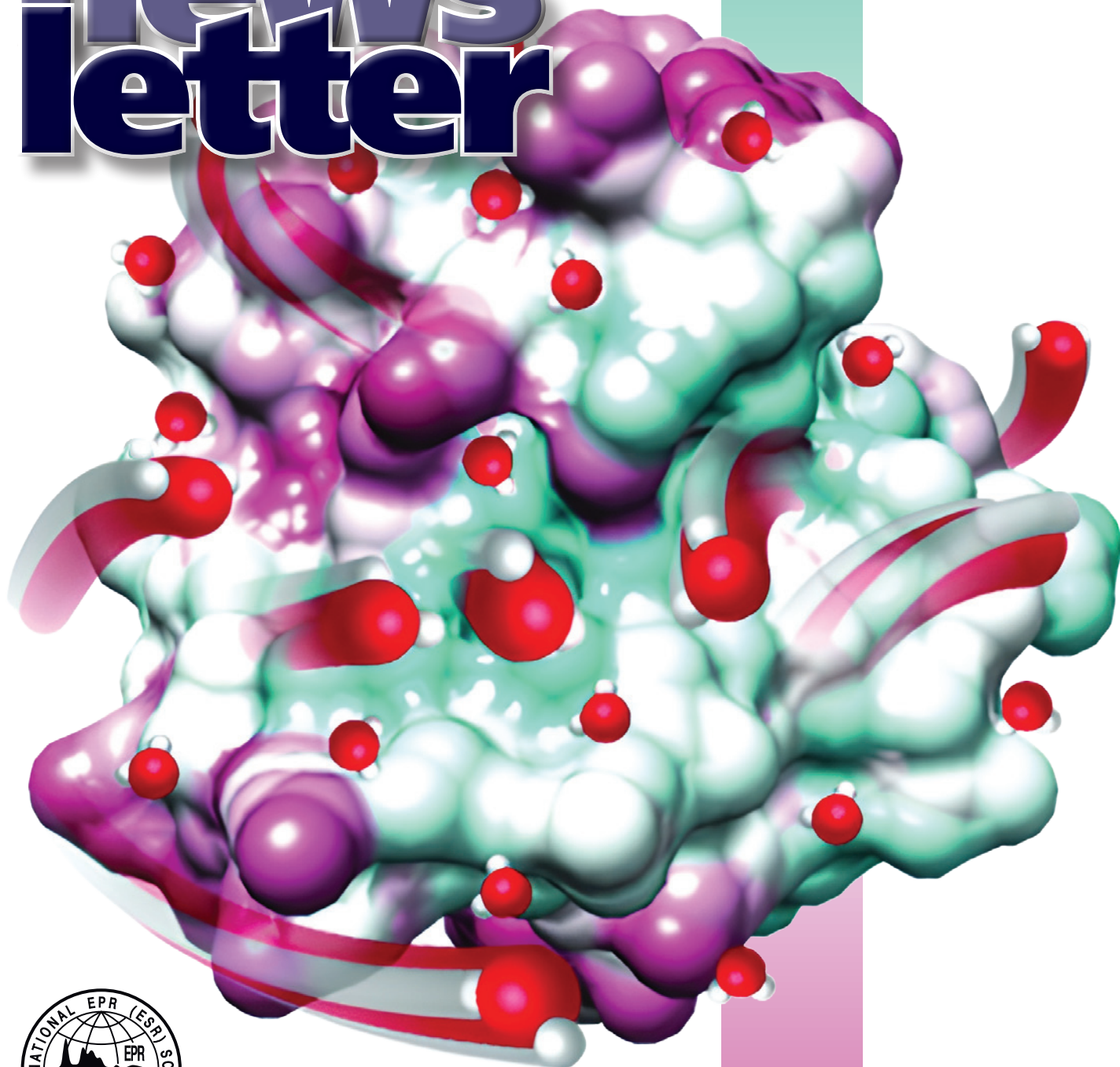


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The Publication of the International
EPR (ESR) Society

HYDROPHILIC



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PRESIDENT

Marina Bennati

University of Göttingen, Department of Chemistry & Max Planck Institute for Multidisciplinary Sciences (Fassberg Campus) Am Fassberg 11 37077 Göttingen, Germany
phone: +49 551 201-1911
e-mail: office.bennati@mpinat.mpg.de
web: <https://www.mpinat.mpg.de/bennati>

VICE PRESIDENTS

Americas

Sunil Saxena

University of Pittsburgh, 711 CHVRN
Chevron Science Center, 219 Parkman Avenue
Pittsburgh, PA 15260, USA
e-mail: sksaxena@pitt.edu
web: <https://www.saxenalab.pitt.edu>

Asia-Pacific

Mi Hee Lim

Korea Advanced Institute of Science and Technology (KAIST), Department of Chemistry
Building E6-6, Rm 504
Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea
e-mail: miheelim@kaist.ac.kr
web: <https://sites.google.com/site/miheelimlab>

Europe

John Morton

London Centre for Nanotechnology
University College London
17-19 Gordon Street, London WC1H 0AH, UK
e-mail: jjl.morton@UCL.ac.uk
web: <https://www.ucl.ac.uk/quantum-spins>

SECRETARY

Janet Lovett

School of Physics and Astronomy, North Haugh, University of St Andrews, St Andrews, KY16 9SS, UK
e-mail: Jel20@st-andrews.ac.uk
web: <https://www.st-andrews.ac.uk/~jel20>

TREASURER

Peter Z. Qin

Department of Chemistry,
University of Southern California, TRF 119,
3430-S. Vermont Ave., Los Angeles, CA 90089-3304, USA
phone: (213) 821-2461, fax: (213) 740-2701
e-mail: pzq@usc.edu

IMMEDIATE PAST PRESIDENT

Song-I Han

Northwestern University Technological Institute J317,
B176 and Silverman Hall B530 2145 Sheridan Rd
Evanston, IL 60208, USA
e-mail: songi.han@northwestern.edu
web: <https://hanlab.northwestern.edu>

FOUNDER PRESIDENT

Harold M. Swartz

Dartmouth Medical School,
Department of Radiology & EPR Center,
7785 Vail Room 702, Hanover, NH 03755-3863, USA
phone: 1-603-650-1955, fax: 1-603-650-1717
e-mail: harold.swartz@dartmouth.edu

Fellows of the International EPR (ESR) Society

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EDITOR

Laila V. Mosina

Zavoisky Physical-Technical Institute
Russian Academy of Sciences
Kazan, Russian Federation
mosina@kfti.knc.ru

ASSOCIATE EDITORS

Candice S. Klug

Medical College of Wisconsin
Milwaukee, WI, USA
candice@mcw.edu

Hitoshi Ohta

Molecular Photoscience Research Center,
Kobe University, Kobe, Japan
hohta@kobe-u.ac.jp

Sabine Van Doorslaer

University of Antwerp, Antwerp, Belgium
sabine.vandoorslaer@uantwerpen.be

TECHNICAL EDITOR

Sergei M. Akhmin

Zavoisky Physical-Technical Institute
Russian Academy of Sciences
Kazan, Russian Federation
akhmin@inbox.ru

FOUNDING EDITOR

R. Linn Belford

(1931–2015)

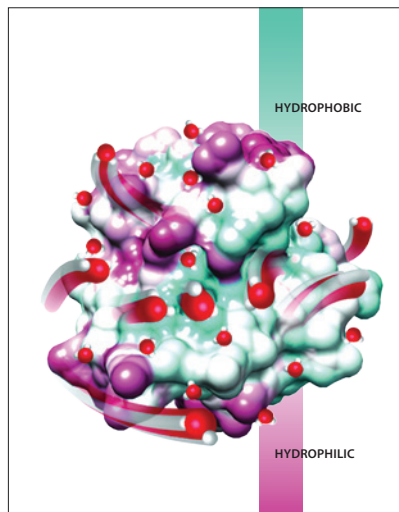
EDITORIAL OFFICE

Zavoisky Physical-Technical Institute
Russian Academy of Sciences
Sibirsky trakt 10/7, Kazan 420029
Russian Federation
phone: 7-843-2319096
fax: 7-843-2725075

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

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The cover picture illustrates aspects of the research of Songi Han, recipient of the 2024 Bruker Prize. It is an illustration that shows the first high-resolution experimental map of water structure and dynamics around a protein surface in solution state that is highly heterogeneous or “colorful” (<https://doi.org/10.1021/jacs.7b08606>). These measurements were made possible by Overhauser dynamic nuclear polarization that relies on the electron spin precession to select the temporal window for ^1H NMR relaxivity in the sub-nanosecond regime. It turns out water forms clathrate-like arches around active sites with greater tetrahedrality, lower density, and higher entropy than bulk water, making such water more “active” as they store entropy and can be readily released when a stronger binding partner comes along.



epr news letter

The Publication of the International EPR (ESR) Society

volume 34 number 1-2 2024

2 Editorial *by Laila Mosina*

IES business

- 3 Letter of the President
by Marina Bennati
- 4 New IES Executives
- 7 Interviews with Former IES Presidents
by Harold Swartz, Keith McLauchlan, James Norris, John Pilbrow, Wolfgang Lubitz, Jack Freed, Hitoshi Ohta, Lawrence J. Berliner, Klaus Möbius, Thomas Prisner, and Songi Han
- 14 Interview with Professor Gunnar Jeschke
- 14 Interview with Professor Jiangfeng Du
- 15 Interview with Doctor Frédéric Jaspard and Doctor Sylwia Kacprzak

Awards

- 17 Interview with Dr. Paolo Bruzzese on the Occasion of His IES Best Paper Award 2023
- 18 Interview with Dr. Nino Wili on the Occasion of His Bruker Thesis Prize 2023 and Raymond Andrew Prize 2023
- 19 JEOL 2023 and IES Poster Prize at the 9th EFEPR Summer School: Sebastian Gorgon
- 20 IES Poster Prize at the 2023 Euromar: Laura Rimmel
- 21 IES Poster Prize at the RMC2023: Roxanna Martinez
- 22 IES Poster Prize at the RMC2023: Austin MacRae
- 23 IES Poster Prize at the 9th EFEPR Summer School: Julia Haak
- 24 IES Poster Prize at the 9th EFEPR Summer School: Radhika Kataria
- 25 IES Poster Prize at the 9th EFEPR Summer School: Orit Nir-Arad
- 26 IES Poster Prize at the 2023 RSC Meeting: Yasmin Ben-Ishay

Another passion

- 28 Sailing
by R. David Britt

Anniversaries

- 30 80 Years Young
by S. S. Eaton, G. R. Eaton, and K. M. Salikhov

In memoriam

- 33 Asako Kawamori (1935–2024)
by Hiroyuki Mino

Editorial

Dear colleagues,

As you know, every cover of the *EPR newsletter* is designed to illustrate research of an outstanding scientist awarded with a distinction of the magnetic resonance community. Once upon a time, a faithful reader of the *EPR newsletter*, who liked our publication nearly as much as I do, told me that the first thing he does when he gets a copy of a new issue is trying to guess whose research is illustrated in its cover. I do not remember if he ever told me how often he succeeded to guess it but I wonder if he was lucky with the cover of the current issue. It illustrates the research of Songi Han, immediate past IES President, recipient of the 2024 Bruker Award for her contributions to the development and application of magnetic resonance techniques. Heartfelt congratulations to Songi!

How do you like this quiz? I understand that if you are reading this editorial, you already know the answer for the current issue, but you may try to solve this quiz when you get the next issue of our publication, and please let me know if you succeed.

This double issue is devoted to the 80th anniversary of the discovery of EPR by Evgeny Zavoisky. The IES Executive team for the years 2024–2026 is also introduced (pp. 3–6).

Marina Bennati, IES President, congratulates the EPR community on the 35th birthday of the IES, whose main goal is to advance knowledge as well as to stimulate developments and applications of EPR/ESR spectroscopy, formulates the ongoing activities of the IES and the ways to implement them.

At the end of 2023, the IES Awardees 2024 were announced: IES Medal for Chemistry to Christiane Timmel for her seminal contribution to advancing the field of EPR for Chemistry applications; IES Medal for Instrumentation and Methods Development to Hiroshi Hirata for his seminal contributions to advancing

EPR spectroscopic mapping techniques and low-field EPR spectrometers for biomedical applications, and John Weil Young Investigator Award to Alexey Bogdanov for the significant contributions to EPR spectroscopy. Heartfelt congratulations to them all!

Special congratulations to Jim Norris, IES President (1996–1999), on his Spin Chemistry Life Time Achievement Award for his pioneering work in time resolved EPR, optical spectroscopy and magnetic field effects in the elucidation of the molecular structure and dynamics of paramagnetic species!

Last but not least, an enormous thank-you to all contributors to the *EPR newsletter*!

Laila Mosina

Conference reports

34 The 62nd Rocky Mountain Conference on Magnetic Resonance

by Dane McCamey and Songi Han

35 ISMAR 2023 as seen by Songi Han

36 9th EFEP Summer School on fundamental theory and state-of-the-art applications of EPR Spectroscopy

by Enrica Bordignon, Daniel Klose and Gunnar Jeschke

36 The 62nd Annual Meeting of the Society of Electron Spin Science & Technology

by Susumu Okubo, Yasuhiro Kobori and Hitoshi Ohta

38

Faculty on the move

BRIDGE THE THz GAP

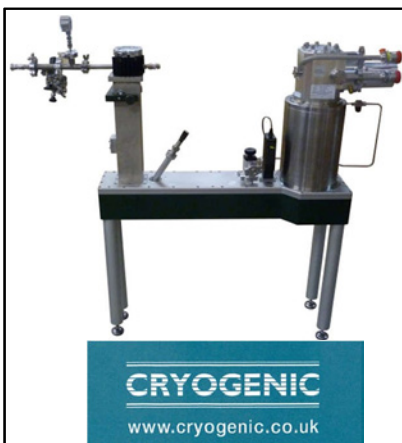
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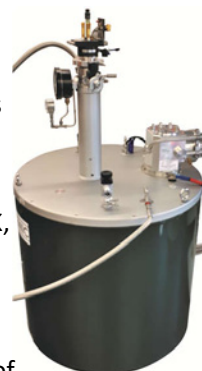
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Letter of the President

Dear EPR colleagues,

Earlier this year, the IES has elected a new Executive Committee for 2024–2026, and I am very honored to serve as new President of the Society for this term. The three newly elected Vice Presidents for America, Asia and Europe are Sunil Saxena (Univ. of Pittsburgh), Mi Hee Lim (Korea Advanced Institute of Science and Technology, KAIST) and John Morton (Univ. College London), respectively. We also have a new Secretary of the Society, Janet Lovett (Univ. of St. Andrews), who has taken over the office from Aharon Blank (Technion Haifa). Peter Qin (Univ. of Southern California) will continue to serve as Treasurer. We are also pleased that Laila Mosina (Zavoisky Institute Kazan) will continue as Editor of the EPR Newsletter and Song-I Han will remain on the Executive Board as the Immediate Past President. In addition, the IES Board has voted to add a new Virtual Media Officer to the IES Executive Board in future, with an election anticipated in 2024. I would like to thank all IES members for their trust in electing this new Board, which is eager to represent this impactful and diverse Society, as well as to support its growth and increasing visibility in the international scientific landscape.

I would like to begin this letter by acknowledging the past Officers for their dedicated service to the Society. First of all, a special thank you to our former President Song-I Han, who took over the Office during the very difficult time of the pandemic, and managed to establish new communication platforms through virtual media, with enthusiastic feedback from the community. I'm very much looking forward to working with her in this upcoming term. Of course, we are also indebted to Maxie Roessler, Michael Wasielewski and Yasuhiro Kobori as former Vice Presidents for Europe, America and Asia, respectively, for their engagement in

many decisions and representing our Society at several international conferences. Another special thanks goes to Aharon Blank for his excellent work as Secretary over so many years (2014–2023). Of course, I'm also grateful to Laila Mosina for her engagement in the EPR Newsletters as well as to Peter Qin as Treasurer, both of whom will remain on the new Board. This will support the new Executive Board members and ensure continuity in future.

This year marks the 35th birthday of the International EPR Society, whose main goal is to advance knowledge as well as to stimulate developments and applications of EPR/ESR spectroscopy. Its members are scientists across academia and industry, from a wide range of disciplines and from countries worldwide. The Society collaborates with many successful local societies around the world. Thus, IES provides a unique, exciting platform for all EPR scientists to exchange and cross-fertilize their research. I will do my best to contribute in this mission, in particular by supporting IES and EPR research to face new challenges of modern societies, which are continuously and unexpectedly changing.

EPR, discovered by Zavoisky 80 years ago, has grown in many fields as the indispensable method to detect paramagnetic centers in biology, chemistry and material science. However, recent developments in high-field EPR, inter spin distance measurements, single-molecule detection, microcircuit design, spin chemistry and more, have shown that EPR has tremendous potential to drive modern and sustainable research fields, such as for instance catalysis for new energy science, structural biology for medical research and quantum information technology. However, tackling enormous challenges is rarely feasible by individual scientists. It requires the concerted efforts by a scientific community that are accompanied

by a strongly supportive environment. This is where, I believe, the IES has and will play key role in everybody's future research.

We should encourage ourselves, our colleagues and students to take advantage of IES, attending EPR conferences and interacting through many communication platforms, including the IES website and the newly established social media. Particularly, I would like to thank all the dedicated young people who have been running the IES Virtual EPR meetings (IVEM), initiated by Nino Wili in April 2020 and now continued by Thomas Schmidt and the IVEM team. This wonderful initiative has become a major forum for young scientists in EPR. But we should also reach out to the larger magnetic resonance community, where developments in EPR combined with other magnetic resonance techniques are currently pushing new research fields.

An impressive example arises from the field of hyperpolarization, which is revolutionizing magnetic resonance. Dynamic nuclear polarization (DNP) from electron to nuclear spins in conjunction with rapid sample dissolution can increase nuclear spin polarization up to four orders of magnitude, the method is now being used in clinical studies for cancer diagnostics. In DNP, electron spins have to be manipulated not only at low but particularly at high magnetic fields, pushing mutual developments in EPR and NMR spectroscopy for instrumentation, theory, pulse sequences and experimental design.

Several other synergies are emerging, for instance between the field of spin chemistry and NMR hyperpolarization via photoexcited states, or with the field of quantum sensing and quantum information technology. There is a strong momentum in new research that we all should exploit by participating at conferences such as EUROMAR, the Spin Chemistry Meeting or ISMAR.

One of my main goals will be to increase the visibility of EPR through IES activities at these conferences. In addition, it is really important



