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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 Stefan Stoll, recipient of the IES Silver Medal for Instrumentation and Methods 2021. It shows the logo of EasySpin, a free and open-source software created by Stefan Stoll for simulating and fitting EPR spectra. You can take EasySpin to get almost anywhere in the EPR world!

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Editorial





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Editorial

Dear colleagues,

It is a great pleasure to start this issue of the *EPR newsletter* with the words of gratitude from our President, Songi Han, to our long-term sponsors, Bruker BioSpin and JEOL, for their 30-year support of the IES (p. 3). Support from our sponsors is extremely important for the IES and enables us to implement all our diverse activities. It is great that our sponsors realize that to support science is a win-win situation and I'm sure our members agree. In their statements, Falko Busse, President Bruker BioSpin, and Takahiro Anai, President of JEOL RESONANCE Inc, said that they are proud to contribute to the IES and will continue to support scientists (pp. 2, 3).

Over the last thirty years the list of sponsors has varied quite a lot, but irrespective of the level or the duration of the support, our society is grateful to all of them.

In the *EPR newsletter* 3/1-4 of 1991, Bruker and JEOL were announced as sponsors of the newly born International EPR (ESR) society, the same as Medical Advances, Oxford Instruments, Wilmad Glass Co., Norell Inc., Micronow Instruments, CRC Press Inc., Scientific Software Services, and Sumitomo Special Metals Co., Ltd. Some company profiles were published (see 3/4, pp. 11–14). It was a good idea to give personal touch to the presentation of our sponsors in addition to advertisements published in each issue of our publication, the same as latterly we have regular columns featuring prima donnas of magnetic resonance, and young researchers, who make the first steps to the heights of their scientific careers. To this end, in the forthcoming issues, we plan to include interviews of our current sponsors. We will start learning about their companies from Jeffrey Jeffrey Hesler (Virginia Diodes) and Thorsten Maly (Bridge12).

One may anticipate interesting revelations. For example, Reef (Philip D., II) Morse, founder of Scientific Software Services (its profile was published in the *EPR newsletter* 3/4, p. 11), shared with our readership his passion for teaching EPR to middle or high school students (see, e.g., 26/2, p. 25). Judging by an EPR Haiku Reef recently sent me, he seems also to be interested in Japanese poetry:

> Electrons spinning In a magnetic field. I sense their presence.

Well said, isn't it?

You are welcome to take a flight with EasySpin (a terrific cover designed by Sergei Akhmin!) and read the success story of Stefan Stoll, IES Silver Medal Awardee 2021 and yes, Stefan is true to himself: never tired of submitting material for his Software column! This time it is "LongDistances – A Program to Analyze DEER Data" by Christian Altenbach. Czesław Rudowicz and Piotr Pietrzyk present a detailed story about the development of the Polish EMR group (pp. 6–8). This story may be considered as a preamble of a story "EPR in Poland", which is under preparation by the same coauthors for publication in the *EPR newsletter*.

In this issue, we say farewell to Konstantin Ivanov, brilliant scientist, great colleague, and dear friend Kostya (p. 9). In the prime of Konstantin's creativity and scientific potential, the thread of his life was mercilessly torn by coronavirus. Our heavy loss is irreplaceable. Our grateful memory will keep Kostya alive for the years to come.

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: https://ieprs.org.





Falko Busse, President Bruker BioSpin:

"Bruker is so proud to be a long-time partner of IES. With new innovations like our Magnettech ESR5000 and the Rapid Scan unit, continued advancements in various EPR applications, and a brand new customer experience center opening in Ettlingen, Germany,



we look forward to what the future holds not only for Bruker, but for the EPR community."

IES Business

30 Years of Bruker BioSpin and JEOL Sponsorship of the IES

A s the President of the IES, it is my great pleasure to use our *EPR newsletter* as a forum to highlight the important contributions of our corporate sponsors to our society. A special shoutout goes to our long-term sponsors, Bruker BioSpin and JEOL. Let me highlight their contributions to the IES and the EPR community.

First of all, congratulations to 60 years of Bruker BioSpin! The IES celebrated 50 years of Bruker with a special issue of our publication (https://ieprs.org/newsletter/vol-20-4) in 2011, and here we are again, with the EPR community looking as vibrant as ever and the importance of EPR in research and commercial enterprises steadily gaining in profile. The current issue of the *EPR newsletter* includes a highlight of Bruker EPR products developed over the last ten years and important milestones of Bruker Magnetic Resonance from the past 60 years (third and fourth cover pages).

Bruker was founded in 1960 and the IES society was formed in 1989. As early as January 1991, it was published in the *EPR newsletter* 3/1 that "The IES is pleased to announce that Bruker Instruments has joined the Society as a Patron". Hence, as of today, Bruker is a patron of the IES for 30 years.

The contribution by Bruker BioSpin to the EPR community includes the Bruker Prize (established in 1986), awarded in 2021 to Michael Wasielewski ("Exploiting Photogenerated Radical Pairs as Electron Spin Qubits for Quantum Information Applications" http:// www.esr-group.org/bruker-lectures), as well as the Bruker Thesis Prize (established in 2015), with the 7th Bruker Thesis Prize awarded in 2021 to Daphné Lupert-Percuel ("Combining Film Design and Spectroscopic Strategies to Elucidate Triplet Dynamics in Molecular Systems" http://www.esr-group.org/brukerthesis-prize). Bruker BioSpin also supports many magnetic resonance conferences.

JEOL is another 30-year sponsor of the IES, starting its support in 1991 as a contributor and becoming a major sponsor in 2010. JEOL's contribution to the EPR community includes support for many magnetic resonance conferences. In 1997, JEOL established the JEOL prize focused on highlighting the accomplishments of the next generation scientists (http://www.esr-group.org/jeol-lectures). The 2021 winner of the JEOL prize is Nino Wili on "Dressing up electron spins to (un) lock their potential: Application to distance measurements between trityl radicals" with



Annalisa Pierro and Katherine Richardson as the runner ups.

The IES is grateful to its long-term sponsors, as well as its many other corporate sponsors small and big, and knows that a robust exchange of research, development and talent flowing between the research community and corporations is a critical backbone of our EPR community. We look forward to highlighting innovative developments, products and services by other corporate sponsors in future *EPR newsletter* issues.

Songi Han



Takahiro Anai, President of JEOL RESONANCE Inc.: "JEOL is a rare company in the world that has been developing and selling ESR equipment for 64 years since it started selling JES-1 ESR

equipment in 1957. JEOL has many types of analytical instruments, and as a member of the JEOL Group, JEOL RESONANCE is a com-



pany that specializes in the development and manufacture of NMR and ESR equipment, and supplies equipment all over the world. We are proud to have contributed to IES as a sponsor, and will continue to support scientists who are conducting research using ESR and contribute to the development of science."

2021 IES Silver Medal for Instrumentation and Methods

Stefan Stoll

It is a great honor for me to receive the 2021 Silver Medal for Instrumentation and Methods from the International EPR Society. According to the citation, the Medal is awarded predominantly for my contribution to the EPR community for developing and maintaining EasySpin, a Matlab-based software package for the simulation and analysis of EPR spectra, so I would like to focus this article on that.

EasySpin has become an important computational tool for many EPR researchers in physics, chemistry, biology, materials science, and related fields. The development of new tools and instruments is a crucial driver of scientific progress. As chemist and inventor Sir Humphry Davy writes in his Elements of Chemical Philosophy (1812), "Nothing tends so much to the advancement of knowledge as the application of a new instrument." (Introduction, p.54) Interestingly, the 2021 Silver Medal for Instrumentation and Methods is the first one awarded for a computational tool, as all the previous Medals honored the development of novel instrumentational methodology. In my view, this parallels the increasingly important role of computation in science in general, particularly since the turn of the century. EasySpin, although only a small package in a small field, is evidence of this trend.

