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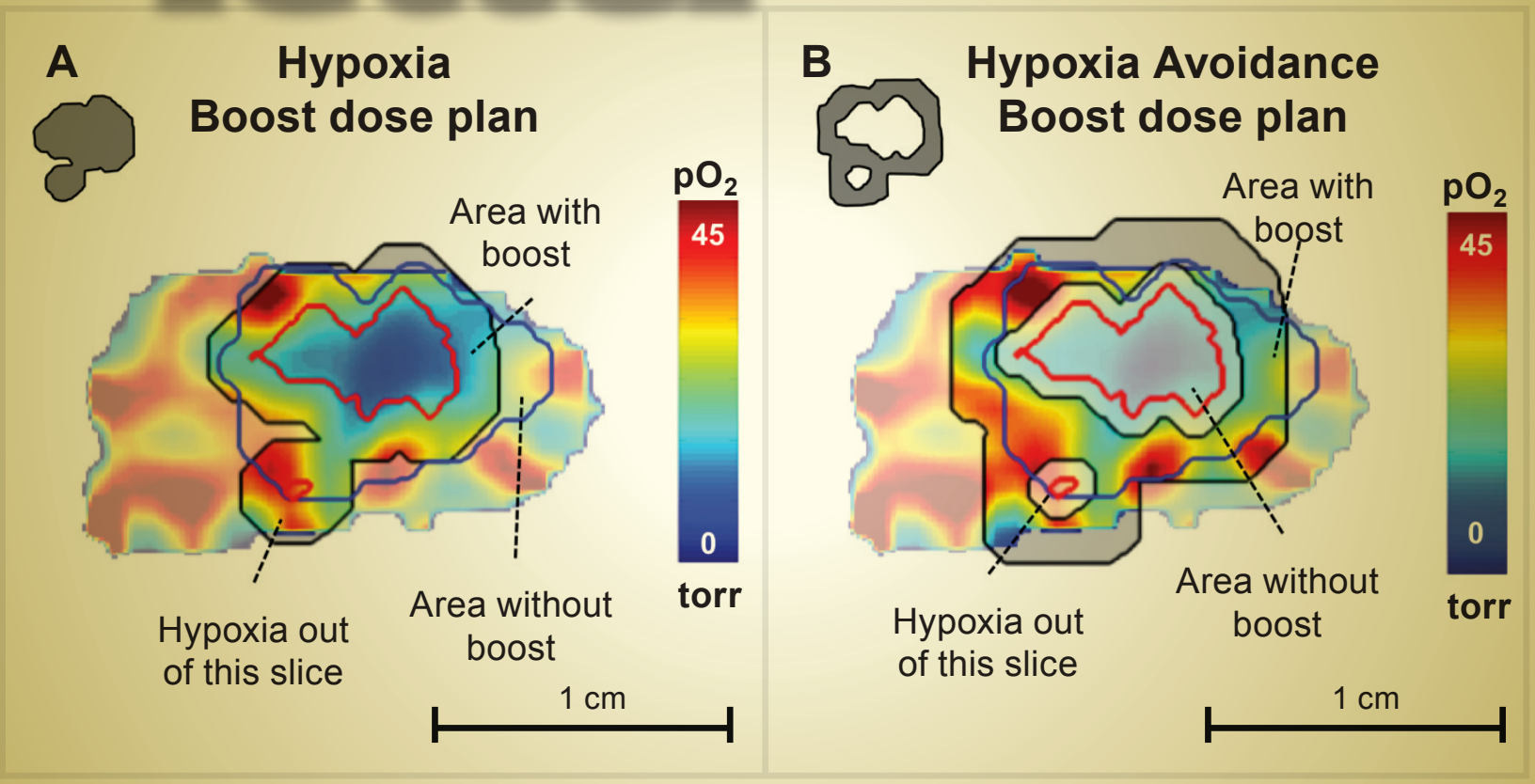

The Publication of the International EPR (ESR) Society

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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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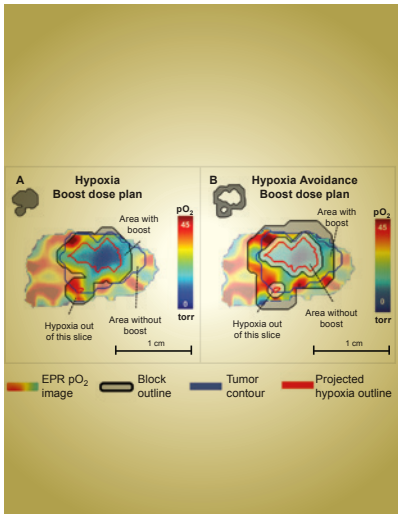

The cover picture illustrates aspects of the research of Howard Halpern, recipient of the IES Fellowship 2023. It shows EPR spin lattice relaxation image slices of the relaxation rates of a trityl spin probe (OX071) scaled to the equivalent molecular oxygen partial pressure at the midplane from the leg of a mouse bearing a malignant tumor shown as a blue contour in both images. Projected onto the slice of both images in red is all of the hypoxic volumes in the tumor defined as those regions with a pO2 of less than or equal to 10 torr. The entire tumor has been treated to a radiation dose sufficient to control 20% of tumors in both images A and B. A boost is randomly selected to deliver a boost radiation dose to the tumor in either the fashion of image A or B. In image A the boost is to the hypoxia expanded by 1.2 mm for setup uncertainty. In image B a roughly equivalent integral volume is delivered to well oxygenated tumor, avoiding the hypoxia. In both images A and B a pO2 color bar is shown for this particular tumor image. Reference* shows the Kaplan-Meier control probability from the randomized treatments using either A or B boosts. It shows a highly significant increase in control from hypoxic boosts, a validation of the use OX071 spin lattice relaxation imaging of tumor oxygenation in the extraordinarily complex tumor environment.

* Gertsenshteyn I, Epel B, Giurcanu M, Barth E, Lukens J, Hall K, et al. Absolute oxygen-guided radiation therapy improves tumor control in three preclinical tumor models. Front Med (Lausanne). 2023;10:1269689.

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The Publication of the International EPR (ESR) Society

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Are you interested to become a member of the International EPR (ESR) Society? Please find the registration/information form for new/continuing members of the IES for individual members on this Web site: https://ieprs.org.

Editorial

Dear colleagues,

It is not surprising that all of you know that the coming year 2024 marks the 80th anniversary of EPR: you could have hardly missed the relevant announcement about a special issue of *Applied Magnetic Resonance* "EPR at 80" under Guest Editorship of Gareth Eaton, Sandra Eaton, and Kev Salikhov devoted to this event (33/3, p. 11). Moreover, 2024 also marks 35 years of the International EPR/ESR Society.

To be prepared to this celebration, it might be good to refresh knowledge about the details of the rich history of the EPR discovery by Evgeny Zavoisky and the development of EPR methods and applications. Being a passionate enthusiast of our publication, my first uncontrollable reaction is to recommend reading all issues of the *EPR newsletter*, since our publication is a perfect forum for all EPR-related materials. However, I realize that you have only 24 hours per day for all your activities, therefore, to start with, I would propose materials from the early days of EPR: presentation of the reconstructed experimental setup of E. K. Zavoisky (14/4, pp. 12, 13); some personal details about Evgeny Zavoisky (13/1-2, pp. 13, 14) and a story about his fascination by the avant-garde art (14/4, pp. 6, 7); articles on his 100th anniversary (17/4, pp. 4, 5) and his participation in the Soviet atomic project (17/4, p. 7).

It is my pleasure to thank all contributors to the *EPR newsletter*, CEOs of the IES, Associate Editors Candice Klug, Hitoshi Ohta and Sabine Van Doorslaer. Special thanks go to editors of long-lived columns: John Pilbrow (EPR newsletter Anecdotes), Candice Klug (New EPR Faculty), Wolfgang Lubitz (Guest of the Issue), and Stefan Stoll (Software), and Sergei Akhmin, our Technical Editor.

Happy New Year 2024 and meet you soon!

