn between a degree in chemistry or one in music. I ended up going with chemistry and enrolled at the ETH Zurich. I guess that the strong research culture at ETH Zurich (that you can feel even as an undergraduate student) gave me the final push to pursue a career in science.

Who introduced you into magnetic resonance?

I first heard about magnetic resonance (specifically NMR) briefly in undergrad analytical chemistry courses. However, it was not until a couple of years later that I attended a proper course on magnetic resonance imparted by Matthias Ernst and Gunnar Jeschke (where I first heard about EPR). While I was overwhelmed by the complexity of EPR, Gunnar's lecture convinced me to start my first undergrad research project in EPR with Gunnar, where I had my first research experience in EPR, which involved trying to understand Bloch-Siegert shifts in adiabatic passage pulses in AWG spectrometers. In fact, as of today, I think I still do not understand it, but the experience was satisfactory enough to convince me to stay in the field of EPR for my master thesis and later for my PhD.

What are you main interests of work in magnetic resonance?

My primary field of work is data analysis and modeling of dipolar EPR spectroscopy. I like working with theoretical models and the accuracy for describing phenomena that they provide. Applying these models to extract complex information from experimental data via data analysis methods is very rewarding. Another particular interest of mine is software development. Depending on what occupies me, I ask myself whether I am more of a researcher or a research software engineer. I believe that good scientific software is a cornerstone of any scientific community, particularly in this age of computers. Our software DeerLab has been a result of both of my main interests and will hopefully provide useful tools and support for our community.

What does your typical lab day look like?

My work requires basically a laptop, a chair, and a table. I seldom visit the lab to do experiments (except when strictly necessary). I find this workstyle to be quite flexible. For example, when I was visiting Stefan Stoll's lab in Seattle, I could continue working without problems by just bringing my laptop along. Still, I do enjoy putting the screen away pausing to chat with my colleagues and friends or going for a run outside to clear my head after too much math or code.

What is your message to your colleagues – the young generation of magnetic resonance researchers?

▶

We live probably in a golden age for magnetic resonance (particularly EPR). Both computers and technology have reached a state that allows us to pursue otherwise wild or unfeasible ideas. Follow your creativity, and do not fear to challenge pre-established ideas in the process. You will contribute to science both by finding out that an old notion is still bullet-proof or by ending up with a better new idea. After all, it is the nature of scientific discipline to evolve.

Stefan Stoll:

Luis Fábregas-Ibáñez received the IES Best Paper Award 2020-21 for his Magn. Reson. paper on DeerLab (DOI 10.5194/mr-1-209-2020). He wrote this paper, and the associated open-source software, as part of a collaboration between Gunnar Jeschke's lab at ETH Zurich and my lab at the University of Washington in Seattle. Luis already reported about DeerLab in a recent issue of the Newsletter (31/1, p. 12). The original idea was to rewrite the backend of DeerAnalysis, the trusted MATLAB-based software for analyzing DEER data, in order to incorporate some of the more recent advances, some of which were developed by Luis. He was ideally suited for this project, with his combination of mathematical knowledge and coding skills. The first impressive thing that Luis did for this was to raise the big question of which programming language should be used for this. He coded prototype implementations in MATLAB, Python and Julia and evaluated performance, usability, and UI capabilities. He argued for free and open-source Python, and we went along. Luis then essentially single-handedly implemented around 50k lines of high-quality Python code, including documentation and tests. This a truly monumental amount of work! Luis' productivity, resourcefulness and initiative are extraordinary and impressive. It is no exaggeration to say that DeerLab opens up a whole new world of data analysis – for example, we recently ran a new analysis methodology on all the DEER data acquired in my lab (several hundred datasets) with a single script. It is therefore clear that it is not just the paper but more importantly the software that is impactful. The DeerLab paper is already receiving citations (12 after 11 months published, according to Google Scholar). One annoyance for Luis is that his name would sometimes be spelled incorrectly. Like many Iberians, he has two surnames. Not everybody in the scientific community is sufficiently aware of this. To avoid this confusion, he recently started hyphenating the two, Fábregas-Ibáñez. Luis keeps having new ideas, so he continues to drive the collaboration between Gunnar's and my lab, and he can be considered somewhat "delocalized" between Zurich and Seattle. Luis spent the summer of 2019 in my lab in Seattle, and had planned to do the same in 2020 and 2021, but the COVID-19 pandemic (plus some travel restrictions not purely based on public-health considerations) has prevented this. In a dramatic twist in June 2021, he was already at Zurich airport, when he was denied boarding the plane to the US. And although he stayed grounded on that occasion, his overall scientific career is definitely taking off.

