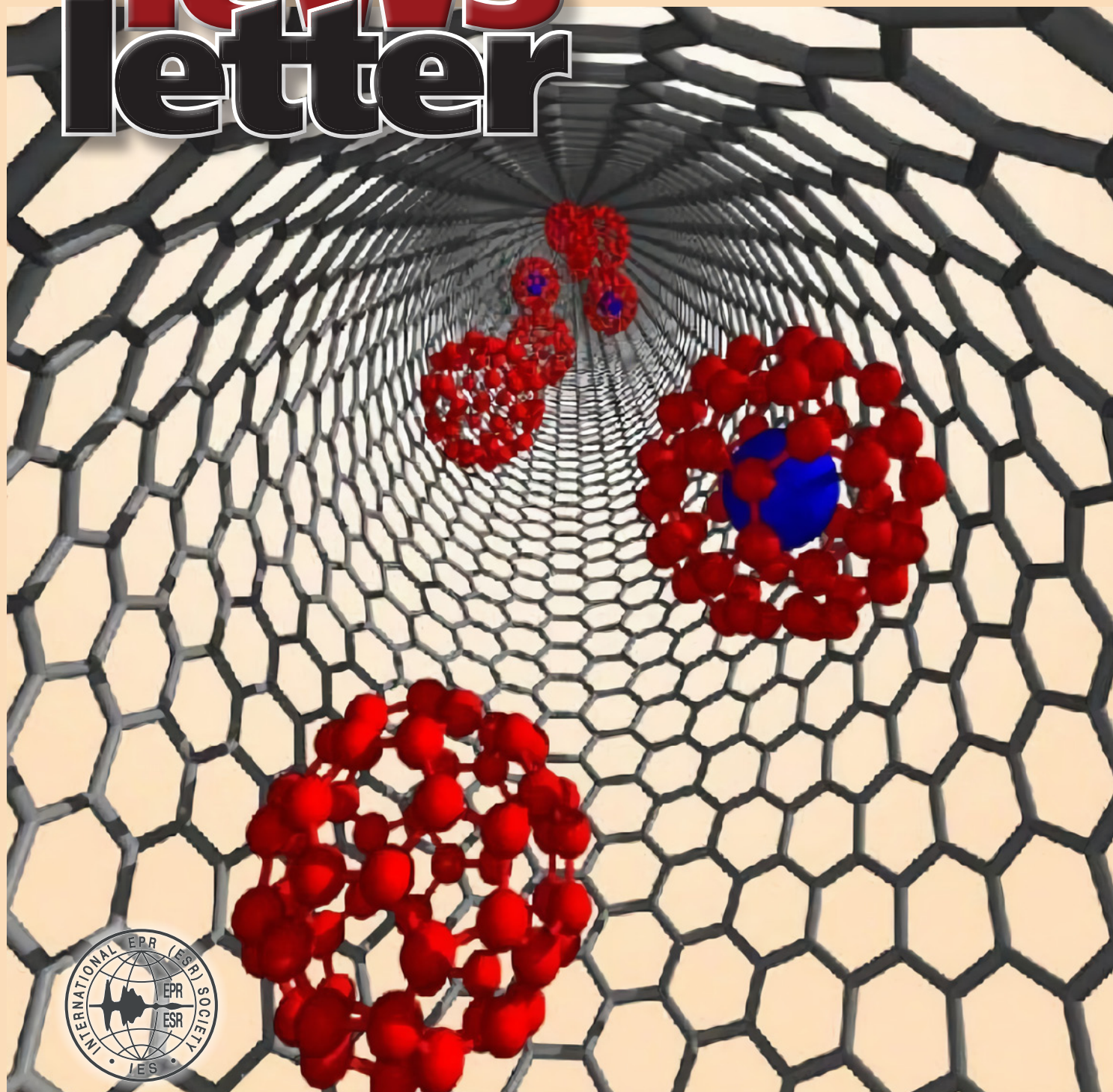


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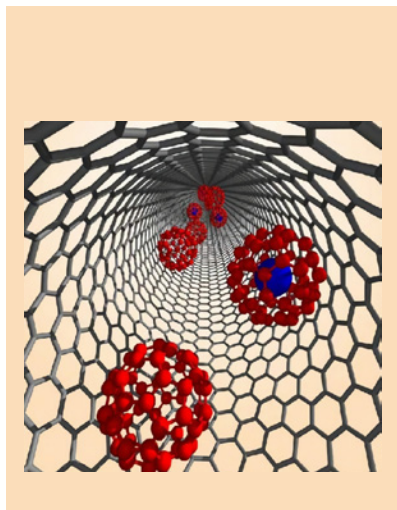
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Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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The cover picture illustrates aspects of research carried out by Klaus-Peter Dinse, recipient of the Zavoisky Award 2020. It shows an artist's impression of C60 and Endofullerenes enclosed in a Carbon Nanotube.