Let me recount some of the context that led EasySpin to its place today. Some technical (but by now a bit outdated) details about EasySpin have appeared in a separate issue 25/3-4 of the EPR Newsletter in 2015. The journey for EasySpin started long ago, when I was a graduate student in Arthur Schweiger's lab at ETH Zürich (1998-2003). At the time, research projects in the Schweiger lab were revolving around developing new pulse EPR sequences to measure spin Hamiltonian parameters more accurately. Most investigated samples where test systems like irradiated malonic acid and the E' center in quartz, but a few projects were application focused and investigated transition metal complexes obtained through collaborators. One of these projects was mine, involving the study of the electronic structure of a series of cobalt complexes with resolved nitrogen ligand superhyperfine splittings. After obtaining a series of frozen-solution CW EPR spectra, I looked for software to fit a spin Hamiltonian model



to these spectra. To my surprise, it turned out that nobody in the lab had an adequate program for simulating solid-state CW EPR spectra of transition metal complexes. Most people were using Mathematica or the C++ library Gamma to calculate and simulate density matrix dynamics. So, driven by my need for a CW EPR simulation program, I set out to write one, and on the way developed some novel algorithmic approaches. Soon, a few other labs started using it for their CW EPR simulation needs. I even recall an instance where some senior folks from Bruker BioSpin were sitting down with me at my desk at ETH Zürich to learn more about EasySpin.

Since my graduate times, EasySpin has grown substantially and organically, with new features added over the years based on my needs and the needs of others: liquids EPR, ENDOR, pulse EPR, slow-motion EPR, magnetometry, molecular-dynamics-based EPR, and most recently rapid-scan EPR. As a result, EasySpin has become more comprehensive over time, almost to a fault: It is becoming increasingly difficult for a single person to maintain the code base. There are so many different concepts and algorithms implemented in EasySpin that is impossible to have all of them mentally present at all times. Tracking down subtle bugs in some of the more complex areas of the code base, such as molecular-dynamics-based EPR and pulse EPR, has become a nontrivial and time-consuming activity.

Prior to my appointment at the University of Washington in Fall 2011, the entire EasySpin code base has been written by me. Since then, EasySpin has seen significant contributions from others as well. Peter Martin, then a graduate student in Dave Thomas' lab at University of Minnesota, incorporated his work on molecular-dynamics-based EPR simulations into EasySpin. He had to learn Matlab for this, as his original code base was written in Python. Stephan Pribitzer, then a graduate student with Gunnar Jeschke at ETH Zürich and now a postdoc in my group, incorporated his advanced pulse EPR simulation software Spidyan into EasySpin. In both cases, it was their initiative, and the main intent was to preserve the work for posterity and to make sure the EPR community will have continued access to it. Claudia Tait, a postdoc in my group and now at University of Oxford, contributed all the pulse shaping capabilities. Joscha Nehrkorn, another postdoc in my group, contributed support for orbital angular momenta and spin-orbit coupling in the Hamiltonian. Further contributions came from Matt Krzyaniak (Northwestern) and Luis Fabregás-Ibáñez (ETH Zürich).

Any released version of EasySpin has a oneto-two-year expiration date, meaning that after this time it ceases to work and a new version needs to be downloaded. Initially, this generated some complaints from users, as it was disrupting their workflow. The main reason behind this "time bomb" mechanism is to prevent potentially buggy old versions of EasySpin, and possibly incorrect simulations and scientific conclusions, to persist in the community. Originally, the source code was kept close for the same purpose. Thankfully, EasySpin was tested well enough from the beginning so that the scenario of a serious bug never materialized. Therefore, after extending and reinforcing our test system, in March 2020 we decided to make EasySpin open source via a GitHub repository (https://github.com/ StollLab/EasySpin). This is for developers only; tested and packaged versions suitable for users continue to be available via EasySpin's main website (https://easyspin.org). Going open source hopefully encourages other EPR researchers to contribute to the code, be it as bug fixes, new features, additional examples, or improvements in the documentation. Eventually, this will mean that my unlimited decision power as the "benevolent dictator for life" (a role common in many small and large opensource software projects) of EasySpin might be transferred to a larger core development team, possibly supported by a more strategically oriented steering committee. I truly hope that community engagement will increase to a level where such a transition makes sense.

It is impossible to overemphasize the roles users play in improving EasySpin. Users have identified countless weaknesses and bugs in EasySpin and reported them either by email or via the EasySpin user forum. EPR conferences and, in particular, the EPR summer schools organized by the European Federation of EPR groups (EFEPR) have been very important venues for feedback collection. At these events, I personally hear from many users about their issues and qualms with EasySpin. While I am able to help in many cases right away, there is always a series of issues that need to be jotted down and addressed when back in my office in Seattle. Participants in the 2019 and 2020 editions of the EasySpin Academy also provided an immense amount of usability insight and feedback. Both eventbased and online user feedback is crucially important and catalyzes changes that make EasySpin better for everyone.

One aspect that is often underappreciated by outsiders is how much infrastructure work is involved in making software tools like EasySpin production-ready, so that they can be used by others. It requires extensive and automated testing, packaging, thorough documentation, maintenance, and lots of time available for support via the forum and via email. To picture this, imagine all development you would need to do and processes you would need to implement in order to turn your home-built spectrometer into a successful commercial spectrometer that can be set up and run in many labs.

Unfortunately, most research funding mechanisms do not support this infrastructure work necessary to create and maintain widely deployable scientific tools. In fact, EasySpin never has had dedicated funding. It was developed as a tool in the context of and alongside with other specific research projects. Only recently have funding agencies in the United States started to recognize the importance of investing into well maintained computational infrastructure for the scientific enterprise. Therefore, it looks feasible in the near future to apply for some dedicated funding for EasySpin.

Where does the field of EPR stand in terms of software infrastructure? In my view, there is an urgent need for more EPR community tools. Many of the essential computational tools in EPR have been and are products of the amazing dedication of focused individuals (Ilya Kuprov with Spinach, Gregor Hagelueken with mtsslSuite, Gunnar Jeschke with MMM and DeerAnalysis, Boris Epel with SpecMan4Epr, and many others present and past). It is very concerning that there is not a single community-developed EPR software. If past experience is any guide for the future, this does not bode well. Software packages stop being developed once the main person behind changes focus, loses interest, retires, or deceases – prime examples are John Weil's EPRNMR and Graeme Hanson's Sophe.

To avoid such destiny, community-based approaches are needed. I think efforts in that direction should be undertaken, either through bodies like the International EPR Society, or through community funding mechanism. There is no lack of ideas or needs. For example, it would be tremendously beneficial to have a curated and richly annotated searchable database of experimental continuous-wave EPR spectra that can be integrated with simulation tools such as EasySpin. The DEER community also needs a database for depositing experimental DEER data that integrates with analysis software. It might be tempting to think that this should be the purview of commercial efforts. While some EPR tool development such as spectrometers and resonators is commercially sustainable, EPR-dedicated scientific software does not lend itself to a sustainable business model, mostly because the total addressable market is fairly small and consists mostly of cash-strapped academic labs. Therefore, the community needs to come together to find ways to fund, develop, and maintain free open source software tools. These are crucial in enabling, supporting and increasing the productivity of researchers that use EPR spectroscopy.

IES Best paper Award, 2020/2021

Luis Fábregas Ibáñez ETH Zuerich

DeerLab: a comprehensive software package for analyzing dipolar electron paramagnetic resonance spectroscopy data. J. Magn. Reson. 1,2020. Additional authors: Gunnar Jeschke, and Stefan Stoll

Michal Kern

University of Stuttgart

Hybrid Spintronic Materials from Conducting Polymers with Molecular Quantum Bits. Adv. Funct. Mater. 31, 2020. Additional authors: Lorenzo Tesi, David Neusser, Nadine Rußegger, Mario Winkler, Alexander Allgaier, Yannic M. Gross, Stefan Bechler, Hannes S. Funk, Li-Te Chang, Jörg Schulze, Sabine Ludwigs, and Joris van Slageren

Nandita Abhankar

University of Maryland, NIST Scalable microresonators for room-temperature detection of electron spin resonance from dilute, sub-nanoliter volume solids. Science Advances 6, 2020. Additional authors: Amit Agrawal, Pragya Shrestha, Russell Maier, Robert D. McMichael, Jason Campbell, and Veronika Szalai

2021 Bruker Prize

Professor Michael Wasielewski Northwestern University, Evanston, IL USA

Awarded for the development and application of Electron Paramagnetic Resonance to the study of photochemical and photophysical processes.