Zavoisky Award 2021

Sergei V. Demishev

Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia.

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

University of Stuttgart,
Stuttgart, Germany.

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.

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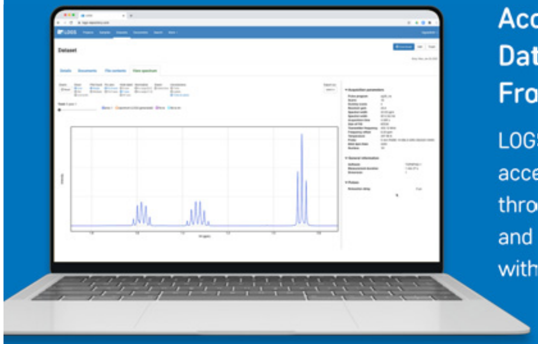

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BRIDGE 12

Jack Peisach (1932–2021)

The EPR community lost one of its early pioneers and practitioners, Jack Peisach on March 4, 2021. Jack was awarded the International EPR Society's Silver Medal in Biology in 1999. He was born on August 23, 1932 to immigrant parents, Harry and Yetta Peisach, grew up in the Bronx and was a life-long resident of New York City. Jack received a B.S. degree in Chemistry from City College of New York in 1953 and a PhD. in Organic Chemistry from Columbia University in 1958. His graduate work was done under the direction of Cheves Walling and involved the characterization of organic reactions under high pressure. This may seem like an odd beginning for a scientist who would be involved in several cutting-edge developments in EPR spectroscopy, but Jack was motivated by problems in biochemistry and realized early in his career that EPR spectroscopy could provide solutions. His enthusiasm for science was contagious and it allowed him to convince two physicists at Bell Telephone Laboratories (BTL), William E. Blumberg and William B. Mims, both experts in the young field of EPR spectroscopy, that problems in biology were worthy of their efforts. Jack was an active participant in these two collaborations that helped launch his 53-year academic career at the Albert Einstein College of Medicine (AECOM) and led to the development of methods that are now routine in EPR labs worldwide. This success is a testimony to Jack Peisach's scholarship, extraordinary patience, practical approach to scientific problems and persistence.

Introduction to EPR Spectroscopy

Jack started his appointment in the Biochemistry Department at AECOM in 1959 as a National Institutes of Health (NIH) – sponsored postdoctoral fellow. His expertise in organic chemistry led to a productive collaboration with Walter Levine, an Assistant Professor in the Pharmacology Department, who was working on characterizing oxidation reactions catalyzed by ceruloplasmin, a multi-copper oxidase. As part of this study, Jack began a collaboration with William E. Blumberg at BTL for the purpose of obtaining EPR spectra of the Cu(II) sites in the enzyme. Blumberg had been a postdoctoral researcher with George Feher at BTL in the late 1950's and had taken charge of Feher's EPR lab after he left BTL for a position in academia. The EPR instrument at BTL was essentially the X-band super-heterodyne instrument built by Feher in the mid 1950's with an added Varian magnetic field modulation and detection system that allowed for the study of biological samples at cryogenic and ambient temperatures [1]. It is likely that the connection between Jack Peisach and Bill Blumberg was made through Phil Aisen, a fellow post-doc at AECOM, who in the early 1960's was also engaged in collaborative EPR studies of ceruloplasmin with Blumberg [2]. While their early studies on ceruloplasmin and other Cu enzymes involved correlating changes in the protein's optical spectrum with Cu oxidation state, it didn't take Jack long to start bringing a variety of copper proteins to Blumberg's lab for EPR analysis. One of their early publications features EPR spectra collected at 1.95 and 77 K of a multi-copper oxidase, *Rhus vernicifera* laccase, showing a mixture of Cu(II) paramagnetic centers, and the spectrum from a newly isolated, mono-nuclear Cu(II) protein, "blue copper protein" from *Rhus vernicifera* [3]. Jack would eventually rename this "blue copper protein" stellacyanin after his then girlfriend, and future wife, Estelle [4].

By the end of the 1960's, numerous EPR studies of Cu(II) model complexes and proteins had been reported in the literature. Based on theoretical studies of Cu(II) square planar complexes, it had been proposed that the spin Hamiltonian parameters, $g_{||}$ and $A_{||}$, measured directly from the EPR spectrum could allow for the determination of the coordinated atoms [5]. In a 1972 review article, Vänngård showed that if one constructed correlation plots of copper $A_{||}$ vs. $g_{||}$ values for Type 1 and Type 2 Cu(II) sites from proteins and structurally related model complexes, they fell in distinct regions [6]. Peisach and Blumberg refined this approach by focusing strictly on EPR results from the Type 2 Cu(II) centers of proteins, and model complexes known to form tetragonally distorted octahedral structures. Furthermore, they grouped the data from model complexes according to the identity of their equatorially – bound atoms and the overall charge of the complex.

