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

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The cover picture illustrates aspects of research carried out by Peter Hoefer, recipient of the Bruker Prize 2017. It shows the first 2D HYSCORE spectrum from 1986 measured on a deuterated single crystal of squaric acid. Since then HYSCORE has become one of the most popular tools for hyperfine spectroscopy and is standard on all Bruker pulse-EPR instruments.







The Publication of the International EPR (ESR) Society

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Market place

Editorial

Dear colleagues,

All of us knew about the 50th Jubilee Annual International Conference of the RSC EPR Group to be held in April, 2017 in Oxford, UK. It is one of the major events in the life of magnetic resonance community also hosting the Bruker Prize, Bruker Thesis Prize, and the JEOL Prize. Therefore it is not surprising that having met with Graham Smith in August 2016 by chance on the way to the APES2016 meeting at the Lake Baikal, among other topics we discussed the possibility of preparing an issue of the EPR newsletter with the relevant event-oriented columns.

It is just great that Eric McInnes, Chairman of Committee, RSC Spectroscopy Group, and the Committee members supported this idea and contributed a lot to this issue of the *EPR newsletter*: the interview with Peter Höfer, Bruker Prize 2017 recipient, success stories of Andrin Doll, Bruker Thesis Prize 2017 recipient (see also 22/4, p.18) and Jason Sidabras, JEOL Prize 2017, a laudation for David Collison on his 65th birthday; Nicholas Chilton's software article and Ilya Kuprov's report on the 50th Jubilee Annual International Conference of the RSC EPR Group; introduction of a cohort of brilliant new EPR faculty – Christos Pliotas, Chris Wedge, Maxie Roessler, Nicholas Chilton, and Emma Richards, and of a book Electron Paramagnetic Resonance written by V. Chechik, E. Carter, and D. Murphy. Dear Eric, thanks a lot for your help and support!

We shift the event-oriented EPR newsletter Anecdotes column to the next issue 27/4 (2017): Les Sutcliffe kindly agreed to share with us his reminiscences of the Annual International Conferences of the RSC EPR Group (see also his story on magnetic resonance in Britain in 1956 (16/2-3, pp. 13, 14). In the meantime, you may enjoy a retrospect on the related material already published in the EPR newsletter: John Pilbrow recalls the Clarendon Laboratory in Oxford in the early 1960s (13/1-2, pp. 16, 17) supplemented by a story of Mark Newton on his early days of ENDOR in the Clarendon Laboratory (16/2-3, p. 8); Michael Baker tells about the beginning of EPR in Oxford (15/2, pp. 7–9); Anatole Abragam shares a story of his discovery of EPR (what does he mean?!) during two happy years in Oxford (15/2, p. 9); Shirley Fairhurst invites us to celebrate the 40th anniversary of the RSC ESR Group (19/1-2, pp. 24, 25). And if you continue surfing on the issues of the *EPR newsletter* on your own, you will find more exciting information on different aspects of the life of the magnetic resonance community in UK.

I anticipate your pleasure on reading the article "Looking backward – How EPR research was done 65 years ago" by Harvey A. Buckmaster. As for me, I enjoyed it tremendously. Thank you, Harvey! I dare to quote your words: "Hopefully, other older EPR researchers will be stimulated to write about their early research experiences." This is exactly what I hope for! These contributions are precious gems of the history of EPR invaluable for the younger generation of magnetic resonance researchers. Dear colleagues, you are more than welcome!

Laila Mosina



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Interview with Doctor Peter Höfer on the Occasion of His Bruker Prize 2017

EPR newsletter: Dear Doctor Höfer, on behalf of the readers of the EPR newsletter we congratulate you on your Bruker Prize 2017. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?

I have started with the decision to study physics at the University of Konstanz. Although I did not know before what physics really is, it turned out to be a good decision. The real scientific part came during the diploma work where I investigated micro clusters by time-of-flight mass spectroscopy. It was an intriguing topic and the experience of developing, applying and understanding founded my enthusiasm for science.

Who introduced you into magnetic resonance?

I was introduced to magnetic resonance as a PhD student at the institute of Prof. Michael Mehring at the University of Stuttgart. The institute at that time was equally focused on NMR and EPR and I have learnt already from the beginning how to translate NMR concepts to pulse-EPR, which was still in its infancy in the 1980's. It was, for example, a very logical process to think about 2D spectroscopy or how to measure nuclear coherences via EPR. With Michael Mehring I had an excellent teacher with a deep understanding of all aspects of magnetic resonance, be it in NMR or EPR. It was a very fruitful time period during which I also developed my passion for magnetic resonance. However, I have also learnt something which seems to be a general aspect of science: success doesn't always come with the first shot and a good degree of endurance and a long term vision is very helpful! My work concentrated on hyperfine spectroscopy and I started building a pulse-ENDOR accessory for the home built pulse-EPR instrument which was maturing in parallel. The first paper coming out of this was about Spinor ENDOR. It was followed by papers about Bloch-Siegert shift and Rabi oscillations, pulse-TRIPLE, EPR detected nuclear coherences and multiple quantum ENDOR. I was eager to apply these new pulse-ENDOR methods and spent some extra time to investigate the soliton spin density distribution in polyacetylene. In parallel to my ENDOR activities we had a project about 2D spectroscopy and my task was to apply 2D methods to ESEEM. I had studied the concepts of correlation spectroscopy as already applied in NMR and was able to translate it to ESEEM. The result was the paper about hyperfine sublevel correlation spectroscopy, a method we named HYSCORE.

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

The development of instrumentation and methods has my strongest focus. Both topics go hand in hand, new ideas about methods trigger new instrument developments and vice versa. A good example of this is the arbitrary waveform generator; a new technology which became available for EPR and which already has triggered several EPR groups to develop new methods to improve the sensitivity of EPR.

What is the driving motivation for you in your research?

It is all about discovery and understanding and then making something useful out of it. I am in the lucky position, and I feel very privileged about this, that I can help turning ideas into products which find use in science and lead to an improvement of life. The close in-



teraction with our customers and fellow scientists provides a lot of inspiration and is a strong motivation driver as well.

What is it to be EPR Business Line Manager of Bruker BioSpin, the firm producing the highest quality magnetic resonance spectrometers? How do you see the mission of Bruker BioSpin?

Even after almost 30 years it is still fun and also full of challenges to work in EPR at Bruker. The core of our business understanding is to enable scientists to be successful by building the highest quality and performance magnetic resonance spectrometers. To help our customers to do research at the forefront of science we aim to provide always the latest technology, like, for example, the rapid scan unit which we are currently developing. We want to make magnetic resonance the tool of choice in analytics and spread it to a wider world of users. To achieve this goal we design solutions to make the instrumentation more accessible and easier to site and use. Our bench-top system, the EMXnano, reflects this vision. It has been specifically designed for those fields of science where EPR is just one of many other analytical tools.

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

Magnetic resonance spectroscopy is a fascinating method which provides unparalleled insight into matter. To be able to use this richness to its full extend one needs to understand the fundamentals of the method. I would therefore recommend not to follow the "black box" approach but know what goes on inside.

Awards

Bruker Thesis Prize 2017



Andrin Doll:

The 50th anniversary RSC meeting in Oxford was a very nice conference. I enjoyed the rich scientific program as well as the ambiance of Oxford, which was well underlined by the authentic venue in Keble college. The organizers really made this jubilee meeting an unforgettable experience!

In addition to this setting, I had the exceptional honor to receive the Bruker thesis prize at the RSC meeting. I thus had the opportunity to give an overview of my activities during my PhD thesis entitled "Frequency-swept microwave pulses for electron spin resonance" in Gunnar Jeschke's group at ETH Zürich [1]. In total, I stayed in Gunnar's lab from January 2012 until June 2016 and defended around March 2016. In brief, I would describe my activities as follows: Implementing frequency swept microwave pulses at X- and Q-band by means of arbitrary waveform generators (AWG) and then playing around with them while trying to understand what is going on.

At the very beginning of my thesis, my main concern was to make such frequency-swept pulses available in Bruker Elexsys spectrometers at X-band and collect initial experience. In the first few experiments, it became immediately clear that there is quite some room for improving the excitation bandwidth when changing from monochromatic excitation pulses to frequency-swept excitation pulses. For a number of pulsed EPR experiments where excitation bandwidth is a limitation, frequency-swept excitation pulses thus became an interesting alternative to evaluate. This initial observation was of course very much according to our expectations, since the advantages in terms of excitation bandwidth are well known in NMR. However, this advantage in excitation bandwidth is paired with a potential limitation of these pulses, namely that they are longer than the monochromatic counterparts and excite the spins frequencyprogressive. Different spin packets are therefore excited at different times. Accordingly, when replacing monochromatic pulses in established EPR experiments by frequency-swept pulses, the experiment may no longer behave as with ordinary pulses.

A picturesque example of the advantages and limitations of frequency-swept pulses is when using them as pump pulse in DEER. In principle, the inversion efficiency of a frequency-swept pump pulse can be enhanced when prolonging the pulse duration, thus enhancing the DEER modulation depth. However, the pump pulse in DEER should be short compared to the dipolar oscillation period of the involved distances. Loosely speaking, DEER with such pulses is about finding a suitable balance between uncertainty in fast dipolar frequencies (short distances) and sensitivity. If one has an idea about the expected distance range ahead of the experiment, one can make the pulse short enough to stay in the 'comfort zone', where the distance range of interest is not affected by the frequency-progressive excitation of the pump pulse. This is rather easily achieved when determining long distances, where long pulse durations well beyond 100 ns are admissible. Accordingly, large modulation depths on broad spectra may be achieved. In my thesis, I demonstrated this with Gd-Gd rulers having long distances up to 8.6 nm. A series of two pump pulses with a total duration of 384 ns achieved Q-band DEER modulation depths beyond 7%. As these long-distance experiments yielded only small echo amplitudes, even for model compounds at dilute concentration (50 μ M), the echo signals were enhanced by a factor of two by reshuffling the populations within the S =7/2 sub-levels of the observer spin.

The requirements are different for short Gd-Gd distances on the order of 2 nm. These short distances do not only require short pump pulses, but also a large frequency separation between pump and observer is advisable, since pseudo-secular contributions when dealing with S = 7/2 spin pairs could severely distort distance distributions. To cope with these requirements, I used a pulse sequence that 'freezes' evolution during the application of the pump pulse by longitudinal storage (CIDME). Accordingly, a Gd-Gd modulation depth beyond 10% without significant broadening due to pseudo-secular contributions became possible, while pumping the spins on an extended time period of 1 µs.