Bruker Thesis Prize 2021

Dr. Daphné Lubert-Perquel Imperial College London, UK Awarded for her talk "Combining Film Design and Spectroscopic Strategies to Elucidate Triplet Dynamics in Molecular Systems"

JEOL Prize 2021

Nino Wili ETH Zurich, Switzerland Awarded for his talk "Dressing up electron spins to (un)lock their potential: Application to distance measurements between trityl radicals"

2021 EAS Award

Professor Song-I Han University of California Santa Barbara, CA USA for Outstanding Achievements in Magnetic Resonance.

JEOL Prize 2020

Dr. Gabriel Moise University of Oxford, UK Awarded for his talk "Spin delocalisation and fine-structure mysteries of the photoexcited triplet state of metalloporphyrins"

The Polish EMR Group reaching maturity at 10th+ Anniversary

The 10th anniversary of establishment of L the Polish Electron Magnetic Resonance Group (PL EMR Group) is a suitable occasion to briefly present the history and current status of the Group. The Group came into being during the Inaugural Meeting held during the First Forum EMR-PL in Rzeszów on 20th of May 2010 (see, Fig. 1). The Meeting was attended by the thirty-seven researchers from all major EPR research centers from all over Poland. The two major goals of the Forum were: (i) to discuss scientific, organizational and financial matters related to the planned new shape of the Polish EPR Society and (ii) to integrate the community of Polish scientists who used EMR spectroscopy in their research, and people working on the development of instrumentation or industrial applications of EMR techniques. A complementary, yet very important, goal was to commemorate Professor Jan Stankowski, who died in September 2009. Prof. Stankowski had spearheaded establishment of the Institute of Molecular Physics (IMP) in Poznań as an independent institution of Polish Academy of Science (IMP PAS). He was highly regarded as pioneer and later doyen of EPR research in Poland, a scientist with significant achievements and wide recognition in the world.

The Polish EMR Group has succeeded the Polish EPR Society, which had existed with varying success from 1995 until 2010. The idea of the then Polish Society for Research in EPR was first floated at the 1st EPR Meeting organized by Profs. Hanna Ambroż and Jacek Michalik in Zakopane in 1993. The Founding Board was formed with Prof. Ambroż as the President and Profs. Zbigniew Kęcki and Jacek Michalik as members. The Founding Meeting of the new Society was held in 1995, whereas its first Congress was organized in Warsaw in 1996 (presentations given at this Congress were published in Nukleonika in 1997). A new Board of the Society was elected in 1998 and Prof. Stankowski became its President. Therefore, the seat of the Society moved to the IMP PAS in Poznań. Informal meetings of the Society's members were held during subsequent RAMIS. According to Prof. Andrzej Więckowski, who was the then Society's Treasurer, the penultimate formal Meeting of the Society took place in 2001, whereas the last one at RAMIS-07 in Bedlewo in April 2007. At the latter Meeting one of the Authors of this note (Cz. R.) become elected as the Polish EPR Society President at the recommendation of Prof. Stankowski.

Two personal (Cz. R.) remarks are pertinent to explain the background for the idea of the transition from the Society (PL EPR Society) to the Group (PL EMR Group). While in Poznań, visiting his mother's grave before All Saints' Day (1 November) in a close-by main alley, he noticed a new grave with the familiar name: Jan Stankowski. What a shock, as the news about untimely passing away of Prof. Stankowski in September 2009 did not reach him. Later it has transpired that the



Fig. 1. Group photo of the Inaugural Meeting participants at the First Forum EMR-PL



general information sent by the IMP PAS in Poznań, also to his then workplace - Institute of Physics at West Pomeranian University of Technology in Szczecin, has not been passed by the Secretary. In addition, the two years' experience as the PL EPR Society President has amply shown that having a formal Statute and the membership fees proved to be a highly impractical solution for a small professional Society. The above events have triggered this idea.

The participants of the Inaugural PL EMR Group Meeting in Rzeszów have unanimously approved the proposal, put forward by Prof. Czesław Rudowicz to transform the Society into its modern reincarnation based on newly devised principles. The change of name from 'EPR' (20 votes) to 'EMR' (15 votes) has gained a mixed support at the Meeting and the new name was adopted later based on the polls from the whole EMR (EPR) community in the country. Interestingly, similar attitudes were noted during the formation of the Asia-Pacific EPR/ESR Society. Back than in 1997 it was also hard to achieve consensus and it was decided to retain both EPR/ESR in the name of the fledging Society. It is also reflected in the APES logo. However, the more general name, electron magnetic resonance (EMR), which corresponds well to the more ubiquitous NMR (nuclear magnetic resonance), has gained wider usage nowadays. The name EMR encompasses the historically original names: electron paramagnetic/spin resonance (EPR/ ESR) and other related techniques such as, e.g. ferromagnetic/antiferromagnetic resonance (FMR/AFMR).

At the Inaugural PL EMR Group Meeting, the participants have adopted a non-profit model where no membership fees are charged and resigned from having a formal Statute. The informal membership in the Group has been extended to all persons, also outside academia, involved in the broader subject of EMR (EPR/ESR) research or who have an interest in the practical applications of the EMR techniques. The organizational structure of the PL EMR Group Council included the following positions: Chairman, 1st Vice Chairman (the person organizing a given Forum), 2nd Vice Chairman (the person organizing next Forum), and Secretary. This structure has ensured smooth activities of the Council as well as organization of the subsequent Fora.

Both initiatives, the foundation of the Polish EMR Group and the series of the Forum EMR-PL organized under the Group auspices every other year by an Organizing Committee from different EMR laboratory in Poland, have originated from the previous 'Far-East Asian' experience of Prof. Rudowicz. To a large extent, there is a pronounced parallel, although on a smaller scale, between Polish initiatives and the Asia-Pacific EPR/ESR Society (APES) established by Prof. Rudowicz with support of a group of eminent researchers from this geographical region during the First Asia-Pacific EPR/ESR Symposium (APES'97) held at the City University of Hong Kong, 20-24 January 1997. The APES organizational model has served very well the regional Asia-Pacific as well as the international EPR/ ESR community. The Asia-Pacific EPR/ESR Society is in full strength and celebrated its 20th+ Anniversary. The Commemorative Symposium APES'18 was held in Brisbane, Australia, in September 2018 (see, the article in EPR newsletter 2019 vol. 29 no. 1, p. 10).

It is a great satisfaction to all members that the Polish EMR Group is 'alive and kicking' after more than 10+ years in existence and suits well the needs of the Polish EPR/ESR community. The + sign at the numbers: 20+ and 10+ requires some explanations. Interestingly this (+) constitutes another parallel between the APES and the PL EMR Group since history repeats itself. Because of the SARS epidemic in South-East Asia during early 2003, the APES Council decided to move the 2003 events to November 2004. Hence, starting from the APES'04 the Symposia moved to even-number years, resulting in a one-year shift in our subsequent anniversaries. Thus, the 20th APES anniversary was falling in 2018 instead of 2017. At the 4th APES'04 held at the Indian Institute of Science, Bangalore, India, November 2004, Prof. Rudowicz stepped down as the APES President after three terms of office (one as the Provisional and two as the elected President) as stipulated by the APES Constitution. Then he became the Founder President and the ex-officio member of the APES Council. In February 2005 he returned to native country to take position at the West Pomeranian University of Technology in Szczecin.

Organization of the First Forum EMR-PL, as well as all subsequent Fora, had been implemented successfully due to dedicated efforts of researchers working as members of the respective Local Organizing Committees (LOC) and Scientific Committees. The fact that the First Forum was organized from scratch in the span of about half a year is in itself a success. This was largely due to Dr. Ireneusz Stefaniuk as the LOC Chairman and his team at the University of Rzeszów as well as financial support, especially, from the Institute of Physics of that university, the IMP PAS, and the Institute of Physics of the West Pomeranian University of Technology in Szczecin. Apart from regular EPR talks, a commemorative session dedicated to Prof. Jan Stankowski was organized. Nearly 50 papers out of all presented at the First Forum EMR-PL have been published in the Special Issue of Current Topics in Biophysics online (CTBo): "Current status and perspectives of EMR (EPR/ESR) research in Poland". This Issue may be considered as a success of the Polish EMR community and, to a great extent, as Prof. Stankowski's legacy. Shortly after its inception, the PL EMR Group became affiliated with the European Federation of EPR Groups (EFEPR).

