# epr newsletter

2022
volume 32 number 3-4


The Publication of the International
EPR (ESR) Society

## Officers of the International EPR (ESR) Society



## Fellows of the International EPR (ESR) Society

Anatole Abragam (1914–2011)
John Michael Baker (1930–2017)
Lawrence J. Berliner
Brebis Bleaney (1915–2006)
James R. Bolton
R. David Britt
Harvey A. Buckmaster (1929–2018)
Klaus-Peter Dinse
Anders Ehrenberg
Gareth R. Eaton
Sandra S. Eaton
George Feher (1924–2017)
George Fraenkel (1921–2009)
Jack H. Freed
Betty J. Gaffney
Daniella Goldfarb
Robert Griffin
Edgar Groenen
Erwin Hahn (1921–2016)
Karl Hausser (1919–2001)
Kalman Hideg (1934–2018)
Noboru Hirota
Brian Hoffman
Wayne Hubbell
Clyde A. Hutchison, Jr. (1913–2005)
James S. Hyde (1932–2022)
Asako Kawamori
Lowell Kispert
Daniel Kivelson (1929–2003)
Melvin P. Klein (1921–2000)
Harry Kurreck (1932–2015)
Wolfgang Lubitz
August H. Maki (1930–2008)
Harden McConnell (1927–2014)
Bruce R. McGarvey
Keith A. McLauchlan
Michael Mehring
Klaus Möbius
Yuriy N. Molin
James R. Norris
John R. Pilbrow
Charles P. Poole, Jr. (1927–2015)
Aleksandr M. Prokhorov (1916–2002)
Arnold M. Raitsimring
Kev M. Salikhov
Tengiz I. Sanadze (1930–2011)
Charles P. Scholes
Arthur Schweiger (1946–2006)
Charles P. Slichter (1924–2018)
Sankaran Subramanian
Leslie H. Sutcliffe (1924–2020)
Harold M. Swartz
Martyn C. R. Symons (1925–2002)
Takeji Takui
Wolfgang E. Trommer
Yuri D. Tsvetkov (1933–2018)
Hideo Utsumi
Joan H. van der Waals (1920–2022)
George D. Watkins
John A. Weil (1929–2010)
Samuel I. Weissman (1912–2007)
David Whiffen (1922–2002)
Hans C. Wolf


epr newsletter

https://ieprs.org/newsletterpage/

The official publication of the International EPR (ESR) Society is supported by the Society, by corporate and other donors, and the Zavoisky Physical-Technical Institute of the Russian Academy of Sciences, Kazan, Russian Federation.

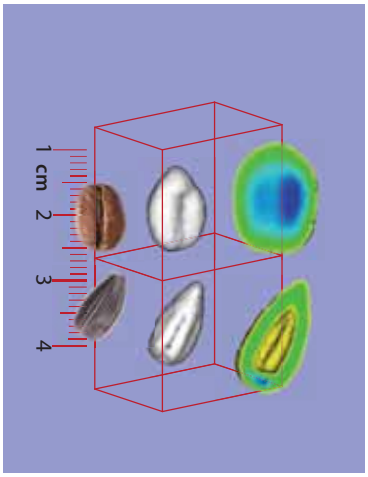



Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.


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

ISSN 1094-5571

TECHNION | PRINTING UNIT




**The cover picture illustrates** aspects of research of Bernard Gallez, recipient of the IES Silver Medal Biology/Medicine 2022 (see also the article "Playing with Oxygen (and others)" by Bernard Gallez, *EPR newsletter*, 32/2, pp. 3, 4). The cover picture shows EPR images recorded in food. Roasted coffee bean (top) and sunflower fruit (bottom) with 3D EPR surface view and cross section view of spin density. Color scale: blue (highest intensity) > green > yellow (lowest intensity).


# epr newsletter

The Publication of the International EPR (ESR) Society

volume 32 number 3-4 2022




continued on page 2

# Editorial



Dear colleagues,

Could you please take a nice cup of coffee or tea or whatever drink you prefer in the time of the day when you venture to read the latest issue of the *EPR newsletter*, make yourself comfortable at your desk and anticipate a long exciting reading: we collected lots of news for you. To start with, this cover invites you to refresh the article by Bernard Gallez, IES Silver Medal Biology/Medicine 2022 (32/2, pp. 3, 4). You must be accustomed to the idea that the cover of an issue celebrates an awardee featured in the issue, but in this case, Marina Bennati, IES Silver Medal Physics/Materials Science 2022 (pp. 11–13) has already been celebrated by her cover as the Bruker Prize 2019 awardee (29/3, p. 3).

It is almost impossible to specify the highlight of this newsletter issue. I feel, it is a newsletter issue full of highlights and the sequence of reading is your choice. Undoubtedly, one of them is the report about the IES Annual General Meeting for 2022, which was held online at the 17th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena 2022 (pp. 3–6). You may judge for yourself how efficient the Society functioned in this time period and the newsletter issues are always available to give you all necessary details. It is really amazing how fruitful the year 2022 was for the society mainly due to the development of all initiatives conceived and implemented by the IES CEOs and supported by the IES members. A good balance between age and youth, and experience and passion was maintained, which we are aimed at permanently.

It is very tempting to tell you what we plan for the future issues to make your mouth water but I prefer let you be excited by the promise that your great expectations won't be cheated. I may give you a slight hint by mentioning some of the names: Jack Freed, Sandy Eaton, David Cafiso, Takeji Takui, Wayne Hubbell, Tobias Hett, Emily Dowker, Zongyu Yang, Thomas Schmidt, Janne Soetbeer, Fabian Hecker, etc. When you will get the forthcoming issue 33/1 (2023), you will see, if you guessed it right. However, according to Patrick Süskind: there is no such human fantasy that reality would not surpass effortlessly. Let us wait and see!

It is my pleasure to thank all contributors to the *EPR newsletter*, CEOs of the IES, Associate Editors Candice Klug, Hitoshi Ohta and Sabine Van Doorslaer. Special thanks go to editors of long-lived columns: John Pilbrow (EPR newsletter Anecdotes), Candice Klug (New EPR Faculty), Wolfgang Lubitz (Guest of the Issue), and Stefan Stoll (Software), and Sergei Akhmin, Technical Editor, a magician of creativity and perfection. It is amazing to collaborate with researchers all over the world and to see our field of research flourish.

Happy New Year 2023!

Laila Mosina

# IES ANNUAL GENERAL MEETING 2022

Minutes of the Annual General Meeting of the International EPR/ESR Society for 2022 held online at the 17th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena, August 31, 2022 (Held in-person and via Zoom).

**Agenda:**

1. Introducing the IES Executives (2021–2023) (Songi Han)
2. Announcement of the 2022 IES Awards (Songi Han)
3. Report of IES online activities 2022 (Songi Han)
4. Report of the *EPR newsletter* Editor (Laila Mosina)
5. In Memoriam of the Giants of EPR (Songi Han)
6. Sponsors and Patrons of the IES 2022 (Songi Han)
7. Report of the Secretary (Aharon Blank)
8. Report of the Treasurer (Peter Qin)
9. Planned Activities for the next year (Songi Han)
10. Questions, Discussion, and Suggestions (Songi Han)

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

Dear Colleagues,

On behalf of the IES Executive Board I wish to welcome all participants of the online IES Annual General Meeting 2022.

*IES executives (2021–2023)*

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

### 2. Announcement of the 2022 IES Awards (Songi Han)

**2022 IES Best Paper Award**

Dr. Katherine Richardson, Imperial College London.

"*Functional basis of electron transport within photosynthetic complex I*", *Nature Communications* 2021, 12, 5387. See *EPR newsletter* 32/3-4, p. 18 (2022)

**2022 John Weil Young Investigator Award**

Dr. Asif Equbal, Assistant Professor, NYU Abu Dhabi.

Award Lecture delivered at the 2022 Rocky Mountain Conference.

"*Dipolar Order in Electron Spins: An EPR Signature of Thermal Mixing DNP*". See *EPR newsletter* 32/3-4, pp. 14, 15 (2022)

**2022 IES Silver Medal in Biology and Medicine**

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

Prof. Bernard Gallez, Biomedical Magnetic Resonance Research Group, Louvain Drug Research Institute (LDRI), Belgium.

Award Lecture to be delivered at the XII International Workshop on EPR in Biology and Medicine (Krakow, Poland), 10–13 October 2022 (organized by Martyna Elas).

His longstanding contributions are to the field of in vivo EPR spectroscopy since the early 1990s and continuing to the present time. He made seminal contributions to the field of characterizing the tumor microenvironment (physiologic and metabolic) using EPR methods in mouse models of human cancer. See *EPR newsletter* 32/2, pp. 3, 4 (2022)

Prof. David Cafiso, Alfred Burger Professor of Chemistry and Molecular Physiology and Biological Physics, University of Virginia, USA.

Award Lecture location: TBD

For his fundamental contribution to apply EPR spectroscopy and site-directed spin labeling to study reversible membrane-protein electrostatic interactions that function in cell signaling systems and in membrane trafficking of relevance to human disease states and neurotransmitter release, and membrane protein structure and function for transport mechanisms.

**2022 IES Silver Medal in Physics**

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

Prof. Marina Bennati, Research Group Leader of the MPI for Interdisciplinary Research and Professor at the University of Göttingen, Germany.

Award Lecture was delivered at 55th ESR Spectroscopy Group of the Royal Society of Chemistry Meeting for EPR, St. Andrews, June 6–10, 2022.

Honored for her fundamental contributions to advance the physics of electron-nuclear double resonance (ENDOR) and liquid-state dynamic nuclear polarization (DNP) spectroscopy at high magnetic fields, and their application for the study of paramagnetic molecular systems. See *EPR newsletter* 32/3-4, pp.11–13 (2022)

**2021 IES Silver Medal in Methods**

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

Prof. Stefan Stoll, Professor at the University of Washington, Seattle, USA.

Award Lecture was delivered at 55th ESR Spectroscopy Group of the Royal Society of Chemistry Meeting for EPR, St. Andrews, June 6–10, 2022.

Honored for his seminal contributions to computational EPR spectroscopy and analysis. Stoll initiated the development of the first generally applicable package for simulating and fitting EPR data. EasySpin is now a mainstay of the field of EPR and an essential tool used by virtually all modern EPR laboratories around the world. Remarkably, Professor Stoll has invested significant effort and resources into making EasySpin a freely available and accessible tool, while he continues to contribute to dissemination of this important software tool through ongoing training workshops for spectroscopists of all backgrounds, and regular upgrades to the software packet. See *EPR newsletter* 31/2, pp. 4, 5 (2021)

**2022 IES Fellow**

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

Asako Kawamori, retired Professor, NPO Agape Kabutoyama Medical Research Institute in Nishinomiya, Japan.

Award and Award Lecture to be delivered in person (TBD). See *EPR newsletter* 32/3-4, p. 13 (2022)

**2022 Best Poster Prizes (to date)**

***2022 RSC ESR Spectroscopy Group Conference (St. Andrews)***

Ciaran Rogers, University of Manchester: "*Modelling Conformational Flexibility in a Spectrally Addressable Multi Spin Molecular Qubit Model System*".

Orit Nir-Arad, Tel-Aviv University: "*Design and Construction of 14 Tesla DNP/EPR spectrometer*". See *EPR newsletter* 32/3-4, p. 19 (2022)

***EUROMAR2022 Conference Utrecht***

Tobias Hett, University of Bonn: "*Influence of Spin Label Conformer Ensembles on Pulsed Dipolar EPR Distance Distributions*".

Mantas Simènas, Vilnius University: "*ESEEM spectroscopy of methyl group quantum tunneling in Co-doped dimethylammonium zinc formate*".

***2022 RMC EPR Copper Mountain***

Xiaowei Bogetti, University of Pittsburgh: *"Newly Developed dHis-Cu$^{2+}$ Force Fields Establish Cost-Efficient Protocol for DEER Measurements at Q-band"*.

Cooper Selco, University of Southern California: *"Non-Markovian Spin-Bath Dynamics of a Single Nitrogen Vacancy Center in Diamond"*. See *EPR newsletter* 32/3-4, p. 20 (2022)

Euan N. Bassey, University of Cambridge: *"Revealing Redox Processes and Probing Phase Transformations in Sodium-Ion Battery Cathodes using EPR and NMR Spectroscopy"*. See *EPR newsletter* 32/3-4, p. 21 (2022)

***2022 Spin Chemistry Meeting***

Emily Dowker, Furman University: "*Effects of hydrophobic modification and electrostatic interactions on sensitivity of riboflavin-ascorbic acid radical pairs to weak magnetic fields*".

Janko Hergenhahn, Oxford: "*Electron spin delocalization in radical anions of porphyrin molecular wires*".

**3. Report of IES online activities 2022 (Songi Han)**

Short Report of the previous Minutes of the Annual General Meeting of the International EPR/ESR Society for 2021 held online at ISMAR-APNMR, 23:05–23:45 (JST) August 24, 2021 (Held via Zoom). AGMs recording can be found in: https://ieprs.org/on-line-activities. See *EPR newsletter* 31/3 (2021) pp. 3–6.

**IES Virtual EPR Meeting (IVEM)**

Biweekly meeting, Signup: https://forms.gle/Usv8sbj3LUr7QvcE8
All IVEM speakers get opportunity to be highlighted in the *EPR newsletter*. https://ieprs.org/on-line-activities
Run and organized by students and young researchers
*IVEM Chairs*: Zhongyu Yang (North Dakota State University, USA), Thomas Schmidt (NIH, USA)
*IVEM Committee*: Tomas Orlando, Joseph McPeak, Yujie Zhao

***Biomolecular***: Malte Dreschner "*In-cell EPR techniques*"; Joshua Casto "*Structural Link in the Transcription Cycle of a Metalloregulator*"; Michael Lerch "*High-pressure EPR toolkit*".
***Chemistry***: Jasleen Brinda "*Dielectric Transition and Molecular Dynamics in the Metal–Organic*"; Josh Biller "*EPR and Corrosion*"; Rebekah Taylor "*para-Xylene Oxidation Catalyst*".
***Chemistry***: Andrei Kuzhelev "Solid-like Dynamic Nuclear Polarization Observed in the Fluid Phase".
***Instrumentation***: Nandita Abhyankar "*Scalable microresonators for room temperature*"; Yaron Artzi "*High-Temperature Superconducting Surface Micro-Resonators*"; Shutian Lu "*Quantum biosensor for DNA aptamers and NV centers*".
***Software***: Madhur Srivastava "*Two-dimensional reconstruction of distance distributions*"; Anna Matveeva "*Data collection approach in PELDOR/DEER: how can it be optimized*".

IES Virtual EPR Meetings (IVEM) are broadcasted via Twitter and Emails: IES Twitter (https://twitter.com/EPR_ESR)

843 Followers, 94 Following

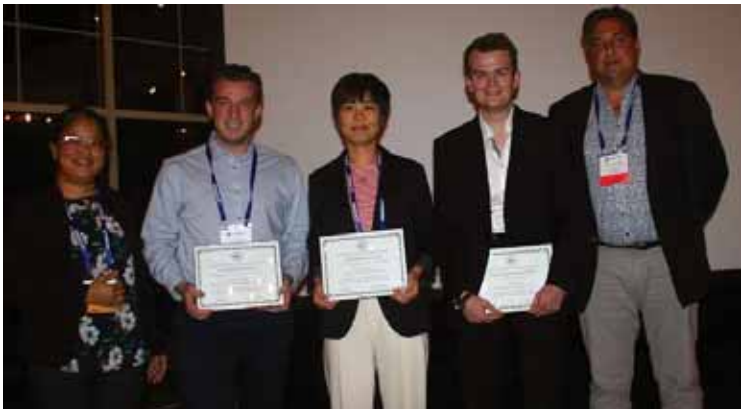
Wanted: New Social Media Officer for the IES.

Critical medium to reach young scientists and a broader audience.

EPR_ESR tweets are embedded on several webpages (ieprs, RSC EPR group, etc.)

Join and follow us @EPR_ESR

Encourage your students to follow @EPR_ESR and stay active



From left to right: Songi Han, Cooper Selco, Xiaowei Bogetti, Euan N. Bassey and Fraser McMillan.

From left to right: Fraser McMillan, Asif Equbal and Songi Han.

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

Since the previous AGM of the IES in 2021 at ISMAR-APNMR, we published 31/3, 31/4, 32/1 and 32/2. We hope you had a look at these copies on the IES website and got color copies.

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

Now we work on the forthcoming issue 32/3-4. To remind you, we present the columns of the newsletter:

Columns of the *EPR newsletter* 32/3-4 (2022)
– Editorial
– IES business
– Awards
– IES Young Investigator Award Revisited
– Another Passion
– Anniversaries
– EPR newsletter Anecdotes
– In Memoriam
– Present Meets Future
– Software
– Tips and Techniques
– Notices of Meetings
– Conference Reports
– New EPR Faculty
– New Books and Journals (including EPR Hot Science)
– Market Place
– Reader's Corner
– Guest of the Issue

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

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

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





**5. In Memoriam of the Giants of EPR**

Jack Peisach (1932–2021) *EPR newsletter* 31/3, 18–20 (2021)
Richard Ernst (1933–2021) *EPR newsletter* 31/4, 9 (2021)
Shimon Vega (1943–2021) *EPR newsletter* 32/1, 14, 15 (2022)
R. W. Quine (1943–2021) *EPR newsletter* 32/2, 15, 16 (2022)
Massimo Martinelli (1943–2021) *EPR newsletter* 32/2, 13, 14 (2022)
Joan van der Waals (1920–2022) *EPR newsletter* 30/3, 5–10 (2020)
James S. Hyde (1932–2022) to be published in the *EPR newsletter* 33/1 (2023)

**6. Sponsors and Patrons of the IES 2022 (Songi Han)**

| | |
|---|---|
| Bruker | Virginia Diodes |
| GMW Associates | Springer / Applied Magnetic Resonance |
| L&M Supplies | JEOL |
| Rotunda | Bridge 12 |
| LOGS | CIQTEC |
| Cryogenic | ACERT |

**7. Report of the Secretary (Aharon Blank)**

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

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

**Major tasks over the last year:**

1. Continued updating of IES webpage
2. Recruit speakers to present EPR tutorials at Bruker Webinars

**From left to right: Songi Han, Janko Hergenhahn and Aharon Blank.**

**From left to right: Songi Han, Emily Dowker and Aharon Blank.**

3. Handling of Awards, fellowships and the "Best paper Award" new initiative
4. Updating of the IES twitter page (with Songi Han, the IES Social Media Officer)
5. Printing and distribution of *EPR newsletter* (with Secretary's kids)
6. Adding new sponsors

**Website updates**

Collection of all Newsletters (Now done, from Vol. 1-1987) (pdfs of Volumes 1-12 are courtesy of the late Arthur Schweiger, Fellow of the IES)

Upgrading details on Awardees – all new Awardees have their photo and citation page, and also past Awardees (on-going...)

**8. Report of the Treasurer (Peter Qin)**

| | |
|---|---|
| 2021 Financial Report ($) | |
| **Balance on January 1, 2021** | **56,155.70** |
| ***Deposits:*** | |
| Membership | 4,436.12 |
| Sponsor Contributions | 25,600.00 |
| TOTAL deposits: | 30,036.12 |
| ***Expenditures:*** | |
| Internet Commerce & Merchant Services, Banking | 682.49 |
| IES Community Support (Conferences, Training, Poster Awards) | 4,820.00 |
| IES Operation (Web, Printing, Editorial) | 26,594.50 |
| Misc (Registration, Postage, etc.) | 75.00 |
| TOTAL expenditures: | 32,171.99 |
| **Balance as on 12/31/2020** | **54,019.83** |
| | |
| 2022 January-June Financial Report ($) | |
| **Balance on January 1, 2022** | **54,019.83** |
| ***Deposits:*** | |
| Membership | 2,130.00 |
| Sponsorship | 7,430.00 |
| Misc (tranfer from John Weil Fund to cover payment for 2021 YIA) | 1,000.00 |
| TOTAL deposits: | 10,560.00 |
| ***Expenditures:*** | |
| Financial Service Fees (Merchant Services, Banking) | 378.43 |
| IES Community Support (Virtual Gp Mtg) | 600.00 |
| IES Operation (Web, Printing, Editorial) | 21,173.80 |
| Misc (Registration) | 133.75 |
| Total expenditures: | 22,285.98 |
| **Balance on June 30, 2022** | **42,293.85** |

**From left to right: Ciaragn Rogers and Orit Nir-Arad.**

**John Weil Fund**

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

| | |
|---|---|
| **Starting Balance on 01/01/2021:** | **$ 21,913.58** |
| Interest Income: | $ 266.65 |
| Distributions for 2021 YIA: | $ (0.00)* |
| **Ending Balance on 12/31/2020:** | **$ 21,913.58** |

* 2021 YIA award ($ 1,000) paid from the general account on 12/2021 fund transferred from the John Weil account in 01/2022.

Thank you, IES members, Thank you, sponsors: Bruker BioSpin, JEOL, Bridge 12, CIQTEK, GMW Associates, L&M EPR Supplies, Rotunda Scientific Technologies, Springer/Appl. Magn. Reson., Virginia Diodes, Signals.

**9. Planned Activities for the next year (Songi Han)**

**Gold Medal of the IES**

**Fellows of the IES**

**John Weil Young Investigator Award**

Deadline for nominations: November 1, 2022; Nominations by active IES members; 100–150 word citation; CV; Publication list.

**IES Best Paper Award (for young scientists)**

Deadline for nominations March 2023; Self nomination; First author with support letter from corresponding author/ supervisor which explains the contribution of first author.

**IES AGM 2023 to be held at the 56th RSC EPR Meeting 23–30 March 2023, University of Leeds, UK**

Local Organizer: Christis Pliotas

**IES Membership Drive: WE NEED YOU!**

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

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

**10. Questions, Discussion, and Suggestions (Songi Han)**

Create more visibility of the Society – also for **young researchers!**
– Invite young scientists (YIA/Poster Prize winners) to the IES Board Meeting – **at real meetings** ...
– Create an interactive Communication Platform on our Webpage – **Twitter** ...
– Put links to tutorials, special articles on our new Webpage
– Create a directory of EPR groups
Host EPR database – first for Dipolar EPR Data base

The meeting was attended by all the Spin Chemistry 2022 International Meeting participants from the field of EPR.

