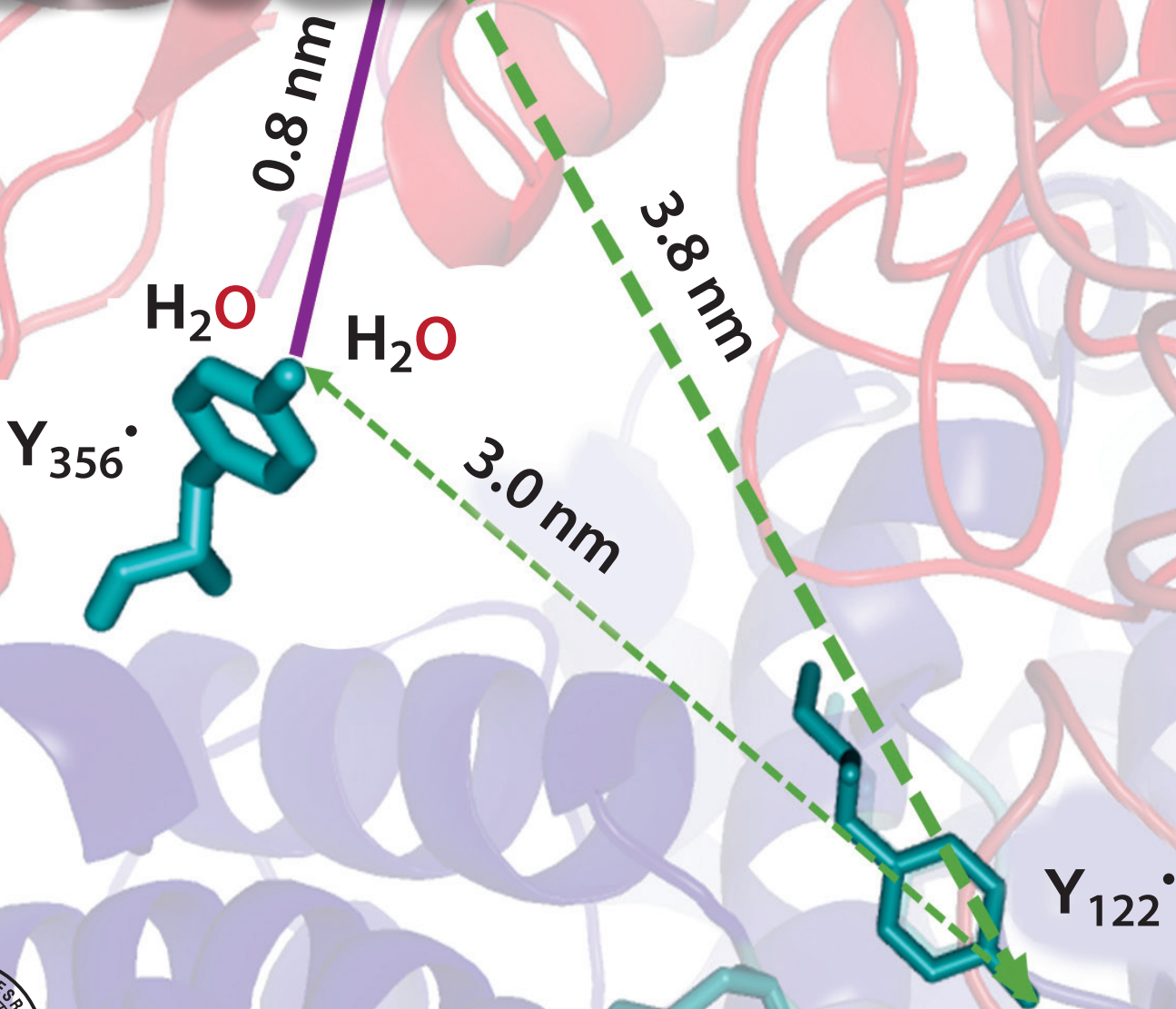


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2019

volume 29 number 3

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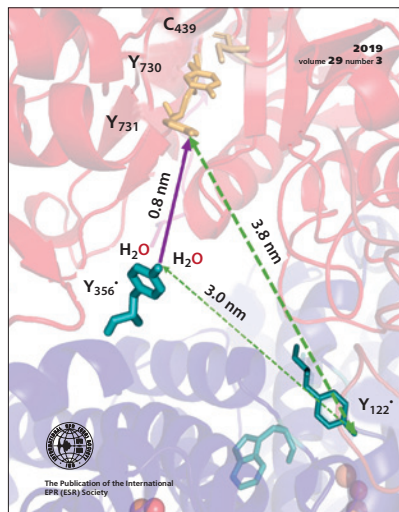
Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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The cover picture illustrates aspects of research carried out by Marina Bennati, recipient of the Bruker Prize 2019. It shows the transient tyrosyl radical intermediate generated in the catalytic cycle of *E. coli* ribonucleotide reductase, which is invisible in the X-ray structure. Distances determined by PELDOR/DEER and ^{19}F ENDOR spectroscopy were used to localize the radical whereas ^{17}O ENDOR revealed that the coordination to water molecules at the protein interface.

epr news letter

The Publication of the International EPR (ESR) Society

volume 29 number 3 2019

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by *Laila Mosina*

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Editorial

Dear colleagues,

Many winners of the prestigious magnetic resonance awards were happy to get the relevant awards for young researchers in the beginning of their professional career. And Marina Bennati, who is featured in this issue as the recipient of the Bruker Prize 2019 (the cover picture illustrates some aspects of her relevant research and you find her interview on p. 3), belongs to this cohort of outstanding researchers. In her interview, Marina mentions: "As I wrote at some occasion in the past, this was the best lecture I ever attended as a student and afterwards I decided to pursue this field." Not to keep you wondering, we give you an explanation of what occasion in the past is meant. In 2002, Marina won the IES Young Investigator Award and in 2013, she kindly agreed to contribute to the IES Young Investigator Award Revisited column (23/2, pp. 6, 7) with a story about her life before and after this distinction. In her current interview, Marina means this

very article. It was an exciting story about the many people who taught and inspired her, a breathtaking description of the research she carried out and an implementation of a motto "Never give up!"

It is good reading for the younger generation of the magnetic resonance researchers, e.g., for Daphné Lubert-Perquel (the Inaugural IES Best Paper award 2019, p. 4), Shunsuke Furuya (IES Young Investigator John Weil Award 2018, pp. 7, 8), and Motoi Kimata (SEST Young Investigator Award 2018, p. 11) and many others not yet featured in the newsletter. It is good reading and inspiring as well, the same as the interview of Larry Berliner, IES Fellow 2019 (p. 5), the article by Thomas Prisner about Michael Mehring, IES Fellow 2019, p. 6), and a success story by Hidekazu Tanaka (SEST Award 2018, pp. 9, 10).

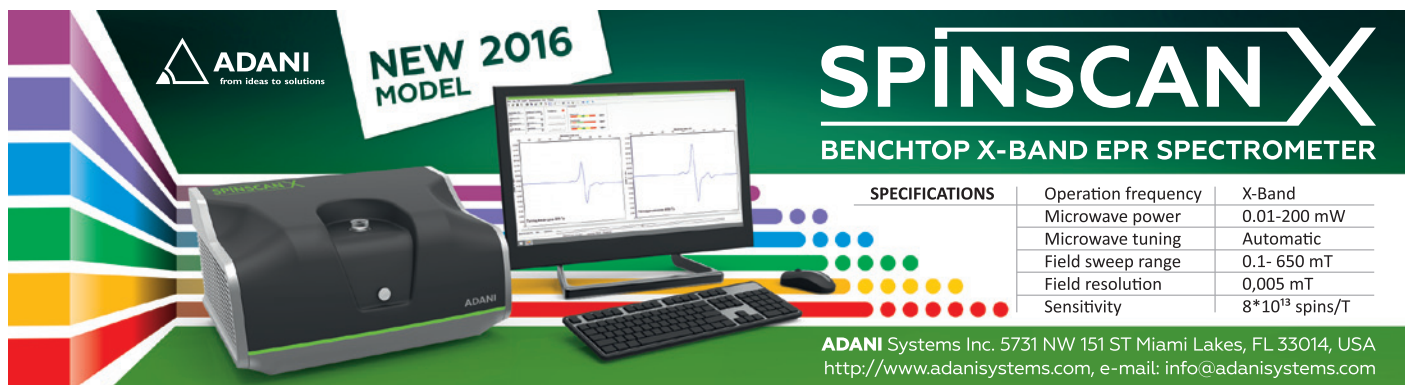
Two great dates being celebrated this year, 75 years of the discovery of EPR and 30 years of the IES, are often mentioned at the international conferences on magnetic resonance, e.g., at the 60th Rocky Moun-

tain Conference on Magnetic Resonance: EPR Symposium (pp. 21–23). The conference celebrated the 30th IES anniversary at the conference banquet with a special presentation, titled "EPR: Past, Current and Future", moderated by Thomas Prisner (IES President) and consisting of talks by Christoph Boehme (Physics/Materials Science), Gareth Eaton (Chemistry/Instrumentation) and Harold Swartz (Biology/Medicine). Moreover, Lawrence Berliner (University of Denver) was honored on his IES Fellowship. Tatyana Smirnova (North Carolina State University) was honored for many years of service as IES Treasurer. Dr. Arthur H. Heiss, one of the EPR community's strong supporters, was thanked by attendees of the conference for a half century of his activities in the field on the occasion of the transition from his position in Bruker, Patron of the IES. Undoubtedly, we all join in sending best wishes and heartfelt thanks to Art. More details will be published in the forthcoming issue of the *EPR newsletter*.

Laila Mosina



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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Interview with Professor Marina Bennati on the Occasion of Her Bruker Prize 2019



where I started learning spin relaxation theory. For the PhD, I moved to Michael Mehring's lab in Stuttgart. He offered me to work on pulse EPR and that is where my long career journey started. Michael has been a terrific magnetic resonance leader and teacher, without his supervision I would not have reached so far. I was particularly delighted to hear that he became the 2019 IES fellow!

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

This is not an easy question because I enjoy listening to or reading about different topics related to magnetic resonance. But perhaps what I like most is trying to understand the physical principle and the mechanism of an experiment, which has been a major driving force in my latest research. If I can describe experimental observations through physical models and catch their parameters with numbers, I feel that I come close to their essence.

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

Magnetic resonance is a fascinating, unique technique with multiple facets and powerful applications across all natural sciences. There is still so much to discover and improve. The new generation might expand applications on the one hand, but should also continue to develop our method repertoire, which is our strength. It is important to follow your own instinct and ideas, from which one can take motivation to search deeper and deeper. It is also important to be fair and recognize other people's merits. It has often been rather a team or community work than that of a single person, which has led to significant progress in science.

EPR newsletter: *Dear Professor Bennati, on behalf of the readers of the EPR newsletter we congratulate you on your Bruker Prize 2019. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

Since I was a teenager, I have always been curious to understand how nature works and fascinated by the micro-cosmos of molecules and atoms. For that reason, I considered becoming a scientist. Besides this, I grew up in a family, in which both parents were scientists and this had influence on my decisions. Many years later, I realized that a career in science is quite different from youth dreams, yet interest and dreams are most likely the best motivation. But it was the support and

the intellectual exchange with supervisors, colleagues and friends that finally made me pursue my career.