Laila Mosina

IES Executives 2024–2026

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For details, see forthcoming EPR newsletter 34/1 (2024)

Letter of the President

All good things have an end, and this also means there are always new beginnings. I cannot believe that the three years that I served as the President of the International EPR society (IES) are coming to an end. When Thomas Prisner approached me whether I would be willing to stand for election, I really did not know what my contributions could be to such a storied history and community with long held traditions, but I agreed anyway because Thomas was very persuasive that as a scientist who is coming from sideways with expertise in-between disciplines would be of great value. Turns out, there were many meaningful contributions that I could help the IES make for the community, but my focus was one that Thomas had emphasized as the single most important goal of the IES. Bring young scientists on board, and make the IES relevant to as many scientists as possible, but especially the younger generation who will bring new ideas and activities. Interestingly, it was the young scientists who came up with the brilliant idea of how to engage the community by holding the IES Virtual EPR meetings (IVEM) despite the Covid-19 restrictions that continued for much longer than anybody had anticipated. I am glad to report to you that the IVEM that Nino Wili started in April 2020 and was continued by Zhongyu Yang and Thomas Schmidt is still going strong with additional support from Yujie Zhao, Tomas Orlando and Robert McPeak. The IVEM now has become a major forum for young scientists in EPR to present their highlights, for poster and talk prize winners to have another platform, and for the *EPR Newsletter* to feature the speakers. The Covid-19 pandemic whose aftermath we are still fighting has taught that both, there are creative ways to keep going and that we cannot replace the magic of in person human interactions that conferences and meetings bring about, no matter how good the technology. We brainstormed and implemented many new ideas, while continuing all important existing traditions of the IES. I felt that the key to success is that every activity that we launch is organized to be sustainable for years to come. A modern society has to engage young scientists and we will need to use all platforms necessary to connect. My request for help was met by additional reinforcements from the new Twitter team consisting of Nandita Abhyankar, Aleksey Bogdanov and Nino Wili. Two of them have never tweeted before but joined to help for the sake of the IES. The IES board also voted to include a Virtual Media officer in the IES Executive Board in the future, with an election anticipated in 2024, to help support and sustain these virtual activities. It will be my duty and pleasure to help support these activities for three more years as the IES constitution demands of the immediate past President. An important principle that I believe is true for any scientific society is that its main purpose is to support its people to achieve their scientific advancement and success. That includes support for the committed vendors whose products are critical for the vitality of the community. The vendors of EPR have a special place in our hearts. We value them greatly and see the urgent need to help expand the landscape to have more innovators and entrepreneurs to increase their portfolio and enter the market. The vendors of EPR are not just vendors, they often come from the EPR community and are deeply committed to our cause, because many products are a result of innovative and out of the box ideas developed by the innovators themselves. This is why the IES treasures their contributions and feels that there is a critical relationship between the users and the vendors. A greater user community will benefit the vendors, and greater product variety and quality will benefit the community. We are grateful for the record-breaking contributions in the past few years from all of our sponsors who shared this vision and helped us have strong financial support that allow us to spread our wings just a bit wider for our community.

Last, but not least let me share with you my strong conviction that the future of the EPR is exceptionally bright. We have not even begun to scratch the surface of how EPR can help revolutionize research in energy science, catalysis, cancer research, structural biology to quantum information science. To fully seize this potential, we also must recognize the power of communication to inspire others. We must make EPR experiments become easier to grasp, understand, conduct, and interpret. Any additional undergraduate and graduate student recruited and retained to get excited about EPR is fuel for our community that is in 2024 celebrating the 80th birthday of EPR and marking the 35th anniversary of our society. It is our job to convey the excitement and the potential of EPR to a broader community. Help us do it better!

My best wishes to everyone and look forward working with you for many years to come.

Songi Han

Interview with Professor Howard Halpern on the Occasion of His IES Fellowship 2023

EPR newsletter: *Dear Professor Halpern, on behalf of the readers of the EPR newsletter we congratulate you on your IES Fellowship 2023. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I suppose that when I was very young, both the reproducibility of measurements with various instruments around the house and the simplicity of physical systems as described to me seemed to be a respite from the chaos about me.

My grandfather didn't finish high school but found a job as a draftsman for the General Electric Co plant in Charlestown MA. Periodically Charles Steinmetz visited the plant. He was the great GE engineer who brought the Heaviside Calculus/Laplace Transform technology which simplified the simultaneous description of mechanical and electromagnetic energy from Europe, which led to the design of many GE products. My grandfather could make Steinmetz laugh and quickly draft suggested improvements.

My grandfather encouraged me to learn algebra and geometry when I was in grammar school and guided me into physics. I earned my Ph.D. from the University of Wisconsin-Madison in High Energy physics where my thesis project involved the production of massive particles (mesons with the mass of protons) from polarized high energy light. I was working at Argonne National Laboratory when it became clear that experimental work in the field would involve large consortia excluding smaller group benchtop experiments so I chose the family business, medicine.

While completing my residency in Radiation Oncology and learning about the presence of low levels of molecular oxygen in some malignant tumors, hypoxia, that created hypoxic resistance to radiation, I found the paper by CS Lai and Jim Hyde describing quantification of oxygen with the superhyperfine EPR linewidths of nitroxides. I sought the advice of Bill Moore, an MRI radiologist at the Brigham Hospital in Boston who had worked with EPR, on the possibility of quantitative imaging molecular oxygen with EPR. He recommended a paper by DeCorps and Fric on the construction of a 10 mT EPR spectrometer. The low field permitted RF excitation at frequencies sufficiently low to access lossy tissues deep in human subjects. I realized that with magnetic field gradients it was possible to derive spectroscopic images. Meanwhile, my grandfather had taught his three brothers-in-law how to run local Boston hardware stores, providing a source of structural advice, and me how to draft machinist specifications. The low frequency imager was conceived.

Who introduced you into magnetic resonance?

Initially, my introduction into magnetic resonance required a good deal of retreading and self-teaching. Dave Ritson with whom I worked for my high energy thesis project at the Stanford Linear Accelerator Center, Group F, taught me to be a particle physicist at SLAC among the groups that won 3 Nobel prizes from work done at least in part while I was there. I have had help and advice from Bill Moore at Harvard; I was first taught to rapidly match and tune a spectrometer by Bob Pound. Paul Horowitz advised me on electronics and to consult the American Radio Relay League Handbook (bible of the HAM radio operators). I have benefitted from my colleagues Mike Bowman, Gareth and Sandy Eaton, Gerry Rosen, Boris Epel and Viresh Rawal. I found that I needed to relearn resonance physics myself through Abragam, Slichter, Poole and the MIT Radiation Laboratory series, paying as close attention to the maintenance of the truth of the equal sign as I could. Learning to appreciate the local rules of chemistry and the wonderful complexity of chemical structures and systems has been a journey of discovery.

What is your idea of teamwork in science?

Teamwork and the progress it produces require the most delicate balance and patience in our community of researchers. It can be argued the truth is polished to mirror clarity by abrasion but it can be shattered by abuse. The optimal balance point is often difficult to define. And at its heart is iteration, the group willingness and patience to redo it better and often finding the opposite from what we expect. Science should know no political or geographic boundaries. It can be defeated by tribalism although tribal perspective needs to be respected in the comfort brought by repetition. It should strive for, as much as possible, consensual agreement reflected in repeatable results in the process of gaining general understanding. And this eases the formation of a universal team.

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

Probably the most important words are patience with yourself (the willingness to go back to long ago learned but less clearly remembered concepts), persistence (stubbornness and the need for iteration), openness to new perspectives (realizing you had an entire concept wrong). As an example, my initial career was as a particle physicist with mass/energy resonance centroids and nuclear energy states and optical absorption/emission energies measured with multiple significant figures: I believed that quantum energy spectra were condition independent. I later read Slichter (one of the authors of the first paper on the effect of spin exchange and chemical exchange on spectra). Another landmark paper author (Harden McConnell) visited my lab to the consternation of my colleagues in our Chemistry Department. And of course I wore out the paper edges of Kev's chapter 2 in the Molin, Salikhov, Zamaraev, *Spin Exchange*. As a result, some of my first papers dealt with the linearity of the migration of the apparent spectral splittings with the conditional concentration effect on the spectral line separations. My initial misunderstanding led to important papers.