# Interview with Dr. Yu He, CEO, CIQTEK

**EPR newsletter:** *Dear Dr. He, the IES greatly appreciates the support of Chinainstru & Quantumtech (Hefei) Co.,Ltd., which contributes to the EPR community by generating products of importance to our community. We are most appreciative that you agreed to answer the questions of this interview. How the idea to found a company was conceived?*

In the past hundred years, nearly 70% of the groundbreaking work and discoveries leading to Nobel Prizes in the Natural Sciences were made with the help of scientific instruments, and the development of physics and chemistry was even more dependent on them. I am familiar with scientific instruments because I have loved physics and chemistry experiments from a very young age.

In 2009, I was admitted to the School of the Gifted Young (SGY) of the University of Science and Technology of China (USTC). Compared with my classmates, I was a little bit "out of the loop" – not only did I like to study various scientific instruments, but I was also keen on organizing practical physics activities on campus. In 2010, I enrolled in a lecture given by Professor Jiangfeng Du, an internationally renowned physicist, and learned that 60% of China's annual investment of hundreds of billions of dollars in fixed assets for scientific research was spent on equipment imports. The scientific research team led by Professor Du achieved a series of original results in the fields of microscale NMR and EPR/ESR spectroscopy, biology, and physics. More than 60 related papers were published in journals such as Science and Nature, which showed me there was a serious shortage of scientific instruments in China and also the possibility of closing the gap through our efforts. I found that I could turn the discoveries of scientists into scientific products and then help them to better explore the mysteries of the universe and the future of mankind. After the lecture, my sense of mission to broaden the boundaries of human knowledge and the responsibility to improve scientific research gave me the faith and strength to start my own business.

*What is your educational and /or research background?*

As mentioned, I went to study in the SGY of the USTC when I was 16. The School was specially designed for the most talented young students. Proposed by Professor Tsung-Dao Lee, a Nobel Prize laureate, SGY was established in 1978, and has since grown in both size and recognition as the premiere honors program in Chinese academia. Its purpose is to explore the ways to train outstanding talents in the fields of science and technology in China, to cultivate outstanding talents in science and technology and other fields, and to promote the development of China's science and technology, education and economic development. In 2010, I approached Professor Du to join the CAS Key Laboratory of Microscopic Magnetic Resonance under his leadership, and in 2013, I became his graduate student and continued my Ph.D. studies after obtaining the M.S. degree with a research focus on physical electronics.

The research and development of EPR spectrometers is very important to me. Since 2010, with the continuous support of the research equipment development program of the Chinese Academy of Sciences, USTC has been exploring the path of independent development and industrialization of China's electron paramagnetic resonance spectrometer. After joining the laboratory, I participated in the development of a prototype of EPR spectrometer, and itremains my research area until now. I am also still working part-time as an EPR product manager in order to provide customers with higher reliability, applicability, productivility and maintainability of the device.

*What were the stages of the formation and development of your company?*

Before the company was formally established, I led an association at school and met many like-minded members. On one occasion, we were inspired by a teacher's talk about interactive instruments used in Harvard and MIT classrooms and this then led the development of a question-answering device that tested whether students understood or not.

In July 2013, Dr. Will Zhang, the co-founder and I set up our first company. Zhang was the backbone of the association, is our vice president of CIQTEK today. He is in charge of the R&D center, which accounts for 70% of the company's Staff. Founded in 2016, CIQTEK is the first national high-tech enterprise in China with quantum precision measurement as its core technology, mainly engaged in the development, production, and sales of quantum measurement, quantum computing, high-end scientific instruments, and related products. The first product was the EPR spectrometer in October 2018, and we officially brought the product, from the original prototype to the market after nearly 2 years of engineering and commercialization. Since then, our EPR spectrometer has evolved and gained recognition from top Chinese universities, such as Tsinghua University, Peking University, and Chinese Academy of Sciences.

We have received a total investment of about 1 billion CNY (150 million USD) from many well-known investment institutions since es-

## Chinainstru & Quantumtech (Hefei) Co., Ltd.

**Our mission.** CIQTEK is dedicated to helping customers to promote the development of technology more efficiently, explore and create the future of mankind.

**Our products.** EPR spectrometer, ODMR spectrometer, quantum computing device, scanning electron microscope, quantum diamond atomic force microscope (QDAFM), quantum magnetic imaging analyzer, specific surface area analyzer (BET), electronic test & measurement.

**Our history.** Chinainstru & Quantumtech (Hefei) Co., Ltd, known as CIQTEK, a high-tech enterprise with quantum precision measurements as the core technology, was founded in December, 2016 at its headquarters in Hefei, China. Now with over 650 employees are committed to providing high-end scientific instruments to the world.

In 2021, CIQTEK finished a C round finance, and financial valuation reached 1 billion US dollar, also was named as a "unicorn" company by Chinese government.

It is devoted to providing products and services to enterprises, governments, and research institutions around the world, including core devices represented by enhanced quantum sensors, advanced instruments, equipment for analysis and test, technical solutions for enabling industry applications, etc.

tablishment, and have launched three world firsts: the world's first "Diamond Quantum Computer for Education", the world's first "Quantum Experiment Platform" based on the principle of NV-center spin magnetic resonance, and the world's first "Quantum Diamond Atomic Force Microscope" based on NV-center and AFM scanning imaging technology. We have also achieved four China firsts: China's first commercial "Pulsed EPR spectrometer", China's first "W-Band High-frequency EPR spectrometer", China's first commercial "Multi Qubits Ion-trap Quantum Computer", and China's first commercial "LWD-NMR". The products have been delivered to hundreds of customers worldwide, including overseas customers such as the University of California, Berkeley, Stony Brook University, New York, University Mainz, Germany, the University of Queensland and Macquarie University, Australia, and Nanyang Technological University, Singapore. A German professor wrote to us "You have made it possible to greatly reduce the cost of research engaged in quantum computing and quantum precision measurement, which is something that benefits all of humanity".

*What obstacles you encountered with and what was the way to overcome them?*

In the beginning, our management and market development ability were very inadequate, then we kept adjusting the promotion direction and upgrading the products. At that time, we met customers during the day and wrote code at night. Later, we found a top-ranking educational institution and sold more than 200,000 sets of our question-answering devices. With the increasing popularity of tablet devices, the function of this product was replaced, which led to its discontinuation. But in this process, our ability was enhanced and the relevant experience played an important role in the development of the diamond quantum computer for education. Now, this computer has gone into dozens of Chinese universities and high schools. It has also been recognized in global markets such as the United States and Australia. With over 100 units shipped worldwide, this is the largest number of quantum computing devices ever shipped.

Since the establishment of CIQTEK, obtaining excellently talented Staff has always been our top priority. We strive to create a "simple and sincere" corporate culture and have set up an evaluation mechanism for core talents with high technical capability . Those who are selected can get options that can be cashed in in the future. In addition, they will get at least three to five years of salary working here. Being open to talking about material benefits is one of our priorities regarding rewarding talent. When one's innovation ability is reflected in the material reward, he/she can concentrate on innovation wholeheartedly. Resisting temptation and guarding against arrogance and impatience, of course, needs to be borne in mind.

The development model of the scientific instrument industry is not like the business model of the internet, where a good idea and the introduction of capital, can immediately contribute to an explosive growth of the industry. We need to devote years and years to research, keep innovating, and truly become skilled "artisans" in order to create one instrument after another that will change industry. I am ready to fight for this for the next 30 or 40 years.

*What is your idea about the secret of business success?*

First, there must be a high-level entrepreneurial team. I was fortunate to meet excellent peers along the journey, such as our Vice President, Dr. Will Zhang, who has been my partner for 10 years, and another Vice President, Dony Feng, who was an executive in a petroleum instrument company and a senior engineer who received his undergraduate degree from Tsinghua University and obtained a double master's degree. There is no absolute right or wrong in the process of entrepreneurship, and sometimes it means decisions have to be made. Everyone in the team needs to complement each other so that one plus one is greater than two.

Then, it is important to focus on one area of development. The scientific instrument industry has emerged several "Fortune Global 500" companies, such as Thermo Fisher and Danaher. We plan to stick to our main business and do a good job with our instruments and services for researchers.

Lastly, I think we must insist on continuously creating value for our customers. We oppose low quality and low price and pursue the aim to provide high-quality products and services to our customers. We will continuously explore the internal potential and use all the resources at our disposal to bring value to our customers and provide them with more valuable services. At the same time, we will restrain the greed for profits, and not sacrifice long-term goals in pursuit of short-term goals.

*What is your message to the magnetic resonance community?*

Electron paramagnetic resonance technology is a very valuable scientific research method. In China, EPR spectrometers have achieved many world-recognised research results in the fields of physics, chemistry, materials science, life science, medicine, and environmental science. We are looking forward to further exchanges with international scholars in these research fields to continuously promote the development of EPR technology. Over the years, based on the profound technology accumulation and excellent spectrometer engineering capability in the field of EPR, CIQTEK has launched a full series of X-band and W-band EPR spectrometers, with customers covering the fields of physics, chemistry, materials, life science, and medicine, etc. The research topics involve structural analysis of transition metal complexes, chemical synthesis, in situ catalysis, polymers, magnetic materials, free radicals, etc. We are pleased to provide first-class products and services to world-wide l EPR specialists.

# Interview with Dr. Eugeny Kryukov, Head of Magnetic Resonance Department, Cryogenic Ltd

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

I received my PhD in NMR from Kazan State University, Kazan, Russia in 1997. My dissertation was about electron phase separation and charge stripes in high temperature superconductors. In 2002, I moved to the UK where I held three postdoc positions. The first position was at the University of Nottingham, where I was working on a brute force method to make high xenon nuclear polarization at millikelvin range temperatures and high magnetic field. This method was considered as a high production outcome of hyperpolarized gas for lung MRI. The second position was in Sheffield University where I developed hyperpolarized gas MRI and ultrafast echo MRI. The third position was at Warwick University where I studied liquid and solid state DNP. In 2011, I joined Cryogenic Ltd, London, UK and now work as Head of the Magnetic Resonance (MR) department where I work with Dr. Alexander Karabanov and Dr. Denis Langlais.

*How was the idea conceived to found Cryogenic?*

Cryogenic Ltd was started by Dr. Jeremy Good, who has over 50 years of experience in the design and manufacture of Cryogenic equipment for research, industrial and scientific applications. The company commenced trading in January 1992 and has since developed unique products, which have influenced research in the scientific community. This is because it made research into high magnetic fields and at cryogenic temperatures widely available around the world, as described below. The company has extended from just five people to 93 staff covering all aspects of design, manufacture and testing of the equipment produced. Sales are made to all corners of the world, and the company is fortunate to have staff of many nationalities who can support its wide customer base.

*What were the stages of the development of your company production?*

Cryogenic Ltd specialises in the production of superconducting magnets and their applications in research, science and industry. To retain its position as an elite market leader, Cryogenic Ltd has constantly developed its products and markets. The work in the eponymous field, the science of low temperatures, is world-leading and has seen rapid progress over the past 50 years. Historically, liquid helium has been an expensive consumable with scarce availability, although it was previously the only method of achieving the required low temperatures. Cryogenic pioneered the research and development of 'dry' systems that utilise mechanical refrigeration and do not require the purchase of liquid helium to cool down superconducting magnet systems. As a result, the demand for the company's products rapidly expanded and changed the scope of world-wide laboratory research. The company has applied its cryogen-free magnet technology in a broad range of applications, including magnetometry, X-ray and neutron scattering, NMR and EPR. 3D vector magnet systems, $^3$He and dilution refrigerator units for temperatures down to 30 mK are also produced for use in STM experiments.

In 2010, the company extended its business into the area of NMR. The production for EPR now consists of cryostats for use with resistive 2.5 T magnets for X- and Q-bands EPR, 6 T horizontal field magnets with integrated variable temperature insert (VTI) for W-band EPR and solenoids up to 18 Tesla.

The idea of an integrated VTI appeared to be very effective, where the same cryocooler is used for both applications: to cool the magnet to below 4 K and to control the sample temperature between 1.5 K and 400 K. The mechanism incorporates separated helium gas in a closed cycle configuration, circulated in the VTI by an oil-free pump. It is also convenient that cryogen-free magnets are always ready for field ramping, so the same magnet can be used at different static fields or in field sweep mode.

All Cryogenic systems are delivered with power supplies for the main magnets, shims and sweep coils. The company production is flexible so it can make solenoid magnets for higher fields (up to 18 T) or non-standard ▶

## Cryogenic Ltd

**Mission.** Cryogenic Ltd is the leading supplier of high field superconducting magnets and low temperature measurement systems which operate without liquid helium.
**Products.** Measurement systems with VSM, AC susceptibility, resistivity, Hall effect, heat capacity, thermal conductivity and Seebeck effect. / SQUID instruments for highly sensitive magnetometers and QHR metrology. / Research magnet systems with fields to 20 Tesla in NbSn and to 25 Tesla or more using HTS insert coils. / NMR, MRI and ESR magnets and systems including gradient coils, RF probes and consoles. / UHV beam-line target magnets and Neutron setting magnets. / Ultra low temperature $^3$He and DR systems to 10 mK with rotating platforms. / Low temperature platforms for STM and AFM systems to 30 mK.
**History.** Cryogenic Ltd commenced trading in January 1992 and won the DTI sponsored 'SMART' award in 1992, 1993 and 1998. As a result, the company developed unique products, which gained rapid applications in the scientific research community. Over the years Cryogenic have been world leaders in product innovation. These include our wide range of Cryogen-Free Magnet systems and Variable Temperature Inserts which are easy to operate and offer significant operational cost benefits. ●

magnets, for gyrotron or beamline applications, for instance.

Additionally, the company is manufacturing magnets for dissolution DNP, where with a more powerful pump used for the VTI a base sample temperature of 1.2 K can be achieved. The company is also making MRI magnets of various sizes, for applications ranging from head imaging down to small systems for preclinical research.

One of the recent developed products is the magnets for solid state magic angle spinning (MAS) NMR applications. The company developed a technique which allowed users to use our magnets at different static magnetic fields on a day to day basis, without compromising the resolution of the measurements. One side effect of the cryocoolers is the mechanical vibration that is converted into temporal magnetic field instability. Cryogenic studied and developed a technique to reduce the field instability down to the level of one part per billion (ppb), an acceptable level for most MAS NMR applications. Currently we offer a full MAS NMR systems up to 600 MHz.

*How could you characterize your interaction with your customers?*

Cryogenic Limited works closely with customers to implement new ideas and tailor our production to specific customer requirements. The total number of systems sold for MR applications worldwide is now close to 100, driven by an ongoing crisis of liquid helium unavailability which continues to fuel demand for cryogen-free technology.

*What are the plans of the Magnetic Resonance Department for the future development?*

The next logical step for the MR department will be to combine the high resolution MAS NMR magnet with an integrated VTI and use the circulating helium gas for both simultaneous sample cooling and sample magic angle spinning. This will extend the temperature range of the MAS NMR experiments and hopefully allow for greater sample rotation rate.

# IES Silver Medal in Physics/Materials Science 2022

## Marina Bennati

It was a great honor for me to receive the 2022 Silver Medal in Physics from the International EPR Society. This distinction was only possible thanks to many talented coworkers, students as well as outstanding collaborators, who contributed to my research work. My independent academic career started end of 2006 at the Max Planck Institute for Multidisciplinary Science (previous MPI for Biophysical Chemistry) and since then, my group and I have been developing and applying pulsed double resonance techniques at increasingly microwave frequencies and polarizing fields. Particularly two techniques have been in focus, ENDOR and dynamic nuclear polarization (DNP), which polarize and detect nuclear spins in the vicinity of paramagnetic centers. These two methods can profit from a strong synergy as they both utilize hyperfine interactions and gain in sensitivity and resolution at high magnetic fields. The direction has allowed us to implement shared high-frequency EPR and DNP instrumentation up to 263 GHz/9.4 Tesla.

Initially, my motivation for ENDOR emerged from studies of paramagnetic enzymes, particularly studies of the activation mechanism, subunit interactions and inhibition of ribonucleotide reductases (RNRs), which are important targets of cancer drugs. RNRs use a radical-based mechanism to catalyze the reduction of nucleotides into deoxynucleotides, the DNA building blocks in all living organisms. Using 94 GHz $^{2}H/^{1}H$ ENDOR we were able to elucidate the hydrogen bond network essential for subunits communication in *E. coli* RNR, the prototype for human RNR [1, 2]. Later on, we could detect water molecules hydrogen bonded to tyrosyl radical intermediates [3]. The tiny $^{17}O$ hyperfine coupling of water coordinated to amino acid radicals was resolved by a combination of 94 and 263 GHz $^{17}O$ ENDOR, where narrowing of the $^{17}O$ hyperfine central transition ($+1/2 \rightarrow -1/2$) at high fields played a key role. Recently we achieved an important milestone in elucidating the most puzzling step in the RNR activation mechanism, i.e. the radical transfer across two protein subunits. Here, two tyrosyl radicals were supposed to communicate via proton-coupled electron transfer (PCET) across the subunit interface. However, this communication remained elusive in all available X-ray and cryo-EM structures [4]. Using PELDOR spectroscopy, we first observed an unexpected displacement of one of the two tyrosines toward the subunit interface [5]. Subsequently, our long-standing collaborator J. Stubbe labelled this tyrosine with fluorine. Using 94 GHz $^{19}F$ ENDOR, we could measure the distance between the fluorinated tyrosine in one subunit, and the radical intermediate on the partner tyrosine in the second subunit. In contrast to other biophysical methods, ENDOR gave clear evidence for the superposition of a long (8 Å) and a short (3 Å) distance, consistent with a conformational change that allows for radical propagation [6].

The mentioned spectroscopic results wouldn't have been feasible without development and optimization of hardware and experimental design. Implementation of pulsed EPR and ENDOR in the quasi-optical regime (263 GHz/9.4 T) permitted us to considerably expand the information content and explore new phenomena [7]. Three intrinsic effects were observed so far in 263 GHz ENDOR spectra: 1) narrowing of ENDOR lines in orientation selected spectra, which uncovered hidden distributions of hyperfine couplings; 2) narrowing of central $^{17}O$ nuclear transition in the range of the ENDOR line width (<100 kHz); 3) resolution of chemical shift (CSA) tensors. Particularly, the 263 GHz $^{1}H$ spectra of the tyrosyl radical in *E. coli* RNR provided the basis to improve the analysis of high-frequency ENDOR data. Indeed, those spectra displayed broad features close to the baseline and raised the question about how to distinguish baseline distortions, due to hardware and RF heating, from real signal. The question was addressed in collaboration with the Department of Mathematics at Göttingen University and UCL London. We started a comprehensive statistical analysis of the ENDOR signal and presented a new processing method that circumvents spectral averaging, i.e. by storing each individual spectrum in a 2D matrix [8]. A mathematical model of the ENDOR signal allowed for a reconstruction of the most-likely signal, i.e. a separation of signal from baseline drifts during long acquisition times [8]. Moreover, modeling of the noise permitted to compute statistical uncertainties in the data points using the Bootstrap method. Application of the method unraveled a conformational distribution of the tyrosyl radical in *E. coli* RNR [9].

Also, the fluorine nucleus provided unique opportunities for high field EPR and ENDOR. The nucleus is rare in biological systems and possess a gyromagnetic ratio very close to the proton, from which the resonances can be resolved at 94 or 263 GHz. Using $^{19}F$, we were able to explore the accessible distance range in hyperfine spectroscopy, and demonstrated that the lower limit of PELDOR/DEER measurements can be complemented by ENDOR from about 0.5 to 1.5 nm [10]. In contrast to $^{19}F$ NMR, $^{19}F$ ENDOR takes advantage of the large electron spin polarization, thus offering larger sensitivity and selectivity. Interestingly, $^{19}F$ ENDOR spectra at 263 GHz/9.4 T unexpectedly appeared asymmetric. Simulations and careful referencing of the nuclear frequen-

cies showed that these features arise from the chemical shift anisotropy (CSA) of $^{19}$F, which is present also at 94 GHz/3.4 T, albeit to a much smaller extent. The CSA tensor parameters could be extracted from ENDOR and turned out well consistent with DFT predicted values and NMR data, thereby providing additional information about geometrical and electronic structure of the spin system [11].

My interest in ENDOR spectroscopy goes back to the time spent in the laboratory of Robert Griffin at MIT. There, I learned that ENDOR polarization transfer schemes are of great interest also for dynamic nuclear polarization. In one of our early studies, we utilized ENDOR to monitor electron depolarization that accompanies the build up of nuclear polarization in DNP [12]. The successful observation of cross-polarization between electrons and weakly coupled nuclear spins (called eNCP), motivated us to explore eNCP for stronger coupled nuclei, which are usually relevant in ENDOR. In collaboration with Shimon Vega and Ilya Kaminker we introduced a new ENDOR scheme, in which eNCP is used as initial polarization transfer step prior to a conventional pulse ENDOR read out [13]. We were able to analytically derive eNCP matching conditions and predict ENDOR intensities for a $I = 1/2$ and for a $I = 1$ nucleus, using single transition operator formalisms [14]. In collaboration with Steffen Glaser from the Technical University of Munich, we started implementing numerical simulation tools, based on the density operator formalism, to predict various polarization transfer schemes [14]. The tools will provide a framework to optimize ENDOR sequences and implement time-optimized sequences.

Finally, the synergy between EPR and NMR in studies of pulse polarization schemes led me to step into the neighbor field of dynamic nuclear polarization. However, this step wouldn't have been possible without the initial collaboration with Thomas Prisner and Peter Höfer, who shared with me this interest [15, 16]. DNP can significantly enhance NMR signals by transferring the higher spin polarization of a paramagnetic center to target nuclei of interest. Differently than in the solid state, DNP in liquids is based on cross-relaxation, where the correlation time modulates the hyperfine interaction on the order of the inverse of the electron Larmor frequency ($\omega_e\tau_c \approx 1$). Initial studies on $^1$H DNP in water and organic solvents demonstrated that $^1$H signal enhancements decrease considerably at high magnetic fields (≥1 Tesla) due to intrinsic dipolar relaxation dispersion [15, 16]. However, examination of the Overhauser equations suggested us that, under certain conditions, scalar (isotropic) hyperfine relaxation can lead to DNP effects almost independently of the external magnetic field. Screening of $^{13}$C DNP in liquid organic small molecules led us to the discovery of huge $^{13}$C signal enhancements (up to ~$10^3$) at magnetic fields of 3.4 Tesla [17]. Notably, signal acquisition time scales with the square of signal enhancement. Therefore, an enhancement of $10^3$ corresponds to a gain in signal acquisition time of $10^6$!