Who introduced you into magnetic resonance?

I became interested in magnetic resonance during my studies of physical chemistry at the University of Münster when I attended the lecture of Werner Müller-Warmuth on spectroscopy and magnetic resonance. As I wrote at some occasion in the past, this was the best lecture I ever attended as a student and afterwards I decided to pursue this field. Interestingly, Müller-Warmuth has been one of the pioneers in the field of liquid DNP but at that time I was not aware of it, now I'm discovering all his most fundamental work. For the Diploma thesis I joined his NMR group,

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The Inaugural IES Best Paper Award 2019



TAKEN BY THOMAS ANGUS (IMPERIAL COLLEGE PHOTOGRAPHER)

Daphné Lubert-Perquel:

I am honoured to have received the IES Best Paper Prize 2018 for the Nature Communications publication titled “Identifying triplet pathways in dilute pentacene films” [1]. This research was part of my PhD investigating the photophysical processes in molecular films, jointly supervised by Professor Sandrine Heutz at Imperial College London and Professor Chris Kay at University College London (UCL). The EPR measurements in this project were carried out at a variety of institutions: at UCL with Dr Enrico Salvadori and Professor Chris Kay, the Molecular Photoscience Research Center at Kobe University with Professor Yasuhiro Kobori, and at the University of Saarland with Professor Chris Kay. I would also like to acknowledge my studentship from the UK Engineering and Physical Sciences Research Council (EPSRC) with the Centre for Doctoral Training for the Advanced Characterisation of Materials (EP/L015277/1), which funded this research.

The aim of this project is to understand the effects of molecular aggregation and orientation on the triplet states and their dynamics in order to optimise thin film devices. Of particular interest is the singlet fission (SF) mechanism whereby a singlet excited state generates two triplet states of half its energy. The latter is critical for photovoltaic applications due its ability to overcome the Shockley-Queisser limit and achieve quantum efficiencies greater than 100%.

In this work, thin films of pentacene in p-terphenyl at various level of doping were grown via organic molecular beam deposition. The methodology was developed and refined resulting in a film design that can be extended to other compatible host-dopant systems for optoelectronic applications [2]. This system provides a unique material platform to fully exploit the capabilities of EPR spectroscopy. In our p-terphenyl/pentacene films, a complete rotation pattern was obtained using time-resolved (TR) EPR building on previous work using TR EPR on triplets in polymer thin films [3] and steady-state CW EPR on copper phthalocyanine thin films [4]. This experiment again demonstrates the efficacy of EPR for determining molecular orientation when other characterisation techniques are insufficient. In the films, two configurations of pentacene dimers could be identified, with differing zero-field splitting parameters and exchange couplings, which are recognised by the angle between the molecules, with pairs either in a collinear or herringbone arrangement.

The triplets generated by SF are strongly-coupled allowing population of higher-spin states, namely quintets, that can be uniquely identified using pulsed EPR spectroscopy to perform nutation experiments. Kinetic modelling of the TR EPR data enabled the elucidation of triplet dynamics according to the dimer geometries. Although this technique has been applied to SF previously [5, 6], this was the first time it was used for ordered thin films and at room temperature.

This orientation control and identification of dynamics according to a chosen orientation could be helpful for a broad range of research areas where EPR plays a useful role. From nanotechnology and molecular magnetism to biochemistry, this approach could be applied where decoupling the effect of geometry from the fundamental photophysics processes is important for resolving fundamental questions of structure and function.

Since completing my PhD, I have started a postdoctoral position as part of the US Department of Energy funded Center for Molecular Magnetic Quantum Materials, working with Professor Stephen Hill at the National High Magnetic Field Laboratory. The research I will be carrying out as part of this new venture will be focused on high-field EPR spectroscopy of molecular nanomagnets of potential interest for next-generation quantum technologies, in-

cluding measurements under external stimuli such as high-pressure and optical excitation.

1. D. Lubert-Perquel, et al.: Nat. Comm. 9, 4222 (2018)
2. D. Lubert-Perquel, et al.: J. Mat. Chem. C 7, 289 (2019)
3. T. Biskup, et al.: Angew. Chem. Int. Ed. 54, 7707 (2015)
4. M. Warner, et al.: ACS Nano 6, 10808 (2012)
5. M. Tayebjee, et al.: Nat. Phys. 13, 182 (2017)
6. L. R. Weiss, et al.: Nat. Phys. 13, 176 (2017)

Chris Kay:

Daphné Lubert-Perquel graduated with a Masters in Physics from the University of Exeter before gaining a place on the joint UCL/Imperial College *Centre for Doctoral Training for the Advanced Characterisation of Materials* in 2015.

As her PhD co-supervisor together with Professor Sandrine Heutz (Imperial College), I had the pleasure of working with Daphné on a project using time-resolved EPR spectroscopy to investigate the mechanism of singlet fission in thin films of organic semiconductors, which is the subject of the paper for which she was awarded this prize. Prior to her PhD, Daphné had experience neither of organic molecular beam deposition for the growth of thin films nor of EPR spectroscopy. It is, therefore, a testament to her dedication and intellect that she became an adept at both methodologies during her PhD.

In addition to her excellent writing, Daphné is a talented verbal communicator and has presented her work at multiple international scientific conferences and symposia as well as several outreach events. During her PhD, she developed and managed an outreach exhibit publicising our project to build a MASER (see Oxborrow et al. Nature 2012, Breeze et al. Nature 2018) which we presented at the Summer Science Exhibition at the Royal Society and London Science Museum in 2017.

Daphné is also an excellent team player and as such has developed links to other groups at UCL and Imperial College as well as with international collaborators, such as the group of Professor Yasuhiro Kobori at Kobe University.

Following a successful defence of her thesis, Daphné has recently moved to Tallahassee for a postdoc with Professor Stephen Hill at the Maglab working on high-field EPR spectroscopy of molecular nanomagnets. I wish her all the best for the next stage of her career.

Interview with Professor Lawrence Berliner on the Occasion of His IES Fellowship 2019



EPR newsletter: *Dear Professor Berliner, on behalf of the readers of the EPR newsletter we congratulate you on your IES Fellowship 2019. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I was always fascinated with magic and discovered that chemistry was used in lots of magic tricks and demonstrations. I started playing with chemistry sets and purchasing from a chemical supply house in order to explore more. Many of us who have indulged in this way in our childhood would not recommend that to young people today due to safety issues (several of us had “interesting” experiences that we wouldn’t wish on other people).

Who introduced you into magnetic resonance?

My introduction to magnetic resonance, particularly EPR, was a bit futuristic. In the summer after my last year as an undergraduate at UCLA I worked for the Chevron Research company, the large oil company based in California. At the time industry labs had very academic research; my supervisor was a Harvard graduate who had worked for George Kistiakowsky. We were studying the Semenov cool flame reaction and hydrocarbon oxidation. Amazingly, this involves free radical chemistry that we now understand quite well today.

I will never forget the PhD scientist who I worked with running EPR experiments for me as he had the name of an early American president, Dr. John Quincy Adams! To be honest, I never thought I would be involved in magnetic resonance after then.

I entered Stanford as a PhD student and was not completely interested in the faculty physical chemistry research that was apparent at the time. A friend told me that a new professor, Harden McConnell, would be joining the department the following autumn. My interest at the time was instrumentation which encompassed a major part of his research program. My first project was building a low-field (L-band) spectrometer to study phase transitions in charge transfers crystals at high pressure. About a year later, due to a mixture of circumstances, I decided to switch my research to something more biological. McConnell had just started to shift part his program into spin labels and he assigned me a project of my own. Little did I know that I would be involved in that field for the whole 50 years of my academic career!

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

This is a more difficult question to answer because research should always be fun and

stimulating, not simply routine hard work. We were involved in synthesizing new spin levels in the early days (I was not a synthetic organic chemist; fortunately had two roommates first at Stanford who were synthetic chemists and then I learned from my colleagues at Ohio State). We were able to probe protein and enzyme structure at a time when crystallographic methods were somewhat limited and just coming out. Perhaps our two most notable accomplishments were presenting the reversible thiol reagent MTSL and doing some of the early EPR work on animals. We had designed the MTSL label, but not being synthetic chemists, were unable to arrive at it until after we collaborated with the late Kalman Hideg. We wanted a reversible label since we were studying a highly valuable enzymes that involved several weeks of isolation for a yield of a few milligrams. We weren’t smart enough to see the application to site directed mutagenesis that my former labmate Wayne Hubbell pioneered with spin labels. SDSL most probably spirited a renaissance in this aspect of biological EPR. Our second accomplishment was probably the demonstration of EPR imaging of live biological samples, including mice and rats. Our initial equipment was fairly primitive, but several colleagues followed up with higher resolution, more sensitive instrumentation.

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

This, to me, is the most important part of this interview. There are several messages:

1. Try to always work on important problems, even if they are both very risky and challenging. Unfortunately the incentive/reward system today values grant funding over significance and impact. Pursuing the former is at best boring, hard work and ‘safe’ science.
2. Share your work with others. Secrecy doesn’t promote scientific advancement.
3. Life isn’t just always working in the laboratory. Engaging in discussions with others and having broad interests can sometimes enhance your creativity.

IES Fellowship 2019 to Professor Michael Mehring



Besides of his many important contributions in the field of solid-state NMR spectroscopy and its applications to material sciences, Prof. Michael Mehring also pioneered important aspects of pulsed EPR methodology, especially in the field of pulsed hyperfine spectroscopy. Michael Mehring, together with his group members Grupp, Höfer and Nebenfuhr, invented the HYSOCORE (Hyperfine Sublevel Correlation Spectroscopy) experiment first published in 1986 [Grupp, Höfer, Nebenfuhr, Mehring, Chem. Phys. Lett. 132, 279], the mostly used pulsed hyperfine method for the characterization of solids. This paper has been cited more than 400 times and was for many years (and still is) the prototype of a modern 2D-experiment

in the field of EPR spectroscopy. Besides of this, his research group in Stuttgart also explored numerous further pulsed ENDOR experiments (with advanced coherence and multi-coherence detection of NMR spins), which he also explored in view of potential applications to quantum computing. His research fields are very broad, ranging from quantum theoretical treatment of dynamics of atoms and molecules, methodical development in the field of solid state NMR and EPR, to general aspects of solid-state physics and material sciences.

Michael Mehring used pulsed NMR and EPR methods for a variety of applications, ranging from organic chemical compounds, to organic conductors, high-TC superconductors and other inorganic materials, polymers and fullerenes. Many of his publications are a fascinating combination of quantum theoretical treatment of the underlying spin system, a description of new methodical and experimental aspects and interesting results on the investigated material, demonstrating the power of MR methods.

Michael Mehring studied Physics in Münster (Germany). After his PhD in solid-state NMR spectroscopy, he went to the well-known research group of John Waugh at MIT (Cambridge, USA), where he contributed to much of the pioneering work in modern solid-state MAS NMR together with other eminent scientists in this group at that time. After his return to Germany, he soon became Professor at the Technical University of Dortmund. In 1983, he moved to the University of Stuttgart, where he became director of the 2. Physical Institute, where he stayed until his retirement.