Important milestones in the PL EMR Group's history may be summarized as follows. Each subsequent Forum EMR-PL, starting from the Second one, was organized under the auspices of the Group. The members of the PL EMR Group Council were serving on either the LOC or the Scientific Committee. During each Forum the General Meeting of the PL EMR Group were conducted that included Chairman's Report, discussion, selection of the venue for next Forum, and election of the new Council.

The Second Forum EMR-PL was organized by the LOC headed by Prof. Kazimierz Dziliński from the Institute of Physics, Częstochowa University of Technology. It was held on May 16-18, 2012 in Hucisko (scenic part of Jura Krakowsko-Częstochowska Nature Park). All together 19 talks and 46 posters were presented at this Forum. Selected papers were published in the Special Issue of Nukleonika (International Journal of Nuclear Research). At the General Meeting the organizational structure of the PL EMR Group Council was amended by including three additional positions: Previous Immediate Past Chairman (position to be filled if the next Chairman is elected), Member, non-elective Member (website administrator).

The Third Forum EMR-PL was organized by the LOC headed by Prof. Zbigniew Sojka from the Faculty of Chemistry, Jagiellonian University. It was held on 23–25 June 2014

> in Kraków. The special occasion of the 650th anniversary of establishment of the Jagiellonian University, the historically first University in Poland added special importance to the Third Forum EMR-PL. Two invited speakers Profs. Jerzy Krzystek and Andrzej Ożarowski (the National High Magnetic Field Laboratory, Florida State University, Tallahassee, USA) were special guests of the Third Forum. The scientific program (36 talks and 43 posters) included materials session, physical and instrumentation session, chemical and biological sessions, all devoted to the applications of EMR, followed by MagComp theoretical and computational session. Papers



Fig. 2. Group photo of the participants of the Fourth Forum EMR-PL.



Fig. 3. Group photo of the Fifth Forum EMR-PL participants during the mountain trip.

presented at that Forum were published in the Special Issue of Nukleonika.

The Fourth EMR-PL Forum was organized by the LOC co-headed by Profs. Wojciech Kempiński (IMP PAS in Poznań) and Ryszard Krzyminiewski (Faculty of Physics, Adam Mickiewicz University in Poznań). It was held on June 27-29, 2016 at the Morasko University campus (see, Fig. 2). Two eminent EMR researchers from abroad were invited as plenary speakers: Profs. Hitoshi Ohta (President of the International EPR/ESR Society and Head of the Molecular Photoscience Research Center at Kobe University, Japan) and Klaus Lips (Vice-President of the European Society for Quantum Solar Energy Conversion and Head of the Energy Materials In-situ Laboratory Berlin at Free University Berlin, Germany). Twenty-seven oral and thirty-two poster contributions were arranged into the scientific sessions devoted to: modern EMR techniques, EMR in physics, chemistry and material research, quantum-chemical modelling and spectra simulation, EMR in biology and medicine, physical fundamentals and novel topics in EMR. Proceedings of the Fourth Forum EMR-PL have appeared in the Special Issue of Acta Physica Polonica A.

The Fifth EMR-PL Forum was organized by the LOC headed by Profs. Maria Jerzykiewicz and Julia Jezierska from the University of Wrocław. It was held on June 5-8, 2018, in the picturesque mountain spa resort Kudowa Zdrój (see, Fig. 3). One invited speaker Prof. Ram Kripal (Department of Physics, University of Allahabad, Allahabad in India) was special guest of the Forum. Twenty talks and twenty-nine posters were presented. Topics included EMR of transition-metal ions and nanoparticles, spin labelling, modelling of spin Hamiltonian parameters, free radical chemistry, high-field EPR. Due to Prof. Kev M. Salikhov, Chief Editor of Applied Magnetic Resonance (AMR), selected refereed papers presented at this Forum were published in the Special AMR Issue dedicated to Polish EMR Group meeting 2018. Two important decisions have been taken at the General Meeting of the PL EMR Group held during this Forum. Prof. Piotr Pietrzyk (Faculty of Chemistry, Jagiellonian University) has been unanimously elected the Chairman-Elect. In view of the pending resignation of the current Chairman, it was envisaged to create a new position in the PL EMR Group Council: Founder Chairman.

The Commemorative Sixth Forum EMR-PL was to be held in Szczecin, Poland, 2-5 June 2020. Its organization by the LOC headed by Prof. Nikos Guskos was in full swing from the end of 2019. That Forum was to be very special, as we would be celebrating the 10th Anniversary of our existence. Two researchers from neighboring countries have accepted our invitation as Plenary Speakers: Prof. Vlasta Brezova, Slovak University of Technology, Bratislava, Slovakia, and Dr. Peter Neugebauer, Central European Institute of Technology (CEITEC), Brno, Czech Republic. Regrettably, because of the SARS-Cov19 pandemic in Poland and all over the world, in spring 2020 the PL EMR Group Council was forced to postpone the Sixth Forum till 2021. In view of the outbreak of pandemic in 2020, the decision to elect Prof. Piotr Pietrzyk as the Chairman-Elect during preceding Forum in 2018 has proved crucial for smooth transition. However, with the second and possibly the third wave of pandemic looming, we may not be able to organize the next Forum in the usual mode in the foreseeable future. Hence, contingency planning to hold the Sixth Forum EMR-PL on-line are under way.

Over the first 10+ years the Polish EMR Group has evolved becoming a virtual professional Group, i.e. with a flexible organization model encompassing all researchers working in EMR/EPR/ESR and related areas, but importantly having a real presence in the Polish EMR community. For more information on the PL EMR Group activities and the next Forum EMR-PL please visit our websites: <http://pgemr.org> and <http://emr6.zut. edu.pl>, respectively.

Czesław Rudowicz Chairman, Polish EMR Group Piotr Pietrzyk Chairman-Elect, Polish EMR Group (In consultation and on behalf of the members of the PL EMR Group Council)

Konstantin L'vovich Ivanov (1977–2021)

"The candle that burns twice as bright, burns half as long"

On March 5th, after a brave two-weeks struggle against COVID in intense care, our friend and colleague, Professor Konstantin L'vovich Ivanov, known to his friends as Kostya, passed away in hospital at the age of only 44. We mourn for Kostya not only as the most talented Magnetic Resonance Theoretician of his generation, but also as a good friend, an excellent collaborator, a great colleague, and a scientist who actively stimulated and organized contacts between his home institute, the International Tomography Center in Akademgorodok, the scientific district of Novosibirsk, Russia, and many scientific institutions all over the globe.

Kostya was born in Akademgorodok on January 10, 1977. He studied Physics at the

Novosibirsk State University (NSU), specializing on Chemical Physics. In June 1998 he obtained his Bachelor's degree under the supervision of Dr E. M. Glebov and Prof. V. F. Plyusnin studying a photo-reaction in solutions and two years later his Master's degree under the supervision of Prof. N. N. Lukzen in the group of Theoretical Chemistry, who would become his scientific mentor for the next few years. Only two years later Kostya successfully defended his PhD thesis «Kinetics of diffusion-controlled reactions of radical recombination and energy and electron transfer processes», supervised by R. Z. Sagdeev and N. N. Lukzen at the International Tomography Center (ITC) and graduated Summa cum Laude. In the same year he married with Elena Kargapoltzeva, and in 2010 their daughter Kseniya was born.