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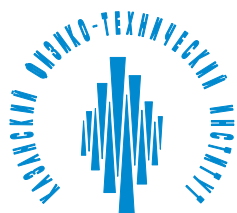
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Editorial

Dear colleagues,

Finally, there is light at the end of the tunnel. The increasing vaccination rate all over the world gives us hope for 2021 that herd immunity against COVID-19 will be achieved soon. As a result, the coronavirus restrictions will be cancelled and we will be able to enjoy our personal contacts we missed so much in 2020. Even if most magnetic resonance conferences in 2021 will use the online format (RSC EPR Meeting, April 12–16, Cardiff UK, <http://www.esr-group.org/conferences/2021-conference-cardiff/>; 43rd International EPR Symposium at the 61st Annual Rocky Mountain Conference on Magnetic Resonance July 25–29, Denver, Colorado, <https://rockychem.com/>; ISMAR-APNMR 2021 August 22–27, Osaka, Japan <https://www.ismar-apnmr2021.org> (ISMAR-APNMR 2021 will also host the IES Annual General Meeting), the Annual conference “Modern Development of Magnetic Resonance 2021”, November 1–5, Kazan, Russia, www.kfti.knc.ru/mdmr/2021 has announced real-life participation keeping online participation as an option. You all are welcome!

This issue of the *EPR newsletter* introduces to you the IES Executive team for the years

2021–2023 (pp. 3–6). In her Letter of the President, Songi Han formulates the ongoing activities of the IES and the ways in which you can engage.

Our heartfelt congratulations to Songi Han on the 2021 EAS Award for outstanding achievements in magnetic resonance and Michael Wasielewski on the 2021 Bruker Award for the development and application of electron paramagnetic resonance to the study of photochemical and photophysical processes. All are also welcome to congratulate Elena Bagryanskaya, Stefan Stoll, Klaus-Peter Dinse and Thomas Schmidt on their awards (pp. 8, 9). We will feature them in future issues of the newsletter but in the meantime you may already meet them in our publications. Michael Wasielewski's interview on the occasion of his IES Silver Medal for Chemistry 2018 is available in 29/1-2, pp. 6, 7. The dreams and expectations of Elena Bagryanskaya are confronted with those of Olesya Krumkacheva, whose mentor she was, in the Present Meets Future column edited by Sabine Van Doorslaer (26/1, pp. 4–7). Klaus-Peter Dinse tells about a magic triangle, consisting of the words: “people, instrumentation, and topics” that proved fruitful during his scientific life (pp. 7, 8). Thomas Schmidt is one of the first to participate in the IES Virtual EPR

Meetings with a talk “Sub-millisecond freezing permits cryoprotectant-free EPR double electron-electron resonance spectroscopy” (30/1-2, pp. 31, 32).

I am glad to use this event to add my personal congratulations to Stefan Stoll and to say a very big heartfelt thank you to him. If I remember right, his first appearance on the pages of the *EPR newsletter* was in 2003. Stefan was featured as the JEOL Prize 2003 winner (13/1-2, p. 9). And exactly in this very issue he published his first article “EPR Easy Spin: a Software Package for the Computation of EPR and ENDOR Spectra” in the then Computer Corner column (pp. 24–26).

Since then he kindly agreed to edit this column (now Software column) and in these nineteen years he is enthusiastic and tireless in finding more and more contributors to his column, which is one of the most long-lived and frequent columns in the newsletter. This issue is not an exception, and you find the Software column with an article “DeerLab, new flavor in dipolar EPR data analysis” by Luis Fábregas Ibáñez (pp. 12–14).

Dear Stefan, your help and support with the *EPR newsletter* is gratefully appreciated and I am looking forward, with greatest anticipation, to the continuation of our collaboration!

Laila Mosina

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Letter of the President

Dear EPR Colleagues,

As the newly elected President of the International EPR(ESR) Society (IES) I would like to greet you all to a new term of the IES that has begun with the New Year of 2021. Thank you to the members of the IES for entrusting in me the ambassadorship for the society. Welcome to those who are not yet members, hear me out why we are worth your membership and help us be the society that represents the vibrant, impactful and diverse EPR community that we are and aspire to be.