Michael Mehring received many awards for his scientific achievements. The most distinguished one in the field of EPR spectroscopy is certainly the Zavoisky Award, which was given to Michael Mehring in the year 2008. Many well-known scientists collaborated, worked and published with Michael Mehring within his scientific career in Cambridge, Dortmund and Stuttgart. Peter Höfer (Bruker), Stephan Appelt (Research Center Jülich) and Marina Bennati (MPI Göttingen) emerged from his research group in Stuttgart, just to name a few of them. He contributed to several books related to magnetic resonance, as *Object-oriented Magnetic Resonance* from Academic Press and *High-Resolution NMR Spectroscopy in Solids* from Springer.

Finally, Michael Mehring was always an impressive person at conferences, giving not only superb talks but also contributing to the discussion with stimulating questions and helpful comments. I gratefully remember very interesting discussions with him at the spring meeting of the German Physical Chemical Society and at the regular magnetic resonance discussion group meetings at the border of the Alps. With his intellectual brilliance, he stimulated and inspired many young scientists working in the field of methodical magnetic resonance in Germany and beyond. Therefore, I am very happy and proud to congratulate Michael Mehring to becoming a Fellow of the International EPR (ESR) society this year.

Thomas Prisner
IES President

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IES Young Investigator John Weil Award 2018



Shunsuke Furuya:

It is an honor for me to receive SEST prize for the development of model materials of quantum spin systems and exploring quantum many-body effects. I would like to thank the members of prize selection committee, officers and all the members of the Society Electron Spin Science and Technology (SEST). In what follows, I would like to introduce two subjects of my research.

(1) Dimerized quantum magnets

Spin pair coupled by a strong antiferromagnetic exchange interaction J is called spin dimer. Dimerized quantum magnet is a quantum magnet, in which these spin dimers are coupled via weak exchange interaction J' . TlCuCl_3 is a spin-1/2 dimerized quantum magnet, which has a singlet ground state with an excitation gap [1, 2]. Magnetic excitations in the dimerized quantum magnet is singlet-triplet excitations called triplons. Excited triplon can hop to neighboring dimer via the transverse components of the interdimer exchange interaction. Consequently, the triplon excitations have dispersion relations. The center of the excitation energy and the width of the triplon band are determined by the intradimer and interdimer exchange interactions, respectively. In TlCuCl_3 , the wave vector that gives the lowest excitation corresponding to the excitation gap is $Q = (0, 0, 1)$ [3]. In a magnetic field, the gap decreases and closes at a critical field H_c , which leads to magnetic ordering. This field-induced magnetic ordering is a typical quantum phase transition (QPT). TlCuCl_3 undergoes the field-induced magnetic ordering above $H_c \approx 5.0$ T. [4–6] The

ordered state is characterized by the coherent superposition of the singlet $|0, 0\rangle$ and triplet $|1, +1\rangle$ states. Thus, the field-induced magnetic ordering can be regarded as the Bose-Einstein condensation (BEC) of triplons [4]. In the ordered state, spins are ordered perpendicular to the external magnetic field [5]. With decreasing temperature in magnetic field higher than H_c , magnetization exhibits the cusplike minimum at the transition temperature T_N . For $T > T_N$, the magnetization is given by the number of thermally excited triplons, which decreases with decreasing temperature. The BEC of triplons occurs at T_N , and below T_N , the number of condensed triplons increases with lowering temperature. The increase of the condensed triplons surpasses the decrease of thermally excited triplons. For this reason, the magnetization has the minimum at T_N . The boundary between paramagnetic and BEC phases in the magnetic field vs temperature phase diagram is excellently described by the triplon BEC theory [6].

TlCuCl_3 undergoes the magnetic ordering also under hydrostatic pressure [7, 8]. This pressure-induced QPT arises from the continuous change in the ratio of the interdimer interaction to the intradimer interaction J'/J . The value of J'/J increases with increasing pressure, which leads to the decrease in the excitation gap. The gap closes at the critical pressure $P_c \approx 0.42$ kbar in TlCuCl_3 [8]. The pressure-induced ordered state is characterized by the coherent superposition of the singlet state $|0, 0\rangle$ and two triplets states $|0, +1\rangle$ and $|0, -1\rangle$. Notable feature of the magnetic excitations is that at P_c , three triplet excitations are reconstructed into two phase modes and one amplitude mode [9]. The phase modes correspond to spin waves in conventional magnets, whereas the amplitude mode is a mode that is observable only near the quantum critical point P_c , where the size of the ordered moment is sufficiently small. With increasing pressure above P_c , the energy of the amplitude mode increases from zero and its intensity decreases. Thus, the amplitude mode cannot be observed in conventional magnets. The amplitude mode was actually observed in TlCuCl_3 by inelastic neutron scattering experiment under pressure [10]. Later, it was theoretically demonstrated that the phase mode and the amplitude mode are equivalent to the Nambu-Goldstone mode and Higgs mode in particle physics, respectively [11].

$\text{Ba}_2\text{MSi}_2\text{O}_6\text{Cl}_2$ ($M = \text{Co}, \text{Cu}$) is a family of the dimerized quantum magnet [12–15]. In $\text{Ba}_2\text{CoSi}_2\text{O}_6\text{Cl}_2$, triplons are localized owing to the almost perfect frustration of interdimer exchange interactions [13]. The magnetization process is stepwise and exhibits plateau at one-half of the saturation magnetization, where triplons occupy the dimer sites alternately to avoid the repulsive interaction between triplons [12]. In $\text{Ba}_2\text{CuSi}_2\text{O}_6\text{Cl}_2$, the splitting of the triplon band owing to the alternation of the interdimer exchange interactions was observed [15]. It was found that the topological property of the dispersion relations near the band gap produces a topologically-protected edge states [15].

(2) Frustrated quantum magnets

A spin-1/2 triangular-lattice antiferromagnet (TLAF) with only the nearest-neighbor isotropic exchange interaction is a prototypical frustrated quantum magnet. At present, the theoretical consensus is that the ground state is not a quantum disordered state such as a spin liquid but an ordered state with the 120° spin structure. Although the zero-field ground state of the spin-1/2 Heisenberg TLAFs is qualitatively the same as that for the classical spin, several quantum spin states that are unstable in the classical spin model are stabilized in magnetic fields with the help of the quantum fluctuation. The most noticeable quantum effect is that an up-up-down (UUD) spin state is stabilized in a finite magnetic field range, causing a magnetization plateau at one-third of the saturation magnetization [16]. The quantum 1/3-magnetization plateau was found in spin-1/2 Heisenberg-like TLAFs Cs_2CuBr_4 with a spatially anisotropic triangular lattice [17] and $\text{Ba}_3\text{CoSb}_2\text{O}_9$ with uniform triangular lattice [18, 19]. The magnetization process observed in $\text{Ba}_3\text{CoSb}_2\text{O}_9$ for magnetic field parallel to the triangular layer is in an excellent agreement with theory [19]. This indicates that $\text{Ba}_3\text{CoSb}_2\text{O}_9$ is close to the ideal spin-1/2 Heisenberg TLAF.

Although the ground state properties of a spin-1/2 Heisenberg-like TLAF with a uniform triangular lattice are well understood both theoretically and experimentally, its magnetic excitations are less well understood. The theoretical consensus is limited for single-magnon excitations. Magnetic excitations in the spin-1/2 Heisenberg-like TLAF $\text{Ba}_3\text{CoSb}_2\text{O}_9$ were investigated by inelastic neutron scattering experiments [20]. Unusual dynamical properties of single-magnon excitations predicted by

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theory such as the large downward quantum renormalization of excitation energies and a roton-like minimum at the M point were confirmed. A notable feature of the magnetic excitations observed in $\text{Ba}_3\text{CoSb}_2\text{O}_9$ is a three-stage energy structure including intense dispersive excitation continua extending to a high energy six times the exchange constant, which cannot be described by the current theory. These experimental results strongly suggest fractionalized spin excitations because the intense excitation continua cannot be explained in terms of conventional two-magnon excitations [20].

Collective magnetic excitations of $\text{Ba}_3\text{CoSb}_2\text{O}_9$ in magnetic fields perpendicular to the triangular layer were investigated by multifrequency high magnetic field ESR [19]. Because the dispersion curves near the Bragg point (K point) can be described by the linear spin wave theory (LSWT), we analyzed the ESR data using LSWT and obtained the exchange anisotropy and the weak interlayer exchange interaction [19].

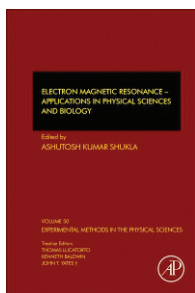
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Electron Magnetic Resonance: Applications in Physical Sciences and Biology describes the principles and recent trends in different experimental methods of Electron Magnetic Resonance (EMR) spectroscopy. In addition to principles, experimental methods and applications, each chapter contains a complete list of references that guide the reader to relevant literature. The book is intended for both skilled and novice researchers in academia, professional fields, scientists and students without any geographical limitations. It is useful for both beginners and experts in the field of Electron Spin Resonance who are looking for recent experimental methods of EMR techniques.

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SEST Award 2018



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SEST Young Investigator Award 2018



Motoi Kimata:

It is my great pleasure to receive the Young Investigator Award of the Society of Electron Spin Science and Technology (SEST). First of all, I would like to acknowledge all the members of SEST, and all the collaborators of my research work. Also, I would like to thank the International EPR Society to give me an opportunity to present my recent research. My research topics are the development of advanced EPR equipment and the study of new type of spintronics phenomena. Here, I will introduce my selected results which are related to spintronics.

1) Spin transport mechanism of pure spin current in a organic polymer film [1]

Spin current (the flow electron spins) is one of the most important ingredients in recent spintronics since it is a promising candidate for efficient information carrier with low energy dissipation. However, in general, the spin current is never conserved in a solid due to the presence of spin orbit coupling. And thus, the search for the long-distance spin transport material is quite important issue for the next generation spintronics.

Since the magnitude of spin orbit interaction of heavy elements are large compared with the light elements, the organic semiconductors, which mainly consist of relatively light elements such as carbon, hydrogen, and sulfur, are promising candidates for long distance spin current transport due to their small spin orbit coupling. However, the spin transport mechanism in organic semiconductors are not fully understood due to the lack of comprehensive

studies of spin transport using multiple experimental probes. In this study, we have determined three key parameters of spin transport (spin lifetime, spin relaxation length, and diffusion coefficient) in heavily doped organic polymer poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT/PSS) from EPR, spin pumping, and charge transport experiments. The most striking feature of this material is the long spin lifetime in the order of nanosecond, which is originating from small spin orbit coupling. In conventional metals, the spin lifetime is typically in the order of picosecond. Also, we showed that these three parameters are consistently explained by a hopping transport model where the spin angular momentum is almost preserved within the hopping process.

2) Experimental observation of magnetic contribution to the spin Hall effect [2].

In addition to the spin transport material, the generation of spin current is also the important topic in spintronics. The spin Hall effect is a main mechanism to make spin current, where the charge current in a metal is converted to the transverse spin current due to the spin-dependent bending of electron trajectories. In this effect, the spin orbit coupling plays an essential role, so that the metallic materials with heavy elements, such as platinum and tungsten, are mainly attracted much attention so far. However, the previous studies are mostly concentrated on the non-magnetic materials. In general, the magnetic spin structure is also important factor to determine the material properties, but the study of spin Hall properties of magnetic materials have been quite limited.