Interview with Professor Murali Cherukuri on the Occasion of His IES Fellowship 2023

EPR newsletter: *Dear Professor Cherukuri, on behalf of the readers of the EPR newsletter we congratulate you on your IES Fellowship 2023. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I was in high school from 1969 to 1973. During this time, I had very good lecturers in Physics and Chemistry which made me develop a strong interest in pursuing education in basic sciences. My father was a prominent physician and though he would have liked me to follow his education/career path, I was encouraged to follow my interests. I went to a Jesuit college (Loyola College) in my home state, and it had a very good science faculty which further strengthened my interests and I continued towards Bachelor's and Master's degrees in Science. During my Master's degree I saw the importance of spectroscopy in chemical physics/physical chemistry.

Who introduced you into magnetic resonance?

I joined the Indian Institute of Technology, Madras in 1979 for my PhD in the Physics department. I initially started my research in solid state physics, growing single crystals to study phase transitions using Electron Paramagnetic Resonance and UV Visible Spectroscopy. However, the lack of adequate facilities and funds to grow large single crystals at that time (early 1980s) made me change my research to the studies of transition metal ions doped in single crystals. The crystals I chose to use for these studies were easily grown using slow evaporation methods removing challenges in growing crystals by melting the starting materials >1200 °C and slowly cooling. My thesis work involved the study of Ni(II) doped in Zn(II) host crystals and studying the formation of Ni(I) and Ni(III) after high-energy radiation of the crystals. The interesting finding was both Ni(I) and Ni(III) were Jahn-Teller distortion systems with similar g-values. To identify the valence states formed after radiation, I had to use ^{61}Ni to further support the interpretation. These studies, though of basic interest, trained me well in EPR spectroscopy and interpretation of complex spectra. I joined NIH in Bethesda after my PhD for my post-doctoral fellowship where I was introduced to EPR spin trapping to study free radical intermediates in radiation chemistry, photochemistry and sonochemistry, modalities relevant in cancer treatment. These EPR studies helped in understanding some mechanistic aspects of these methods used in treatments.

After obtaining my tenure at NIH in 1992–1993, I switched to developing EPR imaging to study tumor physiology. Tumor oxygen status determines response to radiation treatment and knowing the oxygen status (low or high) is necessary. Efforts from our group and others have now made EPR imaging for in vivo applications practical.

What is your idea of teamwork in science?

I can't emphasize more strongly that teamwork is essential in modern day research. My own career trajectory is an example. My collaborative work with Prof. Takashi Kondo (now at Toyama University), Prof. Amram Samuni (Hebrew University of Jerusalem), Dr. Angelo Russo (NIH) and Dr. James Mitchell (NIH) were crucial in strengthening my own case for tenure at NIH, a very competitive place. After my tenure, I have worked as a team with Prof. Sankaran Subramanian, Dr. Ram Murugesan, and Mr. Deva Devasahayam to advance the field of in vivo EPR imaging. This was followed by younger team members such as Drs. Ken Ichiro Matsumoto, Fuminori Hyodo, Shingo Matsumoto, Hironobu Yasui, Masayuki Matsuo, Yoichi Takakusagi, and Shun Kishimoto.

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

Whether you are a graduate student studying for PhD or a post-doctoral researcher, it is always necessary to be creative, develop original concepts within your research environment, and seek out synergistic collaborations.

Interview with Professor Stefan Stoll on the Occasion of His Bruker Prize 2023

EPR newsletter: *Dear Professor Stoll, on behalf of the readers of the EPR newsletter we congratulate you on your Bruker Prize 2023. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

One day in the summer after 10th grade, my high school chemistry teacher Ina Schenk (she just turned 98 this year!) ran into my father by chance. She asked whether I would be interested in doing some extra chemistry in the summer. He asked me, and I agreed. And I started going to the high school chemistry lab several times a week. A few weeks later, after many exciting experiments in the lab, I was hooked on science. In hindsight, this is an impressive lesson for me that illustrates how much effect a teacher can have on students. That is one of the main reasons why I am also a passionate educator.

Who introduced you into magnetic resonance?

It was a bit serendipitous. As a student at the Technical University Graz, I was interested in spending some time abroad at another university, and I started asking around for available student exchange programs. One of them was with Eastern European countries, and Prof. Günter Grampp, an EPR spectroscopist, was the local coordinator in Graz. He arranged for me to go to the Bulgarian Academy of Sciences in Sofia to work with Prof. Nicola Yordanov. That's where I first worked on an EPR spectrometer. My project there was to interface a PC to an old Varian spectrometer to enable digital data acquisition.

What is your idea of teamwork in science?

Science is a team sport! In chemistry, we often talk about the distinction between makers (those that synthesize materials), measurers (those that apply a variety of instrumental tools, from microscopy to magnetic resonance, to examine materials) and modelers (those that use computers, or just paper and pencil, to build and test models that help us explain observations and make predictions). Depending on the science question, you need all three kinds of scientists on your team. And it is always worthwhile looking around for an expert to join your team, instead of doing every aspect of a research project yourself. Teams accelerate scientific discovery. But a crucial aspect for teamwork is the need for soft skills like communication. Unfortunately, young scientists are often not systematically trained in these regards.

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

Electron spins are amazing! They are central to so many molecular processes in our world. I encourage everybody working in magnetic resonance to see the broader significance of what they are working on, and to talk to scientists in adjacent fields as much as possible to make them aware of what powerful tools could be available to them, and to join their teams to answer new and broader scientific questions.

What do like to do outside of science?

Spending time with my family is a top priority. Besides that, I really enjoy being in the mountains. This takes me away from the day-to-day hustle and busywork, and it reminds me as a human of my place in the universe. While I have been hiking and mountaineering since my childhood, during the COVID pandemic I started taking up long-distance trail running, clocking in up to 50 miles (80 km) per week for training. My longest project so far was 56 miles (90 km), but I hope to run even longer distances. All in the mountains, of course.

You play the flute. Tell us more.

I was a passionate classical flautist, and in fact I got a degree in performing arts in parallel to my degree in Chemical Engineering. With lots of practice, I managed to qualify for a series of international music competitions (though I never won one!), and through my teacher, who was one of the Principal Flautists at the Vienna Philharmonic, I had the honor to play many projects with that orchestra under world-famous conductors. But a day only has 24 hours, and human energy is limited, so eventually I had to pick between music and science. My passion for science prevailed. I still play flute from time to time, and I listen to a lot of classical music. As I am writing this, Bach's solo violin partitas and sonatas are running the background.

IES Best Poster Presentation at the SEMRC2022

Katie Whitcomb:

I am honored by the International EPR Society for awarding me the Best Poster Presentation at the 2022 Southeastern Magnetic Resonance Conference (SEMRC) in Tallahassee, FL, and it is my pleasure to be able to share our research with you in this Newsletter. This research would not have been possible if not for the efforts of members of the laboratory of Prof. Kurt Warncke, at Emory University, in pioneering our electron paramagnetic resonance (EPR) spin probe methodology [1–4]. It is with this foundation, that we were able to study the anomalous coupled protein-solvent dynamics of alpha-synuclein (α-syn) under confinement.

α-Syn is a protein (140 amino acids, 14.5 kDa) that has an, as yet, unspecified functional role in neurotransmitter release in brain neurons, and dysfunction, that is associated with Parkinson's disease (PD) pathology in humans and animal models [5]. Free α-syn is an intrinsically-disordered protein (IDP), whose primary structure includes three domains: an N-terminal domain (NTD), "non-amyloid-β component" (NAC), and a dynamically disordered C-terminal domain (CTD).

Toward understanding the molecular mechanistic properties that motivate α-syn function and dysfunction, our established EPR spin probe methodology was applied to the study of coupled protein and solvent dynamics in oligomeric and pre-formed fibrillar forms of α-syn. Controlled-temperature ice-boundary confinement in frozen aqueous solutions was used to localize the motionally-sensitive spin probe, TEMPOL, to solvent phases specifically associated with α-syn.