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data = dnp.fourier_transform(data)
data = dnp.autophase(data)
dnp.fancy_plot(data)
```

BRIDGE
12

Letter of the President

to communicate our results and knowledge also to other communities for instance in physics, chemistry and biology. This will greatly increase the visibility of EPR at funding agencies, in hiring committees, and enhance the likelihood to publish our results in high-impact journals.

The IES offers several important tools to support careers and recognize research of students, young scientists and colleagues. Besides poster awards at international EPR or magnetic resonance conferences, IES awards prestigious prizes and fellowships for new developments of EPR in the various disciplines, from physics up to medicine. The individual prizes in each category are announced via email to the

active IES members as well as through the IES webpage. Additionally, the Best Paper Award may be given to up to two outstanding publications per year. The first author, who should be a young scientist, is recognized by this award. Since all activities and prizes are financed by the IES, it is important to encourage everyone, including young students, to become active members. The Society is not its Executive Board, but its members!

Last, but not least, I would like to highlight the very special role of the EPR Newsletters, edited by Laila Mosina, which reports latest news from our community and provides a framework for vendors to announce their

products. In this regard, I would like to express our special commitment to interact with vendors, who are vital to our community. I would like to encourage their participation in conferences and also their closer collaborations with research labs.

I will be delighted to serve the IES for the next three years. I'm looking forward to new developments and I'm very open for suggestions, ideas or wishes. Thus, please do not hesitate to contact me or one of my fellow Officers, whose contact details are listed on the cover of this Newsletter.

With best regards and on behalf of the entire Executive Officer Board of our Society,

Marina Bennati
President of the IES

New IES Executives



Marina Bennati,
IES President

Marina Bennati is full Professor for Physical Chemistry at the University of Göttingen and Head of the Research Group "Electron-Spin Resonance Spectroscopy" at the Max Planck Institute for Multidisciplinary Sciences. After her studies of Chemistry at the University of Münster, she moved to Stuttgart where she received her PhD in Physics with Michael Mehring as her supervisor. In 1996 she earned a DFG Postdoctoral Fellowship to work at the MIT/Harvard Center for Magnetic Resonance, Cambridge. Here, in the lab of Bob Griffin, she developed high frequency 140 GHz ENDOR spectroscopy and its application for enzymatic catalysis. After her return in Germany, she pursued her career by habilitating in Physical Chemistry at Goethe University in Frankfurt in the lab of Thomas Prisner. In 2007 she was appointed as an Independent Research Group Leader at the Max Planck

Institute for Biophysical Chemistry, and then as Professor at the Department of Chemistry of Göttingen University, where she moved to a full position since. Her research focuses on high frequency EPR and related double resonance techniques, particularly ENDOR and dynamic nuclear polarization. In 2011 she was one initiator of the German Research Council (DFG) priority program '*New frontiers in EPR spectroscopy: from molecular cells to nano materials*', which she chaired until 2019 with annual meetings of the German and International EPR community. In 2021, she has been awarded an ERC Advanced Grant to develop methods at the interface between EPR and NMR.

In the past, she served on the EUROMAR board of trustee as well as on the board of the German Magnetic Resonance Society, representing the German EPR groups therein and at the European Federation of EPR groups (EFEPR). Currently, she is a member of the Editorial Advisory Board of *Journal of Magnetic Resonance* and *Journal of the American Chemical Society*^{AU} as well as of the Review Board of the German Research Council. She also actively participates in recruitment and education of young scientists as a board member of the Göttingen Graduate School.

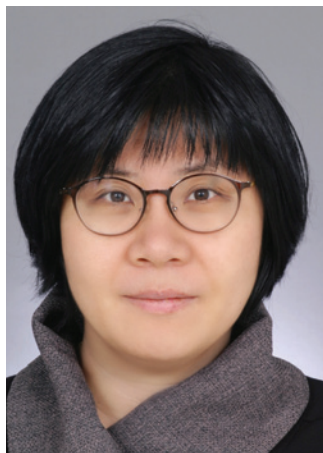
She was co-organizer of several meetings, such as the Telluride workshops on DNP and paramagnetic MR, the EMBO/Chianti workshops, the annual meetings of the German Society of Magnetic Resonance as well as of EUROMAR, EFEPR, and HYP. For her scientific work she received several prizes: The Young Investigator Award of IES, the IES Medal in Physics, the Bruker Lecture Award, and she is Fellow of ISMAR.



Sunil Saxena,
IES Vice-President Americas

Sunil Saxena obtained a B.Sc. (Hons) and a M.Sc. in Chemistry from St. Stephen's College, and the Indian Institute of Technology at Kanpur, respectively. Thereafter he started his graduate work at Cornell University where he developed 2D ESR and pulsed dipolar spectroscopy. His graduate work foreshadowed the rapid development of distance methodology which has had far reaching applications in biophysics. He received his PhD in Chemistry from Cornell University in 1997. Thereafter he performed postdoctoral research at Caltech and at UC Berkeley, where he worked on SS NMR and optical pumping and SQUID detected ultra-low field NMR and MRI technology, respectively. He started his independent career at University of Pittsburgh in 2001, where he rose through the ranks and is currently a Professor of Chemistry. Between 2017–2023 he served as the Chair of Chemistry.

At Pitt, his research interests focus on the development of ESR spectroscopy and its applications to biophysics, including protein-DNA interactions and metals in biology. In earlier work his group developed the conceptual basis for pulsed dipolar spectroscopy for Cu(II) ions and the biophysical research exploited this technology to understand the role of Cu(II) ions in the mediation of protein-DNA interactions as well as aggregation in amyloids. In recent years, his group has developed site-directed Cu(II) labeling of proteins and nucleic acids and established the enhanced fidelity of these labels to measure biomolecular structure, dynamics, and function. He is a recipient of the NSF CAREER Award, the Tina and David Bellet Teaching Excellence Award at Pitt, and the Crano Memorial Award and Lecture from the Akron section of American Chemical Society. He is also an Associate Editor of *Applied Magnetic Resonance*, and on the Editorial Advisory Board of *Analysis and Sensing*.



Mi Hee Lim,
IES Vice-President Asia-Pacific

Mi Hee Lim is a KAIST Endowed Chair Professor and the Director of the Center for MetalloNeuroProteinoChemistry in the Department of Chemistry at the Korea Advanced Institute of Science and Technology (KAIST). She received her B.Sc. in Chemistry from Ewha Womans University, Seoul, Korea, in 1999 and her M.Sc. in 2001 under the direction of Professor Wonwoo Nam. In 2002, she moved to MIT where she obtained her PhD under the supervision of Professor Stephen J. Lippard. She then pursued her postdoctoral research in the laboratory of Professor Jacqueline K. Barton at Caltech. In 2008, she began her independent career as an Assistant Professor of Chemistry and

Research Assistant Professor in the Life Sciences Institute at the University of Michigan, Ann Arbor, USA. In 2013, Mi Hee moved to the Ulsan National University of Science and Technology (UNIST), Ulsan, Korea, as an Associate Professor with tenure. In 2018, Mi Hee joined the Department of Chemistry at KAIST, Daejeon, Korea. Her research interests lie in bioinorganic chemistry, especially focusing on identifying how metal-involved biological networks are linked to dementia, such as Alzheimer's and Parkinson's diseases, and establishing new directions for developing chemical reagents as tools, diagnostics, and therapeutics for such diseases. Mi Hee is a Fellow of the Korean Academy of Science and Technology, a Fellow of the Royal Society of Chemistry, a Member of the Presidential Advisory Council on Science and Technology, a Council Member of the Society of Biological Inorganic Chemistry (SBIC), and a Member of the Samsung Future Technology Association. She also received several awards, including the Award for Women in Science and Technology, the S-Oil Next-Generation Scientist Award, the Asian Biological Inorganic Chemistry (AsBIC) James Hoeschele Award, the Society of Biological Inorganic Chemistry (SBIC) Early Career Award, the Award for '30 Young Scientists of Korea' to lead basic science research for the next 30 years, the Korean Chemical Society (KCS)-Wiley Young Scientist Award, the NSF CAREER Award, and the Alfred P. Sloan Fellowship.



John Morton,
IES Vice-President Europe

John Morton read Natural Sciences and Electrical Engineering at University of Cambridge (UK), and subsequently received his PhD degree at University of Oxford (UK) in 2006 on the topic of decoherence and coherent

control of spins in fullerenes as quantum bits. John was a Royal Society University Research Fellow from 2008-16, establishing a research group at Oxford and subsequently moved to UCL in 2012. He is currently Professor of Nanoelectronics & Nanophotonics at UCL, as well as Director of the UCL Quantum Science and Technology Institute (UCLQ). John's awards include the Nicholas Kurti European Science prize (2008), the Institute of Physics Moseley Medal (2013) in experimental physics, and the Sackler International Prize in Physical Sciences (2016) awarded that year in the field of magnetic resonance. He has held back-to-back European Research Council (ERC) grants.

John's research over the past 20 years has focused on quantum technologies such as quantum computers and quantum sensors, using spins in organic and inorganic materials and devices. He has published over 130 papers with 13,000 citations and has an h-index of 52. He has co-founded three companies in the field of quantum technology, covering quantum computing hardware and software and is active in the public engagement of science.



Janet Lovett, IES Secretary

Janet Lovett is a Senior Lecturer in the School of Physics and Astronomy at the University of St Andrews, UK. Janet completed her degree in Chemistry and DPhil in Physical Chemistry (2006) at the University of Oxford with the supervision of Professor Christiane Timmel. At this time Oxford did not have much in the way of EPR spectrometers. Therefore, to aid the investigation of EPR for biology to underpin Prof Timmel's application for a pulsed EPR suite, she visited various laboratories for experiments, in particular Professor Gunnar Jeschke, then at the MPI for Polymer Research in Mainz, ▶

New IES Executives

and six months at the University of Leiden with Professors Edgar Groenen and Martina Huber on a Marie Curie Training Site Fellowship. In 2006 Janet was awarded the JEOL prize at the RSC ESR conference for the best talk given by a young scientist. Janet's post-doctoral studies saw her move to the Sir William Dunn School of Pathology also in Oxford where she learned more about protein handling and structural biology (while still principally using EPR spectroscopy) in the laboratory of Professor Susan Lea. She held this post concurrently with a Junior Research Fellowship from University College Oxford. In 2010 she was awarded a Royal Society University Research Fellowship and started her own group in the School of Chemistry at the University of Edinburgh. In 2014 she moved to her present position. She is currently the Director for Equality, Diversity and Inclusion in her department and organized the 2022 RSC ESR conference in St Andrews. Janet's research focuses on utilizing EPR, particularly PDS, for structural biology through its application and methodological improvements.



Peter Z. Qin, IES Treasurer

Peter Z. Qin received his B.S. degree in Physics from Peking University in China in 1991. He carried out his graduate study on RNA folding and catalysis under the mentorship of Professor Anna Marie Pyle at Columbia University in the City of New York, and received his Ph.D. degree in 1999. From 1999 to 2002, Dr. Qin carried out postdoc-

toral research work with Professor Wayne L. Hubbell at University of California, Los Angeles, developing methods of Site-Directed Spin Labeling to study RNA. In 2002, Dr. Qin joined the faculty of the Department of Chemistry, University of Southern California, at which he was promoted through the rank and currently holds a tenured full professor appointment. Dr. Qin's research focuses on understanding mechanisms of nucleic acid recognition by studying the relationship between structure, dynamics, and function of nucleic acids and protein/nucleic acid complexes. The Qin group develops and applies Site-Directed Spin Labeling techniques, both in bulk and at the single-molecule level, to monitor structure and dynamics of nucleic acids and protein-nucleic acid complexes under physiological conditions. Current projects in the Qin group focus on using spin-labeling in conjunction with other techniques to investigate mechanisms of target recognition by the programmable CRISPR nucleases that are revolutionizing genome engineering.

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Interviews with Former IES Presidents

EPR newsletter: To mark the 80th anniversary of the EPR discovery by Evgeny Zavoisky and the 35th anniversary of the IES, could you please share with us your opinion about the future of EPR and the development of its applications and methods, and the role of the IES in this process?



Harold Swartz,
Founding President (1989–1993):

I think that the future of EPR is very bright, because of the quality of the young investigators and the remarkable technical developments which continue to occur and evolve, expanding its applications and scientific discoveries. My comments are directed toward developments that have impacted the usefulness of EPR for measurements in living systems to extend basic biological investigations and improve clinical care. But I am confident that similar developments are occurring with other applications.

EPR studies in living systems, including in people (i.e., “clinical applications”), provide uniquely important information. They also face important challenges, some more uniquely *a propos* to magnetic resonance techniques like EPR such as that living systems have large amounts of water (and hence are lossy) and that samples interrogated in vivo can exhibit several types of motion due to physiological processes and voluntary movements. Great

progress has been made to address these issues through on-going technical developments, especially improvement of equipment including resonators and improvement of software for data handling and instrumental operation.

Both spectroscopic and imaging approaches continue to be very valuable, based either on static (e.g., anatomical) and/or dynamic (e.g., redox status) parameters. Full imaging techniques, usually utilizing soluble imaging agents, can provide a lot of spatially dependent information. Spectroscopic approaches usually use particulate EPR sensors (e.g., oxygen-sensing carbon particles) which can provide some spatial information but especially importantly, allow repeated measurements. Pulse has been invaluable for the imaging approaches. Rapid scan is likely to have a major impact on spectroscopic approaches.

There already are several separate and potentially very large and important areas using EPR applications to solve major biomedical problems. Focusing on potential clinical applications, at least three major areas of applications based on measurements by EPR in living subjects have been developed and are rapidly advancing: oximetry, dosimetry, and metabolism. While clinical applications potentially provide the greatest opportunity for EPR to become more widely used, potentially approaching the use of MRI, their use in the clinic is challenging because of the needs to meet regulatory requirements for use in human subjects. In spite of this hurdle, very significant advances are continuing to occur.

Clinical applications of EPR oximetry have already reached the clinic in the form of NIH sponsored clinical studies of cancer. Several groups are attempting to actively advance this area. Another area of great promise is for peripheral vascular disease, especially in diabetics, where EPR oximetry could provide unique and very useful assessments of regions of the body where lack of adequate oxygen could help explain progression of disease. In addition EPR oximetry could provide effective data-based evaluations of interventions intended to increase the oxygen in the compromised tissues.

In dosimetry, EPR has a prominent role for measurements of radiation dose after an unexpected exposure. This application is possible because ionizing radiation induces free radicals, some of which become stabilized for a moderately long time (e.g., for weeks following exposure in fingernails, toenails and living bones) while others stabilize almost indefinitely (e.g., in teeth and in bones that are no longer present in a live organism such as fossils). EPR measurements of radiation-induced free radicals in teeth have become an established part of the responses to unplanned exposures to ionizing radiation. For epidemiological studies from environmental exposures, such as leaks of radiation into streams, EPR measurements of isolated teeth are perhaps the most dependable way to determine the amount of radiation exposure, and any subsequent links to health risks. In the response to acute large events, such as the detonation of a nuclear device by terrorists, in vivo EPR measurements of fingernails and toenails and/or teeth may provide the critical information for triage, i.e., the determination of who is at risk of having a life-threatening response to radiation so that treatments can be directed to the fraction of the population who could benefit from them.

The developments that make these measurements possible have occurred through very productive collaborations between experts in EPR technology and EPR scientists whose background is principally biological.

The IES has been instrumental to these developments in clinical applications in two important ways. It provides opportunities for scientists who develop instrumentation and new technical approaches to connect with scientists carrying out the studies in living systems. These connections have led to cross-disciplinary collaborations that synergistically advance the understanding of the experimental needs and the technical developments to meet those needs. Second, IES has facilitated EPR by disseminating these important contributions to all members in the field and by advocating more broadly to increase the understanding and recognition of EPR's role in addressing these issues. Nonetheless, it would behoove the field for IES to expand on these roles and enhance opportunities for scientists from various related disciplines to interact and learn from each other.





Keith McLauchlan,
IES President (1993–1996):

When the IES was formed by Hal Swartz it filled a void for EPR scientists. A number of Magnetic Resonance societies existed but within them NMR understandably dominated because of its much wider application. A few ESR ones did, notably the ESRDG of the UK Chemical Society. Several people published in the general area but their work was dispersed over several meetings. The main applications remained the study of transition metal compounds and free radicals stabilized within crystal lattices.

The creation of the IES enabled us all to come together and realize that major advances were being made in technique and application. With the former one remembers Jakob Lebedev and Joan Van der Waals in particular and the arrival of the Bruker company into ESR. Jack Freed published important theory throughout. Free radicals were only studied in steady state concentrations, which ignored their true characteristic of reactivity.

This ended with the introduction of pulsed radiolysis and flash photolysis (FP), both depending on the novel principle of repetitive pulses and fast sampling of the signals. The FP method relied on use of computing techniques before commercial personal computers were available, although individual cards were.

The study of transient radicals enabled them to be observed on a sub-microsecond timescale and led to the discovery of Electron Spin Polarization (known erroneously as CIDEP) in radical reactions, a new physical phenomenon. Its interpretation provided direct evidence for reactions happening in solution much faster than the familiar diffusion controlled ones, something predicted by W. A. Noyes. The kinetics community has never acknowledges this gift from ESR! More significantly it suggested that free radical combinations should be

affected by magnetic fields. No conventional chemist believed this but it led to a fundamentally new subject area, Spin Chemistry, now the subject of wide research.

Much of the early work was determined by people building their own equipment, but this is no longer common as commercial instruments have accommodated the newer experiments.

I always believed that if one thought of something new to do it then one should give it a go whether suitable equipment could be purchased or not. A corollary was that the moment a new experiment worked you should already be thinking of the next one. This is the best advice for anyone.

It has been my privilege to know and learn from a wonderful group of international scientists. I am grateful to them all.



James Norris,
IES President (1996–1999):

I consider myself to be a second-generation user of EPR having studied under Sam Weissman, a pioneer of chemical applications of EPR. That EPR is 80 years old this year is hard for me to believe. EPR is an essential and fundamental tool for probing matter on a molecular level with applications in chemistry, physics and biology, yet the field has never been awarded a Nobel Prize. The fundamental nature of EPR will ensure a future for EPR, certainly academically, but what can be expected in terms of its user base numbers?

Years ago, my friend and late colleague Gerhard Closs and I frequently discussed what scientific achievements should be awarded the Nobel Prize. Several of our predictions came to pass, a reasonable outcome since we started with a selective list supported by others as well. However, predicting the future of EPR is more difficult for me. NMR users are

considerably more common than EPR users, an imbalance sure to continue in the future. Today the term EPR includes many extensions and related variations such as ENDOR, pulsed EPR, time resolved EPR, electron spin echo, to name just a few. The general development of sophisticated instrumentation taking place today is very exciting and surely will make EPR more accessible to several new user bases.

In part to compensate for the disparity in the size of the user base, the International EPR Society (IES) was formed in 1989. Since then, the IES has been a major asset in expanding the applications and user base of EPR. Especially significant to the development of EPR was and is the role played by the international meetings organized and hosted by the IES where new techniques and applications were and still are presented and discussed. These international meetings provide a crucial platform to exhibit cutting edge science and expand the user base to compete with the more numerous NMR users. These meetings also exhibited important routine applications of EPR involved in many fields of science. Crucially, the IES played the dominant and vital role in bringing worldwide EPR users together for the first time despite east-west international political divide. While I knew that EPR was invented in Russia by Evgeny Zavoisky, I was totally unfamiliar with any of the important studies and papers pursued and published by Russian scientists. The international meetings held by the IES established not only the true international user base but also many new friendships were born. I personally had enlightening discussions with these new friends and developed a great respect for their sophisticated understanding and development of EPR and its applications.

Currently the EPR user base is expanding modestly via commercial applications, suggesting an optimistic future for users of EPR. One such example of a commercial use of EPR comes from a former PhD student, Richard Rustandi. Richard is employed by Merck & Co. and has used EPR in the development of vaccines. One of the vaccines he helped develop is for adult pneumonia, one for human papillomavirus and one for Ebola. Because of his publications he has recently been invited to lecture at a university on his work. This important application of EPR demonstrates that this latest generation of EPR users is not only expanding the user base but also the applications of EPR. Again, the IES can aid in this expansion of the EPR user base by a more involved interaction with industrial users by inviting them to participate in IES meetings. ►

Finally, like many other fields, EPR will incorporate smaller, more powerful and faster computers with more memory. Also, AI will likely play a role in the design and manufacture of new EPR. Even the direct implantation of AI into the operation of the EPR instrument can be expected. AI will be an attractive and exciting feature for new as well as experienced EPR users. Such EPR developments will guarantee an exciting future for EPR as well as an expanding user base.