Relaxation theory provided a quantitative explanation for this observation [18]. Specifically, scalar relaxation requires modulation of an isotropic hyperfine interaction between the polarizer molecule and a $^{13}$C nucleus on a target molecule. This occurs via formation of a transient polarizer-target complex, in which a suited orbital overlap transfers unpaired spin density to the $^{13}$C nucleus. Such overlap can be modulated with correlation times on the sub-picosecond time scale, for instance via fast collisions in liquids. Calculations of coupling factors using suited spectral density functions for dipolar and scalar relaxation together with analysis of $^{13}$C relaxation dispersion indicated that these fast correlation times can reproduce the observed DNP enhancements. The time dependence of the scalar mechanism is substantially different than the one in the dipolar mechanism, as the latter is modulated by slower molecular diffusion (tens of ps to ns).

A more systematic study over a field range of 10 Tesla revealed that $^{13}$C NMR signal enhancements also strongly depend on the $^{13}$C chemical environment [19] and can be favoured by halogen atoms attached to the target $^{13}$C nucleus. Moreover, the structure and dynamics of the paramagnetic molecule have also substantial impact on the enhancements [20]. $^{13}$C enhancements were also observed in $^{13}CH_2$ and $^{13}CH_3$ groups at 9.4 Tesla. These enhancements of 20–30 represent a reduction in acquisition time on the order $10^2$–$10^3$, and open appealing perspectives for a broader application of liquid DNP. Following our reports at 3 and 9 Tesla, $^{13}$C signal enhancements up to two orders of magnitudes have been confirmed up to 14 Tesla ($^1$H 600 MHz) by other laboratories. Our goal is to examine possibilities to integrate DNP in routine liquid NMR, and thus contribute to the development of the next generation of combined EPR/NMR methods.

At the end of this brief article, I would like to thank again all fantastic and motivated people who have contributed to this work, particularly Dr. Igor Tkach as long-standing research scientist in my group, my present and former PhD students and postdocs, all my collaborators and mentors as well as my husband and my family. I hope that we will continue this exciting collaboration in future.

1. Argirevic T., Riplinger C., Stubbe J., Neese F., Bennati M. (2012), J. Am. Chem. Soc. 134, 17661–17670.
2. Nick T.U., Lee W., Koßmann S., Neese F., Stubbe J., Bennati M. (2015), J. Am. Chem. Soc. 137(1), 289–298.
3. Hecker F., Stubbe J., Bennati M. (2021), J. Am. Chem. Soc. 143, 7237–7241.
4. Greene B.L., Kang G., Cui C., Bennati M., Nocera D.G., Drennan C.L., Stubbe J. (2020), Annu. Rev. Biochem. 89, 45–75.

5. Kasanmascheff M., Lee W., Nick T., Stubbe J., Bennati M. (2016), Chem. Sci. 7, 2170–2178.
6. Meyer A., Kehl A., Cui C., Reichardt F.A.K., Hecker F., Funk L.-M., Gosh M.K., Pan K.-T., Urlaub H., Tittmann K., Stubbe J., Bennati M. (2022), J. Am. Chem. Soc. doi: 10.1021/jacs.2c02906
7. Tkach I., Bejenke I., Hecker F., Kehl A., Kasanmascheff M., Gromov I., Prisecaru I., Hoefer P., Hiller M., Bennati M. (2019), J. Magn. Reson. 303, 17–27.
8. Pokern Y., Eltzner B., Huckemann S.F., Beeken C., Stubbe J., Tkach I., Bennati M., Hiller M. (2021), Proc. Nat. Acad. Sci. 118, e2023615118.
9. Hiller M., Tkach I., Wiechers H., Eltzner B., Huckemann S., Pokern Y., Bennati M. (2021), Appl. Magn. Reson. doi.org/10.1007/s00723-021-01411-5.
10. Meyer A., Dechert S., Dey S., Höbartner C., Bennati M. (2020), Angew. Chem. Int. Ed. 59, 373–379.
11. Kehl A., Hiller M., Hecker F., Tkach I., Dechert S., Bennati M., Meyer A. (2021), J. Magn. Reson. 333, 107091.
12. Weis V., Bennati M., Rosay M., Griffin R. (2000), J. Chem. Phys. 113, 6795–6802.
13. Rizzato R., Kaminker I., Vega S., Bennati M. (2013), Mol. Phys. 111 (18-19), 2809–2823.
14. Bejenke I., Zeier R., Rizzato R., Glaser S., Bennati M. (2020), Mol. Phys. doi: 10.1080/00268976.2020.1763490.
15. Griesinger C., Bennati M., Vieth H.M., Luchinat C., Parigi G., Höfer P., Engelke F., Glaser S., Denysenkov V., Prisner T. (2012), Prog. Nucl. Magn. Reson. Spectrosc. 64, 4–28.
16. Höfer P., Parigi G., Luchinat C., Carl P., Guthausen G., Reese M., Carlomagno T., Griesinger C., Bennati M. (2008), J. Am. Chem. Soc. 130 (11), 3254–3255.
17. Liu G., Levien M., Karschin N., Parigi G., Luchinat C., Bennati M. (2017), Nature Chemistry 9 (7), 676–680.
18. Bennati M., Orlando T. (2019), eMagRes doi: 10.1002/9780470034590.emrstm1581
19. Orlando T., Dervisoglu R., Levien M., Tkach I., Prisner T.F., Andreas L., Denysenkov V.P., Bennati M. (2019), Angew. Chem. Int. Ed. 58 (5), 1402–1406.
20. Levien M., Reinhard M., Hiller M., Tkach I., Bennati M., Orlando T. (2021), Phys. Chem. Chem. Phys. 23 (8), 4480–4485.


# IES Fellowship 2022 Awarded to Professor Asako Kawamori

Prof. Asako Kawamori is awarded the IES Fellowship 2022 for her pioneering EPR works.

She obtained her PhD degree (1962) under Prof. Junkichi Itoh, Department of Physics, Osaka University (Japan). Prof. Ito (1924–2009) was a Japanese pioneer in magnetic resonance studies and was also a mentor for many Japanese magnetic resonance researchers in condensed matter physics. Dr. Kawamori's PhD thesis was 'the study of $^{35}Cl$ nuclear magnetic resonance in $NaClO_3$ crystal'. After she graduated from Osaka University, she obtained a position in the newly founded Faculty of Science, Kwansei Gakuin University (1962). Her early interest was in the properties of dielectric materials using magnetic resonance. She focused on the properties of Wurster's blue/copper acetate.

In the 1980s, she started biophysical studies. The main target was the function and structure of photosystem II, a protein complex involved in oxygen evolution. The reaction mechanism and structure of photosystem II were unknown. Prof. Kawamori investigated the magnetic structures of the oxygen-evolving complex using ENDOR/pulsed EPR techniques. She has determined the relative positions of the redox active components in photosystem II with various techniques such as traditional $T_1$ measurements, 2+1 method, hole-burning, etc. Her most impactful studies used electron-electron double resonance (PELDOR/DEER). Prof. Kawamori succeeded in the measurement of relative distances between redox components in photosystem II (1994). It was the first case of an application to biophysical studies, showing the validity of the PELDOR/DEER technique to the application of the protein structure. It gave pulsed EPR a new application in the field of biophysics.

In 2011, a group at Okayama University succeeded in solving the X-ray crystal structure of photosystem II, and the arrangement of the redox components obtained by Prof. Kawamori was extremely accurate.

After she retired from Kwansei Gakuin University in 2003, she founded the NPO Agape Kabutoyama Medical Research Institute in Nishinomiya (Japan). She applied the new application of the EPR method to the medical field. She has been working on the advancement of magnetic resonance in physics, chemistry, biophysics and humans. Even at 70 years old, her passion for the new methodology was still very high. After her retirement, the Institute was closed (2015).

Prof. Kawamori is currently living in a facility for the elderly. She enjoys her new life. The facility is now strongly restricting visitors because of COVID-19, and so we only connect by phone. Maybe the pandemic will soon be over, and so we are looking forward to seeing her in person soon!

Hiroyuki Mino

# Interview with Dr. Asif Equbal on the Occasion of His John Weil Young Investigator Award 2022

**EPR newsletter:** *Dear Dr. Equbal, on behalf of the readers of the EPR newsletter we congratulate you on your John Weil Young Investigator Award 2022. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I didn't know much about science and research until I got into my undergraduate college. I grew up in India, in a city famous for its steel factory, where most of the people around me were engineers. I admired them and aspired to become one myself. In India, 2.5 million students take the Joint Entrance Examination (JEE) for engineering colleges every year, and only less than 10,000 are selected for the top colleges. I was selected, but I didn't get the computer science or electronics major I wanted. Retrospectively, I am happy that I didn't.

That same year, the Indian government established the Indian Institute of Science Education and Research (IISER) in Mohali, a premier science institute that attracted students from across the JEE qualified pool to consider a career in science. I had the choice of choosing other engineering disciplines or pursuing a BS-MS dual degree in basic science at IISER with full scholarships and monthly stipends.

I chose science over engineering, perhaps because the free tuition and monthly stipends appealed to me at the time. My parents and family friends were concerned about my decision because they had no idea what prospects a basic science degree offered. In a developing country like India, there are limited opportunities in non-technical disciplines like science. Reluctantly, my parents allowed me to join the science program almost two weeks after the semester had started. Our BS-MS curriculum at IISER was unique in that it included both education and research elements. Half of the program was focused on active research from day one. I enjoyed going to the lab, sometimes at midnight to check on cell growth, or sitting in a dark room for hours to align a laser and watch diffraction and interference patterns. I realized that science is a great career choice for curious and persistent people who want to satisfy their curiosity. Plus, you get paid to understand the world you live in, and you have the opportunity to travel the world. Science is more global than any other profession in this world. Even though I may have chosen science accidently, I can't imagine a better profession than this for myself.

*Who introduced you into magnetic resonance?*

I was introduced to magnetic resonance by Professor Ramesh Ramachandran, who was previously a researcher in Bob Griffin's lab at MIT. It was during my summer internship in his lab that he and members of his lab (RVS Rao and Zeba Qadri) taught me basic theoretical concepts of magnetic resonance. Later, I had the opportunity to do my master project at ETH Zurich, in the laboratory of Matthias Ernst, Beat Meier and Nobel laureate Richard Ernst. I worked on a very complicated project to select a particular coherence transfer pathway while attenuating all other pathways in order to precisely measure weak (long-range) interactions between heteroatoms in a protein molecule. Although the problem remains unsolved to this day, it was a great opportunity for me to learn Floquet theory and experimental magic angle spinning NMR, powerful tools that I still use in my research. What fascinated me the most was realizing that designing a magnetic resonance pulse sequence is like playing with lego blocks. Subsequently, I did my PhD on solid-state NMR in the lab of Prof. Niels Chr Nielsen in Denmark, and then moved to the US as a postdoctoral fellow to explore nuclear spin hyperpolarization in the lab of Prof. Songi Han. I also had the chance to work with many other prominent researchers, including Professor P K Madhu and Professor Shimon Vega.

*What is your current research topic?*

My current research is on development of Dynamic Nuclear Polarization which is a technique to potentially increase NMR sensitivity by orders of magnitude. Using DNP it's possible to measure NMR spectrum in a few minutes which otherwise might take days or even months. However the practically achieved goals of DNP is far below its full potential. My focus has been to understand the working mechanism of DNP. One of the major challenges is the lack of insight into the dynamics of electron spins which are the source of DNP. EPR is the best tool to understand electron spin dynamics. It's ironic that NMR and EPR are fundamentally the same yet there is very little exchange of ideas

between the two research communities. I was privileged to have done my postdoc in the lab of Prof. Songi Han who has a unique dual NMR-EPR instrument. I have been working on understanding and development of DNP using pulsed EPR measurements under the DNP condition. Lately I have explored photochemistry of organic chromophores in the lab of Prof. Michael Wasielewski at Northwestern University, Chicago. Chromophores are great candidates not just for opto-electronics but also room temperature DNP for bio-medical imaging which has remained a challenge with conventional persistent-radical based DNP.

*What is your strength and weakness in magnetic resonance?*

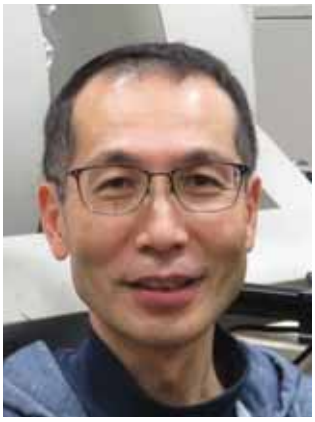
I think my greatest strength is the rigorous education and research training I have acquired, from the analytical theory of solid state NMR (with Professors Shimon Vega and Matthias Ernst) to numerical simulations (with Niels Chr. Nielsen and Thomas Vosegaard), through the magic angle rotation experiment (with P K Madhu), then the theory and instrumentation of nuclear hyperpolarization and pulsed EPR (with Songi Han) and, more recently, light-activated EPR (with Michael Wasielewski). The learning experience over the past ten years has been incredible. It will help me tremendously in developing quantum materials using integrated optical magnetic resonance spectroscopy that I am aiming for next.

My weakness is that I have not been able to read the older books and literature on magnetic resonance, mainly because of lack of time, but also because of the complexity of their writing style, which is different from todays. They contain many hidden treasures that were not explored in the past because the necessary technology was lacking, but which can now be explored thanks to advanced high power radio frequency, microwave and cryogenic technologies. The most striking example is the DNP, which was conceived in the 1950s but was not put into practice until the early 2000s.

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

If I were to suggest something to the younger generation, it would be to spend enough time learning the basics of magnetic resonance, especially from the perspective of spin physics. This may seem daunting, but persistence is the key. The learning curve for MR is steeper than for other spectroscopic tools, but once it is mastered, it can be applied in many fields, whether it is for characterizing and designing new materials, studying biomolecular dynamics, developing new quantum technologies, or even fundamentally understanding the subatomic world. Having an interdisciplinary approach to research will greatly contribute to a successful career in academia or even industry related to magnetic resonance.

# SEST Award 2021



Tadaaki Ikoma
Institute of Science and Technology,
Niigata University, Niigata, Japan

I am greatly honoured to have received the 2021 SEST award for my work entitled "Magnetic Structure and Spin Dynamics of Excited States in Molecular Materials". This research has been carried out not only with my colleagues, who are Prof. S. Tero-Kubota and Prof. K. Akiyama at Tohoku University and Prof. T. Miura, Dr. Y. Wakikawa, Prof. C. Tsai, Prof. W. Jia and Prof. J. H. Jorolan at Niigata University, and many students at Niigata University but also with a lot of external collaborators. This award was a good opportunity for me to reflect on the progress of my research. With the motto "Toward Control from Observation", I had intended to conduct research involving electron spins, but I sometimes realized that things were not progressing as originaly planned. While keenly aware of my own inadequacy, I was fortunate enough to change and expand my study, guided by the unexpected results obtained through some joint research. I deeply appreciate those who have reseached together. I have mainly been studying on three topics of molecular materials, which are Photogenerated Electron-hole (E-h) Pairs, Triplet Harvesting and Organic Solar Cells (OSC), by using multi-frequency/time-resolved ESR spectroscopy and measuring various electrical/optical responses due to the external magnetic field.

**a) Photogenerated E-h Pairs.** In this project which were mostly done at Tohoku Univ., I investigated carrier generation in photoconductive polyvinylcarbazole (PVCz) thin films doped with electron acceptors. By using the time-resolved ESR method, we have succeeded in directly observing photogenerated e-h pairs for the first time. The detected e-h pair is spin polarized trapped pair formed by an electron (e) held at the electron acceptor and a hole (h) captured by trap site of PVCz during the photocarrier generation process. The spin polarization mechanism of trapped e-h pairs was clarified by multi-frequency ESR experiments. Tunnel recombination of the trapped e-h pairs was elucidated by the observed time depednece of spin polarization. In addition, by investigating the photocarrier generation in PVCz thin films from magnetoconductance and magnetoluminescence, it was shown that free carriers are generated by stepwise hole migration. In this research project, we were also able to report new optoelectronic properties of organic semiconductors such as giant magnetoconductance effect and low-field magnetoluminescence effect. Currently, we are studying the dynamics of various spin pairs generated by carrier transport by simultaneous optical and electrical detection (SOED) at Niigata University. Encounter with Prof. K. Okada of Osaka City University oriented my knowledge of the spin dynamics of photogenerated e-h pairs in organic solids toward a challenge to lengthen the lifetime of charge-separated (CS) state, which is an important issue for artificial photosynthesis. Using a ternary compound in which an electron-donar (D) and an electron-acceptor (A) are combined with a platinum complex, we attempted to extend the lifetime of the CS state by utilizing the electron transfer from the lowest excited triplet ($T_1$) state. By controlling the effects of external magnetic fields and molecular motions on electron spin dynamics, we were able to significantly increase the formation yield and decay lifetime of the CS state.

**b) Triplet Harvesting.** The triplet harvesting, meaning effective utilization of the $T_1$ state, is an important point for improving the efficiency of organic electroluminescent diodes (OLEDs). Therefore, we worked on the triplet harvesting

with a view to OLED applications. Prof. T. Fukushima of Tokyo Institute of Technology gave me a chance to study on the $T_1$ state of a four-membered ring boron nitride (BN) compound that is an isoelectronic compound of cyclobutadiene. We found that his molecule emits blue phosphorescence in fluid solutions at room temperature despite the absence of heavy atoms. A key mechanism for the room-temperature blue phosphorescence was the spin-orbit interaction of the nitrogen nuclei. The energy difference between the $\sigma$ orbital of the BN bonds and the lone pair orbitals of the N atoms is reduced by the hyperconjugation with substituents and the large electronegativity of nitrogen. This small energy gap makes the spin-orbit interaction on the nitrogen nuclei effective. I also studied on the $T_1$ state of a compound showing thermally activated delayed fluorescence (TADF), which is caused by the reverse intersystem crossing to the lowest excited singlet ($S_1$) state from the $T_1$ state at room temperature. Introduction of TADF by Mr. Ogiwara, who often visited my lab for a joint research with a company, was the first for me to know TADF. We found that some of TADF molecules undergo the forward intersystem crossing by not only the spin-orbit but also the hyperfine interactions. We are currently studying the effect of the conformation between the D and A in TADF molecules on the intersystem crossing. Once Prof. F. Ito of Shinshu University visited me to show photon upconversion emission by triplet fusion, in which two $T_1$ molecules merge their electronic energies to produce a single $S_1$ molecule. His demonstration of the photon upconversion that can be useful for the triplet harvesting led to my study of triplet fusion using triplet sensitization. We elucidated that the reaction efficiency of triplet fusion depends on the spin dynamics as well as the spin statistics in the transition state regime. Recently we descovered a simple aqueous system showing the photon upconversion with an extremely low threshhold energy and detected triplet-triplet pair corresponding to the activated complex. Currently we are working on control of the triplet fusion based on spin manipulation of the active complexes.

**c) OSC.** Because I have always been interested in photovoltaic effect from a viewpoint of application of photoredox reaction, I could luckily participate in a joint research project of OSC organized by Prof. H. Yamada of Nara Institute of Science and Technology. In this project, I was in charge of development of a new operando measurement method based on the magnetoconductance effect for detecting the spin-selective charge recombination at the p/n-junction area, which is known as one of main factors decreasing the energy conversion efficiency of OSC. Using a Pentacene|$C_{60}$ single-junction OSC, we could quantitatively clarify the trapping/detrapping process of exciton-carrier pairs in the charge transport layer and the singlet fission in the pentacene layer as well as the charge recombination. Furthermore, we elucidated a drastic change of the spin-selectivity in the charge recombination in P3HT:PCBM bulk heterojunction OSC, which is understood by the reorganization energy depending on the fullerene structure of PCBM. We continue this OSC project studying the exciton and carrier dynamics by means of the SOED and the magnetoimpedance measurement.

# SEST Young Investigator Award 2021

Hiroki Nagashima
Department of Chemistry, Graduate School of Science and Engineering, Saitama University, Saitama, Japan

I am honored to have been awarded the SEST Young Investigator Award 2021 for my work entitled "Distance Measurements between Spins and Elucidation of Structures Surrounding Electron Spin by Electron Spin Resonance". This includes my Ph.D. research which focused on photosynthesis at Nagoya University supervised by Prof. Hiroyuki Mino and my postdoctoral research that focused on singlet fission at Kobe University supervised by Prof. Yasuhiro Kobori. I am also grateful to all collaborators in the Prof. Jian-Ren Shen group at Okayama University, Prof. Hiroshi Ikeda group at Osaka Prefecture University (now, Osaka Metropolitan University), and Prof. Taku Hasobe Group at Keio University.

Reaction intermediates are the most important states for understanding chemical reactions. In addition, some chemical reactions, charge recombination for example, reflect their magnetic properties. My interest in these projects is characterizing the magnetic and geometric structure of intermediate states of water oxidation of manganese (Mn) clusters in photosystem II and singlet fission using EPR.