Simulation [6] of TEMPOL rotational mobility in the presence of α-syn produced two distinct components at all temperatures from 220–265 K, as for soluble globular proteins [4], indicating the existence of two solvent phases: the protein associated domain (PAD) and the mesodomain, which forms between the PAD and ice boundary. However, there were three deviations in the behavior of the coupled solvent phases around α-syn oligomers and fibrils, compared to folded, globular proteins: (1) Rotational correlation times revealed dramatically higher fluidity. (2) Partitioning of TEMPOL between the two solvent phases varied significantly with temperature change. Decreasing temperature led to a reduction in the population of TEMPOL in the mesophase, indicating relative compressibility of that phase. (3) The correlation times and component weights showed hysteresis for directional temperature change. For increasing temperature, slower mobility and a larger slow component weight prevailed over a range of approximately 230–250 K, when compared to values obtained in the direction of decreasing temperature.

Interpretation of these results, along with information from previous high-resolution structural characterizations, suggest a model, in which the dynamically disordered CTD, oriented outwardly from the NAC core of oligomeric and fibrillar structures, creates a compressible phase that maintains high fluidity under confinement. Hysteresis is proposed to arise from the compaction of the CTD around the NAC core with decreasing temperature, and crystallization of expelled water along the encroaching ice front. Upon return of the sample to higher temperatures, the ice layer resists melting and repopulation of the compressed CTD solvent region. Our work, now in press [7], shows that confinement-resistant dynamics and compressibility are fundamental, molecular-mechanical properties manifested by the oligomeric and fibrillar states of α-syn. The special dynamical properties of the CTD region may contribute to *in vivo* function of membrane-associated α-syn, by enabling the synaptic vesicle liquid phase in the neuron bouton, and dysfunction, through membrane destabilization and permeation by aggregate forms. This work is supported by NIH GM142113.

1. Nforneh and Warncke, *J. Phys. Chem. B*, 2019, *123*, 5395.
2. Ionescu et al., *J. Chem. Phys*., 2021, *154*, 175101.
3. Li et al., *Meth. Enzymol.*, 2022, *666*, 25.
4. Li et al., *Phys. Chem. Chem. Phys.*, 2022, *24*, 23919.
5. Lashuel et al., *Nat. Rev. Neurosci.*, 2013, *14*, 38.
6. Stoll and Schweiger, *J. Magn. Reson.*, 2006, *178*, 42.
7. Whitcomb and Warncke, *ACS Chem. Neurosci.* (in press).

Kurt Warncke:

Katie Whitcomb came to the Department of Physics at Emory with a desire to apply her physics undergraduate degree and biophysics research experience to elucidate the molecular underpinnings of human pathologies caused by proteins that errantly form amyloid structures. Her arrival coincided with the expansion of our group's low-temperature, controlled-confinement system, for EPR spin probe assessment of protein-solvent dynamical coupling, beyond globular proteins, to encompass all classes. She quickly assimilated the requisite EPR sample preparation, measurement and EasySpin-coded simulation methodologies, and contributed as a coauthor to two publications. Katie then embarked on her own, independent inquiry into the solvent-coupled dynamics of the α-synuclein protein, which functions in signal transduction in neurons, and is associated with Parkinson's disease, when present in amyloid forms. Katie's deft manipulations of this system led to the discovery, that α-synuclein's protein-solvent dynamical coupling in oligomers and fibrils differs dramatically from globular proteins examined previously, showing robust persistence under confinement and a distinctive thermal hysteresis in phase mobilities. This work, along with Katie's presentation skills, were honored by the Best Poster Presentation award at the 2022 SEMRC. The results, and proposals for how the EPR-detected dynamical properties of α-synuclein contribute to physiological function and dysfunction, were subsequently published in *ACS Chemical Neuroscience*. Now the senior graduate student in the laboratory, Katie is training the next generation of students in our EPR methods, as she insightfully continues investigations of the origin of the thermal hysteresis, and the dynamics of α-synuclein in functional monomer and small-multimer forms.

IES Best Oral Presentation at the SEMRC2022

Alvaro Montoya Jr.:

It was delightful to attend the Southeastern Magnetic Conference (SEMRC) in-person in 2022 for the first time in a few years. I got to see many familiar faces while also making some new connections. For my talk at the conference, I presented studies involved in uncovering aspects of the mechanism of Oxalate Decarboxylase (OxDC) from *Bacillus subtilis*. In the organism, the enzyme functions as an acid stress-regulator in the cytosol. The presence of oxalate lowers the cytosolic pH which prompts the organism to express OxDC to catalyze the disproportionation reaction of oxalate to formate, thereby returning the pH to stable conditions. My interest lies in the mechanism of the enzyme itself. Catalysis is mediated by a redox process involving two Mn(II), where one is located in the active site, and molecular oxygen [1]. In the literature, the mechanism shows substrate and oxygen are bound to the active site Mn(II) which forces oxalate into a monodentate conformation despite there being no experimental evidence. Therefore, a portion of my dissertation was focused on characterizing the nature of the enzyme-substrate complex. My hypothesis is that oxalate binds bidentate to the active site, and I tested this with a two-pronged Pulse-EPR approach and through use of a mutant of OxDC, W96F, which possesses very low activity but maintains structural fidelity to the wild-type (WT) [2].

The first approach involved using Three-pulse Electron Spin Echo Envelope Modulation (3p-ESEEM) in an effort to measure the levels of hydration around the active site Mn(II), also known as water counting [3]. In the resting state of the enzyme, two water molecules can be found bound to the metal, completing a pseudo-octahedral geometry. We probed the displacement of the water molecules in W96F mutant upon addition of substrate to the enzyme solution (pH 5.00) via the modulation depth of 3p-ESEEM time traces. Enzyme was prepared in deuterated buffer solutions since deuterium produces much larger oscillations in ESEEM compared to protons at X-band frequencies, allowing for a tractable change in modulation depth. From the experiments, we observed a large decrease in modulation depth upon addition of substrate, indicating the substrate is displacing the D_2O molecules bound to active site Mn(II). The results also showed a good match to Mn-DTPA, which we used as a model for a Mn(II) center with no inner-sphere D_2O contributions to the ESEEM. The second approach involves the use of Pulse-ENDOR at X-band to directly probe the binding of oxalate to Mn(II) in the active site of W96F. Isotopic labeling of the two carbon atoms to ^{13}C affords us a detectable hyperfine coupling to the Mn(II) electrons, and should provide a clear picture of the enzyme-substrate complex. The enzyme samples with substrate produce an ENDOR spectrum centered at the Larmor frequency of ^{13}C. DFT calculations performed by our group provide a baseline for magnetic parameters of monodentate and bidentate oxalate bound to Mn(II) in the active site. The EPR spectra produced from theory show that the bidentate model better matches the experimental data, whilst the monodentate model matches poorly. Refinement of the hyperfine couplings with the bidentate model leads to more accurate reproduction of the experimental spectrum. Electron-nuclear distances are then derived at values of 3.14 and 2.92 angstroms for the ^{13}C nuclei to the Mn(II) electrons. Approximately equidistant carbons further indicated a bidentate mode for oxalate.

Through Pulse-EPR studies, we showed that the water molecules in the active site are displaced in the active site due to oxalate being bound bidentate to Mn(II). This discovery points toward oxygen playing its role elsewhere in the enzyme, perhaps at the other Mn(II) site where recent studies suggest it plays a larger role in catalysis [2, 4]. The results of these studies have major implications to the mechanism found in the literature for OxDC and warrants revision. I would like to thank The International EPR Society for awarding me the prize of Best Oral Presentation at SEMRC and allowing me to write about my research here. I also want to thank my Ph.D. advisor, Professor Alex Angerhofer, and my lab-mate, Dr. Tony Pastore, for their excellent mentorship during my time at the University of Florida and for introducing me to both EPR spectroscopy and biochemistry.