John Pilbrow,
IES President (1999–2022),
Hon Sec IES (1997–1999):

To begin at the beginning, I am by training a Physicist and ‘cut my teeth’ in EPR as a Masters Student in NZ followed by three years at the Clarendon Lab in Oxford – the scene of much of the early development of EPR. The early 1960’s was a time when the Physics Community was beginning to realise that the centre of gravity of EPR was moving towards Chemistry. At that time books about EPR were rare. Apart from the published literature, I recall the two books by David Ingram [*Spectroscopy at Radio and Microwave Frequencies* 1955 & *Free Radicals as studied by Electron Spin Resonance* 1959] and William Low’s *Paramagnetic Resonance in Solids* 1959. George Feher’s famous paper regarding EPR detection sensitivity could be found in the *Bell System Technical Journal* [1957] and of course we were aware of his early ENDOR from P in Si in *Physical Review* [1955].

I now refer to *The International Symposium on Electron & Nuclear Magnetic Resonance* held at Monash University in 1969, the third in a series of ‘one-off’ magnetic resonance conferences, the earlier ones having been in Brazil and Japan. I had joined the Monash Physics Department in 1965 and in 1967

was appointed Symposium Secretary. Key international players included Herb Gutowsky, Charlie Slichter, Raymond Andrew & Robert Blinc, and by far the majority of papers and participants represented NMR.

At the end of the Symposium, Daniel Fiat chaired an informal meeting which I believe represented the beginnings of ISMAR. I sensed that ISMAR would turn out to be significantly dominated by NMR and that was confirmed at ISMAR Conferences that I attended years later in Sydney [1995] and Poznan [2002]. I also recall two major AMPERE Congresses [Rome 1986 & Berlin 1998] where the same situation applied. This is in no way a criticism of either ISMAR or AMPERE given that there are many more working in NMR than in EPR.

EPR did not remain simply as a CW technique applied to transition metal and rare earth ions in crystal matrices, dominated by physics. Increasingly, studies of free radicals, spin labels & metal ions in biological molecules assisted the transition into biology. The demand for better techniques to explore biological systems naturally led to a greater and greater involvement of pulse techniques. By the early 1970’s NMR pulse methodology had increasingly become the norm. However, translating NMR techniques across to EPR wasn’t entirely straightforward due in part to the very different operating frequencies and different relaxation processes.

By the time Hal Swartz established IES about 35 years ago, there were of course several regular EPR meetings in the UK, Europe and the USA, particularly the Annual Rocky Mountain EPR Conference held in Denver. A parallel development was creation of the EPR Newsletter at the University of Illinois, edited by my old friend, the late Linn Belford. The EPR community began to have a voice. And of course that role has been continued since 2002 under the very competent editorship of Laila Mosina.

In 2002 during the Voevodsky EPR Conference in Novosibirsk, I sat down with Laila to ask her to consider becoming Editor of the EPR Newsletter. She eventually agreed and I believe we’d all want to say to her, congratulations for an exceptional job! As we all know, the published literature continues to expand and it is impossible for any of us to keep abreast of all new developments. Thus the EPR Newsletter continues to alert us to all sorts of new research methodologies through carefully chosen and well-crafted articles. This is an important role for the Newsletter and ensures that readers can investigate new

developments without necessarily having to comb through a lot of published research first.

As the EPR community is much smaller than the NMR community, IES, and through the agency of The EPR Newsletter, helps to give EPR spectroscopy its own identity and voice.



Wolfgang Lubitz,
IES President (2005–2008):

This year we are celebrating the 80th anniversary of the discovery of EPR by Evgeny K. Zavoisky in Kazan – a good reason to look back at the development of the method, its applications and future perspectives. The EPR community is small – but very active with regular annual meetings held in different countries in Europe, Asia/Pacific and the Americas. In 1989, 35 years ago, the international EPR Society (IES) was founded, intended to foster the development and application of the method across the scientific disciplines, to communicate information and news about EPR, and stimulate education through the organization of EPR schools, workshops and seminars. The work of the society and the dissemination of news via the EPR Newsletter has been a great success during the last ≈20 years. The EPR meetings are very important; they provide opportunities for the presentation and intense discussion of novel results, future ideas and the free exchange of knowledge, in particular about the rather complex EPR instrumentation and methodology. Here, visits and joint projects are often initiated, technical help is provided and the exchange of postdocs and doctoral students arranged. Without doubt it is mandatory to continue and strengthen all these activities in the future.

The development of EPR since the seminal work of Zavoisky in 1944 and its impact on various fields of the sciences is amazing. The combination of EPR with other methods like

NMR (ENDOR, DNP) and optical spectroscopy (ODMR) has for example widely opened new vistas of applications. The transition to high field EPR significantly increased the spectral resolution of the technique. Very high frequency (THz) EPR experiments paved the way for studying systems that were not accessible to standard EPR methods so far. Different instrumental developments led to a very significant enhancement of the EPR sensitivity resulting in the detection of smaller and smaller numbers of spins, which initiated interesting applications in material science, physics, chemistry, and the biosciences, e.g. in sensing, spin quantum technologies, and in-situ/in-cell and operando EPR – to name only a few. The introduction of pulsed EPR opened the door to various types of time domain experiments with a resolution down to the nanosecond regime. Pulsed dipolar EPR spectroscopy (PELDOR/DEER) has successfully found its way into structural biology research. The method invaded the “diamagnetic world” via spin labeling using paramagnetic tags like stable radicals, metal complexes or triplet state molecules. The field of photochemistry has seen many important EPR applications on excited triplets, higher spin states and radical pairs. Applications in photosynthesis led to a better understanding of light-induced charge separation, transmembrane electron and proton transfer and water splitting catalysis. Enzymes containing metal centers often pass through paramagnetic states in their reaction cycles. Prominent example are the complex transition metal centers in water oxidase, nitrogenase and hydrogenase where EPR has delivered key results. Hand in hand with theory the electronic structure of molecules is now becoming available even for short-lived species, information that is indispensable to fully understand chemical reactions and the structure, dynamics and function of catalysts involved in reaction sequences. These can now often be followed in-situ in real time via operando

EPR. In this context, the miniaturization of EPR set-ups, which can easily be used in the chemical laboratory, has been pursued. Here, the activities around the idea “EPR-on-a-Chip” are highly interesting. Last but not least the interpretation of EPR spectra has been greatly facilitated by the development of smart spectral simulation methods (e.g. “EasySpin”).

This is only a limited, personal selection of some developments and applications in the field of EPR, there are many more, e.g. in spin physics/chemistry, material science, in imaging and in the medical sciences. Many of the mentioned activities are ongoing and promise to become increasingly valuable for the scientific community. The breadth of EPR applications has always been amazing – and I am sure this truly crossdisciplinary trend will continue. The next generation of EPR scientists has a fabulous machinery at hand to attack and solve future problems, in which paramagnetic systems play a role. I therefore believe that EPR and all its variants have a bright future in particular if accompanied by expert theoretical treatments and calculations and the necessary complementary techniques.

There is, however, a caveat in all this. The great success of EPR across the scientific disciplines has only been possible in the past by international collaborations and a free exchange of knowledge concerning instrumentation, methodology and new applications. In recent years this has become very difficult due to several geopolitical conflicts, e.g. in East Europe, in the Middle East, and in Asia. These conflicts are strongly impacting the sciences. They have led, for the first time in several decades, to serious restrictions of international travel, visits of conferences and laboratories and even to the termination of many international cooperations including the use of specialized instrumentation and the important exchange of postdocs and doctoral students. This is poisoning the scientific relationship between countries and very sadly it is cutting grown

ties between many research institutions and laboratories. I strongly believe that we must do everything possible to come back in the foreseeable future to sustainable cooperations and a mutual exchange of ideas and people for the benefit of our science and the next generation of young scientists.



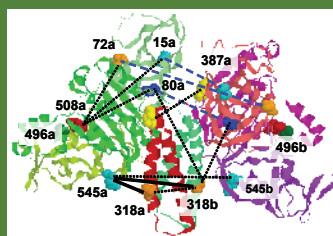
Jack Freed,
IES President (2008–2011):

As it happens we at ACERT just completed a Workshop entitled “Benefits of Electron Spin Resonance Spectroscopy” with the future of ESR in mind. The objective was to interest young researchers at Cornell to realize the great potential of modern ESR methods and the different ways it can greatly aid them in their research projects. It is our feeling here at ACERT that it is very important for the future of ESR to advertise its many potentials to a wide audience to expand the range of scientists benefiting from ESR. To paraphrase a senior participant at the Workshop: after one tries the other biophysical techniques such as crystallography, cryo-EM, NMR, etc., and fails to succeed, then one should try ESR with its record of successes where these other methods could not succeed. We addressed the utility of



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Dept. of Chemistry &
Chemical Biology
259 Feeney Way
Cornell University
Ithaca, NY 14853, U.S.A.

+1-(607)-255-4632

www.acert.cornell.edu

ESR in chemistry, materials science, biology, plant science and medicine, industrial research and testing, dosimetry, as well as archeology, geology, and paleontology. We expect in coming years the applications of ESR in these fields will continue to expand, and ACERT will continue to play a role in this.

There are many new developments of ESR technology and applications – too many for one person to call attention to. I will thus confine myself to ones that we at ACERT feel are important to develop and plan to do so. First is the development of double quantum coherence (DQC) ESR for protein structural studies. Although DEER has been the main technique for this purpose, DQC has some key virtues: it can provide much higher sensitivity (in fact the ability to study a protein at 25 nM has recently been reported), and at micromolar concentrations there is virtually no baseline to subtract. Also we now have a complete theory including all the intermolecular contributions for DQC. Currently DQC is limited to radical pairs and not to clusters, but we hope to extend the method to higher order coherences.

Another area for technology development is in high field ESR. In conjunction with standard field ESR it can provide snapshots of motion at different timescales to help extract the complex motions of proteins and other macromolecules. The field of 2D ESR is also very useful for studying dynamics and needs to be extended to high fields providing orientational resolution. Also, at 95 GHz one can perform 2D exchange experiments analogous to 2D NMR exchange, but covering much faster exchange rates occurring in the microsecond to nanosecond range. There are still challenges to be able to perform such experiments on proteins to observe internal modes of motion occurring on that time scale.

Next I would like to point out the further development of processing ESR data. Here at ACERT we have made considerable progress in denoising noisy signals which can greatly shorten the time of experiments (i.e., much less signal averaging). Also in Pulse Dipolar ESR experiments (e.g., DEER and DQC) we can directly solve the inverse equation needed to obtain the distance distributions, instead of using least squares fitting that all the other methods depend on. It is more direct and can lead to more accurate and more detailed results.

Thus, first and foremost is the objective of interesting a wider audience in the capabilities of ESR. That will create many opportunities for advancing ESR methods and applications.



Hitoshi Ohta, IES President
(October 1, 2012 – June 30, 2013;
2015–2017)

The development of EPR will continue to go into the high-frequency and high-field like NMR with higher sensitivity because it will give the high spectral resolution. It will also solve the remaining issues to observe the zero-field splitting of metal proteins etc. For the high-frequency sources in the range of THz, the high power gyrotron or the quantum cascade laser will come into this field. Moreover, the superconducting magnet beyond 30 T is coming in very near future, which will also support the high-frequency and high-field EPR. Therefore, the development of high-frequency and high-field EPR is very promising.

The EPR detection by the ODMR of NV⁻ center of diamond is becoming very promising after the inventive process to get the high-quality diamond films or nano-particles. It is very useful to detect the biological systems at room temperature. However, it is applicable to extremely small samples at any temperature because of its extremely high sensitivity. This advantage can be applied to many kinds of extreme conditions, and we are trying to apply this method to the EPR detection of sample under extreme conditions, such as very high pressure beyond 4 GPa using the diamond anvil pressure cell. The EPR detection of the amount of sample in less than 0.5 mm diameter space of the diamond anvil pressure cell is not possible by the conventional detection methods. Therefore, the EPR detection by the ODMR of NV⁻ center of diamond is very much promising.

IES is the interdisciplinary society including Physics, Chemistry, Biology and Medicine. In order to solve the issues written above, the cooperation of very wide fields is required. IES is the only society of EPR with very wide

fields of scientists. Therefore, IES is the unique EPR society, which has the role to solve the above mentioned issues.



Lawrence J. Berliner, IES President
(July 1, 2013 – March 31, 2014):

I had the distinct pleasure to participate in the 50th anniversary symposium of the discovery of EPR in Kazan and several other meetings in this great Zavoisky institute. It was amazing to tour the University museum and see equipment that some of us refined in later years, particularly low field EPR.

As to the future of EPR, I have, more than once, offered a pessimistic at view of where would be going; and obviously I've been wrong every time! Having been a graduate student at the beginning of the spin labeling technique (Harden McConnell had some postdoctorates working on this, I was his first 'spin labeling graduate student'). It really appeared that, without synthetic advances, the technique would suffer real limits. People were very active in the former Soviet Union, Japan, France, Hungary and other countries in the European area. But little did I know that when we and the late Kalman Hideg prepared a thiol specific spin level for one of our hands-on projects, did I realize that Wayne Hubbell saw much more into the future and launched the site specific spin labeling (SDSL) technique. That was, in my opinion, a renaissance for EPR applications in biology, etc. Another major advance was the use of high field measurements with superconducting magnets, first developed in Moscow and rapidly picked up around the world. It was again a renaissance, particularly in terms of spectral resolution and time domain characterization. At the very low field end in-vivo EPR has been a reality. Lastly, pulsed EPR has really added versatility to many biological problems. Years ago we had great difficulty in

studying membrane proteins, disordered proteins etc. Now that has been overcome and molecular weights have not become a limiting factor in looking at structure and dynamics in macromolecular systems. Another great advance has been in the studies of the photosystems, where electron-electron interactions and other features of metal centers that were more challenging earlier have become accessible.

So, in the end, am I going to make predictions for the future? I, like other researchers have had dreams about the feasibility of new applications, but I don't want to make the same mistake of being somewhat pessimistic again! While my research involved other areas of magnetic resonance and optical techniques I was "born" with EPR and it will always be my first love. It is clear that journals such as AMR, JMR, MRM, Biophysical Journal, J. Scientific Instruments and several others will be the appropriate 'sounding boards' fostering future advances in this field.



Klaus Möbius, IES President
(April 1, 2014 – December 31, 2014):

Reflecting on the 80th anniversary of Evgeny Zavoisky's discovery of EPR, I conclude that he made his epochal invention under the worst possible circumstances:

It is well documented that in the period between 1939 and 1941, E. Zavoisky, together with S. Altshuler and B. Kozyrev, had searched for *nuclear* and *electron* magnetic resonances in Kazan. However, after the invasion of the USSR by Nazi Germany in 1941, the Second World War prevented Zavoisky from completing this work. He had to disassemble the experimental set-up with which he had observed the first signals. Altshuler later recalled that the inferior experimental equipment, specifically the low quality of the "old-fashioned electromagnet", prevented success. "If Zavoisky had

had 2-3 months more time for the experiments, he would undoubtedly have found the reason for the poor reproducibility of the results." During World War II, Zavoisky continued his research in Kazan.

In May 1944, Evgeny Zavoisky submitted his doctoral dissertation to the P. N. Lebedev Physical Institute of the USSR Academy of Sciences in Moscow. To his disappointment, the responsible scientific committee of the Institute did not recognize the relevance of his discovery. The committee requested more evidence for the reproducibility of Zavoisky's data.

In a second attempt, Evgeny Zavoisky turned to the Institute of Physical Problems in Moscow. There, Academician Pyotr Kapitsa (who was later awarded the 1978 Nobel Prize in Physics) gave him the opportunity to assemble another EPR experimental set-up and carry out his magnetic resonance experiments again. On January 30, 1945, Evgeny Zavoisky defended successfully in Moscow his dissertation for the degree of Doctor of Physical and Mathematical Sciences.

During his lifetime in the Cold War, Evgeny Zavoisky was not adequately recognized and honored by the international magnetic resonance community. One reason was, perhaps, that he had published almost exclusively in Russian journals, which went largely unnoticed in the West. During this period, it was also very difficult for scientists in the USSR to establish contacts with Western colleagues. But eventually, in May 1977, at the occasion of the 6th Meeting of the International Society of Magnetic Resonance (ISMAR) in Banff, Canada, it was planned to honor Evgeny Zavoisky with the ISMAR Award. Tragically, Zavoisky could not personally come to Banff to receive the Award, even though he had travel visa from the Soviet and Canadian authorities. He had passed away in Moscow in October 1976 at the age of only 69. Just after having been informed about the decision of the international ISMAR Prize Committee.

So, when you ask me for my opinion on the future of the EPR and the development of its applications and methods, and the role of the IES in this process, my answer is:

Given the current worrying times, I remain firmly convinced that a flourishing science can only be achieved through the international exchange of creative ideas.

It should be the mission of the IES to support this process to the best of its ability – in accordance with the statutes of its founders since its inception in 1989: "The Society aims to stimulate scientific development of EPR, facilitate communication among EPR researchers, and encourage the use of EPR techniques

in a variety of research areas". For example, in materials science, molecular biology, chemical kinetics or medical imaging. In all these areas, novel applications of EPR are in full bloom.

I would like to emphasize once again that only if these objectives are further pursued can we hope that the EPR community will continue to make new excellent inventions under the best possible circumstances.



Thomas Prisner,
IES President (2018–2019):

EPR spectroscopy has made significant progress over the last 80 years, boasting a diverse array of techniques such as cw-EPR, ENDOR, pulse dipolar and hyperfine spectroscopy, high-field and frequency-swept EPR, miniaturized EPR, time-resolved EPR, electrical and optical detected EPR, spatial resolved EPR among others. These methods have greatly contributed to studying of paramagnetic species, reaction intermediates, transition metal complexes and enzymes and, by spin-labeling techniques, also large diamagnetic macromolecules and complexes. Developments of the last decades, such as high-field EPR allowed to fully exploit the additional information content of g-tensor values in combination with accurate quantum-chemical calculations. Pulse dipolar spectroscopy developed to a well appreciated tool for structural elucidation.

Looking ahead, numerous opportunities await the EPR community. There are several mature fruits ready to be harvested which will spread EPR into a broader community. Initiatives like PDB-dev, a prototype archiving system for structural models, asked the EPR community to create an open accessible EPR databank for dipolar spectroscopy facilitating the integration of EPR data into structural modeling. The International EPR society (IES) will host such a database and help to manage the supervision

process once created and installed. Similarly, demands from various scientific fields underscore the need for a broader access to cw-EPR data (as well as to accessible instrumentation!).

Moreover, I see a number of blossoms which might lead to revolutionary changes in the field of EPR. Increased sensitivity and performance enhancements may lead to redesigned spectrometers, even for analytical applications! This also holds for data analysis. In parallel, recent developments in DNP and microwave pulse shaping capabilities herald new possibilities, including pulse DNP at sub-THz frequencies and single electron-spin detection, combining EPR spectroscopy with NMR, optical spectroscopy or quantum electronics.

Despite its 80-year history, EPR is still young and remains a vibrant field ripe for innovation. Contrary to early perceptions of its maturity, the future holds promise for inventive advancements. EPR is a dynamic research area, attracting young scientists with its interdisciplinary nature encompassing experimental hardware, method development, quantum theoretical calculations, and its combination with various complementary spectroscopic techniques.

In conclusion, EPR remains vibrant, offering thrilling opportunities for interdisciplinary research and collaborations. For me, working within this research domain has been and continues to be immensely enjoyable, offering abundant avenues for exploration.



Songi Han,
IES President (2021–2023):

As we celebrate significant milestones for the International ESR/EPR Society (IES), our view turns towards the future of EPR and its unfolding potential. The journey of scientific discovery has always been marked by the advent of new tools that offer deeper insights into the unseen world. From the first telescopes

to the sophisticated cryogenic electron microscopy, each innovation has expanded our understanding of the universe. Today, we stand on the cusp of a quantum leap in molecular visualization, particularly in the life sciences, where the magnetic resonance properties of spins hold the key to reporting on dynamic molecular events with unprecedented resolution and clarity.

