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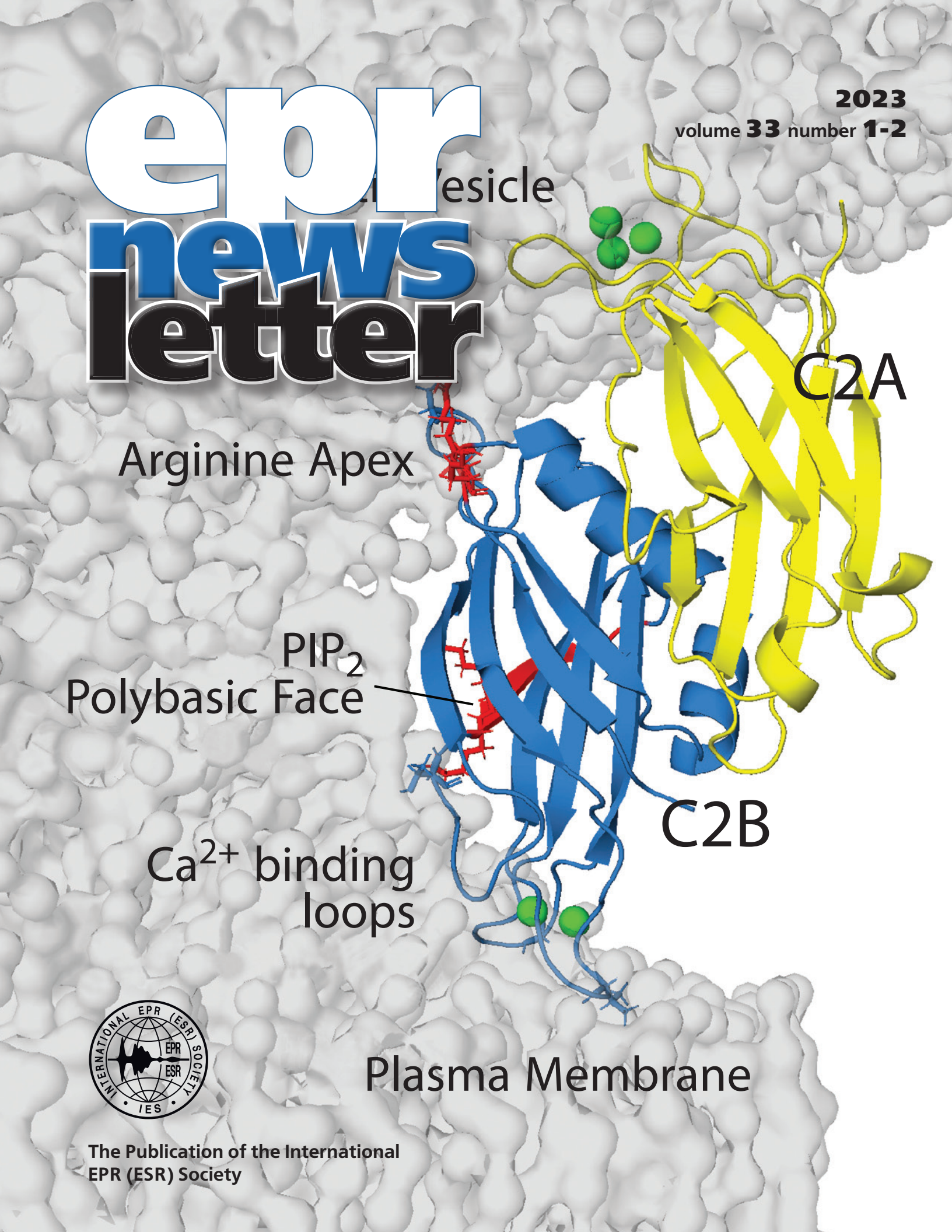

The Publication of the International
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Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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

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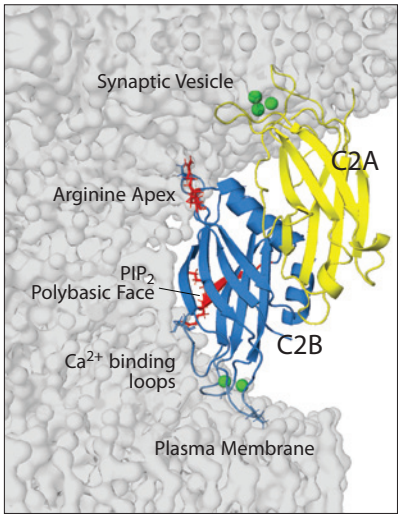

The cover picture illustrates aspects of the research of David Cafiso, recipient of the IES Silver Medal Biology/Medicine 2022. It shows the two C2 domains of Synaptotagmin-1, which functions as the calcium sensor for neuronal exocytosis, interacting with a highly curved membrane intermediate during the fusion process. Conserved regions of the C2 domains have been shown to insert into the membrane and to drive the expansion of the fusion pore, thereby promoting a rapid release of neurotransmitter from the synaptic vesicle to the synapse. See also David Cafiso's interview on the occasion of his Piette Award 2013, *EPR newsletter*, 23/3 p. 7 (2013).

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Editorial

Dear colleagues,

I'm hoping that you feel it is time for the *EPR newsletter* to celebrate its 35th anniversary, and you might have expected to see the cover of this public issue 33/1 composed of the covers of preceding issues as we did for the issue 28/1-2 or something of this kind. However, our motto is "be always unexpected!" and we present to you the cover picture illustrating the research of David Cafiso, recipient of the IES Silver Medal Biology/Medicine 2022. You might also be expecting to see an interview or article from David in this issue telling his success story?! Off the target! Not in this issue of our publication! For the time being, I may only quote David's message to young scientists from his interview on the occasion of his Piette Award in 2013: "I think it is very important for any scientist to not be discouraged by a result that they do not expect or by a result that does not fit their theory. If the experiment is correctly designed, it is telling you something about the way things work, and if the result does not fit your expectations, you now have the opportunity to learn something". Well said indeed!

Our anniversary gives me a nice excuse to remind you that the International EPR Society is actually two years younger than the *EPR newsletter* and that the main celebration is still ahead. Look forward to it!

There is a theory that any two people on our planet are separated by no more than five common acquaintances (six levels of connection). In the case of the EPR community, I presume this number of common acquaintances is even less, maybe two or three?! What do you think? In fact, our community is a big family. Some families are traditionally sending out their family letters in the end of the year telling about their life. I would say that the *EPR newsletter* is the family letter of the IES and the only difference is that its periodicity is higher than once per year.

Well... maybe not the only difference. All issues of the *EPR newsletter* compose an encyclopedia of all aspects of the research carried out by the EPR community and diverse activities of our society and also show that there is life beyond EPR. In our issues, you can find any EPR-related information you are interested in. You will also meet with pioneers of magnetic resonance and learn how great discoveries were made, get an insight into great minds who share their ideas with us, read success stories of laureates of different magnetic resonance awards, look into the eyes of newcomers who make their first steps in the career in science and be charmed by their enthusiasm and vigor, to name a few.

The key word here is "be interested in". All depends on you! And we strive at our best. Welcome to the *EPR newsletter*!

Laila Mosina

Letter of the President

Dear Friends, Colleagues and Students of the international EPR/ESR society (IES).

We have our foot into the year 2023 and are more hopeful than ever that we have all learned how to live our lives, do our science, teach our students, collaborate across the globe and exchange our ideas at conferences, while carrying the lessons and scars of the global pandemic that has become the one defining common experience together. We have come to learn to embrace the virtue of virtual meetings as a tool, but also learned that "virtual" is only a tool, and that absolutely nothing can replace real human interactions that bring friendship, humanity, spontaneity, and unexpected twists into our scientific stories. Science is human, and that is also what we wish to be the guiding principle of our International EPR/ESR society. The role of our society is to support the people in the EPR community, the student who has just begun to grasp the beauty of EPR, the young scientist who is brave enough to launch an academic career, the science innovators of our society who push the frontier of EPR, the entrepreneur who is widening the science scope of our community and the Fellows who have spent their academic lifetime to solidify the impact of EPR spectroscopy to advance chemistry, life sciences, physics, materials science and medicine.

First, I would like to congratulate the following 2023 IES Awardees. Congratulations!

- 2023 IES John Weil Young Investigator Award: Mantas Simenas for his innovative work in developing EPR cryoprobe and other instrumentation
- 2023 IES Gold Medal: awarded to Gunnar Jeschke for his impact on establishing pulsed EPR methods for the study of biological and chemical systems
- 2023 IES Fellow: jointly awarded to Howard Halpern and Murali K. Cherukuri Krishna for their lifetime and seminal contributions to push the field of biomedical EPR towards clinical translational research

We are so pleased of the 2023 Poster Prize winners: Ciaran Rogers and Orit Nir-Arad of the 2022 RSC EPR conference in St. Andrews, Tobias Hett and Mantas Simenas of the 2022 EUROMAR, Xiaowei Bogetti, Cooper Selco and Euan N. Bassey of the 2022 RMC EPR conference, Katie Whitcomb of the 50th edition of the Southeastern Magnetic Resonance Conference (SEMRC), and Chloe Buyse of the International Workshop on EPR in Biology and Medicine. Each poster prize winner receives an award, an invitation to the IES Virtual EPR meeting (IVEM) and an invitation to be featured at our EPR newsletter. Keep up the good work!

The next IES award selection is another one focused on honoring the accomplishments of junior and senior EPR scientists around the world, *the IES Best Paper Award of 2023*, with deadline of March 31, 2023. The IES acknowledges each year up to two publications as "best papers" in the field of EPR. The first author is recognized with this award and a monetary award. The expectation is that the first author be a young scientist. The nomination material should include the publication in PDF and a Letter by the advisor or collaborator explaining the role of the nominee in generating this paper, as well as the impact of this publication to the field of EPR and be sent to ab359@technion.ac.il.

We are so impressed of the leadership of the young scientists of our EPR community who are already forging a way forward, as reflected in the first ever Young Investigators in Magnetic Resonance workshop, taking place on September 21–22, 2023 in Konstanz Germany, organized by Annalisa Pierro, Angeliki Giannoulis, Alessio Bonucci and Dinar Abdullin. The IES is proud to be offering support and encouragements.

You can hear all about our initiatives and provide feedback at our next Annual General Meeting (AGM) that will be held at the IES designated meeting the 56th RSC EPR meeting taking place during March 27–30 2023 in Leeds, UK. A Zoom link will be shared with all members. Please join us, or even better, register for the RSC EPR meeting and come in person. It will be a wonderful meeting.

Topics of discussion at the AGM will include an update on the initiative led by Thomas Prisner on generating the infrastructure for a shared EPR data base for our community, a proposal by the IES to add a new position to the IES executive board, a Virtual Media Officer, to help broaden our reach, efforts to partner with regional and worldwide magnetic resonance communities and a new election for the President and Vice-Presidents of the IES whose terms are ending on December 31, 2023. The role of the IES Executive board is critical. We need your input to prepare excellent nominations for the new term starting on January 1, 2024 and ending on December 31, 2026. Please think of nominees and reach out to us.

We are exceptionally proud of the IVEM activities led by Zhongyu Yang and Thomas Schmidt together with the IVEM committee who are doing a fabulous job keeping this important forum lively and exciting. You are so welcome to sign up to give a talk or a tutorial lesson using the sign-up sheet: https://forms.gle/Usv8sbj3LUr7QvcE8, and stay updated on IVEM's next events on https://sites.google.com/view/ie-ivem-online-activities/home or https://ieprs.org/on-line-activities.

The IES also recognizes the critical role that our commercial vendors play by allowing the scientists to use state of the art technology for conducting science. We see the passion of the people offering products for the scientists and are working hard to shine a bright line on them using our EPR newsletter platform. The EPR newsletter covers all aspects of the IES activities and far beyond. We welcome those who are interested in the life of the magnetic resonance community to our publication (https://ieprs.org/newsletterpage). Be our guest!

Most importantly, we strive to serve the community and stay active and dynamic. We believe in the critical importance of working towards supporting a much more diverse science community than we are currently representing. A more diverse cohort of scientists, considering geography, ethnicity, gender and otherwise, will be the generator of creativity and innovative ideas. The IES is determined to diversify its leadership and membership. Help us get there. Help us nominate new names for the leadership in the future, awards and get involved with your ideas. We are all ears.

With that, I look forward to seeing many of you in 2023!

Songi Han

Interview with Professor Jack H. Freed, Director & Principal Investigator, on the New National ESR Resource

EPR newsletter: *Dear Professor Freed, the IES greatly appreciates the support of ACERT, which contributes to the EPR community by generating services of importance to our community. We are most appreciative that you agreed to answer the questions of this interview. You are embarking on a new resource; how does it differ from the ESR Center that you ran for 20 years?*

Indeed, our new National Biomedical Resource for Advanced ESR Spectroscopy is an outgrowth of our ESR Center that we ran from September 2001 till March 2022. In fact, we have kept the original acronym: ACERT, although our objectives are somewhat different. Our past ACERT was heavily involved with ESR technology development, whereas the new Resource places greater emphasis on service to the national ESR community. This transition can be summarized by noting that many ESR technologies developed previously (some even unique in the world) are now available to the ESR community in the form of training on the new concepts and on the use of the latest spectrometers, software, and their capabilities, and making them available to the community as users and/or for us to run the samples, analyze them, and supply the useful results to the community. In this new endeavor my distinguished structural biology colleague, Professor Brian Crane, is joining me as co-PI.

Are you offering a full range of ESR technologies to both beginners and advanced ESR researchers?

Yes indeed! We hope to be a "one-stop shop" for ESR research. We are providing access to technologies that enable the study of structure and dynamics, especially of biomolecules, for a wide range of distances and time scales. At the "beginners" level we will provide ESR cw spectra of samples of all types including their analysis. Somewhat more sophisticated is the use of ESR for the study of the dynamics of biomolecules. This can be done by obtaining simple 1D ESR spectra, by obtaining the spectra over a range of ESR frequencies (9 to 240 GHz), and also by two-dimensional (2D) ESR, which is the most informative and advanced. Along with the capabilities for all these experiments we have the software for analyzing and interpreting them.

In recent years ESR has been very successfully applied in the field of structural biology, i.e., protein structure. What do you offer for this important application?

The two most powerful experimental ESR technologies are DEER and DQC. We have spectrometers that cover several frequencies and that perform state-of-the-art experiments for both approaches. In the past we have published numerous papers elucidating the structures of a wide range of proteins, so we are very experienced in this activity. We also have a biosynthesis lab with which we can spin label the proteins of interest. It can also be utilized by users who visit our Resource. In addition we believe we have developed the most powerful data processing methods for relating experiments on bilabeled proteins to distributions of distances between the labels, which is the desired result for the application of ESR to structural biology. This has become ▶

National Biomedical Resource for Advanced ESR Spectroscopy (ACERT)

Our mission. To provide an extensive range of modern ESR facilities for biomedical researchers. It is based on our 30-plus years in the development of ESR for biomedical studies. Our instruments provide the capabilities of studying protein structure/function as well as protein and membrane dynamics using the techniques of spin labeling. Our instruments are highly sensitive and constantly being improved, yet our signal processing methods enable us to recover excellent signals from even weak experimental ones, such as for spin trapping and many other ESR applications. These facilities and technologies are available to all users. We will conduct experiments on our instruments as needed and/or train the user on their use, and we will provide the data and their interpretation. Please contact us or make a request for services.

Our facilities. Our ESR spectrometers include a Bruker ELEXSYS 500 spectrometer with X-band bridge, for different 1D/2D cw ESR experiments over a temperature range of 4–450 K; a Bruker ELEXSYS 580 pulse EPR/ENDOR spectrometer operating at 9 and 35 GHz, for a variety of ENDOR and pulse/cw experiments including PDS, ESEEM, T_1/T_2 measurements etc. at a temperature range of 10–400 K; a vintage pulsed, FT and 2D-FT spectrometer operating at 9 and 17 GHz and dedicated mainly to PDS (Pulse Dipolar Spectroscopy); a new state-of-the-art 8–18 GHz pulsed and 2D-FT spectrometer mainly dedicated to 2D-ELDOR; a new 35 GHz pulsed, FT, and 2D-FT-ESR Spectrometer dedicated mainly to PDS; a 95 GHz high-power pulsed 2D-FT-ESR, and cw spectrometer with low-temperature VTI; 93 GHz pulsed-ESR spectrometer mainly for micro-samples; and a 170/240 GHz ESR cw and pulse spectrometer.

In addition, there are computing center workstations for theoretical simulation of ESR spectra; a wet chemistry and biochemistry lab for sample preparation and synthesis; electronics and machining facilities; and extensive downloadable software.

Our history. This new ACERT NIH Resource was funded in July, 2022. It is an outgrowth of the 20 years (Sept. 2001 – Mar. 2022) of ACERT as a P41 NIH-funded ESR Technology Center at Cornell University, Ithaca, NY. It is an R24 National and Regional Resource Center, funded by the National Institute of General Medical Sciences (NIGMS) of the National Institutes of Health (NIH), occupying 613+ sq. meters (6,600 sq. ft.). The Resource Director is Jack H. Freed and the Co-Director is Brian R. Crane. It is the only user Resource of its type in the United States providing ESR services to all potential users. The primary purpose of the Resource is to provide collaborations and service to a wide base of users.

a very popular methodology, and we are now receiving requests from first-time users.

What will you be offering the ESR community in terms of user training and outreach?

ESR is not widely available, and there are researchers, especially young investigators who lack relevant resources, for whom ACERT can act as a "home family." Since ACERT is funded by the NIH, the services we provide are mostly free of charge. Much of contemporary ESR requires a high level of sophistication both in experimental and compositional methods. We plan a regular series of workshops to be devoted to training students and researchers in the latest technologies. These workshops not only provide advanced training, but also serve as an effective means to disseminate much of the specialized knowledge and understanding that our staff has acquired. They also better prepare for collaborative and service work with ACERT, for appreciating the value of our advanced methods, and for enabling some of them to develop such technologies in their own laboratories. Planned workshops include: Dynamics of Biomolecules by ESR; ESR for Structural Biology; Data Processing in ESR; and Computational Methods in ESR.

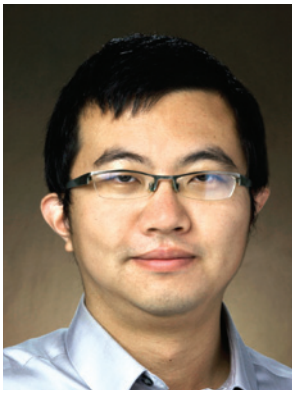
In addition to Workshops, what outreach is planned?

First of all let me announce that ACERT has become a New Major Patron of the International EPR(ESR) Society. In fact, the workshops planned by ACERT will be sponsored by the IES with additional focus on first-time users by offering participant support and fellowships. ACERT researchers will be contributing a series of seminar talks through the auspices of IES to share technical know-how of ACERT capabilities through the IES Virtual EPR Meeting (IVEM) mechanism. We plan to create a central video repository of ESR seminars available via YouTube and the IES website, workshops, and tutorials so that researchers can benefit from the knowledge that is otherwise inaccessible.

How should one arrange for planned visits and/or for your various facilities?

The best way to initiate communication is by contacting our ACERT manager Art Samplaski, either by phone (+1-607-255-4632) or email (acert@cornell.edu; please put "IES query" at the start of the subject line).

International Virtual ESR/EPR Meeting (IVEM): a new avenue to connect the International ESR/EPR Society (IES) and ESR/EPR community



Thomas Schmidt and Zhongyu Yang

The concept of International Virtual ESR/EPR Meeting (IVEM) was originally conceived by a few active and talented graduate students and postdocs, including Nino Wili, Lizzy Canarie, and Shreya Ghosh, from Europe and United States, with the motivation of connecting the students and postdocs in the community during the COVID-19 pandemic. During this time the IVEM served to satisfy the exchange of ideas that previously was embodied by conferences and collaborations. This was of specific value as institutions/research groups are widely spread over 5 continents, Asia, Australia, Europe, North America, and South America. Even travel within the same continent became extremely difficult, if not impossible. With a growing demand for EPR/ESR application to all facets of research IVEM serves as a platform that enables the exchange of ideas, promotes discussions and supports the next generation of EPR researchers. Thus, the first IVEM committee was formed and immediately received extremely positive feedback from postdocs and graduate students in the community. Starting with Dennis Bücker, our very first IVEM speaker, on March 20th, 2020, this biweekly online activity has successfully invited over 25 speakers and promoted over a dozen videos online in the first year, thanks to the rapid development of the community due to the tireless training of new generations of ESR/EPR workforce by pioneers!