Besides these distance measurements that were all recorded by Bruker Elexsys spectrometers extended by frequency-swept pulses, I also looked into enhanced detection bandwidth and FT-EPR techniques. To this end, I designed a home-built AWG spectrometer that is operational at both X- and Q-band. This spectrometer is geared towards experiments where all involved pulses are frequency-swept and result in echoes of broad bandwidths. As opposed to the DEER type of experiments described above, the frequency-swept pulses are here not only used to invert population, but also to excite and refocus coherence. An important ingredient here is that spins can be excited uniformly. As an example, when exciting the entire nitroxide spectrum by a frequency-swept $\pi/2$ pulse, all spins should end up in the transverse plane. In this respect, pulses that compensate for the resonator response function turned out very useful. In fact, distortions in FT-EPR spectra computed from broadband echoes are minimized if all involved pulses excite the spins uniformly. While the criterion for uniform excitation is evident for $\pi/2$ pulses that excite coherence over broad bandwidths, the situation is more intricate for frequency-swept refocusing pulses. In particular, these result in considerable Bloch-Siegert shifts, which can introduce losses if the B_1 field felt by the sample is spatially inhomogeneous or if the excitation is not uniform.

Using this home-built spectrometer and uniform excitation pulses, a number of twodimensional FT-EPR experiments became possible. In particular, the FT-EPR spectrum was correlated to (i) longitudinal relaxation, (ii) nuclear modulation, and (iii) dipolar electron-electron modulation. Besides these two-dimensional spectra, the spectrometer also allowed for critical testing of theory of frequency-swept excitation pulses against experiments [2]. Later on, after I defended my thesis, I also implemented an experiment that unifies broadband frequency-swept refocusing pulses and monochromatic pulses to perform an alternative type of DEER experiment (nonselective DEER), which shows interesting spin dynamics and appears to scale favorably for dynamical decoupling schemes [3].

For all the support during my PhD project, I am very thankful to Gunnar Jeschke. He gave me the very generous opportunity of a PhD project tailored to my skills as electrical engineer and my interest in physics. Moreover, I need to thank a number of other people with whom I directly worked together during my project. Spin dynamics simulations were always very important for understanding and interpreting the experiments, such that I am grateful for all interactions with Stephan Pribitzer, who is the core developer of SPin DYnamics Analysis (SPIDYAN) which can be downloaded from our website (www.epr.ethz. ch). Furthermore, I thank Takuya Segawa for his fruitful work on hyperfine spectroscopy and his role as 'test-dummy' as first user of my spectrometer. During my project, I also got to explore a number of interesting subprojects during semester and master theses. Here I am grateful to the work of several eager students, namely Bettina Basel, Nino Wili, Andreas Dounas, Janne Soetbeer and Stephan Pribitzer. Finally, I am very grateful for the series of Gd-rulers synthesized by Mian Qi in the group of Prof. Adelheid Godt. Without these rulers, the optimization of Gd-Gd distance measurements would not have been possible.

With respect to the Bruker Prize and the RSC meeting in Oxford, I want to thank all the organizers for making this possible, in particular Bruker for funding of the prize and the reviewers for taking their time for reviewing entire PhD theses.

Since July 2016, I am doing a post-doc at CEA Paris-Saclay in the nano-magnetism group of Claude Fermon. I am there investigating on how magneto-resistive sensors can be applied in magnetic resonance, mostly in NMR

at low frequencies and small volumes. These are the type of sensors that are nowadays used as read-heads in hard-disks and for numerous types of magnetic sensors in the automotive industry. In my absence from pulsed EPR spectroscopy, of course, I am following the recent literature with a lot of enthusiasm, in particular on shaped pulses that are becoming available to an increasing number of users.

- 1. A. Doll, Frequency-swept microwave pulses for electron spin resonance, Diss. ETH Zürich, http:// dx.doi.org/10.3929/ethz-a-010670425
- 2. A. Doll, G. Jeschke, Wideband frequency-swept excitation in pulsed EPR spectroscopy, JMR 280, 2017, 46-62
- 3. A. Doll, G. Jeschke, Double electron-electron resonance with multiple non-selective chirp refocusing, PCCP 19, 2017, 1039-1053



The JEOL Prize 2017



Jason Sidabras:

would like thank the organizers of the 50th Lannual international Royal Society of Chemistry EPR Meeting and the JEOL Competition Talk judges for inviting me to talk about Planar Micro-Resonators and Micro-Helix Geometries for Studying Protein Single Crystals with X-band EPR. I would also like to thank JEOL for sponsoring this prestigious annual competition. This year the competing talks

were exceptional and I am honored to have __been awarded the prize.

My start in EPR began in the summer of 2003 where I found a home in the Department $\nabla \times H = \frac{\partial D}{\partial t} +$ of Biophysics at the National Biomedical Link Genter at the Medical College of Wisconsin. For 12 years, 2003–2015, I studied under Prof. James S. Hyde and Dr. Richard R. Mett who were indispensable mentors and with whom I share a number of publications. While I was a full-time research engineer at the Medical College of Wisconsin, I obtained a Master's of Science in Electrical Engineering (2005–2010) from Marquette University under the direction of Prof. James E. Richie, who specializes in electromagnetics and numerical techniques. My Master's thesis used a formal Green's function approach to better understand the physics of a modulation slot and to optimize the slot geometry for production of a uniform 100 kHz field modulation profile over the sample region. This work has recently been published and illustrates the opportunity of designing a uniform-field excitation in solid body cavities with modulation slots [1]. This may be of importance when designing cavities for rapid scan applications at high frequencies.

> As of March 2016, I moved to Germany to pursue an exciting and prestigious career in the Department of Biophysical Chemistry at the Max Planck for Chemical Energy Conversion under Dr. Edward J. Reijerse and Prof. Wolfgang

Lubitz. At MPI-CEC I will lead the development of EPR resonator probe developments for the study of [FeFe]-hydrogenase protein single crystals. These single crystals are in the sub-nanoliter volume $(0.3 \times 0.3 \times 0.4 \text{ mm typical})$ geometries) and require novel resonator development to increase the EPR sensitivity. In May of 2017 I was awarded an EU Funded Horizon 2020 Marie Skłodowska-Curie Individual Fellowship, Act-EPR (http://act-epr.org), specifically on the development of EPR resonator and instrumentation technology to study protein single crystals at X-band. This fellowship also provides me with a path to obtain my PhD in physics under Prof. Dieter Suter at the Technical University in Dortmund.

The use of computer modeling of structures continues to be integral to the field of resonator development where computer simulations probe the relationships between sample properties and electromagnetics using boundary-value numerical methods such as finite-element modeling mixed with analytical models. This field of study represents an interface between electromagnetic theory and laboratory experiments.

Using commercially available programs, such as Ansys High Frequency Structure Simulator (HFSS), the EPR signal intensity can be calculated and compared to other designs [2]. These "computer experiments" save hours of bench time and allow one to design resonators, not only for general-purpose experiments, but also for specific applications and samples.

Along with numerical computation, ultrahigh precision machining techniques such as

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electric discharge machining (EDM) allow for the fabrication of complex structures that are not feasible with traditional fine-mechanics. EDM has positional tolerances of 0.001 microns with features as small as 0.03 mm. Since wire-erosion EDM and die-sink EDM is generally considered a no-force machining, small feature become practical.

This increase in precision and tolerance enabled the W-band (94 GHz) loop-gap resonator [3]. When the complexity goes beyond that of EDM or traditional fine mechanics, electroforming can be used. For instance, complex designs such as corrugated waveguide or hyperbolic tapers for reduction of waveguide insertion loss at high-frequencies. In the design of hyperbolic tapers, wire-erosion EDM was used to create the aluminum mandrel that was electroformed [4]. Finally, as new technology in 3D printing emerges, the transfer from computer design to fabrication becomes even more straight-forward. The next generation 3D printers allow for fine-resolution (0.05 mm) fabrication with complex shapes formed in ABS plastic that can be silver-plated [4]. Currently, commercial 3D printing manufactures, such as ShapeWays (http://www.shapeways.com), also provide the ability to print a wax mold and form a solid-silver geometry. The resolution and tolerances of ShapeWays is good enough for Q-band loop-gap resonators.

Due to the advancements of computer-aided modeling and fabrication techniques, resonator development has moved from generalpurpose resonators for commercial viability to application-specific resonators. At the Medical College of Wisconsin, I started my career in designing resonators for aqueous samples. It would have been simple to engineer new resonators and only increase the number of resonators, not the underlying technology. Instead, my colleagues and I strived for fundamental understandings to the relationships between microwave cavities and the EPR sample. For instance, an in-depth paper was written on microwave leakage issues caused by mode coupling in a TE_{011} resonator with a round iris [5]. This new understanding of modes eventually led us to the superior long-slot capacitance coupling [6]. From the mixture of analytical and numerical modeling, an understanding of the synergy between the waveguide-to-iris-to-resonator can be established.

At the Max Planck for Chemical Energy Conversion I am combining my experience under Prof. Hyde with a new exciting field of biological hydrogen conversion. The hydrogenase catalytic cycle has various redox states and several are paramagnetic. By studying these states we can obtain the basic understanding of the role of abundant transition-metals (Fe and Ni) in hydrogen conversion [7]. The use of single-crystal proteins allow for the disentanglement of angular dependencies of g- and A-tensors and gives insights into molecular interactions at the active site by relating to the X-ray Crystal Structure. It is also important for the understanding of Quantum Chemical Calculations of the catalytic mechanism using the full g-tensor axis. EPR tensor data helps develop the calculations which can yield insights into the catalytic activity.

Single-crystal work on the [NiFe] hydrogenase has been performed with great success and provides the experimental methodology for my work [8]. However, crystals of [FeFe] hydrogenase are 10–50 times smaller in volume comparted to [NiFe] hydrogenase crystals. Because of this significant volume limitation, to date no single crystal studies have been performed on [FeFe] Hydrogenase using EPR at X-band. Using FTIR, EPR, NMR, Raman, and NRVS a convincing catalytic cycle of [FeFe] Hydrogenase has been hypothesized. However, it is very difficult to hypothesize the F-clusters and *g*-tensors axis, and therefore, single-crystal protein studies are needed.