Historically, the evolution of human consciousness and scientific advancement has been intertwined with our ability to observe and understand our environment through increasingly refined “lenses”. These lenses, ranging from the human eye to modern high-resolution imaging techniques, have progressively unlocked the mysteries of both the cosmos and the minutiae of life. The next frontier in “seeing” is quantum sensing of coupled spins that reflect on the intricate molecular world that it represents – a frontier that has been pushed by the magnetic resonance field, and the ESR/EPR field in particular, and one that requires special attention today.

Life’s processes, intricate and dynamic, unfold in aqueous environments where traditional characterization methods reach their limits. The unique capability of EPR to sense molecular dynamics in water, to image oxygen consumption under physiological conditions, and to measure distances between molecular sites with atomic precision in vitrified solution makes EPR an indispensable tool for probing the complexities of molecular communication and assembly under physiological conditions.

Despite the profound potential of magnetic resonance, the relatively low sensitivity of both electron and nuclear spins is their weak point. Electron spins still have an edge over nuclear spins when it comes to signal sensitivity. Only electron spin’s magnetic ground state can be polarized at near unity under accessible conditions of 9 Tesla and temperatures below 4 K. Only electrons, with their spins paired in the singlet or triplet ground state, can be excited by light followed by intersystem crossing to generate highly polarized electron spin signal that is 1000-fold greater than thermally polarized EPR signal. This edge is crucial for advancing our understanding and applications of quantum sensing – a field that is receiving considerable attention and investment from both industry and government sectors. Ironically, many core EPR studies, including techniques like pulsed Electron-Nuclear Double Resonance (ENDOR), out-of-phase Electron Spin Echo Envelope Modulation (ESEEM), and Dynamic Nuclear Polarization (DNP), inherently meet the criteria for quantum sens-

ing. Yet, they often do not enjoy the heightened visibility or support that comes with the quantum information revolution. This gap is a missed opportunity not only for the magnetic resonance field but also for the broader quantum information community. By harnessing the quantum properties of spins and their interactions with other spins and light, we can dream of achieving a level of sensitivity and information content not available to date, as epitomized in the dream of measuring molecular dynamics, protein structure and/or water dynamics in a single cell under stress.

Participation in the quantum revolution is vital for several reasons: it’s where significant investment is coming from both government agencies and industry; it represents a modern “Sputnik moment” with countries like China, Germany, and the USA prioritizing quantum computing capabilities as a national goal; and it offers future job prospects around the world for PhD graduates from EPR laboratories. The lack of magnetic resonance experts in the quantum information science and technology field is an issue that can and should be addressed. Our unmatched expertise in coherent control, polarization transfer, relaxation theory, and spin order measurement position us well. But to have an impact, it is crucial to have an open mind to this new trend in quantum information science. Optical hyperpolarization combined with optical readout offers the blueprint towards highly sensitive magnetic resonance in the optical limit. However, for optical detection of Magnetic Resonance (ODMR), the benefit of relying on the nitrogen vacancy (NV⁻) is unmatched, a reason why “quantum sensing” has become nearly synonymous with ODMR using NV⁻. In this landscape, EPR experts have the potential to surpass the current capabilities and technology by leveraging the high field limit, exploiting advanced EPR cavity available to us, taking advantage of high-power microwave amplifiers, and resonant amplification of analyte’s NMR signal through DNP.

The International ESR/EPR Society (IES)’s role in this effort is crucial, by enhancing collaboration, supporting research, and promoting the education of EPR principles and applications. This effort includes recognizing the need for a broader diversity in topics and membership within the IES and supporting efforts to help make EPR applications more accessible and engaging to non-experts. The future of EPR is very bright, with the potential to open new understanding in the life sciences and beyond. As we celebrate our achievements, we must also commit to fostering the innovations that will define our future. ●

Interview with Professor Gunnar Jeschke

President ad interim of the European Federation of EPR groups

EPR newsletter: *Dear Professor Jeschke, thank you for your continuing collaboration with the EPR newsletter. Could you please share with us your opinion about the future of EPR and the development of its applications and methods, and the role of the EFEPR in this process?*



During most of its history, EPR spectroscopy has stood in the shadow of its slightly younger sister NMR. The main reasons were the much larger abundance of diamagnetic materials of interest as compared to paramagnetic materials and the later development of sufficiently fast electronics and of microwave technology as compared to radiofrequency technology. Hence, the EPR scientific community remained much smaller than the NMR community. This in turn limited our advances in theory, experimental techniques, and instrumentation. Paradoxically, after eight decades this now works in our favour. EPR methodology is far from maturation. The problems to which EPR is applicable remained underexplored. In other words, now we do not have a sufficient number of scientists and labs for addressing all application problems that should be addressed by EPR spectroscopy.

Without disregarding other application fields, I currently see the largest potential for EPR in catalysis, in characterization of partially disordered proteins, and in the general direction of spintronics. I very generously define the last field as including organic conductors, molecular magnets, and conversion of solar to electric energy. One of the major active lines of research in NMR spectroscopy, dynamic nuclear polarization (DNP), could profit strongly from better understanding of electron spin dynamics and relaxation.

Catalysis has always been an important branch of chemistry. Since its early days, EPR spectroscopy strongly contributed to this field. The necessity to transform chemical industry to new feedstocks and new energy inputs has led to a surge of catalysis research. This surge is fueled by new preparation methods for tailored catalysts and by emerging methods for characterizing their structure and action in operando. Too few EPR groups pursue operando EPR as well as its connection with advanced pulsed EPR techniques for detailed characterization of active sites. Go operando, young EPR spectroscopists!

Recently, protein structure prediction has achieved an accuracy and precision that can compete with most experimental techniques. It is fast, too. Structures for the whole human proteome have been predicted by AlphaFold2. Paradoxically, this revealed a large prevalence of intrinsically disordered regions, whose ensemble structure AlphaFold2 cannot predict. Biological EPR spectroscopists know that for many membrane proteins, where AlphaFold2 does confidently predict a single structure, reality is far from that. For most proteins that consist of more than a single, small globular domain, function depends

on *distributed* structure. By providing access to distance distribution restraints, EPR spectroscopy can play a unique role in a new era of ensemble structural biology.

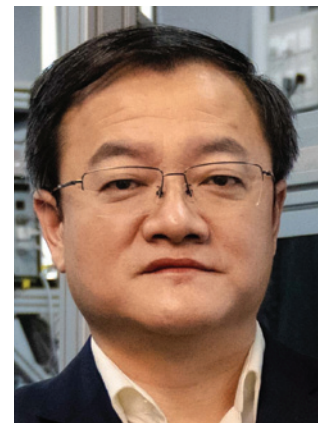
EPR spectroscopy is clearly an important technique for all materials where charge carriers or magnetic moments are either isolated or form small clusters. Further miniaturization of information-processing devices and sensors will force us to use such materials increasingly. The phenomena must be studied that enable or limit such applications. EPR spectroscopists are in a good position to contribute.

Application work is what sells in modern science. However, foundational work provides the ideas and expertise for opening up new application fields and for tailoring techniques. This applies on the level of individual scientists, who need to learn the foundations when they are young. Learning by doing is often the best way. We need to pursue projects on basics of EPR and this means we need to find funding for them. As a community, once we stop work on basics of our field, we decide that this field will become mature and then decline. We should avoid this.

What can EFEPR do? Science is driven by people. People do not like to be bored. First of all, we should excite the young generation by our summer schools and by interesting conferences. When we are excited, we can generate excitement in others. To extend as a community, we need resources. If more EPR groups are needed, we need to lobby for appointments to be made at universities and other research institutions. To attract anything, we first need to be seen. EFEPR should enhance visibility of EPR spectroscopy in European science and its institutions, such as the European Science Foundation. We need to reach out. No President can do this alone, only the community can.

Interview with Professor Jiangfeng Du

President of the Asia-Pacific EPR Society



EPR newsletter: *Dear Professor Du, thank you for your continuing collaboration with the EPR newsletter. Could you please share with us your opinion about the future of EPR and the development of its applications and methods, and the role of the APES in this process?*

In principle, the physical foundation of EPR has been thoroughly unveiled up to date. As for the technology advance, the higher sensitivity of EPR might be one aspect to be developed, e.g., less sample for the cw-EPR, or weaker electron-nuclear spin interaction in ENDOR or weaker electron-electron spin interaction in DEER/PELDOR. The high-field EPR technique from W-band to 250 GHz are necessary because the anisotropic interaction provide the orientation dependence in more detail. All these progresses have to rely on the high-level education and training of the junior scientists in this field. In the past decade, the development and application in Asia were made mainly in China, Japan, South Korea and other countries.

Except for the conventional EPR techniques, the quantum sensing based on the nitrogen-vacancy center (NV) in diamond opens a new door for EPR. Measuring the magnetic resonance spectrum of single molecules/nanoscale materials had been an elusive goal until diamond-based magnetic resonance technology came to us. I believe that single-molecule EPR technology will bring new broadly applications and vitality to EPR. We are working together with scientists from around the world to continuously promote the development of this direction. To attract more researchers and push the field forward together, we summarize the progress and outlook on the new field with the topic of 'Single-molecule scale magnetic resonance spectroscopy using quantum diamond sensors' [Review of Modern Physics 96, 025001 (2024)].

For the international cooperation and affairs, after the 2nd, 8th and 12th Asia-Pacific EPR symposiums had been succeeded in China, more and more international co-operations had been enhanced. Upon the progress, the Asia-Pacific EPR Society plays as a bridging role. In the coming October, we hope more and more researchers to attend the 14th Asia-Pacific EPR symposium to be co-organized by Zhejiang University & University of Science and Technology of China in Hangzhou city, China.

The application of EPR in China has achieved a great progress. The full-time EPR researchers have grown rapidly in China. Since 2011, an annual EPR symposium has been found with ~30 attendees, which lately becomes an effective scholar platform in domestic China. In 2023, about 230 attendees took part in this symposium. In 2022 March, a monograph titled Electron Paramagnetic Resonance Spectroscopy – Principles and Applications by Prof. Ji-Hu Su and Prof. Jiang-Feng Du had been published by Science Press in Chinese. We focus on developing technology and instruments to enable more researchers in China and even the world to use high-performance and affordable equipment. The W-band spectrometer has become available commercially now from the CIQTEK (Chinainstru & Quantumtech (Hefei) Co., Ltd.), a Chinese company found in 2016 in addition to their X-band EPR spectrometer commercialized in 2018. We will give a detailed story about all these achievements in China later in a forthcoming issue of the EPR newsletter.

Interview with Doctor Frédéric Jaspard EPR Business Line Manager, and Doctor Sylwia Kacprzak EPR Market Product Manager (Bruker BioSpin)



EPR newsletter: Dear Doctor Jaspard and Doctor Kacprzak, we are grateful to Bruker BioSpin, Patron of the IES, for the continuing help and support of the IES and collaboration with the EPR newsletter. Could you please share with us your opinion about the future of EPR and the development of its applications and methods, and the role of Bruker Biospin in this process?

Bruker commercial solutions have served the EPR community since the late sixties when its first commercial EPR spectrometer was built. Since then, Bruker has continuously supported researchers in their scientific efforts with advanced technologies. As result, Bruker Analytik GmbH was distinguished with the Zavoisky Award in 2000 for its achievements in the development of instrumentation, especially high-speed acquisition of pulse ELEXSYS 580 and high-field W-band spectrometers, leading to novel applications of the electron paramagnetic resonance technique. Numerous breakthrough technologies were introduced over the years with the goal of enabling our customers to stay at forefront of science. Many of these new developments were a result of the proximity and connections between Bruker and the EPR community. Like in the past, the tradition of collaboration and partnership plays a fundamental role in triggering and guiding new developments in EPR today. A deep understanding of the user needs and







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sharing of expertise led recently to introduction of successful products such as the Q-band FT standalone bridge, the SpinJet AWG and the Rapid Scan accessory. Working in close collaboration with EPR community is certainly a tradition that we cherish and not only plan to continue but also strengthen in the future. With our history and as market leader for EPR technology, Bruker has the privilege but also the responsibility to continue providing high-performance scientific instruments fulfilling customers' needs and enabling their success. An important example of this continuity is Bruker's investment to provide future solutions for the expanding cleantech research area. The development of specific solutions in energy storage and energy conversion as well as environmental studies will push the frontier of the high-field spectrometers down to compact low field equipment.

For the coming years, our vision is driven by the motto: **"Make magnetic resonance more relevant"** for a wide world of users. In this direction, our long legacy of supporting the EPR community to disseminate the scientific knowledge will continue and strengthen by our new platform **#Educate2Resonate**. With this new tool, we dedicate special effort to spread knowledge and understanding about Magnetic Resonance and we invite the whole EPR community to join us in inspiring future generations. To "Make magnetic resonance more relevant", we believe it is as important to provide high-end EPR instrumentation for advanced researchers and their breakthrough discoveries as to provide easy-to-use instrumentation for daily analytical tasks of routine

users. A fundamental aspect of the accessibility and ease of use is the user interaction with the instrument, especially towards the software experience. Software control with optimized workflows combined with automation will enhance both acquisition and data processing phases. In the last few years, Bruker has invested significantly into this digital transformation. With the recently launched software platform **SciY** (platform of advanced scientific and automation software solutions) Bruker intends to enhance the full potential of research data.

The modern instrumentation should combine an increased user accessibility and a reduced footprint following the current trends of miniaturization in technological developments. However, extreme compactness would result in reduced versatility, limiting function to dedicated methods and applications.

Following the newest technological developments, we eagerly anticipate the future implementation of Artificial Intelligence (AI) in EPR. As AI is improving and assisting in various aspects of life, it is justifiably envisioned to enhance as well EPR applications. Machine learning models could offer insight to optimize and control the way to operate the instrument. We could imagine that complex EPR sequences could be optimized to reduce measuring time and prevent operator mistakes. In addition, the data processing phase can greatly benefit from improved decision making in spectrum analysis with availability of structured databases. This assisted acquisition and data analysis will be especially a strong support for non-expert and benchtop routine users.



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Offers unique insights into systems in which NMR is not possible

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Interview with Dr. Paolo Bruzzese on the Occasion of His IES Best Paper Award 2023



EPR newsletter: Dear Dr. Paolo Bruzzese, on behalf of the readers of the EPR newsletter we congratulate you on your IES Best Paper Award 2023. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?

I started my career in academia because of my insatiable curiosity. Ever since I was younger, I was fascinated on how science allows one to rationalize phenomena by decrypting their inmost nature with laws and models. The discovery of relationships belonging to the microscopic world that explain evidences from the macroscopic world is what I most like of my daily research.

Who introduced you into magnetic resonance?

The first time I bumped into magnetic resonance was during my first year of my Master in the University of Turin. There was a mandatory course entitled “Magnetic Resonances” held

by Prof. Mario Chiesa. I remained completely astonished when Mario showed me for the first time the spin Hamiltonian formalism. The elegance and conciseness of using few parameters to explain magnetic resonance spectroscopy ... it is amazing!

What are your main interests of work in magnetic resonance?

I employ EPR techniques for identifying and characterizing active sites in homogenous, heterogeneous and single-site heterogeneous catalysts. In particular, within our group led by Dr. Alexander Schnegg in the Max-Planck Institute for Chemical Energy Conversion, I am interested at understanding selected chemical reactions that might contribute to the transformation of our energy system.

What is the most difficult task of your work in magnetic resonance?

As a spectroscopist, the most arduous and crucial part of my work is the interpretation of EPR spectra to correlate them with the atomistic structure of the systems investigated. Sometimes this analysis may take more time than what we expect (even several weeks!). Nevertheless, I always embrace this challenge with enthusiasm, eager to decipher what the electron and nuclear spins tell us through spectroscopy.

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

I believe our generation is facing considerable challenges in pursuing a career in research. Securing funds, precarious employments and moving far from the own affections are just some of the obstacles that we inevitably experience in our path. I think that the best answer to such adversities is disseminating our scientific activity to wider audiences in a clear and meaningful way. This allows the general public to understand the importance of promoting research in the magnetic reso-

nance field. Even though our findings do not necessarily provide immediate solutions to the energetic crisis or environmental emergency, they surely put the basis to enable effective responses to such global issues.

Mario Chiesa and Andreas Pöppel:

Paolo Bruzzese obtained his Master's degree in Chemistry from the University of Torino in 2018, working on the computational modelling of MgCl_2 -based Ziegler-Natta catalyst. At that time, the two of us had a position for a joined PhD between Leipzig and Torino, funded within the framework of the ITN project Paracat. Paolo was brave enough to leave the field of computational chemistry and accept our offer to join our experimental teams.

During his PhD, Paolo focused on applying hyperfine techniques to elucidate the structure of copper species in zeolite materials, a very relevant topic in the field of heterogeneous catalysis and his ability to integrate experimental and theoretical approaches was instrumental in advancing our understanding of these complex systems.

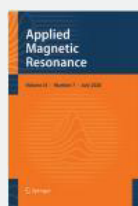
Paolo's work involved meticulous synthetic procedures at the Erlangen Center for Interface Research and Catalysis (ECRC), in collaboration with Prof. Martin Hartmann. His careful synthesis of zeolite materials with controlled Si/Al/Cu composition laid the foundation for selectively isolating specific copper species. Additionally, Paolo developed novel protocols for enriching the zeolite framework with ^{17}O , a significant achievement enabling the precise monitoring of metal-framework interactions using ^{17}O ENDOR /HYSCORE techniques.

Through these efforts, Paolo made groundbreaking contributions to the field by successfully determining elusive monomeric copper hydroxo intermediates via EPR spectroscopy. His application of advanced quantum mechanical methods translated spectroscopic results into atomistic structures, resolving longstanding issues surrounding these intermediates



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Applied Magnetic Resonance



Call for papers: Special Issue – EPR at 80

By the time of the 80th anniversary of the discovery of EPR by Zavoisky, EPR has become an indispensable tool for studying a wide range of chemical and physical phenomena. EPR plays a major role in understanding the mechanisms of chemical, catalytic, and enzymatic reactions, the mechanism of solar energy assimilation, etc. Understanding how to control electron spin relaxation will be key to developing spin technology. EPR spectroscopy will contribute to development of spin technologies not yet imagined.

This Special Issue welcomes reports that both confirm the youthfulness of EPR and point toward even more exciting future developments.

Papers can be submitted between 1 November 2023 and 30 May 2024. Please make sure to choose the special issue article tab “S.I.: EPR at 80”.

Guest Editors:

Prof. Gareth Eaton, University of Denver, email geaton@du.edu

Prof. Sandra Eaton, University of Denver, email seaton@du.edu

Prof. Kev Salikhov, Zavoisky Physical-Technical Institute, email kevsalikhov@mail.ru

crucial to oxidation catalysis by zeolite and enzyme catalysts.

Nothing was routine in Paolo's work and he truly provided new insights that are poised to make lasting impacts in catalysis research and further strengthen the role of EPR spectroscopy in the field. We are delighted that Paolo's achievements have been recognized with the prestigious IES Award.

On a personal note, what we find even more remarkable is Paolo's inclusive and supportive demeanour, always willing to assist his colleagues and share his expertise generously, something we value just as his scientific skills.

Interview with Dr. Nino Wili on the Occasion of His Bruker Thesis Prize 2023 and Raymond Andrew Prize 2023



EPR newsletter: Dear Dr. Nino Wili, on behalf of the readers of the EPR newsletter we congratulate you on your Bruker Thesis Prize 2023 and Raymond Andrew Prize 2023. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?

Difficult to say why exactly. I have always been good at school, and I did like the scientific subjects. I remember liking biology early on, and then later I had a really good chemistry teacher. I had the skills and the interests, so I considered science as an option quite early

on. However, in my last year before university, I seriously considered studying music at a local Jazz school. I played electric bass in several bands, including two big bands, and I practised my scales, studied music theory, etc. Anyway, one afternoon, about a month before the deadline, I signed up to study at ETH Zurich (there is no entrance exam for people with a Swiss "Matura"). I don't remember a particular reason, it was just a gut decision. It turned out to be the right decision, I think. Like this I could do science, and still made a lot of music, both during my undergrad and during the PhD. Unfortunately, Covid, writing the thesis, and moving for my Postdoc interfered quite strongly with playing in a band and playing live. I hope that comes back some day.