At the end of 2020 the current IES president, Dr. Songi Han, promoted the idea to permanently engage the IVEM in the IES with the goal of ensuring a vibrant and well connected EPR community. This was accomplished by recruiting us as co-chairs of the IVEM committee and therefore creating a fluency of continued service. This will not only provide the stability of this important avenue to connect the society but also free up some burdens of graduate students and postdocs whose major goals would still be graduation, publications and finding jobs. Both of us were common attendees and were invited to give talks at IVEM giving a rough introduction to its organization and seminar architecture. Further, extensive help was given by the first IVEM committee, especially Dr. Nino Wili, the IES and Dr. Han. However, upon initiating the seminar series it became self-evident that additional help was needed; we were surprised by the amount of workload that was needed to establish a list of contacts, securely announce upcoming activities through the internet, and subsequently document the completed activities, raising even further the degree of appreciation towards the graduate students and postdocs in the first generation of the IVEM committee!

As mentioned, we came to the realization that we could not and should not organize the IVEM alone, not only because of the workload but also the limited connections and therefore missed opportunities to embrace the community, of which the latter was the original motivation of the IVEM! Thus, we formed the second generation of the IVEM committee, Nir Dayan (Technicon/Israel), Annalisa Pierro (French National Centre for Scientific Research/France), Julien Langley (Australian National University/Australia), Li Feng Lim (Australian National University/Australia), Jana Eisermann (Imperial College/England), Zhigjie Li (University of Science and Technology of China/China), Jaideep Singh (University of Southern California/USA), and Jing Jin (Boston College/USA). This 2021–2022 committee included graduate students and staff scientists from 4 continents working at research institutions, national labs, and universities. Some of the members also served in the first term, which permitted a smooth "transition" and significantly helped to reduce our workload. The creation and subsequent sharing of online forms permitted that everyone could schedule future speakers and upload relevant information, therefore elevating a transparent organization across the committee. One of the primary tasks for the committee consisted in recruiting potential speakers in their institutions/countries/networks and hosting individual IVEM seminars. The usual recruitment process consisted of an invitation a few months before and upon confirmation of interest, we quickly set up a date and time with the speaker. Further, key information for the talk was requested such as title, abstract, TOC figure, and a recent photo 2 weeks before the presentation date with submission date one week prior to the talk. The talk was further announced and promoted by circulating a flier of the upcoming IVEM talk to over 210 contacts as well as through the IES twitter account. After a meeting, we usually post a link of the recorded video record on a free website which permits further distribution of a wealth of information (also adapted from the first term of the IVEM committee). While the given task seemed initially trivial,

we did face challenges such as coordinating the presentation time and the recruitment of the audience. The presentation time became rather challenging as the goal was to include audiences from all over the world while respecting their time zones. The final result was a two time slot presentation system permitting a presenter to choose which schedule causes the least conflict. Yet with patience, flexibility and some intensive work, another 25 speakers were successfully invited and presented their research work at IVEM in the past year.

Now IVEM has begun the 3rd year's operation, which is our second year running the committee. Due to students' graduation and corresponding instability, with sincere appreciation to the "transition" committee and help from IES, we have recruited a new term of IVEM committee, Dr. Tomas Orlando (High Field National Labs/USA), Yujie Zhao (University of St. Andrews/Scotland), and Dr. Joseph McPeak (Helmholtz-Zentrum Berlin für Materialien und Energie/Germany). Through this term we are looking for improvements on our website and record sharing channels that will ultimately benefit new audience members. To do so, Dr. Tomas Orlando has already updated and polished our website (https://sites.google.com/view/ie-ivem-online-activities/home) which contains all the information about the previous and upcoming IVEM meetings as well as the link to a YouTube channel which will specifically post the recordings of IVEM talks. This channel can essentially be used as an educational tool as well for new graduate students to learn EPR. Another goal of this term is to make the already high-quality IVEM talks more interesting and competitive so that we are rewarding up to five IVEM best talks each year with monetary prizes, thanks to the generous support from the IES. We will include this exciting news to our invitation emails and announcement emails. The third goal is to broaden the diversity of speakers' fields and continents. We are thrilled to look for IVEM speakers in materials, biomedical, biophysics, structural biology, green/sustainable chemistry, chemical education, and physics research from all over the world with special priority to Asia and Australia. Our fourth goal is to improve the audience and their participation in the IVEM talks. We will strive our best to adjust timing so that more people from our community can attend conveniently. We welcome comments and nominations of best IVEM talk awards from the audience! Lastly, we want to help broadcast exciting news/papers/position openings in the field during our seminar. We also want to encourage every IVEM speaker to write a brief synopsis to your IVEM talk and publish it in IES newsletters.

With the original and always-be motivation of offering an opportunity for junior scientists to present their work to experts in the field without financial and travel burdens in a friendly environment, we believe the IVEM activity is critical for junior scientists to grow and perhaps choose ESR/EPR as their lifetime careers. As in all fields and all species, new generations are the future! IVEM is a bridge that directs a talented graduate student or postdoc to a successful investigator or industrial scientist. Although we are committed to our best, we cannot do this alone. We would appreciate it if more pioneers and masters in the field can attend IVEM, ask some questions, share with junior scientists your wisdoms and experience, or even just show us your smile which will connect your big names from prestigious journal publications to a real person. This may potentially help you find good postdocs as well! We are also deeply grateful if more PIs in the field can broadcast and encourage your students and postdocs to participate as speakers and/or audience, which will really make a big difference to unify our small community!

Interview with Professor Sandra Eaton, Bruker Prize 2002 and IES Fellow 2008

EPR newsletter: *Dear Professor Eaton, recently IES President Songi Han suggested that long standing IES Fellows be featured in our publication on their current research endeavors. It is fifteen years ago that you were granted the IES Fellowship, the highest designation and distinction of the IES, and you are continuing to innovate in science and have an impact on our society. We are most appreciative that you agreed to be interviewed. Why did you start towards your career in science?*

My parents were both scientists, but they made it clear to my brother and me that we could pursue whatever careers we wanted. They instilled a love of books, learning, and curiosity. My brother and I did science fair projects, each learned to play a musical instrument, and met people from many other countries because of my father's position at Harvard Dental School. In high school I could not decide whether I would pursue my interests in French, math, or chemistry. When I started college I quickly learned that other people were much more talented in French than I was, so I focused on math and chemistry. My undergraduate research project quickly convinced me that chemistry had lots of exciting opportunities.

Who introduced you into magnetic resonance?

As an undergraduate at Wellesley College I was encouraged to being research early in my degree. In the summer after my first year I worked full-time in the research group of Prof. Emily Dudek. Her enthusiasm for chemistry was infectious. I was one of three undergraduates preparing nickel(II) complexes of salicylaldimine ligands. Varying the bulkiness of substituents changed the geometry between square planar and tetrahedral limits. We studied the electron spin delocalization by NMR. We did our syntheses and basic characterization of the products at Wellesley. We had the great advantage that Dr. Dudek's husband was the manager of the magnetic resonance lab at Harvard, which was about 30 min away by car. When we had convinced Dr. Dudek that we had a pure sample she drove us (on Saturday) to run NMR spectra using equipment at Harvard University. I continued working on that project until I graduated and was able to publish my first scientific paper. Having a paper published in a 'real' journal was very exciting.

In graduate school my project used NMR to characterize the mechanism of rearrangement of tris chelate complexes. Prior members of the research group had separated isomers of Co(III) complexes by chromatography. I used dynamic NMR to monitor interconversion of isomers for complexes in which the rate of interconversion was much too fast to separate by chromatography. I was getting glimpses of the power of magnetic resonance to address fascinating questions.

After finding academic positions in Denver, Gareth and I decided we wanted to do something different from our graduate work and started doing EPR more than NMR. We were very fortunate that a Department Chair and Dean at the University of Denver were willing to invest in an EPR spectrometer to get us started, even though we did not yet have a track record in EPR. To keep a stream of publications going our first projects involved NMR studies of dynamic processes in metalloporphyrins. Meanwhile we were starting EPR studies of spin-spin interactions in metal-nitroxide complexes.

Could you please give an example of an event that shaped your attitude toward experiments?

My graduate research project was in collaboration with Dr. Earl Muetterties at Dupont Central Research. He had told my advisor (Dr. Richard Holm) that he would provide a ligand (a tropolone derivative) for me to study that would be isolated from the sap of a Japanese tree. I was totally distraught when I got a phone call that the cleaning crew at Dupont had accidentally thrown away the world's supply of the sap from which my ligand should have been isolated. Apparently the jar of sap had not been labeled and was left in the vicinity of a sink! Lesson 1– label everything that is valuable. To my further dismay my advisor responded by telling me to read the literature and find a synthetic route to the ligand. I had not planned to do organic synthesis, but realized I either had to abandon the project or find a synthesis. Fortunately I found a synthetic route that produced not only the ligand I had planned to study but also another derivative that proved very useful in sorting out the rearrangement mechanism. Lesson 2 – Alternates may be better than your first idea. Or perhaps I should say that persistence is key to success.

What part of your research is most dear to your heart and why?

It's very hard to answer this question because there are so many aspects of what we do that are important to me.

Over the years I have worked with many students. It is both rewarding, and humbling, to see a student develop from a tentative beginner to a young scientist with creative contributions to a project. It is wonderful to hear from students years after they have graduated and learn about what they are doing now.

I very much enjoy the interplay between experiment and data analysis. Looking carefully at data points out features that we don't understand and leads to the design of new experiments. Sharing what we have learned with other scientists and helping them answer their questions is both challenging and rewarding.

What are your most recent innovations you are most proud of?

Over the years Gareth and I have written many scientific papers that we hope have provided information that is useful to colleagues in various fields such as quantitative EPR and electron spin relaxation mechanisms. Seeing our results used in studies by other people, sometimes many years later, is gratifying.

Gareth and I were intrigued by the NMR experiments by Dadok and co-workers in which the magnetic field was swept through resonance at a rate that was faster than nuclear relaxation. They showed promise of substantial improvements in signal-to-noise. Shortly thereafter FT NMR became feasible and became dominant in NMR. For various reasons we thought that rapid scan might have major advantages in EPR and began working to implement it in our lab. This required developments in both hardware and software that were rewarding to accomplish. We showed that for many types of samples, especially ones with longer spin lattice relaxation times, rapid scan provided substantial advantages in signal-to-noise. We worked with Bruker BioSpin to implement this method as an accessory for their spectrometers. Other researchers are also implementing this method in their instruments. It is very rewarding to see something we developed in our lab become available for use by colleagues.

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

Research in any area provides never-ending opportunities to address new challenges. This is especially true in magnetic resonance because we have such a range of experimental methods from which to choose – CW, rapid scan, or pulse, variable temperature, different frequencies. We can contribute to many areas of science.

A supportive spouse is a treasure – nuture each other's aspirations and celebrate each other's accomplishments.

It is important to have a core set of expertise that can provide the basis for grant funding. Without external funding it is very difficult to have the resources to pursue interesting ideas in an academic setting, but then you should explore new arenas that you do not understand.

I have learned a great deal by talking with colleagues about the questions they want to answer and discussing how EPR might provide insights.

What is the secret of your never-ceasing passion for science and creativity?

Each time we answer a research question, it points to new questions. There is no end of interesting new opportunities.

Problem solving is fun!

Each new academic year brings new cohorts of undergraduate and graduate students.

The Bruker Thesis Prize 2022

Janne Soetbeer:

The RSC ESR conference in St. Andrews last June was a great experience. After two years of virtual meetings and talks, it was truly refreshing to finally meet again in person as a scientific community. It was an immense honor to receive the Bruker Thesis Prize 2022 on this occasion. Having given several virtual talks and defended my thesis from the comfort of my living room, it was very rewarding to present the prize lecture entitled *Dynamical Decoupling in EPR Spectroscopy for quantitative decoherence analysis via noise spectroscopy* to a live audience.

My doctoral research work at ETH Zürich, in the group of Gunnar Jeschke, addresses the process of phase memory loss that is central to pulsed EPR spectroscopy as it limits the achievable resolution and/or sensitivity of an experiment but also reports on the decoherence-inducing spin environment. For this reason, it is of great interest to be able to manipulate and understand the driving mechanism. Pulsed manipulation by n refocusing pulses, i.e. dynamical decoupling (DD), is known since the introduction of the Carr-Purcell (CP) sequence to prolong the phase-memory time T_m. Instead, EPR spectroscopists conventionally rely on the Hahn echo experiment to determine T_m and infer qualitative information about the spin environment from the associated echo envelope decay.

My thesis explores DD for EPR spectroscopy by applying the CP and Uhrig $n = 1–5$ sequences to relevant spin systems for chemical and biological EPR application work, namely spin labels in the glassy, frozen state. The low-temperature and low-spin concentration regime allows for the largest DD gains by freezing out decoherence-inducing dynamics and limiting non-refocusable interactions between electron spins. Besides identifying these optimal experimental conditions for pulsed manipulation, I demonstrate how to utilize DD as a spectroscopic method in itself by means of noise spectroscopy. This concept originates from the field of quantum information processing and views repeated refocusing of the central electron spin in time as applying a filter function to the so called noise spectrum $S(\omega)$ in the frequency domain. Inversely, dynamical decoupling noise spectroscopy (DDNS) infers $S(\omega)$ from DD data. However, $S(\omega)$ reconstructions have been limited to qubit-like spin systems given their inherently long phase-memory times and many applicable pulses. By introducing regularized DDNS I lift these limitations to access $S(\omega)$ from DD traces of common EPR spin labels recorded with $n \leq 5$.

The obtained noise spectra quantify the frequency range of the contributing stochastic processes, enabling a concise and tangible decoherence description that reflects variations in temperature, paramagnetic species, matrix, deuteration and spin concentration. For nitroxide radicals in glassy *o*-terphenyl and water-glycerol the low-temperature noise spectra consist of two distinct spectral features. Deuterating the nitroxide's methyl groups enables the assignment of the high-frequency noise spectral component to a spin-center induced process that is driven by rotational tunneling. The second, low-frequency component extends up to a matrix-specific cut-off frequency that reduces upon solvent deuteration. This cut-off frequency provides an effective description of the driving nuclear spin diffusion process, determines T_m, the achievable T_m/n slope and rationalizes DD performance differences observed for CP and Uhrig interpulse delays. Evidently, $S(\omega)$ provides the connecting link between a comprehensive description and a rational manipulation of the decoherence process.

In summary, my doctoral research work demonstrates how to utilize DD to address the double relevance of decoherence for pulsed EPR spectroscopy. First, DD extends T_m and thus serves as a resolution- and/or sensitivity-enhancing building block. Second, via noise spectroscopy DD enables a tangible and quantitative decoherence analysis – beyond the conventionally employed Hahn echo sequence.

Finally, I wish to thank Bruker for sponsoring the thesis prize as a wonderful recognition of doctoral students' contribution to the body of EPR research, the reviewers for the time and effort they spent in evaluating my thesis and the organizing committee of the RSC meeting in St. Andrews for enabling the conference. Thanks also go to Gunnar for the very creative Laudatio speech he gave on this occasion and for supporting me and my research work.

Gunnar Jeschke:

Janne Soetbeer earned a bachelor degree in chemistry and a master degree in interdisciplinary sciences at ETH Zürich. Her master thesis on dynamical decoupling in distance measurements was awarded with an ETH Medal. After a research stay at MIT with Bob Griffin she returned to ETH Zürich to work on coherence loss mechanisms of dilute electron spins at low temperatures, where spatial dynamics does not significantly contribute to transverse relaxation. Her thesis, completed in 2021, was awarded with an ETH Medal as well.

When Janne worked with me, I was particularly impressed by her thorough and thoughtful approach, but also by her great skills in presenting large amounts of data and complicated concepts clearly. Probably related to her interest in art, she strives for aesthetically pleasing visualizations. All this and her helpful attitude make her an excellent teacher.

From my perspective, Janne has advanced an already well-researched field through three quite distinct achievements. First, she acquired a large set of very high quality data and analyzed them very carefully by an empirical approach. These results are a treasure trove for further developments beyond her dissertation project. Second, Janne developed regularized noise spectroscopy by overcoming problems of the original approach that arise for a small number of refocusing pulses from electronic noise. Thus, she could quantify contributions to decoherence in various samples. These results became a stepping stone for understanding the possibilities and limitations of noise spectroscopy in pulsed EPR. Third, Janne demonstrated that a fast contribution to decoherence, which she had discovered in her data, arises from tunneling of the methyl groups of nitroxide spin labels. We currently build on this in another dissertation project. Janne did not only generate a lot of understanding herself, she also opened up new research directions.

JEOL Prize 2022

Fabian Hecker:

The first RSC meeting I attended and where I got to experience the fantastic community of the EPR groups in the UK and Europe, took place in Glasgow in 2019. Then Corona hit, and no in-person conferences took place. Thankfully, we could still experience the meeting online in 2021, and the JEOL competition went on without interruption. When it became clear that the conference would finally be an offline experience again, I was even more excited to go to St. Andrews. I had observed the JEOL competition over the last four years with amazement at the quality of research and how it was presented, and I felt honored to be able to participate in the 2022 edition together with Luis Fábregas-Ibáñez, Arnau Bertran, Yujie Zhao, and Shari Meichsner. Christiane Timmel, head of the RSC EPR group, announced that I had won the JEOL competition with my talk "^{17}O hyperfine spectroscopy to detect water binding to biologically relevant radicals" by quoting the German proverb: "*Er kocht auch nur mit Wasser*" – which translates to "*he is also just cooking with water*". I agree with her on the figurative meaning, which refers to the fact that there was no magic to our work - instead, it was good EPR spectroscopy. However, I would argue with the literal meaning since we certainly tried to avoid cooking the biological samples – which tends to be less of an issue when the measurements are performed in frozen solutions at 50 K. I would also append the saying - "*cooking with expensive water*" – as the 90% ^{17}O-labeled water we used was rather costly.

The work I presented in the JEOL competition focused on detecting ^{17}O-labeled water molecules around tyrosyl and nitroxide radicals with modern EPR hyperfine (hf) spectroscopy methods. This was the focus of my Ph.D. project, which, as with so many things in science, wasn't planned. It came about around half a year into my original Ph.D. project when my supervisor Marina Bennati came into my office and asked me whether I would like to join her and her long long-time collaborator JoAnne Stubbe on a trip to Frank Neese in Mühlheim for a discussion meeting on future work concerning ribonucleotide reductase (RNR). Of course, I said yes without thinking twice. A short time later, I found myself in a room at the MPI für Kohlenforschung, discussing experimental strategies to detect specific water molecules inside the active enzyme complex of *E. coli* class 1a RNR.

Water molecules in this enzyme had been proposed based on ^{1}H ENDOR experiments of trapped tyrosyl radicals on the radical transfer pathway [1]. Yet the abundance of protons in the biomolecule made the assignment challenging, and direct experimental evidence was missing. Marina's idea was to use ^{17}O labeling of the water since the low natural abundance of this isotope makes the assignment of spectral signatures unambiguous. We agreed it would be the best option but also realized that it would come with several challenges: The low gyromagnetic ratio and the high nuclear spin I = 5/2 of ^{17}O contribute to the nucleus's low sensitivity in magnetic resonance experiments. Several people, including Marina, had successfully used $H_2{}^{17}O$ to investigate its coordination to metal ions with ENDOR [2], HYSCORE [3], and EDNMR [4]. However, we were considering it for organic tyrosyl radicals, which adds the difficulty of longer distances between the radical and the ^{17}O nucleus due to the coordination via an H-bond, resulting in smaller and less easily detectable hyperfine interactions.