The resulting $A_{||}$ vs. $g_{||}$ correlation plots showed distinct regions allowing one to predict the metal ion's primary coordination sphere from parameters that were readily obtained from the EPR spectrum. These findings were reported in an article entitled, "Structural Implications Derived from the Analysis of Electron Paramagnetic Resonance Spectra of Natural and Artificial Copper Proteins," that appeared in *Archives of Biochemistry and Biophysics* in 1974 [7]. According to Jack, this article, which has been cited approximately 750 times, was rejected by multiple journals before submission to "Archives"!

Pulsed EPR Spectroscopy

Jack Peisach probably met Bill Mims on one of his first trips to BTL in the early 1960's. At that time, the labs were located in a complex on West Street in lower Manhattan and Mims' pulsed EPR spectrometer shared a 12-inch electromagnet with Blumberg's cw-EPR instrument. There was a miniature track system that allowed the magnet to be moved between the two spectrometers. Jack took particular delight in telling his students that when BTL was moved to Murray Hill, New Jersey in the mid-1960's, the magnet stayed behind at 463 West Street because of the cost associated with removing it from the building. While Mims had published articles on the nuclear modulation effect (ESEEM) and electron spin echo (ESE) -detected ENDOR in the early to mid-1960's, his primary focus at that time was using pulsed EPR and ESE to study the effect of applied electric fields on electron spin dynamics. In their 1967 paper on the characterization of the unusual Cu(II) site in stellacyanin, Peisach and Blumberg point to the possibility of using Mims' methodology for further characterizing the metal binding site. Early attempts at such experiments were disappointing, but they presented a challenge to both Blumberg and Mims who were convinced that ESE methods could deliver much more information on metalloprotein structure than conventional cw-EPR spectroscopy. By 1974, the pulsed EPR spectrometer in the Mims lab at Murray Hill had been completely rebuilt. The microwave transmitter now featured a 1 kW grid-pulsed traveling wave tube amplifier, resulting in an order of magnitude reduction in microwave pulse widths from 200 to 20 ns, a sensitive homodyne detection system that allowed for a reduced dead time [8], and a novel stripline transmission cavity that provided a 20-fold increase in sample filling factor and featured a geometry that allowed for straightforward application of electric field pulses to frozen solution samples [9].

It was at about this time that Jack Peisach and Bill Mims began a regular collaboration that was to last until Mims retired from BTL in 1985. Specifically, Peisach would travel to Murray Hill every Thursday for the purpose of conducting pulsed EPR experiments on samples that had been prepared in his lab at AECOM, or by collaborators at other institutions. The success of this arrangement, especially in those early days, was due to the persistence of both men as they worked to develop measurement methods and evaluate their usefulness. The improved pulsed EPR spectrometer facilitated Linear Electric Field Effect (LEFE) measurements on frozen solution samples. While they didn't provide the precise measure of crystal field parameters that Mims had hoped for, they did yield magnetic field profiles, measurements of electric field or g-value shift versus magnetic field, that could be used qualitatively. For example, in a series of experiments with William and Nanette Orme-Johnson, a method for using these LEFE magnetic field profiles to classify iron-sulfur clusters was developed [10].

LEFE studies of the Cu(II) site in stellacyanin, an experimental goal that had helped drive the instrumentation development of the early 1970's, proved less interesting as the measured electric field induced shifts in g-value proved to be too small to warrant in-depth study. However, the protein showed deep low frequency nuclear modulations (ESEEM), most likely from weak ^{14}N ligand hyperfine coupling. To better characterize this coupling, Mims proposed an ESE-detected ENDOR experiment using a 3-pulse, or stimulated echo approach that he had developed in the mid-1960's. To their surprise, when recording 3-pulse ESEEM data from stellacyanin, they found that the echo modulation persisted well beyond 10 µs. These data were much more amenable to frequency analysis than 2-pulse ESEEM data and the ENDOR approach was dropped in favor of trying to analyze the coupling using ESEEM. The initial approach to this analysis was typical of Jack Peisach – study a group of inorganic model complexes for the Cu(II) site and compare the resulting ESEEM data to that obtained from stellacyanin. It didn't take long to find a model that matched perfectly, Cu(II)(diethylenetriamine)(imidazole), and the ^{14}N ESEEM from stellacyanin was assigned to the bound imidazole side chain of a histidine [11]. For Mims, satisfaction would come soon thereafter when ^{14}N-imidazole in the above model complex was replaced with its ^{15}N-labeled counterpart and the persistent modulations, referred to above, disappeared. At that point, one could understand the experiment from the point of view of a spin Hamiltonian and both chemist and physicist were satisfied! [12, 13].