Who introduced you into magnetic resonance?

I heard about NMR in the first year of studies, and with some googling I found out that Richard Ernst and Kurt Wüthrich have been at ETH and apparently quite important. Then the first lectures about interpreting NMR spectra I heard by Oli Ebert. I liked it back then, but I don't think I was all in already at that point. In the second year, I had a course in quantum mechanics by Beat Meier and Matthias Ernst, and of course they used spins as model systems quite often. In my third year, I heard the lecture in Magnetic Resonance theory by Beat Meier and Gunnar Jeschke, and I absolutely loved it. I only really appreciated years later how deep (and difficult...) that lecture was, and how unique it was that NMR and EPR are just taught side-by-side. I recorded my first EPR spectrum in a practical course with Ines Rubio-Garcia (shout-out to her!) more than 10 years ago, that's a third of my life, which is quite crazy.

What are your main interests of work in magnetic resonance?

I guess there are two answers. One is the elevator-pitch one, where I need to show a "profile". For this I would say my interests lie in the interface of EPR and NMR. In the theory and method development. This spans hyperfine spectroscopy and dynamic nuclear polarization, and includes building instrumentation and theoretical and numerical modelling.

The second answer is that I just love spins, and I am amazed how much they can tell us about nature. I have yet to find a subfield of magnetic resonance I find truly boring. There is so much. Light-induced stuff, low-field or even zero-field NMR, MRI, solid-state NMR with magic-angle spinning, all these crazy relaxation-analysis in Bio-NMR, and so on.

When at ETH, you were one of two presidents of the union that defends interests of doctoral students. Could you please tell us about this part of your life?

At ETH, the doctoral students of the department are represented by a union. But this is not really a union in the sense that there is a collective bargaining agreement or anything. But it has seats in the department conference, the teaching conference and so on. Additionally, it helps integrating new PhD students and Postdocs in the department life and tries to help solve conflicts. It has a quite important social function I would say. I was co-president of this union for two years (one year with Janne Soetbeer, another with Agathe Vanas, who you might know from EPR conferences as well). This time gave me some interesting insights into university politics, both good and bad. I still care a lot about how PhD students are treated, at ETH and elsewhere. They are essential for academic research and teaching, and I think there are plenty of problems regarding the treatment of PhD students that should be solved, at ETH and elsewhere.

It is well-known that you are the initiator of the International on-line seminar for young scientists. How this idea was conceived?

That is quickly told. I just asked some Twitter colleagues if they would be interested to discuss their research, because all the conferences were cancelled. "Conceived" is a big word for that, I just rolled with the flow. I also have to point out that starting such a thing is very easy, the hard part is keeping it running. Currently the committee includes Thomas Schmidt, Joseph McPeak, Tomas Orlando, and Yujie Zhao. I am pretty sure they have organized more seminars than I have!

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

First of all definitely don't listen to me. I make all important decisions with my gut, and I don't think you should listen to that. Other than that I hope that we can go back to communicating science honestly, instead of "selling" it to an audience. It's ok if your EPR experiment does not cure cancer, does not solve the climate crisis, and doesn't provide scalable and fault-tolerant quantum computing. On the other hand, if you want to cure cancer, solve the climate crisis, or build a quantum computer, go ahead! If you can use EPR for it – even better!

JEOL 2023 and IES Poster Prize at the 9th EFEPR Summer School



Sebastian Gorgon:

Luminescent radicals with high-spin states

Whereas most stable radicals are non-emissive, there is now a class of radicals that offer fully spin-allowed luminescence entirely within the doublet spin manifold. Record efficiencies for deep red and infrared light-emitting diodes were recently reached in trityl-based radicals linked to carbazole electron donors [1].

I started exploring interconversion between different spin states in the context of organic materials for light emitting diodes using photophysical methods during my PhD under Prof. Sir Richard Friend at the University of Cambridge. I showed that tris(2,4,6-trichlorophenyl) methyl (TTM) radicals can efficiently harvest triplet states on neighbouring closed-shell molecules. By tuning the molecular en-

ergetics, I established conditions under which this process occurs either unusually fast, or reversibly [2, 3]. These observations inspired me to explore covalently bound structures, to take advantage of stronger through-bond, instead of through-space, interactions between luminescent radicals and triplets. These luminescent radical-acene (R-A) molecules, synthesised by the group of Prof. Feng Li at Jilin University in China, provide a fantastic platform for exploring the interplay between spin and exciton dynamics.

While pump-probe spectroscopy allows tracking the excitons across over 10 orders of magnitude in time, optical wavelengths do not offer sufficient precision to resolve all states involved in our materials, as, by design, the energy gaps are minimised. Therefore, I initiated and conducted a parallel experimental stream using EPR as a visitor at the Centre for Advanced ESR (CAESR) at the University of Oxford. I was very lucky to be guided into this rich world of ESR by Dr. Emrys Evans, now at Swansea University, and Dr. Will Myers at CAESR.

This combination of techniques grants unparalleled access to the mechanistic behaviour of excited states of paramagnetic materials. In this case, the key insight was the match in the temperature-dependence of the high-spin state polarisation inversion seen in transient EPR and of the delayed photoluminescence revealed the key features of the mechanism.

Taking all the experimental data together allowed us to construct an excited state diagram and mechanism for luminescent R-A compounds, which we have now published in a recent article in Nature [4]. Eliminating the energy gap between the photogenerated state and high-spin state allows their interconversion in either direction, which is mediated by the available thermal energy. This approach simultaneously supports a high efficiency of initialisation, spin manipulations and light-based readout.

Magnetic resonance provided many key insights for this work, from the detection of characteristic quartet and quintet half-field signals to the signatures of exchange coupling regimes from lineshapes at X-, Q- and W-band. Additionally, the Optically Detected Magnetic Resonance (ODMR) experiments by Dr. Jeannine Grüne then confirmed the high-spin state is linked with the radical emission at both cryogenic and room temperatures.

This modular mechanism has allowed me to design a light-spin switch based on a biradical, where control the spin information between electrons in both the excited and ground states via contrasting exchange interactions. The radical spin pair is uncorrelated in the ground state. After absorbing light, strong correlation is switched on, mediated by two electrons on the bridge. Following light emission, the spin information is relayed from the excited state to the ground state. Therefore, a spin polarised ground-state can be prepared in R-A-R solely by the intrinsic exciton dynamics under photoexcitation, without any use of microwave driving. This makes it a fully-organic, room-temperature analogue of semiconductor colour centres, such as the NV in diamond.

Through this work we have taken the first steps towards a fully-organic modular platform for room-temperature molecular quantum information science interfaced with light, as recognised by a Quantum Creators Prize from the University of Chicago.

Careful engineering of energy levels leads to a reversible mechanism connecting high-spin and bright states. Crucially, the energetic separation between these states is large on magnetic scales, but accessible on optical scales. This balance allows both robust spin manipulations via microwaves and read-out using visible light.

The tunability exemplified through the extension from monoradical R-A to biradical R-A-R shows the generality of our luminescent high-spin materials approach, and extensive



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possibilities for control in polymeric multi-radical systems that remain to be explored. Broader emission wavelength range is achievable by employing emerging luminescent radical families which are being actively developed.

Access to magnetic information via a luminescent channel at room temperature opens a path towards ambitious future applications, such as biological quantum sensing of local fields at physiological conditions and information relay on the nanometre level.

Having arrived at the problem originally from a different direction, I am very grateful for the input from the EPR community and encouragement through the JEOL award at the RSC ESR conference and poster prize at the EFEPR School. I am excited to push these research ideas further over the coming years as a Research Fellow at Emmanuel College in Cambridge.

1. Ai, X., Evans, E., Dong, S. et al. Efficient radical-based light-emitting diodes with doublet emission. *Nature* 563, 536–540 (2018).
2. Cho, H.-H., Gorgon, S., Hung, H. et al. Efficient near-infrared organic light-emitting diodes with emission from spin doublet excitons. arXiv:2308.02355, *Nature Photonics*, in press.
3. Gu, Q., Gorgon, S., Romanov, A. et al. Spin control with triplet and doublet excitons in organic semiconductors. arXiv:2312.10595
4. Gorgon, S., Lv, K., Grüne, J. et al. Reversible spin-optical interface in luminescent organic radicals. *Nature* 620, 538–544 (2023).

Emrys Evans:

Sebastian has discovered a new class of molecular materials exhibiting spin and photo-physics that could enable future quantum technologies. He demonstrated that molecules containing luminescent organic radicals and chromophore groups – with energy resonant excitons – can enable coupling of light absorption and emission to multi-electron correlated, high spin ($S > 1$) states at room temperature.

Sebastian had to develop into a ‘triple threat’ scientist to probe the spin, optical and magnetic properties. He performed time-resolved optical spectroscopy that showed the exciton dynamics following photoexcitation was extremely fast and led to a long-lived, emissive state. ESR was critical for revealing the exciton transfer mechanisms and that quartet ($S = 3/2$) high spin states were formed in the monoradicals. His measurements at CAESR (Oxford) gave very strong evidence of this in the dipolar-induced width of the transient ESR signal and spin-dependent nutation frequency experiments. Sebastian was not satisfied and

went further to measure double quantum ESR transitions at half field that could only be present in quartet states. This meticulous approach to science was adopted throughout his PhD. By working with an international team of collaborators it was possible to have close links between design, characterization and exploitation to advance the exciting new materials platform. Feedback from understanding how the monoradicals worked led to the biradical system that showed potential exploitation in a light switch that turns on coupling of electron spins in the ground state. This approach will lead to innovation of new materials in future.

The broader implications of the work is that molecular materials with quantum-ready properties could be designed by chemical modifications to target spin-optical behaviour. It could provide a starting point to explore molecular quantum technology applications in sensors and networks, which needs more ‘triple threat’ scientists.

IES Poster Prize at the 2023 Euromar



Laura Remmel:

At the Euromar 2023 I had the great pleasure to present my research on the fluoride binding riboswitch and to be awarded the IES Poster prize. It was a great honour to receive this prize, especially in Scotland, where for me this whole project began. I would, therefore, like to thank the IES for selecting my research work for this prize, and for giving me the opportunity to describe this work in this Newsletter. I would also like to express my gratitude to Bela Bode as well as Marina Ben-

nati for their continuing support throughout this project as well as everyone else working with me during this time.

At high concentrations, fluoride ions act toxic to cells. Fluoride binding riboswitches are a safety mechanism of nature. Upon high fluoride concentrations the RNA binds fluoride ions, which leads to a change in the structure of the RNA, initiating the production of fluoride exporters to protect the cell from being harmed [1]. I started working on the investigation of the fluoride riboswitch from *Thermotoga petrophila* as a project during my Ph.D. with Bela Bode at the University of St Andrews. Performing ^1H NMR measurements we found that the riboswitch undergoes a transition from a free, via a magnesium-bound to a fluoride-bound state, indicated by the presence of different signals in the NMR spectrum. By performing PELDOR measurements we could show that this transition is only going along with a subtle change in the overall fold. We see broad and barely changing distance distributions for all three states, independent of the labelling positions we looked into. These findings agree with the presence of a pre-organised structure.

Nevertheless, to gather more insight into the fluoride binding by the riboswitch, which is crucial to its whole biological functionality, we could not solely look into the overall-fold itself, but needed additional insight into the fluoride binding pocket of the RNA.

In September 2019 a paper on ^{19}F ENDOR measurements, allowing the determination of distances between a spin label and a ^{19}F nucleus, was published by Andreas Meyer and Marina Bennati [2]. We saw a great potential in this as the riboswitch is designed to bind fluoride ions by nature. It happened to be the case that only a few weeks later, in November 2019, I had the chance to meet and speak to Marina at the EFEPR school in Brno, where we set the cornerstone for a collaboration. I designed the constructs we wanted to investigate and discussed potential travel options for me to Göttingen to learn about ^{19}F ENDOR measurements when Covid came and all travel stopped. It took another 1.5 years until I was finally able to travel to Göttingen and to perform the ^{19}F ENDOR measurements together with Andreas. We all knew that because of its complexity the fluoride riboswitch might not be an easy system to investigate and were very happy when we saw the first spectra with a visible splitting allowing us to determine distances between the nitroxide spin label and the fluoride ion. ►

Nonetheless, the analysis of such complex systems with more flexible spin labels, causing the presence of multiple conformations of the spin label, is a challenging task I continued to work on as a member of Marina's group. This work is now allowing us to simulate sum spectra based on Gaussian distance distributions and, in presence of a suitable model, also orientation selective spectra based on the various rotamers obtained from *in silico* labelling. Both simulation routines were performed using our home-written simulation program SimSpec [3]. The results showed us that the model we had built using the crystal structure as a template is in one case matching, in one case partially matching and in one case mismatching the measured data. This shows that we seem to have a deviation between the crystal structure and the solution structure and highlights that ^{19}F ENDOR is capable of picking up even these small differences.

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Bela Bode:

I first met Laura during a visit to my alma mater, the Goethe University in Frankfurt am Main. Laura had applied for a PhD studentship funded by the Wellcome Trust Institutional Strategic Support Fund, and her experience in magnetic resonance and molecular biology that she had gained during her Master's Thesis in the group of Prof. Harald Schwalbe made her a perfect fit for the project. A few weeks later Laura embarked on her PhD journey at the University of St Andrews in Scotland. Laura made excellent progress on a number of very different and very challenging projects ranging from the investigation of structure, conformational dynamics and multimerization behaviour of soluble and membrane proteins to fluoride sensing riboswitches. The latter topic had proved difficult before Laura's arrival, but Laura immediately designed a folding protocol and used her NMR experience to establish optimum conditions and verify correct folding. With the folding established Laura performed an *in silico* labelling study, established the phosphorothioate-based site-specific labelling of the RNA, confirmed the fold of the labelled constructs and studied the structure of the folded riboswitch using pulse

dipolar EPR and ENDOR – all of these are firsts in my group in St Andrews and testament to the step-change her hard work has brought. For ^{19}F ENDOR Laura visited Prof. Marina Bennati and Dr Andreas Meyer in Göttingen on a Royal Society International Exchanges Grant. This was a great success all round and after graduating in St Andrews Laura has joined the group in Göttingen working on modelling of ENDOR data of biomolecules. Her skills in the lab, her open and friendly nature and the home-baked treats she occasionally shared with the group are all dearly missed. It is great to see Laura go from strength to strength, and I wish her all the best for her future.

IES Poster Prize at the RMC2023



Roxanna Martinez:

Molecular complexes are promising candidates for spin-based applications spanning from magnetic resonance imaging to quantum information processing. A key challenge in advancing these applications is understanding how to generate long electron spin relaxation times (T_1 , T_m) in magnetic environments. A major obstacle to reaching this goal is the presence of other magnetic nuclei in the environment, because these nuclei shorten spin relaxation times. Current approaches to mitigate this issue are to reduce or completely remove nuclear spins from the environment. Although this can increase relaxation times, it is not an ideal strategy for applications where there will be a magnetic environment present. The aim of my research is to utilize the chemical tunabil-

ity of molecular complexes to fundamentally understand what features of nuclei control their influences on relaxation time.

On my poster at the Rocky Mountain Conference on Magnetic Resonance 2023, I presented the impact of ligand chlorination and counterion tuning at high field/high frequency in V(IV) complexes. In a previous study by our group (*Chem. Sci.* **2019**, 10, 8447–8454), we found that different substitutional patterns of ^1H ($I = 1/2$, $2.79\mu\text{N}$) and $^{79/81}\text{Br}$ (^{79}Br : $I = 3/2$, $2.11\mu\text{N}$; ^{81}Br : $I = 3/2$, $2.27\mu\text{N}$) magnetic nuclei in the ligand shell can produce up to 50% variation in T_m at high field/frequency. From that study we had several remaining questions. First, is spin diffusion in ligand ^1H atoms really responsible for suppressing T_m ? Could it be the Br spins instead? Or, could a slight change in geometry around the V(IV) ion be responsible? Finally, could the difference in T_m be related to a change in counterion binding groups dictated by the Br atoms on the ligand? Our prior work showed that, at X-band frequencies, the CH_3 groups of the R_3NH^+ counterions dictate T_m , but it wasn't clear if that was the case in the described compounds.

To answer these questions, I prepared V(IV) complexes with $^{35/37}\text{Cl}$ nuclear spins on the ligand shell, $(n\text{-Bu}_3\text{NH})_2[\text{V}(\text{C}_6\text{H}_{4-x}\text{Cl}_x\text{O}_2)_3]$ and two additional complexes, $(\text{Et}_3\text{NH})_2[\text{V}(\text{C}_6\text{H}_4\text{O}_2)_3]$ and $(n\text{-Hex}_3\text{NH})_2[\text{V}(\text{C}_6\text{H}_4\text{O}_2)_3]$ to vary counterion methyl group distance from the V(IV) center. Single-crystal diffraction analyses showed that all complexes exhibit similar structures, demonstrating that structural changes were not responsible for the originally observed changes in T_m . Continuous-wave and echo-detected EPR spectra (at X-band and 120 GHz frequency) revealed g and A values that are consistent across all compounds, also precluding electronic structure changes as the source for the initially reported variations in T_m .

Finally, we performed two-pulse Hahn-echo experiments to test the impact of the different substitutional patterns on the phase memory relaxation times, T_m , the T_m for the complexes at 5 K ranged from 4–5 μs . The chloro analogue to $[\text{V}(\text{C}_6\text{H}_2\text{-4,5-Br}_2\text{O}_2)_3]^{2-}$ did not show a short T_m time compared to the rest of the series. This indicated that the slight change in geometry and the spin diffusion of the ligand ^1H atoms are not responsible for the shortening of T_m exhibited. We also collected Hahn-echo decay data of the complexes with different trialkylammonium counterions (Et_3NH , $n\text{-Bu}_3\text{NH}$, $n\text{-Hex}_3\text{NH}$) ►

Awards

to test the role of these chemical species on T_m at high field/frequency. The values of T_m at 5 K range from 3.6–4.0 μ s and increase as CH_3 group moves away from V(IV) ion, but with a diminished effect compared to data collected X-band. From these latter results we rule out that the counterion is a major contributor to T_m at high field/high frequency.

Our results left us with the question of why $^{79/81}\text{Br}$ nuclear spins have a particularly negative impact on the V(IV) T_m when at the 4,5-position vs. $^{35/37}\text{Cl}$? We propose that the quadrupole coupling interactions of the $^{79/81}\text{Br}$ could be impacting the V(IV) T_m in a particularly potent way. But, we still have a long way to go and more exciting EPR to do until we fully understand the effect.

A portion of this work was performed at the National High Magnetic Field Laboratory in collaboration with Dr. Johan van Tol. This work has been published in *Dalton Transactions* (*Dalton Trans.*, 2023, 52, 10805–10816).

Joe Zadrozny:

Roxanna is an outstanding member of my research group. Roxanna's research mission is to understand magnetic noise at the molecular level. She has been putting a lot of effort into using synthetic chemistry to do so. It's really fun science, because she does all the work that synthetic inorganic chemists do: change ligand sets, swap out different counterions, etc. So we get to think about a lot of fun inorganic chemistry together. But at the end of these studies, she uses magnetic resonance to see how those chemical alterations affect how a metal-based electron spin "sees" the environment. So we also get to think about weird spin physics. Our group has made some exciting discoveries that show that the molecule itself can produce noise that overpowers noise generated by the tens of thousands of external, solvent-based nuclei. Roxanna's work is now going a step deeper. Inorganic chemists have a multitude of design parameters for alter-

ing a molecule's properties by adding chemical functional groups that modify electron density. Roxanna is pioneering a new set of design parameters that instead focus on magnetic noise. It's really exciting work and we continue to see new and unexpected effects.

Roxanna was also instrumental to moving our lab this past fall to Ohio State University. She actually moved ahead of the main laboratory equipment and personnel so that she could be out here to receive the equipment and start setting up the lab, and she's been a real leader in this effort. Our lab is almost set up now and she is fired up to get going here, so be on the lookout for papers from her in the near future!

IES Poster Prize at the RMC2023



Austin MacRae:

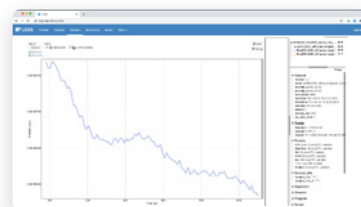
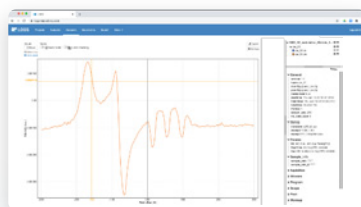
I want to start by thanking the International EPR (ESR) Society for awarding my poster presentation at the Denver Rocky Mountain Conference in June 2023. The conference was an outstanding opportunity to connect with fellow scientists utilizing EPR for novel discoveries. I presented on the effects of Metal-