Nevertheless, we decided it was worth a try and were surprised when we looked at the first 94 GHz Mims ENDOR spectra of the tyrosyl radical $Y_{356}^{\bullet}$ in an RNR sample containing a ^{17}O labeled buffer. It showed a well-resolved hyperfine spectrum with sharp coupling features, which we could link to a ^{17}O nucleus coupled with a significant isotropic hyperfine coupling of ~0.6 MHz. It turns out that hydrogen-bonding also results in the transfer of spin density onto the water's oxygen nucleus, rendering the coupling resolvable by high-field Mims ENDOR [5]. We could detect such couplings for three different (amino)tyrosyl radicals in RNR and, with quantum chemical calculations on the DFT level, link it to a common, in-plane coordination of water molecules to these radicals since the hyperfine coupling is highly sensitive towards the binding geometry. The high-magnetic field was advantageous in limiting the effects of nuclear quadrupole broadening, yet the method is also applicable at 34 GHz and can detect the fingerprint of in-plane water.

We then turned our attention to one of the favorite radicals of the EPR spectroscopy world: nitroxides. $H_2{}^{17}O$ and EDNMR had been used to quantify the hydration level of a spin-labeled protein, but information about the structure of water molecules around the nitroxides had yet to be reported [6]. We re-

corded HYSCORE, EDNMR, and ENDOR spectra of two representative nitroxide radicals in bulk $H_2{}^{17}O$ at different magnetic fields to study their hydration structure and find the best method to detect the ^{17}O hf couplings. We observed quite a different picture compared to the tyrosyls, namely much larger hyperfine couplings up to 8 MHz and broad hf spectra with distinct differences between pyrrolidine and piperidine-based nitroxides. A quantitative analysis of the spectra based on MD simulations and DFT predicted hf parameters was consistent with a distribution of close solvating water molecules around the NO group in the nitroxide radicals, in which the coordination geometry is influenced by subtle steric effects of the ring and the methyl group substituents [7].

The two studies showed how much structural information about the hydration of organic radicals can be gained by ^{17}O hyperfine spectroscopy and how radicals can be used as probes for water structure in biomolecules and on material surfaces.

I want to thank the organizing committee of the 2023 RSC EPR conference for selecting me for this prize and especially JEOL for sponsoring it. In addition, my gratitude goes to Marina Bennati for being a fantastic mentor, Lisa Fries and Markus Hiller from our group, who worked with me on the project, Mario Chiesa, who taught me ^{17}O HYSCORE and JoAnne Stubbe, who introduced me to the wonderful world of ribonucleotide reductase.

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Marina Bennati:

It was a pleasure for me to work with Fabian over many years. I'm very proud that he won the hard JEOL talk competition, thanks to his excellent scientific and communication skills. During his PhD thesis he developed an ambitious EPR spectroscopic approach to detect water molecules in the first and potentially also in the second ligation sphere of biologically relevant organic radicals, such as the important redox-active tyrosyls and the widespread nitroxide radicals. He demonstrated that, against our initial expectations, a tiny spin density (on the order of 0.1% or less) transferred from a radical site to the oxygen nucleus of a water over a hydrogen bond, generates well-resolved hyperfine splitting in ENDOR. He then examined the repertoire of hyperfine spectroscopic techniques to identify the most suited methods for water detection. His work corroborated the significance of the oxygen nucleus as a selective reporter for electronic and structural information at molecular level.

Fabian was able to acquire and cross-fertilize a wide spectrum of expertise from protein biochemistry, advanced EPR spectroscopy up to spectral analysis and programming. His engagement to science led him also to develop a strong enthusiasm in teaching, through which he shared his knowledge with several young students. The JEOL prize is a well-deserved recognition for all this engagement and contributions. I'm happy that his success is motivating him for a postdoctoral position in magnetic resonance. He will get the opportunity to learn more techniques and will hopefully contribute to next generation of scientists.

IES Poster Prize at the Euromar 2022

Tobias Hett:

First, I would like to express my sincere gratitude to the International EPR (ESR) Society for awarding me a poster prize at Euromar 2022 in Utrecht, The Netherlands, and for the opportunity to present my research in the IES newsletter. On my poster, I showed a combination of Pulsed Electron-Electron Double Resonance (PELDOR/DEER)[1] spectroscopy and microsecond freeze-hyperquenching (MHQ) [2] to study the conformational change of a protein with spatiotemporal resolution. Monitoring conformational changes is of particular interest, as they are key to protein function. Here, we studied a helix movement induced by cyclic adenosine monophosphate (cAMP) in a cyclic-nucleotide binding domain (CNBD) [3]. Using PELDOR and site-directed spin-labelling, we identified a protein construct that reflects the transition from the ligand-free *apo* state to the cAMP-bound *holo* state as a distance change of 1.9 nm. To track the conformational change, we used a freeze-quench device (MHQ) that mixes and freezes the CNBD and cAMP on a microsecond time scale. By preparing MHQ samples at aging times between 82 and 668 µs and performing PELDOR, the trajectory from the *apo* to the *holo* state could be sampled. The distance distributions revealed a gradual depletion of the *apo* state and a simultaneous build-up of the *holo* state. However, neither additional peaks could be observed that would indicate intermediate states nor a gradual shift of the distribution along the distance axis from the *apo* state to the *holo* state, which would be expected for monitoring the helix movement. This finding suggests that the conformational change occurs on a sub-microsecond time scale and thus could not be resolved by MHQ/PELDOR. Molecular dynamics simulation of the *apo*-to-*holo* transition corroborates this notion by showing that the helix movement proceeds within a few nanoseconds. To scrutinize whether MHQ/PELDOR monitored mere ligand binding, we prepared MHQ samples at different cAMP concentrations while keeping the CNBD concentration and the aging time constant. At ligand-to-protein ratios above 67, the CNBD was found to be saturated with cAMP within the dead time of the MHQ device. As the MHQ samples at the different aging times had been prepared at 100-fold ligand excess, cAMP binding could be excluded as a potential cause of the population shift.

Mechanistically, the experimental and computational findings were interpreted in terms of a dwell-time distribution. In a simplified picture, the trajectory from the *apo* to the *holo* state contains two free-energy barriers, ligand binding and the conformational change, which are both crossed within nanoseconds if the cAMP concentration is high enough to rapidly saturate the CNBD. After crossing the first barrier, the protein and the ligand form an *apo*-ligand-complex, in which the protein is structurally still in the *apo* state but with the ligand at the binding site. During the dwell time, the *apo*-ligand-complex accumulates thermal energy to cross the second barrier and to transit to the *holo* state. This dwell time is in the microsecond range and therefore rate-determining on the trajectory from *apo* to *holo*. Being individually long for each protein molecule, the dwell time is statistically distributed, and longer aging times permit a larger fraction of protein molecules to transit to the *holo* state. Thus, using MHQ/PELDOR, we could resolve the dwell-time distribution of the *apo*-ligand-complex and thereby shed light on the mechanism of ligand-activated conformational changes [4].

This work is the result of a collaboration between Professor Olav Schiemann (University of Bonn, Germany), Professor U. Benjamin Kaupp (Max Planck Institute for Neurobiology of Behavior – caesar, Bonn), Professor Helmut Grubmüller (Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany), and their workgroups and has been published in the Journal of the American Chemical Society (*J. Am. Chem. Soc.* **2021**, 143, 6981–6989, DOI: 10.1021/jacs.1c01081). I would like to thank my supervisor, Professor Olav Schiemann, for his continuous support and our collaborators for their efforts and valuable contributions to the project.

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Olav Schiemann:

Tobias Hett, or better Tobi, is an important pillar of my research group. He is always available to discuss with or answer questions from other group members, he helps in setting up pulsed EPR experiments, and advises in computational things. Besides all this support for others, he very successfully runs his own research. Over the years this led to a group's inventory number appearing on him, because whenever one of us came to lab, Tobi was already or still there (we are not sure which of both).

I first got to know Tobi in 2015, when he joined my group for his Bachelor Thesis. At that time, he tested and calibrated a flow through resonator from Bruker using a Fenton like reaction as the test system. He fought his way through the kinetics and was able to publish the work in JMR. To my joy, he came back to my lab for his Master Thesis in 2017, where he started to work on Microsecond Freeze-Hyperquenching (MHQ) in combination with site directed spin labeling and Pulsed Electron-Electron Double Resonance (PELDOR or DEER). He continued this work through to his PhD because this project did indeed turn out to be an Apollo-like project as our close collaboration partner Benjamin Kaupp from Caesar (now a Senior Professor in my lab) termed it. In later stages of the project, Tobi also performed MD simulations in collaboration with Helmut Grubmüller, a collaboration we are very fond of to continue. During the years Tobi received a few awards, e.g., the Ernst award of the FGMR and the Peyerimhoff-Research Prize of the University of Bonn. In addition, he is since many years a well-regarded tutor in both physical chemistry practicals. Beyond science, Tobi is, although he appears to be on first sight a rather quiet character, an adventurous guy. During his school time, he spent a couple of weeks as an exchange student in China and he thoroughly enjoys cross country cycling. While writing this, Tobi is on his way to the Weizmann Institute to check out a postdoc stay in the lab of Lucio Frydman. Knowing that Lucio is also a tough cyclist, I hope for dramatic, but not too dramatic, photos from the Negev. Tobi, we are very proud of you having received the IES poster prize at the EUROMAR2022, keep on rolling.

IES Poster Prize at the 2022 Spin Chemistry Meeting

Emily Dowker:

Spin correlated radical pairs (SCRP) produced from photochemical reactions are susceptible to changes in their spin dynamics in the presence of a magnetic field. This quantum mechanical phenomenon is known as a Magnetic Field Effect (MFE) and can be observed physically through the altered reaction rates or product yield of the radical pair. Under the right conditions, these radical pairs are sensitive to both the magnitude and direction of the external field, effectively operating as a molecular compass. In practice, most spin correlated radical pairs that have been studied do not meet these criteria. The aim of this work is to identify the specific conditions required to optimize the sensitivity of radical pairs to low strength magnetic fields on the order of the Earth's natural field (50–100 μT). Flavin-based radical pairs incorporated into a micellar environment have shown promising magnetic field effects at weak field strengths, otherwise known as Low Field Effects (LFE). In contrast to higher field MFEs, Low Field Effects arise due to electron-nuclear spin-spin interactions. As the weak field lifts the degeneracy of the spin states, the number of pathways for singlet to triplet interconversion (and efficiency) is increased. For the magnetic field to have an effect on the system however, radical pairs must have a high probability of re-encounter after adequate time for singlet-triplet mixing has occurred (10 ns). This effect is therefore highly dependent on the environment of the molecules in question. A micellar environment lends itself particularly nicely to these conditions as it provides optimally sized supramolecular structure (1 nm) for effective radical interactions. Furthermore, we can harness the physical properties of the micelle, such as its hydrophobic core and charged Stern layer, to further confine the radicals, increasing the probability of recombination after diffusion. To understand the conditions required for an LFE more concretely, we have undertaken a systematic study of a series of flavin acceptor molecules and ascorbic acid donors in ionic micelles under various conditions, including modifying the charge and hydrophobicity of the donor and acceptor, as well as monitoring factors such as pH, micelle size, and diffusion rate. Because the environment surrounding a radical pair greatly influences the effects of a magnetic field, we are analyzing the location of each molecule in the system. To locate the ascorbic acid donors, we are employing a hydrophobic electron acceptor that can only exist in the micellar phase. Similarly, we can localize the flavin electron acceptors by quenching with an ion that cannot associate with the micelle due to charge repulsion. We can then extract locational information by comparing quenching rates across these experiments. MFE measurements were taken by prompt fluorescence magnetically altered reaction yield (PF-MARY). This instrument monitors changes in the fluorescence intensity of the singlet molecular precursor to the radical pair in the presence or absence of a magnetic field. Low Field Effects will produce a positive percent MFE due to the increase in S-T mixing. Understanding the conditions required for maximizing the LFE may give important insight into the quantum mechanical and classical interactions of radical pairs that are crucial for the observation of compass behavior. If harnessed effectively, this understanding could be utilized to create chemical compass systems as alternatives to current global positioning systems.

Lauren Jarocha:

It is my absolute pleasure to write to all of you today to introduce you to a talented young researcher in the field of spin chemistry. Emily Dowker is an undergraduate student at Furman University. For those of you who may not know Furman yet, it is a primarily undergraduate institution located in Greenville, South Carolina, USA. Emily is one in a long line of promising young spin chemists that have come out of the Furman Chemistry Department's research program, which is one of the largest undergraduate research programs in the country. She joined my lab in the Summer of 2020, after only her first year of college and in-spite of a raging pandemic that forced us to work remotely. During that time, she learned the computer programming language LabVIEW so she could contribute to the construction of a purpose built instrument in the lab to measure magnetic field effects on chemical reactions. We also tackled some complex topics in quantum mechanics, photochemistry, and kinetics. Emily excelled with this difficult material, and quickly picked up the programming languages we needed in the lab. All of this effort established a strong foundation; she hit the ground running when we were finally able to return to the lab in person the following summer. I have worked with Emily now for three years, during which time she has been investigating the interplay between hydrophobicity and electrostatic interactions on the observation of low-field effects in radical reactions occurring in micelles. It has been a pleasure to watch her grow as a scientist, and take ownership of her research. Her enthusiasm and diligence have produced promising results, which she shared at the most recent Spin Chemistry Meeting at Northwestern. I want to end by thanking the IES for recognizing Emily for her outstanding work, and giving her the opportunity to share it with you.

Interview with Dr. Fei Kong on the Occasion of His APES Young Scientist Award 2002

EPR newsletter: *Dear Dr. Fei Kong, on behalf of the readers of the EPR newsletter we congratulate you on your APES Young Scientist 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 would like to thank the Asia-Pacific EPR/ESR committee for giving me the Young Scientist Award and providing the opportunity to present my recent work. It is a great honor and an affirmation of my work. I am also grateful to Prof. Elena Bagryanskaya and Prof. Yong Li for the recommendations. Although it's a pity we can't communicate face to face due to the pandemic, I still learned a lot during the online symposium.

When I was growing up, I had access to a lot of mechanical and electronic components, including electric motors, radios, TV sets and so on. There was great satisfaction in the process of disassembly and assembly over and over again. At the same time, I wondered what is the power behind such a sophisticated operation? It was only after education that I learned that this power is called science. What is even more exciting is that the process of learning science is endless, so it is worthy of being a lifelong career.

You were featured in the EPR newsletter 30/4, 13, 14 (2020) as the IES Best paper Awardee 2019/2020. How were your first steps into magnetic resonance under co-supervision of Professors Jiangfeng Du and Fazhan Shi?

I joined Professor Jiangfeng Du's group as a graduate student because of the strong interest in the fascinating quantum phenomenon. During the first two years, I focused on quantum simulation based on solid-state spin defects, and learned a lot about quantum controls. When I started my PhD, Dr. Fazhan Shi suggested that the spin defect is a promising quantum sensor for magnetic resonance sensing, which can substantially improve the spin sensitivity to even single-spin level. I then switched to this area and started my first magnetic resonance research on single-DNA EPR spectroscopy.

Why did you choose a somewhat overlooked territory in the range of EPR techniques?

My first EPR research was single-spin EPR based on quantum sensors. Although it was very impressive to promote the sensitivity from billions of spins to single spins, the spectrum we get looked no better than conventional one. It meant one can hardly get more information from the single-molecule spectrum. In order to make this technique more useful, I needed to improve the spectral resolution, and I found zero-field EPR is a direct way to do so. It was overlooked because of the low sensitivity, which can be naturally avoided by our single-spin technique. So I think the combination of zero-field EPR and single-spin EPR is promising.

What is the main content of your APES Young Scientist Award 2022 lecture?

I have introduced a zero-field EPR technique. Different from conventional EPR, the sensor we used is a spin defect in diamond named NV center. The EPR signal comes from the dipolar field generated by the sample spins, which decays rapidly with the sample-sensor distance. The NV center is atomic-scale, and thus can be very close (several nanometers) to the sample to detect even single spin. More importantly, the NV sensor detects the variance of the dipolar field rather than net field. The former is magnetic-field independent. So the zero-field NV-EPR does not suffer from low sensitivity, while maintains high spectral resolution.

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

EPR spectra are usually complicated. How to understand them requires a great deal of experience. Instead of trying an experiment again and again, I suggest the young researcher spend more time on reading textbooks, reviews and research papers. The difficulties you face should have been encountered by others. So you can always find a solution there. Although it takes times, it will finally save a lot of time throughout the PhD.

Slow sports

Gunnar Jeschke

ETH Zürich, Switzerland

There is fast food and there is slow food. I have always been slow at sports. In high school, I did not excel, to put it mildly, and accordingly I hated these lessons. I didn't break a sweat in other subjects, and while I was slow at sports, I was lightning fast at homework. Hence, I had a lot of spare time to spend with swimming and cycling, which I enjoyed. Running felt wrong at the time. After earning a doctoral degree, I stopped swimming and cycling. Although I still went for hikes, I gained and gained and gained weight.

At the age of 37, I was suddenly seized by another passion. This one would be clearly beyond the scope of this article, except that it also made me love sports. I slimmed so fast that the company doctor of the institute became worried. My kilometer time in swimming, which I had taken up again, did not improve beyond the one in my youth. This would only happen years later, when I learned to crawl 2000 metres in a row. What was new: I now loved running. At this time, I lived in Mainz. I gradually extended my runs from my apartment north of the city center to the Rhine, then along the Rhine, across the Rhine and into the fields. I did not think about races. It was a given that I was too slow for races.

My first exploit came three months later. It was while cycling solo on an alpine pass. I took a day off and a direct train from Mainz to Ötztal station in Austria. The next day I made it up to Timmelsjoch (2474 m), cycling the last kilometer still with short clothes in light snowfall. Oncoming motorists greeted with their flashers. In the restaurant on top, I had, in this sequence, warm clothes, a soup, and a hot chocolate.

This experience turned me into a pass cycling addict. Since then, I take two weeks off every year in June or September and ride my bike through the Alps or the Pyrenees. This is not about speed. When I cycled from Alpe d'Huez via Col du Galibier and Col du Télégraphe to Saint-Michel-de-Maurienne in 2018, I climbed Galibier at about a third of the pace of the professionals, who did it a few weeks later during the Tour de France. Still, it felt very good.

The day before I had just missed the experience of being overtaken by Chris Froome on the climb to Alpe d'Huez. He was training there, which had not been known before. My English hosts in a small chalet near the road told me only in the evening. In 2015, I did cycle in a race with one of the giants in cycling history, the Belgian hero of the 1960s and 1970s, Eddy Merckx. Granted, it was an unlicensed race, Eddy Merckx had celebrated his 70th birthday a few months earlier and he was doing this for fun. I did not even make it to the finish line of the 2015 Eddy Merckx Classic near Salzburg in Austria. About 20 kilometers into the race I crashed so badly that I thought it prudent to donate my severely damaged bicycle to the Paraplegic Foundation.

Yes, at some point I had started racing, slowly. In 2010 my research group at ETH Zurich took part in the SOLA stage run. It was the first race in my life. The first runner out of 14 starts in the morning. After the team has covered 115 kilometers and 2747 meters altitude difference, the last runner arrives in the late afternoon. And then the team parties. For a slow runner, this is a very good way of starting to compete. The race is definitely for fun, except for a few top teams. There are even two categories: fast teams and slow teams.

SOLA encouraged me to sign up for my first half marathon in Lucerne in 2011. I am now at eleven Lucerne Swiss City (Half-)Marathons and still counting. Later, SOLA encouraged me to try trail running. Some of the SOLA stages have substantial ascents. I noticed that I could overtake some runners in these ascents, who had overtaken me in flat sections. In mountain runs, slowly, I graduated from Zugerberg

Alps cycling in 2018.

Classic via Blüemlisalp-Lauf to Zermatt half marathon.