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Alex Angerhofer:

It gives me great pleasure to introduce Dr. Alvaro Montoya to our EPR community. Alvaro graduated in 2017 as the first college graduate in his family with his B.S. degree in Chemistry from Susquehanna University in Pennsylvania, a small private liberal arts college in the Appalachian highlands about two and a half hours drive from Philadelphia. At Susquehanna, he performed undergraduate research in the laser lab under the direction of Dr. Wade Johnson. Alvaro applied to the University of Florida (UF) graduate program in chemistry and joined the 2017 incoming class in the physical chemistry division. He received a Graduate Student Fellowship from UF which allowed him to focus on his course work and his research with only minimal teaching responsibilities. I am very fortunate that Alvaro decided to join my group in the fall of 2017. We work on the interface between chemical biology and physical chemistry and incoming students first learn to prepare and purify protein including site-directed mutagenesis. This is followed by an introduction to EPR and other spectroscopic techniques. Alvaro enjoyed the challenge of working in two different disciplines. He became proficient in making his own mutants of oxalate decarboxylase, including the introduction of unnatural amino acids into the protein. He also became quickly comfortable operating our CW X-band instrument, using it for his research, and helping others with theirs. He cherished the opportunity to visit the NHMFL in Tallahassee on several occasions to perform high-field EPR on his samples. In the fall of 2019, he attended the 8th Summer School of the European Federation of EPR groups on Advanced EPR in Brno, Czech Republic. It was an immensely enriching experience for him, and he came back motivated to dive into pulsed EPR and ENDOR which became an important aspect of his thesis. As my senior EPR student, Alvaro also became proficient in repairing and maintaining our aging Elexsys E580 spectrometer. When it came time for him to graduate and look for employment, he had options in the biotechnology industry as well as in magnetic resonance. I am happy for him and for our community that he chose to accept Bruker's offer to join the Billerica team as an EPR Applications Scientist. He understands the challenges of chemical biology and will be very helpful to that community in exploring EPR to solve their problems. Let me close this note by thanking the International EPR Society for recognizing Alvaro on his oral presentation at the 50th SEMRC in Tallahassee, Florida.

2023 IES PhD Thesis Prize of the French EPR Society

Loïc Soriano:

My doctoral research was conducted at the Institut Matériaux Microélectronique pour les Nanosciences de Provence (IM2NP) in Marseille, under the supervision of Dr. Sylvain Bertaina in the magnetism group. I would like to express my gratitude to Dr. Bertaina and the entire research team for their unwavering support, trust, and guidance throughout my research journey. Being awarded the 2023 IES PhD Thesis Prize by the French EPR Society for my thesis titled "Electron Paramagnetic Resonance Study of Spin Coherence in Organic Compounds (o-DMTTF)$_2$X (X = Cl, Br, I, NO_2, and NO_3)" is a tremendous honor. I am immensely proud to receive recognition from such a vibrant and compassionate community. Currently, I am pursuing a postdoctoral position in NMR, and I hope Dr. Bertaina forgives me for turning to the dark side of magnetic resonance.

My doctoral research focuses on the study of impurities within organic spin chain compounds, specifically (o-DMTTF)$_2$X (where X = Cl, Br, I, NO_2, and NO_3). These mixed valence salts function as one-dimensional conductors with uniform antiferromagnetic spin 1/2 chains at room temperature. Below the critical temperature T_{SP}, they undergo a spin-Peierls transition, resulting in a magnetic and structural transition from uniform to dimerized spin chains [1]. Infinite dimerized spin chains have a non magnetic ground state, consequently spin susceptibility must be zero at low temperature. However, numerous theoretical studies have indicated that a translational symmetry breaking can lead to a s = 1/2 ground state [2–5]. This s = 1/2 magnetization is localized around impurities and extends over tens of lattice sites, forming a magnetic soliton. Recently, the first recorded

Rabi oscillations of pinned solitons were reported in $(TMTTF)_2X$ salts (where X = PF_6, AsF_6) [6], an analog compound to $(o\text{-}DMTTF)_2X$. In magnetic systems, decoherence is typically influenced by spin-bath dipole-dipole interactions, and the observation of Rabi oscillations necessitates spin dilution. In this context, we explore an alternative approach for electron spin qubits, considering strong correlations as a potential paradigm.

EPR spectroscopy is a particularly pertinent technique for examining these impurities due to its sensitivity as a local probe measurement. Through a meticulous analysis of single crystal spectra, we are able to discern the microscopic structure of the chains, such as uniform exchange coupling, dimerization of the chains or coupling between chains. We identify a paramagnetic signal at low temperatures originating from s = 1/2 impurities. By employing a combination of EPR spectroscopy, Density Matrix Renormalization Group and Quantum Monte-Carlo calculations, two highly efficient methods for low-dimensional systems, we demonstrate that these defects are intrinsic to the chains [7–9].

The second part of my thesis work centers on the dynamics of pinned solitons. Single crystals of $(o\text{-}DMTTF)_2X$ yield a robust spin echo signal at low temperatures, affording the opportunity to use advanced pulse sequences. Our investigation of the temperature and field dependence of T_1 relaxation time reveals a prevalence of spin-phonon processes. Subsequently, we explore decoherence mechanisms using techniques such as Hahn echo decay, dynamical decoupling, and hyperfine spectroscopy sequences like ESEEM and HYSCORE. It becomes evident that conventional models for diluted spin systems fall short in describing our system. We conclude this work by discussing on the potential influence of strong correlations on spin decoherence.

Finally, I would like to thank all my collaborators: Marc Fourmigué and Olivier Jeannin for the single crystals synthesis, Hervé Vezin and Guillaume Gerbaud for generously providing access to their pulsed EPR platform and their precious advices, Maylis Orio for Density Functional Theory calculations and Michel Giorgi for the X-ray diffraction measurements.

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6. S. Bertaina & al., Physical Review B **90**, 60404 (2014)
7. J. Zeisner & al., Physical Review B **100**, 224414 (2019)
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Sylvain Bertaina:

I met Loïc during his Master's internship, when he became interested in the continuous-wave EPR study of charge-transfer organic compounds. Very committed to this first contact with the academic world, he started a PhD thesis on the coherent dynamics of defects in spin chains. The aim was to study the spin dynamics of solitons formed by translational symmetry breaking. This experimental thesis became a real challenge during the COVID-19 period. He took advantage of this period to develop theoretical models based on exact diagonalization, DMRG and quantum montecarlo to explain many of the experimental results observed to date. This intellectual curiosity enabled him to obtain remarkable results in the EPR field of strongly correlated defects. Wishing to continue his career in the field of magnetic resonance, but open to other methods, he is now a post-doctoral fellow at LNCMI in Grenoble, where he is working on NMR in superconducting materials.

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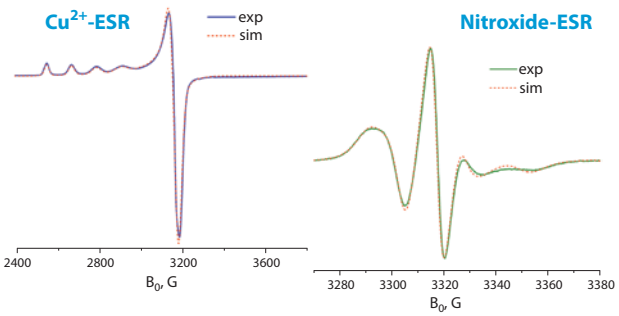
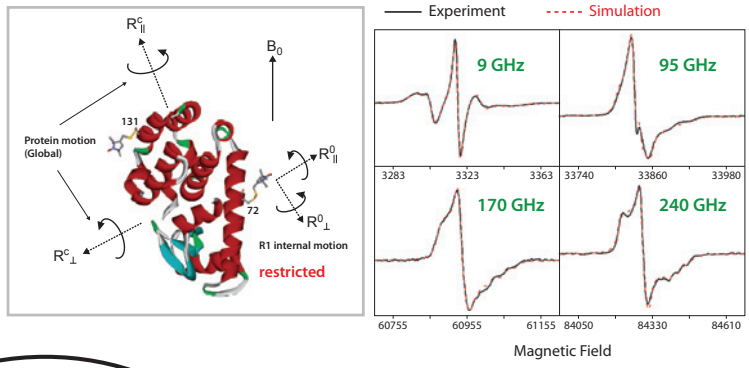


Multifrequency ESR



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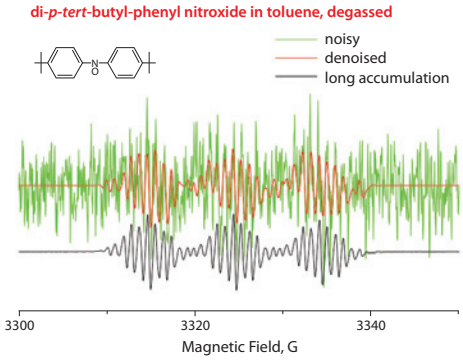