Organic Framework (MOF) crystallinity on encapsulated protein orientation and dynamics. Enzyme encapsulation in MOFs can be challenging for large enzymes, large substrate enzymes, and enzyme clusters. Our group utilizes methods such as co-crystallization in aqueous solutions to overcome this challenge. Co-crystallization is beneficial for protein encapsulation because larger proteins or protein clusters can be encapsulated with this green synthetic method by forming the material around the proteins under benign conditions. However, this method has drawbacks for the MOFs formed compared to their highly stable, solvothermal counterparts such as reduced crystallinity. This drawback of co-crystallization raises concerns about the crystal packing quality in these MOFs and how it impacts enzyme performance.

In this project, we expanded on our recent discoveries of multiple aqueous-phase co-crystallized MOFs with varying metal ions (Zn^{2+} , Al^{3+} , Zr^{4+} , Ni^{2+}) and two varying aromatic ligands (BDC, BPDC). The crystallinity of these materials ranges from highly ordered single crystals and less ordered multi-phase crystals to less ordered amorphous or gel-like crystals. We are utilizing site-directed spin labeling (SDSL) – Electron Paramagnetic Resonance (EPR) spectroscopy to probe enzyme dynamics and restriction of encapsulated T4 phage lysozyme labeled with the MTSL spin label. This technique probes protein backbone motions that are related to the local crystal packing quality and density. A rough connection between protein mobility/dynamics and MOF crystallinity was found through these EPR studies and simulations. The restriction of motional dynamics of 8 separately labeled surface T4L sites is increased with higher crystal packing quality/density of the encapsulating MOF. We also found that the ligand affects the crystal packing and motional dynamics of the labeled side chain when looking at



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MOFs of the same metal ion. The MOFs with biphenyl dicarboxylic (BPDC) ligands create densely packed, 2D layer-by-layer Metal-Organic Materials (MOMs) with the increased restriction and immobilization of the spin label. However, when we form gel-like, less crystalline materials with extended BPDC ligands, the restriction is lower than the benzene dicarboxylic (BDC) counterparts. When analyzing the overall data and giving insight into the mobility of the spin label at each labeled site, we found some of the protein surface residues are more likely to be exposed above the surface of the material. This allowed us to elucidate the residues of protein most likely to be exposed and general protein orientation in the materials. We roughly connected the exposure of the protein's active site with the catalytic activity of the large-substrate lysozyme. For example, materials with a higher probability of having the active site exposed above the surface of the MOF have higher activity. Overall, this work suggests a connection between MOF crystal packing/density and protein mobility that could guide future material design for enzyme immobilization.

This work is published in *ACS Applied Materials & Interfaces* (*ACS Appl. Mater. Interfaces* **2023**, 15(31), 38124–38131, DOI: 10.1021/acsami.3c07870). I would like to thank my advisor for guiding me through this project, Dr. Zhongyu Yang, and my colleague, Zoe Armstrong, who co-authored this work and guided me through the operation of the instrument since this was my first project working with EPR.

Zhongyu Yang:

Austin MacRae originally grew up in Shakopee, Minnesota, roughly 30 minutes away from Minneapolis-St. Paul (the Twin Cities). He then went to Bemidji State University for a bachelor's degree in chemistry

with an emphasis in Biochemistry from 2014–2018. In 2018, he started his Ph.D. at North Dakota State University (NDSU) in 2018. Originally, he was interested in inorganic chemistry and inorganic chemical catalysis. He then became interested in enzymes and biocatalysis after the Pandemic and was looking for a tool to connect chemical catalysis and biocatalysis. So, I recruited him as a graduate student about 1.5 years ago because my group happens to have the tool he was looking for, metal-organic frameworks (MOFs). Here we immobilize enzymes in MOF scaffolds through biomineralization (co-crystallization) so that metals/ligands in MOFs may participate in enzyme biocatalysis. The challenges are to ensure sufficient stability of the resultant enzyme@MOF composites, understand the structure relationship of enzymes on MOFs, and correlate crystallinity with enzyme structure-function-dynamics. Austin took the challenge and revealed such correlation, which essentially resulted in his award.

He then graduated from NDSU and decided to stay in my group as a postdoc due to his passion about using MOF to bridge chemical and biocatalysis. Austin is not only a successful independent scientist but also a great team leader. He is always the go-to person whenever a group member has questions or runs into trouble in research. He is always available to chat about science no matter if it is a Sunday morning or after midnight. He is also a great educator because of his significant contribution to the upper division Inorganic Chemistry Laboratory course. He has won multiple awards in the past single year including the Roy Milde scholarship and the Travel Award from NDSU. His passion in science truly moved everyone in my group and I am just so lucky to keep him in my group after he graduated. We are all thrilled by his IES Poster Award at the RMC2023, and we all know that he can do more than that! Keep up the good work, Austin!

IES Poster Prize at the 9th EFEPR Summer School



Julia Haak:

Mapping out the active site of lytic polysaccharide monooxygenases using hyperfine spectroscopy

First, I would like to thank the International EPR (ESR) Society for awarding me a poster prize at the 9th EFEPR Summer School in Geneva and for giving me the opportunity to discuss some of my current research in the IES newsletter. I am currently pursuing my Ph.D. at the Max Planck Institute for Chemical Energy Conversion, where our research targets the exploitation of renewable energy sources, and thereby the replacement of fossil resources, a task of increasing urgency in the context of climate change.

One prominent approach for harnessing renewable fuels involves the conversion of biomass into biofuels [1]. Although cellulose and chitin are the two most abundant polysaccharides in nature, making them desirable starting materials,

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their recalcitrant character constitutes fundamental difficulties for biorefinery processes. In this regard, the relatively recent discovery of Lytic Polysaccharide Monooxygenases (LPMOs) has opened new avenues for the industrial breakdown of biomass [2], as this class of enzymes is able to catalyze the oxidative cleavage of glycosidic bonds in these polysaccharides.

LPMOs are copper-dependent enzymes, that have a highly conserved active site, consisting of a mono-copper center surrounded by the T-shaped *Histidine-Brace* [3, 4]. This motif comprises a bidentate *N*-terminal histidine, coordinating via its amine function and the δ -nitrogen of its imidazole ring, and an additional histidine side chain coordinating via its ϵ -nitrogen. During catalytic turnover LPMOs activate a co-substrate (either H_2O_2 or O_2 [5]) to generate highly-oxidizing intermediates, which perform the challenging C-H bond activation in the crystalline polysaccharides (~ 95 – 104 kcal/mol) [6, 7].

The ability of the Histidine-Brace to stabilize such highly-reactive intermediates, prompts the question what its essential electronic and structural features are that enable the unique and intriguing reactivity of LPMOs. Motivated by this question and its importance not just for fundamental research, but also biological and industrial applications, we used a range of spectroscopic techniques in combination with isotopic labeling (^{15}N , ^2H , ^{63}Cu) to gain detailed insights into the resting active site of the AA10 LPMO *SmAA10A* from *Serratia marcescens* (CBP21).

UV-Vis and electron paramagnetic resonance (EPR) spectroscopy revealed a strong pH-dependency of the active site, showing several chemical transitions associated with a total of five species, between pH 4.0 and pH 12.5. Surprisingly, even under the most extreme alkaline conditions surveyed, we did not observe degradation of *SmAA10A*. Instead the protein's specific activity on chitin could be fully recovered after its incubation at these high pH values, demonstrating the reversibility of the observed transitions.

To further study the individual species emerging over the studied pH range, we employed a variety of pulsed EPR techniques, aiding to resolve smaller superhyperfine and nuclear quadrupole interactions. While the first transition is associated with a change of the coordinating solvent molecules (from two coordinating waters to one hydroxo ligand), leaving the Histidine-Brace widely unchanged, the subsequent transitions are attributed to deprotonation events at the two coordinating histidine residues. This includes the deprotonation of the remote nitrogen nuclei of the two imidazole moieties, which is observed in electron spin echo envelope modulation (ESEEM) and hyperfine sublevel correla-

tion (HYSCORE) experiments. Additionally, electron nuclear double resonance (ENDOR) experiments show that the coordinated amine function is deprotonated at $\text{pH} > 11.5$.

We hope that understanding both the protonation states and the electronic structure through advanced EPR techniques will shed light on these protein's ability to activate oxygen and perform some of nature's most difficult C-H bond activations. By studying this flexibility in the Histidine-Brace, as modulated by pH, we are also laying a spectroscopic foundation for the study of LPMO interaction with lignocellulose substrate and potential trapped intermediates.

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George Cutsail:

I am very excited and proud to see Julia receive the IES poster award for presenting her research at the recent EPR Summer School in Geneva. Since Julia has joined my group, she has pushed our knowledge, techniques, and understanding of copper hyperfine spectroscopy applied to both copper proteins and mononuclear copper catalyst centers. Much of her PhD thesis research consists of applying techniques such as ENDOR, ESEEM, HYSCORE and EDNMR to bioinorganic systems. This includes her current work on lytic polysaccharide monooxygenases, where she has taken a very deep dive into the spectroscopic features of these proteins so that we can better understand how their electronics of their active may be tuned for reactivity. But don't let this fool you, she has knack for tackling diverse and challenging problems. Recently, she has also pushed our understanding of main-group radicals and as taught our group how to best employ both multi-frequency EPR and parallel-mode EPR spectroscopy for these systems with giant hyperfine couplings.

Knowing her high level of curiosity in science and her excitement to talk about research, this recognition comes as little surprise to me. She is doing fantastic research and I am confident for her success in the future. Kudos Julia!

IES Poster Prize at the 9th EFEPR Summer School



Radhika Kataria:

Enabling electrical readout of molecular quantum bits

I extend my sincere appreciation to the International EPR Society for the recognition of my work with the poster prize at the 9th EFEPR Summer School in Geneva and for the opportunity to disseminate my research findings through the EPR Newsletter.

EPR or Electron Paramagnetic Resonance is a well-established technique for investigating spin transitions in various systems. However, its limited sensitivity due to the low energy of microwave photons requires ensembles of spins for detection, hindering direct device applications. Converting spin transitions to high-energy transitions via electrical [1] or optical [2] means can enable much more sensitive detection, potentially down to the single qubit limit. This paradigm shift has been demonstrated in diverse systems including donor atoms in semiconductors, nitrogen-vacancy centers in diamonds, quantum dots, and nuclear spins in molecules.

Molecular quantum bits (MQBs), based on electron spins in molecules, offer a competitive qubit system with relatively long coherence times of hundreds of microseconds at temperatures as high as 100 K [3]. Moreover, the high chemical versatility of these qubits allows for tailored functionality and selective analyte sensitivity, making them highly attractive for quantum sensing applications. Furthermore, molecules provide superior scalability and positioning capabilities compared to other qubit systems.

IES Poster Prize at the 9th EFEPR Summer School

In this project, we aim to enable the electrical readout of such qubits by integrating them with organic semiconductors (OS). Organic semiconductors exhibit weak spin-orbit and hyperfine interactions, promoting extended coherence times, and their compatibility with semiconductor-based control electronics streamlines device integration. The proposed readout mechanism relies on a spin-dependent interaction between charge carriers in the OS and MQBs, with proof-of-concept involving observing changes in electrical conductivity upon exciting qubit spin transitions.

We utilize the high mobility semiconducting polymer poly[2,5-bis(3-tetradecylthiophen-2-yl)thieno[3,2-*b*]thiophene] (PBTTT) as the OS and molybdenum tris[1-(methoxycarbonyl)-2-(trifluoromethyl)ethane-1,2-dithiolene] ($\text{Mo}(\text{tfd}-\text{CO}_2\text{Me})_3$) as a potential qubit. The similar energy of the HOMO of the polymer and the LUMO of the qubit enable efficient charge transfer, inducing mobile polaronic charge carriers in the polymer backbone. UV-Vis-NIR spectroscopy and conductivity measurements assess doping efficiency across various concentrations.

EPR spectroscopy confirms the viability of $\text{Mo}(\text{tfd}-\text{CO}_2\text{Me})_3$ anion as an MQB, exhibiting ligand-based spin density and phase memory times of a few microseconds up to 75 K. Temperature-dependent charge transport measurements reveal significantly enhanced conductivity upon doping, even at low temperatures, facilitating simultaneous electrical conductivity and coherence.

CW-EPR measurements on $\text{Mo}(\text{tfd}-\text{CO}_2\text{Me})_3$ -doped PBTTT films revealed a single signal across a wide temperature range (4 K to room temperature), unlike the two separate signals expected from polarons and qubits. High-field EPR spectroscopy at 360 GHz was employed to enhance g-resolution, revealing a slight axial g-anisotropy. However, it was uncertain whether this stemmed from a single spin type or an interaction between spin types, inhibiting the possibility to specifically excite the qubit spins. To address this, we are simultaneously exploring a transition metal-based qubit as an alternative for our system.

Having successfully characterized the individual components and the hybrid qubit-semiconductor system, our current focus is on developing a setup for electrically detected magnetic resonance measurements at our X-band EPR spectrometer. This will allow us to investigate signatures of qubit-charge carrier interactions.

In summary, this study lays the groundwork for integrating MQBs with OS for enabling

electrical readout, offering a promising avenue for quantum sensing applications. Finally, I would like to thank Prof. Joris van Slageren for being a wonderful and supportive supervisor and my research group for ensuring an encouraging and stimulating work environment. Last but not least, I would like to express my immense gratitude to Dr. Ute Zschieschang and Dr. Hagen Klauk from the Max Planck Institute for Solid State Research for extending their varied knowledge and experience in organic electronics to me.

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Joris van Slageren:

In 2020, Radhika applied to the prestigious International Max Planck Research School in Condensed Matter Science in Stuttgart. Because of her impressive CV, she was selected as a candidate. After an impressive interview, I offered Radhika a position in my group, which thankfully she accepted. Once in Stuttgart, Radhika quickly revealed herself to be an extraordinary scientist and person. Having carried out a Masters thesis on a spintronics topic in physics, she was now embarking on a topic dealing with organic semiconductors and molecular quantum bits in a chemistry department. However, Radhika was undaunted by the steep learning curve, and quickly settled in. In the years that Radhika has now been in my group, she has learned a wide range of things, from thin film preparation to microstructuring of substrates to contacting these fragile structures. The truly amazing moment was when Radhika decided she was also going to learn chemical synthesis and prepare the dopant molecule that was no longer commercially available. Almost needless to say, she also carried this off successfully. Radhika's thesis project has been very challenging, and progress has been slow – but steady. We are now at the verge of making important breakthrough advances in the electrical readout of molecular qubits. This has only been possible, because Radhika is such an enormously self-motivated, goal-oriented and frustration-tolerant person. She is also very open and sociable and has contributed substantially to the understanding of physics of the group. I am very happy and thankful that Radhika's qualities have now been recognized by the IES Poster Award.



Orit Nir-Arad:

I am honored to receive the IES poster prize during the last EFEPR summer school, where I showed our recent pulsed EPR and Dynamic Nuclear Polarization (DNP) results acquired using our home-built 7 and 14 Tesla DNP/EPR spectrometer, at Dr. Ilia Kaminker's group at Tel-Aviv University. I want to thank the organizers of the summer school for the opportunity to learn more about EPR and to meet all the amazing teachers and other students in the field.

In my poster, I showed the design and construction of the dual DNP/EPR spectrometer and presented our recent results on paramagnetic centers in diamonds, focusing on substitutional nitrogen centers (P1 centers) in HPHT single-crystal diamonds.

I joined the group of Dr. Kaminker during my undergraduate studies in chemistry three and half years ago as a research assistant. At that time, we were only two students in the group, both of us undergraduates, trying to learn as much as we could about EPR. A short time after I joined, the superconducting magnet was delivered, and we had to combine all the various components of the spectrometer and learn how to install the magnet on our own due to the COVID-19 restrictions.

After completing my B.Sc. in chemistry, Summa cum Laude, I continued my work in the group as a Ph.D. student in the direct Ph.D. track. During that time, we continued to install, test, and optimize the different parts of the spectrometer. The group research is centered around the development of new DNP methods through a deeper understanding of

the DNP mechanisms from the electron spin perspective. To achieve this, we needed to construct both the Nuclear Magnetic Resonance (NMR) and the EPR sides of the spectrometer, which operated at both 7 and 14 Tesla (200 and 400 GHz) and at 8–300 K.

DNP has been a rapidly developing field in the past two decades. It is used to enhance NMR signals by orders of magnitude, allowing for experimental time savings of up to four orders of magnitude. It completely transformed the solid-state NMR field allowing for experiments previously deemed impossible. The DNP enhancement relies on polarization transfer from electron spins to nuclear spins. It must be performed at high magnetic fields to achieve the resolution expected from modern NMR experiments.

A detailed understanding of the polarization transfer process is a prerequisite for the rational design of improved DNP experiments. To understand this complex quantum mechanical process, we must be able to probe both nuclear and electron spins. EPR experiments, such as electron-electron double resonance (ELDOR), performed under DNP conditions (high magnetic field and low temperatures), were shown to provide a wealth of information about the DNP mechanisms. Since electron spin properties such as spectral width, relaxation times, and electron spectral diffusion (eSD) rate are field- and temperature-dependent, it is necessary to perform the EPR measurements under DNP conditions.

Last year we performed our first DNP experiments using P1 centers in diamond. P1 centers were recently shown to be an efficient source of ^{13}C hyperpolarization in DNP experiments performed at 3.3 T. Using our home-built instrument we determined that P1-DNP remains very efficient at both 7 and 14 T and is mediated by multiple DNP mechanisms in a complex interplay. Our investigations of the underlying DNP mechanisms, using pulsed EPR performed with the same instrument and conditions, revealed an unexpected broad EPR signal between the sharp P1 peaks, centered around the same g-factor and exhibiting distinct T_1 relaxation times. We assigned the unexpected signal to exchange-coupled P1 centers and were able to simulate the EPR line at both high fields and at X-band using the same parameters. The simulations allowed us to quantify the ratios between the various populations of P1 centers in the diamond. Using ELDOR experiments, we showed both populations interact and provide an efficient mechanism for eSD by connecting populations of dif-

ferent crystallographic sites and ^{14}N states. These results were published recently in the Journal of the American Chemical Society.

I wish to thank the Ariane de Rothschild women's doctoral program for funding my Ph.D. studies and the Israel Science Foundation (grant No. 2149/19) for funding the research. I also wish to thank the rest of the group for their contribution to this work, and my Ph.D. supervisor Dr. Ilia Kaminker.

IES Poster Prize at the 2023 RSC Meeting



Yasmin Ben-Ishay:

Revealing the dual behavior of PpiB in cells compared to in solution using EPR spectroscopy

The RSC ESR meetings are always a great pleasure to attend. The last meeting hosted by Dr. Christos Pliotas in Leeds was a major success, including fascinating talks by invited speakers and innovative student presentations. Personally, the cherry on top was to be awarded with the best poster prize entitled 'Probing Protein Dynamics and Structure of PpiB in Living Bacterial Cells using EPR' by the International EPR (ESR) Society (IES) and organizing committee. I'm truly honoured to receive this prize and would like to take this opportunity to express my sincere gratitude to the IES committee for awarding me.

As in all good love stories, a side character becomes the love interest. The work that granted me the eligible award was not differ-

ent – It started as a side project and unfolded to be the main one. Namely, the selected protein was used for methodology development purposes yet reveals an intriguing structural behavior and became the main theme of my studies in the past year.

The motivation to probe the structure and dynamics of proteins in living cells derived from a profound notion in biology that the native environment of a protein may affect its dynamics, stability, structure and, subsequently, functionality. The transient interactions of the proteins' surface with cell components, which co-evolve and jointly adapted through evolution, govern the elucidative fifth level of protein structural organization termed the 'quinary structure'. The relatively novel concept of a protein quinary structure was conceived in the 70s yet is still ambiguous due to the lack of extensive experimental data. In recent years, pieces of evidence started to accumulate thanks to the implementation of the in-cell approach in current biophysical methods. Among these techniques, EPR combined with site-directed spin labeling (SDSL) has become a powerful tool for investigating protein structural changes and dynamics in living cells.

In this work, we aim to explore potential manifestations of the quinary structure on a well-structured globular protein exploiting EPR techniques. We focus on *Escherichia coli* (*E. coli*) peptidyl-prolyl *cis/trans* isomerase B (PpiB) and investigate its dynamics and conformational changes in *E. coli* cells and in solution. The main cytosolic chaperone, PpiB, plays a key role in the maturation process of folded proteins and possesses a pivotal contribution to cell survival and adaptation to new environments. Utilizing the advantages of nitroxide and Gd(III) spin labels, we probe PpiB dynamics and structure by combining nitroxide-based X-band EPR at ambient temperatures and high-field (95 GHz) double electron-electron resonance (DEER) on frozen solution, respectively. Two pre-chosen labeling sites, located on alpha-helix and loop motifs, were interrogated exploiting a variety of different spin labels and labeling chemistry, including the orthogonal Gd(III)-NO counterparts via incorporation of unnatural amino acid. We observed a significant decrease in the residue-specific mobility for both labeling sites in the cellular milieu compared to in solution. Moreover, a broadening of the distance distribution was solely observed in *E. coli* cells and absence when the same variant was measured in solution or delivered to a non-native cellular environment, i.e. hu-