In my first Zermatt half marathon I was starting in the elite group. This happened by mistake, due to signing up with a completely unrealistic finish time. Though I realized at the very start that I should not run the pace of this group, my hunting instinct got the upper hand on me – at least as long as it would last. I still made it to the finish line on Riffelberg after 1334 m uphill, with only slight cramps. The time was decent for my real abilities. It took me slightly more than a week to recover, most of which I spent at the EUROMAR conference 2016 in Aarhus. My third Zermatt half marathon in 2018 I did well. It came one week after the cycling tour mentioned above. My basic endurance was at its peak and my body fat at its low. In my age category, I finished 43rd out of 68 runners, without cramps, feeling gorgeous. On the evening after this race, I signed up for my first Glacier 3000 run. This is the run where you can see Edelweiss flowers near the track.

In 2012, a doctoral student presented me with an extremely convincing argument. After having competed in a half marathon, and being a passionate swimmer and cyclist, I absolutely had to try myself in an Olympic-distance triathlon. This involves 1.5 km swimming, 40 km cycling, and 10 km running. During these years, the major Swiss triathlon took place in Zürich. I took the advice and competed four times in a row in the Zürich triathlon.

When I changed to mountain triathlons, they turned out to be games of chances. It took me three attempts to complete the triathlon from Sierre (533 m) to Gemmi pass (2268 m). The first two times, they diverted us to an alternative running route in Leukerbad. Once, the wind was to fierce and too cold on top and once icy rain was predicted on top. The alternative route was scenic, too, but not quite what I desired. In the Davos Challenge 2021, the lake had a water temperature of 15°C and the air was at 10°C. The organizers did not dare to let us swim. Instead, they converted the race to a duathlon. Swimming was replaced by a run around the lake. This was followed by the original cycling route up and down Flüelapass, and the original 10 km run in Davos. During cycling, short clothes were strictly forbidden, as was going downhill from the pass without a jacket. And then the sun came out during the final run. Pure bliss.

Slow sportsmen can cope with their students beating them by half an hour on the 10 miles and 700 m ascent of Blüemlisalplauf. What they still dread is DNF – "Did not finish". I produced three of them so far. You have already read about the one in the Eddy Merckx Classic. The second one came 2021 in my second participation in the Glacier 3000 run. It was the weather again, which turned bad faster than metereologists – and hence the organizers – had assumed. The time limit at the last checkpoint in Cabane was shortened by a whopping 45 minutes. I arrived there during a cold downpour and pitied the helpers, who had to wait for other runners, while I could take the cablecar down to Col du Pillon. Formally, it was not even a DNF in the results list. The organizers decided to declare everybody a finisher, who had made it to Cabane.

My third DNF was a real one. It happened last year on the 35 km variant of Eiger Trail Run. At the RSC Conference about two months earlier, Stefan Stoll had warned me about downhill. I had trained some downhill, but not after fast uphill. It happened what had to happen. The first uphill to Spätenalp went well. The first downhill to Wengen was OK. I did better than expected from Wengen up to Männlichen. From Männlichen to Kleine Scheidegg it is a strolling mile. From Kleine Scheidegg to Eigergletscher it took some effort, but I reached Eigergletscher with ample time left for the last 15 km down to Grindelwald.

Or so I thought. The excruciating pain in my legs started almost immediately on the downhill. My poles carried me until Alpiglen at kilometer 26, where I missed the time limit by a large margin.

A friend, who arrived to Grindelwald in the early evening, met a devastated copy of mine for dinner. She talked me into registering for the Glacier 3000 run that would take place three weeks later. She even tried to make me do this already next morning in a cable car. I finally did it next evening. It was the right thing to do.

I knew that I could not afford a second DNF in a row. This race I planned strategically. I never exceeded my target heart rate for more than 30 seconds. On the first 15 km from Gstaad to Reusch I never let my heart rate drop far below the target. I had been faster to Reusch before, but I was well within my plan. In Reusch, the steep part starts. Passing some better runners in this part made me confident. I felt well at Oldenegg, where the technically most difficult part starts. At Cabane I knew that it would work out. To be sure, I did not make it by a very large margin. I had eleven minutes left of a time limit of five hours. When you are slow in sports and you are getting older, time limits become an important criterion in selecting races.

I prefer slow food over fast food. I am still slow at sports and I am now getting slower by the year. My passion for sports, though, appears to be a long-distance runner.

Glacier 3000 run near Scex Rouge in 2022.

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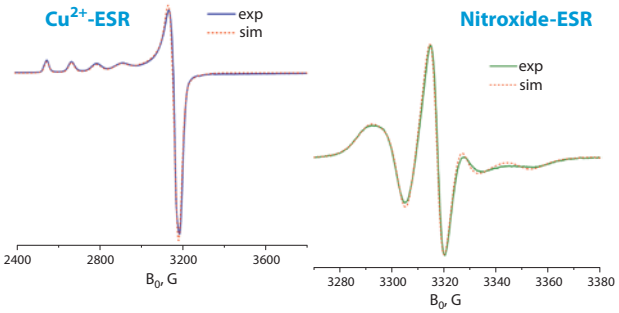
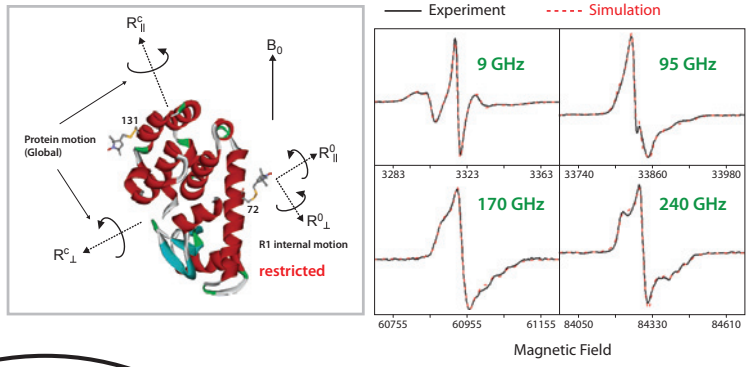
ESR Spectral Fitting



Multifrequency ESR



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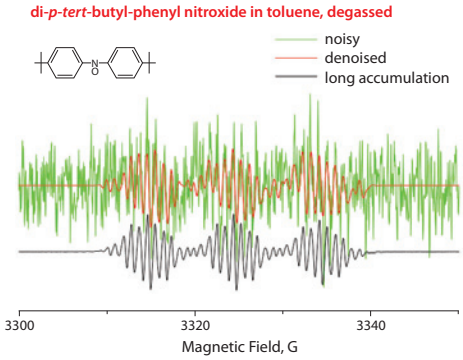

1) Perform
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2) ESR Data Analysis
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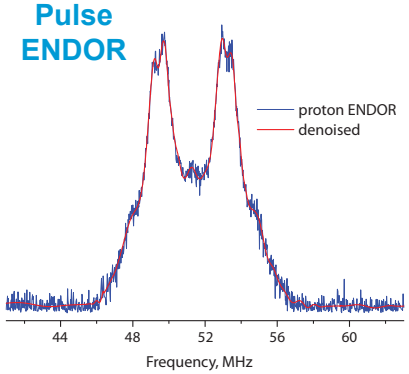
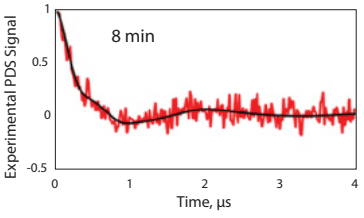
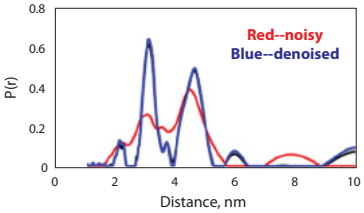
4) Standard Samples
5) Contact Info Above

Pulse ENDOR

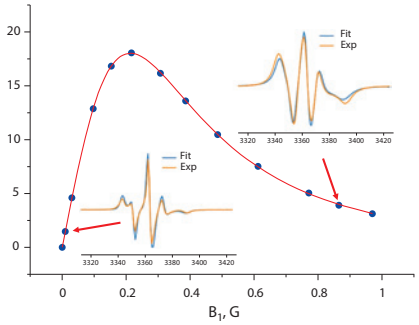


DEER & DQC



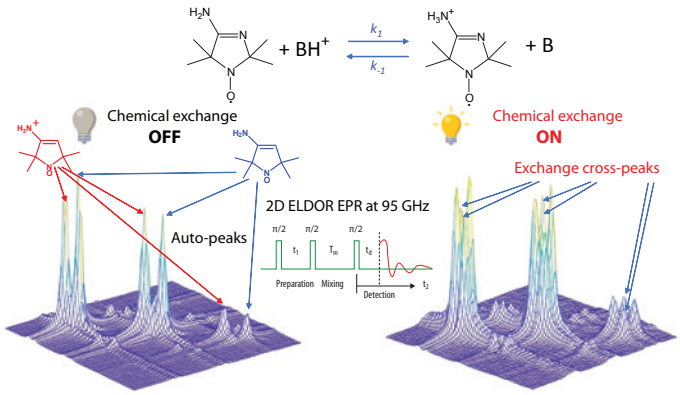


Simulation



Saturation Curve

2D ELDOR



Past Technology Achievements of ACERT after 20 Years while a P41 NIH Technology Center

For the fifth anniversary of our National Biomedical Center for Advanced ESR Technology (ACERT), which was launched in September, 2001, with support from the NIH, I wrote an article for the *EPR newsletter* (vol. 16, #4, 2007) on its 5th anniversary expressing the philosophy and perspectives of ACERT. We received funding from the NIH for the limit of 20 years, which concluded this year (April, 2022). It seems appropriate to review some of ACERT's technical accomplishments during that period. I outline below 20 such accomplishments in chronological order. (Our extensive collaborative work is outlined on our web-site: www.acert.cornell.edu.)

1 Protein Structure Determination by PDS [1]: Eight T4 lysozyme doubly-labeled mutants were studied at 9 and 17 GHz by Double Quantum Coherence ESR (DQC) with distances ranging from 20 Å to 50 Å yielding excellent distance distributions. Those distances were readily rationalized in terms of the known crystal structure, characteristic conformers of the nitroxide side chains, and molecular modeling. This study set the stage for the use of DQC-ESR for determining the tertiary structure of large proteins with just a few long-distance constraints.

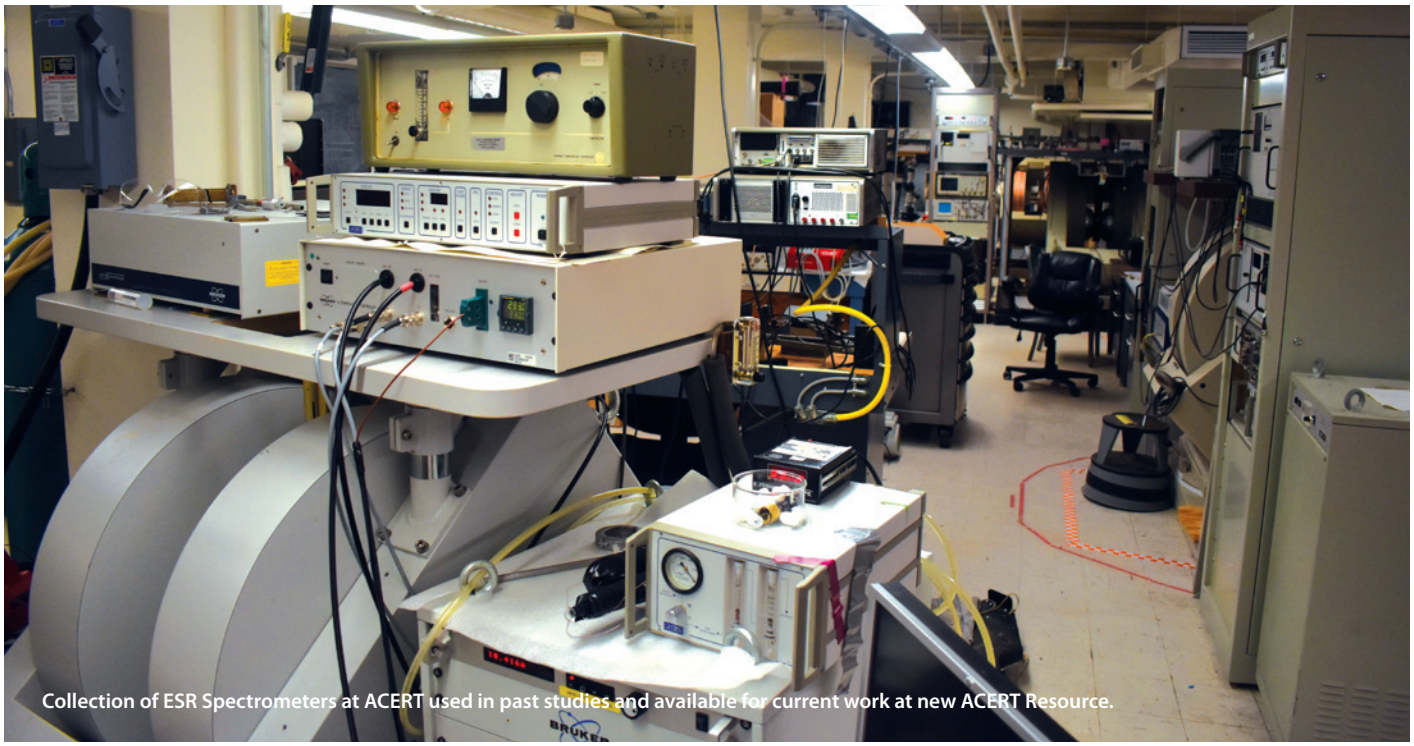
2 17 GHz High Resolution Pulse Spectrometer for PDS: Protein Structure [2–5]: We implemented highly-sensitive DQC and DEER at 17 GHz to dozens of studies on protein structure and function with a number of them noted on our web site. Here we mention the first PDS studies on oriented lipid bilayers and on bicelles. We also first applied PDS to deuterated solutions and lipids, and to deuterated proteins to help measure distances greater than 50 Å.

3 95 GHz High Power Spectrometer for 2D-ELDOR [6]: We reported on the design and implementation of a high power (1.2 kW) high bandwidth pulse ESR spectrometer operating at 95 GHz. The high power pulses were needed to perform two-dimensional (2D)-FTESR experiments that can unravel the dynamics of a spin system in great detail. A principal design goal was the ability to investigate dynamic processes in aqueous solution at physiological temperatures with the intent to study biological samples.

4 ESR Microscopy with Micron Resolution[7, 8]: We showed through theoretical prediction and initial experiments that ESR microscopy can improve upon resolution limits of NMR and successfully undertake the 1 μm resolution challenge. The three-dimensional (3D) ESR microimaging system operating in pulse mode at 9 GHz enabled the acquisition of spatially resolved magnetic resonance signals of free radicals in solid or liquid samples with a resolution of up to 3.5×7×10 μm in 20 minutes of acquisition. With a detection sensitivity at RT of 10^9 spins/√Hz one can measure ca. 2×10^7 spins in each voxel after 1 hr. of acquisition.

5 170/240 GHz Spectrometer with Quasioptical Induction Mode Bridge [9]: Our spectrometers at high field (≥3 T) are based on quasioptical design techniques. A key feature of quasioptical systems is that the optics conserves the polarization state of the incident beam. We exploited this to encode the ESR response of the sample for ease of detection; it is the quasioptical analog of induction-mode detection at microwave frequencies. ESR spectra of labeled T4 Lysozyme were obtained at 170 and 240 GHz (as well as 9 and 95 GHz), showing their strong dependence on magnetic field.

6 Development of Tikhonov and Maximum Entropy for PDS Analysis[10, 11]: Tikhonov regularization was demonstrated as a powerful and valuable method for the



Collection of ESR Spectrometers at ACERT used in past studies and available for current work at new ACERT Resource.

determination of distance distributions of spin-pairs in PDS-ESR. Tikhonov Regularization with regularization parameter determined by the L-curve criterion was described and tested, confirming its accuracy and reliability on DQC and DEER experiments. However, the distribution obtained tends to exhibit oscillatory excursions with negative portions in the presence of finite noise. The Shannon-Jaynes entropy of a probability distribution provides an intrinsic non-negativity constraint in an unbiased way. We showed how the maximum entropy method (MEM) may be used in conjunction with Tikhonov to ensure positive pair distributions, thereby enhancing the accuracy of TIKR.

7 Multifrequency ESR Spectra of a Spin-labeled Protein Calculated from Molecular Dynamics Simulations [12]: Relating the features of the observed ESR spectra to the underlying molecular motions and interactions is challenging. We performed extensive molecular dynamics (MD) simulations of fully solvated spin-labeled T4 lysozyme. To extend the time window of the MD simulations, stochastic Markov models were constructed from the trajectories. The calculated multifrequency ESR spectra are in very good agreement with experiments at different field strengths.

8 Sensitive Determination of Local Ordering in Lipid-Protein Mixtures[13, 14]: Several chain spin labels and a spin-labeled cholestane were used to study the dynamic structure of plasma membrane vesicles (PMV) prepared from RB1-2H3 mast cells. These results indicated that a liquid-ordered-like region (the abundant component) and a liquid-crystalline region (the less abundant component) coexist in the PMV. This suggested that membrane-associated proteins are important for the coexistence of these regions. In another spin-labeling study of a fusion peptide from the flu virus with a lipid membrane we found the ordering effect on the headgroup and the acyl chains near the headgroup increased significantly in a manner consistent with a cooperative phenomenon. However, changes in order near the end of the acyl chain were negligible. These observations were later found to apply to a wide range of viral fusion peptides.

9 Application of MOMD and SRLS to Dynamic NMR Spectra[15]: Protein dynamics in fluids can readily be studied by NMR relaxation methods. The primary issue is how to address the great complexity of protein dynamics. NMR spin relaxation in liquids pertains to the Redfield limit where only relaxation parameters can be measured. It was shown how the slowly-relaxing local structure (SRLS) model is an effective means for analysis of these NMR data. It is based on a coupling of tensorial properties, including those of the magnetic interactions, which are included in SRLS. The SRLS approach is used to analyze extensive NMR relaxation data.

10 Determination of Tie-Line Fields for Coexisting (Lipid) Phases [16]: Tie lines are used to determine the compositions of phases that are in equilibrium. We pointed out that there are a continuum of non-intersecting tie lines; hence, they form a "field". It corresponds to a unique mathematical parameterization called a "ruled surface". We developed an experimental method to globally determine a tie-line field, as opposed to fitting one tie-line at a time. This method was illustrated by interpreting ESR data on a mixed lipid and cholesterol system exhibiting a two-phase region.

11 Rapid Freezing of samples in PDS [17]: Pulsed dipolar ESR requires frozen samples. An important issue in the biological application is how the freezing rate and cryoprotectant could affect the conformation of biomacromolecule and/or spin label. In a comparison of results from rapidly freeze-quenched ($\lesssim$100 μs) samples to those from commonly shock-frozen (1 s or longer) samples, the inter-spin distance distributions were broader for rapidly-frozen than for slowly frozen samples. This is ascribed to rapid freezing trapping a larger ensemble of spin-labeled rotamers. Also, rapidly frozen samples needed lower concentrations of cryoprotectant (e.g., glycerol) to obtain decreased local spin concentrations due to insufficient solvent vitrification.

12 Distance Geometry in PDS [18]: A method for determining precisely how a lipid molecule locates in a lipoxygenase enzyme was developed. Based on the known x-ray structure, five natural side chains were replaced with spin labels yielding ten pairwise distances. These 10 distances were measured between these labeled sites to establish a framework. The location of a lipid spin could then be determined by "triangulation" by measuring the distance of the lipid spin from each of the five framework labels. The extensive distance measurements could be sped up by the use of DQC.

13 Long Distance Measurements by Five-Pulse DEER [19]: Standard DEER contains four pulses. We introduced a new version of DEER in which an extra pulse at the pump frequency is included. This significantly reduces the effect of nuclear-spin-diffusion on the electron-spin phase relaxation, thereby enabling longer dipolar evolution times that are required to measure longer distances. This enables a significant increase in the measurable distances, improved distance resolution, or both.