After his doctorate he entered in collaboration with experimental groups at ITC (A. Yurkovskaya) and FU Berlin (H. M. Vieth) the scientific field of hyperpolarization, in which he soon developed into one of the leading players of the field by developing a series of important theoretical concepts which shaped the field and lead the development of new and more efficient experimental tools. The result of this scientific endeavor was not only his Second Doctorate (the Russian equivalent to the habilitation, known in German speaking countries) with his masterly thesis "Kinetics of multistage liquid phase processes involving particles with spin degrees of freedom" but also the establishment of several large scale international collaborations such as the EU COST action of hyperpolarization, where he headed the theoretical group, the EU DNPdesign evaluation and many others and the realization of the roles of scalar interactions and Level Anti-Crossings in SABRE and related techniques. In 2016 Kostya was finally appointed to Professor of Physics and in 2018 he became the Director of the ITC.

With his never-ending enthusiasm and energy, he established and successfully conducted new joint projects with many groups ranging from T. Takui and K. Sato in Japan, over P. Madhu in India, G. Buntkowsky in Germany, G. Bodenhausen, France, R. Kaptein in the Netherlands, D. Abergel and F. Ferrage, France to M. Levitt, UK, to name just a few of them. The most important of these collaborations is a "megagrant" from the Russian government, which enabled Kostya together with Rob Kaptein to renew the scientific infrastructure of the ITC and transform it into one of the leading places of hyperpolarization research in the world.

His scientific work was honored by several important prizes and awards, including a Fellowship of the Alexander von Humboldt Foundation (Germany) in 2008, the Medal of the European Academy of Science (Europea Academia Prize) in 2010, a Fellowship of the Japanese Society for Promotion of Science in 2016 and the Laukien Prize in 2020.

With all his enthusiasm in scientific collaboration and exchange, it is not surprising that Kostya was also the spiritual father and one of the four organizers (together with D. Abergel, G. Buntkowsky, P. Madhu) of the "Intercontinental NMR Seminar", ICONS, which was after his untimely death renamed after him. This series of "Zoom-Seminars" and virtual conferences was his answer to the break-down of scientific communication and exchange caused by the COVID pandemic, the disease which finally extinguished Kostya's brilliant flame.

> G. Buntkowsky, H. M. Vieth, and A. Yurkovskaya

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LongDistances – A Program to Analyze DEER Data

Christian Altenbach

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LongDistances is a full-featured and easy-touse standalone program for the analysis of common pulsed EPR DEER (or PELDOR) data in terms of inter-spin distance distributions. Once downloaded and installed, it is ready to use. First released to the public in 2014, it is still under active development.

Historical background. The introduction of EPR pulse methods to determine inter-spin distances (see Jeschke, 2012 for a review) was a revolutionary development for the field of site directed spin labeling because the final result is a deceptively simple distance distribution. Using multiple distances, global structure can be monitored as a function of protein state (Altenbach et al, 2008). The power of the method has energized collaborations between EPR labs and many fields in protein chemistry, pharmacology and others. It is now often used in collaboration with researchers that are not very familiar with EPR spectroscopy and they might not be aware of the fundamental power as well as the fundamental limitations of the method. LongDistances can be used by anyone, no EPR domain expertise or coding experience necessary.

The user interface. The graphical user interface is shown in Fig. 1 and is organized into tabs on the left and a display area on the right. The prime design goal was for the LongDistances program to be fully interactive and mousecentric, rarely requiring any keyboard input. All parameters have reasonable defaults, all choices are primarily automatic to take out the guesswork, but anything can be manually adjusted if the expert user wants to explore. Any interaction (e.g. trimming data, changing background, modifying parameters) is fully interactive and causes recalculation of all displays for instant visual feedback. Scaling is applied to be most intuitive (e.g. the background is scaled to [1-modulation depth] to naturally follow the data if overlaid on the same graph).

Direct interaction with cursors requires graphs of reasonable size, making it impossible to place everything on one panel. The current display always shows global information on the right, while the main user interactions take place on task-specific tab pages on the left. The order of the tab pages mirrors the typical workflow where analysis progresses from left to right. Starting on the first tab to load the data (or generate a simulated dataset!), we progress through trimming, background determination, and regularization to get the distance distribution. The remaining tabs are for additional exploration (L-curve, error analysis), to glance under the hood (internal data), or to configure aspects of the analysis and algorithms. Note that milliseconds after new data is loaded, a good guess of the resulting distance distribution is already shown, based on reasonable assumptions and nonnegative Tikhonov regularization. All other steps are optional and just serve as refinement. Once the analysis is complete, a rich collection of output files is created automatically, including a summary picture that can be emailed to collaborators.

It can be daunting for the new user to be confronted with so many controls and indicators, but extensive help is available: Most objects have tip strips that appear when hovering over them with the mouse, and many also have defined "Context Help" that can be toggled by pressing Ctrl+h to show a detailed description of the item currently under the mouse. For even more assistance, the prominent [Help] button on the front panel will open the online help in the default web browser.

Simulation tool. During algorithm development, it was important to be able to quickly simulate any possible data scenario to test algorithms, performance, robustness, and gauge limitations. The simulation engine is a core part of the program and has important uses:

(1) To provide intuitive "learning by doing", even if there is no experimental data available. There are plenty of textbooks and publications that describe the theory in detail, but it might be hard to really understand what it all means in practicality. How does the dipolar data change if we change the center of the distance distribution? What if we change the width of the distance distribution? What if there are multiple peaks? How much noise is too much?

(2) For understanding the limitations of the methods if basic principles of signal processing are violated. What happens to very short distances if the time spacing is too

Figure 1: The fitting tab page of LongDistances showing the current result as well as a rich choice of models and options. Even a complicated model-free fit typically completes in under one second. The right side always displays global data.

Figure 2: A view into the internal data used by LongDistances to calculate the distance-to-time transforms. The kernel matrix is shown as an intensity graph. The vertical axis corresponds to the given time points of the dipolar data under analysis. Note the symmetry about the zero time point. The horizontal axis corresponds to the freely chosen linear distance ramp as defined by lower/upper limits and number of points. Each array element contains the theoretical signal intensity for a given distance and time encoded as color according to the z scale. Calculating the dipolar signal for any given distance distribution vector is a simple matrix-vector multiplication. The inverse problem needs to solve a linear system of equations, which is typically ill-posed and requires regularization.

wide? What happens to very long distances if the length of the dipolar trace is too short? How does the quality of the recovered result deteriorate as a function of noise or modulation depth?

Experts in the field can glance at dipolar data and immediately tell if it is suitable for analysis and if so, even guess the approximate distance(s) and width. Extensive "playing" with the simulation tool will allow anyone to get a similar understanding.

The math. The continuous dipolar evolution function is an integral transform of the distance distribution. As with anything involving digital processing, we are dealing with a discrete approximation: The dipolar evolution function is sampled at discrete equidistant time points spaced in the low nanoseconds and we are interested in a distance distribution with sufficient range and spacing to answer important questions about global protein structure. We don't need subatomic resolution and the upper and lower distance limits are given by the limitations of the method. In a nutshell, we are typically dealing with up to a few hundred points in each domain. A detailed description of all implemented algorithms is available in the help section of the product website.

Error analysis. The method itself is extremely accurate because we measure frequencies that depend on the inverse third power of the distance. A 20% change in distance causes a change in frequency (and the period of the associated oscillation) by about a factor of two. Frequencies are easy to measure accurately and this makes the theoretical precision well below subatomic scales. It follows that any spread in width is a real distance distribution, not an "error", as long as we are near the sweet spot of time spacing and duration for the given distance. Error analysis deals with the question how uncertainties in the input (time domain data) translate into uncertainties in the output (distance domain). In general, noise in the time domain will influence the distance distribution in a complicated fashion. In addition, we have errors caused by uncertainties in the background and zero point, by the finite length of the acquired dipolar trace, as well as other factors such as potential experimental and instrumental artifacts.

The error analysis tab provides a rich interface where many aspects can be randomly varied repeatedly while accumulating statistics. Most perturbations are scaled to the estimated noise in the data. The simplest is to add additional Gaussian noise to the data while the analysis is repeated and accumulated in a 2D histogram.

Epilogue. This article was only able to show the tip of the iceberg in terms of features. Much more details are available online at the link given below. Please download the program and have fun using it! Requests for new features and enhancements are always accepted. Please report all suspected bugs.