Higher plants and cyanobacteria produce oxygen and carbohydrates from water and carbon dioxide through photosynthesis. The Mn cluster in the photosystem II protein complex of the thylakoid membrane is a catalyst for water splitting and oxygen evolution in photosynthesis. When the reaction center in photosystem II is excited by absorption of a photon, an electron transfer occurs and oxidizes the Mn cluster via a tyrosine residue ($Y_Z$). The Mn cluster has five different redox states ($S_0$–$S_4$) during the water oxidation cycle. The most stable $S_1$ state structure was revealed by X-ray crystallography with 1.9 Å resolution [1]. However, hydrogen bond structures surrounding Mn cluster was unclear. Thus, we performed electron nuclear double resonance (ENDOR) spectroscopy on the $S_2$ state Mn cluster to detect hydrogen-bond structures. To characterize the geometry, I made an oriented Photosystem II membrane sample [2] and measured the orientation dependence. The obtained ENDOR spectra were analyzed based on the X-ray crystal structure [3]. The assignments were also confirmed by $Ca^{2+}$-depletion and $Ca^{2+}/Sr^{2+}$-substitutions. It was concluded that the roles of $Ca^{2+}$ involve the maintenance of the hydrogen bond network near the $Ca^{2+}$ site and the electron transfer pathway between Mn cluster and $Y_Z$ [4]. Additionally, the methanol binding site, which was thought to compete with water molecules bound to the Mn cluster, were clarified by the $^1$H-ENDOR spectroscopy [5]. These results are key to discuss how the Mn cluster generate O=O bond formation, deprotonate water molecules, and release protons outside of photosystem II.

After I received my Ph.D., I moved to Kobe University and started a project on singlet fission reactions. Singlet fission, which generates two triplet excitons (TT) from one photon, enables the theoretical limit of the photovoltaic

efficiency to be exceeded [6]. We found singlet fission occurs in 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-pentacene) aggregates in frozen solution. Singlet-fission-born quintet state $^5(TT)$ excitons were observed by time-resolved EPR spectroscopy. Existence of the quintet state was proven by a spin nutation experiment. The time-resolved EPR (TREPR) spectra were asymmetric due to the strong absorption signals and weak emission signals. They are different with previous reports for covalently linked TIPS-pentacene dimers and TIPS-tetracene thin films, in which the $^5(TT)_0$ state is populated by $^1(TT)$-$^5(TT)_0$ mixing [7, 8]. Spin nutation experiments revealed that there are not only $^5(TT)_0 \leftrightarrow {}^5(TT)_{\pm1}$, but also $^5(TT)_{\pm2} \leftrightarrow {}^5(TT)_{\pm1}$ transitions. TREPR spectra were well reproduced by spectral simulations assuming preferentially populated lower sublevels of quintet states $^5(TT)_{-1}$ and $^5(TT)_{-2}$ and ignorable populations in higher sublevels $^5(TT)_{+1}$ and $^5(TT)_{+2}$. The molecular geometry of two pentacene molecules forming multiexcitons were determined from the Euler angles of the magnetic parameters. We suggested that sublevel selective spin conversion occurred during the triplet-exciton diffusions within geminate multiexcitons. These findings for the quintet generations show a strong impact of coexistence of molecularly ordered 'hot spot' and disordered regions for the exergonic SQ mixings driven by entropy [9].

I am currently studying the structure and dynamics of radical pairs in proteins related to the field effect, which is thought to be involved in the magnetoreception of migratory birds. I am developing a reaction yield detected magnetic resonance (RYDMR) system combined with the conventional pulsed EPR system to control spin-dependent reactions using local optimization theory to understand the structure and dynamics of intermediate species more precisely [10].


1. Umena, Y., et al., *Nature* (2011)
2. Asada, M., et al., *Biochim. Biophys. Acta* (2013)
3. Nagashima, H.; Mino, H., *Biochim. Biophys. Acta* (2013)
4. Nagashima, H., et al., *J. Biol. Chem.* (2015)
5. Nagashima, H.; Mino, H., *J. Phys. Chem. Lett.* (2017)
6. Smith, M. B.; Michl, J., *Chem. Rev.* (2010)
7. Tayebjee, M. J. Y., et al., *Nat. Phys.* (2017)
8. Weiss, L. R., et al., *Nat. Phys.* (2017)
9. Nagashima, H., et al., *J. Phys. Chem. Lett.* (2018)
10. Masuzawa, K., et al., *J. Chem. Phys.* (2020)


# SEST Young Investigator Award 2021


Yusuke Wakikawa
Shizuoka Institute of Science and Technology, Fukuroi, Shizuoka, Japan


I am very honored to receive the Young Investigator Award from the Society of Electron Spin Science and Technology (SEST) for my research entitled "Spin Dynamics of Charge Carriers and Excitons in Organic Semiconductor Materials and Devices". I would like to thank the SEST committees for this award and the International EPR Society for providing me with this opportunity to present my research.

Electronic devices composed of organic semiconductor materials are less expensive and more flexible than devices based on conventional inorganic semiconductors. The performance of organic electronic devices is influenced by the crucial elementary processes of spin-dependent charge-carrier generation and transport that occur in the device. Free carriers are mainly lost through spin-dependent recombination in Coulombic-bound electron–hole (e–h) pairs formed by an interaction between two carriers with opposite charges. Therefore, it is important to evaluate these elementary processes under operating conditions to facilitate the development of materials and devices. To investigate the spin-dependent processes in organic semiconductor materials, we used magnetoconduction (MC) and electrically detected magnetic resonance (EDMR) techniques, which measure changes in conductivity owing to external magnetic fields and electron spin resonance, respectively. I would like to present studies on carrier recombination in thin films of supramolecular-assemblies [1–4] and organic optoelectronic devices [5, 6].

The recombination processes in the charge-carrier generation and transport in supramolecular assemblies of hexabenzocoronene and oligothiophene, two promising next-generation solar cell materials, were investigated [1–4]. The MC effects in supramolecular thin films were investigated, and it was found that nano-controlled donor-acceptor junction structures completely suppressed recombination during charge-carrier generation. Additionally, it was demonstrated that the structure of the supramolecular assemblies provides a shallow trap, which is favorable for charge-carrier transport [4].

Combining EDMR and capacitively detected magnetic resonance (CDMR), the recombination of photogenerated carriers in devices composed of regioregular poly(3-hexylthiophene-2,5-diyl) (P3HT) was investigated [5]. The EDMR and CDMR spectra owing to the e–h pair, a precursor for recombination, were observed. The modulation frequency dependencies of EDMR and CDMR revealed the rapid recombination of free carriers in the bulk P3HT film and the slow one of space charges at the Schottky junction between P3HT and an aluminum electrode. The space-charge recombination is responsible for photocurrent enhancement. These findings for amorphous organic solids will contribute to the development of technologies for optoelectronic devices.


For this award, I would like to express my deepest gratitude to Prof. Tadaaki Ikoma of Niigata University for his guidance during the research study and to my collaborators for their kind support. Furthermore, I am very grateful to my wife and children for their unconditional support.



1. Y. Wakikawa, T. Ikoma, Y. Yamamoto, T. Fukushima and T. Aida, Synthetic Metals, 160, 275–279, 2010.
2. S. Yagai, T. Seki, H. Murayama, Y. Wakikawa, T. Ikoma, Y. Kikkawa, T. Karatsu, A. Kitamura, Y. Honsho and S. Seki, Small, 6, 2731–2740, 2010.
3. Y. Wakikawa, T. Ikoma, Y. Yamamoto, T. Fukushima, T. Aida, and K. Akiyama, J. Phys. Chem. C, 117, 15295–15305, 2013.
4. Y. Wakikawa, T. Ikoma, Y. Yamamoto, T. Fukushima and K. Akiyama, ACS Omega, 2, 3260–3266, 2017.
5. Y. Wakikawa, and T. Ikoma, J. Phys. Chem. C, 124, 19945–19952, 2020.
6. Y. Wakikawa, and T. Ikoma, J. Phys. Chem. C, 125, 26613-26618, 2021.

# Interview with Dr. Katherine Richardson on the Occasion of Her IES Best Paper Award 2022

**EPR newsletter:** *Dear Dr. Richardson, on behalf of the readers of the EPR newsletter we congratulate you on your IES Best Paper Award 2022. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I have always relished logic, reasoning and solving puzzles therefore, while I was growing up I was drawn to studying Mathematics. By the time I came to choosing my undergraduate degree I had become increasingly interested in what felt like a more practical, hands-on way of applying problem solving to the real world, science. To keep my options open I chose a degree in Natural Sciences at UCL, which allowed me to pick courses from various departments. This provided a solid interdisciplinary foundation for my career. I have also always enjoyed the notion that in studying science I can prove myself right, or indeed wrong!

*Who introduced you into magnetic resonance?*

Dr. Maxie Roessler introduced me to the power of EPR spectroscopy. Although I had fleetingly come across both EPR and NMR during my undergraduate degree, I did not know the wealth of information it is possible to gain about biological systems using such techniques. During my PhD under Maxie's supervision, I learnt how EPR techniques can provide mechanistic and structural information about enzymes. In particular, those which transfer single electrons in the essential reactions which sustain life. I learnt a wealth of techniques that can be used to understand the chemistry and physics underlying biological processes, and the unique information EPR spectroscopy can provide in the study of respiration and photosynthesis. I was immediately fascinated by the complexity of EPR spectrometers and have taken great pleasure in learning how they work.

*What are your main interests of work in magnetic resonance?*

My main interest is in applying EPR techniques to the study of bioenergetic processes which balance and optimise photosynthesis, and understanding the physics that underpins them. I am curious about the development of EPR based methods and technology which are capable of studying the often unstable, fleeting or low concentration samples obtained from biological materials. I am always looking for ways to exploit the ability of EPR spectroscopy to answer interesting and fundamental questions about electron transfer within proteins that cannot be provided by other techniques.

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

I have found that some of the best ideas and breakthroughs come from learning from different disciplines or research areas. I would recommend listening to talks and attending conferences, even if you are not sure they are directly relevant to your work. You never know what you will learn or who you might meet. Discuss and collaborate with other members of the community and engage with their science, you may find insights you would not come across otherwise, or an exciting new application for your research.

Maxie Roessler:

Katherine came to us (to me and my then colleague and now collaborator Guy Hanke) with the perhaps more unusual path of having worked as a technician in the protein production facility at Queen Mary University (QMUL) for a couple of years before starting her PhD on the highly competitive London Interdisciplinary Doctoral Training programme. It turned out that her strong background – perhaps more accurately affinity for and agility with – proteins, combined with her chemistry studies as part of her undergraduate natural sciences degree at UCL, were instrumental to Katherine's success during her PhD. She truly rose to the challenges of a very interdisciplinary project: making photosynthetic complex I (the enzyme Katherine worked on) from scratch – with no established procedure in either my or Guy's lab – is no mean task in itself, but working with tiny quantities to get the enzyme into the right state and then performing pulse EPR experiments is quite another achievement.

Katherine did all this in a highly delocalised state (truly embracing the delocalised iron-sulfur cluster spin centres she worked with!) between QMUL, Imperial College (where I moved to in the first year of her PhD) and University College (UCL). At QMUL, she effectively became in charge of the EPR instruments there and the to-go-to authority when anything went wrong or required fixing. At UCL, in John Morton's lab, she worked with cryogenic preamplifiers to tease out the DEER traces at the spectral 'edges', achieving a signal-to-noise ratio that made is possible to interpret the data reliably. This work was instrumental to Katherine piecing together the energetics of electron transfer in photosynthetic complex I that ultimately led to her best paper award.

Besides having been the one to approach for everything to do with proteins for all my group members, Katherine taught me a lot about photosynthesis, and that it is possible to determine (with much determination!) the magnetic parameters of different iron-sulfur clusters whose spectra all overlap and whose relaxation properties and reduction potentials are very similar. She has left us with many interesting leads to follow up on and has opened up a new research direction in my group. I am sure that she will continue to thrive working on a different photosynthetic enzyme in Sheffield now – and I am delighted to see that she is still making use of EPR in her work!

# IES Poster Prize at the 2022 RSC meeting St. Andrews

Orit Nir-Arad:

I'm honored to receive the IES poster prize at the RSC meeting this year for my part in the design and construction of a 14 Tesla DNP/EPR spectrometer for the investigation of Dynamic Nuclear Polarization (DNP), at Dr. Ilia Kaminker's group at Tel-Aviv University. I also had the honor to be invited to give a talk about my work at the International Virtual EPR Meeting.

I joined the group two years ago, as a research assistant, during my undergraduate degree in chemistry. I continued my work at the group as a Ph.D. student in Physical Chemistry, in the direct Ph.D. track, earlier this year, after completing my B.Sc. Summa cum Laude.

The group research is centered around the development of new DNP methods. One of the core projects in the group aims at understanding DNP mechanisms from the electron spin perspective. DNP has been a rapidly developing field in the past two decades due to its potential to enhance Nuclear Magnetic Resonance (NMR) signals by orders of magnitude, allowing for experimental time savings of up to four orders of magnitude, thus completely transforming the field. DNP relies on polarization transfer from electron spins to nuclear spins. To maximize the benefits of DNP experiments, they must be performed at high magnetic fields to achieve the resolution expected from modern NMR experiments.

Polarization transfer is a complex quantum mechanical process, a detailed understanding thereof is a prerequisite for the rational design of improved DNP experiments. 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, $T_1$ and $T_2$ relaxation times, and electron spectral diffusion rate are field and temperature dependent, it is necessary to perform the EPR measurements at the DNP conditions – high magnetic field and low temperature.

Such EPR measurements require dedicated instrumentation. During the past three years, such an instrument has been built in our group. The dual DNP (NMR) / EPR instrument allows for EPR and DNP (NMR) experiments at 14 Tesla (400 GHz) and 8–300 K.

In my poster, I showcased the CW-EPR capabilities at 14 Tesla and the full temperature range available for our system. I presented the latest configuration of the spectrometer as well as some of the developments we made during the two years since I joined the group. The spectrometer allows for the acquisition of frequency and field-swept EPR spectra at 400 GHz, which I demonstrated using samples of P1 centers in diamond, BDPA in polystyrene, and $Li_2ZnGeO_4$ doped with $Mn^{2+}$, from Dr. Michal Leskes's group at the Weizmann Institute of Science in Rehovot, Israel.

The spectrometer is built around a 14 T cryo-free magnet with 1 ppm field homogeneity. It is equipped with 7 shim coils and a sweep coil and is well-suited for both EPR and solid-state NMR experiments. Our spectrometer combines a 400 GHz amplifier multiplication chain transmitter (from Virginia Diodes Inc.), a quasi-optical (QO) bridge with induction mode EPR detection (using Bridge12 components), and a phase-sensitive superheterodyne receiver (home built). All of the different components of the spectrometer are controlled by SpecMan4EPR software, created and maintained by Dr. Boris Epel. The unique feature of our spectrometer is the position of the QO bridge below the magnet with 400 GHz radiation transmitted through the specially designed windows at the bottom of the cryostat. This allows for a reduced heat load on the cryostat, ample space in the probe for the DNP RF circuitry, and rapid sample exchange. I showed our CW-EPR probe, designed in collaboration with Bridge12. The probe allows for a fast sample exchange at cryogenic temperatures. We showed that the temperature stabilizes within ~ 15 min upon sample exchange at 10 K.

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 lastly my Ph.D. supervisor Dr. Ilia Kaminker.

Ilia Kaminker:

I first met Orit when she took the General Chemistry II course as a first-year undergraduate student. (Sometimes it is worth teaching those first-year courses). She immediately stood out from the crowd as an exceptional student. At the end of Orit's first undergraduate year, I offered her to join my group as an undergraduate research assistant. She has been a central figure in the group since then. After completing her undergraduate studies in chemistry with all possible distinctions, last year she started her PhD in the direct PhD track, becoming my first graduate student.

The 14 Tesla EPR / DNP spectrometer in my laboratory is a complex, home-built instrument consisting of multiple components by various manufacturers assembled on-site. Orit was involved in all stages of the equipment assembly, installation, calibration and setting, and in running the experiments. This was especially challenging during the COVID-19 pandemic, as with no international travel we had to perform all installations ourselves without any technicians on-site.

The 2022 RSC ESR group meeting, during which Orit received the IES poster prize for her work on 14 Tesla EPR instrumentation, was the first international conference she attended. This fall, Orit was selected to participate in the prestigious Ariane De Rothschild Women Doctoral Program for which only four PhD students are selected every year across all disciplines on campus. I am looking forward to continue working with Orit for the remainder of her PhD and watching her becoming a brilliant independent scientist.

# IES Poster Prize at the 2022 Rocky Mountain Conference

Cooper Selco:

For EPR spectroscopy and many other experiments in quantum information science, it is essential to understand how a spin of interest behaves and how its behavior changes over time by interacting with surrounding environments. However, the understanding of the dynamics through a direct measurement of the spin and an analysis using a many-body system model can be very challenging because there are various types of couplings between the spin and its environments, and the measurement of those dynamics is usually done under temporal, spatial and ensemble averaging. Therefore, we often employ a statistical model to extract the spin dynamics from the measurement result with averaging. There are two types of statistical processes for spin dynamics: Markovian and non-Markovian processes. A Markovian process is a process in which future outcomes are predicted based only on the current state. In other words, knowing the current state holds the same predictive power as knowing the system's full history. Such processes are said to be "memoryless" since one does not need a memory of previous system states to predict future states. For example, gambling can be considered a Markovian process, since your chances of winning only depend on the cards you currently hold and does not depend on past hands (if the deck is shuffled). On the other hand, a non-Markovian process is one that is not Markovian, i.e., one where future outcomes depend not only on the current state but on past states as well. Such processes are said to have "memory effects" since a memory of previous system states is needed to have full predictive power. For example, suppose there is a jar that contains two red marbles and one blue marble. In one case, a marble is removed from the jar that you are not allowed to see. Then, you remove a marble yourself which is red. You are then asked, what is the probability that the last marble in the jar is blue. The best you can say is one-half. However, if you are allowed access to what the color was of the first marble that was removed (say, red) then you can say with certainty that the last marble left in the jar is blue. In this case, the probability that the last marble is blue depends not only on information of the current state (the most recent marble that was removed), but on the entire history of all past states as well. Therefore, it is non-Markovian. Another way to see this is that knowing information of previous states allowed for more predictive power, which means the process is non-Markovian.

In quantum physics, we often study only a small part of a much larger system. For example, if we study optically addressable spin qubits in diamond, we can only experimentally probe the qubit and cannot directly observe interactions between the qubit and the environment. Qubits coupled to a large number of other quantum particles are called open quantum systems, where the qubit is referred to as "the system" and the environment is referred to as "the bath". It would be infeasible to write down all the microscopic interactions between the system and the bath. So, physicists develop models to try to reproduce and explain the coupling between the system and the bath that is observed in experiments. To model system-bath interactions physicists most often use Markovian models, where the spin-bath dynamics only depend on the current state of the system. However, it is possible for non-Markovian effects to be present in open quantum systems. In this case, one would need a non-Markovian model to accurately predict and understand the spin-bath dynamics. Such models are said to include "memory effects" coming from the bath since the bath retains a memory of previous system states.

The nitrogen vacancy (NV) center in diamond consists of a single substitutional nitrogen impurity next to a vacancy defect in the diamond lattice. Single NV centers can be optically initialized and readout with a high degree of quantum control at room temperature. They are ideal candidates for quantum sensing applications due to their long coherence times and high sensitivity to external magnetic fields.

In this project, we are working on techniques to experimentally probe the non-Markovian spin-bath dynamics present in single NV centers in diamond. We study NV centers in both type-Ib and type-IIa diamond crystals where dipolar interactions are dominated by nitrogen electron spins and $^{13}C$ nuclei respectively. We perform optically detected magnetic resonance experiments to study the spin-dynamics of the NV center under the influence of different environmental spin-baths. To model and understand the spin-bath dynamics, we use the post-Markovian master equation (PMME). In this equation, the time derivative of the system density matrix is given by an integral over past system states. Since the current spin-bath dynamics depend on previous system states, the PMME is non-Markovian and captures memory effects coming from the bath. We can further probe the non-Markovian dynamics by calculating the trace-norm distance between two different initial states. The trace-norm distance is a quantity which represents the amount of information that is known about the system. In the non-Markovian case, since the bath has a memory for retaining information about previous system states, we can use the trace-norm distance to calculate the information present in the system and see if there is any information backflow between the system and the bath.

For pulsed electron paramagnetic resonance spectroscopy and many other experiments in quantum information science, it is essential to protect quantum coherence from environmental decoherence sources. Non-Markovian environmental bath dynamics can present a perspective for understanding and combating quantum decoherence. Furthermore, non-Markovian effects may arise from quantum entanglement due to coherent couplings between the qubit and the bath. Therefore, understanding non-Markovian dynamics has the potential to provide new ways to probe quantum entanglement between a qubit and surrounding baths. This could allow for the creation of entangled states between the NV center and surrounding bath spins which could be used for enhanced quantum sensing with sensitivity beyond the standard quantum limit.

Susumu Takahashi:

Cooper Selco is currently an undergraduate student at University of Southern California, Los Angeles, CA, USA. He has received many awards in his undergraduate research, including IES best poster award, the RMC travel award, and USC provost awards. He is expected to graduate with B.S. in Physics in Spring 2023 and plans to attend a Physics Ph.D. program. He has already demonstrated himself to be an exceptional experimentalist who can perform highly sophisticated experiments with perfect control, can interpret experimental results with a strong grasp of the theory, and can build strategic collaborations.

# IES Poster Prize at the 2022 Rocky Mountain Conference

Euan Bassey:

First commercialized in 1991, lithium-ion batteries (LIBs) have become a mainstay of modern technology: we depend upon them for powering our devices, our transportation and even load levelling renewable energy sources on the grid. These batteries operate *via* a simple mechanism: $Li^+$ ions shuttle from the positive electrode (the cathode) to the negative (the anode), *via* an ionically conductive but electrically insulating electrolyte. When $Li^+$ is removed or inserted at an electrode, an electron compensates the change in charge by travelling *via* the external circuit, providing power. The long lifetimes, fast charge-discharge rates and the large amount of energy they can store (known as the capacity) of LIBs have driven their increasing use. This increase in demand, however, has come alongside a substantial increase in their cost: indeed, in 2022 alone, the cost of raw materials for LIBs has almost trebled. If batteries are to be used in the future – especially on the grid – a cheaper, more sustainable alternative is required. Rather than reinventing the wheel, one can simply move down a period in the periodic table: from lithium to sodium.

Sodium-ion batteries (NIBs) rely on (almost) the same chemistry at a fraction of the cost, a consequence of the higher natural abundance of sodium than lithium. As such, NIBs are poised to play a vital role in future grid-based energy storage. To date, the capacities of NIBs – limited by the cathode – are too low for many real-world applications, and the sources of NIB degradation (leading to shorter battery lifetimes) have not received the attention that LIBs have. If we are to address the energy storage problem and improve the electrochemical performance of NIB cathodes, we need to understand the sources of capacity losses in terms of the structural changes these cathodes undergo during charge and discharge.