14 New Denoising Method for cw and pulse ESR [20 , 21]: A new wavelet method was developed to denoise 1D experimental signals. The new method a) enables the selection of the number of decomposition levels to denoise, b) uses a new formula to calculate noise thresholds, c) applies denoising to the approximation component, and d) allows flexibility to adjust the noise thresholds. When applied to cw ESR spectra, it was shown to increase SNR by more than 32 db without distorting the signal. This method was adapted to pulse-dipolar electron-spin resonance spectroscopy (PDS). Signal averaging times could be reduced by as much as 2 orders of magnitude. Excellent signal recovery was achieved when the initial noisy signal has an SNR $\gtrsim$ 3.

15 A New SVD Method to Determine Distance Distributions in PDS[22, 23]: Regularization is often utilized to elicit the desired physical results from experimental data containing noise. We developed a new SVD method that yields very accurate distance distributions ($P(r)$) and their uncertainties in the analysis of PDS experiments. It is based on the following. First, one applies the SVD approach separately for each value in order to obtain its respective $P(r_i)$. As one adds singular value contributions, starting with the largest singular value, the value of $P(r_i)$ converges to a plateau value but eventually diverges. The correct $P(r_i)$ is the average over the plateau values, and the uncertainty is given by fluctuations in the plateau values. These convergence properties differ for different values of r_i. Excellent results for PDS are obtained without the introduction of a regularization parameter.

16 Microsecond Exchange Processes for Nitroxide-Labeled Species by 2D-ELDOR at 95 GHz [24]: Exchange processes are routinely studied by 2D exchange NMR techniques by observing the development of exchange cross-peaks. Whereas 2D NMR enables the real time study of millisecond and slower processes, 2D ESR in the form of 2D-ELDOR has the potential for such studies over the nanosecond to microsecond real time scale. Unfortunately for ESR, at typical frequencies the exchanging states ▶

yield ESR signals that are not resolved from each other within their respective line widths. We showed by 2D-ELDOR at 95 GHz it is now possible to resolve them in many cases because of the increased g-factor resolution. These capabilities were demonstrated by 1) the protonation/deprotonation process for a pH-sensitive spin label and 2) a nitroxide radical partitioning between polar (aqueous) and nonpolar (lipid) environments.

17 Improved Computation of Dynamics of Proteins by 2D-ELDOR [25]: Recent developments permitting experiments at 95 GHz provide molecular orientational resolution, enabling a clearer description of the nature of the motions. However, we found that the existing theoretical methods for computing 2D-ELDOR experiments at higher frequencies over a wide motional range begin to fail seriously when applied to very slow motions characteristic of proteins in solution. One reason is the failure to obtain accurate eigenvectors and eigenvalues of the complex symmetric SLE matrices describing the experiment in the range of very slow motion. Also, these matrices are "non-normal" and cannot even yield reliable results for very slow motions. We have employed algorithms that overcome both issues. Their use is illustrated for very slowly tumbling proteins with somewhat faster domain motions, showing how they can lead to cross-peaks that inform about the nature of the domain motions.

18 Construction of New High Resolution Pulse Spectrometer at 35 GHz for PDS/ELDOR, with 1 kW Pulses: The new 35 GHz pulse spectrometer was built to replace our vintage Ku band PDS spectrometer by providing more convenient operation but also higher sensitivity and additional options. The recently installed cryogen-free system greatly facilitates round-the-clock unattended operation. The 1 kW TWTA is sufficient for DQC and a class of shaped pulses like Hermite pulses. It allows us to excite more spins in a larger volume with uniform-B_1 DR or TE102 cylindrical resonators, thus further increasing sensitivity.

19 Construction of New High Power 17 GHz 2D-ELDOR and PDS spectrometer: This is equipped with a 4 kW TWTA for 2D-ELDOR. It can generate short intense pulses needed for 2D-ELDOR or DQC. Its high-speed pulse-forming channels with quadrature modulators can also function as I/Q phase modulators to generate pulse chirping and shaped pulses. MW pulse generation is quite flexible. It is tunable over 8–18 GHz in five bands. The bridge includes an up/down converter for Ka band function. The pulse-forming system is based on a custom 1 ns resolution 12 channel PCI card.

20 New 93 GHz Swept cw/Pulse ESR Spectrometer: This spectrometer operates at low power (20 mW) in cw mode and up to 1 W in pulse mode. It includes a variable-temperature insert (VTI) that is operational down to 10 K and is intended for a) experiments with novel configurations of microfluidic and conventional micro-resonators, b) experiments with wide field sweep, and c) fundamental-mode cavity experiments including ENDOR and DNP. On this instrument it is possible to perform pulsed spectroscopy experiments where power is not a critical concern (e.g., frozen samples for DEER).

Jack H. Freed

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- Sweep echo detection
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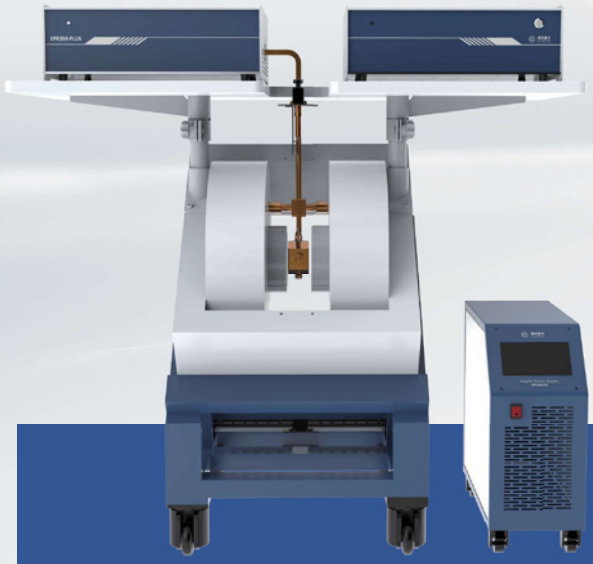
- ENDOR experiment

X-Band Pulse / Continuous Wave Electron Paramagnetic Resonance Spectrometer

EPR100



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- Irradiation experiment

X-Band Continuous Wave Electron Paramagnetic Resonance Spectrometer

EPR200-Plus

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Desktop EPR

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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	5×10^{9} spins/(G√Hz)

Applications

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

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James S. Hyde (1932–2022)

The many facets of James S. Hyde: Tributes from some of his many admirers

While we are all saddened by the loss of this great scientist, it is important to also focus on his many contributions and celebrate them. In this spirit we have reached out to his colleagues and friends tasking them to comment on their remembrances of Jim. The response has been outstanding and is included in full, after this introduction considering the many facets of Jim. Jim himself provided us with a very illuminating description of his views on his career in an autobiography published in a special issue of Applied Magnetic Resonance in his honor in 2017 (Appl. Magn. Reson. 2017 Dec; 48(11-12): 1103–1147. doi: 10.1007/s00723-017-0950-5. Epub 2017 Oct 27).

My first in-person interaction with Jim was in his role as an austere magnetic resonance physicist, when I attended one of the legendary Varian workshops in the early 1960s. With my background as an MD with an inclination to biophysics, I had recently inherited a magnetic resonance laboratory at the Walter Reed Army Institute for Research in 1962. I knew I needed to quickly and proficiently learn more of the fundamentals of the instruments I was now supposed to utilize and manage. Gratefully, I learned about the Varian Workshops, which were advertised as doing just that.

The Workshop was indeed a very useful and enjoyable experience and provided my first introduction to Jim and his insightful but esoteric understanding of the physics underlying magnetic resonance. My remembrance of Jim at this workshop was of someone who gave an impressive (but mostly incomprehensible) and highly accurate description of the physics of EPR and how physical principles impacted the EPR spectra obtained with the Varian EPR spectrometers that were then available. I gradually came to grasp some of the elements of physics that Jim was illuminating as I went over my notes and read and reread the "EPR at Work" series, which Jim developed to make these principles accessible to users like me.

The next several years provided opportunities to know Jim better and to further appreciate his vast expertise as well as to begin to understand the depth and breadth of the very interesting and complex person he was. I was especially surprised and very delighted when, in late 1974, I received a note from Jim indicating he was exploring the possibility of moving from Varian to a university.

I had by then moved to the Medical College of Wisconsin (MCW) in Milwaukee, WI as a research oncologist/radiologist and scientist. Encouraged by this exciting opportunity to continue my research interests and advance magnetic resonance research, I investigated a program (Research Resources) at NIH that was designed to provide wide access to very sophisticated expertise and instrumentation. The program was intended to support centers of excellence, each representing unique and special technical scientific competence, with the intent to not only support the special expertise of the personnel of the center, but to make the technology widely available to multiple users who could train at these centers and then disseminate the knowledge and technology broadly.

I corresponded with Jim about this opportunity to create a joint adventure for both of us, and we both became very enthusiastic. On Dec. 25, 1974 (yeah, flights were cheaper on Christmas day and fine with me), I flew to California. Jim and I spent the next couple of days working out the details for what became the first NIH-sponsored Research Resource on EPR. Meanwhile, I was able to convince the Dean's office at MCW and the Department of Radiology that recruiting Jim would be a very productive step. They agreed and offered him an appointment with guaranteed salary (with the expectation we could compete successfully for NIH support that would in fact cover his salary). This investment proved very wise, as Jim brought multiple large and smaller grants to MCW and established it as a widely recognized center of excellence, not only in EPR but later in MRI as well. The essence of the enthusiasm for the original funding was perhaps best expressed by the Chair of our Advisory Committee for the Program at MCW, Helmut Beinert, who proclaimed, "Jim is a national asset that we need to support to help many investigators".

The four years that we co-directed the EPR Center at MCW were among the most enjoyable and productive of my academic life. Jim and I were the perfect academic "odd couple," i.e., we had complementary areas of expertise and interests so, as a result, we had minimal areas of rivalry or conflict. We developed a warm and enduring personal relationship, with multiple visits between our households as well as for scientific collaborations. More details on Jim and the ESR Center at MCW are available in H. M. Swartz, "An Incomplete History of Jim Hyde and the EPR Center at MCW" in Biomedical ESR, a volume in the Biological Magnetic Resonance Series. S. S. Eaton, G. R. Eaton, L. J. Berliner (eds.) The Netherlands: Kluwer Publisher, Chapter 2, pp. 7–22 (2004).

Before I left MCW to become an Associate Dean at the U. of Illinois College of Medicine in Urbana-Champaign (UIUC-Medicine), Jim began to explore an area of research that became another cornerstone of his academic achievements. I convinced him that magnetic resonance imaging (MRI) was a ground-breaking modality that was likely to have a large impact in clinical medicine and basic research. After some further investigation, Jim enthusiastically joined into that area of research.

He since developed many new concepts in MRI that have become very, very important (see his autobiography for some details). As my career evolved, first at the UIUC-Medicine and then at Dartmouth College (in the Schools of Medicine and Engineering), Jim continued to be an extremely valuable advisor and collaborator. Each of the new EPR Centers I later founded (at UIUC and Dartmouth) had an Advisory Committee that Jim was always willing to serve on and in every instance made monumental contributions to our progress. In a complementary manner, after leaving MCW, I became a member of the Advisory Committee for Jim's EPR Center at MCW. In that sense, we each served a span of 40+ years of leading NIH funded EPR centers. I like to think that he and I continued

during that time to provide complementary viewpoints that kept our EPR Centers on paths pertinent to biomedical applications.

I have many fond memories of the science we did together, the many dialogs and debates we had, the many contributions of Jim made to my own research program, and especially of the many and warm personal interactions Ann and I have had through the years with Jim and Karen. We will greatly miss Jim.

We also will continue to enjoy our memories of Jim the friend and mentor, Jim the proud and happy patriarch, Jim the epicure of great food and excellent wine, Jim the art supporter, Jim the outdoor enthusiast, and of course Jim the scientist and Jim the organizer and portrayer of imaginative research enterprises.

These themes are echoed and expanded in the many tributes to Jim from Jim's colleagues that follow in their entirety as submitted. The breadth of them is mind-boggling!

Harold M. Swartz

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• Family man

(Note: *See also many references to his family in his notes from his colleagues. Sarah Hyde, his daughter, summarized this aspect of her father very nicely.* [HMS])

Jim took great pleasure in seeing everyone, asking about the future plans of his grandchildren, enjoying the antics and chatter of great grandchildren, and of course, making sure we all had plenty of champagne. We are all so grateful for this time we had together before his unexpected passing in August.

Sarah Hyde

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• Research mentor

(Note: *See also the many references to Jim's very significant mentoring in other notes from his colleagues*. [HMS])

Jim Hyde was an amazing scientist, professor, and member of the community, open minded with boundless enthusiasm for new questions, discoveries, and endeavors, generous and deeply supportive, and a heartfelt, joyful smile. I was Jim's first graduate student, beginning after my second year of medical school. My work used saturation recovery and electron electron double resonance methods to study bimolecular collision rates and diffusion in spin-labeled model membranes. After graduating, I would go on to the University of Pennsylvania departments of radiology and then psychiatry. Here I would shift to MRI studies, which were just becoming clinically available, and eventually go to Emory University to help establish a functional MRI program. In the meantime, Jim and his graduate students had become trailblazing leaders in functional MRI. Jim introduced me to one of the students, Allen Song, who would later join our group at Emory and go on to Duke University where he became director of the Brain Imaging and Analysis Center. Thinking about memorable quotes from Jim, the most remarkable is something quite rare – silence. When I would go to Jim to discuss something or ask a question, or he would begin a discussion, he would often begin with a very long pause of silence. Very, very long pause, longer than I have ever known with anyone else (except perhaps one other). These were moments of relaxed anticipation and clear attentiveness. When he would begin to speak it was always very engaging and invariably interesting. There was a sense that he took the question as the basis to think about something that could become important, valuable, that it was worth time to think about this slowly, carefully, creatively, at that moment, before speaking. This may be a general reflection of how Jim was ready to give his time and energy to others. Alongside his scientific achievements, with his wife Karen, Jim would become an art collector and supporter of the local Museum of Wisconsin Art, which he helped grow and expand in wonderful ways to benefit the community. Jim was generous with his time, energy, creativity, and a diversity of supportive activities. For all these, I am most grateful.

Carol Popp Weingarten

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Professor Hyde observed the world through the eyes of a spin. His contributions to the magnetic resonance community were many and will continue to provide fruitful avenues of research l for years to come. I am proud to have had him as a mentor and owe him a lifetime of gratitude for the many travels and thoughtful discussions that I enjoyed with him.

Jason Sidabras

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Always signal-to-noise ratios!!

I worked with Jim for about 2.5 years as a postdoc between 1979 and 1982, but we continued our collaborative research, and the last paper we wrote together, which was our 14th, was published in 2007. I got busy working on single fluorescent-molecule imaging and fluorescence lifetime observations under the microscope since 1990 and have not done very much EPR work since then. However, our interactions continued throughout our lives, including two memorable visits of all my family members to Jim and Karen at their home (a farm!!) and their visit to our home in Tokyo. I am extremely thankful, particularly to Karen, for the warm welcome at their home. I will cherish these special memories till the end of my life.

When I first arrived at Jim's lab as a postdoc, my first and biggest surprise was that Jim was always talking about signal-to-noise ratios. Consequently, I also ended up discussing them whenever I got together with Jim, which was almost every day over lunch at the canteen at the Medical College of Wisconsin. Initially, I wanted to talk more about science than technology, but in time, I started enjoying the discussions about the signal-to-noise

From left. Front: John Elrod (grandson), Karen Hyde (wife), Kate Hyde (great granddaughter) , Jim Hyde, Carl Tucker (grandson). Back: Julia Elrod (granddaughter), Matt Elrod (son-in-law), Elizabeth Elrod (daughter), Doug Hyde (grandson), Laurel Hyde (daughter-in-law), David Hyde (son), Sarah Hyde (daughter), Ernie Tucker (son-in-law), Claire Tucker (granddaughter), Ben Haas (partner of granddaughter).

ratios, mostly due to the extremely high-level insights that Jim shared in these discussions.

I would like to list the four most important lessons about signal-to-noise ratios I learned from Jim, which I hope might also be useful to the readers. Please endure the inclusion of my own prejudices here.

1. Science is limited by what you can measure and/or observe, which is constrained by the signal-to-noise ratio. This is true even for biochemical measurements, like western blot gel patterns. Therefore, talking about the methodology is almost the same as talking about the signal-to-noise ratio that the method provides.

2. When you think about the signal-to-noise ratio, you must always consider signal and noise separately.

3. Noise can often tell you as much as the signal. Noise usually represents the essential part of the specimen and your measurements. Enjoying looking at error bars rather than the mean values has thus become one of my basic habits when I read papers and manuscripts now.

4. When the detector is noisy, like microwave detectors, place an amplifier before the detector to enhance both the signal and noise up to the level where the enhanced "noise" (be careful, this must be noise and not signal) becomes greater than the detector noise. I recently used this principle to develop an ultrafast camera system enabling the fastest single fluorescent-molecule imaging to date (33 kHz; Fujiwara et al. bioRxiv 10.26.465864).

I now feel that I was quite lucky that the non-linear EPR spectroscopy I learned in Jim's lab at the beginning of my scientific career was a technology with low signal-to-noise ratios. Compared with visible-light optical absorption spectroscopy, which deals with electromagnetic fields (light) of ~500 nm wavelengths, EPR tends to deal with those of ~1 cm. Accordingly, the energy level involved in EPR spectroscopy is about 10,000x ~ 100,000x lower. Therefore, whereas noise is often difficult to detect in the optical absorption spectra, in the pulsed EPR spectroscopy (saturation recovery EPR) I was involved in developing, I had to deal with saturation recovery curves with signal-to-noise ratios generally between 2.5 and 6.

I never expected that getting accustomed to low signal-to-noise ratios in my data would become useful later on. While I was working on ultrafast single-particle tracking and single fluorescent-molecule imaging, many other scientists gave up due to the very low signal-to-noise ratios involved in these technologies. The signal-to-noise ratios (more precisely, the noise part contains both the noise in the signal and the noise in the background) were often between 2 and 3; namely, the data were always on the verge between useful and useless observations. However, this was OK with me because I became familiar with low signal-to-noise data and I knew that one could still use such methods effectively. Therefore, I was not afraid of or overly worried about the signal-to-noise ratios of the images we obtained, even when they were only a little higher than 2. Indeed, we kept managing to obtain exciting data in this field.

In conventional EPR spectroscopy, Jim used to talk about a magic factor of 2.5 (which even included a psychological factor), invented by his previous Varian colleagues for describing the signal-to-noise ratios of conventional EPR spectra, but it did not seem to work well for the saturation recovery curves. Once I gave a talk in Prof. Jack H. Freed's lab at Cornell and said that the signal-to-noise ratio I was generally getting in my saturation recovery curves was about 10. One of Jack's postdocs was very skeptical, and he insisted that the signal-to-noise ratio I was getting must be about 4. I reluctantly had to accept his point, and from that time, I stopped using the magic factor of 2.5 for my saturation recovery curves.

The signal-to-noise ratios in single fluorescent-molecule images we obtain in my lab are generally about 2.5. Interestingly, other labs often state that the signal-to-noise ratios they are getting are about 6, which is a difference by a factor of about 2.4. I know that we are using a very precise and strict definition of the signal-to-noise ratio in my lab. I feel quite amused to consider that other labs might also have invented their own magic factor of 2.5.

I am now extremely thankful to Jim and will be even more thankful to Jim in the future, for introducing me to such scientifically important concepts and sources of amusement.

However, rather than only talking about signal-to-noise ratios, I wish to mention one of the scientifically important findings that Jim and I made in 1982. We published the EPR detection of transient dimers of rhodopsin, a G-protein-coupled receptor (GPCR), which was the first finding that a GPCR can continually form metastable homodimers/oligomers. It took almost 30 years until this concept became quite popular in the GPCR field. Now, using single fluorescent-molecule imaging, my group has further characterized metastable GPCR homodimers and their functions (Kasai et al., 2010, 2016; Kasai et al. bioRxiv 2020.02.10.929588). This is a good example of a situation where considering signal-to-noise ratios has paid off handsomely.