The use of planar micro-resonators (PMR) is promising technology [9] to increase the sensitivity for volume-limited samples. By decreasing the overall size of the resonator the efficiency parameter can be significant increased (2.4 mT/W^{1/2}), while maintaining a good Q-value (approx. 190), yielding an increased signal by a factor of 3 compared to the Bruker MD5 dielectric resonator is possible. However, due to the planar geometry, the B_1 distribution tends to be non-uniform over the sample volume, leaving room for improvement.

In order to increase the magnetic field homogeneity and increase EPR signal intensity, I am proposing the use of a self-resonant microhelix. This 6 turn, 0.4 mm I.D., and 1.2 mm length resonator provides a strong B_1 field (4.2 mT/W^{1/2}) with a much more homogeneous magnetic field. The new micro-helix geometry increases the B_1 by a factor of 2 and the Q-value (approx. 360 for self-resonant micro-helix) by a factor of 2. Moreover, the 1.2 mm resonator length provides easier sample placement.

The self-resonant micro-helix is coupled inductively by a resonant loop. The coupling scheme is directly related to a recent MRI surface-probe development where the coupling of two resonant modes provides an impedance transformation which increases the MR signal intensity due to the change in magnetic susceptibly during resonance condition [10]. This work was introduced at 400 MHz and through the design of the MRI surface probe and coupling a factor of 8 was theoretically and experimentally shown.

By using a resonant coupling loop, placing the micro-helix at a point of maximum mutual inductance, and critically coupling the microhelix one can theoretically gain another factor of 2 in EPR signal intensity. Overall a theoretical factor of 24 compared to the Bruker MD5 dielectric resonator for a volume-limited sample of $0.3 \times 0.3 \times 0.3$ mm³ is possible. Preliminary results show a factor of 15 with room for improvement. Overall, this technology opens up the possibility to do single-crystal protein work on [FeFe] Hydrogenase and other volume-limited samples, such as materials research, samples



of limited availability, and even systems on a chip/microfluidics.

With insights gained from previous experience, near-field antenna research, and computer-guided optimization (such as genetic algorithms), I believe application-specific resonator development remains a fruitful research topic. I look forward to working with many of you as micro-resonator technology develops further. Please follow my work at http://act-epr.org.

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IES Young Investigator Award 2016



Sergey Veber:

First of all, it is my pleasure to thank the International EPR Society for such a high evaluation of my scientific results. Without exaggeration, this is the highest award I ever received to date. This award means the responsibility for the current research and also implies certain expectations for the future one.

When attending the international EPR conferences, I was always impressed by the activity of the International EPR Society and the local EPR societies. Such activity accelerates the progress in EPR, initiates joint projects and makes the EPR community more visible. Interestingly, for the first time I presented my EPR results at the 3rd EPR Summer School of EFEPR in Wiesbaden, Germany and I was greatly impressed by the highest level of its organization and the participation of top EPR experts. I would say that the size of the EPR community and the versatility of EPR are optimal for a fruitful performance of the IES and relevant societies: the EPR community is not too large and all active scientists know each other; on the other hand, it is not too small and there is place for the fantastic variety of developed approaches and objects under the study to flourish.

In this multi-faceted world of EPR spectroscopy I was mainly focused on the application of EPR to the investigation of thermo- and photo-switchable magnetoactive Cu(hfac)₂L^R compounds based on nitroxide radicals (L^R) and copper(II) ions. Although we cannot apply the pulsed EPR techniques but we can use only the continuous-wave and time-resolved EPR technique, the bistability of such complexes is an appealing property which attracts me so far. Starting this project as early as in 2006, we published more than 20 articles on EPR spectroscopy of these complexes. As the result, we understand EPR of temperature-induced magnetostructural transitions in Cu(hfac)₂L^R, and also discovered the ability of Cu(hfac)₂L^R to photoswitching at very low temperatures (T <25 K) to the metastable state. At the present time we continue to investigate the metastable state of photoswitchable copper(II)-nitroxide complexes aimed at revealing the relationship between their chemical structure and the temperature stability of the photoinduced state. We also develop approaches for the manipulation with light of the magnetostructural state of $Cu(hfac)_2L^R$.

I would like to use this happy opportunity to thank near and dear people who helped me during the last decade and thus enabled these investigations. First of all, I thank my supervisors Prof. Elena Bagryanskaya and Prof. Matvey Fedin who guided me during my studentship and with whom I gladly cooperate at the present time. Elena is an outstanding supervisor with extremely high internal standards and all-embracing care of people around her. She understands the supervision in a comprehensive way and takes into account not only the scientific success of a student but also understands his internal problems. I dare say that on this side it is important a student salary, which is not very high, can be increased to a reasonable amount only due to supervisor's efforts who should spend a lot of time applying to different foundations for additional money. In my case I could concentrate solely on the research without thinking on money problems. I am grateful to Elena very much for that. Although we have no close collaboration over the last few years, I am infinitely grateful to Elena for her impact on my development not only as a scientist but also as a personality.

Matvey Fedin, who is head of the laboratory I am currently working at, was my PhD supervisor. It is a pleasure for me to continue my collaboration with him. Having a lot of new ideas he initiates and develops a large number of projects. However he never restricts my activities to the participation only in these projects but also lets me have free time for the implementation of my own ideas. Moreover, as head of a lab, he shields me from the bureaucracy obligations releasing some more time for new projects. Of course, I am not the only person who was lucky to work in this team: I am sure that more than 20 former students who worked together with Elena and Matvey have similar memory.

Awards

Елена Григорьевна, Матвей, большое вам спасибо за потраченное на меня время, очень это ценю и дорожу отношениями с вами.*

Almost a half of research mentioned above was carried out within the international collaboration. The possibility to perform research at the high-level world-known EPR laboratories gave me the precious practical experience and the chance to communicate with distinguished scientists, which I consider as a prerequisite for every student in order to find his/her own way. I'm thankful to Prof. Klaus Mobius and Dr. Anton Savitsky, to Prof. Daniella Goldfarb and Dr. Alexey Potapov, to Prof. Wolfgang Lubitz and Dr. Edward J. Reijerse, to Prof. Klaus Lips and Dr. Alexander Schnegg and to their colleagues I was working with during my visits to their laboratories. The opportunity to use unique equipment there allowed me to obtain high-level new experimental results revealing the processes taking place in the studied compounds. Again, these close collaborations were possible due to personal contacts of my supervisors with colleagues abroad, which is partially the result of the IES activity. The novelty of my research is due to the originality $Cu(hfac)_2 L^R$ magnetoactive complexes I study. This type of the complexes is synthesized at the International Tomography Center. I am most appreciative of Prof. Victor Ovcharenko and his colleagues at the laboratory of multispin coordination compounds for the close collaboration over these years.

And last but not least, I am infinitely grateful to my wife Veronica Veber, whom I love very dearly, for supporting my activity all these years and for our two daughters (and I still hope for a son in the future).

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^{*} Elena Grigor'evna, Matvey, thank you very much for your time, I really appreciate it and cherish the collaboration with you.

Anniversaries

Celebrating the 65th birthday of Prof David Collison



This issue of the IES newsletter in part celebrates the 50th Annual International Conference of the Royal Society of Chemistry ESR Group, which was held in Oxford earlier this year. This isn't the only notable anniversary in UK EPR this year - my friend and colleague Prof David Collison celebrated his 65th birthday in March. The IES newsletter has a nice tradition of marking such events and Laila Mosina suggested that we ask David to write something in celebration of his career. My problem with this was that I knew David would be far too modest to write such a thing. This was resolved by (i) David instead agreeing to write a Future-Meets-Present piece for this issue, and (ii) me writing a bit about David's career, which he won't know about until he receives this issue in the post.

David has made many important contributions to transition metal, and inorganic more generally, EPR. He was born in 1952, the same year in which Bleaney and Bowers published their landmark EPR paper on the "anomalous paramagnetism of copper acetate" [1] – this was obviously a portent! He graduated with a BSc in Chemistry in 1976, then a PhD in 1979, both from Manchester. Surprisingly, EPR was not involved at this stage - his doctoral work involved polarized single crystal electronic spectroscopy of terminal-oxo and -nitrido coordination compounds. He picked up EPR in a post-doctoral spell with Frank Mabbs, again in Manchester, where he wrote what was amongst the first matrix diagonalisation software for spin >1/2 species driven by the need to model the EPR and magnetic properties of biologically relevant FeS and FeMoS clusters and nitrogenase [2]. In 1984 he was awarded a prestigious Royal Society university research fellowship, to stay in Manchester (for a Lancastrian he seems quite fond of the place) where he ultimately rose through the ranks to a personal chair. In early work he extended his passion for single crystal spectroscopy to EPR, and the use of multiple frequencies, probing low symmetry effects in $Mo^{\hat{V}}/V^{IV}=O$ compounds [3] including weakly exchange coupled systems [4]. Some imaginative chemistry was developed to enable this work, e.g. using ${GaCl}^{2+}$ as an isomorphous host for $\{VO\}^{2+}$, or $\{SnCl\}^{3+}$ for $\{MoO\}^{3+}$. The driver for much of this work was bioinorganic chemistry (including work on multi-copper enzymes) [5], and together with Mabbs and Dave Garner, important developments were made in molybdo-oxido/sulfido chemistry, and metal dithiolenes, leading towards the pterin cofactors of molybdo- and tungstoenzymes [6]. Other notable work included the identification of the chemical nature and electronic structure of amavadin [7], the nonoxo vanadium(IV) species found in Amanita mushrooms. David also became significantly involved in the use of XAS and EXAFS to probe metal coordination environments, modeling copper corrosion inhibition, and the development of uranyl coordination chemistry.

In 1993, Frank and David published their textbook, a 1300-page treatise on transition metal EPR [8]. One novelty was the huge library of simulated spectra for S > 1/2 complexes to enable initial interpretation of experimental spectra. [I am reliably told that

Frank and David were initially commissioned to write "a short text on the chemistry of tungsten". To be fair, some tungsten(V) EPR spectra are mentioned on page 289.] He has been an important "father of the house" figure in the UK EPR community and, in my view, played a particularly important role in keeping interest in the technique alive in the UK during a spell when it was somewhat unfashionable. In 1995 he and Frank established the EPSRC-funded National Facility for EPR Spectroscopy, which is still going strong, providing a centre of expertise and equipment for multi-frequency EPR to the UK academic community. In the 25 years or so that I have known him it has been very obvious that his real passion has been in working with and mentoring young researchers, and he is rightly proud of the many scientists who have worked with him from undergraduate levels onwards. I was one of the beneficiaries of this, first meeting David around 1992 when I visited Manchester to do some Q-band measurements during my PhD (Manchester had one of only two Q-band spectrometers in the UK at the time, and the only one that worked!), then enjoying a post-doctoral spell with him and Frank Mabbs. I always appreciated his (near) infinite patience, good nature and enthusiasm. It has been a pleasure to collaborate with him over the years since then, and I am still learning from him. So, many happy returns David, and thanks for all the tea and biscuits!