Perhaps the most promising class of NIB cathode is the layered sodium manganese oxides, $Na_xMnO_2$, in which edge-sharing $MnO_6$ octahedra are arranged into layers, between which $Na^+$ ions sit, enabling relatively high $Na^+$ ion mobility and hence fast charge/discharge rates. Conventionally, on charging and discharging the battery, charge is compensated by Mn redox reactions (in the case of $Na_xMnO_2$, the $Mn^{3+/4+}$ redox couple); put simply, the amount of capacity available in a battery is a function of the number of energetically accessible electrons available for redox. In practice, this capacity also depends on the phase transformations a cathode undergoes during charge and discharge: one can readily imagine that, on removing $Na^+$ ions from the cathode, the structure will likely change; the reversibility of these changes impacts how much reversible the battery is capable of from one cycle to the next.

Tackling the capacity problem is therefore nontrivial, as one must ensure: there are sufficient redox centres are present to give reasonable capacities; that the structure is sufficiently stable to repeated removal and insertion of $Na^+$ ions and that the materials used in the battery are cheap, sustainable and nontoxic, in keeping with the NIB ethos. The "easiest" of these symptoms to remedy is perhaps structure stabilization: indeed, it has been demonstrated on numerous occasions that, by adding a metal cation dopant (e.g., $Li^+$, $Zn^{2+}$, $Mg^{2+}$, ...) to the Mn layer, the number of phase transformations the cathode experiences drastically falls. In the case of Mg-doped $Na_xMnO_2$, $Na_xMg_yMn_{1-y}O_2$, the number of phase transformations drops from seven down to two. A major concern about this material, however, was the decrease in the number of Mn centres and consequent decrease in capacity. Against all odds, however, the opposite occurs: the addition of Mg into the lattice increases the net capacity of the material relative to the $Na_xMnO_2$ parent.

It is here that you may be asking "why is this article in an EPR magazine? The author hasn't mentioned the technique once!" Have no fear, because it is in EPR that the answer to the curious capacity increase lies. To understand the redox processes taking place, my research has focused on the application of EPR, in conjunction with magnetometry and NMR, to understand the redox processes in $Na_{0.67}[Mg_{0.28}Mn_{0.72}]O_2$ (affectionately referred to as NMMO). By using *operando* X-band EPR – in which an electrochemical cell of NMMO was cycled whilst simultaneously recording EPR spectra – it was noticed that the signal intensity increased on initial charging, consistent with magnetometry measurements of an oxidation of $Mn^{3+}$ to $Mn^{4+}$, but this intensity significantly decreased over the region of increased capacity. The formation of unstable $Mn^{5+}$ was ruled out from $^{23}Na$, $^{17}O$ and $^{25}Mg$ NMR spectroscopy, leaving the only culprit as partial O oxidation (i.e., $O^{2-} \rightarrow O^{n-}$, $n < 2$), followed by strong antiferromagnetic spin-pairing with $Mn^{4+}$, also consistent with magnetometry data. Further evidence for this mechanism was also obtained from variable-temperature, *ex situ* high-frequency EPR ($\nu$ = 383 GHz), in which a significant loss of signal intensity was again observed in the anomalous capacity region. This intensity dropped even further on cooling the sample to 5 K, indicative of a strongly coupled antiferromagnetic ground state, consistent with the proposed charge compensation mechanism.

Whilst other techniques such X-ray absorption spectroscopy may be used as probes of battery materials' electronic structure, EPR provides a non-invasive handle on not only the location of unpaired spins, but also the magnetic interactions within the lattice. Indeed, without EPR, the charge compensation mechanism of NMMO would likely remain unclear. The unique perspective of EPR on a device material with such a large number of strongly interacting spins is critical in understanding the performance of the material and the relationship between its properties and chemical structure.

Clare P. Grey:

Euan first came to me as a masters student, working on a systematic exploration of the magnetic properties of a range of new layered inorganic coordination polymers. It was at this point I was aware of his enthusiasm, ability and keen interest in exploring structure-property relationships of materials. As a PhD student with me, he focused on understanding the NMR and EPR spectra of a set of complex Na-ion and Li-ion battery materials, principally working with the compound he describes in his article below. Through a diligent combination of these experimental techniques as well as *ab initio* calculations of EPR and NMR properties, Euan was able to tease out the complex degradation mechanisms, redox processes and $Na^+$ ion hopping dynamics in the aforementioned material. His careful, meticulous and unique approach to tackling these problems has expanded the fields of both paramagnetic NMR and EPR of condensed paramagnetic systems and his work lays the ground for future generations. Euan gave numerous tutorials on paramagnetic NMR, EPR and *ab initio* calculations and advised several group members over the years. Without doubt, he has been one of the star performers of the group and has helped us to grow both scientifically and intellectually during his time as part of my group. I look forward to seeing his career progress over the coming years.

# Celebrating the 60th Anniversary of SEST,

## the society serving scientific communities of electron spin science/technology and electron magnetic resonance/molecular magnetism in Japan

On the occasion of Joint International Conference, ISMAR-APNMR-NMRJ-SEST 2021, held in Osaka, Japan from August 22 to 27, 2021, SEST (The Society of Electron Spin Science and Technology) celebrated the 60th anniversary of ESR/EPR communities of Japan, noting that the ESR/EPR communities were reformed as the current organization scheme of SEST, which was founded in 2001: The SEST predecessor organization as ESR Meeting of CSJ (The Chemical Society of Japan) was founded in 1961. The first general assembly of SEST was held in Ocha-No-Mizu, Tokyo on October 29, 2002. SEST has been legally registered as well-recognized academic General Incorporated Association in Japan and operated in conformity according to Act on General Incorporated Associations and General Foundations since 2015.

The reformation has been underlain by emerging diverse scientific topics relevant to rapidly developing microwave technology and particular advance in materials science and quantum chemistry for magnetic tensors, attempting to anticipate further developments in ESR/EPR, termed Electron Spin Science and Quantum Technology. The representatives of the existing ESR/EPR communities in the fields of medical, pharmaceutical and biological science, geology, physics, and chemistry in Japan had kept discussing the reformation procedure, reformed scheme of the organization and formal foundation of SEST for two years until 2001. SEST as a consequence of the reformation has provided a unique platform for scientific communities which until now has been able to cover wide research areas relevant to ESR/EPR, from both the experimental and theoretical sides, in natural science/technology such as physics, chemistry, biology, geology, dentistry, medicine/medical science, food science, environmentology, mathematical science, and quantum information/computing science including advanced quantum spin technology.

In memory of the foundation of SEST, the first edition of a book, "Introduction to Electron Spin Science and Spin Technology" (Gakkai Publishing Co., Tokyo) editorially supervised by SEST was issued as part of the SEST publishing project on Nov. 30, 2003, and the enlarged and revised version (Yoneda Publishers, Chiba) on May, 21, 2011. The book gives a comprehensive treatise on Electron Spin Science and Spin Technology until the early 2000's in an introductory and comprehensive manner. The revised version of the book was written by 29 specialists including late Prof. Yu. V. Yablokov, who had greatly contributed to the Prof. E. K. Zavoisky's pioneering work relevant to ESR/EPR in Russia (note that Prof. Yablokov had made his special contribution, at the request of SEST Founder President and Dr. Laila Mosina, Kazan, to a chapter of the book while staying at Institute for Molecular Physics, Poznan, Poland). We have noted that Prof. Hiroshi Sakurai, a Board Director of SEST and Prof. Toshikazu Nakamura, a Board Director of SEST made their enormous efforts to edit the first and revised edition of the book, respectively. We also emphasize that particularly the revised version has extensively been used as a textbook for SEST Summer School for students and young scientist every year since published, hoping that the book will be updated in terms of further progress in experiment and theory of Electron Spin Science and Spin Technology. It should be noted that the enormous achievements in particular topics relevant to pseudo Jahn-Teller genuine organic radicals, both experimentally and theoretically made by the late Prof. Machio Iwasaki and coworker, Dr. Kazumi Toriyama, have not fully been included in the book, unfortunately.

After the reformation of the ESR/EPR communities in Japan, it seems that the post-reformation generation have shown up until recently in many important fields relevant to ESR/EPR, and most of such generation have inherited, more or less in terms of their own science, from predecessors or pioneers in the communities, the locations of whose groups are indicated in Figure 1 depicted below.

Importantly, we have noted that particularly in chemistry and related fields those predecessors or pioneering leaders of ESR Meeting of JSC were the contributors of the volumes for ESR spectroscopy in all "The Series of Experimental Chemistry" regularly published, until the 5th edition printed in 2007 under the editorial supervision of CSJ, by Maruzen Publishing Co. Similar series of Solid-State Physics, in which the volumes of ESR/NMR spectroscopy for researchers in physics were published by other scientific publishers such as Kyoritsu Publishing Co. These volumes of "The Series of Experimental Chemistry" except the one of the 5th edition of the series have given advanced and comprehensive treatises on electron magnetic resonance from the experimental side. The 5th one has included an advanced treatise on quantum chemical calculations of magnetic tensors appearing in true spin Hamiltonians relevant to ESR/EPR spectroscopy. Noticeably, scientific influence of all the volumes dealing with ESR/EPR on students, beginners and newcomers to the ESR/EPR fields has kept underlying the development of the ESR/EPR communities in Japan until recently. In this context, we also note that there have been published several monographs for ESR/EPR spectroscopy; "An Introduction to Electron Spin Resonance" (Kodansha Publishers, 1975) by Yukio Kurita, "Electron Spin Resonance" (Baifukan Publishers, 1978) by Muneyuki Date, "An Introduction to Elec-

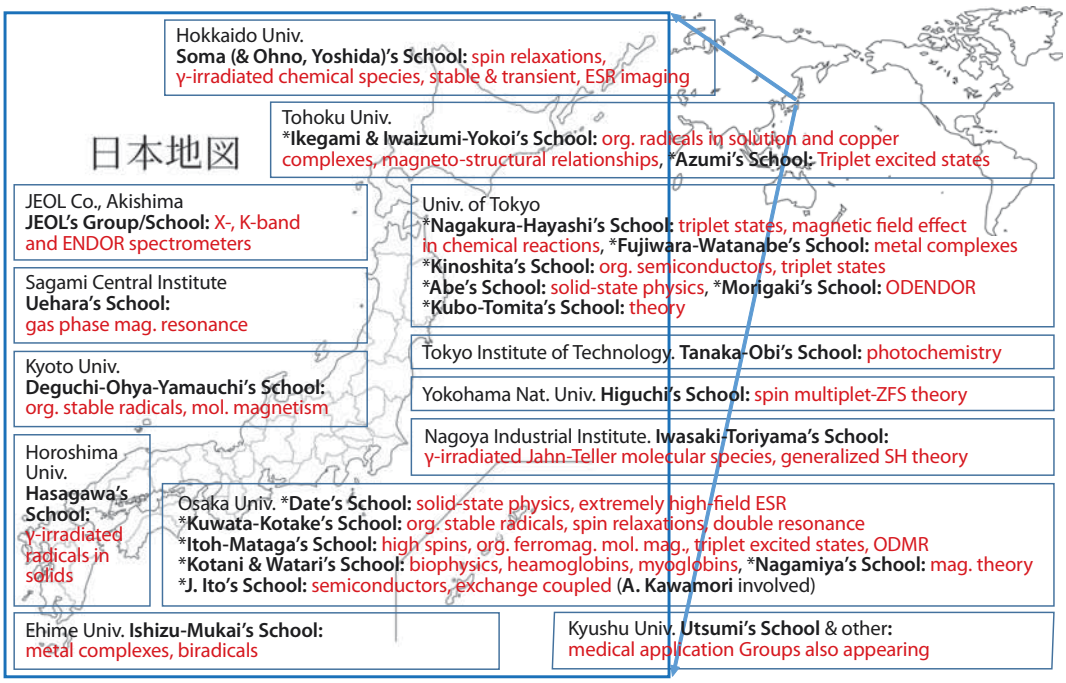



**Figure 1.** A brief sketch of the early stage in the development of ESR/EPR schools (the first generation) dominating across Japan in 1960's. Figure was uploaded on Aug. 22, 2021 during the opening address of Joint International Conference, ISMAR-APNMR-NMRJ-SEST 2021, held in Osaka, Japan from Aug. 22 to 27, 2021. We note that in addition to Dr. Kawamori, there were two leading women scientists in the early days of ESR/EPR communities in Japan, i.e., Dr. Tokuko Watanabe (Professor, Tokyo Univ. of Fisheries, appointed from The Univ. of Tokyo and retired) who has made pioneering achievements in the theoretical analysis of ESR/EPR parameters for open-shell metal complexes) and Dr. Kazumi Toriyama, Nagoya Industrial Institute who made the enormous achievements in particular topics relevant to pseudo Jahn-Teller genuine organic radicals, both experimentally and theoretically, with the late Prof. Machio Iwasaki and coworkers.

tron Spin Resonance" (Nankohdo Publishers, 1980) by Keiji Kuwata and Koichi Itoh, "An Introduction to Practical ESR" (Kodansha Publishers, 1981) by Kazuhiko Ishizu, "Electron Spin Resonance" (Kodansha Publishers, 1989) by Hiroaki Ohya and Jun Yamauchi, "ESR Microscopy" (Springer-Verlag, Tokyo, 1992) by Motoji Ikeya and Toshikatsu Miki, "New Applications of Electron Spin Resonance – Dating, Dosimetry and Microscopy" (in English, World Scientific Publishing Co., 1993) by Motoji Ikeya, "Bio-science ESR" (Hirokawa Shoten Publishers, 1996) by Hiroshi Sakurai, "Dynamic Spin Chemistry: Magnetic Controls and Spin Dynamics of Chemical Reactions" (in English, Kodansha Publishers, 1999) edited by Saburo Nagakura, Hisaharu Hayashi and Tohru Azumi, "Molecular Magnetism, New Magnetic Materials" (in English, Kodansha Publishers, and Gordon & Breach Scientific Publishers, 2000) edited by Koichi Itoh and Minoru Kinoshita, "Introduction to Dynamic Spin Chemistry: Magnetic Field Effects on Chemical And Biochemical Reactions" (World Scientific Publishing Co., 2004) by Hisaharu Hayashi, and "Introduction to Electron Spin Science for Biochemists" (Kodansha Publishers, 2011) by Masahiro Kohno, Toshikazu Yoshikawa and Toshihiko Ozawa.

The authors of the monographs described above were leaders in the ESR/EPR communities or pioneers in their fields of ESR/EPR. We also notice that many SEST Board Directors and SEST members contributed to the chapters of "EPR of Free Radicals in Solids, Trends in Methods and Applications" (Kluwer Academic Publishers, First Ed,, 2003, Second Ed., 2012) edited by Anders Lund and Masaru Shiotani (a SEST Board Director) and to several chapters of "Electron Spin Resonance (ESR) Based Quantum Computing" (in English, Springer Nature, 2016) edited by Takeji Takui, Lawrence Berliner and the late Graeme Hanson.

Indeed, the book publishing projects above (domestic) such as "The Series of Experimental Chemistry" have provided excellent comprehensive treatises and monographs relevant to updated ESR/EPR spectroscopy, but they were Japanese editions except a few, unfortunately. The Japanese editions have had their own right in the scientific communities in Japan, but from the global viewpoint such unique projects have not fully been underscored so far. In this context, we believe that the best plan for the continued book publishing project of SEST will be to attempt to achieve the global publication in English, which helps us contribute to further progress in emerging fields of electron spin science/technology and share our achievements with the global ESR/EPR communities and respect the academic legacies which we have inherited from our and global predecessors of their fields.

The post-reformation generation of SEST are the third generation across the country, and some groups have inherited from their predecessors, developing their particular fields but the current research topics relevant to the emerging generation are diverse. Figure 1 gives a brief sketch of the early stage in the development of ESR/EPR schools (the first generation) dominating across the country in 1960's. The focus of their research subject of each group is given only briefly in the figure, and we are afraid that some leaders' names might be missing. Among or prior to the first generation there were pioneers who had gone across the Pacific and the Atlantic and stayed overseas, and some had come back to Japan after leaving their permanent positions; Ichiro Miyagawa, Professor of Physics, The University of Alabama, who left his associate professorship at The University of Tokyo in 1962 and stayed in Tuscaloosa since 1965, having heading a NASA Project relevant to crystal growth in space (passed away on April 5, 2018); Minoru Fujimoto, Professor of Physics, The University of Guelph, who left

Osaka University and accepted a faculty appointment in 1968 after working with Varian Associates Lab.'s and Oxford Groups, and has been a pioneer in the fields of structural phase transitions of matter in terms of ESR/EPR spectroscopy and Prof. Fujimoto is the author of "The Physics of Structural Phase Transitions" (Springer-Verlag, 1997) and "Introduction to the Mathematical Physics of Nonlinear Waves" (IOP Science, 2014 (First Ed.); Jiro Higuchi, the late Professor of Chemistry, Yokohama National University, who had stayed at Bell Telephone Lab. during the years of 60's and achieved the first theoretical work on the electronic structures in the electron spin multiplets of organic molecules; Noboru Hirota (retired), Professor of Chemistry, Kyoto University (since 1975), who worked with Prof. Samuel I. Weismann at Washington University, St. Louis and later with Prof. Clyde A. Hutchison Jr. at The University of Chicago and accepted a faculty appointment at The State University of New York until 1975, and who has been a pioneer of laser-utilized time-resolved ESR/EPR spectroscopy and its first application to chemical reactions, and Prof. Hirota is the author of "A History of Modern Chemistry" (in English, Kyoto Univ. Press, 2016).

Fortunately, Dr. Laila Mosina, the editor of the IES EPR newsletter gave recent Awardees of SEST a chance to make contributions of their own stories of relevant research to the current issue. Their contributions exemplify recent trends of emerging research achieved by new generation of SEST after the reformation.

Finally and importantly, we note that many academic societies have been aware of the issues of diversity/inclusion for them to further progress, and during the opening ceremony of Joint International Conference, ISMAR-APNMR-NMRJ-SEST 2021, held in Osaka, Founder President of SEST raised the importance of the awareness for our ESR/EPR communities, exemplifying the lesser recognition of the achievements made by Dr. Asako Kawamori, Emeritus Professor of Kwansei Gakuin University, in the early stage of modern pulse-ESR/EPR spectroscopy. IES President, Prof. Songi Han, Chemistry and Biochemistry Department, The University of California - Santa Barbara, announced on Feb. 11, 2022 in her official message to Friends, Colleagues and Students of IES that Award for 2022 IES Fellow would go to Prof. Asako Kawamori "for her seminal contributions in the early days of modern pulsed EPR and its application to the study of photosynthesis systems" (cited from her message). We also congratulate Prof. Kawamori on her receiving the Award, empathizing with her challenges as a scientist and what she was going through in her life. This encourages us to make continued efforts to improve our knowledge about the diversity/inclusion issues in our academic societies, which is relevant to "breaking the bias habit" (the habit of unconscious biases) (cited from the title of a Workshop, WISELI, UW-Madison: https://wiseli.wisc.edu/workshops/bbh-inclusive-campus). We believe that to help capable women scientists/researchers out of the shadow is essential for nowadays academic communities.

Founder President of SEST
Takeji Takui,
Emeritus Professor & Senior URA,
Department of Chemistry and Molecular Materials Science, Graduate School of Science, Osaka Metropolitan University/Osaka City University, Osaka 558-8585, Japan
University Administration Division, Research Administration Department/University Research Administration Center, Osaka Metropolitan University/Osaka City University, Osaka 558-8585, Japan

# Jan Schmidt: on the Occasion of His 85th Birthday

Twenty years after his retirement as a professor of physics at Leiden University, Jan is still the active, friendly and supportive person as the EPR community knows him. While the instrumentation in the laboratory had his full attention in those days, nowadays he is in the lead of solving technical problems that show up in the apartment building he lives in.

Jan Schmidt grew up in Amsterdam, where he studied physics. After his graduation in 1961 and his military service, he was employed as a research scientist at the Royal Dutch Shell Laboratory in Amsterdam. During this period he worked for two years in the laboratory of Professor Lionel Solomon at the Ecole Polytechnique in Paris, from 1964 till 1966. His stay in this vibrant magnetic-resonance environment has had a great impact on his career. Back in Amsterdam, he decided, in 1968, to follow Joan van der Waals, who was appointed a professor at Leiden University, as a PhD student in the Department of Physics. Soon after, he enjoyed his first great scientific achievement with the optical detection of microwave transitions between the spin sublevels of the triplet state of organic molecules in the absence of a magnetic field. This ODMR experiment in zero-field concerned a breakthrough in the study of photo-excited triplet states, and inspired many research groups worldwide. June 1971, Jan defended his thesis 'Modulation of phosphorescence by microwaves', in which he described both steady-state and transient experiments on the phosphorescent triplet states of quinoline, quinoxaline and naphthalene, each present as a guest in a single crystal of durene.