Akihiro Kusumi

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I was a grad student at Stanford from 1971–1975. My official advisor was Harden McConnell world-famous biophysical chemist at Stanford, but my actual advisor for most of my research was Jim Hyde, senior scientist at Varian, a few miles from the Stanford Campus. I was a physicist, and Jim taught me chemistry and biophysics, which has led me to a productive career as Professor of Biophysics at the University of Minnesota (1979 – present) and President of Photonic Parma LLC (2014 – present). He welcomed me to his lab at Varian, and he also welcomed me to his beautiful family, Karen, David, Sarah, and Elizabeth. From them, I learned many important lessons about life, including how to enjoy wilderness camping and fishing. Most importantly, Jim taught me, by his example, how to be a teacher, entrepreneur, husband, father, and friend. I am forever grateful to Jim and his family.

David D. Thomas

PhD graduation of David D. Thomas (1975). From left: Dave Thomas, Harden McConnell, and Jim Hyde.

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• Collaborations with scientists from Poland and the former Soviet Union

(Note: *Jim built incredibly on associations that I had initiated in the 1970s. These connections became of great importance in terms both of their productivity and scientific creativity, which also led to close personal connections lasting many decades. Jim was immensely proud of being awarded an honorary doctorate from the Jagiellonian University*. [HMS])

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It is difficult to accept the passing of a good friend forever and the fact that I will never be able to simply talk to him again. In this tribute to Jim, I would like to say a few words about him as a man who was a good friend. Jim was a great scientist. Indeed, his publication record is truly impressive. It consists of over 400 publications that have already been cited about 50,000 times. It is worth mentioning that already in 1989, he was appointed Doctor Honoris Causa of the Jagiellonian University in Cracow, my university which is one of the oldest European universities.

I met Jim for the first time in 1967 in Moscow at the Institute of Virology where an exhibition of scientific equipment made by Varian was organized. Jim Hyde was a member of the Varian team serving the exhibition. I got permission to use the E-3 spectrometer for the whole week of the exhibition to collect data for my master thesis. Ten years later, I met Jim again when I came to the Medical College of Wisconsin for the first time. Since then, I have made about 50 visits to Jim's lab, staying there for a total of about 10 years.

During these multiple visits to Jim's lab, a total of about 100 collaborative articles were published, the most cited of which is the publication describing the concept of a new resonator called the loop-gap resonator. During the writing of this publication, Jim's excellent ability to extract important results in research, as well as the ability to name and clearly describe them, was revealed.

I have always been impressed by his ability to clearly write publications and grant proposals. Undoubtedly, he was helped by his exceptional knowledge of grammar, which I found out for myself. I loved our lunches together where we talked about various things. One time during a lunch time conversation, I asked him about the rules for using a hyphen in English. After a moment's thought, Jim enumerated all the rules that I accidentally knew back then from my wife who was taking an English grammar course. None of my other American friends could list those rules. It was amazing to me that Jim, as he said himself, remembered the grammar rules of high school well.

My visits to Jim's home will always be remembered. Once upon a time Jim, showing me his home furniture projects, aroused my interest in woodworking, thanks to which I made some furniture myself. These are just a few examples that come to my mind right now and that have shaped my relationship with Jim, they will remain in my memory forever.

In addition to the things mentioned above, I am very grateful to Jim for having met many wonderful people. I would especially like to mention my good friend Wayne Hubbell, as well as Harold Swartz and Richard Stevens.

I am very sorry to have lost such a good friend.

Wojciech Froncisz

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Forty-two years of collaboration with Jim Hyde!

My collaboration with Jim Hyde started in 1980 when I, in March 1980, came to the United States as visiting scientist for research training at the National Biomedical EPR Center. We published together thirty-eight experimental papers and six reviews and book chapters. According to Google Scholar, seven of these publications have been cited more than one-hundred times. I am very happy with these scientific achievements. Beyond our scientific collaboration, which can be expressed in numbers, I developed a close friendship with Jim, which helped me greatly in establishing my permanent life here in America. Jim supported and mentored me during that time.

During the first twenty years of our collaboration (that is, between 1980 and 2000), I visited the EPR Center twenty-one times, and Jim always welcomed me very warmly and in the most friendly manner. It alleviated all the stress, which – especially during our first visits – most of us Polish scholars felt due to being abroad and working with such a world-famous scientist.

In all our years of working together, one of the most memorable events for all of us was when Jim received a degree of Doctor Honoris Causa from Jagiellonian University. The ceremony took place at the Collegium Maius, Jagiellonian University's oldest building, which dates back to the fourteenth century. That very traditional and grandiose ceremony was followed by a somewhat relaxed party. The master of the ceremony made the first toast, talking about collaboration, science, and so on. The next toast, which was made by Jim, somewhat surprised people, including me. He pronounced, "To my wife Karen, who shares this day with us". Now I understand that it was one of the best toasts I've ever heard, warm and coming directly from Jim's heart.

To commemorate this ceremony, we organized the Workshop on Newest Applications of ESR in Biomedical Research. That way, thanks to Jim, we established the tradition of these workshops, which take place in the Jagiellonian University every three years. Jim was always the honorary guest. Three years ago, during the 11th Workshop in October 2019, Jim and Karen walked happily through the streets of Old Krakow. I believe that Jim's spirit will bring EPR scientists from all over the world together for many returns of the workshops in Krakow.

At the end of 2000, I relocated permanently to the United States. It was very difficult decision, and I was somewhat lost as to what I would have to do to set up my life in Milwaukee and my work in the Department of Biophysics (in the EPR Center). I asked Jim for major advice. After thinking about it for a while (and talking with Karen, who was also present), he said, "First, you have to buy a house; next, you have to put all your free money in retirement funds; and third, you have to get grants". After some additional thinking, he

W. Karol Subczynski is rising to give a toast during the ceremony for Jim. From left: W. Karol Subczynski, James S. Hyde, and Karen Hyde. (Taken at the 3rd EPR Workshop, Krakow, September 1995.)

added, "Because you have no time to save enough for the retirement, I suggest that you also play the lottery". Five years later, I protested to Jim that his advice is not working. I bought a house, I put all available money into my retirement funds, and even I got my first R01 grant. However, until then, I had not managed to win anything playing the lottery! Today, I take back my protest. When I sent in my grant for competitive renewal last year, it dawned on me that getting it is somewhat like the lottery and connected – not in a small part – with the personal luck. My third renewal was funded through May 2020. In that way, I think that I fulfilled all four limbs of Jim's advice.

About ten years ago, Jim and I established a new, rather personal tradition. Several times a year (maybe even once a month), at the end of the work week, we would have one (or sometimes two) drinks of something tasty and unusual. We started with cognacs from Turkmenistan (interestingly, this Muslim country produces excellent cognacs, comparable with the best French cognacs). We had rums directly from Guyana, and balsams (a drink made of local herbs) from Siberia (an area of Amur), Turkmenistan, and Latvia. Most of our supplies came from my daughter, who frequently travels all over the world. During these approximately thirty-minute breaks, we would talk about good drinks and good food, about unconventional travel and travel experiences we have had, and – of course – about interesting people we have met. We almost never discussed research. Thanks to Jim and his support, I have many memorable moments. I know that these good times will not return, but I will keep and cherish these special memories for the rest of my life.

Witold Karol Subczynski

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I first met Jim Hyde in 1967 when he came to the Varian show in Moscow. I worked then in the laboratory of V. V. Voevodsky, in the group of Ya. S. Lebedev. In my opinion, we then achieved a certain progress in the development and application of the EPR method in the study of chemical reactions in the gas and solid phases. A. G. Semyonov's group completed the development of the first domestic EPR spectrometer. Using this spectrometer, I was able to study in detail the kinetics of radical pairs recombination in butyronitrile. Jim then, despite being busy at the show, spent several days in our laboratory. The first thing we did was to compare the sensitivities of our spectrometer and the Varian spectrometer using the Weak Pitch sample that Jim had brought with him. Comparison under optimal conditions for each spectrometer was not in our favor, which we easily explained by the much more powerful klystron of the Varian spectrometer. And then at the lab meeting were extensive discussions of the results, which we rushed to share with Jim. It was the time when the search for new ways of developing EPR technology began. In particular, there was great interest in the ELDOR technique. In this method, the optimal resonator is most important. We talked at this meeting about our two versions of the resonator, volume cavity and spiral resonator, developed by V. A. Bendersky. Jim presented his volume cavity. Each promoted his own resonator and everybody remained with his own opinion. As far as I remember, Jim was particularly interested in Lebedev's report on the effect of concentration of the microwave power of a wire loop placed inside a cavity. I suspect the discussion of this effect may have contributed to Jim's development of the loop-gap resonator later. This event made a deep impression on me, still a young researcher. Jim instantly grasped the main idea of any presentation, gave his original evaluation of it, and provided possible further technical development.

Jim Hyde has always amazed me by many-sided interests at a very high professional level. As I found out later, as a rabbit breeder, Jim even bred a new breed of rabbits. I recall our meeting in September 1989, when Jim stopped in Moscow for a couple of days on his way to Novosibirsk for the conference dedicated to the memory of V. V. Voevodsky. I was appointed as the so-called "escort", i.e., during the visit, I was supposed to be a guide and accompany Jim everywhere. Jim's first desire was to visit the Pushkin Museum of fine Art. This is a relatively small museum, in which they collected unique paintings by famous artists. When we finally got to the museum (for Jim and Karen it was a very unusual journey in a crowded trolley bus), Jim immediately headed to a certain hall where he wanted to gaze upon two famous impressionist paintings (unfortunately I don't remember the name of the painter). When we finally found ourselves in that hall, the required paintings were not there. We asked the museum staff. They provided a strange response, i.e., that these paintings were never in that hall. Jim was very disappointed. He insisted that, by his knowledge of catalogs, these paintings must be there and said that he had just arrived from America to gaze upon the original works. The manager who was summoned attempted to pull the wool over our eyes, insisting that either the paintings were taken away for storage or restoration or they were simply taken away somewhere. So, perestroika was then already at full speed and even museums had begun to move into a state of chaos. After this unsuccessful attempt, we spent some time visiting various exhibition shops. Jim tried to purchase any original paintings and/or carpets. However, very quickly Jim understood that as soon as the sellers recognized that the buyer was American, they did their best to 'circle him around their fingers'.. I was amazed at how well Jim understands modern painters and carpet patterns (especially compared to me). Therefore, no one managed to fool him, despite many attempts.

In 1989, my Moscow laboratory manager Lebedev agreed with Jim Hyde that he would take me to the MCW laboratory for one year as a visiting scientist. To say that it was a big challenge for me is an understatement. The first foreign trip in my life and to stay for a year, and even going to such a laboratory! The laboratory really turned out to be more than any of my expectations in every sense. Of course, I do not mean the fantastic laboratory space that many people have heard about. Above all praise is the convenience and organization of the work of the entire laboratory team, which contributed to the high efficiency of research. Excellent relations between all employees, when everyone is ready to help you. All this left me with the warmest memories of this important period of my life.

I would especially like to mention Jim's light-hand here, which I felt during this visit. For clarification, here I need to say a few words about the purpose of my work, which Jim suggested to me. I was directed to obtain experimental confirmation of Jim's earlier theoretical result: the effect of nuclear relaxation on the saturation recovery of nitroxide radicals under various experimental conditions. To get me up to speed, Jim appointed J. J. (Jun-Jie Yin) as my mentor. But even with his great help, it took me about two months to master the device and all the subtleties of the experiment. By this time, Joy (Joy Joseph) had completed the development of a special program for fitting saturation recovery curves. And the rather time-consuming collection of 12x7 experimental data began. But the more I got data on the systems of interest to us with solutions of radicals with the narrowest spectral lines, the more I did not like the results of fitting processing because of their irreproducibility.

As time went on, when meeting in the hallway, Jim asked if I liked the Midwest climate, if I needed any help, but not a word about ▶

my work (although I'm sure J. J. talked about the state of my research at his regular meetings with Jim). And when I almost gave up hope, I decided to take a break. I asked Hal Swartz permission to visit his lab in UICU. In Hal's laboratory, lithium phthalocyanine crystals were synthesized. This crystal showed amazingly narrow EPR line in the absence of oxygen. Hal kindly allowed me to take some crystals with me to MCW.

Oh, how lucky I was! With the help of this crystal, I was able to find out that the cause of my problems was the result of imperfection of the FID signal suppression coils. I informed Jim and he asked to personally demonstrate him all my evidence on the device. The coils were improved after all, but my visit to the US was already ending. Before my departure, at a laboratory meeting, I could not boast of my scientific success for this year, and I had to talk about my Moscow results. In conclusion, Jim provided an amazing assessment of my visit. He said, "you taught us how to work". And I was so pleased, I got a charge of enthusiasm for the next few years.

Oleg Grinberg

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• Tributes from colleagues at Medical College of Wisconsin

It was an honor and a pleasure to have worked so closely with such an incredible biophysicist and impactful human being for so many years at the National Biomedical EPR Center at the Medical College of Wisconsin. My memories from the more than 25-year journey since I met Jim are too many to capture, but here are a few that stand out: I remember him pacing the halls of Biophysics deep in thought, his influence on my academic career trajectory, his hours-long meetings with the engineers in his lab, his animated discussions (he loved to challenge and be challenged), his silence during a conversation, which meant he was thinking (not that you should fill that silence yourself!), him wearing a suit to work every day, his proud and steadfast support of his trainees, and the satisfaction of eliciting a grand smile from him. I am truly honored and humbled to hold the James S. Hyde Professorship in Biophysics at the Medical College of Wisconsin.

Candice Klug

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• Tributes from many other outstanding EPR scientists

I first met Jim in 1964 when he came to Cornell to lecture on his achievement of liquid state ENDOR with Gus Maki. This inspired me to do a theory of why it works and led to a close friendship with Jim. Together we worked on the development of ENDOR and ELDOR; he, doing the experiments, and me, the theory. This included my visits to Varian in Palo Alto where Jim was working. Our families enjoyed many occasions together. We remember with fondness the time during a Magnetic Resonance Gordon Conference when our families had a working vacation by taking adjoining cottages at a New Hampshire lakeside. When it was time for Jim to leave Varian, I tried to get him to join our Biophysics Department at Cornell. Jim instead moved to Milwaukee where he established a strong Biophysics Department at the Wisconsin Medical Center in Milwaukee. He and his Center prospered. We kept up for many years, and Jim would often send me papers of his excellent accomplishments. My wife Renee and I are very much saddened by his passing.

Jack H. Freed

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I met Jim in 1972 when I visited Varian in Palo Alto to purchase my first EPR spectrometer.

During the tour of the lab, Jim explained the prototype saturation recovery spectrometer that he had constructed. The salesman thought his presentation was deadly and would kill his sale. He kept tugging on my arm, trying to get me out of the room. I thought instead that, if only I had time to ask a couple more questions, I would finally understand what Jim was saying about the spectrometer.

Jim had family in the Denver area and occasionally visited our lab at DU.

After Jim moved to MCW, I visited his lab many times. Knowing that Jim was involved in breeding rabbits, I started one of my visits to MCW with the facetious question whether the rabbit I had just seen as I approached the lab was one of his. The panic expression on Jim's face said I should not have said that! He asked what color, size, etc. Consequently, I was pleased when Helmut Beinert chose to present Jim with a rabbit at the celebration held for him in 2002 at the University of Denver. The following picture is from that event.

From left: Gareth Eaton, Sandy Eaton, Jim Hyde (and rabbit), and Helmut Beinert.

In addition to the many visits as a member of the P41 Science Advisory Board, I spent several productive periods of research at the MCW Center, especially performing S-, K-, Q-, and W-band studies. The S-band studies were done while John Pilbrow was visiting. We used the massive S-band cavity resonator that had to be supported on a lab-jack. Based on the development of the LGR by Jim and Wojciech, I quickly made a S-band and X-band LGR with hand tools in my garage. Now, we all use lumped-circuit resonators rather than cavities for most EPR measurements. In private conversation Jim and I joked about the fact that for many years we had looked at the image of the magnetron on the cover of the volumes in the Rad Lab Series but did not recognize that the loops and gaps would make a good lumped-circuit EPR resonator.

Building on what we learned from Jim about saturation recovery and from Mike Bowman about spin echo, our lab built several time-domain spectrometers at frequencies from 250 MHz to X-band, including several in which the bridge and data systems support both saturation recovery and spin echo in addition to standard CW. When I lectured at the MCW EPR Center about our invention of rapid scan EPR, I pointed out that, although we used magnetic field scan at X-band, it would be feasible to use microwave frequency scan at W-band. I was pleased that Jim quickly performed the W-band frequency sweep experiment, and then extensively developed a sub-field of rapid scan EPR that he called NARS.

The best part of my visits to MCW were the long discussions with Jim about the nature of spins, relaxation, instrumentation, and our shared vision for the future of EPR.

Gareth Eaton

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I have had the good fortune of meeting Jim in 1990, interacting with him in discussions over the years. With deep respect to him, I can summarize him through my interactions:

Jim knew the EPR signal in its variety of incarnations, how to capture the signal and to understand the important scientific questions which can be answered by EPR signals.

This is true in fMRI as well as FcMRI with his pioneering publications.

Murali K. Cherukuri

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I learned that Jim passed away recently. I want to convey my deepest condolences to both the family as well everyone in the Biophysics Department at MCW and to the entire EPR community. It is obvious that much beyond the institutional impact, Jim was a towering figure in the EPR community – his was the first few names one learned as soon as one started into the field.

Sunil Kumar Saxena

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I will be forever grateful to have had Jim Hyde as a mentor, colleague, and friend. Without his involvement over many years, I would have accomplished much less in my career. Even though I did not communicate with him on a regular basis, the knowledge that he was there gave me confidence to proceed in new directions where I would need his help. His passing leaves a serious void in my scientific life which will not be filled. Thanks Jim, wherever you are.

Wayne L. Hubbell

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I feel a deep obligation to express my sadness at the passing of Jim Hyde, this outstanding scientist and human being, by contributing briefly to this Tribute to James S. Hyde in the EPR Newsletter. I know Jim Hyde since a long time, in fact for almost 55 years, experiencing him always as one of the leading magnetic resonance scientists, a stimulating colleague and noble contender in the wide field of advanced EPR spectroscopy. Jim Hyde's research interests in EPR partially overlapped with our own. The careers of Jim Hyde and K. M. [the author] continued to overlap in many ways as their interests shifted gradually from physics to biophysics. For example, to develop advanced EPR instrumentation to extend the ways in which EPR spectroscopy can be applied to new categories of biochemical problems that are not yet accessible by standard spectroscopy techniques. Specifically, double resonance methods with a variety of microwave-frequency/magnetic-field combinations were in the focus, such as ENDOR and ELDOR at X-band and W-band. Interesting spin physics and spin chemistry of biocomplexes could thus be studied, such as membrane proteins embedded in their natural or artificial matrices. Their structure, dynamics and function relationships could be elucidated. By using site-directed spin labelling, SDSL, pioneered by Wayne Hubbell and co-workers at UCLA, the application of EPR methods in the life sciences has been greatly expanded.

In essence, my encounters with Jim Hyde over the years have been characterized by exciting science (very important) and inspiring personal interactions (no less important). I want to thank him for all this.

Jim Hyde is the founder of the National Biomedical EPR Center at the Medical College of Wisconsin in Milwaukee, a US Research Resource supported by NIH. The public grant of the Center has been continuously funded since 1976. He served as Director of the EPR Center from 1980 until his formal retirement in 2016. Jim Hyde's research has been non-stop funded by the public sector for more than forty years – that in itself is an amazing success story.

My first encounter with Jim Hyde was in March1965 when I attended the international EUCHEM Conference on "Chemical Aspects of Electron Spin Resonance" at the Royal Agricultural College in Cirencester (England). It was organized by David H. Whiffen from the National Physical Laboratory (NPL) at Teddington (Middlesex). I have always been grateful to him for having created, via the Cirencester conference, the opportunity to personally meet with so many fascinating EPR scientists, among them Jim Hyde, Jack Freed, Fabian Gerson and Giovanni Giacometti.

My last encounter with Jim Hyde was in October 2019 at the "XI International EPR Workshop on Biology and Medicine" in Krakow (Poland). The workshop was hosted by Tadeusz Sarna of Jagiellonian University in Krakow, Poland, a long-time cooperation partner and close friend of Jim Hyde.