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4) Standard Samples
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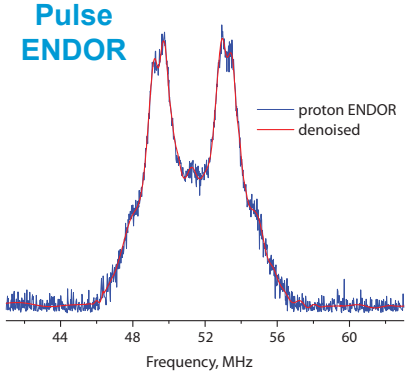
Pulse ENDOR



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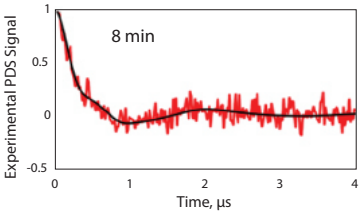

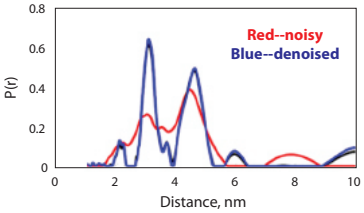

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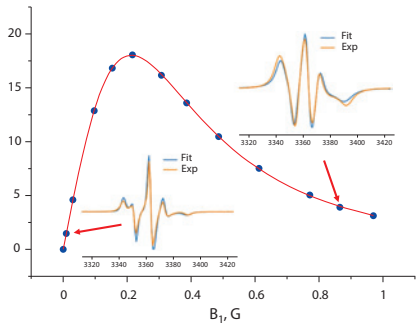

Saturation Curve

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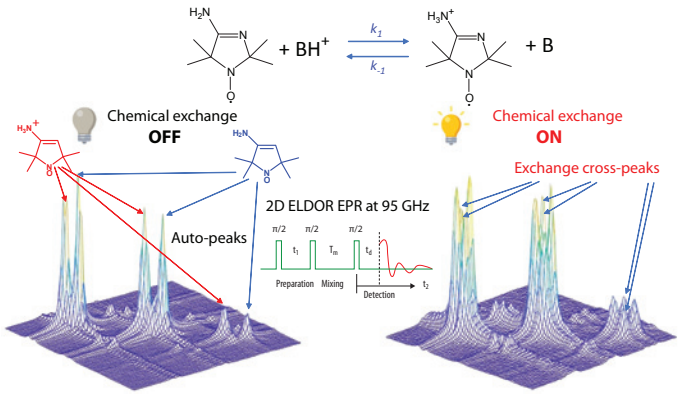

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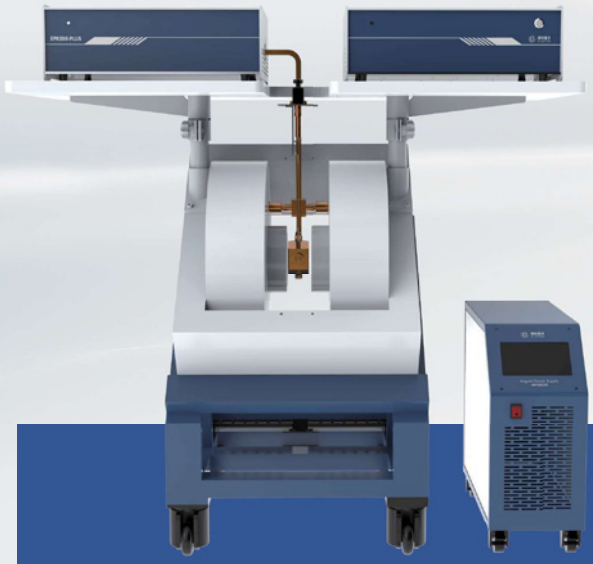

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Uniformity of magnetic field in sample area	Better than 50mG
Detection SN ratio in continuous wave mode	Better than 600:1
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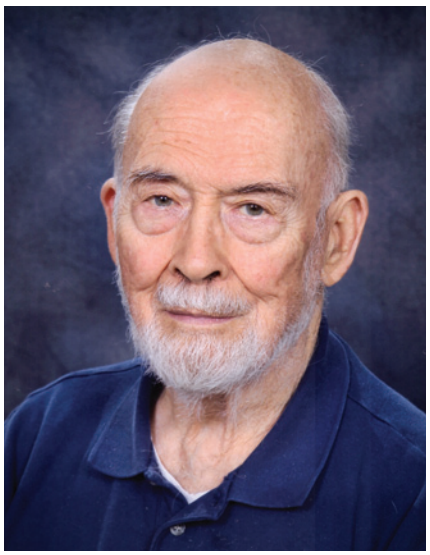

Bruce R. McGarvey (1928–2023)

Bruce R. McGarvey, Professor Emeritus at the University of Windsor, Windsor, Ontario, Canada, died on January 24, 2023 in Windsor. Prof. McGarvey was known for pioneering contributions to both nuclear and electron paramagnetic resonance. He was a Fellow of the IES. He was predeceased by his wife Mathilde who passed away in 2013. He is survived by his children Peter (Maria Carmen "Menchu"), Kathleen (Fred), and Paul, and by two grandchildren and his brother David McGarvey (Judi). Most of the information for this obituary came from Peter McGarvey.

Bruce R. McGarvey was born on March 10, 1928 in Springfield Missouri. His father worked for the S. S. Kresge company, which had a chain of what were called "dime stores". Promotion came with transfers to another bigger store. As a result, the family moved frequently to various smaller cities in Missouri, Iowa, and Illinois. In 1940, they moved to Minneapolis, Minnesota, where they finally remained.

Bruce McGarvey graduated from Southwest High School in Minneapolis in June 1946. He had been interested in airplanes and flying and wanted to become a pilot, so he received an appointment to the US Military Academy, West Point, NY and began there July 1, 1946. By the end of August, he realized he really wanted a career in science, not the military, so he requested a discharge and was accepting into Carleton College in Northfield, Minnesota on short notice. He graduated in 1950 with a major in Chemistry.

In the summer of 1950, McGarvey worked in the Analytical Department of Kodak in Rochester, New York. In September, he began graduate studies at the University of Illinois, Urbana-Champaign. Later that fall, he received an induction notice but was able to postpone being drafted into the US Army until the end of the academic year. He then obtained an Atomic Energy Commission (AEC) scholarship which led to a draft deferment.

Bruce McGarvey chose to do research with Professor Herbert S. Gutowsky in the area of NMR. Two other graduate students, Leon Meyer and David McCall, also joined his group at that time. To get them started, Prof. Gutowsky assigned them two assignments. First, they had to calculate the value of $\sum_i r_i^{-6}$ for sites in the various crystal structures of known metals because this was needed to use the second moment equation of Van Vleck. Second, they were to measure the chemical shifts of ^{19}F in substituted fluorobenzenes. Gutowsky wanted the calculations for a study on the NMR of metals that he eventually assigned to McGarvey. The measurement of fluorine chemical shifts was assigned to all three students to help them learn how to operate the NMR spectrometer and to see if the shifts validated the directional theories of the organic chemists. When they first did the shift measurements, the spectrum was displayed on the oscilloscope using a sinusoidal 30 Hz magnetic field sweep which generated large beat signals that made the resolution of two nearby resonances difficult. After Gutowsky visited Bloch's group in Stanford, they switched to a slow linear saw tooth generator for the magnetic sweep and an oscilloscope with a long persistence phosphor. The resulting paper was the first NMR paper in *JACS* [https://doi.org/10.1021/ja01139a025]. David McCall was assigned to measure ^{31}P shifts and discovered spin-spin splitting in NMR by doing so. Meyer and McCall did a lot of grunt work polishing the permanent magnet's pole faces to get the world's first high resolution NMR spectrometer, which McGarvey was spared because of not requiring high resolution. His assignment was to measure more accurate second moments of the broad NMR lines of solid metal powders and Knight shifts of the same metals [https://doi.org/10.1063/1.1700782 and https://doi.org/10.1063/1.1698794]. The second moments of the metals were larger than predicted by the Van Vleck theory. The explanation was the short T_1 times that made a measurable contribution to the line shape.