The early 1980's brought substantial changes to BTL as the Bell Telephone System was going through a government mandated divestiture. Jack was anxious to continue building on the foundation of pulsed EPR spectroscopy in biology that he and Mims had built over the previous decade. To that end, he applied for NIH funding to construct a new pulsed EPR spectrometer at AECOM. After a couple of rounds with the agency, a 3-year individual investigator grant was awarded in 1982. This was a brave undertaking given that the new instrument would be built at a medical school that lacked the electronics and machining expertise available at BTL. However, Jack had the support of both Blumberg and Mims when it came to spectrometer design. The success of this endeavor, which I was hired to carry out, lead to the establishment of an NIH Research Resource in Pulsed EPR in 1985. By that time, Mims had retired from BTL and Jack forged ahead running a more conventional research group of post-docs and graduate students at AECOM. The nature of his research also began to shift towards using EPR spectroscopy to understand chemical reaction mechanisms. It was no accident that over half of Jack's ~310 publications would come from the period between 1985 and his retirement from AECOM in 2012.

Jack Peisach was a caring mentor. He maintained his role as a teacher long after his students left his laboratory. He excelled at teaching the art of grantsmanship, a skill that is so vital to the survival of a scientist. I can distinctly remember talking to him on the phone about writing a shared instrumentation grant in the mid-1990's. At that time, I had been out of Jack's lab for over 5 years and he still asked me how I was going to justify my request. It probably took about 15 minutes for Jack to distill my reasoning down to one or two points that provided a succinct "justification of need" for the review panel. Jack also understood the importance of family life. On several occasions, I remember him walking into the lab late in the afternoon and telling me to go home. He always asked about my wife and children when our paths crossed at meetings.

Personal Life

Jack and Estelle Peisach were married from 1966, after he had renamed the "blue copper protein" from *Rhus vernicifera* in her honor, until Estelle's death in 2012. Over the course of her career, Estelle served as Professor of Psychology at both NYU and Pratt Institute. She also ran a private practice in lower Manhattan and was very devoted to her patients. Jack and Estelle shared a deep dedication to family life. They raised two sons, Ezra and Daniel, who would both earn doctoral degrees in structural biology or medicine, and go on to successful careers of their own.

Jack had a keen appreciation for classical music and a passion for Jewish history and culture. He was an exceptional storyteller who could draw from what appeared to be an endless knowledge base. I can remember stories that ranged from the building of the subway system in New York City in the 1880's to Columbia University's selection of Dwight Eisenhower as their president. You always learned something when you talked to Jack, and you were always entertained!

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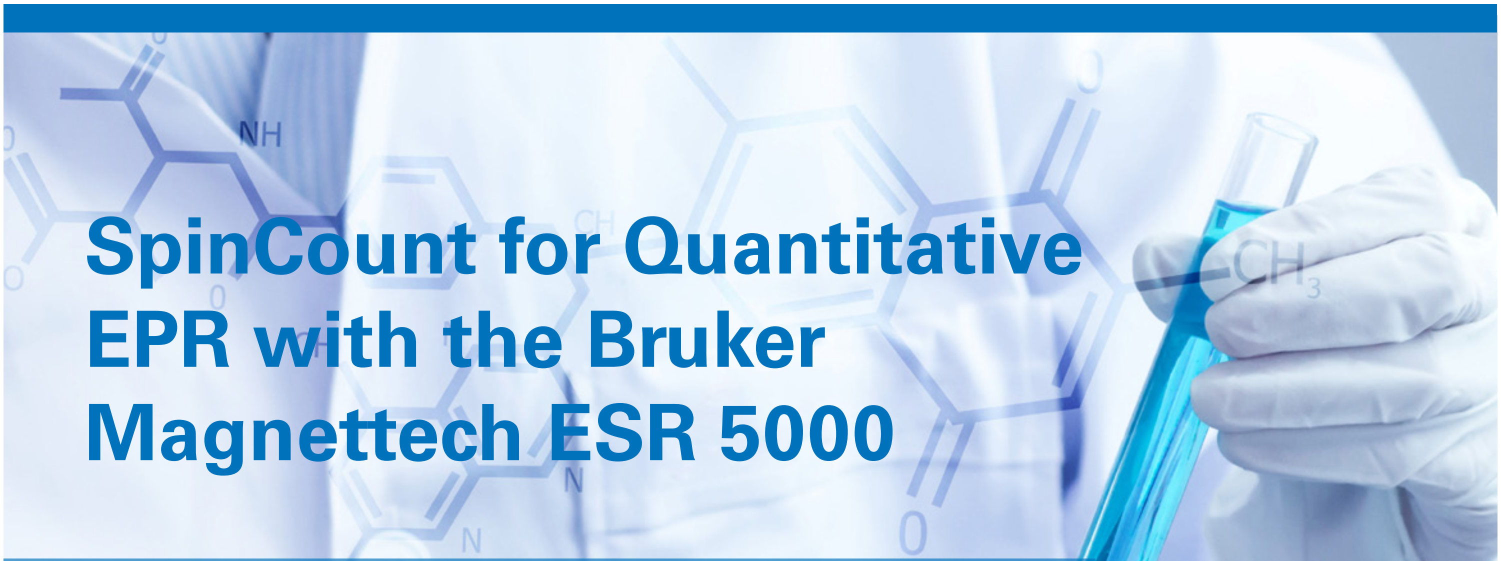
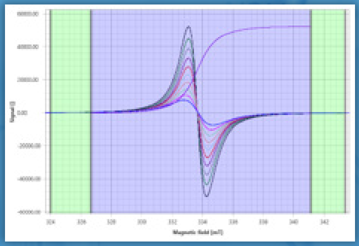
13. Mims W.B.: ESE in Biology. Glen Gardner: NJ **1985**.