During the long period of time between these two key events, I remember many more encounters with Jim Hyde at both sides of the Atlantic. However, I will confine myself here to only two of them that I find particularly indicative for Jim Hyde as a scientist and as a human being:

1) In July 1967, there was the "8th International Symposium on Free Radicals" at Novosibirsk/Akademgorodok (USSR), where I met Jim Hyde and Jack Freed for the second time, two years after our first encounter. Remarkably, ENDOR was one of the main topics of the Akademgorodok conference program. Appropriately, Jim Hyde and Jack Freed were the big stars of ENDOR-in-solution, they were praised with deep admiration for what they had achieved together with Gus Maki from Harvard. Jack Freed had provided the theoretical basis for liquid-phase ENDOR with a series of keynote papers on saturation and relaxation of radicals in solution. Unfortunately, he got sick right at the beginning of the symposium and spent most of the time in hospital in Akademgorodok. Thus, Jim Hyde became the lonely ENDOR central star, always orbited by a flock of admirers of all ages.

It was still the time of the Vietnam war. And every day the conference participants felt the absurd consequences of the existing Iron Curtain, and this even in academic circles. And then, in the evening of the official Conference Dinner, in a hotel in the middle of the Siberian taiga around Akademgorodok, a rather relaxed Jim Hyde once again became the shining star of the evening. Vodka, and more vodka was flowing, helping to exchange old and new ideas, trying to better ▶

Jim Hyde (left) and Klaus Möbius (right) in the garden of Jim and Karen Hyde's house in Milwaukee (2005). Photo by Arthur Schweiger.

understand each other. And to establish new East-West collaborations and friendships, tunneling the Iron Curtain. Some of them are lasting until today, for example Jim Hyde's sustaining EPR connections to Kazan and Krakow. In Kazan, he was distinguished by the 1995 Zavoisky Award for his contributions to the instrumentation and methodology EPR spectroscopy. And, notably, over the years his EPR and MRI research has been carried out with staff engineers and scientists from the Jagiellonian University in Krakow, with his closest collaborator Wojciech Froncisz working at the forefront of EPR innovations of loop-gap resonators.

2) In May 2005, I followed the invitation to participate in the "EPR Instrumentation Workshop" at Milwaukee. The workshop was jointly organized by Jim Hyde from the National Biomedical EPR Center of Medical College of Wisconsin and Arthur Schweiger from the Physical Chemistry Laboratory at the ETH Zurich. Scientifically, the workshop was a great success.

Jim Hyde and his wife Karen were kind enough to take the foreign speakers to their house in the marvelous Wisconsin countryside. There, we could admire not only their collection of historic agricultural instrumentation in the barn and corresponding expertise of farming. But also, their fine art collection of paintings and prints from Wisconsin artists and European expressionists exhibited in their house. Furthermore, Jim Hyde's extraordinary wine cellar, temperature-controlled, well-sorted and well-stocked. As seen in the figure above, serious matter can best be discussed over a glass of wine, even outdoor in the vast stretch of Hyde's garden.

Next day, late in the afternoon, Jim Hyde invited K. M. for a visit of the Milwaukee Art Museum, located directly at Lake Michigan. It is an architectural landmark designed by legendary architects, including Santiago Calatrava. The Museum was already closed. But Jim Hyde, apparently as a prominent sponsor, had open access, also after business hours. Somewhat surprisingly, he took the direct way to the Museum's small, but superb collection of Gabriele Münter, the famous German expressionist artist of the early 20th century. It was one of his favorite collections of the Milwaukee Art Museum, he said, and his insightful commentaries on the exhibits were a delight to listen.

With his family, we share in the mourning for Jim Hyde.

Klaus Möbius

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While I have had many wonderful opportunities to interact with Jim in all types of professional settings, clearly the most important and impressive interactions occurred during my post-doctoral experience as his second post doc at Varian starting in 1966.

My first duty at Varian was to achieve the noise free solution ENDOR SPECTRUM of a radical in liquid using a kw rf source that was claimed locally, in the surrounding labs, to be the reason for ALL New Varian instrument development problems and failures by its rf broadcast interference. However, Richard Ernst, Nobel Prize later in MRI, used it as a remote source to debug his computer next door to me at Varian (the Endor lab where I lived). What a clever person.

Later that year, Jim created the ELDOR cavity, which I used and we published a paper on the resolved EPR spectra of different overlapping radicals produced by X-radiation.

Afterwards, Varian produced the following year, three commercial ELDOR instruments, one went to Russia, one to Brookhaven National lab and one to me at UA, where I used it as the basis for AEC GRANTS for 15 years on X-irradiation chemistry, that developed in to 30 more years of funding on carotenoids by DOE UNTIL 2015, supporting some 20 PhD's, 7 MS and 25 years of NSF funded REU programs for undergraduates. This is the result of the 'can do' ground breaking attitude promoted in Jim's lab at Varian.

To date, I am still publishing with my former students, now professors at universities.

Lowell Kispert

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• Commercial ventures and engineers

(Note: *This was always an important aspect for Jim, starting with his high productivity at Varian; he was very expert in this arena as in so many arenas*. [HMS])

***

Dr. Hyde hired me as a young microwave engineer in 1982 for a summer job to design a solid-state oscillator replacement for a 35 GHz klystron in a Varian E-110 bridge. The microwave engineering endeavors soon expanded into noise reduction in EPR bridges at Q- and X-bands. The development of multiquantum bridges followed in the 1990s, when he also served as my dissertation advisor (he was an Adjunct Professor at Marquette University). The multi-function W-band bridge development and experiments (FM, SR, frequency swept) were an outgrowth, engineering-wise, of these previous accomplishments. In all of these developments, I was impressed with Dr. Hyde's grasp of engineering methodology, knowledge and appreciation of specifications, and his ability to recognize the strategic advantages that new or improved engineering products could bring to EPR. I always enjoyed discussing his new ideas to improve or innovate an EPR experiment with modern technology as an enabling component. He led several engineers in a large variety of efforts far beyond microwave engineering throughout his distinguished career at MCW. I will remember him always for these treasured memories and contributions, and for the summer job that lasted 35 years!

Robert A. Strangeway

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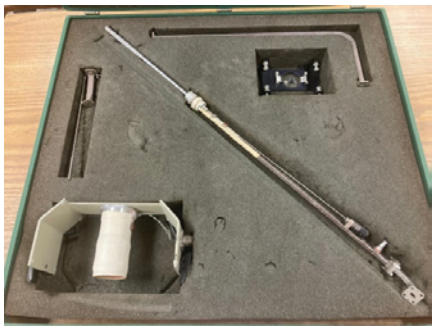
Regarding Jim's elegant resonators

(Note: *Jim was most proud of his achievements in developing unique resonators*. [HMS])

Jim's genius was especially evident in his accomplishments in resonators. Here is a photo of Jim's elegant Varian wire-wound low-temp Q-band resonator. Knowledgeable microwave folk are entranced by it 'on sight'! I know little of its history, except that it was probably purchased in the first half of the 60s. And I thought that this was the only one in existence, but Jim Anderson (see below) also has one – a more advanced version?



Jim's elegant Varian wire-wound low-temp Q-band resonator (~ early 1960s).

Brian Hoffman

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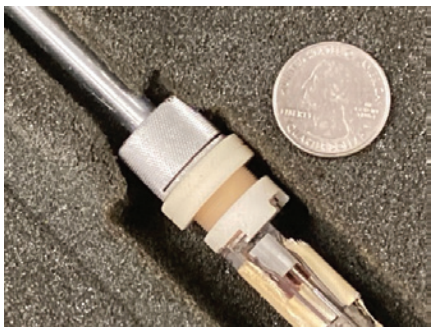
I have one of Jim's elegant resonators also! It came with my Q-band bridge. Their first Q-band bridge was in the sixties I believe. I even made a silver plated graphite replacement when I was at MCW. It was hard to electroplate graphite. Plating was thicker than we liked though. Jim liked the idea enough that he got Wojciech to get a grant to study the feasibility of plating graphite. Conclusion: too many oils embedded on the graphite to reliably plate in thin enough layers. I always wondered if vacuum deposition would have worked. Graphite is easy to machine and still allowed modulation. This version dates to



Jim's elegant Varian wire-wound low-temp Q-band resonator, commercial version (~ 1983).

around 1983. Jim had me develop the method to do wire wound cavities, made at X-band.

Jim Anderson

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I comment from the perspective of knowing and working with James S. Hyde, PhD for 38 years. Jim worked with Bill Zabriskie and me in transferring academic based technology in the name of Electron Spin Resonance (ESR) and Magnetic Resonance Imaging (MRI) to the creation of the company Medical Advances, Inc. In many of the academic technology transfers to commercial enterprises only involves the technology. Jim, since he had worked in the commercial world at the company Varian, very much understood that to make the technology viable in the marketplace the principal inventor must be transferred in intellect and consultation to the newly incorporated enterprise. Jim made his presence with Medical Advances investors, staff members and the engineers/scientists. And at times he was always available to meet with customers. When Medical Advances was acquired by Intermagnetic General Corporation (IGC), a company that was listed on the NASDAQ, Jim was appointed to the IGC board of directors. Though he committed time to the business, he continued to apply his time and intellect to do research in ESR and MRI, writing papers and creating patentable material. As Chairman of the Department of Biophysics Jim continued to lecture, serve as mentor to many students and engage colleagues in ESR and MRI. In the scientific, academic and business world he was truly a man for all ages.

I attended the funeral which had moments of sadness and joy as we remembered Jim. We will miss Jim and what he accomplished.

Three homilies captured contributions from his children with their memories of Jim and what he meant to then, reflections from those who worked with him in biophysics and the application of his discoveries and finally, his contribution to the Museum of Wisconsin Art.

Truly a life well lived.

Rich Stevens

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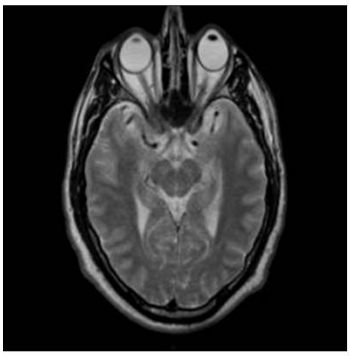
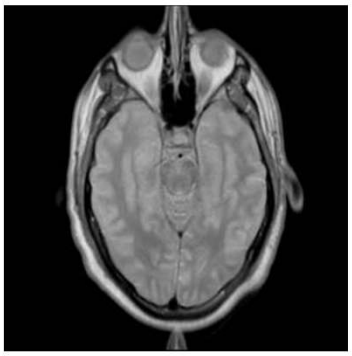
In summary, in these brief tributes to the many facets of Jim Hyde, we have tried to delineate, but cannot really fully summarize, the many ways that Jim has impacted our personal and professional lives. The field is so much richer because of him. And so much poorer now that he is gone. The best way we can show our appreciation is to continue to pursue the paths and the approaches that Jim has illuminated for us.

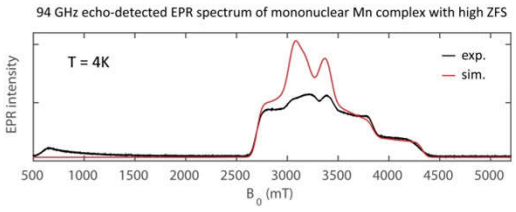
Harold Swartz

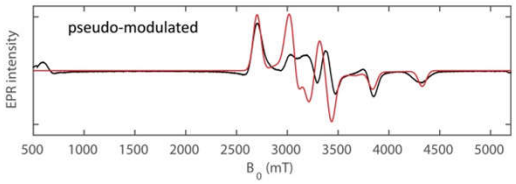
Magnetic Resonance

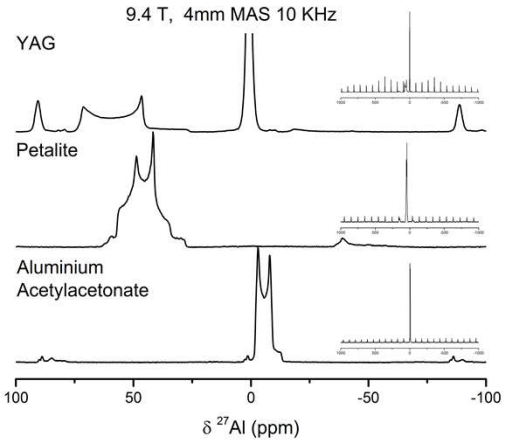
(MRI, EPR, NMR, DNP)

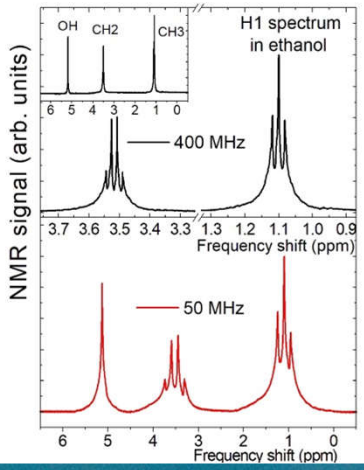












The 12th Asia-Pacific ESR/EPR Symposium (APES2022)

November 4–7, 2022, USTC & ZJU, China

The 12th Asia-Pacific ESR/EPR Symposium was successfully held under the auspices of the Asia-Pacific EPR/ESR Society (APES) in Hefei, China from November 4th to November 7th, 2022. The symposium is jointly organized by University of Science and Technology of China, and Zhejiang University. Due to the pandemic of Covid-19, it was an online event for international speakers and participants, in an unprecedented way in the APES history.

The symposium attracted more than 180 participants (including about 110 domestic participants and 70 from overseas) from 13 countries and regions (Australia, China, Germany, India, Japan, Philippines, Poland, Russia, Slovakia, South Korea, Switzerland, UK, and USA). Totally there were five plenary lectures, 20 invited lectures, one Young Scientist Award and six oral presentations over four days of the conference, focusing on four topics: EPR in Biology, Spin-based Quantum, Technology & Instruments, and Chemical/Molecular Magnetism.

The five plenary lectures were made by world-renowned scientists in the EPR/ESR community, which included: "New methodical approaches for EPR and DNP" by Prof. Thomas Prisner from Germany, "Single molecule magnetic resonance spectroscopy and imaging" by Prof. Jiangfeng Du from China, "Mechanisms of electron spin memory loss in glassy frozen samples" by Prof. Gunnar Jeschke from Switzerland, "Pulse EPR applications of trityl and stable nitroxide radicals" by Prof. Elena Bagryanskaya from Russia, and "Electron spin resonance in single atoms and molecules" by Prof. Taeyoung Choi from South Korea.

During the symposium the participants exchanged their ideas and raised discussions on the forefront of research in all aspects of EPR/ESR, ranging from theoretical and experimental advances in CW/Pulsed EPR, high frequency and high field EPR, ENDOR, PEDLOR/DEER, time resolved EPR, FMR, MRI, ODMR to applications in medicine, biology, chemistry, materials science and nanotechnology. It facilitated collaboration and scientific exchange between the world-acclaimed scientists and Asia-Pacific researchers. Three excellent oral presentation awards were elected, and EPR/ESR equipment manufacturers CIQTEK and Bruker BioSpin introduced their progresses in technologies. The APES Young Scientist Awards this year goes to the young researcher, Dr. Fei Kong from China. Dr. Fei Kong gave the presentation "Zero-field EPR spectroscopy based on quantum sensors".

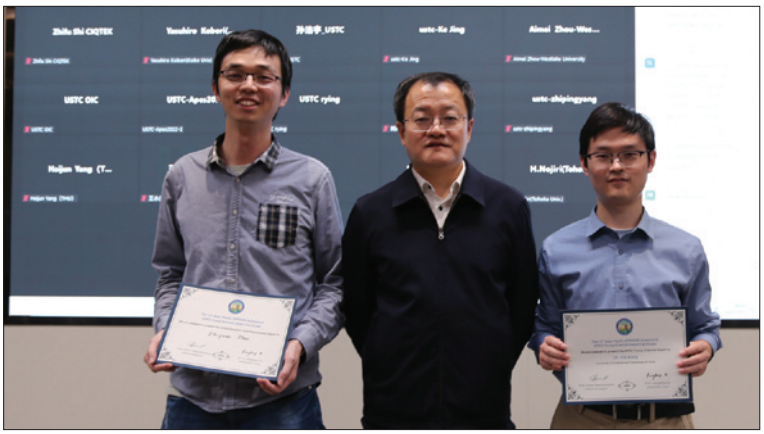
At the online council meeting held on November 6 during the symposium, the following researchers were elected as the APES Council Members for Term 2022–2025.

Officers:
President: Prof. Jiangfeng Du (China)
Vice President: Prof. Pratapchandra Kurup (India)
Vice President: Prof. Fazhan Shi (China)
Immediate Past President: Prof. Elena Bagryanskaya (Russia)
Secretary: Ms. Ying Rui (China)
Founder President: Prof. Czesław Rudowicz (Poland, formerly Hong Kong)
Country/Regional Representatives:
Australia/New Zealand: Dr. Nicholas Cox
China: Prof. Shangda Jiang
India: Prof. Balachandra G Hegde
Japan: Prof. Akio Kawai
Philippines: Dr. Marvin Jose F. Fernandez
Republic of Korea: Prof. Sun Hee Kim
Russia: Prof. Matvey Fedin
Advisory Council Members:
Prof. Hitoshi Ohta (Japan, former President & Vice President APES)
Prof. Hiroshi Hirata (Japan, former Vice President of IES)

The council members also reached a consensus that biennial APES symposia would return to odd-numbered years. APES 2023 will be held in India in 2023. Prof. Prathapachandra Kurup from the Cochin University of Science and Technology will organize the event.

Within the past 25 years, the Society witnessed a fast growth from youth to maturity. A series of symposia have been hold. The symposia provide an excellent platform for exwchanging scientific ideas with strong friendship among the participants not only from Asia-Pacific region, but also from all over the world. The previous symposia in the APES history were successful, thanks to the hard voluntary work and organizational efforts of many colleagues in various countries. These symposia left abundant heritage to the contemporaries and descendants. APES2022 is the 12th symposium following the

Professor Jiangfeng Du at the opening of the Symposium.



From left to right: Zhiyuan Zhao, Professor Jiangfeng Du, and Fei Kong.

successful APES 1997 (Hong Kong, China), APES 1999 (Hangzhou, China), APES 2001 (Kobe, Japan), APES 2004 (Bangalore, India), APES 2006 (Novosibirsk, Russia), APES 2008 (Cairns, Australia), APES 2010 (Jeju, Korea), APES 2012 (Beijing, China), APES 2014 (Nara, Japan), APES 2016 (Listvyanka, Russia), and APES 2018 (Brisbane, Australia). APES 2020 has been postponed since the outbreak of COVID-19 pandemic.

Professor Jiangfeng Du, Chairman, President of the Asia-Pacific EPR/ESR Society, and Ying Rui, Secretary of the Asia-Pacific EPR/ESR Society

The 50th Southeastern Magnetic Resonance Conference

November 4–6, 2022, Tallahassee, Florida, USA

The 50th edition of the annual Southeastern Magnetic Resonance Conference (SEMRC) was held at the Four Points by Sheraton hotel in Tallahassee, Florida, over the weekend of November 4–6, 2022. This regional meeting has a long tradition of bringing together leading scientists to discuss the latest developments in NMR, EPR and MRI, with a focus on exchanges of ideas and recent magnetic resonance research highlights, including new applications and technique development. Particular emphasis is placed on activities in the Southeastern United States, with strong participation of young researchers. The 2022 meeting was organized jointly by the NMR and EPR groups of the US National High Magnetic Field Laboratory (MagLab), with respective User Program Directors Rob Schurko and Stephen Hill serving as conference co-Chairs. This continues the tradition of the MagLab hosting the meeting every two years. The conference program can be found at the following website: https://nationalmaglab.org/semrc.

The conference kicked off on the Friday evening with two Keynote presentations. The first of these, entitled "The Metal Complex as a Magnetic Vessel that Controls Coherence", was given by Professor Joseph Zadrozny from Colorado State University. His talk appealed nicely to both the NMR and EPR audiences, focusing on the role of electron-nuclear interactions in the coherence properties of spins associated with transition metal complexes of interest in wide-ranging applications from quantum technologies to MRI contrast agents. His talk was followed by a career perspective presented by Emeritus Professor Timothy A. Cross from Florida State University, which included some amusing stories behind the decision to move the MagLab to Florida and the subsequent development of the world-class magnets used for high-field magnetic resonance research.