In his first year in graduate school McGarvey decided to get a Master's degree in case he was drafted by the end of the year. To that end he made measurements on the chemical shifts of the thallium resonance in various compounds. Thallium has two isotopes ^{205}Tl and ^{207}Tl, both with $I = 1/2$, and have the third and fourth largest magnetic moments of naturally occurring isotopes; he had detected both in his metal work. Gutowsky suggested measuring the shift between Tl^+ and Tl^{3+} in aqueous solution because the shift could easily be calculated from Ramsey's theory and the wave functions for the two ions in vacuum. However, the measured shift was an order of magnitude larger than the calculated value due to the presence of coordinated water molecules attached to the ions. This showed that the chemical shift in thallium compounds was much larger than what was measured in the NMR of ^{1}H, ^{19}F and ^{31}P. McGarvey's Master's thesis was on the chemical shifts of various thallium compounds and was awarded in September 1951. In 1952, Gutowsky came in with a physics paper that stated it was important to know the ratio of the resonance frequencies for the two isotopes (^{205}Tl / ^{207}Tl) to high precision. They realized this was easy to do because the two frequencies are close together and all that was needed was to measure the difference in frequencies. Gutowsky and McGarvey did this one Saturday afternoon and the results were published in *Physical Review* [https://doi.org/10.1103/PhysRev.91.81]. McGarvey had (co-)authorship on four papers and two letters to the editor in his three years as a graduate student. He was in at the beginning of a major field in Chemistry in which anything one did was new and important. McGarvey received his Ph.D. in June 1953.

He accepted a position as Instructor at the University of California-Berkeley starting July 1. It was a two-year appointment and there was no guarantee that he would be kept on. McGarvey originally intended to construct an NMR spectrometer and continue his solid-state studies but this changed when he discovered that Walter Knight in Physics was starting studies in the exact same area. Melvin Calvin was pushing EPR because of his interest in metal chelates. The Radiation Lab people at Berkeley were also interested in EPR and put up the money to purchase a six-inch electromagnet from Varian. McGarvey then began studying the Montgomery Series of books on microwave electronics, the Radio Amateurs Handbook, a review article by Bleaney on EPR, and borrowing circuit diagrams for the EPR

spectrometer of A. Kip in the Physics Department. It took a year to get the spectrometer built with the help of the machine shop and electronics technicians. McGarvey's first spectrum of powdered copper acetylacetonate was obtained on June 2, 1954. The first spectrum of copper acetylacetonate in dioxane solution was made on September 29. EPR spectra were recorded for various copper chelates in different solvents, which came from Melvin Calvin's lab and were prepared by R. Linn Belford, whom McGarvey knew from the University of Illinois and had been Belford's teaching assistant in physical chemistry. All of these spectra exhibited the four-line hyperfine pattern from the ^{63}Cu and ^{65}Cu nuclei with I = 3/2. The g value and hyperfine splitting varied with change of solvent and ligand. The most surprising feature of the liquid spectra was the different line width of each hyperfine line. McGarvey had no idea why and could get no explanation from anyone in the Chemistry or Physics departments. He did not know that George Pake's group at Stanford were observing the same thing for vanadyl complexes. It was later explained by Harden McConnell who was at Shell Development at the time and had attended a Departmental seminar where McGarvey presented his results. McConnell explained the anisotropy in solution as due to the fact that the tumbling of the solute molecules was not fast enough to average out the broad anisotropic spectrum observed in frozen solutions.

McGarvey grew a single crystal of copper acetylacetonate and determined $g_{\|}$ and $g_{\perp}$. The hyperfine interaction was not visible in the pure crystal due to spin-spin line narrowing interactions with neighboring copper ions. The g values were similar to those found by Bleaney in hydrated copper ions, except they were smaller in magnitude due to the more covalent bonds in the acetylacetonate, where the unpaired electron resides in a $dx^2–y^2$ orbital. This was proof that Pauling's prediction that covalency in the copper chelates would force the unpaired electron to be in the 4pz orbital so that dsp^2 hybridization could take place was incorrect. During this time Pauling came to Berkeley for a month and Ken Pitzer, department head at the time, strongly urged McGarvey to talk to him. Pauling was not particularly pleased when McGarvey suggested that his research was proving Pauling wrong and that the LCMO method of Mulliken was better. Pauling launched into a rapid-fire lecture on how his Atomic Orbital approach could explain what McGarvey was seeing, who could not follow Pauling but felt he did not really understand crystal field theory. In his paper, McGarvey simply stated that Pauling's approach could not explain the experimental results and that the unpaired electron is in a $dx^2–y^2$ type MO.

In 1955 McGarvey was promoted to assistant professor with a two-year contract. After promotion he was allowed to teach a course and was assigned one section of the undergraduate physical chemistry course. He was also informed that he could direct a graduate student, so he took on August (Gus) Maki. Maki had been a starting graduate student under Pitzer's direction but had been drafted. When Maki returned in the fall of 1957, Pitzer was away on sabbatical so Maki elected to work with McGarvey. McGarvey had just succeeded in growing crystals of diamagnetic palladium acetylacetonate doped with small amounts of copper acetylacetonate and Maki performed single crystal EPR studies on these.

Before they could write this work up, McGarvey was let go by the Department. Maki and McGarvey wrote two papers on the work that became Citation Classics in the 1970s [https://doi.org/10.1063/1.1744456; https://doi.org/10.1063/1.1744457; there are also classic papers from that time on EPR of Ti(III): https://doi.org/10.1063/1.1733669 and Cr(III): https://doi.org/10.1063/1.1725209]. McGarvey could not convince any large research universities to hire him so he accepted a position at Kalamazoo College [Kalamazoo, MI, USA] where he built another ESR spectrometer and published three papers. He and the other chemistry professor Kurt Kaufman were the first to get research grants at the College and had great difficulty explaining them to the President and the Finance Administrator.

In 1962 McGarvey moved to Brooklyn Polytechnic, which at the time was a large research department with over 200 graduate students and graduating 60 Ph.D.'s each year. He continued doing EPR and developed an interest in the NMR paramagnetic shift and coauthored with Robert Kurland a paper on the theory of the shifts [https://doi.org/10.1016/0022-2364(70)90100-9]. Earlier theories had made assumptions that were violated by most of the systems studied in the literature. In 1967 McGarvey received a Guggenheim Foundation fellowship to spend a year with Professor Geoffrey Wilkinson at Imperial College in London. Unfortunately, by 1972 Brooklyn Polytechnic was near bankruptcy due to severe cuts in government grants brought on by the Vietnam War [it is now a branch of New York University: https://engineering.nyu.edu/about/brooklyn]. McGarvey accepted a position at the University of Windsor and stayed there until retirement in 1993. In Windsor he did NMR and EPR on lanthanide systems [https://doi.org/10.1021/ic00260a034], spin-crossover systems [https://doi.org/10.1021/ic00277a012], biradicals and triradicals. From 1996 to 2008, he lectured, consulted and did research on ruthenium(III) systems for several months each year at the University of São Paulo at São Carlos in Brazil [https://doi.org/10.1021/ic9914701]. McGarvey also gave a course at the University of Florence. He published over 140 papers and 8 chapters in books, with one of the last ones being with the editor of this obituary [https://doi.org/10.1021/ic201189a].

Joshua Telser

Patrick Carl (1973–2023)

With great sadness and deep sorrow, we have to say goodbye to our colleague and friend Patrick Carl. He had been an invaluable part of Bruker EPR for twenty years. Pat passed away peacefully at home in Karlsruhe, Germany on June 20th at the young age of 49.

He was born in New Hartford, New York, but grew up in Tennessee and Wisconsin.

He graduated from Platteville High School in Wisconsin and continued with further studies at Winona University in Minnesota. This was followed by a Ph.D. in Chemistry at the University of Iowa as the first graduate student of Sarah Larsen, studying the characterization of transition metals in zeolites by EPR.