Notes

LongDistances was developed at UCLA in the laboratory of Professor Wayne Hubbell with support from the Jules Stein Professorship Endowed Chair. Christian Altenbach is a researcher in the Hubbell lab at the Jules Stein Eye Institute and has been deeply involved in the development and analysis of site directed spin labeling from the very beginning. He received his PhD in Biophysics in 1985 from the University of Basel, Switzerland. He learned programming in the early 1970s using punch cards but switched to LabVIEW (National Instruments, Austin, TX) in the mid 1990s. He is a certified LabVIEW developer (CLD) and LabVIEW champion. The LongDistances program is free and can be installed on any modern Windows computer. Images are for version 942 and details can change in the future. It is interesting to note that the entire program was written in pure LabVIEW and does not contain even a single line of code. LabVIEW is a graphical programming language based on dataflow, inherently parallel and very well suited for pure computations as well as interactive user interfaces.

Links

LongDistances download page with links to the program website, online help, and detailed description of all algorithms: http:// www.biochemistry.ucla.edu/Faculty/Hubbell/software.html

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Conference reports

ICONS-Discussions 2021: When Nuclei meet Electronic Spins Online-Z00M https://sites.google.com/view/nmr-seminar-series/icons2021

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P. K. Madhu

ICONS2021, organized during February 10–12, 2021, was the second edition of the online "Intercontinental NMR Seminar" conference on magnetic resonance. The conference series started as an off-shoot of the weekly Intercontinental NMR Seminar Series initiated and organized by Konstantin Ivanov (ITC, Novosibirsk, Russia), Gerd Buntkowsky (TU, Darmstadt, Germany), Daniel Abergel (ENS Paris, France), and P. K. Madhu (TIFR Hyderabad, India) as a response to the lack of live seminars and conferences in the times of the COVID-19 pandemic. Contrary to what "NMR" in the title suggests, both the ICONS seminars and the ICONS conference series cover all aspects of magnetic resonance, including both EPR and NMR, with the goal to foster new developments in magnetic resonance and to enable communication and dissemination of research ideas among the magnetic research community. While the speakers at the conferences are chosen among experienced scientists in the field, the seminar series tries to give a balanced mixture between early-stage researchers and experienced scientists.

So far, in the weekly series, nearly fifty scientists from five different continents have presented their recent results and in the two installments of the conference, 25 talks were presented. While the first ICONS conference in 2020 (for details of the contents of the talks see the report in APMR [1]) was broad in scope, the second conference was focused on fields where the interaction of electron and nuclear spins play a pivotal role with a special emphasis on recent developments in the field of Dynamic Nuclear Polarization. With this focus we wanted to further support and stimulate the interactions between EPR- and NMR-oriented groups as representatives of the field of magnetic resonance. The thirteen invited speakers were in chronological order Fedor Jelezko, Ulm, Akinori Kagawa, Osaka, Olivier Ouari, Marseille, Bob Griffin, Boston, Thomas Prisner, Frankfurt, Kazunobu Sato, Osaka, Sami Jannin, Lyon, Valentin Novikov, Moscow, Songi Han, Santa Barbara, Sabine van Doorslaer, Antwerpen, Dominik Bucher, Munich, Stephen Hill, Tallahassee and Jörg Matysik, Leipzig. In their presentations they spanned a broad range of topics, including the design of stable radicals, technical developments like the application of arbitrary

waveform generators controlling microwave pulses, pulsed EPR and hyperfine spectroscopy and the spectroscopy of nitrogen vacancy centers in nanodiamonds, to Chemically Induced Nuclear Polarization and DNP applications in MRI. Their talks were broadcast across the Zoom and YouTube platforms. The average combined attendance was around 180. For details of the contents of the talks see the report in APMR [2].

The 348 participants of the meeting came from 34 countries on 6 different continents (Europe, North America, South America, Africa, Australia, Asia) and 17 time zones, ranging from Japan in the east over Europe to the West Coast of the United States.

The conference and seminar series were sponsored by Alexander von Humboldt Foundation, Wiley, Springer, HyperSpin, and Adani. The next ICONS conference is planned for September 1–3, 2021. It will again cover the whole width of magnetic resonance. For details and the schedule of upcoming talks see the home page of the meeting ICONS-Seminary.

Finally, it is our very sad duty to mention that our friend and co-organizer, Prof. Konstantin Ivanov from the ITC Novosibirsk, himself became a victim of COVID, and passed away shortly after the conference. Owing to his untimely death it appeared obvious that we must rename the series to "Konstantin Ivanov Intercontinental NMR Seminar Series" in order to honor him as a great friend and an outstanding scientist.

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The 54th Annual International Meeting of the RSC ESR Group April 2021, Cardiff, UK

The 53rd Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry was due to take place at the University of Manchester at the end of March 2020. Having already managed relocation of the event to a new city centre site after cancellation of the originally booked venue of Chancellors Hotel, home of the successful 2012, 2003 and 1998 meetings, our local organisers took the difficult decision to cancel the meeting due to the unfolding global pandemic. While with hindsight the cancellation seems inevitable the decision taken by Prof. Eric McInnes to protect our community and our families was made when messaging from the UK government was business as usual and nearly two weeks before a nationwide lockdown was announced. We thank Eric for his decisive leadership and his whole team at Manchester for their considerable efforts in preparing for the meeting, and look forward to an eventual return of the meeting to Manchester in the future.

After the Manchester conference the 54th Annual International Meeting of the group was due to take place in Cardiff. Having agreed that Eric had been through enough already we continued with this plan and were delighted that Dr Emma Richards agreed to host our first ever virtual meeting in April 2021. Not only did this require planning of the event in an entirely new and untested format, but after cancellation of the Manchester meeting the schedule needed to include not one but two Bruker Lectures and two Bruker Thesis Prizes. along with the IES Young Investigator Award for good measure. Alongside these live award lectures and live plenary and invited talks, in an effort to ease participation from different time-zones the new format compressed the conference into just 4 hours per day using pre-recorded contributed talks with live Q&A sessions. We thank our session chairs for capably running these sessions which managed to achieve discussion of every paper whilst also keeping to time, much to the relief of the organising team. It was even possible to deliver posters online, including pre-recorded flash presentations, contributing to an incredibly high density of excellent science presented throughout the week. The successful conference format allowed participation by an incredible 520 registered delegates from 24 countries, and the meeting included a record

45 contributed talks (viewed over 7000 times on our private YouTube channel) and the total of 55 posters is surpassed in recent times only by conferences in anniversary years. While I'm sure we all long for the opportunity to meet again in person and discuss our research informally over our preferred beverage, Cardiff 2021 will be fondly remembered as a vibrant and enjoyable meeting, a highpoint in an otherwise difficult year. We thank Emma and her team for rising to the challenge of organising our first virtual conference and all who participated to make it a success.

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 EPR spectroscopy. The Bruker Prize 2020 was awarded to Prof. David Collison of the University of Manchester for his seminal contributions to transition metal EPR, spanning both theory and experiment with topics ranging from bioinorganic chemistry to molecular materials. The nominations not only mentioned his authoritative book *Electron Paramagnetic Resonance of d Transition Metal Compounds* but also his work as co-founder and director

Award of: Bruker Prize 2020 to Prof. David Collison (top left), Bruker Prize 2021 to Prof. Michael Wasielewski (top right), Bruker Thesis Prize 2020 to Dr Nabeel Aslam (bottom left) and Bruker Thesis Prize 2021 to Dr Daphné Lubert Perquel (bottom right).

Conference reports

of the EPSRC UK National EPR Facility, fostering collaborations within the EPR community and popularising applications within wider scientific communities. His lecture, "*The attraction of unpaired electrons*", was postponed from 2020 and delivered online during the 2021 Cardiff virtual meeting.

Bruker also sponsor an annual EPR Thesis Prize, set up to recognise outstanding work by PhD students in the field of ESR Spectroscopy. The Committee read thesis summaries and support letters from supervisors and examiners to narrow the field down, a challenging task given the growing application numbers and strength of the submissions, and then ask experts to read and assess each short-listed thesis in depth. The 2020 winner was Dr Nabeel Aslam for his thesis completed at the University of Stuttgart, supervised by Prof. Jörg Wrachtrup. Nabeel, who was granted a Feodor Lynen fellowship and is now undertaking postdoctoral work at Harvard University, delivered an excellent lecture, "Nanoscale NMR with a quantum sensor in diamond", which was also postponed from the 2020 meeting.