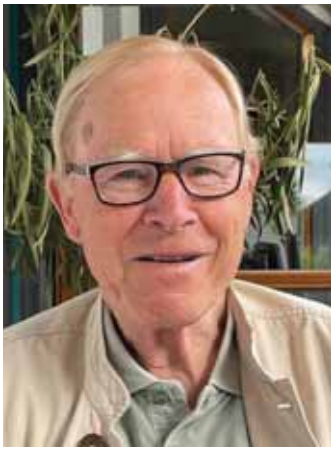
Following a post-doc at the IBM Almaden Research Laboratory in San Jose, California, he continued his work on triplet states. He focused on the elucidation of the spin selectivity of the populating and depopulating of the triplet sublevels and the role of spin-orbit coupling, and introduced, besides ODMR, Electron-spin-echo (ESE) techniques, initially at 9 GHz. In the second half of the eighties, he became fascinated by the spectral resolution that could be gained when working at higher microwave frequency. He developed an ESE spectrometer operating at 95 GHz, with a probe head that contained a cylindrical single-mode cavity, and enabled orientational studies of single crystals, optical excitation, and radio-frequency excitation for pulsed ENDOR experiments. The successful application of this novel spectrometer in a variety of research fields encouraged him to take the next step to 275 GHz. In these pioneering projects Jan's feeling for instrumentation was decisive in combination with his continuous ▶

and inspiring discussions with the fine-mechanical and microwave engineers. His laboratory became internationally recognized as one of the leading groups in high-frequency EPR. On the application side, he switched from the triplet states of molecules to the study of semiconductors and nanoparticles thereof. In 1993, he was among the first to optically detect the EPR signal of a single molecular spin, and single-molecule spectroscopy became the focus of his research. The observation of the excitation spectra of individual light-harvesting complexes of photosynthetic bacteria represents another highlight in his impressive scientific oeuvre. In this context, Jan will be the first to emphasize the contribution of his collaborators and students through the years, but no doubt he was the driving force. For his contributions to EPR he was awarded the Silver Medal for Physics and Instrumentation of the International EPR Society in 1995, the Bruker Prize in 1999, the Ampère Prize in 2000, the Zavoisky Award in 2006, and the Gold Medal of the International EPR Society in 2008. After his retirement he became chairman of the Board of Supervisors of the Leiden Instrumentmakers School, which ones again illustrates his commitment to instrumentation.

When I joined the group, in 1985, I knew Jan's research activities but did not know him personally. Soon after I found out that he was an ideal colleague. I entered a well-organized laboratory, and was offered a project he had started. We closely worked together in harmony for many years and his unselfish character offered me the chance to develop my own research projects. Up till today I appreciate this attitude from which I benefitted a lot.

Edgar Groenen

# Michael Mehring – Fostering the Symbiosis of EPR and NMR: on the Occasion of His 85th Birthday



Celebrating the 85th birthday of Michael on October 7th, it is appropriate to track his scientific path. How was it possible for him to have such an immense impact on the development of Magnetic Resonance – not only in Germany? A few important milestones can be easily identified:

First, it was important that he made the right choice for picking his supervisor – Otmar Kanert (Univ. Münster) – for his PhD study in solid state physics.

Second, after getting his degree in 1969, he exposed himself to the most challenging post doc environment – The NMR group of John Waugh at the MIT. There he met Alex Pines and Robert Griffin, and together they formed a spectacular effective group of young researchers, influencing the later development of solid state NMR. Sabbatical leaves to Boston and Berkeley deepened their friendship, lasting till now!

Third, returning to Germany in 1972, he got his first permanent position at the University Dortmund, a young university developing a new concept for teaching, integrating experimental and theoretical topics from the very beginning. Being exposed to mathematical concepts of high energy theoreticians, his aim for a thorough understanding of the possibilities of spin manipulations was further incited. He showed the benefits of the spinor formalism for the description of coupled spins. He compiled his deep knowledge about multidimensional NMR in his textbook: "Principles of High Resolution NMR in Solids".

It came to no surprise that his interest turned also to electron spins and he succeeded in applying the concepts of pulsed excitation also now in the microwave regime. His direct approach for optimizing the power/field conversion by using a slotted tube cavity proved important for first pulsed EPR experiments in his group (1980). In 1986 he was invited to lecture at the Shanghai University, initiating further magnetic resonance studies in China.

His breakthrough results did not stay unobserved, and he was offered different positions in Germany. He decided to go to Stuttgart University as full professor in 1981 – here also meeting one of the German EPR pioneers H. C. Wolf. Always being interested to interact with leading theoreticians, he co-organized with Hans Kuzmany (University Wien) an International Winterschool in Kirchberg (Austria), which was started in 1985. Mini symposia at the ski tracks and the late evening sessions, followed by informal sessions in the bar, gave students the chance to meet eminent scientists face to face. This gave the opportunity to discuss latest results of pulsed EPR on charge and spin transport – first on conducting charge transfer salts and on conducting polymers, and later on high $T_c$ superconductors. It was to no surprise that HYSCORE was established as landmark method to study these compounds.

The new Carbon phases like $C_{60}$ and graphene were a new playground for pulsed EPR, and clearly Michael took the chance to explore these compounds with advanced methods. His deep knowledge of unitary transformations of density matrices gave room for exploring Qbit tasks also, showing factorization. A fascinating talk at the Kirchberg Winterschool 2007 about quantum computing with subtitle: "Introducing the principles of quantum computing to those who always wanted to know about quantum computing but never dared to ask", was a perfect example about Michael's capability to address complicated topics.

Needless to say that Michael also was active in science management. He served in decision boards of the DFG, and helped to organize NMR and EPR activities at the GHMFL (Grenoble High Magnetic Field Laboratory). He also was active as dean in shaping the Physics department of Stuttgart University.

Being highly visible at the international stage, he was awarded the BRUKER prize, Zavoisky award, and AMPERE prize, to list important ones. He also organized one of the Gordon Conferences on Magnetic Resonance and served as president of ISMAR.

In his free time he enjoyed sailing and skiing, and after retiring he also excelled in painting, examples which can be admired in his beautiful home. For the coming years I wish him and his wife Sabine all the best!

Klaus-Peter Dinse

# Electron-spin transient nutation as transition moment spectroscopy: Messages from spin systems behind electron spin transient phenomena

Kazunobu Sato

Graduate School of Science, Osaka Metropolitan University, Japan

Quantum computers and quantum information science have been attracting wide interest from the viewpoint of an emerging quantum technology that leads to technological innovation in many fields. A qubit (quantum bit) plays an essential role as a minimum information resource in most of the models for quantum computers like superconducting, trapped ion, trapped electron in quantum dot or photon. It seems that the physical state of the qubit with a two-level system can be described by a Bloch sphere and its intrinsic physical idea has become widely accepted by the scientific community. The transient behavior of the qubit is phenomenologically considered by Bloch equations well-known in magnetic resonance spectroscopy. The behavior is consistent with its physical picture based on the quantum theory for the two-level system.

Applications of well-defined open-shell entities such as molecular spins or molecular magnets have been proposed as electron spin qubits which are "matter qubits". Approaches to quantum information by utilizing magnetic materials have emerged recently. In such research the electron spin transient nutation (ESTN) has attracted keen attention as a key event of the qubit behavior. The term "transient nutation" was introduced at an early stage of magnetic resonance spectroscopy by H. C. Torrey in 1949 [1]. The transient nutation phenomena were quantitatively explained based on the Bloch theory. Methodology to measure the transient nutation phenomena in the rotating frame has been developed in NMR/NQR spectroscopy at an early time and has later also appeared in EPR spectroscopy.

The transient nutation phenomena are fundamental responses of a spin system when applying arbitrary irradiation fields and are observed also in optical spectroscopy. The ESTN phenomena in paramagnetic compounds appear in a time domain and thus are observed in pulsed EPR spectroscopy, giving us useful information about the quantum nature of electronic spin systems, which cannot be identified in terms of continuous-wave (cw) EPR spectroscopy. The ESTN phenomena provide straightforward messages from the spin systems having not only the simple two levels but also complicated multiple sublevels, thus exemplifying direct experimental determination of the electron spin quantum numbers $S$ of paramagnetic entities. From the methodological viewpoint, NMR/NQR spectroscopy does not require such spin multiplicity identification. Pioneering results concerning ESTN spectroscopy based on pulsed EPR spectroscopy have been achieved in 1990. J. Isoya, M. K. Bowman and coworkers have determined the effective spin quantum number $S$ to be $S = 3/2$ for a nickel impurity in synthetic diamond [2]. They have shown a distortion of the impurity site from tetrahedral symmetry, which gives rise to non-vanishing ZFS parameters due to the breakdown of symmetry occurring in the crystal. A. V. Astashkin and A. Schweiger have demonstrated that the ESTN method facilitates the spin identification of complicated EPR spectra from transition metal ions in solids by exploiting the nutation frequency dependence of the allowed and forbidden EPR transitions [3]. We have studied the electronic structures of various organic high-spin systems in single crystals as well as in non-oriented media using ESTN spectroscopy for a long time since the early 1990s [4]. In this short article, I would like to review the ESTN method we have applied to various spin systems, only referring to a few examples.

In 1997, we have published results of two-dimensional ESTN (2D-ESTN) experiments applied to polycationic high-spin models for purely organic ferromagnetic metals [5], demonstrating that the transient nutation phenomena of organic high-spin compounds in frozen organic glasses showed a magnetic field dependence. The dependence is due to the difference in EPR transitions involved, giving us EPR transition probabilities relevant to the spin sublevels. We have successfully identified the spin multiplicities and discriminated the EPR transitions in terms of the nutation frequency in the non-oriented media. The technique has been applied to a high-spin polycarbene generated by photo-irradiation of the corresponding precursor at low temperature, whose molecular structure predicts apparently small ZFS parameters [6]. Figure 1 shows a contour plot of the 2D-ESTN spectra of the triscarbene at cryogenic temperature. Discriminated nutation frequencies were attributed to the allowed EPR transitions in the septet spin state. The 2D-ESTN spectroscopy unequivocally enables us to identify that the observed convoluted fine-structure spectrum at X-band is due to a spin-septet state from a purely organic synthetic entity. The magnetic field dependence of the frequencies also corresponds to the angular dependence of the EPR transitions, which is in agreement with the complex simulation of the fine-structure EPR spectrum with random orientation in non-oriented media. It indicates that 2D-ESTN spectroscopy is capable of decomposing the overlapping EPR transitions in cw fine-structure EPR spectra. This differs from the putative advantage of high-field/high-frequency EPR spectroscopy.

The 2D-ESTN spectroscopy has another intrinsic advantage for resolving complicated fine-structure EPR spectra due to the contribution from nuclear spins. The lanthanoid ion, $Eu^{2+}(^8S_{7/2})$, doped in a calcium fluoride ($CaF_2$) single crystal with cubic symmetry is known to give one of the most complicated fine-structure/hyperfine structure EPR spectra ▶

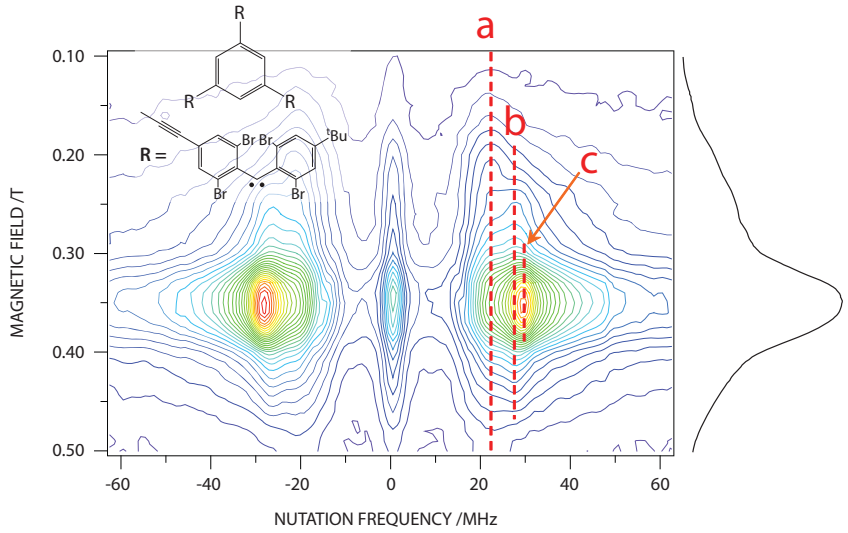



**Figure 1.** Contour plot of field-swept 2D-ESTN spectra of brominated triscarbene observed at $T = 5$ K in a 2-MTHF glass. An electron spin-echo detected fine-structure EPR spectrum of the triscarbene is shown on the right. Three dominant peaks indicated by **a**, **b**, and **c** were discriminated at 22.0, 27.5, and 29.5 MHz, respectively.

(Figure 2). The spin system has an octet spin state ($S = 7/2$) with two nuclear isotopes of nuclear spin $I = 5/2$ in its electronic ground state. The two nuclear isotopes with similar natural abundance complicate the EPR spectrum. In addition, inclusion of higher order terms in the fine-structure spin Hamiltonian is required for reproducing the EPR spectrum. The fourth- and sixth-order terms arise from the high cubic symmetry while the second-order terms vanish. We have applied the 2D-ESTN method to decompose the complex nuclear spin contribution [7]. In the 2D-ESTN spectrum of the $Eu^{2+}$ ion in the single crystal, the nutation frequencies indicated the dependence on hyperfine EPR transitions as well as on the spin quantum number $S$ and $M_S$ manifold. It is demonstrated that the 2D-ESTN method discriminates the hyperfine allowed EPR transitions from the hyperfine forbidden ones and the contributions from the isotopes. Such discrimination of the EPR transitions enables us to make facile assignments of complicated fine-structure/hyperfine structure EPR spectra, in which the transition probabilities play a key role in the complete analysis in terms of the transition moment spectroscopy. The nutation frequencies observed for the hyperfine allowed and forbidden transitions were quantitatively understood with the help of reduced rotation matrix elements for $I = 5/2$.

The nutation frequency is closely related to the spin state, and easily understood by using a simple equation for the nutation frequency in the weak extreme limit of the irradiation field compared to interacting terms appearing in spin Hamiltonians. We have discussed particular ESTN phenomena of weakly exchange-coupled biradical systems, in which it is not appropriate to apply the simple approach for the nutation frequency [8]. For the nutation frequency of such a biradical, we need to categorize the nutation behavior as shown in Figure 3 according to the relative strength between the spin-spin interaction ($D_{12}$) and irradiation field for exciting the spin ($\omega_1$). In the weak extreme limit of the irradiation field ($\omega_1 \ll D_{12}$), the nutation phenomena governed by the $D_{12}$-driven motion are well understood by the first-order approximation for the EPR transition, and in this case the ESTN spectroscopy has a great advantage in characterizing the spin states. On the other hand, in the strong irradiation limit ($\omega_1 \gg D_{12}$), the nutation phenomena in the case of the $\omega_1$-driven nutation motion are governed by the strong irradiation field. This means that it is impossible to discriminate the individual EPR transitions involved. The nutation motion then behaves like a simple doublet spin. In the case of the intermediate irradiation strength ($\omega_1 \approx D_{12}$), the nutation motion depends on both spin-spin interactions and the $\Delta g$-effect in the two-spin system. It is necessary to quantitatively understand the relevant nutation phenomena without simplification in the intermediate case.

Recently, we have treated weakly exchange-coupled heterobiradicals in collaboration with E. Bagryanskaya and coworkers [9]. Continuous-wave EPR spectra of the heterobiradicals which consist of trityl and nitroxide radical moieties show EPR line splittings due to the exchange interaction in solution. The nuta-

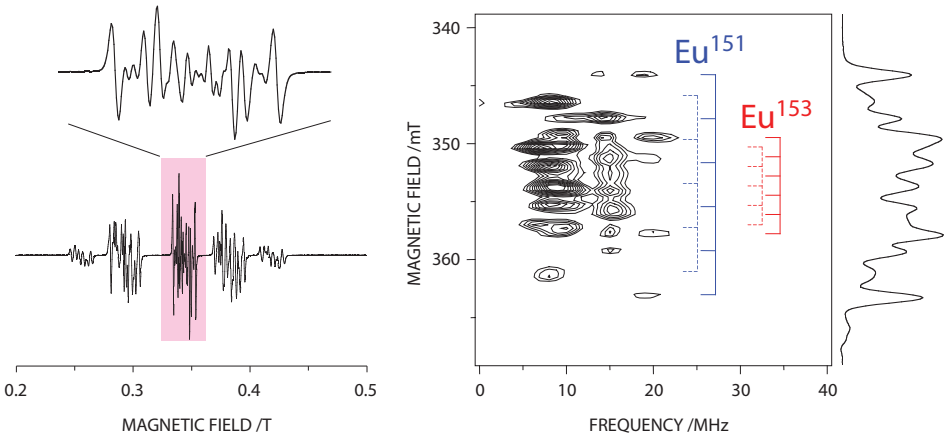



**Figure 2.** Continuous-wave X-band EPR spectrum of $Eu^{2+}$ in a $CaF_2$ single crystal observed at $T = 3.5$ K. On the right, a contour plot of the 2D-ESTN spectra observed from the EPR transitions between $M_S = 1/2$ and $-1/2$ spin sublevels. It indicates that EPR transitions with hyperfine structure have different nutation frequencies.

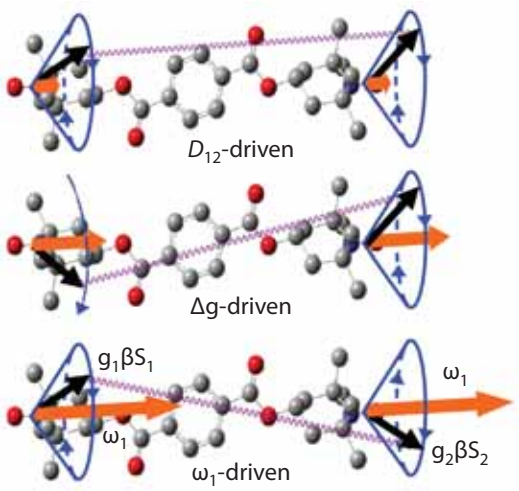



**Figure 3.** Pictorial representations of the nutation motion for exchange-coupled biradical systems with respect to microwave irradiation strength $\omega_1$ given by orange arrows. A dominant term in three different interactions ($D_{12}$-, Δg- and $\omega_1$-driven) governs nutation motion in the rotating frame. The $D_{12}$-driven motion corresponds to the weak extreme irradiation condition. The $\omega_1$-driven nutation motion corresponds to the strong irradiation limit. The Δg-driven motion is an intermediate case. In the Δg-driven motion, the nutation frequency depends on both spin-spin interaction and the Δg-effect in the two-spin system.

tion phenomena of the biradical systems in solution belong to the intermediate case, in which the Δg-driven motion is dominant. Under such conditions, the nutation behavior of the biradicals is not simplified, and they exhibit a variety of nutation phenomena. These nutation phenomena have been investigated based on pulsed EPR spectroscopy with rectangular pulses. In the past decade, arbitrary waveform pulses have become available in the field of pulsed EPR research, using arbitrary waveform generators (AWGs). These pulses enable us to control the nutation motion in a desired manner. The transient spin nutation behavior of matter spin qubits controlled by the pulses is expected to become relevant for quantum information processing.

**References**


1. Torrey, H. C., *Phys. Rev.* **1949**, 76(8), 1059–1068.
2. Isoya, J.; Kanda, H.; Norris, J. R.; Tang, J.; Bowman, M. K., *Phys. Rev. B Condens. Matter* **1990**, 41(7), 3905–3913.
3. Astashkin, A. V.; Schweiger, A., *Chem. Phys. Lett.* **1990**, 174(6), 595–602.
4. Sato, K.; Shiomi, D.; Takui, T.; Itoh, K.; Kaneko, T.; Tsuchida, E.; Nishide, H., *J. Spectroscopic. Soc. Japan* **1994**, 43(5), 280–291.
5. Sato, K.; Yano, M.; Furuichi, M.; Shiomi, D.; Takui, T.; Abe, K.; Itoh, K.; Higuchi, A.; Katsuma, K.; Shirota, Y., *J. Am. Chem. Soc.* **1997**, 119, 6607–6613.
6. Tomioka, H.; Hattori, M.; Hirai, K.; Sato, K.; Shiomi, D.; Takui, T.; Itoh, K., *J. Am. Chem. Soc.* **1998**, 120(5), 1106–1107.
7. Matsuoka, H.; Sato, K.; Shiomi, D.; Takui, T., *Appl. Magn. Reson.* **2003**, 23(3), 517–538.
8. Ayabe, K.; Sato, K.; Nishida, S.; Ise, T.; Nakazawa, S.; Sugisaki, K.; Morita, Y.; Toyota, K.; Shiomi, D.; Kitagawa, M.; Takui, T., *Phys. Chem. Chem. Phys.* **2012**, 14(25), 9137–9148.
9. Sato, K.; Hirao, R.; Timofeev, I.; Krumkacheva, O.; Zaytseva, E.; Rogozhnikova, O.; Tormyshev, V. M.; Trukhin, D.; Bagryanskaya, E.; Gutmann, T.; Klimavicius, V.; Buntkowsky, G.; Sugisaki, K.; Nakazawa, S.; Matsuoka, H.; Toyota, K.; Shiomi, D.; Takui, T., *J. Phys. Chem. A* **2019**, 123(34), 7507–7517.

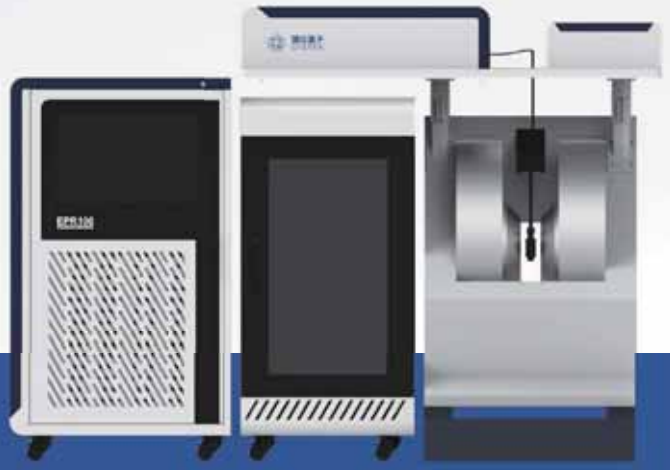
# Electron Paramagnetic Resonance Spectrometer

国仪量子 CIQTEK

## EPR100/EPR200-Plus

### EPR100

- Equipped with all CW mode functions of EPR200-Plus
- Echo / FID measurement
- Relaxation time measurement
- Sweep echo detection
- DEER experiment
- ENDOR experiment



X-Band Pulse / Continuous Wave Electron Paramagnetic Resonance Spectrometer

EPR100

### EPR200-Plus

- 1D magnetic field scanning
- 2D magnetic field-microwave power scanning
- 2D magnetic field-modulation amplitude sweep
- 2D magnetic field-time scanning
- Variable temperature experiment
- Irradiation experiment

X-Band Continuous Wave Electron Paramagnetic Resonance Spectrometer

EPR200-Plus

CIQTEK is a high-tech enterprise with quantum precision measurement as the core technology that is originated from CAS Key Laboratory of Microscale Magnetic Resonance (since 2000) in University of Science and Technology of China. This laboratory focuses on the research of spin quantum control and its applications in novel quantum technologies, with various experimental routes including nuclear magnetic resonance (NMR), electron spin resonance (ESR), optically-detected magnetic resonance (ODMR), magnetic resonance force microscopy (MRFM), and electrically-detected magnetic resonance (EDMR).