man HeLa cells. Hence, the conformational space of PpiB was expanded specifically in its physiological environment, suggested by the combined effect featuring the *E. coli* cell. Intriguingly, crowding agents and cell lysate have failed to recapitulate the fundamental change in dynamics, emphasizing once more the importance of performing in-cell studies. Combining the observation of a significant change in dynamics and conformational populations in the cellular context, we reveal the dual behavior of PpiB in solution and in-cell, suggesting the presence of a quinary structure. For more details on this study, please read our recently published paper [1].

Lastly, I would like to thank my supervisor, Prof. Daniella Goldfarb, for her invaluable and supportive guidance throughout this study. Everyone knows she can move mountains and, indeed with her remarkable admiration for the field, she inspired me to forsake my former academic pursuit and to 'fall in love' with magnetic resonance, particularly EPR. I'm a true believer now.

Daniella Goldfarb:

Yasmin, a dedicated biologist, eagerly joined our research group as a PhD student, driven by her enthusiasm for investigating structural changes in proteins during cellular functions. To begin, Yasmin delved into mastering the intricate procedure of incorporating unnatural amino acids into proteins, which allows for high specificity. My expertise in this is practically non-existent. Yasmin took the lead, selecting a soluble model protein, *E. coli* peptidyl-prolyl cis/trans isomerase B (PpiB). She successfully incorporated alkene-containing lysine-based pyrrolysine at a specific position and labeled it with the azido-derivative of a Gd(III) label.

This endeavor marked a significant success, and Yasmin, with support from experts at in Israel and abroad, navigated the complexities of unnatural amino acid utilization. Additionally, Yasmin introduced a cysteine to which she attached a novel nitroxide spin label, generously provided by our collaborators, resulting in an orthogonally labeled PpiB with both nitroxide and Gd(III) labels. All labeling procedures were conducted in vitro on a purified PpiB variant, and the protein was introduced into *E. coli* cells via

electroporation—an optimization process spearheaded by Yasmin based on published procedures.

Following this, Yasmin conducted extensive EPR measurements on both in vitro and in-cell samples. This involved exploring PpiB's residue-specific dynamics through X-band continuous wave (CW) EPR examining its structure using W-band double electron-electron resonance (DEER). This encompassed Gd(III)-Gd(III), Gd(III)-nitroxide, and nitroxide-nitroxide DEER.

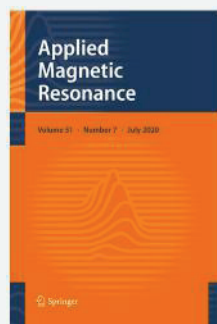
The outcomes and significance of Yasmin's work is described above. Notably, she excelled in three crucial aspects: (i) mastering the biochemistry associated with protein expression (UAA incorporation), purification, and labeling while optimizing click chemistry conditions; (ii) fine-tuning the electroporation procedure for *E. coli* cells (previously accustomed to working with human HeLa cells); and (iii) proficiently recording high-quality CW-EPR and 95 GHz DEER on cell samples. The latter required Yasmin to navigate the intricacies of our custom-built spectrometer, a task that showcased her mastery of its unique characteristics. Congratulations, Yasmin!

1. Ben-Ishay, Y., Barak, Y., Feintuch, A., Ouari, O., Pierro, A., Mileo, E., Su, X.C. & Goldfarb, D. 'Exploring the dynamics and structure of PpiB in living *Escherichia coli* cells using electron paramagnetic resonance spectroscopy'. *Protein Science* vol. 33, issue 3, e4903. DOI: 10.1002/pro.4903 (2024).



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Sailing

R. David Britt

University of California, Davis



I have been sailing and sailboat racing for a number of years. In fact, this started with an EPR connection. I was at a Gordon Research Conference in Rhode Island, and on the afternoon breaks I was sitting with John McCracken on a hillside by the water watching all the nice sailboats, and decided I should try to learn to sail. So I signed up for lessons at Vallejo Yacht Club, one of the closer San Francisco Bay locations to UC Davis. Clubs in part use such “learn to sail” courses to recruit new members and to sign up folks to serve as crew in the various club races, often midweek in the early evening during summer and the flanking long daylight months. So I started crewing on races in Vallejo, on a pretty fast, very technical mid-80s race boat (Olson 29). Eventually I bought a used sailboat myself, an old J/24, to get some experience on the helm, and to learn something about tuning the rig etc.

After some time, I bought a Beneteau 10R (Fig. 1), which we used for a combination of SF Bay and local Pacific Ocean racing. In addition to the main sail, and the smaller headsail up front, this boat, which I called *Split Water* as a bit of a play on our research in photosynthetic water splitting, has big nylon spinnakers (often called kites) for sailing fast downwind (we are going upwind in this photo). I kept this boat in Richmond, most of the time at the excel-

lent Richmond Yacht Club that has a great racing program. Ocean racing in the Pacific off Northern California can be pretty “interesting” given that once you go out the “Golden Gate” you are in the full bore of the Pacific Ocean, which can be pretty hairy at times. In particular, in 2012 we were doing a race around the Farallon Islands about 25 miles offshore from San Francisco, when the boat right behind us cut it too

close to the island and got swamped by a breaking wave, with several tragic deaths. After that the Coast Guard clamped down on offshore racing for a while, making sure all boats in organized racing events were inspected and skippers and crew trained in “Safety at Sea” courses. We were planning a serious race for San Francisco to Hawaii later that summer, so we needed all the at sea safety we could muster!



Fig. 1. The original *Split Water* (Beneteau 10R) bashing out into the Pacific Ocean by the South Tower of the Golden Gate bridge on a Farallon Islands ocean race.



Fig. 2. Trophy ceremony for the 2012 Pacific Cup, with the *Split Water* crew (David Britt, Greg Paxton, Josh Butler, Jesse Corlett (not pictured, Chris Corlett)), and presentation by Miss Hawaii.

The summer before I had taken a training course in the Transpac race from Los Angeles to Hawaii on a big fast Santa Cruz 50, in part to get some experience for doing a similar race, the Pacific Cup, which is from San Francisco to Oahu. I was fortunate to have a great bunch of experienced crew for the race. Racing 24/7 in the open ocean with only a few hours sleep on a rotating schedule is certainly grueling. I did all the

navigation myself, which was an interesting learning experience. In the end, we came in second out of nine boats in our division, <https://pacificcup.org/content/2012-results> so we managed to get a trophy (Fig. 2).

The Beneteau 10R was a fun boat, but it was fairly heavy (good for slamming through ocean waves) but even when powered up with a spinnaker going downwind the hull stays in the water ... this makes it

a “displacement boat” and limits its speed. Some years ago, the sailing world started to see a class of lightweight boats, with a lot of sail area and broad flat sterns, which with enough wind could climb up out of the water and “plane” on the rear part of the boat much like a powered speedboat. So I ended up selling the Beneteau and bought a J/88 sport boat (Fig. 3). This boat could go much faster, but going fast and doing quick maneuvers such as putting up the spinnaker and taking it down quickly in a mark rounding takes a lot of crew skill. With this boat, also called *Split Water*, we did mostly San Francisco Bay racing, most often against other J/88s, in what is called “one design” racing, as all boats are essentially the same. This avoids the handicap racing intrinsic to racing dissimilar boats where the faster boats taking a determined time penalty. The highlight of the J/88 era was in 2019, when we won our J/88 division in the Rolex Big Boat series in San Francisco https://yachtscoring.com/event_results_cumulative.cfm?eid=6241.

Things of course changed in 2020 with the pandemic. All organized crewed sailboat racing was shut down. Most dramatically for me, in August 2020 our house burnt down in one of the notorious California wildfires, which led us to move to Point Richmond Ca, just by the Richmond Yacht club. Maintaining crew at the level needed to compete on the J/88 was not easy, and sometimes seemed like a second job, in parallel with maintaining a research group in advanced EPR spectroscopy. Living near the boat, instead of an hour away, made it more appealing to have simpler boat where I could race with one or two people, or maybe by myself. So after a while I sold the J/88 and bought a 20 year old Alerion 28 (Fig. 4), named *Jewel* by the previous owners. *Jewel* is a full displacement boat, with no spinnaker (at the moment), but we have fun racing because we have a nice one-design fleet at Richmond YC, so even on the Wed night after-work races we have a competitive one-design race within the club. And the fleet keeps growing as folks buy old Alerion 28s from around the country and move them to Richmond YC, which has become quite the Alerion 28 hub. It is a fun boat to sail, not as fast by any means as the J/88, but it is fun competing with the local group of highly experienced Alerion 28 sailors.



Fig. 3. Downwind run back through the Golden Gate on the J/88 *Split Water*, with the spinnaker in action.



Fig. 4. A group of Alerion 28s rounding a mark in a Richmond YC race. *Jewel* is the third boat in line.

80 Years Young

S. S. Eaton, G. R. Eaton, and K. M. Salikhov

Unsuccessful efforts by Gorter to observe magnetic resonance were followed by success in gas-phase NMR by Rabi in 1938, in condensed phase EPR at low frequencies by Zavoisky in 1944, and then NMR in condensed phase by Purcell (solids) and Bloch (liquids) and coworkers in 1946. Independently, the Bleaney lab began measuring energy level splittings in transition metals by EPR at several frequencies, including X-band (Bagguley and Griffiths, 1947). Zavoisky's experiments were cited by Bleaney in the Bagguley and Griffiths announcement of X-band results (Bleaney in *Foundations*, page 37). Stimulated by Gorter, Zavoisky, and Purcell et al. (1946), Cumberow and Halliday (1946) measured paramagnetic absorption by solid $\text{MnSO}_4 \cdot 4\text{H}_2\text{O}$ at 2.93 GHz. The early history of EPR is well-documented in Kochelaev and Y. V. Yablokov (1995) and in *Foundations of Modern EPR* (1998). A relaxation perspective on the history is presented in Eaton and Eaton (2020).

The subsequent development of EPR illustrates strong interaction between selection of spin systems to study, development of instrumentation, and development of theory of spectra and relaxation times. Fundamental theory preceded the search for

resonance (Waller, 1932, and Van Vleck 1932, 1940, 1970).

The instruments used by Zavoisky (Silkin 2005) and by Bleaney differ greatly, supporting independent development, but there is no question that Zavoisky was the first to observe resonance and the first to publish. However, Bleaney's approach was more widely adopted and subsequent EPR measurements were predominantly conducted in the X-band (ca. 9–10 GHz) region.

Jumping ahead a bit in the historical development, the introduction to EPR of the lumped circuit loop-gap resonator by Hyde and Francis (1982) revolutionized many applications of EPR, but it had been forgotten that Zavoisky's original EPR resonator was a loop-gap resonator.

Early papers reported observation of EPR signals from a wide range of paramagnetic species including transition metals, lanthanides, organic radicals, and defect centers in solids. The selection of paramagnetic species provided answers to many fundamental questions and supported interpretation in terms of nuclear hyperfine couplings, g-values, and anisotropy of each. The role of excited electronic states was revealed. In the first two decades many relaxation time

measurements were made. The selection rules that fit these spectra and the interpretation in terms of the direct and Raman processes and then with the addition of the Aminov-Orbach process became the basis for textbook introductions. More recently, there has been more focus on exceptions to the simple arguments and effort to understand the mechanisms of relaxation. For example, the R_2NO moiety called nitroxide or nitroxyl was known before EPR was available to confirm the assignment as a free radical, and the initial spectra also confirmed the molecular orbital picture of bonding that predicted nitrogen nuclear hyperfine interaction. The chemical and biological versatility of nitroxides contributes to a vast literature. Recently Salikhov formulated a new paradigm of spin exchange and its manifestations in EPR spectra shape which gave a good impetus to the development of the theory of paramagnetic relaxation in solutions and the application of EPR in physics, molecular biology, etc. (Salikhov 2019).

Several monographs produced after about two decades of development of EPR brought important features of EPR to the scientific community. Assenheim (1966) provided an introduction to EPR, Wilmshurst (1967) to the spectrometers, while Orton (1968) focused on transition metals and Lancaster (1967) on semiconductors. Ingraham's monograph (1969) emphasized biological and biochemical applications. The extensive multivolume series of books edited by Lawrence Berliner highlighted biological applications of EPR.

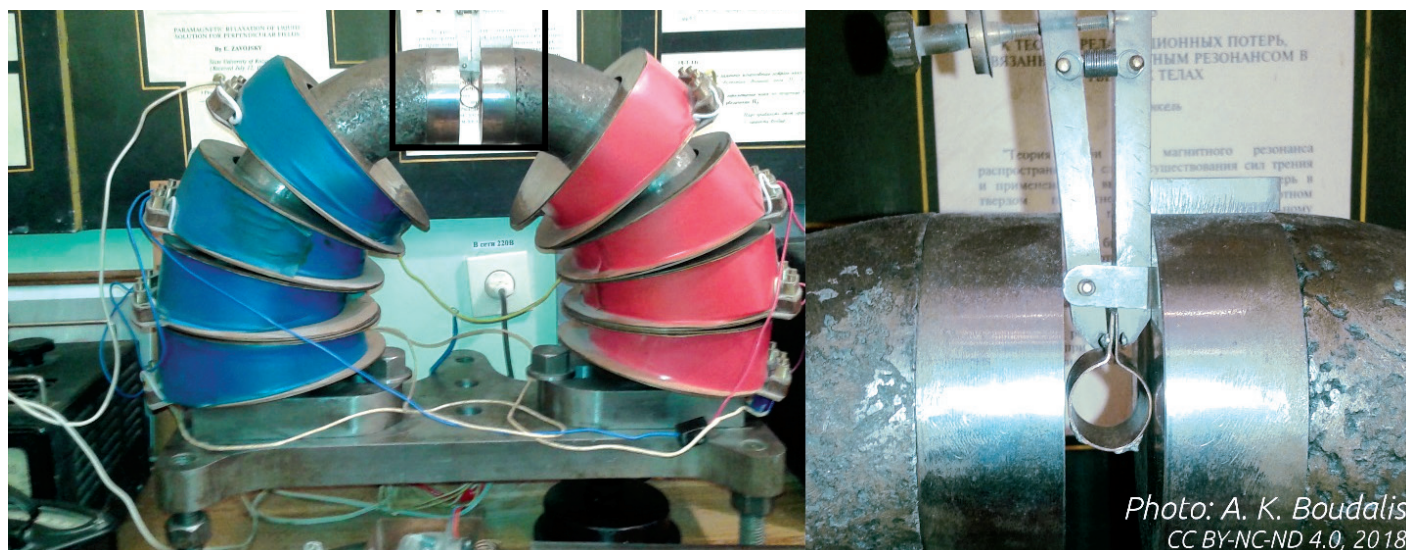
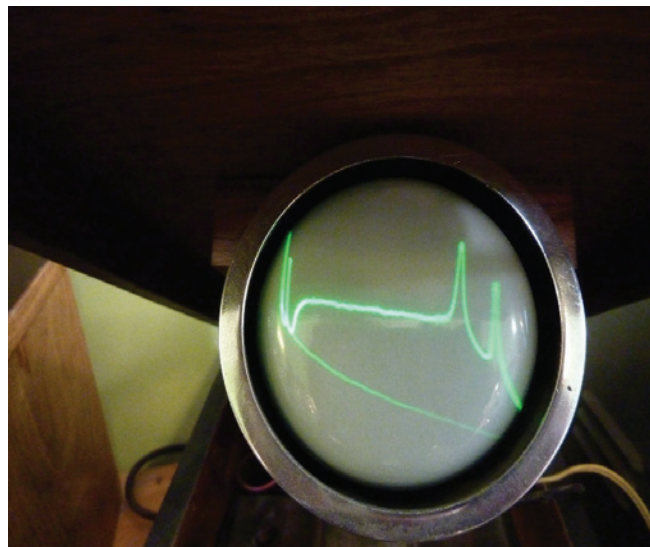
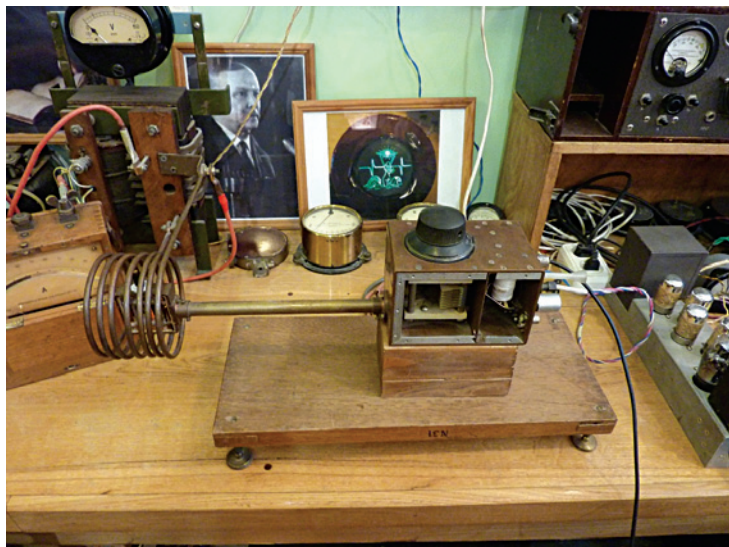


Photo: A. K. Boudalis
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The DuBois electromagnet with a loop-gap resonator in its pole shoe. The plexiglass clamp with the screw was used to tune the resonator. This and subsequent pictures of the Zavoisky spectrometer are of a reconstruction in the Zavoisky museum in Kazan, based on his lab notebooks. The original was disassembled long ago. See Silkin 2005 and <http://chiralqubit.eu/a-visit-to-the-Zavoisky-museum>.



Photographs of the Zavoisky spectrometer measuring DPPH taken Sept. 24, 2019 by GRE

Textbooks such as Al'tshuler and Kozyrev (1964, 1974), Wertz and Bolton (1972) and Atherton (1973) were crucial to expanding the community of scientists that could apply EPR to solving problems. After the Eatons demonstrated the conditions needed to perform CW EPR quantitatively, the *Quantitative EPR* book (2010) became an important introductory text. Research monographs such as Abragam and Bleaney (1970), Standley and Vaughan (1969), and Schweiger and Jeschke (2001) are foundations on which modern EPR is based. Modern research is also enriched by the monographs by Brustolon and Giamello (2009) and by Goldfarb and Stoll (2018). The "bible" for EPR instrumentation and methodology has been Poole's 1967 monograph, with a second edition 1983, and expanded in two volumes of a *Handbook of Electron Spin Resonance* 1994, 1999.

Key instrumental developments were high-Q reflection cavity, magic T and then circulator, low-noise Klystron (now replaced by low-noise Gunn diode sources), reference arm, magnetic field modulation and lock-in detection, high homogeneity magnets with high-stability power supplies, Hall-probe feedback magnetic field control, and solid-state electronics. In modern spectrometers all operations are under computer control.

For many years EPR measurement was predominantly continuous wave (CW) and predominantly X-band (ca. 9–10 GHz). Two types of pulsed EPR were developed, which have become known as saturation recovery and spin echo. Instruments capable of these pulse experiments were all home-built until Bruker developed the ESP380 FT-EPR

spectrometer in 1987. The development of pulse methods has played a major role in the development of EPR spectroscopy and its applications. In the early stages, in the 1960s and 70s, the main driving force was Mims in the U.S. and the Milov, Raitsimring, Salikhov, Tsvetkov, and Yudanov team in Novosibirsk. The triumph of the spin echo method is that it overcomes the masking effect of the inhomogeneous broadening of the EPR spectra and facilitates identifying weak spin interactions. One of the remarkable achievements is the development of nanometrology based on the modulation of the observed electron spin echo signal caused by the dipole-dipole interaction between the spins of unpaired electrons (Milov, et al., 1981) or between unpaired electrons and nuclei (Mims in Geschwind, 1972; Salikhov et al., 1976; Dikanov and Tsvetkov 1992; Schweiger and Jeschke, 2001).

More recently, rapid scan EPR has become the third fundamental method of performing EPR. Rapid scan does away with magnetic field modulation and lock-in detection. For long relaxation times and narrow spin packets, the magnetic field passes through resonance at times short relative to relaxation times. The time on resonance at constant microwave power is similar to the high-power-on time of pulsed EPR, so much higher power can be used with rapid scan EPR resulting in higher signal-to-noise relative to CW EPR. Duty cycle limitations of pulsed EPR usually result in rapid scan EPR providing better signal-to-noise per unit experiment time than pulsed EPR for species for which relaxation times are long enough to record spin echo spectra. Spectrometers

for CW, pulse, and rapid scan method are now commercially available. Benchtop size X-band spectrometers are available from several vendors, making X-band CW EPR accessible to a wide range of users.

X-band resonators were initially transmission, but quickly evolved into the now-common reflection resonator. At X-band a rectangular cavity resonator became standard. The use of lumped circuit resonators facilitated extension of EPR spectrometers to both lower and higher frequency/field than X-band. An historical sidenote on this history is intriguing: A textbook attempting to persuade students about cavity resonators, started with a lumped circuit inductor and capacitor (a loop-gap resonator) and stepwise transformed it into a cavity.

Interactions between spins monitored by EPR inform us about many phenomena. Dipolar interactions between pairs of electron spins native or labeled in polymers, especially biomolecules, has become a major application of EPR. Measurement of defect centers either inherent in objects or the result of radiation, explored by EPR, provides quantitative information about radiation dosimetry, archeological dating, artworks, stone sculpture analysis, and foodstuffs. There is major current effort to design spin systems with long phase memory times and other spectroscopic features that could contribute to quantum information computing.

The development of nuclear magnetic resonance imaging stimulated analogous development in EPR, but the differences in spin concentrations and relaxation times required different technologies. Initial experiments were performed independently

and essentially simultaneously in three labs (see Eaton et al., 1991). In vivo measurement of physiological chemistry was facilitated by the development of EPR spectrometers with frequency less than about 1 GHz. Many of the studies used nitroxide radicals. When triarylmethyl radicals of long-time persistence in vivo became available, their greater sensitivity to collisions with O₂ relative to nitroxides opened new horizons in EPR oximetry (Epel et al., 2014). Both localized spectroscopy and multidimensional imaging contribute importantly to preclinical physiological studies. Aspirations to clinical applications motivate this field. Low-field in vivo imaging has been pioneered by the Halpern and Krishna labs (see, for example, Biomedical EPR Parts A and B).

EPR is a major tool for characterizing persistent organic radicals and transition metal complexes. Many of these studies provide sufficient detail to stimulate very elegant high-order simulations. The success at X-band and the predictions of theory guide major efforts to achieve greater sensitivity and expand to both higher and lower microwave frequency and magnetic field. Extremes of temperature, pressure, and other sample environments are goals of many research teams. In spite of the many applications of EPR the cost of instrumentation has limited acquisition by many laboratories and small sales volume has restrained investment in new spectroscopic capabilities.

EPR instrumentation, commercial or locally built, now encompasses CW, rapid scan and pulse, zero-field to tens of tesla, low RF frequencies to teraHz, and microscopy to in vivo imaging and spectroscopy. Insights from high-field magnetic resonance stimulated major labs in several countries. Ohta and colleagues in Japan push the technological limits of multi-extreme EPR at high frequencies, high magnetic fields, and high pressures (Ohta et al., 2010, 2013; Ohmichi et al., 2021).

Current research will lead the way to quantum computing and health applications in the clinic. The future is limited only by the imagination of the next generation of students.

This brief synopsis of the first 80 years of innovation in EPR is an invitation to the EPR community to participate in celebrations at conferences around the world in 2024. Papers that strengthen the foundations of EPR for the next 80 years will be published in a special issue of *Applied Magnetic Resonance* to be edited by the authors of this article.

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Asako Kawamori (1935–2024)

Doctor Asako Kawamori, Honorary Professor at Kwansei Gakuin University, Fellow of the International EPR Fellow, passed away on January 15, 2024 (at 88 years of age).

Dr. Kawamori was born on March 29, 1935, in Izumi-ohsu, Osaka, Japan. She spent her childhood there. She had entered Osaka University, one of the few female students at that time. She belonged to the laboratory of Dr. Junkichi Ito, who is at the frontier of magnetic resonance research in Japan. After receiving doctoral degree in 1961, she started to work at the Faculty of Science, Kwansei Gakuin University, which had just been founded. She was one of the first faculty members. Her early works focused on solid-state phys-



ics using NQR, MASER, and so on. In the mid-1980s, she began studying biophysics. She focused on the photosystem II (PSII) protein complex. One of the early successful studies

was the first detection of ENDOR in the Mn cluster of PSII. Using distance measurement techniques, including the first application of PELDOR, she succeeded in studying the protein structures.

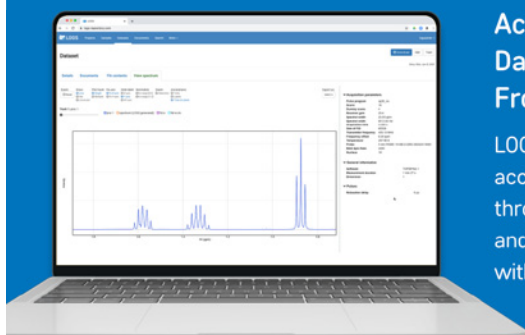
In 2003, Professor Asako Kawamori was distinguished as Honorary Professor at Kwansei Gakuin University. In 2022, she was awarded the IES Fellowship for her pioneering distance measurements in proteins by pulsed dipolar spectroscopy.

After her retirement at the university, she founded Agape Kabutoyama Medical Research Institute, a non-profit organization, and tried to apply EPR to the medical field. After closing the institute in 2016, she moved to a nursing home and spent time there until the end of her life. With many people related to academic society, alumni, and university staff, her funeral was a solemn send-off.

Hiroyuki Mino

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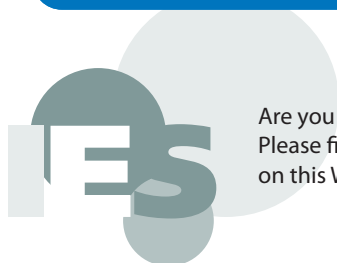


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The 62nd Rocky Mountain Conference on Magnetic Resonance

July 22–27, 2023, Denver, Colorado, USA

This year was an EPR only meeting – the 42nd International EPR Symposium. Attendance of over 120, including a significant number of international representatives, made for a successful gathering. Travel stipends assisted the attendance of 14 students and early career researchers.

The EPR Symposium commenced with two workshops. Thorsten Maly from Bridge 12 gave an informative introduction to resonators and resonator design, with a hands-on demonstration of their open-source PCB-based X-band loop-gap resonator. Stefan Stoll followed with an EasySpin tutorial, introducing several well received new features, including the ability to simulate non-equilibrium (spin-polarized) initial states.

The scientific program ran from Monday to Thursday. The 15 sessions ranged across a wide variety of topics – metals in biology, new approaches for improving DEER sensitivity, spin devices, biomaterials, molecular mechanisms of disease, NV centers and quantum sensing,

singlet fission, quantum systems and decoherence, defects in materials, new chemical motifs, technique development, high and low field measurements, and EPR imaging. It would be remiss of me not to take this opportunity to thank the session chairs for a sterling effort, keeping time admirably and more importantly for facilitating what one attendee noted were “the best discussions they had seen in quite a while”. Lengthening the speaking slots for contributed talks (to 20 rather than 15 minutes) was another factor which contributed to this outcome.

There were two special sessions: the International EPR Society Fellow Award session saw Howard Halpern (University of Chicago) discuss his work on Biologic Confirmation of Pulse Spin Lattice Relaxation EPR pO₂ Images, and the IES Silver Medal session heard from David Cafiso (University of Virginia) about the membrane spin labelling work which led to that award. David also agreed to give the speech at the Conference Banquet, an entertaining and informative retrospective touching on his experiences (and well received anecdotes) ranging from his student days at Berkeley in the 1970’s to now.