After his Ph.D., Pat left the country for a three year post-doc with Daniella Goldfarb at the Weizmann Institute in Israel to explore FT-EPR and high field EPR. Two and half years into the stint at Weizmann she asked him, "What's next?" and he responded, "I want to work for Bruker." Daniella called Peter Höfer and, well the rest is history. He started with us in 2003 as application scientist.

Pat was indispensable in many tasks at Bruker, including writing PulseSPEL programs, python scripts, testing repaired items, and basically scut work we need to perform as application scientists. He particularly excelled in helping the EPR community to get their experiments working, from the mundane to the esoteric. His professionalism, perseverance, and expertise were an invaluable resource to the EPR community. As application scientists at Bruker, we are no longer research scientists, but we have a great passion in promoting the community with technical support and advice for the emerging EPR applications. Pat was our guidepost in this endeavor.

It was always a pleasure to work with Pat. He had an encyclopedic knowledge of EPR, both theory and practice. He was always ready to pitch in and be helpful. Pat's sense of humor and wry wit will be sorely missed.

Pat is survived by his soulmate Oezlen and his sons Domique and Daniel of Karlsruhe Germany, his mother Cindy and brother Mark of Platteville. He is further survived by his nephews, Austin and Ethan Carl and his nieces, Kennedy McMillin and Alayna Carl. He was preceded in death by his father, LeRay.

Pat still came into Bruker until the very end. The applications team was able to enjoy his company a month before his demise. He attended several gatherings during our EPR applications meeting in May.

Throughout his life, he was a passionate advocate for animal welfare, driven by a deep compassion for all creatures. His wish was to have memorials made in his name to the Cancer Society or the Humane Society or Rescue League.

We thank the many community members that offered contributions to the remembrance book we prepared.

Ralph Weber,
Bruker BioSpin Corp., Billerica, USA

Euromar 2023
July 9–13, 2023, Glasgow, United Kingdom

Euromar 2023 took place in the City of Glasgow at the Scottish Events Campus (SEC) organised by Dr. John Parkinson (University of Strathclyde) as main organiser and local organisation co-leads Professor Dr. Sharon Ashbrook (University of St Andrews) and Professor Dr. Frederic Blanc (University of Liverpool). The diverse scientific programme had strong representation of EPR and hyperpolarisation especially when it came to prizes and plenary and invited talks. Also this year the conference was preluded by the Bruker Pre-EUROMAR Symposium before the traditional opening Prize Session. The "Richard R. Ernst Prize in Magnetic Resonance" (The Ernst Prize), named after magnetic resonance pioneer and Nobel Laureate Professor Dr. Richard R. Ernst, recognising 'recent beneficial applications of Magnetic Resonance' was awarded to Professor Dr. Lucia Banci (University of Florence) and Professor Dr. Jack Freed (Cornell University) who shared their work in the respective prize lectures *In-cell NMR: progresses and challenges* and *ESR and Biophysics at ACERT*. The 2023 AMPERE prize was awarded to Professor Dr. Ashok Ajoy (UC Berkeley). The Raymond Andrew Prize is awarded by the Groupement AMPERE in memory of Professor Dr. Raymond Andrew and to honour his pioneering work in the field of magnetic resonance. The outstanding PhD thesis in magnetic resonance selected in 2023 was by Dr. Nino Wili (University of Aarhus) who presented his prize lecture *Spinlocked electrons: From electron electron distance measurements to dynamic nuclear polarization* discussing his PhD. Coincidentally, Dr. Nino Wili's PhD supervisor Professor Dr. Gunnar Jeschke (ETH Zürich) was delivering the next prize lecture celebrating his award with the IES Gold Medal during the Monday morning plenary session. The prize lecture *Distance distribution information for ensemble structural biology* gave deep insights into 25 years of development of pulse dipolar EPR methodology and applications. The award was presented by the IES Vice President – Europe Dr. Maxie Roessler (Imperial College London). Professor Dr. Marina Bennati (University of Göttingen) provided impressive results on fluorine radical distance measurements and resolution of chemical shift anisotropy in high-field ^{19}F ENDOR in her plenary lecture *EPR spectroscopy at the interface to NMR: high field ENDOR and DNP*. A notable new feature of this year's Euromar

Euromar2023 conference chair Dr. John Parkinson opening the conference.

Professor Dr. Ilya Kuprov demystifying AI in magnetic resonance in his tutorial.

were flash talks by poster presenters at the end of four parallel sessions that were very well received. The first tutorial was not concerned with magnetic resonance experiments or analysis but with their publication. Professor Dr. Warren Warren (Duke University) and Professor Dr. Tatyana Polenova (University of Delaware) gave their respective views as journal editors on *Beating the odds on Journal Acceptance* and *Best Practice in Scientific Publishing*. The sometimes light-hearted anecdotal examples must have been very useful for early career researchers and were even insightful for those with a sizeable publication effort of their own. In the second tutorial Professor Dr. Ilya Kuprov (University of Southampton) and Professor Dr. Vladislav Orekhov (University of Gothenburg) embarked on a jargon- and myth-busting exercise relating to artificial intelligence and machine learning in magnetic resonance by relating to well-known mathematical methods. Their tutorial *Artificial intelligence for a busy NMR spectroscopist* provided an overview of AI for data processing and experiment design in the context of magnetic resonance. The conference had two sessions entirely devoted to EPR/ESR featuring invited presentations by Professor Dr. Sharon Ruthstein, Dr. Maxie Roessler, Professor Dr. Mario Chiesa and Professor Dr. Marilena Di Valentin covering the full breadth of modern EPR applications from metal-based transcription factors in-cell and electrochemical EPR to homogeneous catalysis and light-induced pulse dipolar EPR. In parallel the hardware sessions featured updates on EPR-on-a-chip by Professor Dr. Jens Anders (University of Stuttgart) and EPR cryoprobes by Dr. Mantas Šimėnas (Vilnius University). Outgoing chair of the Euromar Board of Trustees Professor Dr. Thomas Prisner noted that many of the contributions on hyperpolarisation,

IES Secretary Professor Dr. Aharon Blank (left) awarding the IES poster prizes to Ms Marina Dajka (right) and Dr. Laura Remmel (center).

paramagnetic NMR and even NMR applications featured related EPR spectra. The strong showing of the EPR community was rounded off by three poster prizes. The IES sponsored awards were won by Ms Marina Dajka (Free University Berlin) and Dr. Laura Remmel (Max Planck Institute for Multidisciplinary Sciences, Göttingen) with posters describing EPR applications in membrane proteins and nucleic acids. The RSC journal Dalton Transactions sponsored poster prize was awarded to Dr. Mikhail Agrachev (ETH Zürich) for work on two-dimensional molybdenum carbide materials. The organisers also provided a rich social programme with the opening night Welcome Reception in the Glasgow Science Centre just across the river Clyde from the SEC. Monday night the traditional Bruker Social Evening was held in the Riverside Museum allowing delegates to explore 3,000 objects on display from skateboards to locomotives, paintings to prams and cars to a Stormtrooper. On the final evening the Gala Dinner & Cèilidh was held at the Kelvingrove Art Gallery & Museum. Here, one could explore displays including natural history, arms, armour and art from many art movements and periods of history before dinner. This was followed by the Cèilidh (traditional Scottish country dancing) and live music providing a very memorable closure to the conference.

Bela Bode
Euromar 2023 Local Organizing Committee

EPR

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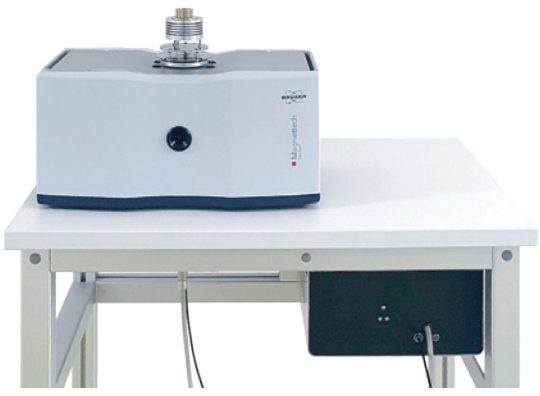

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EPR

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