Contact us / **+86-551-62835225** Chinainstru & Quantumtech (Hefei) Co.,Ltd. | www.ciqtek.com | gylz@ciqtek.com

# Desktop EPR

国仪量子 CIQTEK

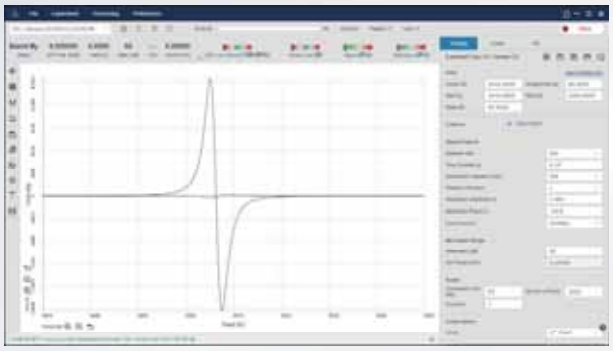
## Electron Paramagnetic Resonance Spectrometer **EPR200M**

### Product Parameter

| Parameter | Value |
|---|---|
| Frequency Range | 9.2-9.9GHz |
| Modulation Field Amplitude | 10 Gauss |
| Magnetic Field Range | 6500 Gauss (Max) |
| Uniformity of magnetic field in sample area | Better than 50mG |
| Detection SN ratio in continuous wave mode | Better than 600:1 |
| Absolute spin number sensitivity | $5\times10^{9}$ spins/(G√Hz) |


### Applications

01 Environment Science
02 Chemistry
03 Physics & Material
04 Biomedical
05 Food Science
06 Industry



Contact us / **+86-551-62835225** Chinainstru & Quantumtech (Hefei) Co.,Ltd. | www.ciqtek.com | gylz@ciqtek.com

# F. Ann Walker (1940–2022)

F. Ann Walker, Regents Professor Emerita at The University of Arizona, died on January 30, 2022, in Spokane, Washington after a long illness. Her significant contributions and leadership in magnetic resonance spectroscopies, especially of heme-containing systems, have been recognized by numerous awards, including: Fellow of the American Association for the Advancement of Science (1984); Garvan-Olin Medal, American Chemical Society (2000); Luigi Sacconi Medal, Inorganic Chemistry Division, Italian Chemical Society (September, 2001; awarded July 2002); Alexander von Humboldt Senior Research Awardee in Science (2003-05, Univ. of Lübeck, Prof. Alfred Trautwein); Alfred Bader Award in Bioinorganic Chemistry, American Chemical Society (2006); Fellow of the American Chemical Society (2011); Eraldo Antonini Lifetime Achievement Award from the Society of Porphyrins and Phthalocyanines (2020).

Photo courtesy of Mary G. Enemark

An account of the career of Professor Walker (known as Ann to colleagues and friends the world over) appeared previously in an article in a 2011 *EPR newsletter* (volume 21, number 1, pages 6-7) celebrating her 70th birthday. Selected portions of that article as well as some of her subsequent activities are summarized below.

Ann was born on May 11, 1940, in Adena, Ohio, USA, a small town in eastern Ohio. She received her B.A. in 1962 from The College of Wooster, with a major in chemistry. She did her graduate work at Brown University in physical inorganic chemistry with Richard L. Carlin and Philip H. Rieger on EPR studies of vanadyl complexes and received her Ph.D. in 1966. She continued research on EPR spectroscopy as an NIH Postdoctoral Associate with Professor Daniel Kivelson at UCLA (1966-67), where she became interested in the magnetic spectroscopies of metalloporphyrin systems. In her faculty positions at Ithaca College (1967-70) and San Francisco State University (1970-90), she demonstrated that the concepts of electron donating or withdrawing properties of substituents on aromatic rings developed by physical organic chemists, can be applied to metalloporphyrins, and that such effects are exquisitely reflected in their spectroscopic properties. During this period, she published 26 papers in the prestigious *Journal of the American Chemical Society*. These manuscripts are characterized by carefully planned experiments, attention to experimental detail, thoughtful discussion, and comprehensive referencing, and they have set high standards for research in metalloporphyrin chemistry.

Upon joining the faculty of the University of Arizona in 1990, Ann provided leadership in establishing an EPR Facility and hiring Dr. Arnold Raitsimring (International Zavoisky Awardee, 2016) to develop state-of-the-art pulsed EPR spectrometers covering the 2–40 GHz range. She pioneered the imaginative application of multi-dimensional NMR, pulsed EPR, $^{57}$Fe NMR and Mössbauer spectroscopies to understand the relationships between structure and function of the heme centers of proteins and model compounds. Ann's ability to forge productive international collaborations was essential for the success of these technically very difficult experiments which provide information about dynamic processes in metalloporphyrin centers. Her comprehensive review articles and chapters on spectroscopic investigations of paramagnetic metalloporphyrins and ferriheme proteins are highly cited and provide valuable insights to both experienced researchers and to those new to the field.

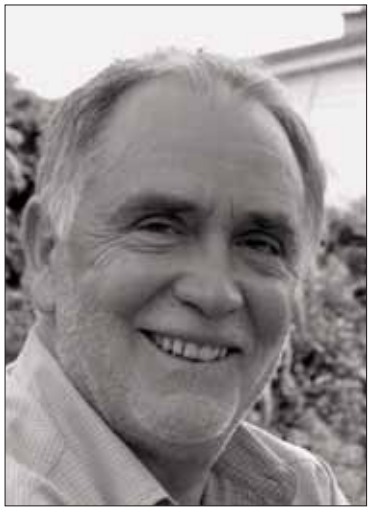
In recent years, her research focused on nitrophorins, novel heme containing proteins from the saliva of the blood sucking insect *Rhodnius prolixus* (the kissing bug) that reversibly bind nitric oxide (NO). These extensive studies, which utilized molecular biology, electrochemistry, pulsed EPR spectroscopy, and multi-dimensional NMR spectroscopy, have attracted wide attention because NO is an important messenger molecule in vasodilation and immune responses and because *R. prolixus* is the host for the parasite that causes Chagas' disease, a fatal incurable wasting of the muscles of the heart and the intestines.

Ann served as an Associate Editor for the *Journal of the American Chemical Society* from 1998-2010, where she handled manuscripts dealing with magnetic resonance. She also was Chair of Inorganic Chemistry Division of the American Chemical Society (2010), Chair of the Gordon Research Conference on Metals in Biology (2003), served on the ACS Presidential Commission on Women in Chemistry (2000-01), and organized three symposia on Porphyrins, Metalloporphyrins and Heme Proteins at National Meetings of the American Chemical Society.

Ann loved to travel! Her world-wide network of research collaborators provided many opportunities to experience different landscapes and cultures. She visited all seven continents, and in 2019 took a four-month cruise around the world. Her annual "Christmas Letter" enabled readers to participate vicariously in her travel adventures.

Ann was a remarkable mentor whose impeccable professionalism enriched the scientific careers of students and colleagues alike. She especially championed female and underrepresented scientists. Ann lived life fully, certain she would leave this world a better place. A memorial service celebrating Ann's life was held in Tucson, Arizona on July 9, 2022. The service was streamed live and is now available online (https://youtu.be/cxAdrTVVBLU).

John Enemark



# Eckhard Bill (1953–2022)

Our dear friend and long-term colleague Eckhard Bill passed away suddenly and unexpectedly on October 6th, 2022. Eckhard was a giant in the field of magnetism, Mössbauer- and EPR spectroscopy applied to open shell transition metal ions.

Eckhard Bill studied physics at the University of Saarland and became enthusiastic about Mössbauer spectroscopy already during his studies. He was one of the first students of Alfred (Ali) Trautwein, who did his habilitation in the group of Uli Gonser and then accepted the call for a professorship at the University of Lübeck in 1983. Enthusiastic about his young student, Ali Trautwein offered Eckhard to work with him in Lübeck and set up a laboratory for Mössbauer spectroscopy there. Thus, in a short time, Eckhard attained the position of laboratory manager, who, with his extensive experimental expertise, supervised a large number of measuring stations for Mössbauer spectroscopy at low temperatures and high magnetic fields.

Eckhard was fascinated by biological and chemical systems in which iron centers have functional roles such as catalysis and transport. His dissertation, still completed at Saarland University, is entitled "Mössbauer Investigations on the Cofactor Iron of Putadimonooxin". After the establishment of the Mössbauer laboratory at the University of Lübeck was completed, Eckhard established EPR spectroscopy in the group of Ali Trautwein and then also magnetometry in the early 1990s. Eckhard Bill was not only an extremely talented experimentalist, he was always an authority in the interpretation of the obtained measurement results and an expert in the use of the spin Hamiltonian formalism, which can be used to describe magnetic properties of metal centers in proteins and chemical complexes.

Countless collaborations made Eckhard Bill a highly visible figure in the Mössbauer-, EPR- and bioinorganic chemistry communities. His always friendly and personable way of dealing with people as well as his high level of expertise and immense enthusiasm for science made him a much sought-after cooperation partner for researchers all over the world.

Hence, it was not surprising that Karl Wieghardt offered him in 1995 to set up a laboratory for Mössbauer and EPR spectroscopy at the then Max Planck Institute for Radiation Chemistry (later Bioinorganic Chemistry, then Chemical Energy Conversion). For almost 30 years, he led the Magnetism, Magnetic and Mössbauer Spectroscopy group there in the departments of Karl Wieghardt (1995–2010), Frank Neese (2011–2017), and Serena DeBeer (2018–2020) and thereby greatly contributed to the international reputation of the Mülheim chemistry campus. Even after his retirement in 2019, Eckhard Bill remained highly active in research and teaching as an advisor to the Institute.

In the EPR community, Eckhard has played a special role by masterfully combining the power of EPR spectroscopy with magnetic characterization techniques and computational quantum chemistry. His comprehensive perspective and complementary approach continue to shape the application of EPR and Mössbauer spectroscopy in fields as diverse as (bio)inorganic chemistry, catalysis research and molecular magnetism.

His scientific work is reflected in more than 500 publications. In 2013, he received the IBAME Science Award for his contributions to biological and chemical Mössbauer spectroscopy. Together with Ali Trautwein and Phillip Gütlich, he co-authored an authoritative and highly influential textbook on the application of the Mössbauer effect in transition metal chemistry.

Eckhard was an extremely kind person who was always happy to share his knowledge with others. He always took a positive perspective on everything and everyone and his interest in the other people was always genuine. Hence, it is not surprising that he was an extremely popular teacher in a variety of summer schools around the world. Eckhard Bill has educated generations of inorganic chemists in the art and science of SQUID magnetometry, EPR and Mössbauer spectroscopy and the analysis of the experimental data on the basis of spin Hamiltonians. At the same time, he was a ingenious and very popular discussion partner for quantum chemists seeking a closer connection to "real life".

Eckhard Bill has supported a large number of careers by travelling to the laboratories of newly appointed colleagues and helped them setting up their laboratories. In doing so, Eckhard was a true wizard who always knew how to solve problems and do things the right way.

Eckhard is greatly missed by all who knew him. Our sympathy goes out to Eckhard Bill's family, especially his wife Ute Czeromin and his daughter Eva Bill.

Frank Neese, Volker Schünemann,
Alexander Schnegg

# The story of DEERNet

Ilya Kuprov

The phone started ringing 30 seconds after I had clicked *Send*. *"Crikey, what is that thing?"* – Gunnar Jeschke has a time dilation machine at ETH, that's the only explanation I have for that level of efficiency. *"Erm... we just autogenerated a few billion DEER traces and threw them at a neural net. Sorry about that strange pedestal in one of your datasets, we probably didn't train it well enough"* – I was cautiously optimistic; the output looked kinda OK except for that one quirk Steve Worswick and I could not get rid of (Figure 1, right panel). There was a giggle in the phone – *"That 'strange pedestal' is a dataset from Victor Chechik that no Tikhonov method would ever be able to process: a combination of a very sharp and a very broad distribution. That's not an artefact, that's your network beating every model-free tool we have."* Ah... now that's interesting.

In 2017, a major problem was that Steve and I knew next to nothing about the experimental aspects of DEER spectroscopy. For the next three months, Gunnar was patiently babysitting us through generating databases of realistic-looking training data (*"no, the baseline is multiplicative, not additive", "yes, you do need to include these horrendous distance combinations, that's what most biologists actually have"*). The resulting nets were spookily effective at processing DEER traces – a famously difficult task roughly comparable to reconstructing the pig from a sausage. To my surprise, we managed to publish a paper on the strength of that alone [3].

Colleagues were understandably cautious. *"But how does it actually work?"* – Daniella Goldfarb and Akiva Feintuch looked both impressed and suspicious after DEERNet extracted excellent quality distance distributions from their data. *"We haven't the foggiest."* – was my honest reply.

Leverhulme Trust has a lovely policy whereby they would not fund anything that a mainstream funding agency would fund. Well, that'd be us... *"This... thing solves a problem that is not supposed to be solvable; we don't know how. That is fascinating, slightly scary, and goes to the philosophical foundations of what it means to do science in the era of artificial intelligence. Erm... eccentric enough?"* That was the weirdest funding application I had ever submitted. The reviewers waved us through on the sheer optimism of the proposal... explaining a fully connected neural net is a tall order.

By about 2021, we managed. We knew the necessary maths of course. Under the bonnet, neural nets are straightforward linear algebra; spin dynamics people are good at that. Jake Amey, Jake Keeley, and Tajwar Choudhury joined the team and we managed to crack the network open. Another round of fascinated head scratching ensued: the thing apparently invented a bandpass filter, a notch filter, a frequency axis rescaling transformation, frequency division multiplexing, group embedding, spectral filtering regularisation, and a map from harmonic functions into Chebyshev polynomials – in ten minutes of unattended training from a random initial guess [4]. Jake and Taj are still working out the details; the net is not fully transparent yet, but it is translucent.

The strongest side of DEERNet was what it lacked: caveats and adjustable parameters. Turns out biologists hate those. This is how the collaboration with Enrica Bordignon, Laura Galazzo, and Janet Lovett started [2]. It was a dark and stormy night at a drinks reception of the 2019 ESR Group conference, and two exasperated colleagues were staring into a laptop: *"Oh, bless, Gagarin's control panel looked simpler!"* – Enrica and Laura were not well pleased with DEERAnalysis – *"Oh... Hi Ilya, hi Gunnar. Can you make us something that doesn't require a PhD in computer science? Like, data goes in, answer comes out?"*. I googled up the control panel of the Vostok spacecraft. The ladies had a point. *"Well, as it happens, we just made something like that. The only parameter is the file name."*

```
[deer_trace,time_axis]=
elexsys2deernet('file_name');
deernet(deer_trace,time_axis);
```

We did have to go through multiple rounds of the training database updates, Laura's edge cases ventured rather far from mainstream DEER processing situations. But we did man-

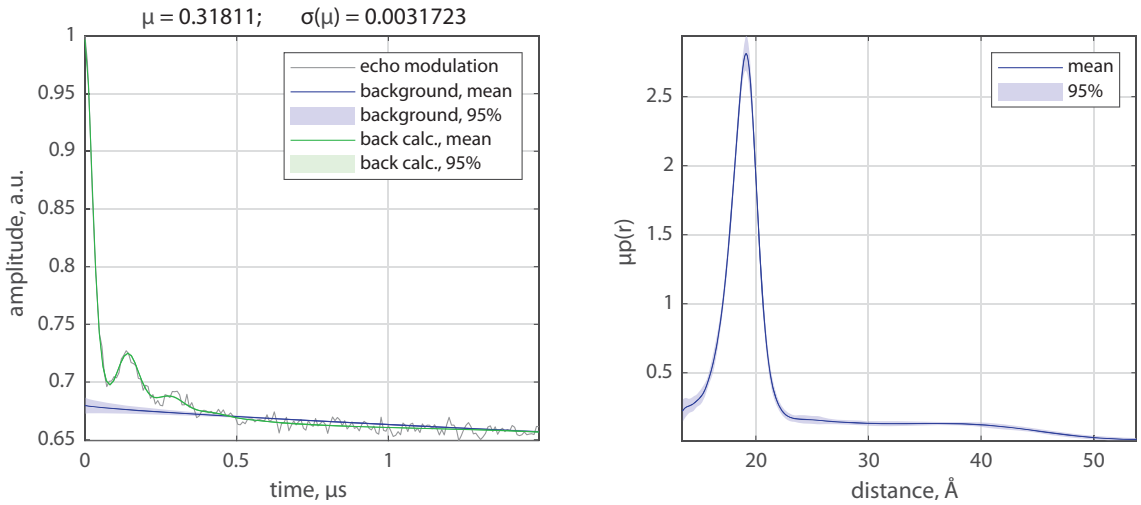



**Figure 1.** Pairs of nitroxide radicals tethered to the surface of gold nanoparticles, with the thiol tether attachment points diffusing on the surface of the nanoparticle (sample Au 3 after solvolysis and heating in [1]). The broad pedestal is real, it matches the analytical model reported in [1]; existing regularisation methods cannot process this dataset without either broadening the peak or introducing clumping artefacts into the pedestal. Reproduced from [2].

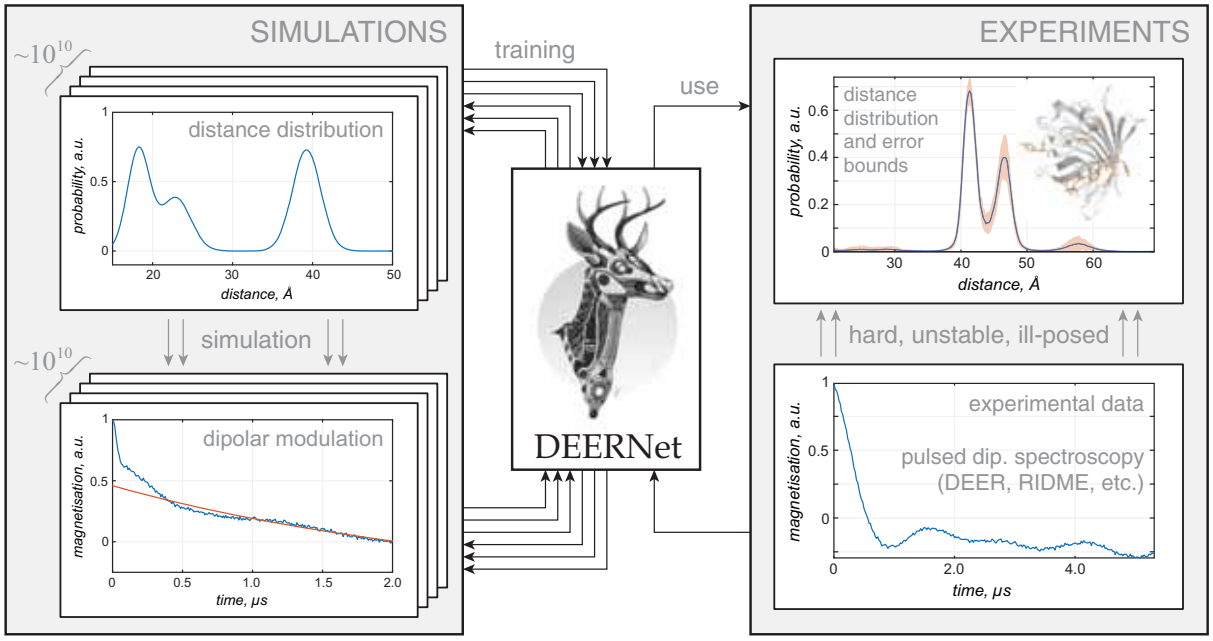



**Figure 2.** DEERNet training and inference flowchart. The block schematic shows the relationship between the computationally generated training database, the neural network, and its practical application in the context of pulsed dipolar spectroscopy distance measurement. To converge the training process, a carefully designed database with many billions of question-answer pairs is necessary; it can only be generated by highly accurate simulations including models of instrumental artefacts and noise. At the point when the network is used, it has no adjustable parameters. Reproduced from [2].

age to retain that key feature – whatever exotica you have (long distances, 3+ distances, multipath artefacts, *etc.*), DEERNet would just do that, no adjustable parameters, same two-line call. So far, common use scenarios have been: (a) in difficult cases where user bias in the choice of baseline and regularisation parameters must be eliminated; (b) as a second opinion alongside Tikhonov or model fitting tools; (c) as a source of initial guesses for Tikhonov or model fitting tools; (d) in situations when the users of DEER spectroscopy have no mathematical physics background and no interest in methodology, and only seek a reliable data processing tool.

More generally, neural nets convert the ability to simulate complex physical phenomena into the ability to interpret experimental data without fitting – at least in the cases where the relationship is a Fredholm integral. Anyone who has ever programmed a two-spin system simulation would find them easy to understand and use. Time to buy a GPU?


1. P. Ionita, A. Volkov, G. Jeschke, V. Chechik, Lateral diffusion of thiol ligands on the surface of Au nanoparticles: an electron paramagnetic resonance study. *Analytical Chemistry* **80**, 95–106 (2008).
2. J. Keeley, T. Choudhury, L. Galazzo, E. Bordignon, A. Feintuch, D. Goldfarb, H. Russell, M. J. Taylor, J. E. Lovett, A. Eggeling, L. Fábregas Ibáñez, K. Keller, M. Yulikov, G. Jeschke, I. Kuprov, Neural networks in pulsed dipolar spectroscopy: a practical guide. *Journal of Magnetic Resonance* **338**, 107186 (2022).
3. S. G. Worswick, J. A. Spencer, G. Jeschke, I. Kuprov, Deep neural network processing of DEER data. *Science Advances* **4**, eaat5218 (2018).
4. J. L. Amey, J. Keeley, T. Choudhury, I. Kuprov, Neural network interpretation using descrambler groups. *Proceedings of the National Academy of Sciences* **118**, e2016917118 (2021).