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Eric McInnes



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Looking Backward – How EPR research was done 65 years ago

Harvey A. Buckmaster, IES Fellow

Thad intended to write about the events L that led to my development of the first high frequency magnetic field modulation paramagnetic resonance (PMR) spectrometer on the 50th anniversary of its successful demonstration but various health and other problems intervened. The original nomenclature PMR became electron paramagnetic/spin resonance (EPR and ESR) when commercial instruments became available. When I started to draft an outline for this manuscript, I realized how much doing physics research has changed since the 1950's and that it would be very difficult for younger researchers using EPR spectroscopy to appreciate the problems I encountered unless I explained how much this technology has changed since then. This article attempts to combine those elements of the state of the technology that existed in the early 1950's which were relevant to my research with those autobiographical details that spanned the period from the summer of 1952 to the end of 1955 that played some role in enabling me to make a significant contribution to the design of PMR spectrometers. Earlier personal educational and economic information is also included to help set the stage. The PMR spectrometer that I designed and built had a sensitivity that was greater by a factor of about hundred than any previous PMR spectrometer and it was the first PMR spectrometer in Canada.

Vacuum tube technology was still used in all electronic instrumentation during the 1950's. Researchers had to design and construct almost all electronic instrumentation. Commercial oscilloscopes and multimeters were only just becoming widely available but expensive and their frequency range was very limited. The WWII development of radar had accelerated the demand for and evolution of such instrumentation. For example, Cossor, an old British electronics company, who had made the first TV's in the 1930's, introduced the first split beam oscilloscope after WWII in 1946 but its upper frequency limit was less than 100 kHz. Single beam oscilloscopes were first manufactured in the U.S.A. by Dumont starting in 1943 but by 1960 Tektronix held a commanding position in this area of instrumentation. The first multimeter, called an Avometer (amps, volts, ohms), was developed in England in 1927. It was rugged and flexible but rather bulky and heavy and only became widely available when the Model 8 was marketed 1946. This model was produced until 2008! Large spring clips were used to attach the Avometer to the circuit under measurement but were too bulky to attach to semiconductor circuitry.

Although the point contact germanium transistor had been demonstrated in 1947, low frequency transistors only started to become available commercially in the late 1950's and silicon transistors with higher frequency performance were unavailable until the 1960's. Commercial instrumentation using semiconductors did not appear until the 1960's. The transition from high voltage, low current devices to low voltage, high current devices had many ramifications for EPR spectrometer design. Probably the most important was in the design of the electronic control circuitry for the electromagnet as the energizing coils which had been previously designed using a large number of turns of about #12 diameter insulated copper wire to carry a current of a few amperes now became a small number of turns of copper tubing insulated to carry a high current for use with high current transistor control circuitry. Cooling problems also required different solutions. Early microwave detector diodes using a wire whisker point contact germanium where replaced in the 1950's by point-contact semiconductor diodes that were more stable and reproducible. However, their low frequency noise spectrum was not known nor studied. The development of transistor technology enabled more sensitive and reliable microwave detectors to be manufactured.

It was the norm that, when physicists, pioneer a new area of research, the specialized instrumentation required had almost always been designed and constructed in-house. When an area such as EPR has matured and its application has become of sufficient interest to chemists and biochemists, then commercial instrumentation becomes economic to market. Physicists who continue to work expanding the frontiers of this field will frequently use some commercial instrumentation when appropriate as well as designing and building what they need since making new or more precise measurements requires innovative instrumentation. Some physicists choose to become metrologists in their area of specialization. I became a metrologist in several areas of microwave technology as a consequence of doing the research described in this paper while continuing to be a theoretical and experimental physicist.

I started to do a PhD in physics at the University of British Columbia (UBC) in Vancouver, BC in the summer of 1952 after completing an MA in applied mathematics at UBC. I had received a BSc (1 Hon) in mathematics at the University of Alberta in Edmonton, AB in 1950 but had taken an equal number of mathematics and physics courses. I slowly realized that I had developed a significant skill base to do research in physics because I had obtained an amateur radio licence in 1946 and was skilled in wood and sheet metal working as well as in photography. I was able to save sufficient funds from what I earned in my photography business to put myself through an undergraduate degree provided that I had a summer job each year and was able to save about \$400. This was necessary as my parents could not afford to send me to university although my mother tried to send me \$10 every month for spending money. Originally, I was interested in a career in mathematics or theoretical physics because I thought that one kept ones hobbies separate from what you did to earn a living. This idea probably came from my mother who considered hobbies as something for children but not adults. After graduating with my BSc in the spring of 1950, I spent the summer working at the Canadian atomic energy laboratory located at Chalk River, ON. I had expected to be assigned to the theoretical physics group but my supervisor, John Bayley, gave me the task of designing and constructing an omegatron. He was amazed by what I had been able to accomplish in the four months that I worked with him and urged me to consider a research career in physics rather than mathematics. He told me he had chosen me on the basis of my hobbies I had listed in my application!

Since I had been awarded a teaching assistantship from the UBC mathematics department, I felt that I should continue along the mathematics route. It paid \$900 for teaching one class of Mathematics 101 and running a remedial mathematics laboratory the first year and \$1100 for teaching two sections of Mathematics 101 the second year. I also received an NRC Summer Student grant of \$400 for the four summer months of 1951 to do my thesis research. This was sufficient to enable me to live in one of the UBC residences which cost about \$80/month room and board with

a single room. After completing two years of graduate level mathematics courses and my MA thesis, I concluded that I was more creative in physics than in mathematics although my thesis yielded a publication which was not then the norm.

I was fortunate to be awarded a National Research Council of Canada (NRC) graduate scholarship valued at \$800 for the winter eight months and \$400 for the summer four months of 1952/3. After a disastrous initial start with another supervisor, Dr. H.E.D. Scovil (Derek), who had just joined the UBC physics department after completing a D. Phil at Oxford in Professor Bleaney's pioneer paramagnetic resonance spectroscopy research group, persuaded me that I should become his PhD student. I felt wanted and the research area intrigued me so I accepted his proposal. It was an excellent decision and I prospered working with him. I have always felt very indebted to Professor Arthur Crooker, an optical, UV and IR spectroscopist at UBC, for encouraging this union as he had a great faith in my intellectual and research skills. He also provided me office space in his research laboratory until I got my life sorted out after my above mentioned unfortunate initial start.

When I became Dr. Scovil's graduate student, I was assigned laboratory space was the northeast quarter of a large room (#100) in the basement of the Henning Physics Building under a large lecture theater. Initially, there was nothing in this space except a desk and

the classic layout of wooden cabinets with glass window doors on the north and east walls above a counter with a sink over lower storage cabinets. The space to the west had been used by a Ph.D. student of Professor van der Ziel who had constructed a microwave gas absorption spectrometer for the 18 to 26 GHz K-band to measure the ammonia gas absorption spectral lines near 23 GHz. He had built all the instrumentation and waveguide components himself as commercial microwave components were then not available although microwave flanges and copper waveguide was available. This student had fabricated microwave attenuators, directional couplers, tunable microwave diode mounts and waveguide elbows using 0.25"×0.50" copper waveguide and the design data in the volumes of the MIT Radiation Laboratory series of books that summarized everything that had those working there been learned

about radar during WWII. This gas absorption spectrometer used a 23-26 GHz 2K33 reflex klystron and a high voltage power supply that he had designed and built. I was told that I could scavenge any components that were not in use but that I could not remove anything from the spectrometer which was to remain operational. Fortunately, a spare high voltage klystron power supply existed so I could use this unit when I started to construct an EPR (PMR) spectrometer. There were also several other invaluable pieces of instrumentation available including a tunable K-band wavemeter with an accuracy of about 0.05% and a wartime signal generator which operated up up to about 40 MHz.

My supervisor was convinced that the sensitivity of a paramagnetic resonance (PMR) spectrometer could be increased if a way could be found to get the high frequency magnetic field modulation inside the microwave resonant cavity where the sample to be studied was mounted. At Oxford, Professor Bleaney's group used the 50 Hz UK power line for this purpose. The use of higher modulation frequencies was limited because of the Foucault current that it induced in a conductor decreased the field inside a conductor and also caused vibrations and heating. Some of the group knew from their wartime experience in the development of radar systems that microwave radar systems using a superheterodyne detector and an intermediate frequency of 30 MHz were very sensitive. They had built a superheterodyne



PMR spectrometer but were unsuccessful in solving the instability problems that arose because the signal reflex klystron had to be kept tuned to the cavity resonant frequency after it had been cooled to liquid hydrogen or helium temperatures and the local oscillator reflex klystrons had to track these changes to generate the 30 MHz intermediate frequency. This approach proved to be unsuccessful and was abandoned. There was also no information about the noise spectra of the microwave 1N21, 1N23 and 1N26 detectors for 2-4, 8-12 and 18–26 GHz waveguide bands available since this was not a problem at 30 MHz. The fact that all semiconductor diodes exhibited a 1/f or flicker noise spectrum at low frequencies was not known as mentioned above.