Having concluded the postponed 2020 Bruker Prize celebrations on Monday evening on Tuesday we were treated to the 2021 prizes. The Bruker Thesis Prize 2021 was awarded to Dr Daphné Lubert-Perquel, for her thesis completed at Imperial College London, supervised by Prof. Sandrine Heutz and Prof. Chris Kay. Her lecture, "Combining Film Design and Spectroscopic Strategies to Elucidate Triplet Dynamics in Molecular Systems", was delivered live from the National High Magnetic Field Laboratory where she is now based. Following on from this was the 2021 Bruker lecture, "Exploiting Photogenerated Radical Pairs as Electron Spin Qubits for Quantum Information Applications", by 2021 Bruker Prize winner, Prof. Michael Wasielewski of Northwestern University. The prize award recognised his marriage of EPR and optical spectroscopy, through which he has made pioneering contributions in the fields of artificial photosynthesis, nanoscale optoelectronics and quantum information science.

Both Bruker award sessions were of exceptional quality, and we note again our gratitude to Bruker for their ongoing support of these prestigious prizes.

JEOL and IES prizes

In the long history of the RSC ESR Group, one of the predictors of a successful scientific career is the JEOL Medal with many past winners currently holding faculty posts at universities across the world. Eligible abstracts submitted for the 2020 meeting were considered for the short-list and eight of the best selected to give a talk at the Manchester meeting. While the 2020 conference was cancelled and other prizes postponed, the committee felt that it would be a great loss if these prize lectures, often given at the culmination of a PhD project, did not take place in a timely manner. We were therefore delighted that JEOL agreed to the prize competition running in an online format, and seven of the eight finalists were able to participate in a stand-alone online event on 27th and 28th May 2020. This successful first foray into online lectures using Zoom attracted an audience of over 130 participants from around the world, and the judging panel were impressed with the quality of delivery given what at that time was a rather unfamiliar experience of lecturing to a camera and computer screen. The winner of the 2020 JEOL medal was Gabriel Moise for his talk "Spin delocalisation and fine-structure mysteries of the photoexcited triplet state of metalloporphyrins" with Kaltum Abdiaziz and Janne Soetbeer runners-up in a tight competition.

The success of the 2020 online JEOL session was a major factor in the decision to run a fully online conference in 2021 once it became clear a face-to-face meeting would again be impossible. It was therefore fitting that the Cardiff Virtual meeting concluded with the 25th annual JEOL prize talk session. Once again there was an incredibly strong field, and it was difficult to short-list just six participants to give prize lectures. All gave excellent talks but in the end the JEOL Medal was awarded to Nino Wili for his talk "Dressing up electron spins to (un)lock their potential: Application to distance measurements between trityl radicals" with Annalisa Pierro and Katherine Richardson runners-up. We thank JEOL for continuing to support the medal and look forward to the 2022 competition.

We were once again pleased to be supported by the International EPR Society at the Conference this year, who awarded not only their traditional poster prizes, but also the John Weil Young Investigator Award. The Young Investigator Award lecture for 2020 was given by Dr Sabine Richert of University of Freiburg and the poster prizes went to Luis Fábregas Ibáñez (for a poster titled "*DeerLab and new aspects in dipolar EPR spectroscopy analysis*") and Fabian Hecker (for a poster titled "¹⁷O ENDOR detection of water molecules on the radical transfer pathway of ribonucleotide reductase").

Committee

Eric McInnes and David Collison have come to the end of their ex officio terms on the committee as organisers of the 2020 Manchester Conference, which completes for Eric a run of service that actually began in 2011 with his election as Secretary and organiser of the 2012 Manchester Conference! The following committee members have also served their full term of office: Gavin Morley, Olav Schiemann, Sylwia Kacprzak, and Ilya Kuprov. We thank them all for their service and as Christiane Timmel noted in her end of conference address, we owe a particular debt of gratitude to Ilya for an exceptionally long stint on the committee that surpasses even Eric's record. Ilya was elected as webmaster in 2009 until becoming secretary in 2016, a progression that now appears to have become the established route to the Secretary position with my own appointment to the role following on from two full terms as web-master since 2016. Running our elections online for the first time using new RSC dictated procedures we had a record number of applicants, and after a rather lengthy process also welcome to the committee Christos Pliotas (University of Leeds) as Ordinary Committee Member, Marilena Di Valentin (University of Padova) as International Representative, Alex Rogerson (Bruker UK) as Industry Representative and Will Myers (University of Oxford) as Webmaster. Janett Lovett (St Andrews) also joins the committee ex officio as organiser of the next conference.

Social Media

The RSC ESR group joined Twitter in September 2020, please follow us @RSC_ESR

Next conference

Dr Janett Lovett is organising the next conference in St Andrews between Monday 6th and Friday 10th June 2022. Please see http://www. esr-group.org/conferences/2022-conferencest-andrews for further information and join the rsc-esr-group@jiscmail.ac.uk mail list to be notified when new details are released. We look forward to a face-to-face meeting with the opportunity to raise a glass to Eric, Emma and their teams for their efforts during the last two years, and to celebrate the achievements of all our prize winners.

> Dr. Chris Wedge, RSC ESR Group Secretary, School of Applied Sciences, University of Huddersfield UK

new Books & Journals

Applied Magnetic Resonance 51/11 (2020) https://link.springer.com/journal/723/ volumes-and-issues/51-11 Dante Gatteschi: On the Occasion of His 75th Anniversary Co-Guest Editors: Lorenzo Sorace, Maria Fittipaldi, Donatella Carbonera

The Special Issue of *Applied Magnetic Resonance* to celebrate Prof. Dante Gatteschi on the occasion of his 75th birthday has been published in November 2020, to honor an outstanding scientist who had a major impact in the field of magnetic resonance. The Spe-

cial Issue contains 23 papers, both original contributions and reviews from friends and colleagues of Prof. Gatteschi. The topics of the contributions provide a glimpse of the different fields touched upon by Dante in his longstanding career, which moved from EPR of exchange coupled systems to the seminal application of High-Field High-Frequency EPR to many different aspects of molecular magnetism.

The subjects of the contributions range from the determination of single-ion anisotropy

in molecular or bio-inorganic compounds, making ample use of ligand field arguments to rationalize the observed results, to the characterization of organic spin chains and high spin organic polymers; from the application of EPR to solve problems in fields as different as catalysis and mineralogy to application of advanced techniques and instrumental developments. Theoretical papers and perspectives on new fields of research are also presented.

Over the years, Prof. Gatteschi was intensely active in promoting the development of appropriate conditions for successful scientific research at a national and international level. This was accomplished with a natural inclination to develop intense human relationships with colleagues and students, as proved by the enthusiasm of contributors to this Special Issue.

To formally offer Dante the Special Issue and to celebrate his 75th birthday a webinar was organized by Maria Fittipaldi and Lorenzo Sorace and supported by the Italian Group of Electron Spin Resonance (GIRSE), of which Dante was one of the founders.

The webinar took place in two afternoons and included both scientific contributions and personal recollections from Dante's collaborators and former students (for the list of the speaker https://www.girse.unifi.it/index.

new Books & Journals

php/events-2/past-events). All talks provided prominent examples of what Dante has taught to many of us and of the breadth and depth of his scientific interests. The number of participants, from all over the world, reached 124: a special thank goes to all of them and to all the speakers who made this webinar possible with their passionate response. To be all together was again the sign of how much Dante has given to the whole scientific community, and it has been extremely nice and important in a moment that is worldwide extremely difficult.

These two days and the Special Issue have been the present that all community offered to Dante for his 75th birthday and it was a great pleasure for all of us to give him back some of the warm and stimulating atmosphere that he has created and supported all around him with his work and his humanity.