The remainder of the roughly two-day program included two full sessions of EPR talks and an additional session on Dynamic Nuclear Polarization (DNP). The first EPR session focused on chemical and biological applications and was headlined by invited speaker, Troy Stich from Wake Forest University; the title of his presentation was "Exploring Mechanism and Plasticity of Radical SAM Enzymes". The 2nd EPR session on technique development, held on Sunday morning, was headlined by invited speaker Mykhaylo Ozerov from the MagLab in Tallahassee; he discussed "Magnetic Resonance in the Far Infrared Spectral Range". Meanwhile, the DNP session was headlined by two invited speakers: Alex Nevzerov from North Carolina State University, who described "A Resonator-Based NMR Probe for DNP of Thin Film Samples and Overhauser DNP"; and Frédéric A. Perras from Ames Laboratory in Iowa, who presented on "Methyl-Driven Overhauser MAS-DNP". These sessions included several presentations by graduate students and postdocs, including: Faith Scott (MagLab, Florida State University), Yifan Quan (MIT), Afnan Jaufer (MagLab, University of Florida), Alvaro Montoya (MagLab, University of Florida), Elvin Salerno (MagLab, Florida State University), and Aulden Jones (Georgia Tech). A two-hour poster session was also held prior to the conference banquet on Saturday evening, featuring presentations primarily by postdocs, graduate students and undergraduates. The conference was fortunate to receive generous financial support from several vendors of EPR/DNP instrumentation, including Bruker, Doty Scientific, JEOL, TECMAG and Bridge12. The International EPR (ESR) Society also supported two awards to junior researchers, including a certificate and $200 cash prize. The first was made for the best oral presentation, given by University of Florida graduate student Alvaro Montoya. Alvaro presented portions of his PhD research on "Enzyme-Substrate Complex in B. Subtilis Oxalate Decarboxylase Revealed by Pulsed EPR Spectroscopy", work that was supervised by Professor Alex Angerhofer. The second award was given for the best poster presentation by graduate student Katie L. Whitcomb from Emory University. Her research on "Protein and Coupled Solvent Dynamics of Oligomeric and Fibrillar Alpha-Synuclein" is supervised by Professor Kurt Warncke.

Photos of graduate students Alvaro Montoya and Katie L. Whitcomb receiving their IES certificates from Professor Stephen Hill for best students presentations at the 50th SEMRC.

Although the SEMRC is usually held annually, the previous edition organized by Louisiana State University had been delayed by a year and was also held virtually due to the COVID pandemic. We were therefore extremely grateful to return to an in-person format, which was attended by over 100 participants, not far below pre-pandemic participation. The 51st SEMRC will be organized by Alex Smirnov, Tatyana Smirnova and Alex Nevzerov at North Carolina State University. They plan to combine the meeting with the Southeastern Regional Meeting of the American Chemical Society, which will be held in Durham, NC, from October 25–28, 2023.

Stephen Hill
Florida State University and National High Magnetic Field Laboratory

IES Virtual EPR Meeting, December 2, 2021

EPR and Corrosion – A New Opportunity

Dr. Joshua R. Biller

Understanding, measuring, and mitigating corrosion, especially for high strength aluminum aerospace alloys, draws considerable interest and research funding since estimates of the impact of corrosion around the globe are about $2.5 trillion annually [1]. Many commonly used aerospace aluminums are alloyed with metals which become EPR active cations as the corrosion reaction proceeds. Despite (1) the large wt% loading of these metals during the alloy process, and (2) the tremendous sensitivity of EPR, the study of EPR active transition metal cations related to corrosion on aerospace aluminum is not commonplace. This presentation described preliminary work done at TDA Research regarding the use of EPR at X-band as a tool for studying and characterizing corrosion on samples taken from actively corroding AA2024 and AA6061 alloys with primer and topcoat coatings applied.

Corrosion is electrochemical reaction characterized by strong pH changes and liberation of EPR active metal cations, and it involves the transfer of electrons between a metal surface and an aqueous electrolyte solution [2]. For example, during corrosion the oxidation of the aluminum (anode) and reduction of oxygen (in the presence of water) forms hydroxide (at the cathode). The traditional focus for the corrosion of aluminum alloys are the following two electrochemical half-cells:

Cathodic: $\frac{1}{2}O_2 + H_2O + 2e^- \rightarrow 2OH^-$ (basic)
Anodic: $Al \rightarrow Al^{3+} + 3e^-$ (acidic)

Because the anodic reaction often occurs in a confined area, the metal ions formed are precipitated as the hydrous oxides and cover the mouth of a "pit" which forms in the metal surface as the aluminum is dissolving. Thus, the solution is trapped which allows the buildup of hydrogen ions. As the corrosion process proceeds, the anode area becomes more acidic while the cathode becomes more basic. Researchers have recognized that pH sensitive materials are great candidates for detecting corrosion. Many analytical techniques, including IR, NIR, and Raman spectroscopy detect spectral changes due to pH.

Underappreciated in the study of corrosion is the fact that many EPR active cations – Fe^{3+}, Co^{2+}, Mn^{2+} or Cu^{2+} for instance – are also generated because of the corrosion process. In copper containing alloys (used often in aerospace applications), solid copper metal grains (Cu^0) are dissolved and re-deposited at secondary sites (which leads to accelerated corrosion) according to the following reactions:

$Cu^0 \rightarrow Cu^{2+} + 2e^-$
(original dissolution at primary copper grain)
$Cu^0 + 2H_2O \rightarrow Cu(OH)_2 + 2H^+$
(reaction of Cu particles in corrosion gel)
$Cu^{2+} + 2e^- \rightarrow Cu^0$
(redeposition of solid copper at secondary sites)

In terms of corrosion monitoring, these EPR active cations may offer the clearest indicator for determining when corrosion has started – in the absence of corrosion, there should be no EPR signal. When corrosion is proceeding, EPR active signals may arise and fall away with time based on the state of corrosion. In addition, the most widely used anti-corrosion measure involves reduction of dichromate (Cr^{6+}) to a chromium oxide (Cr^{3+}) which forms a solid barrier to prevent further oxidation of the surface of the primary metal or the alloying phases. Chromate can be present in the systems either as a conversion coating at the metal surface or loaded into coatings at very high concentrations (i.e up to 30% wt).

Within the different alloys of aluminum, the 2000 series has copper as it's primary alloying element. Addition of the copper results in the highest strength heat treated aluminum alloys available, which makes them widely used in several aerospace applications. The increased strength comes at the expense of reduced ductility and corrosion resistance. For AA-2024 specifically, the alloy can contain up to 4.9% Cu and 0.9% Mn, by weight. In a first experiment, a 3 x 3" panel of AA-2024 was coated with a 0.001" (~25 μm) thick primer layer and allowed to undergo accelerated corrosion according to ASTM B117 salt fog test. As corrosion proceeded, we analyzed a small amount of a clear gel generated from the corroding panel with a benchtop EPR unit. In a single scan a clear spectrum was recorded with contributions from Cu^{2+} and Mn^{2+}, with sufficient SNR such that values of anisotropic values of g- and A- could be fit for each species.

We are just beginning to explore EPR characterization of corrosion as a function of time, alloy type and corrosion prevention mechanism in the lab at TDA. A "holy grail" for the global corrosion mitigation community is an in-field measurement tool capable of detecting corrosion without the addition of any sensors to coatings or metal treatments which require in-service craft to return for retro-fit. The biggest leap may be sweeping a magnetic field wide enough to capture transition metal spectra, although frequency swept transition metal EPR may be a good alternative [3]. EPR has an advantage over other analytical techniques because it can directly sense alloy degradation by the presence and activity of EPR active transition metals.

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2. Buchheit, R.G., et al., *The electrochemistry of intermetallic particles and localized corrosion in Al alloys*. JOM, 2001. **53**(7): p. 29–33.
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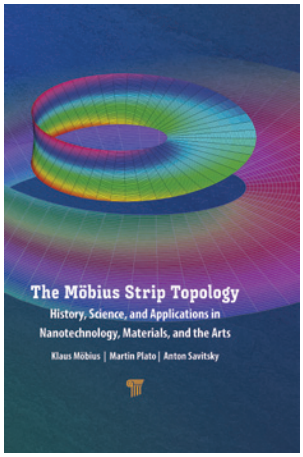

The Möbius Strip Topology: History, Science, and Applications in Nanotechnology, Materials, and the Arts
by Klaus Möbius, Martin Plato and Anton Savitsky
ISBN: 978-981-4968-20-1 (Hardcover, € 216)
ISBN: 978-1-003-25629-8 (eBook, € 162)
Publisher: Jenny Stanford Publishing Pte. Ltd, Singapore, 2023
926 pages

Summary:

This new book reports about the eminent mathematician and astronomer August Ferdinand Möbius (1790–1868) in the mirror of his time with its political and social specificities. It was marked by the devastating Napoleonic Wars in Central Europe and their far-reaching ramifications. The legacy of August Ferdinand Möbius reaches into today's sciences, arts, and architecture. It is rediscovered again and again – leading to new heights of scientific knowledge and cultural aesthetics. The famous one-sided 'Möbius strip', a prototype of non-orientable surfaces, is a paradigmatic example of the fascination and significance of mathematical topology for understanding unexpected consequences of complex object deformations.

In the 19th century, research in the field of pure (abstract) mathematics was reaching its peak in Germany, and Carl Friedrich Gauss (1777–1855) was an epochal example. August Ferdinand Möbius was his doctoral student, and his work was profoundly influenced by C. F. Gauss. In the 18th century, it has been the French school of applied mathematics that dominated and enabled rapid developments of science and technology in Europe and beyond. How did this shift in emphasis from applied to pure mathematics occur, and why in Germany?

It can be argued – and the book provides plenty of evidence – that major reasons were the catastrophic consequences of the Napoleonic Wars in Europe, leading to total defeat of Prussia in 1806. Immediately following this, far-reaching reforms of the entire state system were carried out in Prussia and other German states (keyword "Stein-Hardenberg Reforms", 1807–1815), they affected also the educational system. The leading role in this was played by the brothers Wilhelm and Alexander von Humboldt. Now, freedom of university teaching and research was guaranteed. This attracted many creative people from around the world with new ideas, thereby enabling the "Golden Age" of pure mathematics and fundamental theory in physical sciences.

The new book is the first to present numerous detailed case studies on Möbius topology in mathematics, astronomy, chemistry, molecular medicine, physics and nanomaterial sciences, including aspects from modern computer simulations for molecular design and engineering, literature and music, arts and architecture. They cover highlights from the 18th century up to the present years, taking examples from Europe, America, Australia, and Asia.

The book is richly illustrated with excellent figures to accompany each chapter and section. It is composed of 9 Chapters and an Introduction that is setting the stage for the follow-up Chapters with their discussions about essential scientific discoveries and cultural understandings. This is further supported by an extended Index and a Bibliography after each chapter. The first 3 Chapters deal with the time of August Ferdinand Möbius's early life, academic education, and academic career during the Napoleonic Wars. Chapters 5 to 8 deal with Möbius strip topology and elaborations on Mathematics and Astronomy, as well as applications from Chemistry, Physics and Nanomaterials. In Chapter 9, highlights from the Arts and Architecture are described. It reports, for example, on the spectacular modern architecture of buildings and bridges in Berlin, Amsterdam, Beijing, and Changsha that are inspired by Möbius strip topology.

The book tells illuminating stories on the people around C. F. Gauss and A. F. Möbius. Complicated characters are involved, often in intense competition. For example, the Möbius strip: It was given birth about 160 years ago, but had two legal fathers, August Ferdinand Möbius and Johann Benedict Listing (1808–1882). Both had been students of C. F. Gauss, but the priority of their paternity is still controversial. The stories are telling of extremes of euphoria in case of success alternating with bottomless disappointment in case of failure. Of the researchers' greatest strength and – in not so rare cases – of their human weakness. And even the eminent idol Gauss is not exempt from this.

The book addresses experts and laymen alike: teachers and students, undergraduates and postdoctoral researchers, anybody from the educated public. In short: the book is written for those who believe in the power of new ideas in our culture.

POSITIONS

Two Postdoctoral Positions: Development and Application of Advanced High-Field EPR

Where: The High-Field EPR Group Led by Stephen Hill, National High Magnetic Field Laboratory (MagLab), Tallahassee, FL.

Deadline: Until the positions are filled.

The first position focuses on development and application of pulsed high-field EPR methods at W-band (94 GHz) and potentially higher frequencies. The successful applicant will have at her or his disposal a state-of-the-art high-power (1 kW peak) W-band spectrometer developed at the University of St. Andrews.* This instrument offers true nanosecond time resolution and wideband excitation (1 GHz instantaneous bandwidth), facilitating complex pulse programming using an arbitrary waveform generator, thus enabling a suite of multi-dimensional electron-nuclear (and electron-electron) resonance methodologies. Applicants should be comfortable working on hardware development. However, the end-goal centers on **applications ranging from quantumspin science and materials research to coordination chemistry and structural biology**.

The second position is funded by the **Center for Molecular Magnetic Quantum Materials** (**M^2QM** – efrc.ufl.edu). It involves fundamental high-field EPR investigations of molecular materials developed within M^2QM, and via a worldwide network of collaborators. Areas of interest within M^2QM that are under active investigation at the MagLab include: understanding decoherence processes and the development of strategies for enhancing coherence in molecular spin qubits; demonstration of multi-qubit entanglement and quantum logic operations in magnetic molecules; and exploitation of magnetoelectric coupling and optical activity for realization of electrically and/or optically switchable spin qubits.

The EPR facility at the NHMFL boasts a wide range of unique pulsed and continuous-wave high-field EPR instruments spanning the range from 9 GHz to 2.5 THz, and magnetic fields up to 45 T. The group comprises six faculty-level researchers, an engineer who assists with instrument development, as well as a cohort of graduate students and postdocs. The group also has strong interactions with EPR and NMR experts in chemistry and biology at both Florida State University and the University of Florida in Gainesville. Further information concerning the MagLab EPR group, including links to recent publications, can be found at: http://magnet.fsu.edu/usershub/scientificdivisions/emr/index.html

Minimum qualifications: a Ph.D. in Physics, Materials Science, Chemistry, or a related discipline. Expertise in EPR spectroscopy is certainly an advantage, particularly applications of pulsed and/or high-field EPR, or design/development of magnetic resonance instrumentation (radio frequency, microwave, software/hardware interfaces, etc.). However, strong consideration will also be given to candidates with experience in the application of other spectroscopic or magnetic characterization methods to molecular materials. Familiarity with the following application areas is also desirable: molecular materials, including molecular magnets; quantum spin science, e.g., studies of defect states in semiconductors; spectroscopic studies of coordination compounds; and applications of EPR in structural biology.

Questions regarding the position should be directed to Stephen Hill (shill@magnet.fsu.edu). To apply, please send a CV, a cover letter describing your experience and research interests, and the contact information for three references.

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* Cruikshank et al., Rev. Sci. Inst. **80**, 103102 (2009); https://doi.org/10.1063/1.3239402

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Standard AMCs and MixAMCs have been developed to provide high performance RF drive multiplication and downconversion for full waveguide band coverage. These systems can be used to extend traditional spectrum analyzers and signal generators into the THz and mm-wave ranges. VDI's standard AMC and MixAMCs offer various modes of operation. VDI AMCs can be operated in standard frequency mode (<20GHz, 10dBm nominal) or high frequency RF drive mode (<45GHz, 0dBm nominal). VDI MixAMCs can also operate in standard and high frequency LO drive modes. Customers also have the option to operate MixAMCs for block-downconversion (<20GHz IF) or as a spectrum analyzer extender. Standard AMCs and MixAMCs are available from WR15 (50-75GHz) to WR1.0 (750-1,100GHz).

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EPR

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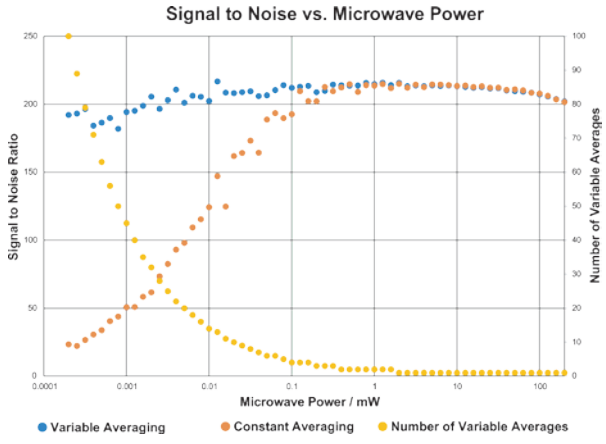

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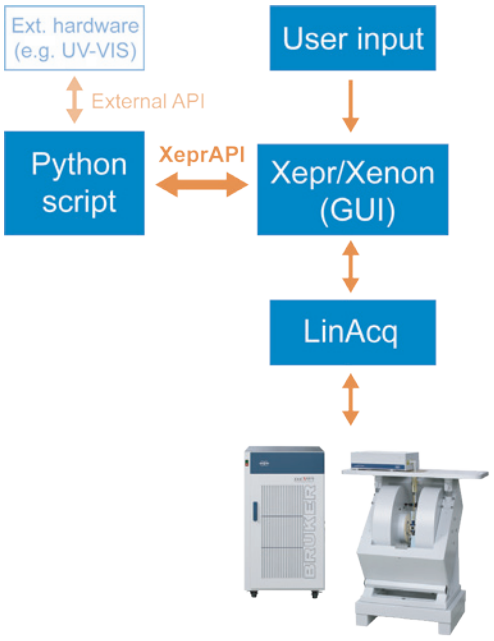

Above: Flowchart showing the XeprAPI

Left: Result of a python script that varies the number of averages to maintain a constant S/N

EPR

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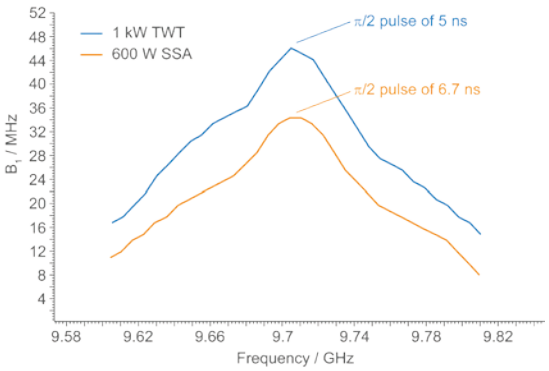
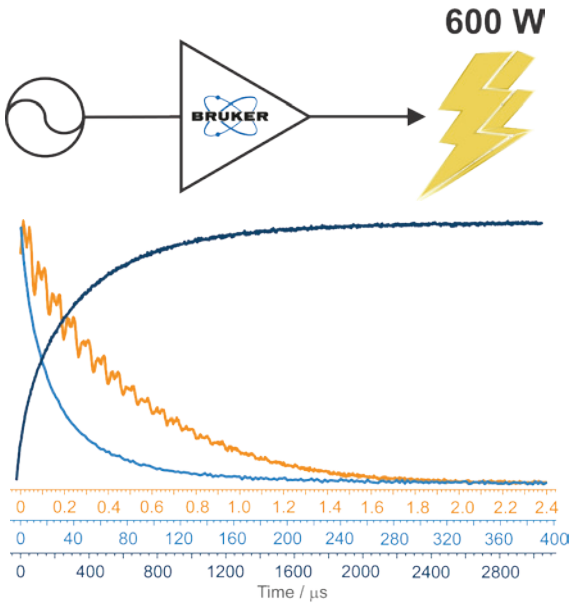


Bandwidth profiles of a MD4 resonator for different amplifiers under identical coupling conditions



Different relaxation time measurements of a solid nitroxide sample with the 600 W SSA.

T_m = 0.51 µs (orange)

$T_{1\rho}$ = 19.8 µs (blue)

T_{1inv} = 280 µs (dark blue)

$T_{1\rho}$ measurements used saturation pulses up to 400 µs

For more information please visit
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