I started by building a simple 24 GHz transmission resonant cavity spectrometer using the information in Dr. Scovil's thesis as a way of learning about microwaves since this was the design used in Oxford and most of the components were available. I could not proceed further until I had an electromagnet which could create a magnetic field of at least 0.9 T (~9,000 gauss) in a 5 cm air gap anticipating that I would need this gap for a double glass dewar to be able to do experiments at liquid helium temperatures (4.2 K). There were no spare electromagnets available in the physics department and Dr. Scovil's NRC (National Research Council of Canada) research grant was insufficient to be able to purchase a commercial unit. Moreover, the commercial mag-

nets that were available were not suitable for my purposes. Someone must have suggested to me that I should contact a local steel foundry to see if they could provide me with the steel billet that would be required to form the frame for an electromagnet. I carefully designed an electromagnet with 100 mm diameter, adjustable air gap pole faces that would meet my experimental requirements and took this design out to the Steel Company of Canada plant in Burnaby, a suburb of Vancouver, to meet with the manager. He turned out to be very helpful and offered to provide me with a billet of soft steel that could be milled into the dimensions in my design (see Figure 1). The machine shop in the physics department had only three people; one of whom only

Figure. 1. Photograph of electromagnet with a dewar in place.

did small projects. I knew that it would be a number of months before the physics department machine shop could start this job so I suggested to Alex Fraser, the head machinist, that he let me do the rough machining using a milling machine to accelerate the creation of my electromagnet. He agreed and had other machinist, Bill Morrison, show me to operate a milling machine and where to start. Bill kept an eye on what I was doing and did the final machining of the components

for the magnet. When all these components and the adjustable spacing magnet poles and shims were completed, an outside machine shop was contracted to make a large flat circular ball bearing base about 30" in diameter for the magnet to be mounted on so it could be rotated by 360 degrees. This feature would enable the angular PMR spectra to be measured and studied without having to rotate the sample under study. It enabled rotational PMR spectral measurements to be made much more accurately than was possible if the sample was rotated inside a microwave resonant cavity. The aluminum forms or spools for the wiring used to control the magnitude of the magnetic field also needed to be wound. By the end of August 1953, I was ready to test the electromagnet that I had designed and constructed using a proton nuclear magnetic resonance magnetometer I constructed using a marginal oscillator. It was a great relief that everything worked as designed as I could observe the spectrum of a DPPH g = 2 sample.

The modulation coils that I designed and constructed used a Bakelite coil former wound with coated copper wire were also fitted on the pole pieces. Plastics were still in their infancy. Bakelite had been available for a number of years and lucite was now available but Teflon



was just becoming available in rods, sheets and thin films. A recent innovation was the replacement of cotton woven insulation on wire by a flexible lacquer. It was possible to generate fields at frequencies up to a few hundred Hertz so I would be able to try and verify one of my supervisor's ideas. The major problem to solve was to design a 24 GHz resonant cavity which would allow low frequency modulation to penetrate its conducting walls. The first trials involved having one of the machinists make a brass cavity with a very thin wall where the paramagnetic sample would be located. These early trials showed that the basic idea was sound. I tried to make a cylindrical silver plated glass cavity with brass end pieces but was unable to get the joints sufficiently conducting to obtain a good microwave Q-factor. I was, however, able to study the attenuation of high frequency modulation signals inside this silver tube. There was no one at UBC who had any experience with making the high quality silver films that were required so this approach was discarded.

Scovil and I spent one long Saturday morning and afternoon in the fall of 1953 kicking this problem around and considering the various cavity mode configurations that might work. Somewhere in this discussion, we realized that

Figure. 2. Photograph of showing the spectrometer head with the H₁₁₁ mode slotted transmission cavity.

slots could be cut in in the cavity which would allow some modes to be excited without reducing the cavity *Q*-factor. This led to the conclusion that the cavity itself could be used as a half turn loop for the high frequency modulation generating current. A crude trial was attempted that indicated that we were on a winning wicket. The microwave current configuration

for a TE₁₁₁ or H₁₁₁ mode resonant cavity was chosen because it was possible to cut an axial slot without degrading the cavity Q-factor (see Figure 2). It took large modulation current to obtain the optimum sensitivity since the peak-to-peak current had to be equal to a half line width of the resonance to be studied. We did not know anything about the noise spectrum of the 1N26 microwave diodes so chose 455 kHz since this frequency was used as the intermediate frequency in AM radios so 455 kHz transformers were available for use in the preamplifier. One further problem remained. The large modulation electromagnetic fields created made it very difficult to detect a resonance as it was swamped by leakage from the generator and loop system so both the 455 kHz high power rf generator and the microwave detection system needed to be very carefully shielded (see Figures 3 and 4). This problem was solved by putting the rf generator in a brass box and the microwave detector and the 455 kHz amplifier in another brass box but insulated from this box. It was found that the leakage through the lid of the detector brass box was still a problem although the level was now much lower. Using a sheet of aluminum foil as a gasket yielded inconsistent results. Eventually, it was found that



tightening the screws for the lid systematicly from one end solved this final problem as this eliminated micro buckles in the brass lid (see Figure 3). Ground loops were another serious problem as 60 Hz interference and noise leads to inconsistent results. Breaking ground loops required using ungrounded two-wire rather than three-wire AC plugs and sockets but there were always other more subtle sources of such ground loops to remove so one became an expert in "cleaning" up the "noise" in an instrumentation system. Ground loops

in the microwave components were broken using thin Teflon sheets and lucite screws.

Such problems are rarely a problem with contemporary semiconductor instrumentation.

The first measurements of an EPR spectrum for a few percent Gd³⁺ ions in lanthanum ethyl sulfate at room temperature confirmed that the sensitivity had been increased by a factor of about hundred. The observation of the $\Delta M = \pm 2$ and ± 3 transitions provided an excellent confirmation of the sensitivity increase as the latter had not been detected previously and the $\Delta M = \pm 2$ had been observed only at orientations near 60° to the crystal symmetry axis. There were still hurdles to be overcome as most measurements would be made at liquid nitrogen or helium temperatures. Allowing the refrigerant to fill the microwave cavity was not a solution since microbubbles inside the cavity caused the resonant frequency to

fluctuate. Araldite, the first epoxy resin, had just become available so it was tried by filling the slot in the resonant cavity. Unfortunately, it was very brittle when set and cracked when immersed in the refrigerant. The heat generated by the rf current in the waveguide to and from the sample microwave cavity was minimized using German silver waveguide that





was silver plated on the outside. This waveguide was made using a tapered stainless steel mandrel to transform tubing into rectangular waveguide approximately 0.150"×0.300". This was a slow tedious job as the German silver was not very malleable. Inserting a length of rectangular Teflon bar into the German silver waveguide and tapered where it entered the air

Figure. 3. Photograph of isolated microwave detector in shielded brass box with lid removed.

filled copper waveguide also required great patience. Fortunately, the Teflon was self lubricating.

A thin wall flexible rubber tube sealed at one seemed to be a feasible solution. Human condoms or contraceptives were initially rejected as I assumed they would not be sufficiently strong to be stretched from the microwave resonant cavity to the top of the brass cap holding the dewars and where the waveguide exited but was insulated from the brass dewar cap. I learned that veterinarians used latex rubber bandages on horses after they were bred so I went and talked

Figure. 4. Photograph of the spectrometer head with the high power 455 kHz amplifier in shielded brass box.

to one. He gave me a bottle of liquid latex rubber to try but warned me that it would not be easy to make a smooth tube with the dimensions I needed. After many trials and failures, I decided, in desperation, to try a human condom. The first trial was successful even when it was stretched to over three times its normal length but I soon discovered that

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only one brand was made with natural rubber latex and it had fewer failures when immersed in liquid nitrogen!

The condom story would not be complete without noting that contraceptives were not displayed on the shelf in a drug store as they are today but kept in a drawer below the sales counter in a pharmacy. On request, the pharmacist would open this drawer so one could choose the brand to purchase. In order to be reimbursed for their purchase, I had to take the receipt to the secretary in physics department office who was responsible for the research grant petty cash. This became widely known in the university as it was a most unusual purchase! Social mores have also certainly changed enormously in Canada since the 1950's!

The Gd³⁺ measurements were repeated at liquid nitrogen (90 K) and again, I was able to confirm the sensitivity increase already discovered, It was now time to start to make the measurements for my Ph.D. thesis (see Figure 5). In reflecting on how I was able to achieve this sensitivity improvement, it seems evident to me that fate played a strange role since the components available to me in the laboratory were K-band 18-26 GHz (0.25"×0.50") waveguide. Had I inherited X-Band 8.2-12.4 GHz $(0.50" \times 1.00")$ waveguide, then many of the technical problems I have described above may not have existed or would have had completely different solutions. In fact, the knowledge that the sensitivity could be increased by increasing the modulation frequency immediately led quickly to the development of the cavity

Figure. 5. Photograph of the PMR(EPR) high frequency spectrometer with the author taking measurements.

design at 9 GHz that is still used. Like most new physics ideas, they are pregnant for some time until someone shows the way forward. I was fortunate to be the first person to find a solution to the EPR sensitivity at low magnetic field modulation frequencies.

Research in the 1940's and 50's focussed on designing and constructing apparatus and getting it to operate with reasonable stability for short periods of time during which measurements could be made. Today, instrumental design is a research field of its own and most experimental research is now focussed on making precision measurements that are repeatable and very accurate. It should not be forgotten that making advances in any area of science frequently involves the design and development of new more sensitive instrumentation or pioneering new approaches. These changes are not surprising as so many aspects of life today have changed due to digital technology, computers and the internet. The author hopes the reader will have gained some appreciation of the changes that have occurred in doing research today by reading about how the author did his PhD research in EPR spectroscopy over sixty years ago. Hopefully, other older EPR researchers will be stimulated to write about their early research experiences.

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Software



Magnetometry has been a mainstay of inorganic chemistry for the better part of a century and was chiefly important in the determination of molecular structure before the advent of X-Ray crystallography. These days, magnetic measurements occupy a rather more niche area, however as we venture further down the periodic table with heavy element chemistry [1, 2], realise ever-more

PHI – A user friendly spin Hamiltonian modelling package

Nicholas F. Chilton, School of Chemistry, The University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

complex polymetallic assemblies [3], or design molecules with staggering magnetic anisotropy [4], our preconceptions of magnetic properties and electronic structure begin to fail, and thus we rely on magnetic measurements to provide crucial information. Because of the thermodynamic nature of the magnetometry experiment, contributions from all populated states are observed which may result in a non-trivial problem that must be reverse engineered; thus, we inherently rely on modelling in order to extract information on the underlying electronic structure. Similarly, as EPR spectroscopists well know, deconvolution of EPR spectra by visual inspection is only possible for the simplest spectra and more commonly simulation is the only way to extract useful information.