In this study, we were focused on an antiferromagnetic metal with non-collinear magnetic structure Mn₃Sn. In this material, the magnetic sublattice spins show inverse triangle order on a kagome lattice. This antiferromagnetic material is quite unique since the large anomalous Hall effect, which normally appear in ferromagnetic materials, is observed with vanishingly small magnetization. Since the origin of anomalous Hall effect and spin Hall effect is closely related each other, the unconventional spin Hall properties would be expected in this material.

In this experiment, we have fabricated micro-structured spintronics device with a help of focused ion beam, and measured the current-induced spin polarization at the surface of single crystalline Mn₃Sn by attached ferromagnetic NiFe alloy electrode. In the conventional spin Hall effect in non-magnetic materials, the direction of current-induced spin polarization is independent of the external magnetic field. However, in the case of Mn₃Sn, the direction of current-induced spin polarization is reversed when the triangle magnetic structure is switched by the external magnetic field. This unexpected effect, which we call the magnetic spin Hall effect, is really the novel type of spintronics functionality, which would contribute to multipurpose and efficient spintronics.

My studies have been performed with many collaborators. Here, I would like to show my gratitude especially for H. Ohta, S. Okubo, T. Sakurai, E. Ohmichi (Kobe University), T. Terashima, S. Uji (NIMS), H. Tajima (University of Hyogo), Y. Niimi (Osaka University), H. Chen (Colorado State University), S. Sugimoto (NIMS), P. K. Muduli (Technische Universität Dresden), A. H. MacDonald (University of Texas at Austin), K. Kondou (RIKEN), M. Ikhlas, T. Tomita, S. Nakatsuji, Y. Otani (University of Tokyo), S. Kimura, H. Nojiri (Tohoku University).

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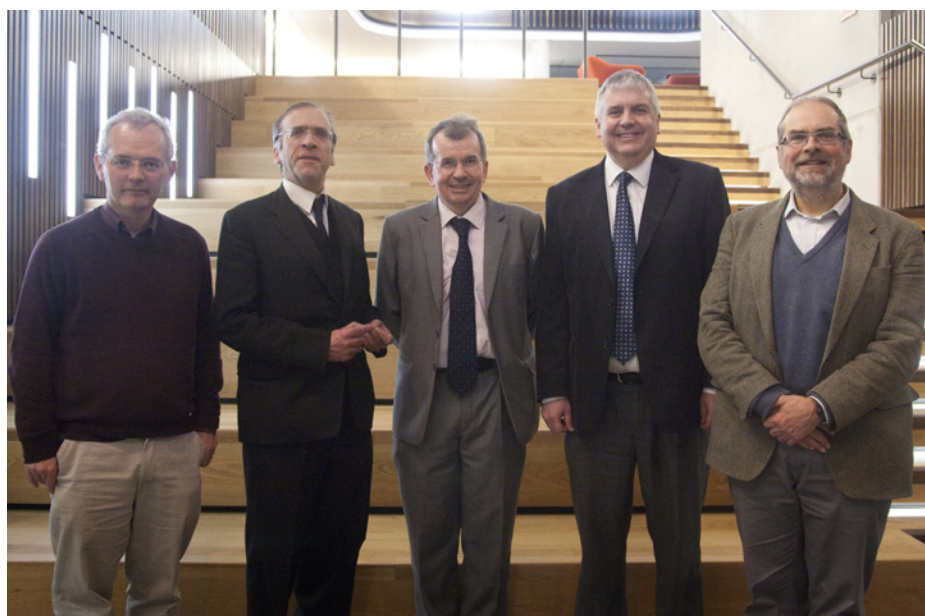
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The Inaugural Brebis Bleaney Memorial Lecture 2019

Mark Newton

February 22nd 2019, Oxford, UK

Professor Brebis Bleaney (1915–2006) was born in London and won scholarships to both Westminster City school and St John's College, Oxford. He was awarded a first-class degree in Physics (1937) at Oxford and went on to do research with Professor Sir Francis Simon. He obtained his doctorate in 1939 and was drafted into the Oxford-based Admiralty team which worked on the development of microwave techniques for radar. He made many contributions to this programme particularly in the development of Klystrons at 10 and 24 GHz. It is well known that following the war Bleaney pioneered the development and application of electron paramagnetic resonance (EPR), exploiting the new microwave technologies for fundamental research, initially unaware that the first EPR experiment had been carried out in 1944 by E. K. Zavoisky at the University of Kazan in the Soviet Union. Bleaney is fondly remembered in Oxford as an inspiring scientist and a man of great kindness and



Michael Baker's two sons (Christopher and Timothy) attended the Inaugural Brebis Bleaney Memorial Lecture endowed by their father. From left to right: Professor Stephen Blundell (University of Oxford, former Head of Condensed Matter Physics and practitioner of muon spin resonance), Timothy Baker (wearing one of his father's suits), Professor Mark Newton (University of Warwick), Professor Robert Taylor (Head of Condensed Matter Physics, Oxford), and Christopher Baker.

warmth. Together with Anatole Abragam, Bleaney published *Electron Paramagnetic Resonance in Transition Ions* (1970) which is still the definitive text book on the subject, and with his wife (Betty Bleaney) he wrote an excellent text book, *Electricity*

and *Magnetism* (1957), known to generations of students as "B and B".

Michael Baker (1930–2017) met Brebis Bleaney as an undergraduate at St. John's College Oxford (Bleaney was his tutor) and after being awarded a first class in Physics



Mark Newton endeavouring to review 75 years of EPR research. The lecture included demonstrations of EPR on plasticine (see EPR of manganese-containing plasticine: Spectral simulation and use as an internal standard for comparison of the signal intensities of various free-radical EPR spectra, P. Rahimi-Moghaddam, Y. Upadrashta, M. J. Nilges, and J. A. Weil, *Applied Magnetic Resonance*, 24(1), 113-125, 2003, DOI: 10.1007/BF03166683) and reviewed the applications of optically defects EPR from the nitrogen vacancy defect in diamond (see Quantum technologies with optically interfaced solid-state spins, D. D. Awschalom, R. Hanson, J. Wrachtrup, and B. B. Zhou, *Nature Photonics*, 12(9), 516-527, 2018, DOI: 10.1038/s41566-018-0232-2).

Finals, joined Bleaney's research group to do research on paramagnetic resonance. Bleaney had an immense influence on Michael Baker's career; they collaborated and discussed science for over 50 years. Michael (elected a Fellow of the International EPR/ESR Society in 2011) was an inspirational and patient teacher who spent nearly all of his research career in Oxford where he nurtured students, and used EPR and ENDOR to study defects in solids and magnetic materials.

Michael endowed an annual lecture commemorating the life and works of Bleaney and the Inaugural Brebis Bleaney Memorial Lecture 'Electron Paramagnetic Resonance: Past, Present and Future' was given by Professor Mark Newton (University of Warwick), himself a student in Baker's research group, this February in the Sir Martin Wood Lecture Theatre in the Department of Physics, Oxford. The lecture described some of the key events in the discovery and development of EPR (and related techniques) but also highlighted how the field is continuing to evolve with the detection of single electron spins

now routine in some systems (e.g. optical detected magnetic resonance from single nitrogen vacancy defect in diamond), such that we can optimistically look forward to applications ranging from studies of single molecules, to enhanced sensitivity and spatial resolution in magnetic resonance imaging. Mark Newton was very grateful to Professor David Collison (Manchester), Professor Graham Smith (St. Andrews), Dr William Myers (Oxford – Centre for Advanced ESR (CÆSR), Oxford), Professor Arzhang Ardavan (Oxford) and Professor John Gregg (Oxford) who all supplied ma-

terial for the lecture which was attended by many scientists who had worked with Bleaney and Baker over the years, as well as new researchers and students using EPR in different branches of science. The lecture was followed by a lively drinks reception and a recording of the lecture is available at <https://podcasts.ox.ac.uk/electron-paramagnetic-resonance-past-present-and-future>.



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Harvey Allen Buckmaster (1929–2018)

I was first aware of the work of Harvey Buckmaster in 1976 when I published a paper that was an improvement on a method of evaluation of spin-Hamiltonian parameters by fitting simultaneously all the single-crystal line positions of the Gd^{3+} ion, obtained for one orientation of the external magnetic field (along the principal axis of the zero-field splitting tensor) to all the spin-Hamiltonian parameters, published by his EPR group at the University of Calgary, Alberta (Canada). I had suggested that one should fit at least the line positions obtained for one more orientation, preferably perpendicular to the z -axis, for orthogonal-axis consistency. Naturally, he was curious as I was the new kid on the block in Canada in the EPR field. This was the beginning of my research career in EPR. We were both investigating experimentally and analyzing single-crystal $Gd(III)$ X-band EPR data. Gradually his respect for my expertise in theoretical EPR grew. His own expertise was predominantly experimental EPR. Indeed, he had built a superheterodyne X-band EPR spectrometer from components, and had a deep knowledge of EPR instrumentation. Because of his non-EPR diverse interests, he ‘missed the boat’ when Charley Poole published his classic book on experimental techniques in 1967. Harvey, in fact, gave a

bad review to that book as a consequence of his missing the boat for publishing his own book on experimental EPR techniques, but in due time realized that he was not objective in that review, and indeed Charley’s book was meritorious and deserved to be considered the bible of experimental EPR techniques. In fact, he developed very warm relations with Charley Poole over time through me, who’d been a good friend of Charley’s for years. Since he always wanted to write on his expertise in experimental EPR, I invited Harvey to write the chapter entitled “*Low Frequency CW-EPR Spectrometers: 10 MHz to 100 GHz*” in the *Multifrequency EPR: Theory and Applications* (Wiley-VCH, Weinheim, Germany, 2011) book, edited by me. He was named a Fellow of the International EPR Society in 2005. (I had the honour of nominating him.) My friendship with Harvey grew over the years. He did not pursue EPR research actively during his post-retirement period at the end of 1990s at the University of Victoria, British Columbia. He settled in Victoria, the heaven of Canadian retirees, where the weather is nice throughout the year. In the end, he bequeathed both his X- and Q-band spectrometers to me, including two magnets, as well as the components to build a 24-GHz spectrometer, which he did not have a chance to put together. This provided him with the opportunity to come to Montreal to set up his spectrometers in my lab. He stayed in my house for two weeks, giving us the opportunity to get to know each other better. We walked a lot and enjoyed the fine cuisine of Montreal and the French culture. He even reviewed my manuscripts under preparation! I benefitted from his expertise in writing. During his stay, Jack and Renée Freed spent one of the weekends in Montreal en route to St. Martins for vacation. It was a great opportunity for all of us to dine at a famous French restaurant and talk about EPR research. When Harvey finally left Montreal to return to Victoria, it was nostalgic to see him leave after so many days. I took him to *Via Rail* train station, situated in the basement of the famous Queen Elizabeth hotel, with very nice shops and restaurants. He wore a nice hat and leather jacket, looking very elegant, being a tall man. He kept in touch with me with keen interest afterwards while back in Victoria to keep track of my research, politics in Quebec and with the EPR news as I was the Secretary of the International EPR Society for six years. I encouraged him to write an article about his instrumentation skills for the *EPR Newsletter*. Finally

he did, and it was published recently in the *EPR Newsletter* entitled “*Looking Backward – How EPR research was done 65 years ago*”. He enjoyed hiking in the Rocky Mountains every summer until the last years of his life, when his body gave up, stopped making red-blood platelets. He passed away peacefully at the age of 89 on November 28, 2018, surrounded by his family. His wife told me that he said at that time that he had no regrets with the life that he passed. I never met Margaret (his wife) but from what she heard of me, she wanted to talk to me on the phone. We did, and she was quite happy to have exchanged a few words with me. I promised her that I would write his obituary for the *EPR Newsletter*. Harvey will be sadly missed in the scene of Canadian and international EPR, where he was a shining star. I will miss him as a good friend, with whom I not only discussed EPR research, but also Canadian politics, among others.