## The 55th Annual International Meeting of the RSC ESR Group

June 2022, St Andrews, UK

Following on from a highly successful virtual meeting in 2021, masterfully organised by Dr Emma Richards of University of Cardiff, the 55th Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry saw a return to an in-person event, coordinated by Dr Janet Lovett. The meeting returned to Scotland, which had also played host to our last pre-pandemic in-person meeting, held in Glasgow in 2019. On this occasion there was no whisky distillery tour but the meeting kicked off after dinner with an informative lecture on scotch whisky. This was followed by a tasting event and drinks reception, providing a welcome opportunity to renew acquaintances in person before the start of the scientific programme. The social programme also included the traditional conference banquet held in the historic Lower College Hall of the University of St Andrews, a venue some may have recognised from our 2014 conference held in nearby Dundee. Prior to the meal guests were treated to Scottish bagpipe music before assembling for a group photograph on the lawn, and after the meal and speeches the more energetic could dance the night away at a traditional Ceilidh in Upper College Hall.

While always clear that the record participation of over 500 delegates for the 2021 online event could not be matched by a physical meeting we were pleased to welcome to St Andrews nearly 140 participants from at least 11 different countries. In a break from group tradition the conference ran from Monday evening to Friday lunchtime, rather than Sunday to Thursday. While this was necessary in part due to limited Sunday train services the shift to a Monday start is planned to continue for future conferences, reducing the intrusion of the meeting and associated travel into valuable weekend time.

During the meeting we received a brief Bruker organisational update introducing Dr Frédéric Jaspard as the EPR Business Line and Product Manager, who noted that Dr Peter Höfer was now semi-retired. Peter has been a regular attendee of the RSC ESR meeting for many years, honoured in 2017 with the award of the Bruker Prize for the invention of 2D HYSCORE and with a legacy that also includes the establishment of the Bruker thesis prize for an outstanding PhD thesis in the field of EPR spectroscopy. Many subsequent speakers noted with gratitude the support they had received from Peter over the years. We offer our best wishes to Peter for a long and happy retirement, and look forward to working with Frédéric and his team in the years to come. We are grateful to Bruker and all the conference sponsors, and thank them for their support without which the meeting would not be possible. In particular JEOL and the International EPR (ESR) Society (IES) sponsor awards given at the meetings as noted below. Other sponsors of the St Andrews meeting were Applied Magnetic Resonance, Bridge 12, CIQTEK, Cryogenic, the Institute of Physics (IOP) Magnetism Group and Magnetochemistry.

### Senior prizes

Prof. Gunnar Jeschke kicked off the scientific programme with his plenary lecture *"To relax or not to relax"*, the first of many speakers during the meeting to discuss the nature of phase memory loss in electron spin systems. Other plenary lectures were presented by Prof. Songi Han (*"Dynamic Nuclear Polarization using Electron Spins Clusters"*), Prof. John Morton (*"Enhanced sensitivity ESR and spin-based quantum memories"*), and Prof. Sunil Saxena (*"A metallic spin on protein dynamics"*). In addition to these plenary lectures and five invited talks the meeting also hosted an IES prize session chaired by IES President Prof. Songi Han. Winner of the 2021 Silver Medal for Instrumentation Prof. Stefan Stoll started the session with his lecture *"Understanding electron spin decoherence"* while Prof. Marina Bennati received the 2022 Silver Medal in Physics/Materials Science and delivered a lecture *"Recent Developments in ENDOR and Liquid DNP spectroscopy"*.

One of the highlights of the RSC ESR group meeting is the award of the prestigious Bruker prize, an annual lectureship and prize, given to a scientist who has made a major contribution to the application of EPR spectroscopy, which Bruker Corporation has generously sponsored since 1986. After both 2020 and 2021 prize lectures were delivered online during the Cardiff virtual meeting, this year saw a welcome return to an in-person prize session and Bruker sponsored celebratory drinks reception. The Bruker Prize 2022 was awarded to Prof. Graham Smith of the University of St Andrews, who gave an excellent lecture *"Sensitivity and Time Resolution in High field EPR"* which highlighted the wide scope of Graham's work spanning both high-field EPR and many other millimeter wave technologies. Most within the EPR community will be aware of the HiPER instrument developed by Graham and his team, which in Graham's own words is a "quasi-optical, AWG-controlled, 94 GHz pulsed EPR spectrometer, which operates at kW power levels over 1 GHz instantaneous bandwidth", and many attendees took the opportunity to join a guided tour of the labs with Graham's team.

**Award of: IES Silver medals to Prof. Stefan Stoll (2021 Instrumentation) and Prof. Marina Bennati (2022 Physics/Materials Science), with IES President Prof. Songi Han (right) and local organizer Dr Janet Lovett (left)**

**Left panel: Award of 2022 Bruker Prize to Prof. Graham Smith (centre), with Dr Frédéric Jaspard of Bruker (left) and RSC ESR group Chair Prof. Christiane Timmel (right). Right panel: Award of 2022 Bruker Thesis Prize to Dr Janne Soetbeer (centre), with her supervisor Prof Gunnar Jeschke (right) and Dr Frédéric Jaspard of Bruker (left).**

### Junior prizes

One of the great traditions of the RSC ESR Group meeting is the JEOL medal which has been running since 1997. The award is open to applications from PhD students and first-year postdoctoral researchers, with participants in the prize lecture session selected from the abstracts submitted. Once again the entries were of a high calibre, presenting a significant challenge to the ESR group committee in both short-listing six speakers and judging the talks which spanned a wide range of EPR topics. The winner of the 2022 JEOL medal was Fabian Hecker of the Max-Planck Institute Göttingen for his talk *"$^{17}O$ hyperfine spectroscopy to detect water binding to biologically relevant radicals"*, with Yujie Zhao of University of St Andrews and Luis Fábregas-Ibáñez of ETH Zurich the runners-up in another tight competition. We thank JEOL for continuing to support the medal, and generously sponsoring an evening drinks reception.

Over 60 posters were presented during the two poster sessions of the meeting and we were once again pleased to be supported by the International EPR Society at the Conference, who awarded poster prizes to Ciarán Rogers of University of Manchester (for a poster titled *"Modelling Conformational Flexibility in a Spectrally Addressable Multi-Spin Molecular Qubit Model System"*) and Orit Nir-Arad of Tel-Aviv University (for a poster titled *"Design and Construction of 14 Tesla DNP / EPR spectrometer"*). The Royal Society of Chemistry ESR group also awarded poster prizes to Jörg W.A. Fischer (ETH Zurich), Lubomir Loci (University of Manchester), Julie Toftelund Lerche (University of Copenhagen), Daniele Panariti (University of Padova) and last but not least Thomas S.C. Macdonald who joined us all the way from Australia (UNSW Sydney)!

While the above-mentioned prizes are awarded for a talk or poster given at the meeting, since 2015 Bruker have generously sponsored a lecture and significant cash prize based on assessment of a full PhD thesis. In the closest competition yet the 8th Bruker Thesis Prize was awarded to Dr Janne Soetbeer for her PhD thesis completed at ETH Zurich. Janne gave an excellent lecture *"Dynamical decoupling for quantitative decoherence analysis via noise spectroscopy"* in which she highlighted a number of possibilities for further exploitation of noise spectroscopy that others in the community might wish to investigate. We note again our gratitude to Bruker for their support of this prize, and the expert reviewers who assisted in the substantial task of assessing a number of full PhD theses.

### Committee

Having steered the committee through a few difficult years to finally oversee the first in-person conference during her term of office Prof. Christiane Timmel has been re-elected as group chair until 2025. As mentioned in her after dinner speech at the conference we owe a huge debt of gratitude to Prof. David Norman who stands down as treasurer, leaving the group accounts in significantly better shape than when he took up the reigns as deputy treasurer in 2017. We wish David well on his retirement, and his successor as treasurer, Dr Emma Richards, well in her new role. Having already shown her impressive managerial ability in organising the 2021 meeting which started as the hoped for in-person event and pivoted to become the ESR groups' first ever full virtual conference, we are confident that the group finances are in safe hands. We also thank Dr Paul Jonsen and Dr Floriana Tuna for their service as general members on the committee, with Paul beginning a second committee term and Floriana standing down at the St Andrews meeting. An RSC managed online nomination system is being used to recruit new ordinary committee members, with nominations due by the end of August 2022.

We thank Janet Lovett and her team from the Department of Physics at the University of St Andrews for organising a highly enjoyable 2022 meeting. Not only did Janet successfully organise the group's first ever meeting in St Andrews, a venue which has long been considered infeasible due to the restricted accommodation options in this small city often filled by golf enthusiasts and other tourists, but she contended admirably with ever changing covid related rules and guidance from multiple organisations during contract negotiations. Janet remains on the committee *ex officio* as past conference organiser to pass on her considerable experience as the next meeting is organised.

### Next conference

Dr Christos Pliotas is organising the next conference in Leeds between Monday 27th and Thursday 30th March 2023, and we are pleased to announce that this will be a joint meeting with the IES. Please see http://www.esr-group.org/conferences/2023-conference-leeds/ for further information and join the RSC-ESR-GROUP@JISCMAIL.AC.UK mail list or follow @RSC_ESR on Twitter to be notified when registration and abstract submission opens.

Dr. Chris Wedge, Secretary
School of Applied Sciences
University of Huddersfield, UK

## ICONS-5: Hyperpolarization and Magnetic Resonance

ICONS-5, organized during August 31 – September 02, 2022, was the fifth edition of the on-line magnetic resonance conference series called Konstantin Ivanov InterCONtinental Magnetic Resonance Seminar [1–5], named after our untimely deceased colleague and friend, Konstantin (Kostya) Ivanov. The ICONS conferences are an off-shoot of the weekly Intercontinental NMR Seminar Series that started on April 8, 2020. This seminar series has contributed to maintain the communication and dissemination of research ideas among the magnetic research community in times of COVID-19 pandemic and will continue to do so beyond. In the framework of the ICONS series, until now, more than 130 scientists from five different continents have presented their latest results. Contrary to what "NMR" in the title suggests, both the ICONS seminars and the ICONS conference series cover all aspects of magnetic resonance, including both EPR and NMR, with the goal to foster new developments in magnetic resonance and to foster communication and dissemination of research ideas among the magnetic resonance community. While the speakers at the half-yearly conferences are chosen among experienced scientists in the field, the weekly seminar series tries to give a balanced mixture between early-stage researchers and experienced scientists. The ICONS-5 conference attracted registrations from nearly 200 people from 30 countries (in the spirit of the meeting, covering 6 continents, Europe, North America, South America, Africa, Australia, and Asia) and spanned 17 time zones from Japan over Europe to the West Coast. The meeting talks were broadcast across the Zoom and YouTube platforms. The average combined attendance was around 120.

Following the tradition that the summer ICONS conferences are broad in scope, we invited a number of cutting-edge speakers from solution-state and solid-state NMR, EPR, Dynamic Nuclear Polarization, Parahydrogen Induced Polarization (PHIP, SABRE), Molecular Dynamics, NMR-diffusometry and -relaxometry and relaxation theory in order to highlight recent developments in these fields. The twelve invited speakers were in chronological order Malcolm Levitt, UK, Björn Corzilius, Germany, Paul Schanda, Austria, Thomas Theis, USA, Jamie Walls, USA, Patrice Bertet, France, Ashok Sekhar, India, Bernhard Blümich, Germany, Nikolai Skrynnikov, Russia, Jean-Pierre Korb, France, Eva Meirovitch, Israel and Thomas Barbara, USA. The presentations spanned a broad range of topics, going from basic spin-physics and experimental technology over applications in chemistry and biochemistry, medical imaging, and investigation of physiological processes. For details of the contents of the talks see the upcoming report in APMR [5].

The conference and seminar series were sponsored by the Alexander von Humboldt Foundation, Wiley, Springer, HyperSpin, and Adani. Following the scheme of a general MR conference in summer alternating with a specialized conference on cutting-edge topics in winter, there are already plans for a specialized ICONS-6 in spring of 2023. For updates and the schedule of upcoming talks see the home page of the meeting ICONS-Seminar.


1. Abergel, D.; Buntkowsky, G.; Ivanov, K. L.; Madhu, P. K., Editorial: Introducing the Intercontinental NMR Seminar ICONS2020. Appl. Magn. Reson. 2021, **52**, 1–4.
2. Abergel, D.; Buntkowsky, G.; Ivanov, K. L.; Madhu, P. K., Editorial: The Second Intercontinental NMR Conference ICONS2021. Appl. Magn. Reson. 2021, **52**, 565-569.
3. Buntkowsky, G.; Abergel, D.; Madhu, P. K., Editorial: The Third Konstantin Ivanov Intercontinental Magnetic Resonance Conference on Methods and Applications ICONS 3, Appl. Magn. Reson. 2021, **52**, 1–4.
4. Buntkowsky, G.; Abergel, D.; Madhu, P. K., Editorial: The Fourth Konstantin Ivanov Intercontinental Magnetic Resonance Conference on Methods and Applications ICONS 4, Appl. Magn. Reson. 2022, **53**, 857–860.
5. Buntkowsky, G.; Abergel, D.; Madhu, P. K., Editorial: The Fifth Konstantin Ivanov Intercontinental Magnetic Resonance Conference on Methods and Applications ICONS 5, Appl. Magn. Reson. 2022, available online, https://doi.org/10.1007/s00723-022-01501-y.


G. Buntkowsky, D. Abergel, P. K. Madhu

**Asif Equbal**

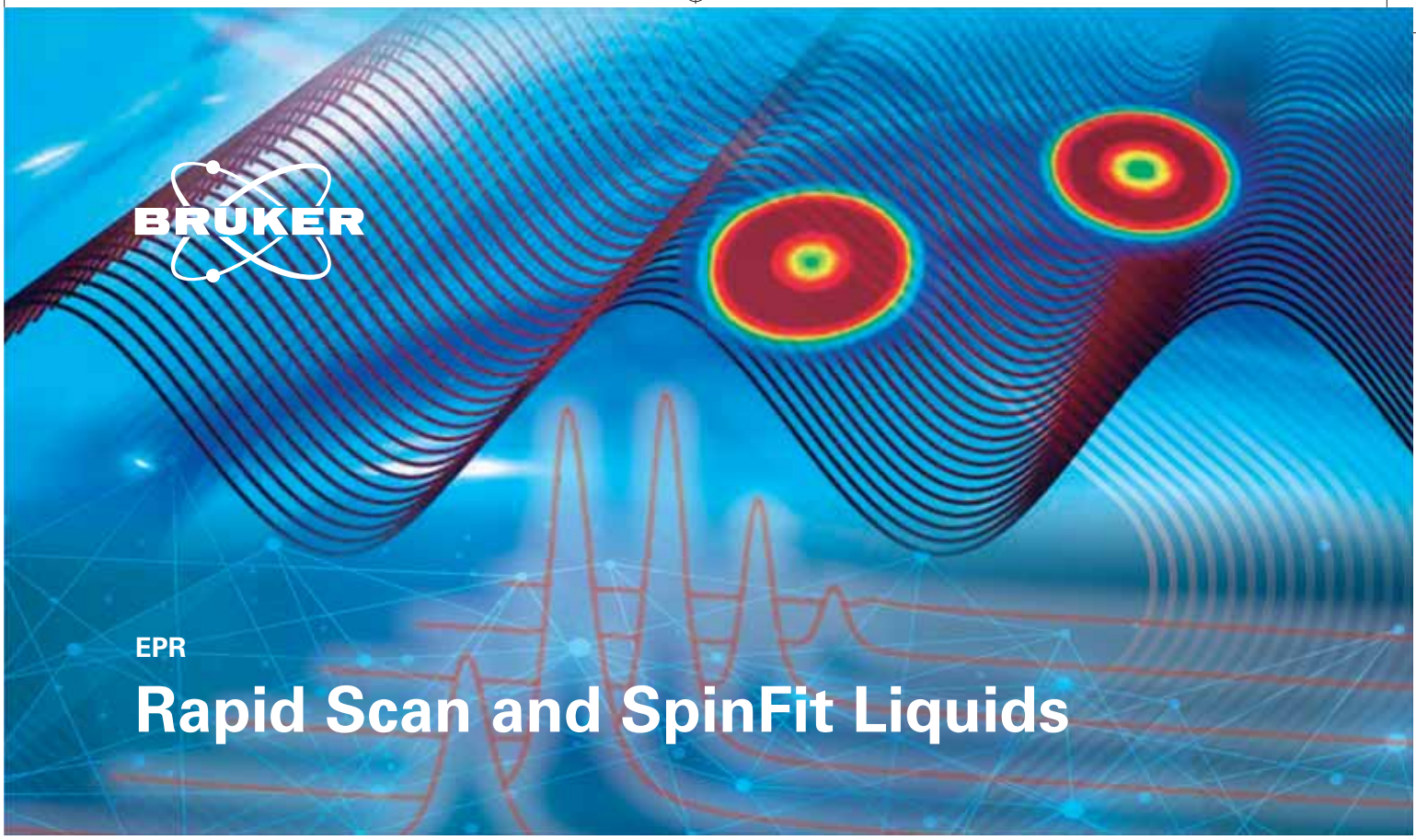
Asif Equbal received the 2022 John Weil Young Investigator Award (YIA) for his outstanding contributions to the field of EPR by applying the understanding of coupled electron and nuclear spins to advance dynamic nuclear polarization (DNP), a technique that combines the sensitivity of EPR and the high spectral resolution of NMR. DNP has transformed many branches of NMR in fundamental ways. Asif Equbal has been instrumental in applying the understanding of electron spin physics to advance the scope of DNP, and has become well known in the magnetic resonance community for his multiple contributions.

He advanced the theoretical understanding of DNP by considering the complexity of interactions between multiple electrons and nuclear spins, discovered the efficiency of thermal mixing DNP using narrow-line radicals at high magnetic fields, and realized the sensitization of fast-relaxing and broad paramagnetic species for DNP by coupling to narrow-line radicals, among other things manifested by the truncated cross effect. This understanding directly contributes to extending the scope of DNP to new spin systems, DNP under magic angle spinning at high magnetic fields, and DNP with optical pumping.

Dr. Equbal has also been playing a lead role in organizing regular web-based seminars under the forum Global NMR Discussion Meetings. These seminars have covered various aspects of magnetic resonance, including key topics of EPR, NMR, DNP, and magnetic resonance instrumentation. The range of speakers and topics this forum has witnessed is also a testimony to Dr. Equbal's knowledge of the field and general standing.

Dr. Equbal did his Master thesis with Prof. Matthias Ernst at the ETH, his PhD studies with Prof. Niels Chr. Nielsen at Aarhus University and with Prof. P. K. Madhu at TIFR, Postdoctoral research with Prof. Songi Han at UC Santa Barbara. He has also explored design of molecular spin qubits for quantum sensing and computation using integrated optical and EPR spectroscopy with Prof. Mike Wasielewski at Northwestern University.

Dr. Equbal is pursuing an independent academic career. He became a Tenure Track Assistant Professor in the Chemistry department at New York University Abu Dhabi in September 2022. His research harnesses the power of EPR to advance the fields of DNP and quantum information science. We wish Dr. Equbal all the best for his future endeavors.



EPR

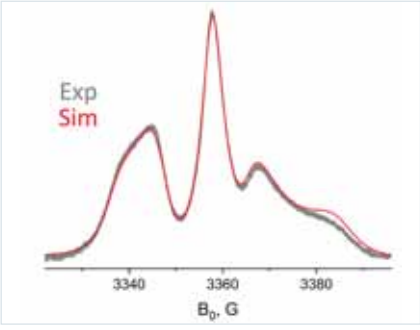
# Rapid Scan and SpinFit Liquids

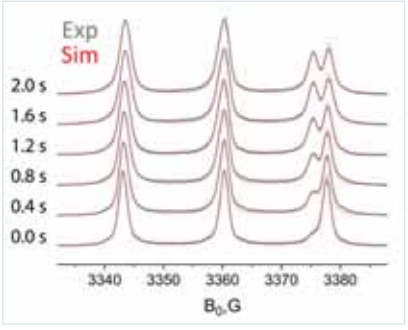
## ... a dynamic duo

**Rapid Scan Accessory**
Enhanced sensitivity and superior time resolution

**SpinFit Liquids**
Detailed lineshape analysis for Rapid Scan EPR spectra

- Simulation of derivative and absorption EPR spectra
- Automatic selection of dynamic regime (slow/fast motion)
- Option for anisotropic diffusion
- Simulation and fitting of 1D and 2D datasets




**Left:** Anisotropic diffusion dominated spectrum of 5-doxyl stearic acid in liposomes
**Right:** Redistribution of TEMPO between water and oil phases

**For more information please visit www.bruker.com**

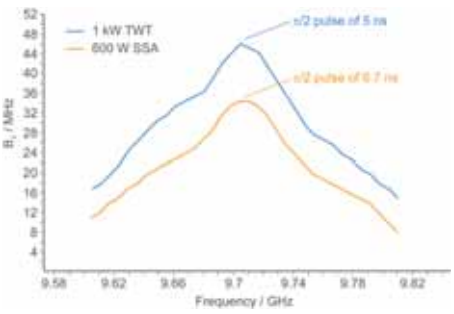
EPR

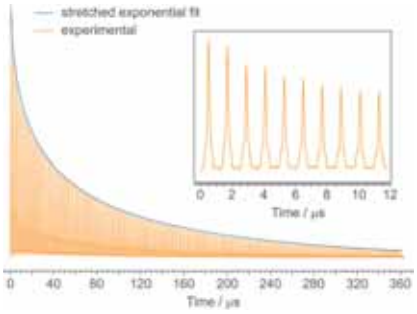
# A new family of Bruker-developed solid-state pulse amplifiers

## … is growing with the 600 W X-band amplifier.

**Features**

- Suitable for **all X-band Flexline resonators**
- For pulsed X-band applications like DEER, ENDOR, ESEEM and HYSCORE
- A new alternative to the 1 kW X-band TWT




**Left:** Bandwidth profiles of a MD4 resonator for different amplifiers under identical coupling conditions;
**Right:** EPR signal of γ-irradiated quartz measured by a CPMG sequence with 300 refocusing pulses

**For more information please visit www.bruker.com**

Innovation with Integrity