The most common form of model employed to interpret magnetic or EPR measurements is the spin Hamiltonian. Initially, such Hamiltonians can appear bewildering to the untrained eye, but once the framework is understood the concept is deceptively simple and yet extraordinarily powerful. Such models derive from the full many-electron Hamiltonian, where knowledge of the radial wavefunction is dispensed and replaced with parameters, and the angular part is considered exactly. This approach is particularly suited to magnetism, as the magnetic properties arise from the angular part of the wavefunction. Thus, the angular momentum of quantum mechanics is the fundamental toolbox for working with spin Hamiltonians, providing a tangible gateway to understanding the practicalities of quantum theory. However, there are downsides of the parameterised spin Hamiltonian method; for example, the choice of basis states may not always be obvious, or sometimes the number of parameters may be too great. Therefore, packages for spin Hamiltonian modelling must be general enough to cope with complex problems, allow simultaneous modelling of data from multiple complementary techniques in order to avoid over-parameterisation, and be simple to operate for the end user.

Historically, there was a distinct absence of a single unified package for spin Hamiltonian calculations that allowed modelling multiple experiments with a flexible Hamiltonian. Most codes also required other software or special expertise in order to operate, and few were freely available on the web. Therefore, PHI [5] was designed to fill this void, providing a freely-available and stand-alone spin Hamiltonian package that allowed anyone, anywhere, to model magnetic and spectroscopic data. It was also designed to be user friendly from the ground up, such that it was approachable by non-experts and amenable to teaching environments. To this end, an integral part of the program has always been the graphical user interface (GUI) that allows instant visualisation and exploration of simulated and experimental data (Figure 1). While PHI operates natively in Windows, Mac and Linux desktop environments, it is also a modern parallel code that can take advantage of high-performance computing infrastructure to distribute work using either the OpenMP or MPI frameworks.

Chief among the capabilities of PHI is the ability to simultaneously fit experimental data from multiple experiments with a single Hamiltonian. Whilst originally designed for magnetometry data, the capability list quickly grew to include magnetisation, magnetic sus-



Figure 1. Fitting a temperature dependent X-band EPR spectrum with an S = 3/2 zero-field splitting Hamiltonian.

ceptibility, the magneto-caloric effect, heat capacity and, importantly, EPR. As there were already very popular and efficient EPR modelling packages available, for example X-Sophe [6] or EasySpin [7], the EPR aspect of PHI was not designed to replicate these codes. Rather, the algorithm in PHI is distinct in that it simulates spectra using a "brute-force" method, similar to that employed by Weihe and co-workers [8, 9], considering transition probabilities between all pairs of explicitly calculated field-dependent eigenstates and does not rely on interpolation or extrapolation methods. The main advantages of this approach are that it makes no assumptions about allowed or disallowed transitions, implicitly includes looping transitions, allows for true frequency space linewidths, and permits simulation of multi-frequency data at no additional cost. The downside of this approach is that many explicit field strength and angular integration points may be required to avoid simulation noise for spectra of highly anisotropic species with sharp lines, which can result in very expensive calculations. Nonetheless, the utility of PHI for EPR simulations and fitting has been proven due to its quick uptake in the community and its use in the literature. In addition to the algorithmic benefits of PHI, there are also a variety of useful features for EPR simulations such as simultaneous multifrequency and multi-temperature modelling, anisotropic pseudo-voigt lineshapes [10], subspace perturbation methods, and anisotropic strain implemented for all spin Hamiltonian parameters. Development has been continuous since the first version and there are plans to include inelastic neutron scattering (INS) simulations, perturbative hyperfine interactions, frequency-domain EPR and also to provide simulations employing the full d_n or f_n microstate basis. At only four years old

and with over 5000 downloads worldwide, the future is bright for PHI.

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The 50th Jubilee Annual International Conference of the RSC EPR Group April, 2017, Oxford, UK

The 50th Jubilee Annual International Conference of the RSC ESR Group was masterfully organised in April 2017 at Keble College of the University of Oxford by Prof Christiane Timmel and Prof Arzhang Ardavan. The conference has set two records in the history of the Group: by attendance (over 170 people from more than 16 countries) and by sponsor participation (19 companies and institutions). Through a heroic sponsor engagement effort, the organisers also managed to keep registration and accommodation costs at the same level as the previous conferences, despite Oxford being second only to Westminster in structural costs. Throughout the organisation and the smooth running of the conference, able assistance was provided by Dr William Myers, Dr Sabine Richert, Dr Alice Bowen, and numerous other members of the Oxford ESR community.



The location was splendid, the food delicious, the program interesting and intense, and the organ recital in the College Chapel by Matthew Golesworthy – a member of Professor Timmel's research group – very memorable. Even the notorious British weather decided to cooperate. The organisers have quite probably signed themselves up for doing the 60th Jubilee meeting too, in ten years' time. It was universally acknowledged that Doppler Effect looks very good on Chris Timmel.

Bruker Prizes

Since 1986, Bruker Corporation has generously sponsored an annual lectureship and prize, given to a scientist who has made a major contribution to the application of ESR spectroscopy in chemical or biological systems. After thorough deliberation and consultation within the academic and industrial ESR community, the ESR Group of the Royal Society of Chemistry informed Bruker that the outstanding scientist whose seminal contributions the members of the Group would like to recognise is, in fact, currently working at Bruker – we were very pleased to award the 2017 Bruker Prize Lecturer to Dr Peter Höfer, the inventor of 2D HYSCORE spectroscopy who has also made major contributions to the development of pulsed ENDOR techniques.

The other annual ESR prize sponsored by Bruker is the Thesis Prize, set up to recognise outstanding work by PhD students in the field of ESR Spectroscopy. The Committee received seven applications from students who had submitted their thesis in the previous two years. By reading the summaries and the support letters from supervisors and examiners, the Committee narrowed the field down to three submissions and then went through the considerable job of reading each thesis in depth. It was abundantly clear that the extraordinary scientific work by Dr Andrin



Doll of ETH Zurich, supervised by Professor Gunnar Jeschke, was the winner. A complimentary note on the margins was about the typographic quality of the thesis – the work could have been published as a book right there and then.

Bruker was a major force behind making the Conference a success: this being the 50th Jubilee meeting, the company has generously agreed to sponsor the participation of all past Bruker Prize winners who were able to come. The result was an extraordinary chance for the participating students and postdoctoral researchers to interact with the people who had defined modern ESR spectroscopy: Jack Freed, Thomas Prisner, Gunnar Jeschke, Daniella Goldfarb, Wolfgang Lubitz, Robert Bittl and others.

JEOL and IES prizes

In the long history of the RSC ESR Group, one of the best predictors of an excellent scientific career is the JEOL medal: many past winners are currently holding faculty posts at universities across the world. All student abstracts were considered for the short-list, the authors of the best five were invited to give a talk. It was very clear to the Committee that the masterpiece of microwave engineering presented by Jason Sidabras, of the Max Planck Institute in Mülheim, was the winner. A representative of the JEOL Corporation presented the medal during the drinks reception, much appreciated by the attending students, that the company also sponsored.

The International EPR Society has traditionally presented two poster prizes during the Conference Dinner: Claudia Tait was recognised for her work on ENDOR with band-selective shaped inversion pulses, and Maria Guilia Dal Farra was awarded the other prize for her poster on light-induced porphyrin-based spectroscopic ruler for nanometre distance measurements.

Scientific highlights

In the admittedly biased view of your intrepid correspondent, Monday morning was a highlight, with a very insightful talk from Stefan Stoll about pulse coherence effects in DEER spectroscopy and a stunning waveletbased data de-noising method described by Jack Freed – because wavelets are a natural basis for many types of ESR signals, the improvements are impressive indeed. All the usual brilliant suspects were also there: Graham Smith with further improvements in the hardware, Mark Newton with another detective-quality diamond story, the DEER/PELDOR gang with their proteins, nucleic acids and lanthanides, Ulrich Steiner with some interesting triplets, Sandra Eaton with the future of rapid scan EPR – one of the heavenly host of the previous Bruker Prize winners contributing their wisdom and insight. Keith McLauchlan has clearly discovered the secret of being eternally 65.

Committee

Graham Smith has retired from the Chair position after the statutory three years at the helm and received a warm laudation during the dinner speech by Eric McInnes, the current Chair. Dima Svistunenko, the organiser of the excellent Colchester conference in 2016, has also rotated off. David Norman, a very experienced past ESR Group officer, was persuaded by the Committee into first weighing the possibility of succeeding Fraser MacMillan as Treasurer in 2018, then into considering it in principle, and finally into accepting the very demanding and paper-intensive job.

Next conference

Maxie Roessler is organising the next conference at Queen Mary University of London between 8th and 12th April 2018. See http://www.esr-group.org/conferences/2018conference-london for further information.

Ilya Kuprov



Christos Pliotas

Christos obtained a BSc in Physics from the University of Athens before moving to Scotland for an MSc in Medical Physics at the University of Aberdeen. That is when he was introduced to the principles of magnetic resonance, under the supervision of David J. Lurie. He was then awarded a studentship from the Institute of Medical Sciences to pursue a PhD in Biochemistry in Ian R. Booth's lab, on membrane proteins and in particular potassium transporters. During this project he used Site Directed Spin Labelling (SDSL) and CW EPR spectroscopy, along with other biophysical methodologies to identify conformational changes occurring upon binding of activating/ inhibiting ligands to these transporters. For his postdoctoral studies, he joined the University of St Andrews, James H. Naismith FRS (structural biology) and Olav Schiemann labs (pulsed-EPR spectroscopy), where he focused on the mechanosensitive ion channel MscS.

In St Andrews, he employed x-ray crystallography along with multiple PELDOR (DEER) measurements to propose a new molecular model for mechanosensation based on MscS, a common mechanism for ion channel regulation. He was the recipient of the Royal Society of Edinburgh Research Fellowship Award 2015, and he is now a principal investigator at the Biomedical Sciences Research Complex, University of St Andrews, focusing his research on ion channels and mechanosensation.

new EPR Faculty

Pliotas group research focus is on integral membrane proteins, particularly mechanosensitive (MS) ion channels. Bacterial MS channels sense membrane lateral tension changes, mediated by lipids to protect the cell against severe osmotic shock and prevent cell lysis. In higher organisms they are involved in hearing, touch and cardiovascular architecture. Due to the their mechanosensing nature, in solution and absence of a lipid bilayer they adopt different conformations and oligomeric states, making their crystallisation challenging. In this concept PELDOR (DEER) spectroscopy combined with SDSL becomes an invaluable tool to identify and structurally characterize important protein's function states, under different stimuli/conditions, prior to crystallisation and maximise success. In addition, PELDOR offers the advantage of characterising structural transitions within lipid environment, a crucial parameter for natural mechanosensors regulated by membrane tension.