Professor Harvey Allen Buckmaster was a pioneer EPR spectroscopist. His PhD thesis at the University of British Columbia involved the construction of the first high sensitivity, wide or narrow band, double field modulation paramagnetic resonance spectrometer in Canada in 1953, and the first demonstration of the sensitivity improvement achievable using high-frequency modulation in 1954. After completing his NRC Overseas Post-doctoral Fellowship in radio astronomy at Cambridge, he pursued EPR research at the University of Alberta in 1957. He moved to the University of Calgary in 1960, retiring as an emeritus professor of physics in 1993. He then joined the University of Victoria as an Adjunct Professor pursuing EPR research for another six years. His experimental research involved introduction of synchronous signal processing and noise suppression techniques, finally constructing a broadband 1–2 GHz CW and pulse EPR spectrometer in 1992. As for theoretical contributions, he exploited application of tensor operators in the spin-Hamiltonian formalism, and investigated application of computers to fit EPR spectra to spin Hamiltonians. Apart from designs, his experimental research in EPR included studies of S-state impurity ion host lattice effects, *in situ* combustion and impurity ions in coals, radiation effects in biological tissue, and medical biophysics studies of hemoglobin and malignant hyperthermia. He has published over 180 scientific publications.

Sushil Misra
Concordia University, Montreal, Canada

Reflections on Harvey Buckmaster

I didn't have the honor of knowing Harvey for as long or extensively as did other colleagues who have offered their personal comments. Nonetheless I can offer some reflections of the man as a person. He was one of the pioneers of the Canadian EPR establishment whose name and national affiliation went hand in hand. Harvey was a dependable attendee at the Rocky Mountain Conferences on Analytical Spectroscopy, particularly the EPR section.

As a person he was very loyal and supportive of his respected colleagues and friends as well as being candid about his severe

health issues. Harvey and I were supporting a colleague for recognition and he was 'on top of it' and concerned right up until the end. He also shared some of the annoying details of his medical treatment with me. These are all the marks of a good friend even though we had more limited personal contact.

We will all miss him dearly.

Larry Berliner
University of Denver, Denver, USA



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Effects of light in everyday life monitored by electron paramagnetic resonance (EPR) spectroscopy

Kalina Ranguelova and Ralph Weber
Bruker Biospin Corp., Billerica, USA

Photochemical reactions are initiated by absorption of energy in the form of light and involve formation of free radicals and transient excited states whose chemical and physical properties differ greatly from the original molecules. For example, one of the most well-known flavor defects in beer across the world is to become skunky or 'lightstruck' after exposure to UV light. The reason for this 'lightstruck flavor' is the photodecomposition of isohumulones, the major flavor components of hops, via a free radical photodegradation mechanism. Free radicals and excited states are often short-lived but play crucial roles in significant photochemical processes such as photooxidation, photodegradation, photostability, photocatalysis, photosynthesis, and polymerization.

Electron Paramagnetic Resonance (EPR) spectroscopy is the only analytical technique capable of detecting species with free radicals and transient excited states in a direct and non-invasive manner. The technique is very versatile as it can be applied to gaseous, liquid, or solid samples over a large range of temperatures. It can be used to detect, quantify, and monitor the intrinsic photogeneration of short-lived species and is therefore extremely useful for detecting free radicals in photochemical reactions in polymer science, pharmaceuticals, environment, etc. The aim of this paper is to present a general overview of the diversity of EPR applications when it comes to photochemical reactions.

I. Photodegradation studies using EPR

Light is an important factor in considering the stability of materials and is important to study and evaluate if light exposure results in unacceptable changes in the final product or compromise its shelf-life. For example, degradation of polymers due to light exposure leads to discoloration and a decrease in the mechanical properties (elasticity, toughness, etc.). To prevent this decomposition, Hindered Amine Light Stabilizers (HALS) are added to the polymer. When the polymer is exposed to UV-irradiation HALS suppresses radical damage in the polymer by forming

a HALS-based nitroxyl radical, i.e. HALS sacrifices itself to protect the polymer molecules. EPR detects the HALS radicals and by monitoring and quantifying the EPR signal, the effectiveness of HALS can be evaluated. This EPR application is successfully used to determine polymer photodegradation in both academic and industrial settings for research and quality control. For example, Ford Motor Company published an EPR study where concentrations of HALS radicals during the early stages of weather exposure provide direct insight into the long-term weathering performance of clearcoat/basecoat automotive paint systems [1].

Skin is a very susceptible target organ to photodegradation (photoaging). UV-light is the main cause of skin disorders including sunburn, premature aging, and photocarcinogenesis, resulting from UV-induced oxidative stress and mediated by short-lived radicals named reactive oxygen species (ROS). Thus, photoprotection is crucial for preventing the undesired effects of sun exposure and is mainly achieved using sunscreens and other

skin care products containing UV-filters, and antioxidants. Their radical scavenging activity can be measured by EPR spectroscopy as well as screening of their efficacy and safety. The product is typically tested under accelerated conditions (UV-irradiation) to increase the rate of photodegradation and the data generated from these stability studies (stress testing) can be transferred to real time stability data. For example, UV-filters are the key ingredients of cosmetic sunscreen formulations that absorb specific wavelengths of ultraviolet radiation [2]. Sunscreens should ideally protect from sunburn/erythema induced by UVB and from the genotoxic/oxidant effects of both UVA and UVB which contribute to skin photodamage. For a sunscreen's optimum performance and efficacy, the first and foremost requirement is that the UV-filters should remain effective during the entire period of exposure. The EPR signal of a stable radical (TEMPO) was followed for 25 min of UV irradiation in the presence of different UV-filters showing their efficiency to reduce the radical (Figure 1). Clearly UV-filter D was the

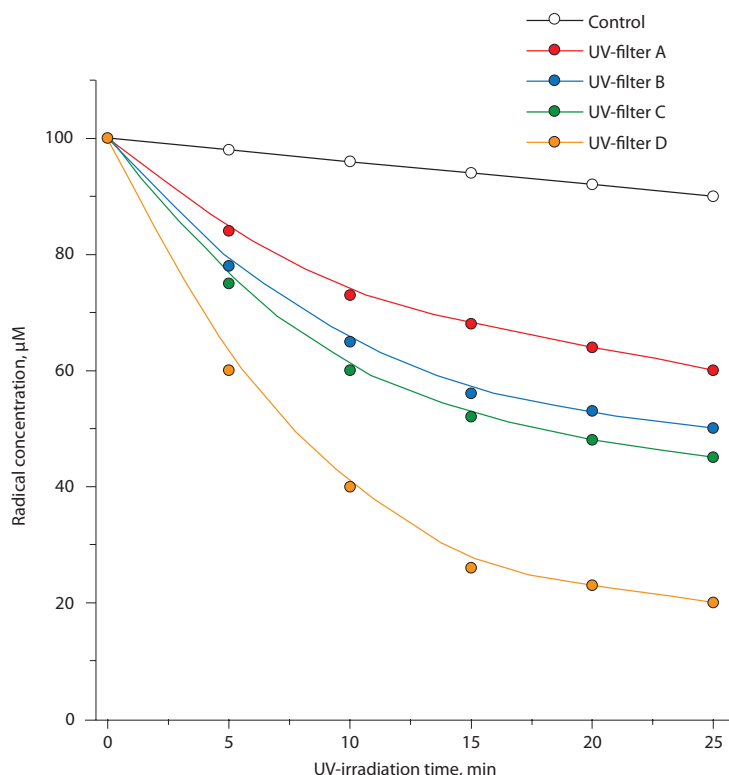


Figure 1. UV-filter efficacy determined by EPR. The ability of the UV-filters to quench free radicals increases in the following order: A < B < C < D.

most effective one at quenching free radicals in the sunscreen formulation.

Free radical photochemical reactions are very common in food and beverages and they play a major role in food photodegradation. In addition, there is strong evidence for the fundamental role free radicals play in many diseases. However, there are also studies showing that free radicals generated during food processing may play key functional roles in texturization, flavor formation, and other reactions contributing to food properties and characteristic qualities. Therefore, identifying and understanding photochemical reactions that are free radical-mediated in foods and beverages, and learning to control these reactions associated with food qualities and shelf-life stability give us sufficient reason to be interested in EPR detecting and studying radicals in foods and beverages.

II. Photocatalysis studies using EPR

Stability, low cost, non-toxicity and appropriate photocatalytic activeness are some of the criteria for a good photocatalyst. Amongst them, titanium dioxide meets these criteria for industrial-scale utilization and is predisposed to a wide range of applications in various areas (photocatalysts, solar cells, thin film capacitors, gas sensors, self-cleaning surfaces, etc.) In general, the photoactivity of TiO_2 is determined by the process of electron/hole pair generation, recombination, interfacial transfer, and by the surface reactions of these charge carriers with the species adsorbed on the surface of the photocatalyst. TiO_2 derives its activity from the fact that when photons of a certain wavelength are incident upon its surface, electrons are promoted from the valence band and transferred to the conduction band. This leaves positive holes in the valence band, which react with the hydroxylated surface to produce $\cdot\text{OH}$ radicals (Figure 2).

The modern chemical industry as well as pharmaceutical and environmental sciences rely heavily on heterogeneous photocatalysts. Understanding the operational mode or reactivity of these catalysts is crucial for improved developments and enhanced performance. Where paramagnetic centers are involved, ranging from transition metal ions to defects and free radicals, EPR spectroscopy is without doubt the technique of choice. Photocatalytic degradation of organic pollutants is frequently carried out using semiconducting polycrystalline TiO_2 forming free radicals by light irradiation. EPR detects and identifies key active species (hydroxyl radicals, superoxide, singlet oxygen) produced in irradiated TiO_2 suspen-

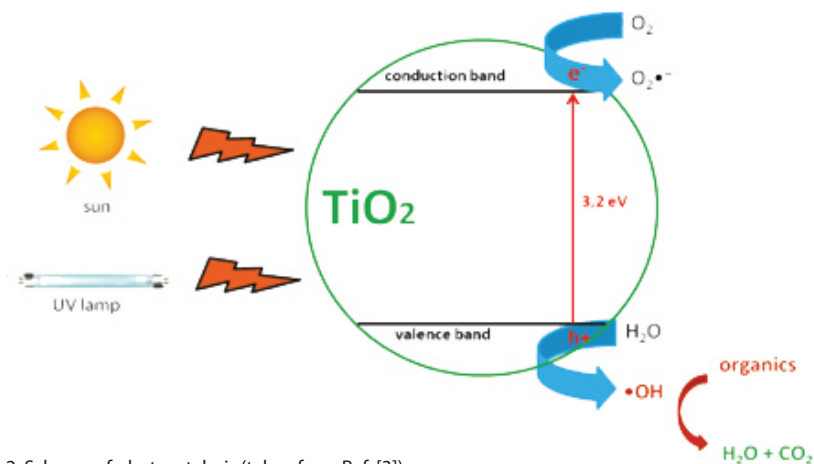


Figure 2. Scheme of photocatalysis (taken from Ref. [3]).

sions. Monitoring the radical intermediates by EPR provides complete characterization of TiO_2 and other photocatalysts' activity (Figure 3).