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ISMAR-APNMR 2021 (Including the IES AGM2021) August 22–27, 2021, Online, Osaka, Japan

https://www.ismar-apnmr2021.org

ISMAR-APNMR 2021 is a joint international conference of 22nd International Society of Magnetic Resonance Conference (ISMAR), 9th Asia-Pacific NMR Symposium (APNMR), 60th Annual Meeting of the Nuclear Magnetic Resonance Society of Japan (NMRSJ), and 60th Annual Meeting of the Society of Electron Spin Science and Technology (SEST). It was originally scheduled at Osaka, Japan but it will be held in principle as online considering the impact of the COVID-19.

ISMAR-APNMR 2021 will cover a wide range of research related to the inherent physics of magnetic resonance and its applications in chemistry, biology and medicine. Individual sessions are devoted to new NMR and EPR methods, applications in material science and biology & medicine, dynamical nuclear polarization, dosimetry/earth science, in vivo NMR and EPR, MRI imaging, to name a few. ISMAR-APNMR 2021 will host the IES

Annual General Meeting.

Chairperson: Prof. Toshimichi Fujiwara If you need a support, you can contact the following email address: ismar-apnmr2021@ jtbcom.co.jp

Modern Development of Magnetic Resonance 2021 (MDMR 2021)

November 1–5, 2021, Kazan, Russian Federation

www.kfti.knc.ru/mdmr/2021

The Zavoisky Physical-Technical Institute of FRC Kazan Scientific Center of RAS, the Academy of Sciences of the Republic of Tatarstan and the Kazan Federal University organize the Week of Science in the period from 1 November till 5 November 2021 including the annual International Conference "Modern Development of Magnetic Resonance 2021" and the anniversary Zavoisky Award 2021 ceremony (www.kfti.knc.ru/ en/zavoisky) supported by the Government of the Republic of Tatarstan.

2021 marks thirty years since the first Zavoisky Award was given to Dr. William B. Mims (USA).

The International EPR/ESR Society granted two IES Student Poster Awards to be selected from EPR-related poster presentations by young researchers.

The conference is organized under the auspices of the Groupement AMPERE.

The celebration of the 85th birthday of Prof. Kev M. Salikhov is planned within the events of the Week of Science.

- The scope of the conference
- Perspectives of magnetic resonance in science and spin technology
- Theory of magnetic resonance
- Low-dimensional systems and nanosystems
- Electron spin based methods for electronic and spatial structure determination in physics, chemistry and biology
- Molecular magnets and liquid crystals
- Spin-based information processing
- Strongly correlated electron systems
- Chemical and biological systems
- Medical physics
- Magnetic resonance imaging
- Other applications of magnetic resonance
- Modern methods of magnetic resonance
- Magnetic resonance instrumentation
- Related phenomena

Co-chairmen:

Alexey A. Kalachev Kev M. Salikhov e-mail: mdmr@knc.ru phone: 7 (843)2720503 fax: 7 (843)2725075

www.bruker.com/epr

POSITIONS

Position at MagLab

Research Faculty position for development and application of high-field Dynamic Nuclear Polarization methods in collaboration with the EPR and NMR groups at the MagLab.

Further details can be found here: https:// nationalmaglab.org/careers/job-opportunities/ research-faculty

Post Doc @ Goldfarb Lab

Post-doctoral positions in the Goldfarb group at the Weizmann Institute of Science.

I have a couple of post-doc positions in my lab on the development and applications of pulse EPR distance measurements on proteins inside cells. The aim is to probe structure of proteins in their native environment, to explore conformational changes due to interaction with other proteins and ligands in the cell, and detect response to cellular processes that may lead to conformational changes. This is based mainly on the use of Gd³⁺ spin labeling schemes, but not only, that are compatible with the reductive environment of the cell. This includes the development of new in-situ labeling schemes, expanding the measurements to include ENDOR (electron-nuclear double resonance) techniques. In terms of specific biological systems we are interested in the focus is the Hsp90 chaperon and its interaction with drugs.

Background required: Molecular Biology/ Biochemistry and/or Magnetic Resonance (NMR or EPR).

Information about the Weizmann Institute and its post-doctoral program can be found at http://www.weizmann.ac.il and https:// www.weizmann.ac.il/feinberg/admissions/ about-program, respectively.

For those who are interested, or have any questions please contact: Professor Daniella Goldfarb, Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, 76100 Israel web: http://www.weizmann.ac.il/chemphys/ EPR_group

e. mail: daniella.goldfarb@weizmann.ac.il

Max-Planck-Institut für biophysikalische Chemie Göttingen

The research group of Electron Paramagnetic Resonance (EPR) spectroscopy (Prof. Dr. Marina Bennati) invites applications for positions as PhD and Postdocs (f/m/d).

The positions are funded by the ERC advanced grant Bio-enMR, which aims at establishing spectroscopic methods at the interface between EPR and NMR spectroscopy. Specifically, we develop electron nuclear double resonance and liquid-state dynamic nuclear polarization for the investigation of bio-macromolecules, for instance the interaction of enzymes with drugs. Work will include collaborative research at the national and international level.

Your Profile:

– Master/PhD or equivalent academic degree in Physics or Chemistry

- background in magnetic resonance spectroscopy

- experience in the field of either EPR or NMR (for a Postdoc position)

Additional Information:

PhD students will have the opportunity to participate in one of several available PhD programs of the Göttingen graduate schools with four years funding, http://www.uni-

goettingen.de/de/56640.

html. Postdoc positions are limited to two years with possibility of extensions. The positions are available from October 2021 but the starting date is flexible. Payment and benefits are based on the TVöD guidelines.

The Max Planck Society is committed to increasing the number of individuals with disabilities in its workforce and therefore encourages applications from such qualified individuals. The Max Planck Society strives for gender and diversity equality. We welcome applications from all backgrounds.

Please submit your application including a short letter of motivation, CV, a list of publications, and email addresses of two referees preferably via e-mail as a single PDF file to ausschreibung16-21@mpibpc.mpg.de

Max Planck Institute for Biophysical Chemistry, Electron Paramagnetic Resonance Spectroscopy, Prof. Dr. Marina Bennati, Am Fassberg 11, 37077 Göttingen, Germany, Web: www.mpibpc.mpg.de/bennati.

Information pursuant to Article 13 DS-GVO on the collection and processing of personal data during the application process can be found on our website below the respective job advertisement.

EQUIPMENT

Wanted: Used Electromagnet and Power Supply

Bridge12 is looking to purchase a used electromagnet and power supply for X-band EPR spectroscopy.

Please contact Thorsten Maly, Bridge12 Technologies, Inc., Framingham, MA USA, at tmaly@bridge12.com if you have a magnet available. US location preferred.

L&M EPR Supplies, Inc.

4152 W. Lisbon Ave., Milwaukee, WI 53208 Phone: (414) 324-1052; Fax: (262) 889-2368 www.lmepr.com sales@lmepr.com

S	TPX Capillaries	EPR Sampling Tubes
U U	Quantity	Price/Part (\$US)
_	1-19	60.00
Ē	20-99	50.00
ш.	100+	40.00

BRUKER 10 Years of EPR Innovations

2010: Spinfit

2013: Q-band power, 150 W TWT with pi-pulses as short as 12 ns with an over coupled resonator.

2016: EMXnano, High performance benchtop EPR spectrometer incorporating SpinFit and SpinCount for simulation and quantification.

2019: Rapid-Scan accessory, a new way of performing EPR overcoming saturation limits, improving signal to noise, and increasing time resolution.

2013: SpinJet-AWG first commercial arbitrary waveform generator for pulse EPR.

2016: SpinFit anistropic

2018: VAMP-III and SpecJet-III, detection bandwidth of 1 GHz with 14-bit amplitude resolution.

2019: Magnettech ESR5000: Bruker's latest benchtop EPR spectrometer, combining a compact design with a wide range of applications.

Innovation with Integrity

Bruker

BRUKER 60 Years of Innovation with Integrity

1960: The Founding of Bruker-Physik AG

1962: The first NMR laboratory with KIS1

1971: WH 90, the first FT-only NMR Spectrometer

1996: EPR ELEXSYS line introduced

2010: World's first commercially available solid-state dynamic nuclear polarization-enhanced NMR system (DNP-NMR)

Bruker

Innovation with Integrity