Pliotas group website: http://synergy.standrews.ac.uk/pliotas

new EPR Faculty



Chris Wedge

Christopher Wedge became a Senior Lecturer in Physical Chemistry at the University of Huddersfield in October 2016. Chris's first encounter with EPR was during a summer project with Prof. Geoffrey Luckhurst (Southampton), probing ordering of liquid crystals. Chris went on to receive his MChem and D.Phil from the University of Oxford, where his Part II (undergraduate project) and doctoral work in the group of Christiane Timmel developed zero- and low-field optically-detected EPR techniques. Through observation of radiofrequency magnetic field effects (MFEs) on radical pair reactions his work revisited fundamentals of magnetic resonance, testing the limits of the rotating frame approximation, observing the cross-over from time-averaged static MFEs to true resonant effects, and investigating radiofrequency spin-locking. Along with studies of a chemical compass molecule this work informed use of low-field EPR in animal behavioural studies seeking to verify the existence of a radical pair based avian compass. Chris stayed on in Oxford spending three years as a Stipendiary Lecturer in Physical Chemistry at St Hilda's College while carrying out postdoctoral projects which investigated molecular magnets as potential spin qubits and reduced MFE detection limits to femtolitre volumes.

In 2013 Chris moved to the University of Warwick as Taught Course Leader for the Integrated Magnetic Resonance Centre for Doctoral Training (iMR CDT), coordinating training in magnetic resonance for PhD students across six partner universities. During this time Chris established a number of fruitful collaborations applying EPR in various areas, some related to his interests in excited state systems such as photoactivated anti-cancer complexes and thermally populated triplet excitons, while others have developed his expertise in spin-trapping. Chris's current research focuses on hyperpolarization and time-resolved EPR, exploiting optically-polarized electronic systems to increase nuclear polarization and hence NMR sensitivity. Having recently demonstrated increased solution-state NMR sensitivity arising from radical-triplet pairs he is now working on increasing enhancements at higher magnetic fields. Chris has been a member of the RSC ESR spectroscopy group committee since 2015 and is currently the group's webmaster.



Maxie Roessler

I was born in the northern German city of Hamburg and grew up in vibrant and everchanging Berlin. Despite my affinity for roman languages in my early years (I lived in Italy and attended a French school), the UK has now been my home for over a decade. I feel lucky to have had the opportunity to complete my chemistry studies in Oxford (with a detour to Beijing for 1.5 years between undergraduate and PhD), a very special place in many respects and one where I first fell in love with EPR spectroscopy. I am now delighted to live in cosmopolitan London with my family and to work in the multicultural Queen Mary University (my current group members come from seven different countries!) in an exceptionally collegiate environment.

As a PhD student in the newly-established EPR centre at Oxford and under the supervision of Prof. Fraser Armstrong and mentored by Prof. Jeffrey Harmer, I primarily investigated hydrogenases – enzymes that are very efficient at interconverting protons and hydrogen using non-precious metals and that are thus of considerable technological interest. I became fascinated by the role that iron-sulfur clusters can play in catalysis and EPR spectroscopic investigations played a major role in the discovery of a new type of iron-sulfur cluster. At Queen Mary University, although I have ventured beyond the Fe and S elements, I continue to investigate iron-sulfur clusters in different enzymes. A major goal of my group is to unravel the "energy-coupling mechanism" of complex I – with the promise that an understanding of the mechanism may, eventually, facilitate tackling the many serious diseases that are associated with the dysfunction of this essential enzyme in respiration.



Nicholas Chilton

Nicholas F. Chilton is currently a Ramsay Memorial Research Fellow at The University of Manchester. Having started his research career at Monash University (Melbourne, Australia) in inorganic synthesis and characterisation of magnetic molecules, he ventured to The University of Manchester for his PhD under the supervision of Profs. Richard E. P. Winpenny and Eric J. L. McInnes. At Manchester he discovered the power of EPR spectroscopy for the investigation of the fine electronic structure of magnetic molecules, allowing the accurate experimental determination of the composition of the low-lying magnetic states. His research involves the use of multiple spectroscopic techniques (EPR, NMR, INS, optical) along with magnetometry to characterise novel magnetic molecules, specifically in the fields of single molecule magnetism, quantum information processing and magnetic shift/contrast agents. He is also heavily involved in the computational and theoretical aspects of molecular magnetism, having developed the leading tool for modelling of magnetic and spectroscopic data (PHI program, see elsewhere in this newsletter), and also regularly employing relativistic complete active space self-consistent field (CASSCF) ab initio methods to support and model experimental data.



Emma Richards

Emma Richards was appointed as a Cardiff University Research Fellow in April 2015. Prior to this, she was a Postdoctoral Research Associate working in the area of asymmetric homogeneous catalysis (2007–2015, Cardiff University). She gained her PhD in 2007, entitled "An EPR Investigation of Stable and Transient Oxygen Centred Radicals over Polycrystalline TiO₂". Emma studied for her BSc(Hons) Natural Sciences at the University of Bath (1999–2003), where she was awarded the Accenture prize for highest graduating student. To date, Emma has authored 48 peer-reviewed articles (citations 844; h-index 16), and two invited book chapters. She is co-author on the introductory level textbook "Electron Paramagnetic Resonance" in the Oxford Chemistry Primers series (OUP, published June 2016). She currently serves as a committee member on the RSC ESR Spectroscopy Group (2015-18).

Her research interests focus on utilizing the powerful technique of Electron Paramagnetic Resonance (EPR) spectroscopy and associated hyperfine methodologies (e.g. ENDOR and HYSCORE) in two main areas of activity: (i) investigating electron transfer processes in condensed matter materials of importance in visible-light activated catalysis, and (ii) determination of reaction mechanisms in homogeneous catalysis, through identification of on/ off-cycle intermediates.

Visible-light Photocatalysis is of fundamental importance in the fields of organic air pollutant remediation, water purification and energy production (in the form of H_2). In recent years, several strategies for improving photocatalysis efficiency have been developed, including metal/non-metal doping, dye sensitisation, and mixed-oxide hetero-junctions. Many of these strategies are aimed towards increasing the visible light absorption of TiO₂ or by increasing the lifetime of the photoexcited electron and hole charge carriers. It is well recognised that these charge carriers can migrate to the surface of the metal oxide, where they participate in redox reactions with surface adsorbed species, generating for example reactive oxygen species (ROS) responsible for organic remediation. Elucidating the mechanistic details of electron transfer processes over well characterised doped metal-oxides is a fundamental requirement for enabling rational design of novel, highly active, photocatalysts – EPR spectroscopy can provide a unique insight to the reaction pathways and intermediates generated under irradiation conditions.

EPR spectroscopy is an extremely versatile technique for determining homogeneous reaction mechanisms, which is important for the design and development of new active catalysts. The paramagnetic parent pre-catalyst, the activated catalyst itself or any resulting reactive intermediates, can all be monitored in-situ in order to delineate the role of the formal metal oxidation state and the influence of ligand structure on the resulting catalytic activity. We have recently focussed on the use of low valent transition metal complexes of formal oxidation states in cross-coupling reactions and ethylene oligomerisation. Our results demonstrate the utility of EPR to probe the structure-reactivity relationships in paramagnetic homogeneous catalysts, providing information not readily accessible by other techniques.

The group is equipped with cw EPR (X-/Q-/W-band), cw ENDOR (X-/Q-band), and pulsed EPR/ENDOR (X-band) facilities.





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and versatile technique for the characterization of paramagnetic species in many fields such as biology, chemistry, materials science, and physics. A thorough analysis of the EPR spectrum can provide an unparalleled and comprehensive description of the chemical identity, structure, symmetry, electronic properties, and dynamics of the spin system. Whilst many spectroscopic and physical chemistry textbooks may provide a short

Electron

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a powerful

Electron Paramagnetic Resonance Authors: V. Chechik, E. Carter, D. Murphy Publisher: Oxford University Press Series: Oxford Chemistry Primers No. of pages: 128, over 150 illustrations, Published: 14.07.2016, Paperback ISBN: 9780198727606, Price: £19.99

> section on EPR, and with several excellent advanced textbooks on the subject, there are few introductory texts available. This book is intended to be a useful entry level text primarily aimed at advanced undergraduate students and for postgraduate students and other novice users of EPR spectroscopy. The book focuses on explaining the basic principles and use of continuous wave (cw) EPR, with a strong emphasis on the interpretation of spectral parameters and how these can be linked to chemical and physical properties of the paramagnetic species. The first three chapters cover a brief overview of the theory and experimental methods in cw EPR. The next three chapters cover different aspects

of single electron spin systems, including isotropic-condition spectra of organic radicals, anisotropic-condition spectra in the solid state, and the intricacies of transition metals ions and inorganic radicals. Systems with multiple unpaired electrons are discussed and the spin Hamiltonian description of a rhombic S=1 system is analysed, in addition to a discussion of linewidth analysis. A brief overview of the type of information available through more advanced pulsed EPR techniques is finally presented. This book closes the gap between the content in general physical chemistry books and the many excellent advanced texts, and will prove useful to scientists working in biochemistry, materials science and catalysis who are increasingly using the power of EPR spectroscopy in their research. Author information: Victor Chechik, Reader, University of York; Emma Carter (now Richards), University Research Fellow, Cardiff University; Damien Murphy, Professor, Cardiff University.

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 and non-credit-card payment instructions for individual members on this Web site: www.epr-newsletter.ethz.ch/contact.html

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- Environmental toxicology
- Bioinorganic chemistry and more

Technical data

Sensitivity: 8 x 10⁹ spins/0.1 mT Magnetic field range: 5 – 600 mT

POSITIONS

Research Specialist Senior Position at West Virginia University

The Department of Biochemistry is searching for a Research Specialist Senior, with a strong background in RF/MW engineering experience. This position is available immediately and will be in the In Vivo EPR Multifunctional Magnetic Resonance center, Department of Biochemistry, Health Sciences Center, West Virginia University in Morgantown, WV. The selected candidate will assist Dr. Tseytlin in designing and manufacturing electron paramagnetic resonance (EPR) spectrometers and imagers. The position will be for one year in length, with a possibility of extension. The duties and responsibilities for this position are: designing, manufacturing, assembling, and experimental testing of EPR spectrometers and imagers. Applicants must hold a minimum of Master's Degree (or foreign equivalents) in Electrical Engineering, Physics or a related field and two years of experience, or a combination of education and experience. Qualifications must be met by time of appointment. All interested, qualified candidates should apply to jobs.wvu.edu with a cover letter of interest and current CV.