of Monochromatic Multi-photon Resonances in a Two-level Spin System Through Magnetic Resonance Spectroscopy with OLEDs”), with a cash prize supported by Bridge 12. Poster Prizes, supported by the International EPR Society, were awarded to Roxanna Martinez (Colorado State University, “Investigating the Role of Nuclear Spin Patterning and Counterion on Spin Relaxation in V(IV) Complexes”) and Austin MacRae (North Dakota State University, “Impact of Metal-Organic Framework Crystallinity on Enzyme Orientation and Dynamics”).

The Scientific committee for the meeting comprised Dane McCamey (Chair, UNSW Sydney), Songi Han (Co-Chair, Northwestern University), Claudia Avalos (New York University), Christoph Boehme (University of Utah), Sandra Eaton (ex-officio, University of Denver), Mrignayani Kotecha (O2M Technologies), Petr Neugebauer (Central European Institute of Technology), Shekar Ramanathan (Dartmouth University) and Sunil Saxena (University of Pittsburgh).

The meeting would not have been possible without the generosity of supporters and exhibitors: Bridge 12 Technologies, Inc., Bruker (who also hosted the traditional Bruker EPR Users’ Meeting & Reception, Cold Technologies, Inc., Cryogenic US LLC, National High Magnetic Field Laboratory, O2M Technologies, LLC, Rotunda Scientific Technologies, Spinflex Technologies, Virginia Diodes, Inc. and the Australian Research Council Centre of Excellence in Exciton Science.

The 63rd Annual Rocky Mountain Conference on Magnetic Resonance will take place August 4–8, 2024, returning to the Copper Conference Center in Copper Mountain, Colorado. The Chair for the EPR Symposium is Prof. Songi Han (Northwestern), with Stephen Hill (NHMFL) taking on the role of Co-Chair.

Dane McCamey
Chair, EPR Symposium 2023



From left to right: Thorsten Maly, Songi Han, Alysia Mandato, Sebastian Atwood, and Dane McCamey.

We were pleased to be able to present awards for the Best Student Talks to Alysia Mandato (University of Pittsburgh, “Improving Sensitivity of Distance Measurements at Nanomolar Protein Concentrations using Double Quantum Coherence”) and Sebastian Atwood (University of Utah, “Electrical Detection



From left to right: Dane McCamey, Austin MacRae, and Songi Han.



From left to right: Songi Han, Roxanna Martinez, and Aharon Blank.

Songi Han, Co-Chair:

We all hold dear what the Rocky Mountain Conference EPR means to us as a special conference for our community. Throughout all the years of its existence, the conference has always been focused on all aspects of EPR, ranging from fundamental sciences (physics, chemistry and biology), method development and all the way to magnetic resonance applications for engineering, materials sciences, medical imaging. We experienced how much spirit there is in the RMC EPR through the tragic and sudden passing away of Mark Stone from Milestone on August 11, 2022 by realizing how much Mark meant to the conference, and at the same time learning how important this conference is to EPR researchers around the world who showed up even with organizational challenges that we faced without Mark's steadfast presence. Mark was not "just" an organizer of the RMC EPR, but the cornerstone who embodied the spirit of the conference. Everyone who has ever participated in the RMC EPR knew Mark as part of the community. There was no problem that he would not solve, no matter how last minute it would be, with a smile on his face. Every par-

ticipant felt the love and the commitment from Mark, as well as his sister Ella who always was there by his side supporting his work. His passing was a shock to the RMC EPR community and organization because Mark made everything work including registration, scheduling the program, organizing vendor needs, to updating the webpage, and suddenly the conference organization needed to be done without his devoted support that we got accustomed to for decades. Chair David McCamey together with the RMC treasurer Sandy Eaton still made the RMC EPR happen in 2023 without any crisis, but there was a challenge from which we learned. The official count of the conference participants was well below the previous year's number until 2 weeks before the conference start date, which made the organizers worry because the finance of a conference depends on the participant number. Luckily, we learned that there is an unbreakable RMC EPR spirit: at the last minute, the conference participant number rose to the same number as in previous years, showing that the community was seeking to participate no matter what. The question was floated whether the community needs an annual RMC EPR or whether this should go to a biannual schedule like the RMC



NMR. Upon polling the audience, the answer was a resounding, "Yes, we absolutely need an annual RMC EPR!"

We now look towards the RMC EPR in 2024 that I will be chairing. The conference will be a special event as 2024 marks the 80th anniversary of Yevgeny Zavoisky's pioneering EPR experiment, a discovery that undeniably paved the way for all modern strides in electron magnetic resonance. We look forward to hosting all of you for this special Birthday EPR conference. ●

ISMAR 2023 as seen by Songi Han

The ISMAR 2023 taking place in Brisbane, Australia, was a fantastic conference. But there are a few aspects that stood out. There were many female plenary speakers some of whom I had never heard give a full lecture before, and it was a truly enjoyable experience. Even though EPR was a small part of ISMAR 2023, there were remarkable presentations worth highlighting. One of them was the plenary lecture by Christiane Timmel from Oxford University who gave a lecture par excellence! Her talk on "Inspired by Nature, Mimicked in the Lab – A Collection of Short Stories on Spin Polarisation" was highly didactic, exceptionally entertaining and truly inspirational. She effectively introduced fundamental and exciting concepts of the spin physics basis of magneto sensing of migratory bird to an audience for whom this was news. I had the privilege to give the Paul Callaghan Award Lecture in the opening night of the ISMAR conference, and even a greater privilege to be introduced by Daniella Goldfarb to the audi-

ence. We both had a huge smile on our faces and insisted that the conference chair snap a photo of us while we were on the stage. When sharing my talk that I entitled "The Shape of Water on Active Surfaces" I thought about what did Paul teach us that I would like to convey to the young scientists in the audience. Here is the story I shared when I was an undergraduate intern in his lab when he was still at Palmerston North at Massey University. I was unhappy that my experiments

were not working, and when I told that to Paul he countered "What do you mean your experiments are not working? You must respect your experiments!". What he meant was that the data tells us something that we must scrutinize with an open mind because that will lead us somewhere, possibly interesting and new, but only if we truly open our eyes to where the experiment lead us.

Another highlight for the EPR community was that Marina Dajka from the Free University of Berlin was selected as the poster winner of both the ISMAR and the IES EPR prize committee for her work on "Dipolar electron spin resonance spectroscopy of the lipopolysaccharide ABC transporter LptB2FG".

And last, but not least, we finally had the opportunity to hand over to Elena Bagranskaya her 2021 IES Medal in Chemistry in person that I carried with me for three years. It was truly a pleasure to hand over the medal and give her a congratulatory hug, thanks to the graciousness of the ISMAR organizers who allowed us to have a small celebratory moment on stage. ●



Professor Dr. Daniella Goldfarb (left) awarding the 2023 Paul Callaghan Prize to Professor Dr. Songi Han (right).

9th EFEPR Summer School on fundamental theory and state-of-the-art applications of EPR Spectroscopy*

September 3–9, 2023, Geneva, Switzerland

Since the first School in 1999 in the Italian city of Caorle, the EFEPR Summer School earned recognition as a traditional core of European education in the field of EPR spectroscopy. Numerous research groups send their PhD and some Master students to the School to learn the state-of-the-art in the field. As for all social events, this tradition was forced to take a break during the Covid-19 pandemic. Following the wish of the European EPR community for a swift restart, the EFEPR decided in November 2022 in an online General Assembly to give it a go to organize the 9th EFEPR Summer School in Geneva, Switzerland, in September 2023, co-organized by Enrica Bordignon, University of Geneva, and Daniel Klose and Gunnar Jeschke, ETH Zurich, together with an international scientific board – backed up locally by a meticulously working blue-cladded team of brave helpers (known as “blue T-shirts”).

As it is tradition on this school, the lecture program was dense, covering a wide range of EPR-topics and providing a formidable deep-dive from the basics of cw EPR, pulse EPR and quantum mechanics to current applications in Structural Biology and Catalysis, including the use of fast arbitrary waveform generators. Thus, the school catered to a wide range of interest groups and application fields from structural biology over coordination chemistry and catalysis to material science – and we thank all

the 24 lecturers (42% female) for these excellent contributions!

The wide range and diversity are also reflected in the 112 participants (45% female), mostly PhD students from 21 countries on 4 continents, who showed their dedication in lively discussions at two evening poster sessions and in hands-on tutorial sessions. These lab sessions, organized and scheduled according to each student's interests, included both real and virtual labs for the first time on our School – which allowed for more demonstrations via remote spectrometers for advanced tutorials such as DQC, ENDOR, HYSORE, and RIDME.

A special lecture dedicated to the James Webb space telescope, given by a scientist from the “Observatoire de Genève”, also met great interest, in particular because it covered the spectroscopy enabled by the telescope. After this evening lecture, participants enjoyed a traditional Swiss specialty: Chocolate fondue – to be added to the several kilos of chocolate distributed during the School! The dense scientific program was interrupted by the traditional relaxation day, which featured a boat tour across the idyllic Lake Geneva to the French village Yvoire. The sunny afternoon was rounded out by a picnic lunch, swimming, and a stroll through the charming medieval town.

On the last evening, we concluded our School with the poster awards for eight excellent young scientists, kindly sponsored by Groupement Ampère (Marvin Lenjer, Bartosz Mozgawa, Femke Reichardt, Maximilian Mayländer) and the IES (Radhika Kataria, Julia Haak, Orit Nir-Arad, Sebastian Gorgon) and the travel grant awards supported by Groupement Ampère. The two groups of Poster Prize winners and their contributions are featured in detail in the AMPERE Bulletin and, for

the IES awards, in this issue (pp. 19, 23–25). The last exchange of ideas was done via a lively forum, in which we addressed fundamental questions (what is SPIN?) and discussed the highlights of the School. We are happy that the participants embraced with great support the theme of sustainability which resonated with the ethos of this School (especially the vegetarian-only food, the absence of plastic bottles, the minimization of printed items, and the Swiss tap water).

Organizing such a lively event within such a short lead time would not have been possible without local support by the University of Geneva and donations from EPR-related and Swiss industries, including the Gold sponsors Bruker Biospin, Mettler-Toledo and Cryogenic.

We are already looking forward to the next EFEPR School 2025 kindly hosted at the University of Manchester, for updates see www.EFEPR.org.

Enrica Bordignon, University of Geneva,
Daniel Klose and Gunnar Jeschke,
ETH Zurich

The 62nd Annual Meeting of the Society of Electron Spin Science & Technology

November 2–4, 2023, Kobe, Japan

The 62nd Annual Meeting of the Society of Electron Spin Science & Technology (SEST2023) was held from November 2nd to 4th, 2023, at the Centennial Hall and Takigawa Memorial Hall, Kobe University, Kobe, Japan. SEST has held a scientific meeting in various cities in Japan every year, and this was the second time to be held at Kobe University since SEST2009 (Chair: Hitoshi Ohta). This year's meeting was held on site in full face-to-face mode including the reception since 2019 (held in Kawasaki, Chair: Akio Kawai). SEST was established in 2002 in Tokyo where the joint conference on the 41st ESR Symposium and the 7th *in vivo* ESR Workshop was held. This establishment was strongly motivated at the Asia-Pacific EPR/ESR Symposium in 2001 (APES2001, Chair: Asako Kawamori) held at Kobe University. SEST is also registered at Kobe University nowadays. Therefore, Kobe is important for SEST in various aspects. The total number of participants in this meeting (SEST2023) was 187 including 80 graduate or undergraduate students. We had 47 oral presentations and 69 poster presentations in addition to 1 plenary lecture, 4 award lectures and 2 mini-symposia (a total of 8 talks).

In the afternoon of November 3rd, the SEST annual general meeting (AGM) was

* Modified from Bulletin du Groupement AMPERE no. 293 (2023).



From left to right: Enrica Bordignon, Gunnar Jeschke, Radhika Kataria, Julia Haak, Orit Nir-Arad, Sebastian Gorgon, and Daniel Klose.

held. Board members of SEST reported the current status & activities, and the future plans of the society to the members. After the AGM, award ceremonies and award lectures for the SEST Awards, SEST Academic Award and Young Investigator Award were held. The SEST Awards were given to two researchers. Prof. Akio Kawai (Kanagawa University) received the SEST Award for his achievement entitled “Development of advanced electron spin probing method and elucidation of dynamic chemical phenomena”, and Prof. Hikomitsu Kikuchi (University of Fukui) received the SEST award for his achievement entitled “Development of spin model materials exhibiting novel magnetic properties”. Newly established SEST Academic Award was given to one researcher. Associate Prof. Shojiro Kimura (Tohoku University) received this award for his achievement entitled “High field ESR studies on quantum magnets”. Furthermore, the Young Investigator Award was given to one researcher. Assistant Prof. Miho C Emoto (Health Sciences University of Hokkaido) received this award for her achievement entitled “Imaging study of oxidative stress states in mouse brain using EPR for pathological insights”.

In this annual meeting, Prof. Christopher Kay (Saarland University) was invited as a speaker for a plenary lecture on Nov. 4. Prof. Kay is an active researcher in quantum sciences. He presented his cutting-edge research on quantum sciences under the title of “From EPR resonators to masers: a dielectric journey”.

We had two mini-symposia. The first mini-symposium in the morning of Nov. 3 was entitled “Frontiers in Magnetic Resonance Instrumentation” organized by Prof. Hitoshi Ohta (Kobe University). After the short in-

roduction by the organizer five speakers were scheduled. They were “Development of nano-diamond-based optically detected magnetic resonance of fluorescent for practical application” by Prof. Masazumi Fujiwara (Okayama University), “Development of high-pressure THz ESR and its application” by Assistant Prof. Takahiro Sakurai (Kobe University), “Development of the force-detected THz ESR technique using gyrotrons and its applications” by Associate Prof. Eiji Ohmichi, “Development and application of very-low-temperature ESR/NMR measurement system” by Associate Prof. Yutaka Fujii, and “Development of NMR spectroscopy using high-field DNP and its application to biological systems” by Prof. Toshimichi Fujiwara. However, Prof. Masazumi Fujiwara was not able to connect the on-line presentation from Germany, and his presentation was shifted to the day after SEST2023. The second mini-symposium in the morning of December 4th was entitled “Manipulation and Measurement of Multiple Spin Quantum System” organized by Prof. Yasuhiro Kobori (Kobe University) which started just after the plenary lecture by Prof. Kay. Three speakers were scheduled. They were “Spin polarization in chromophore assemblies” by Prof. Nobuhiro Yanai, “Electron spin manipulation in weakly coupled spin systems by AWG-ESR method” by Prof. Kazunobu Sato, and “Dynamic nuclear polarization MRI for *in vivo* metabolic imaging” by Prof. Fuminori Hyodo.

SEST recognizes several young members with 2 kinds of presentation awards, the Excellent Presentation Award and Poster Presentation Award, in every annual meeting to encourage young researchers. These awards are judged among the presenters who applied beforehand. The Excellent Presentation Award is given to

students and postdocs who give outstanding oral presentations. This year, this award went to Yuto Shoji (Kobe University) and Haruka Tsutsumi (Osaka Metropolitan University) out of 5 candidates. On the other hand, the Poster Presentation Award is given to students who presented their research results with well-prepared posters. The recipients of this award were Naoko Iizuka (Showa Pharmacy University), Shinya Kosaki (Nagoya University), Yuri Kasu (Saga University), Yohei Kudo (Hokkaido University), Nana Tomita (Hokkaido University), and Taichi Ishimura (Hokkaido University).

The reception of meeting was held at Soshuen restaurant at Mikage near Kobe University in the night of Nov. 3. Purely Japanese-style mansion of the wealthy executive with 5,300 m² garden was built in 1934. The mansion turned into a Chinese restaurant after the World War II. This is the reason why the name “Soshuen” sounds like a Chinese restaurant for Japanese. It is now an Italian restaurant, and the wedding parties were also going on in the other rooms on Nov. 3. Although there was a limitation due to the size of the room, 107 participants enjoyed very much the atmosphere, the food and the drinks. Everybody was very happy to have face-to-face mutual communications at the reception since 2019. SEST will have a next annual meeting in November 2–4, 2024 in Fukui, and such a reception is also expected.

Susumu Okubo,
Associate Professor, Chair, SEST 2023
Yasuhiro Kobori,
Professor, Vice-Chair, SEST 2023
Hitoshi Ohta,
Professor, Adviser, SEST 2023
Molecular Photoscience Research Center,
Kobe University



SEST award winners, from left to right: Hiroyuki Nojiri (SEST President), Akio Kawai, Hikomitsu Kikuchi (SEST Awards), Shojiro Kimura (SEST Academic Award) and Miho C Emoto (Young Investigator Award).



Poster Presentation and Excellent Presentation Award winners, from left to right: Hiroyuki Nojiri (SEST President), Naoko Iizuka, Shinya Kosaki, Yuri Kasu, Yohei Kudo, Nana Tomita (Poster Presentation Awards), Haruka Tsutsumi and Yuto Shoji (Excellent Presentation Award). Taichi Ishimura is not in this photo.



Enrica Bordignon

Enrica Bordignon moved from Ruhr University Bochum (Germany) to the University of Geneva (Switzerland) in September 2021. Dr. Bordignon received her MSc and PhD degrees in chemistry from the University of Padova (Italy). She completed postdoctoral fellowships at the University of Osnabruck (Germany) in the laboratory of Professor Heinz-Jürgen Steinhoff and at ETH Zurich (Switzerland) with Professor Gunnar Jeschke. Dr. Bordignon began her independent career in 2013 first as a W2 Professor of Biophysics at the Free University – Berlin (Germany) and then as a W2 Professor of EPR spectroscopy in the Department of Chemistry and Biochemistry at Ruhr University before being appointed full Professor of Physical Chemistry at the University of Geneva in 2021. She was also appointed Vice Dean of the Faculty of Science at the University of Geneva in July 2023 and has earned awards and honors in the EPR field, including the IES Young Investigator Award in 2011

and the Ampere Prize for Young Investigators in 2016. Dr. Bordignon is a physical chemist with research interests focusing on the study of protein conformational dynamics in vitro and in cells using site-directed spin labeling EPR spectroscopy.



Song-I Han

Song-I Han moved from the University of California – Santa Barbara to Northwestern University in July 2023 to become the Mark and Nancy Ratner Professor of Chemistry. Dr. Han received her undergraduate degree in chemistry from the University of Koln and her PhD in chemistry from the Aachen University of Technology in the lab of Pro-

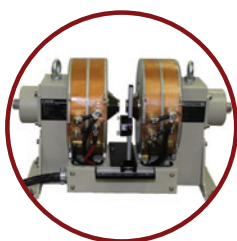
fessor Bernhard Blumich. She then completed a postdoctoral fellowship at the MPI for Polymer Research in the lab of Professor H.-W. Spiess, followed by a fellowship at UC Berkeley with Professor Alex Pines. Dr. Han became an Assistant Professor of Chemistry and Biochemistry at the UC Santa Barbara in 2004, where she rose through the ranks to full professor and remained for nearly 20 years before joining the faculty at Northwestern University to continue her highly productive career in magnetic resonance development. She has earned numerous awards in, and is an active member of, the EPR and NMR fields, including immediate past President of the IEPRS, Executive Council member of ISMAR, Elected Fellow of ISMAR and the 2024 Bruker Prize awardee. The focus of the Han lab is to push the boundary of magnetic resonance spectroscopy to use electron and nuclear spin systems as amplifiers, antennas and sensors to “see” molecular processes in water of biological, biochemical and biomimetic processes. The group’s primary strategy involves developing hardware for dynamic nuclear polarization (DNP) enhanced NMR and EPR at fields ranging from 0.35 Tesla to 7 Tesla. Her group often finds itself focusing on fundamental spin dynamics mechanisms underlying DNP to find new ways for sensitivity enhancements and to extract essential information about molecular organization through the interaction landscape of the coupled electron and nuclear spin network. The overarching goal is to achieve a deeper understanding and control of molecular processes vital to life sciences, focusing on biomedical inquiries and bio-inspired approaches.

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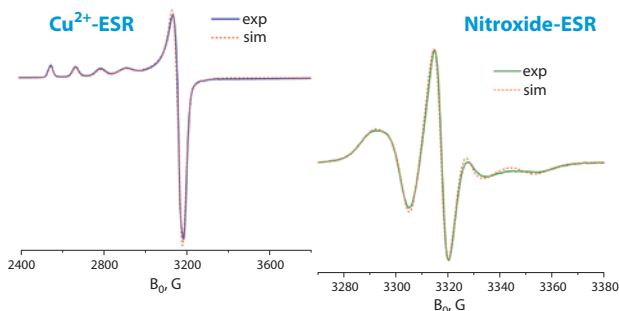
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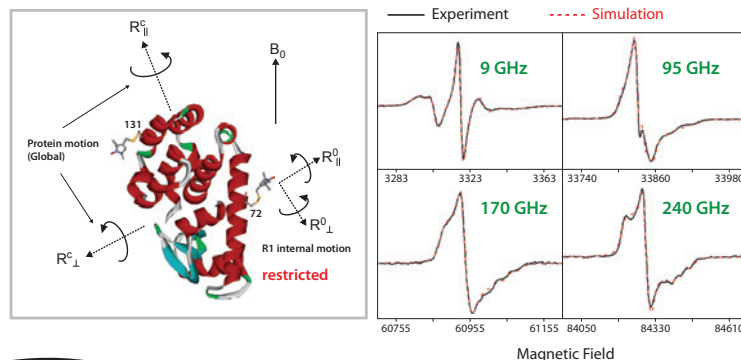
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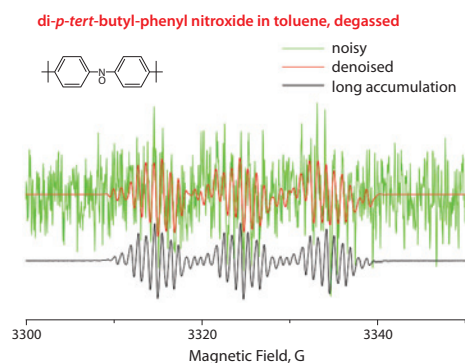
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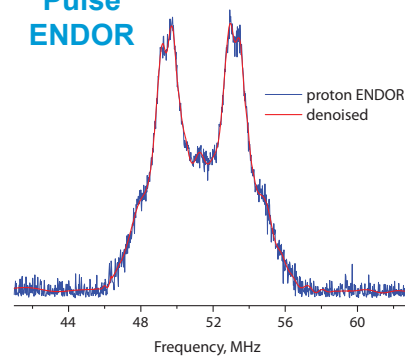


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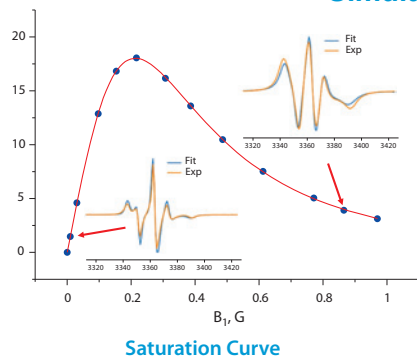


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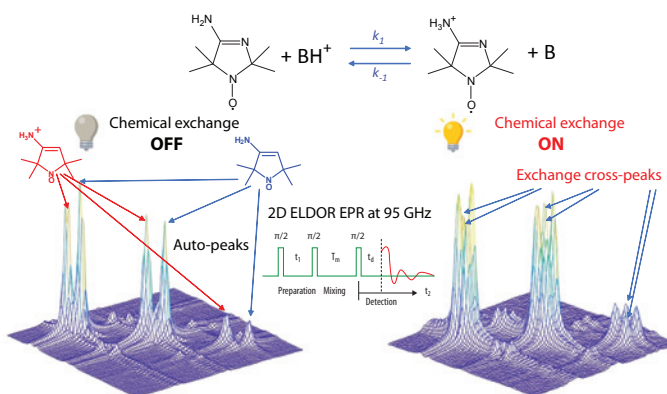
Pulse ENDOR



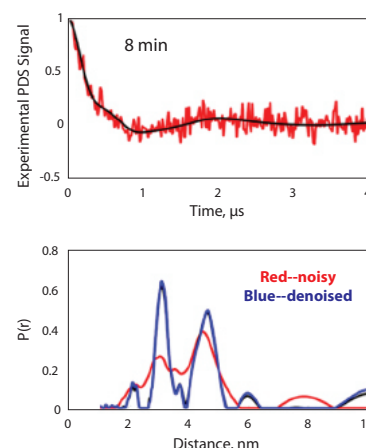
Simulation



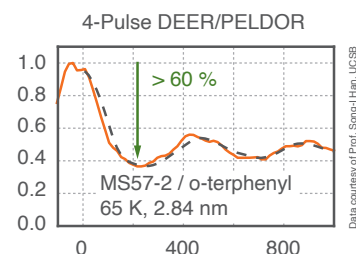
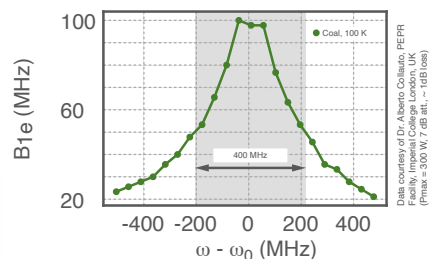
2D ELDOR



DEER & DQC



Loop-Gap Resonator for Pulsed Dipolar EPR Spectroscopy at Q-Band



Large Bandwidth ...

- Resonator Q
- Critically coupled: < 400
 - Overcoupled: < 85
 - Bandwidth: > 400 MHz

... Ideal for PELDOR Spectroscopy

The large bandwidth and conversion factor ensures large modulation depths in PELDOR/DEER experiments.



BRIDGE
12

More information about the Bridge12 QLP at www.bridge12.com/products/qbandprobe

Millimeter-Wave Transmit and Receive Systems for EPR and DNP

VDI offers high power sources up to 3 THz, including:

- up to 1.2 Watts @ 140 GHz
- up to 250mW @ 197 GHz
- up to 220mW @ 263 GHz

These AMCs include high power amplifiers up to ~200 GHz. AMCs with these new amplifiers offer improved amplitude and phase control. Broadband, full waveguide sources up to 1.5 THz are available.

VDI also offers heterodyne and detect receivers up to 3 THz.

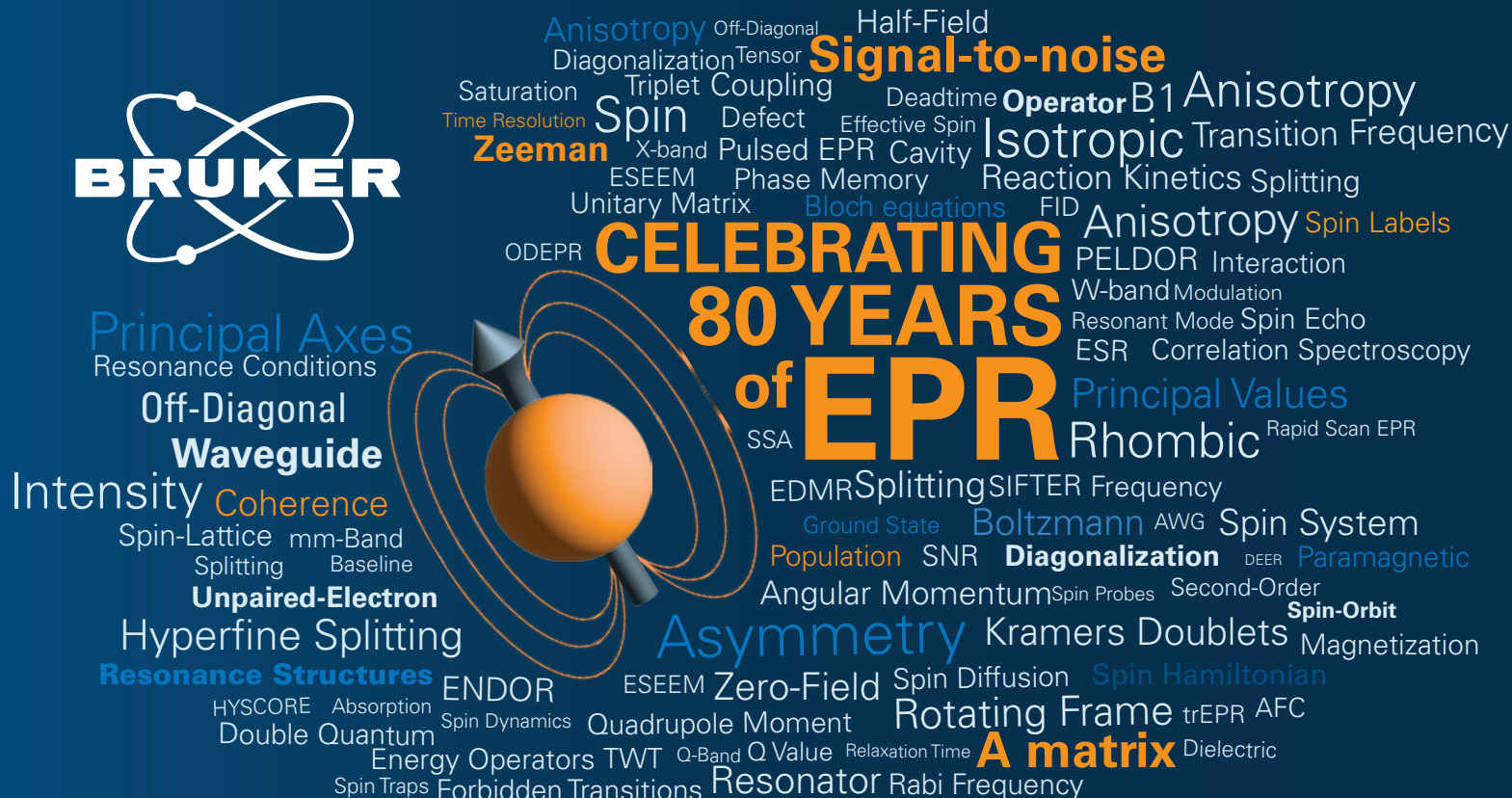
Contact VDI for more information.



Virginia Diodes, Inc.

979 2nd St. SE, Suite 309
Charlottesville, VA 22902
434.297.3257

vadiodes.com



Celebrate 80 Years of EPR with Us

- An EPR portfolio covering all application needs, ranging from benchtop devices to CW and pulse high-frequency EPR
- A worldwide network of EPR Application Scientists and Service Engineers to support customers in technical and scientific questions



Innovation with Integrity



EPR

Multi-Harmonic Detection Accessory

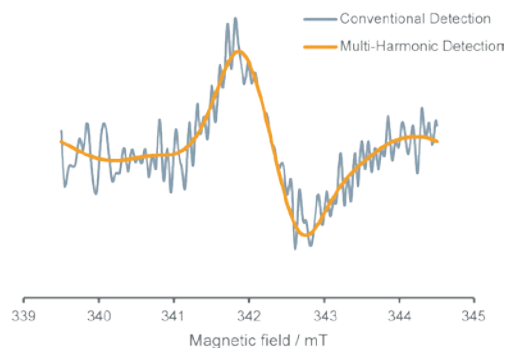
Unlocking the Full Potential of CW-EPR

Bruker is excited to introduce the Multi-Harmonic Detection Accessory into the EPR portfolio.

Key features of the Multi-Harmonic Detection Accessory:

- SNR enhancement for your CW-EPR spectrum leading to reduced acquisition times
- Dedicated software for acquisition and analysis
- Compatible with EMXplus, ELEXSYS and Magnettech ESR5000 spectrometers
- Field-upgradable

For more information please visit www.bruker.com



In-vivo CW-EPR spectra of a single Zebrafish: Conventional detection in grey and multi-harmonic detection in orange. A single Zebrafish embryo is shown above.