Another EPR application in photocatalysis is related to detection of paramagnetic reactive oxygen species (ROS) during photocatalytic activities of nanomaterials. For example, Vankayala et al. reported that singlet oxygen is generated via photo-irradiation of gold nanoparticles which can be used as photothermal agents in treating cancerous tumors [4]. Many micro- and nanomaterials are capable of initiating ROS generation under varying experimental conditions which can be considered as an intrinsic parameter of a given nanomaterial, like other physiochemical properties such as particle size, morphology, etc. EPR is used to develop appropriate ROS-active nanomaterials for specific applications since their photocatalytic and photobiological activity correlates with the ROS concentration monitored by the resonance technique [5].

III. Photopolymerization studies using EPR

Free radical photopolymerization is the most widespread application so far, and modern technologies are constantly looking for new and efficient radical photoinitiators. On absorption of light, a photoinitiator induces free radical chemistry reactions that result in significant changes in the solubility and physical properties of suitable formulations. EPR spectroscopy is used to detect and monitor free radical intermediates shedding light on the underlying mechanisms. For example, EPR methods were successfully applied in development of a novel class of silyl radical generating photoinitiators used for photopolymerization of methacrylates, e.g., in dental materials [6]. Three different radical intermediates were detected and identified by EPR (Figure 4). Furthermore, quantitative EPR analysis provided information about the radical reactivity and photopolymerization efficiency. The data contributed to a starting idea for the development of other photoinitiating systems in this series.

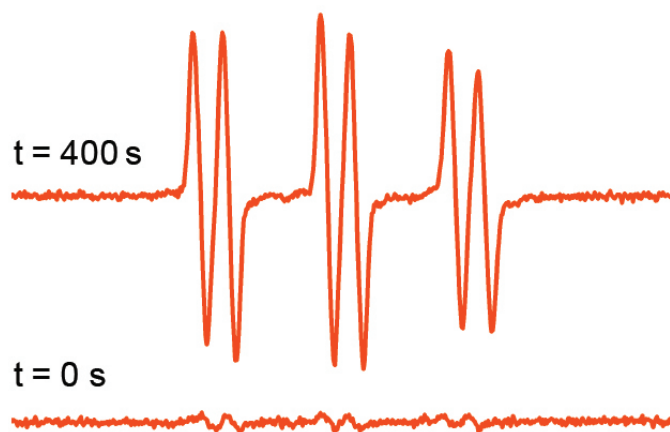


Figure 3. Hydroxyl radical detection by EPR in UV-irradiated TiO_2 after 0 and 400 sec. The spin trapping technique was used to capture the radicals.

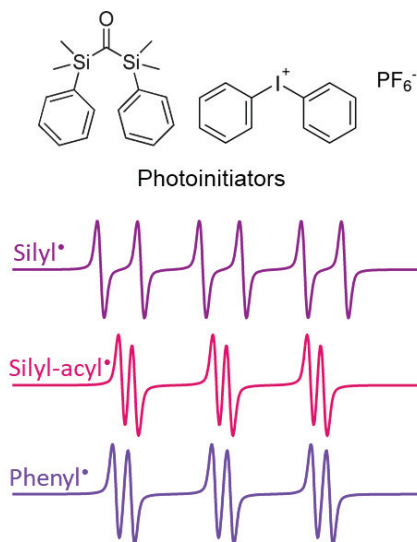


Figure 4. EPR spectra of radical species generated in photoinitiator bis-silylketone used for photopolymerization of methacrylates, e.g., in dental materials.

In summary, understanding photochemical reactions is crucial for many applications in science and technology. EPR provides the unique capability to directly measure the radicals that play a crucial role in these reactions. By detecting, identifying, monitoring, and quantifying radical intermediates, EPR is the solution for better understanding free radical photochemistry reactions and thereby helps to improve products' performance and their shelf-life.

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new EPR Faculty



Ilia Kaminker

Ilia Kaminker became a Senior Lecturer (equivalent to the US assistant professor) in the School of Chemistry at Tel Aviv University in July 2018. Ilia earned a dual-major undergraduate degree in chemistry and biology from Tel Aviv University in 2006. He then joined the Weizmann Institute of Science where he earned his Ph.D. in Chemical Physics in 2012 working on high-field pulsed EPR methodology and its applications to the mechanism of RNA helicases with Daniella Goldfarb. As a postdoc, Ilia first joined Shimon Vega's group where he worked on understanding the spin-dynamics in dynamic nuclear polarization (DNP). After completing a second, four-year postdoctoral fellowship as HFSP fellow in

Song-I Han's laboratory at the University of California - Santa Barbara working on high field EPR and DNP, Ilia joined the faculty of Chemistry at Tel-Aviv University. He received the prestigious IEPRES Young Investigator Award in 2015. His current research focuses on the development of advanced methods in DNP and high-field EPR aimed at understanding the underlying mechanisms and improving

the DNP methodology for the detection of "difficult" nuclei, which is expected to shed light on diverse questions in material science such as the catalysis by surface-bound transition metal complexes, the structure of metal-organic frameworks, determination of solid phases in active pharmaceutical ingredient (API) preparations and more.



Jarett Wilcoxen

Jarett Wilcoxen became an Assistant Professor of Chemistry and Biochemistry at University of Wisconsin - Milwaukee in Au-

gust 2019. Jarett earned his undergraduate degree in Biochemistry from the University of California - Santa Barbara in 2007. He earned his PhD degree in Biochemistry and Molecular Biology at the University of California - Riverside in 2013 in the laboratory of Russ Hille where he studied the Mo- and Co-containing CO dehydrogenase using kinetic, mechanistic, and spectroscopic approaches. Jarett then completed a postdoctoral fellowship in David Britt's lab at the University of California - Davis studying radical SAM enzyme mechanism by EPR, with particular interest in Nitrogenase cofactor biosynthesis. His current research focuses on the roles of metal(s), metal ligands, and nearby amino acid residues play in directing catalysis in radical SAM and molybdenum enzymes.

The 52nd Annual International Meeting of the RSC ESR Group April 2019, Glasgow, UK

The 52nd Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry was masterfully organised by Stephen Sproules in Glasgow in April 2019. The attention to detail was unprecedented – there were taxis waiting at Glasgow airport at the exact time of arrival of each of the participants, and the seemingly omniscient Stephen and his team were there at the hotel entrance to personally greet everyone. The carefully scripted programme featured a ceilidh – a Scottish dance roughly comparable to running a marathon on a Moebius strip; it took the breath away from your intrepid correspondent. At about 5:30 one morning, a very British waiter surveyed a collection of napkins covered in equations and pulse sequences that had accumulated through the night, and inquired “would ladies and gentlemen like some more wine?” We did.

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. The Bruker Prize 2019 was awarded to Marina Bennati of the Max Planck Institute for Biophysical Chemistry for her outstanding work in ESR instrument development (dual mode cavity for W-band, rapid freeze quench for multi-frequency ESR, *etc.*), theoretical and methodological research (CP-ENDOR, orientation selection, *etc.*) and biophysical applications that also included the neighbouring NMR and DNP spectroscopies.

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 twelve (a record so far) applications from the students who had submitted their



Prof Marina Bennati



No trip to Scotland is ever complete without a visit to one of its famous whisky distilleries. The programme included a trip to Auchentoshan, which translates from Gaelic as “corner of the field”; it was less than two miles away from the Conference hotel. The guided tour of the distillery ended with a tasting of their signature single malts.

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 asked external experts to read and assess each thesis in depth.

The winner was Dr Claire Motion for her thesis completed at the University of St Andrews, supervised by Prof Graham Smith. To quote our expert reviewer panel:



Dr Claire Motion

“Dr Motion has significantly enhanced sensitivity of a cutting-edge spectrometer and has demonstrated an incredible sensitivity improvement in low-spin Fe(III)-nitroxide DEER, which no expert would have predicted. This was not just a matter of luck, but a result of meticulous preparation and deep understanding. [...] the thesis of Dr Motion is a convincing demonstration of scholarship [...] it is very impressive how many journal articles she managed to publish.”

All attendees were very impressed and noted, with gratitude, that Bruker was again a major force behind making the Conference a success.

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 six were invited to give a talk. Two presentations stood out – an

applications talk by Sonia Chhabra (*“Application of EPR Methodology Towards Cr/PNP Based Ethylene Tetramerisation Catalysis”*) and a methodology talk by Frauke Breitgoff (*“Pushing for Longer Distances: Frequency-Swept Excitation in Distance Measurements of Spin-1/2 Systems”*). By a very tight margin, the second presentation won the JEOL Medal. A representative of the JEOL Corporation presented the medal during the drinks reception that the company also sponsored.

The International EPR Society has expanded its presence at the Conference this year, awarding not only its traditional poster prizes, but also the Silver Medal. The poster prizes went to Luis Fabregas Ibanez (for a poster titled *“Hyscorean: Measurement, Processing and Analysis of Non-Uniform Sampled HYSCORE”*) and Benjamin Tucker (for a poster titled *“An Investigation of Refocused Out of Phase DEER and RIDME”*).

The IES Silver Medal was awarded to Robert Bittl of the Free University of Berlin (see *EPR newsletter*, 29/1-2, p. 9).

Committee

The following committee members have served their full term of office: Alice Bowen, Bela Bode, Maxie Roessler, Enrico Salvadori, Eric McInnes – the former four were warmly thanked for their service, the latter had a dinner speech by Christiane Timmel dedicated entirely to himself, detailing his very impressive accomplishments as Chair, as well as the long history of the McInnes clan.

Christiane Timmel was unanimously elected Chair for the next three years, Eric McInnes and David Collison (the organisers of the Manchester conference) received their seats *ex officio*. Floriana Tuna (Manchester University) and Paul Jonsen (Talavera Science Ltd.) were elected Ordinary Committee Members by a majority vote.

Conference reports

Next conference

Eric McInnes, David Collison, and Floriana Tuna are organising the next conference in Manchester between 29th March 2nd April 2020. See <http://www.esr-group.org/conferences/2020-conference-manchester/> for further information.

Prof. Ilya Kuprov,
RSC ESR Group Secretary

The 6th Awaji Island International Workshop on Electron Spin Science & Technology: Biological and Materials Science Oriented Applications (AWEST 2019)

June 16–19, 2019, Hyogo, Japan

The 6th Awaji Island International Workshop on Electron Spin Science & Technology: Biological and Materials Science Oriented Applications, AWEST 2019, was held on June 16–19, 2019 at Awaji Yumebutai International Conference Center, Hyogo, Japan.