West Virginia University is an Equal Opportunity/Affirmative Action Employer and the recipient of an NSF ADVANCE award for gender equity. The University values diversity among its faculty, staff and students, and invites applications from all qualified individuals, including minorities, females, individuals with disabilities and veterans.

Postdoc in optical nuclear magnetic resonance, joint Los Alamos/UNM, USA

The quantum nanophotonics and biosensing lab at U. of New Mexico (PI: Victor Acosta) and the atomic magnetometer/NMR/MRI labs at Los Alamos National Lab (PI: Igor Savukov) seek a motivated postdoctoral candidate for a joint UNM/LANL project. The successful candidate will work on a highly multidisciplinary project that combines new techniques in optical nuclear polarization using NV centers in diamond nanostructures with low-field and optically-detected NMR/MRI. The goal is to develop a microfluidic platform operating at room temperature and low magnetic field which can deliver biochemical analytes with a nuclear polarization exceeding that possible using large superconducting magnets and/or cryogenic temperatures.

While working on the project, the postdoc will:

• Apply quantum mechanics, nanophotonics, and biochemistry to emerging new fields.

• Learn semiconductor nanofabrication techniques in world-class cleanrooms (CHTM, CINT).

• Work with partners in academia, national labs (LANL, Sandia), and industry (ODMR Tech).

The position will initially be based in Albuquerque, NM at the UNM lab. There the work will be focused on developing the NV hyperpolarization apparatus. Then the postdoc will transition to conducting NMR/ MRI experiments at LANL to characterize and optimize its performance.

A PhD in Physics, Chemistry, Optical/ Electrical/Chemical/Biomedical Engineering, or a related field is required. Experience in spin physics, biophysics tool development, and/or quantum optics is desired. Experience in magnetometry, semiconductor nanofabrication, and/or solid-state color centers is also helpful. Compensation is commensurate with experience and is expected to increase when work transitions to LANL. Candidates with very strong publication records will have an



opportunity to apply to highly competitive LANL fellowship programs. More information is available on our webpage. Interested candidates, please send Cover letter (describing research interests and career goals) and CV (with complete publication record) to Victor Acosta (vmacosta@unm.edu) and Igor Savukov (isavukov@lanl.gov). UNM and LANL are equal opportunity employers.

Postdoctoral Fellow

The Magnetic Resonance Spectroscopy group at Rensselaer Polytechnic Institute (RPI) is conducting cuttingedge research in the fields of solar energy transduction in natural and artificial systems and the development of novel materials and solar technologies. By performing fundamental and applied research, we work on sustainable solutions for major challenges facing energy and the environment. RPI is committed to the training of future scientists and engineers and is one of the oldest science and engineering universities in the United States. We are looking for a Postdoctoral Fellow for advanced multi-frequency pulsed electron paramagnetic resonance (EPR) spectroscopy of natural and artificial systems.

Your tasks

 Operation and further development of pulsed EPR spectroscopy experiments (including ENDOR, HYSCORE and transient EPR spectroscopy)

- Performance of experiments on redox proteins, metal oxides and thin films

– Analysis and numerical simulation of experimental data

 Presentation of scientific results at national and international conferences

- Publication of scientific results in international journals

 Scientific collaboration with graduate and undergraduate researchers at RPI

Your profile

You are a flexible team member able to work independently on different projects. You have

completed your PhD in chemistry or physics and have experience with pulsed EPR spectroscopy. A good command of various software tools enables you to analyze pulsed EPR spectra readily. You have active interest in experimental work with good practical skills and enjoy working in an interdisciplinary team. Your broad knowledge in physical chemistry and spin physics is a valuable asset to understanding the results of complex experiments. Good communication skills in English are required.

For further information please contact: Prof. K. V. Lakshmi

Department of Chemistry and Chemical Biology and The Baruch '60 Center for Biochemical Solar Energy Research Rensselaer Polytechnic Institute

Troy, NY 12180 e-mail: lakshk@rpi.edu lakshmi@baruch60center.org phone: (518) 698 7976

Please send your application materials to Prof. K. V. Lakshmi through e-mail correspondence.

Cryogenic EPR Postdoctoral Position

A postdoctoral position is available immediately for a collaborative project between Professor Cory's lab at The Institute for Quantum Computing (IQC) and a local startup. The project uses superconducting resonators and Optimal Control Theory (OCT) to increase the sensitivity of pulsed electron spin resonance at cryogenic temperatures. The goal of the project is to also demonstrate applications to molecularly thin samples. This program is expected to reveal new and interesting results of EPR of biochemical processes.

The successful applicant should have an advanced degree (PhD) in chemistry, biochemistry or physics with significant experience in EPR of biomolecules.

The appointment will be for two years with the possibility of renewal. The salary is competitive and commensurate with experience, ranging from \$55,000 to \$70,000. Women and minorities are encouraged to apply.

Apply to grum.teklemariam@highqlp.com.

Post-doctoral research associate

We are looking for post-doctoral associates interested in measurement/instrumentation development of EPR spectroscopy applied to energy and biologically-derived nanomaterials to join us at the Center for Nanoscale Science & Technology (http://cnst.nist.gov) at NIST, a highly interdisciplinary and very well resourced user facility. My laboratory contains a Bruker E580 EPR spectrometer (X-band) as well as a NIST-designed spectrometer (Q-band), both of which are equipped with arbitrary waveform generators for pulse-shaping. UV and visible CW lasers have been interfaced with the instruments to enable photoexcitation of samples. Current work is in the areas of spectroelectrochemical EPR spectroscopy development for solid catalyst materials and nanoscale structural measurements of biomaterials, including DNA-based nanomaterials. The ideal candidate would lead a project that makes use of the CNST nanofabrication capabilities as a means to provide meaningful EPR-based measurements. Typical successful applicants have a strong research background and academic record. Letters of reference are required.

Contact: Dr. Veronika Szalai phone: 301-975-3792; e-mail: veronika.szalai@nist.gov

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Old, but well maintained EPR Spectroscopist, with wide application experience, seeks opportunity to support active research group. EPR- based publications over 5 decades, most recently 2011, mass spectrometry publications to 2014. Experience in the study of transient organic and organometallic free-radicals; transition metal complexes; spin-trapping; spin probe; radical ions; matrix isolation and γ -radiolysis techniques; photocatalysis;



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Please Contact: Phil Barker pba02985@ bigond.net.au or pbarker@uow.edu.au to receive user logbook and publications list.

Postdoctoral Associateships in Magnetics at NIST

We offer postdoctoral opportunities in magnetics at the National Institute of Standards and Technology in Boulder, Colorado, USA. Annual salary is \$65,600 plus benefits. Appointments are for two years. Application deadlines are 1 February and 1 August annually (but inquire earlier).

The application process is competitive. Typical successful applicants have a strong research background and academic record. Letters of reference and an original research proposal are required.

U.S. citizenship and a background investigation are required (no exceptions). www.nist.gov/pml/electromagnetics/magnetics

EPR Specialist Position at Johns Hopkins

Postdoctoral or specialist (staff) position is available immediately to study membrane proteins at the Johns Hopkins University School of Medicine in Baltimore, Maryland, USA. We study conserved membrane enzymes with implications for human health (see Nature Chem Biol 8:759, eLife 1:e00173, and Nature Rev Micro 7:411), and are generously funded by the National Institutes of Health (NIH) and the Howard Hughes Medical Institute (HHMI). The project uses site-directed spin labeling (SDSL) with nitroxide probes to study the dynamics, distance measurements, and saturation kinetics with CW-EPR methods. The applicant must have at least 3 years of prior experience in SDSL, EPR, spectrum simulations, and distance measurements as evidenced by publications. Experience with membrane proteins is preferred but not essential. Position will come with generous salary and benefits, depending on experience and record of achievement. Interested applicants please send detailed CV and contact information for 3 references to rosanna@jhmi.edu.

Bruker BioSpin Corp

Bruker BioSpin Corp is looking for a highly motivated individual to join our EPR Service team to install and support high technology EPR Spectrometer Systems in customer research labs. This individual will install and service our EPR Spectrometer Systems and train customers for basic operation of the equipment. A BS in electrical engineering, electronics or related fields or equivalent experience is required. Experience diagnosing and repairing electronic, electromechanical and/or mechanical equipment is required. General understanding of analog electronics, digital electronics, high voltage circuitry/ circuits, microwave technology, vacuum technology, cryogenics; strong technical skills on analytical instrumentation required.

Please send resume, cover letter and salary requirements to bruker.jobseprfse0620@ bruker-biospin.com

EQUIPMENT

Wanted: Badly needed certain parts of, or even a complete Bruker X-Band microwave unit from the mid-seventies, the one which came with the Bruker B-ER 420 system. Particularly, the klystron heating and protection board, B-E-Z 10. Please contact Prof. Dr. Wolfgang E. Trommer, Department of Chemistry, TU Kaiserslautern, P.O.Box 3049, D-67653 Kaiserslautern, Germany. E-mail: trommer@ chemie.uni-kl.de.

EPR parts, electronics and hardware

Pulse generators, amplifiers, frequency counters, etc. We also offer X-band cavities, waveguide, klystrons, cells, etc. for Varian instruments.

Please contact techepr03@gmail.com for availability and pricing.

Design and construction of EPR electronics

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 kHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field-control units to voltagecontrolled scan operation. A 6-digit 1-ppm frequency counter is available in X-, C-, S-, L-band, or MHz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the University of Denver. **Please contact:** Richard W. Quine, e-mail: rquine@du.edu, phone: 1-303-871-2419

Available: Used Varian EPR equipment

(1) Varian E-104 EPR spectrometer with vertical style bridge and e-line fieldial. (2) Varian E-9 EPR spectrometer. Both available with warranty and continued service support. (3) Varian TM cavity with flat cell holders and flat cells. (4) Varian E-257 variable temperature controller with heater sensor and insert holder. (5) Varian E-272B field/frequency lock accessory.

Please contact: James Anderson, Research Specialties, 1030 S. Main St., Cedar Grove, WI 53013, USA. phone/fax: 1-920-668-9905, e-mail: janderson36@wi.rr.com







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