John McCracken

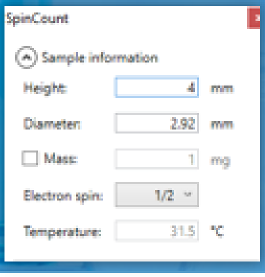


SpinCount for Quantitative EPR with the Bruker Magnettech ESR 5000



High Precision Double Integration

- An easy-to-use high precision method
- Single measurement quantification



Height: 4 mm

Diameter: 2.92 mm

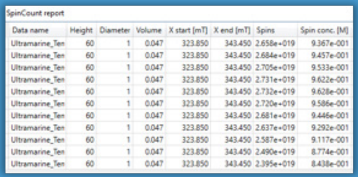
☐ Mass: 1 mg

Electron spin: 1/2

Temperature: 31.5 °C

User Input

- No reference sample required
- One-time factory calibration



SpinCount report

Data name	Height	Diameter	Volume	X start [mT]	X end [mT]	Spins	Spin conc. [M]
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.658e+019	9.367e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.684e+019	9.457e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.705e+019	9.533e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.731e+019	9.622e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.732e+019	9.628e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.720e+019	9.586e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.681e+019	9.446e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.637e+019	9.292e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.587e+019	9.117e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.490e+019	8.774e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.395e+019	8.438e-001

Reporting

- Applies to 1D- and 2D-data

Learn more at:

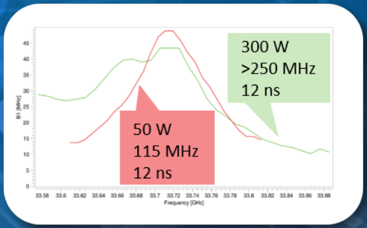
EPR

Innovation with Integrity

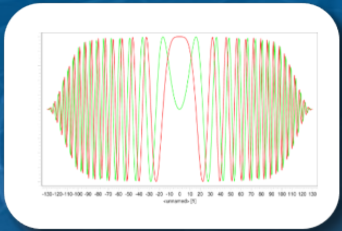
BRUKER
10 Years of EPR Innovations

2010: Spinfit

2013: Q-band power, 150 W TWT with pi-pulses as short as 12 ns with an over coupled resonator.

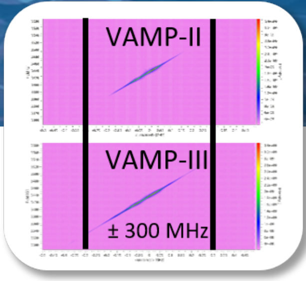


2013: SpinJet-AWG first commercial arbitrary waveform generator for pulse EPR.



2016: EMXnano, High performance benchtop EPR spectrometer incorporating SpinFit and SpinCount for simulation and quantification.

2016: SpinFit anistropic



2018: VAMP-III and SpecJet-III, detection bandwidth of 1 GHz with 14-bit amplitude resolution.

2019: Rapid-Scan accessory, a new way of performing EPR overcoming saturation limits, improving signal to noise, and increasing time resolution.

2019: Magnettech ESR5000: Bruker's latest benchtop EPR spectrometer, combining a compact design with a wide range of applications.

Innovation with Integrity

Bruker