The AWEST has been organized in mid-June every year at the same venue, Awaji Island since 2013. The aim of the AWEST is to provide an international/global forum for discussions of interdisciplinary issues on electron spin science/technology relevant to open shell systems/compounds and electron-mediated phenomena to biologists, chemists, materials scientists, physicists and other scientists with both academic and industrial backgrounds. The AWEST covers wide scientific areas in biology, chemistry, materials science and physics. There are many topics concerning to electron spin science and technology: methodological developments, materials-science oriented applications of electron spins, spin-mediated molecular biology and the others.

This year, there were 60 oral presentations after an opening talk by Prof. Marco Affronte



Conference photo

under a tight schedule in the 6th AWEST. Various emerging topics related to electron spin science were presented: Spin labeling dipolar ESR, Structural determination by DEER, DNP enhanced solid state NMR, time-resolved ESR, pulsed ESR, high-field ESR, and the others. The total number of the participants was 75 from 10 countries, including 15 overseas participants.

In the past AWESTs, we have been awarding young researchers for their excellent poster presentations. This year we awarded an excellent oral presentation with Springer-Verlag's support. The international student award went to Ms. Tatiana Sherstobitova (Hiroshima Univ.) for Springer Award under the review by Award Committee whose members were the overseas invited speakers. Prof. Martin Lemaire (Brock Univ.), who chaired the special session for young researchers, handed Springer Award over to the awardee.

On June 21, there was a conference excursion to the UNESCO world heritage, Himeji Castle, and Japanese garden "Koko-en". The Himeji Castle is nicknamed "Shira-sagi



From left to right: Tatiana Sherstobitova and Martin Lemaire.

(White Heron)" castle built in 1609. After major renovations, the Himeji Castle has been reopened in 2015.

In next June, we plan to organize the 7th Awaji Island Conference (AWEST2020) at the same venue (June 17–20, 2020). We are looking forward to welcoming you from overseas and delivering your recent results.

Kazunobu Sato
Executive Secretary, AWEST Secretariat
Professor Osaka City University
website: <https://qcqis.sci.osaka-cu.ac.jp/awest/2019/>



Creating an Exciting World of EPR...

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SharedEPR/IEPRS EPR summer school July 17–21, 2019, Denver, Colorado

The SharedEPR network, funded by the National Science Foundation in the US, and the International EPR Society jointly organized a 3.5-day long summer school on EPR spectroscopy for non-experts. It was held at the University of Denver, Colorado.

The school consisted of a series of seven lectures, covering the basics of the CW EPR experiments, fundamentals of spin physics, g tensors, hyperfine coupling, high-spin systems, nitroxides, transition metal complexes, and pulse EPR. The instructors were Michael Lerch (Medical College Wisconsin), Eric McInnes (University of Manchester), Glenn Millhauser (University of California Santa Cruz), Thomas Prisner (Goethe University Frankfurt), Enrica Bordignon (Ruhr University Bochum), Kurt Warncke (Emory University), and Troy Stich (Wake Forest University). Stephen Hill from the National High Magnetic Field Laboratory (the MagLab) in Tallahassee gave an evening keynote presentation about the EPR capabilities at the MagLab, including a live video tour of their high-power 95 GHz spectrometer (HiPER).

The lectures were accompanied by small-group laboratory practicals. The lab practicals were based on small groups, with at most 4 students per instrument. This required the use of a total of six spectrometers in parallel (3 Bruker EMXnano, 1 Bruker EMX, 1 Bruker E580, and 1 home-built rapid-scan spectrometer). The practicals were held in the labs of Sandra and Gareth Eaton at the

University of Denver. Laboratory instructors included Debbie Mitchell, Joseph McPeak, Lukas Woodcock (University of Denver) as well as Kalina Rangelova and Ralph Weber (Bruker).

Demand for the school was high. Due to the limited space in the practical labs, the capacity of the school was limited to 40 participants. There were close to 200 applications.

The organizing committee included Gary Gerfen (SharedEPR; Albert Einstein College of Medicine), Thomas Prisner (president, IEPRS; Goethe University Frankfurt), Stefan Stoll (University of Washington, Seattle), Songi Han (University of California Santa Barbara), as well as Sandra and Gareth Eaton (University of Denver).

Besides SharedEPR and the IEPRS, Bruker contributed substantially to the school by loaning two additional EMXnano spectrometers and by providing their application scientists as lab instructors.

Feedback from the participants was overwhelmingly positive: “The school was very interesting, well-organized, had a good variety of materials, did a good job of incorporating different levels of learners, and the instructors were generally approachable and engaging.” “An outstanding tour of modern EPR theory and practice.” “A very informative experience that primed me on basic and practical aspects of EPR.” “With the help of knowledgeable and approachable EPR experts, I gained the theoretical and practical background needed to effectively obtain and interpret EPR spectra.”

Gary Gerfen, Stefan Stoll
SharedEPR network

60th Rocky Mountain Conference on Magnetic Resonance and 42nd International EPR Symposium

July 21–25, 2019, Denver, Colorado

The 42nd International EPR Symposium at the 60th Rocky Mountain Conference on Magnetic Resonance (RMC) was held in the mile-high city Denver, Colorado, United States, from Sunday July 21 to Thursday July 25, 2019. This year RMC was sponsored by Avanti Polar Lipids, Inc., Bridge 12 Technologies, Inc., Bruker, Clin-EPR, LLC, Cryogenic US LLC, Element Six, MagnetTech/Rotunda Scientific Technologies, National High Magnetic Field Laboratory (NHMFL), Virginia Diodes, Inc. and Shared EPR network.

This RMC held only the EPR symposium (no NMR symposium). The number of registered attendees at the EPR Symposium was 160, the highest number of the participants for RMC with only EPR symposium! 80% of the attendees were from the US, the other from abroad. A third of the attendees were students. With the sponsorship from NHMFL and Shared EPR network, 17 travel awards were provided to students and post-doc participants!

The EPR scientific program was held from Monday morning to Thursday noon. It included 16 invited talks (25+5 minutes) and 47 contributed talks (12+3 minutes). The topics of the 14 sessions spanned a large range of topics, including biomacromolecules (structural biology), spin centers in biology and chemistry (enzymology, catalysis and Cu/Gd spin labels), materials (quantum physics





From left to right: Fraser MacMillan (EPR Symposium co-chair), IES Poster Prize winners (Joseph McPeak from University of Denver; Elizabeth Canarie from University of Washington) and Thomas Prisner (IES President).

in molecular spin systems and new defects centers in diamond), spin devices (magnetic resonance using NV centers in diamond and resistively-detected NMR), methods (development of high frequency EPR/Hyperfine spectroscopic techniques), and EPR imaging-clinical. In addition to the scientific program, Lawrence Berliner (University of Denver) was honored for being named the Fellow of the international EPR society (IES). Tatyana Smirnova (North Carolina State University) was being honored for many years of service as treasurer of IES. Moreover, the conference celebrated the 30th IES anniversary at the Wednesday conference banquet with a special

presentation, titled “EPR: Past, Current and Future”, given by Thomas Prisner (IES president, Goethe University Frankfurt), Christoph Boehme (University of Utah), Gareth Eaton (University of Denver) and Harold Swartz (Dartmouth College).

There were poster sessions in the evening of Monday and Tuesday that featured a total of 67 posters. The poster sessions were well attended, and supported by the free drinks that the EPR Symposium was able to offer. Furthermore, student poster prizes were awarded during the banquet on Wednesday. I am proud to mention that this RMC provided 14 poster awards sponsored by IES,



Poster award ceremony. From left to right: Samuel M. Jahn, Joseph E. McPeak, Muhammad Abdullah, Fraser MacMillan, Cassidy E. Jackson, Luis Fábregas Ibáñez, Elizabeth R. Canarie, Susumu Takahashi, Wei Li, Benjamin Fortman, Laura Mugica, Konstantin Herb, Trang T. Tran and Katie M. Dunleavy.



From left to right: Thomas Prisner, Tatyana Smirnova, and Stephen Hill.

Springer-Applied Magnetic Resonance and RMC as well as book donations from Lawrence Berliner (University of Denver) and Stefan Stoll (University of Washington)! The poster committee, comprised of the invited speakers and the scientific committees, awarded the following students; Elizabeth R. Canarie (University of Washington), Joseph E. McPeak (University of Denver), Luis Fábregas Ibáñez (ETH Zürich), Wei Li (Emory University), Spencer Johnson (Colorado State University), and Konstantin Herb (ETH Zürich), Benjamin Fortman (University of Southern California), Justin Huffman (West Virginia University), Trang T. Tran (University of Florida), Cassidy E. Jackson (Colorado State university), Samuel M. Jahn (University of Washington), Ryan C. O’Connell (West Virginia University), Muhammad Abdullah (University of Massachusetts Amherst), Laura Mugica (University of Southern California) and Katie M. Dunleavy (University of Florida).

Before RMC, the three-day EPR summer school (July 18–20, 2019) was successfully held in University of Denver with supports from Shared EPR network, International EPR Society, Bruker BioSpin and University of Denver. In addition, Bruker gave a presentation on new and updated products and hosted an excellent dinner buffet on July, 21, Sunday at University of Denver.

The scientific committee of the EPR Symposium was comprised of Susumu Takahashi (University of Southern California, chair), Fraser MacMillan (University of East Anglia, vice-chair), Ania Bleszynski-Jayich (University of California Santa Barbara), Christoph Boehme (University of Utah), Enrica Bordignon (Ruhr-Universität Bochum), Boris Epel

(University of Chicago), Gail Fanucci (University of Florida), Songi Han (University of California Santa Barbara), Stephen Hill (Florida State University, National High Magnetic Field Lab), Dane McCamey (University of New South Wales), and Chandrasekhar Ramanathan (Dartmouth College). The committee members served as session chairs.

In 2020, the 61th RMC with the 43rd International EPR Symposium will be back to a mountain and ski resort at Copper Mountain, Colorado, July 21–25, 2020. The chair for the 2020 EPR Symposium is Fraser MacMillan (University of East Anglia).

Susumu Takahashi
Chair, EPR Symposium 2019

EPR Transition – Dr. Arthur H. Heiss

One of the EPR community's strongest supporters, Dr. Arthur H. Heiss, is transitioning from his position in Bruker on August 1, 2019. Outstanding performance during an undergraduate research experience with John Weil led to Art joining the research group of Clyde Hutchison, Jr., at the University of Chicago. His 1974 Ph.D. thesis was on "ENDOR of La Nuclei in $\text{LaCl}_3:\text{Sm}^{3+}$." In 1973 Art began working at Bruker, with an early and forward-looking emphasis on computers in EPR.

During 1981–1987, when IBM marketed Bruker instruments in the USA, Art led EPR for IBM (part of our E580 has IBM labels). When IBM terminated the marketing agreement, he returned to Bruker. Dieter Schmalbein's brief "A Bruker EPR History" in Foundations of Modern EPR, World Scientific, 1998, included the following tribute to Art:

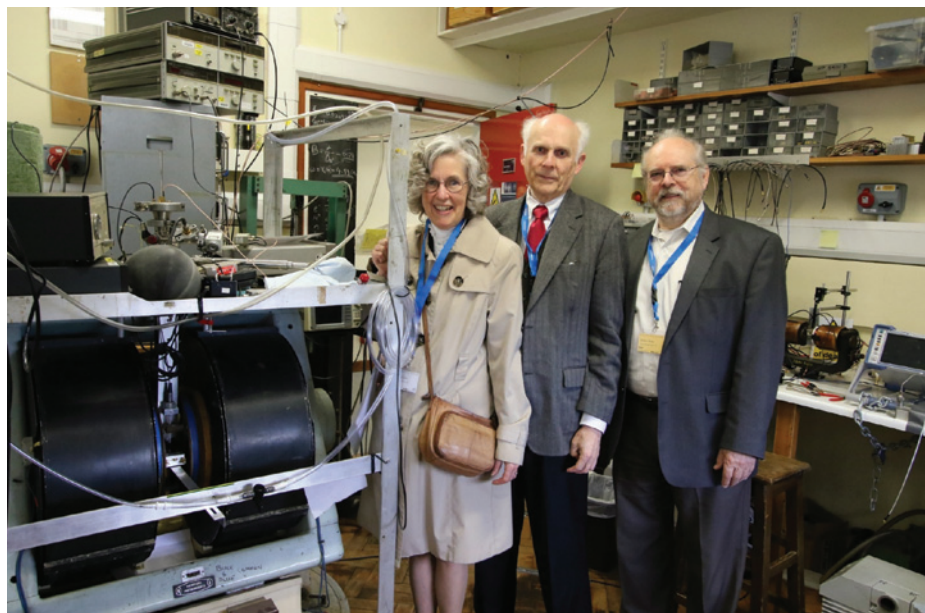
"Dr. Arthur Heiss started his career as the US EPR Manager and it was his task to open this large market for the Bruker product. Art gained a rich experimental experience during his University time in Chicago with Prof. Clyde A. Hutchison Jr. at the Department of

*The EPR community thanks
Dr. Arthur H. Heiss*

for a half century of pushing the frontiers of the field, starting with his study in the laboratory of Professor Clyde Hutchison Jr., followed by 46 years at Bruker. These years provided the community with spectrometers of increasing sensitivity and flexibility of CW and pulsed

EPR performance, and most recently, rapid scan EPR capability. Dr. Heiss also championed new applications of EPR in research and in industry.

With best wishes from colleagues, including the attendees of the 60th Rocky Mountain Conference on Magnetic Resonance, and the 42nd International EPR Symposium.



Photograph of Bleaney's magnet, Sandra S. Eaton, Gareth R. Eaton, and Arthur H. Heiss, during the RSC meeting at Oxford in 2017.

Chemistry. Art knew every detail of the spectrometer and he knew the US EPR customers and their applications. He knew the American market and he did not tire of teaching us what to do and how to behave. Art is not only an excellent sales man, he has been and still is an important member of the development team. He cares honestly about his customers and his input is indispensable." Two decades later, this assessment remains on-target.

Early in the development of EPR Hutchison worked with Bleaney in Oxford, so it was a

pleasure in 2017 to visit the Oxford lab and see that the magnet that Bleaney used was still in service.

Art has been a strong supporter of the annual EPR Symposium (the Denver meeting), so it was apropos that he announced his transition at the Bruker EPR User meeting in Denver July 21, stimulating the following thanks (see plaque) which was signed by many attendees.

Gareth R. Eaton and Sandra S. Eaton

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Conference reports

EasySpin Academy 2019
August 26–28, 2019, Seattle WA,
United States

From Aug 26 to Aug 28, 2019, the research group of Stefan Stoll at the University of Washington in Seattle organized a two-day workshop about using the software package EasySpin to simulate, fit, and analyze EPR spectra. EasySpin is a MATLAB-based toolbox developed by Stefan Stoll and others. The workshop, titled EasySpin Academy 2019, was targeted towards graduate students and postdocs with little or no experience with MATLAB or EasySpin. It was attended by 20 students from various universities and research institutions in the United States.

The workshop covered the basics of MATLAB and EasySpin; data import and export; the simulation of continuous-wave EPR spectra in the liquid state, the solid state (powders and crystals), and the slow-motional regime; least-squares fitting; spin operators, Hamiltonians, and energy level diagrams; the simulation of pulse EPR and ENDOR spectra; the calculation of EPR spectra from molecular dynamics trajectories; interfacing EasySpin to the quantum chemical software ORCA; pulse shaping and advanced spin dynamics.



Participants, instructors, and tutors at the EasySpin Academy 2019 in Seattle.

The workshop was organized into ten hands-on sessions over two days. The sessions were based on worksheets. Instructor demonstrations alternated with participants working

on exercises from the worksheets. Multiple tutors from the Stoll research group assisted students in working through the exercises.

Stephan Pribitzer
University of Washington

Market place

POSITIONS

Bruker EPR Opening

The EPR Division of Bruker BioSpin has two openings for the Billerica, MA, USA office.

Application Scientist

• Ph.D. in the following areas is a prerequisite for this position: Chemistry, Biochemistry, Physics, Molecular Biology.

• Postdoctoral experience is desirable.

• U.S. Citizenship or U.S. Permanent Resident status required.

The official posting is at:

<https://englishcareers-bruker.icims.com/jobs/7800/epr-application-scientist--bruker-biospin-epr-team/job?hub=12&mobile=false&width=940&height=500&bga=true&needsRedirect=false&janIoffset=-300&junIoffset=-240>

<https://englishcareers-bruker.icims.com/jobs/7795/field-service-engineer---bruker-biospin-epr/job?hub=12>

Field Service Engineer

• Minimum 3 years Life Sciences Field Service work experience diagnosing and repairing complex mechanical, electromechanical and/or electronic equipment required with demonstrated mathematical abilities.

• Bachelor Degree desirable in Electrical Engineering, Electronics, Chemistry related fields.

• U.S. Citizenship or U.S. Permanent Resident status required.

The official posting is at:

<https://englishcareers-bruker.icims.com/jobs/7795/field-service-engineer---bruker-biospin-epr/job?hub=12>

EQUIPMENT

Available: Affordable pulsed upgrade to Bruker CW EMX system

NEW! MR lab at the Technion offers a very affordable upgrade of Bruker EMX CW ESR and Varian CW ESR systems to a modern pulse ESR.

For details: <https://mr-lab.technion.ac.il/files/2019/03/Upgrade-of-Bruker-and-Varian-CW-ESR-to-Pulse-ESR-1.pdf>

Aharon Blank, ab359@technion.ac.il

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: 1-920-889-3893, e-mail: janderson36@wi.rr.com

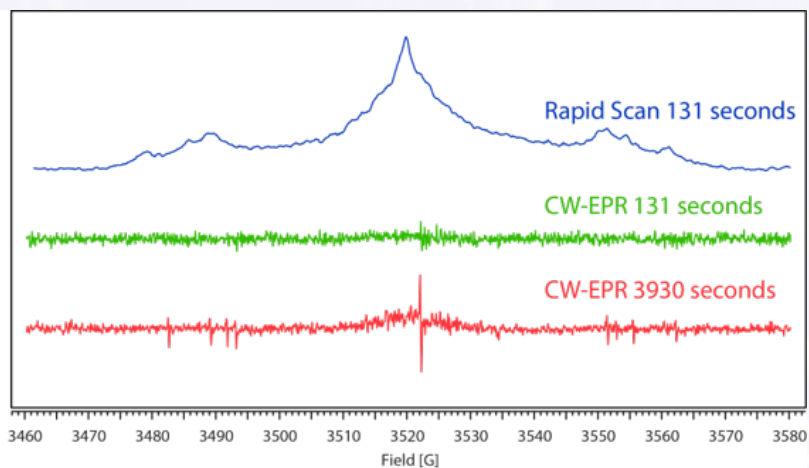
EPR parts, electronics and hardware

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

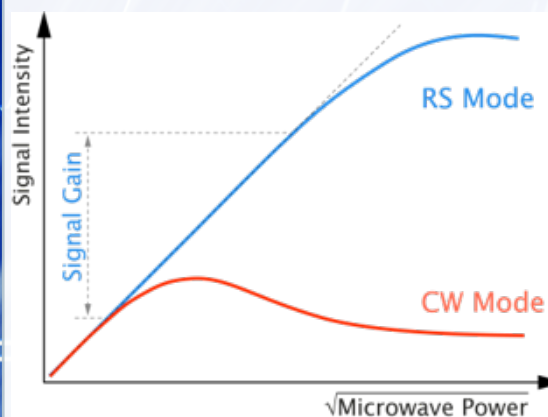
Please contact: techepr03@gmail.com for availability and pricing.



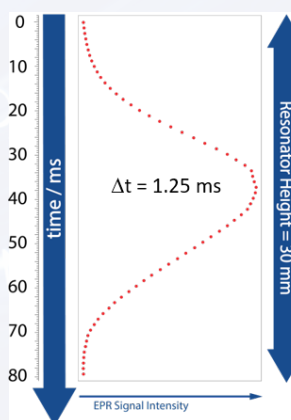
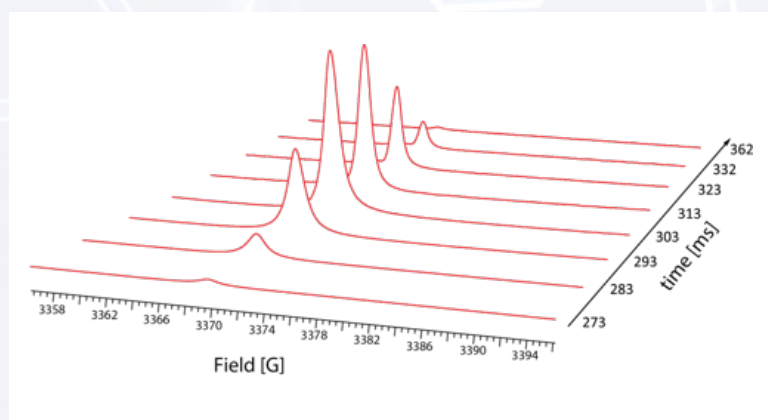
Single Nitrogen Substitution P1 Center in Diamond.



RS-EPR vs. CW-EPR saturation curves.



Free fall of BDPA sample followed by RS-EPR.



A Revolution in EPR - Increasing Sensitivity and Time Resolution

To overcome the limits of sensitivity in conventional CW-EPR, the new Rapid Scan EPR technique takes advantage of the later onset of signal saturation that allows higher microwave powers to be used.

The increase in signal due to the higher power leads to the improvement in signal to noise.

With the high scan rates in RS-EPR the full EPR spectrum of short lived species can be observed and the changes can be followed with unprecedented time resolutions as low as 10 microseconds.

- Sensitivity increase due to later onset of saturation
- High scan rates resulting in high time resolution for full spectrum acquisition



The Rapid Scan accessory comprises the following components :

- | | |
|----------------------------------|---------------------------|
| 1. RS Driver | 5. RS Coils |
| 2. RS Acquisition Unit | 6. Water cooler for coils |
| 3. RS Resonator | 7. Capacitor unit |
| 4. MW Frontend with I/Q Detector | |

A Revolution in EPR - Introducing the Rapid Scan Accessory

RS-EPR is a revolutionary technique that opens new possibilities not previously available with conventional CW-EPR. With an increase in the signal to noise ratio and a decrease in the acquisition time, RS-EPR can probe very low concentrations and very fast reactions.

- Field scan width: up to 200 G per segment
- Field scan times: as low as 10 microseconds
- Compatible with EMXplus and ELEXSYS (10" magnet)
- Compatible with all variable temperature accessories