Let me begin by thanking the executive officers of the last period, as well as introduce the newly elected officers. First and foremost, I would like to thank the immediate past President Thomas Prisner for his dedicated service to the IES. He tirelessly worked on making the IES a bigger tent for the EPR (ESR) community, enhance the visibility of EPR (ESR) research and researchers and put his focus on supporting young scientists by advocating for awards and poster prizes at all magnetic resonance conferences that have an EPR presence, and invested in supporting EPR schools. He had a committed team of executive officers, Gunnar Jeschke, Hiroshi Hirata and myself as Vice Presidents for Europe, Asia and America who worked alongside. Special thanks to Hitoshi Ohta, the past president before Thomas who, per constitution of the IES, served on the executive board of the past term and has been, and continues to be a big champion of the EPR (ESR) society. I am grateful to have three longer serving executives who keep the IES running and organized: Aharon Blank as the Secretary and Peter Qin as the Treasurer of the IES, and Laila Mosina as the Editor of the EPR Newsletter that we regard as a treasure of the IES. We will rely on their wisdom as we start a new term with the newly elected Vice Presidents for Europe, Asia and America: Maxie Roessler, Yasuhiro Kobori and Michael Wasielewski.

You can find the affiliation and contacts of the entire executive board in the cover page of the EPR newsletter, and all of us are happy to be contacted and engage with you. We are committed to continuing and expanding the work and reach of the International EPR(ESR) Society.

The International EPR Society has been active since its inception in 1989, aims to stimulate scientific development of EPR (ESR), facilitate communication among EPR (ESR) researchers, and encourage the use of EPR (ESR) techniques across a wide variety of research fields. The Society maintains a large database of members who are active in EPR (ESR) research. These members

have access to the quarterly EPR newsletter, and are eligible to be nominated to various awards, medals and recognitions. The Society features the IES awards at various magnetic resonance conferences.

Moving forward, I would like to share with you that our utmost priorities will be to increase the number of IES members while increasing the diversity of its membership in terms of research area, geography, gender, race and otherwise, maximize the engagement of young researchers who are entering the field of EPR (ESR), and so enhance the reach and impact of EPR (ESR) research worldwide. The IES is committed to keeping up with the fast pace of research developments, and doing its part to make sure we as a society evolve with its constituents and the new directions that they will lead us to. The EPR Society *is only as good as its Members*, the IES IS its Members. ►

New IES Executives



Song-I Han,
IES President

Dr. Han received her Doctoral Degree in Natural Sciences (Dr.rer.nat) from Aachen University of Technology (RWTH), Germany, in 2001. She pursued her postdoctoral studies at the Max-Planck Institute for Polymer Research, Mainz, Germany sponsored by the Max-Planck Fellowship and the University of California Berkeley sponsored by the Feodor Lynen Fellowship of the Alexander von Humboldt Foundation. Dr. Han joined the faculty at University of California Santa Barbara (UCSB) in 2004, received tenure in

2010 and was promoted to full professor in 2012. She is currently a Professor in the Department of Chemistry and Biochemistry, as well as the Department of Chemical Engineering at UCSB. She is a recipient of the 2004 Camille and Henry Dreyfus New Faculty Award, the 2007 NSF Faculty Early Career Development Award, the 2008 Packard Fellowship for Science and Engineering, the 2010 Dreyfus-Teacher Scholar Award, the 2011 NIH Innovator Award and the 2015 Bessel Prize of the Alexander von Humboldt Foundation. Most recently, Dr. Han was awarded the BPS Innovation Award of 2018, and was elected fellow of the ISMAR, joining a distinguished international group of scientists contributing to advances in magnetic resonance. She was most recently awarded the 2021 EAS Award for Outstanding Achievement in Magnetic Resonance. She is the newly elected President of the International EPR Society effective 2021.

The Han lab is pushing the frontier of electron and nuclear spin magnetic resonance instrumentation and concepts in dynamic nuclear polarization (DNP) amplified nuclear magnetic resonance (NMR), together with precise manipulation of electron and nuclear spin probes located on biomolecular and materials surfaces, to uncover their structure, the design rules for molecular recognition, and the surface structuring and dynamics of hydration water. ●



Letter of the President

I list some of the ongoing activities and news from the IES, and ways in which you can engage:

The IES has an active Twitter account with more than 500 followers and trends increasing. Please follow us @EPR_ESR and encourage your students to do so. We aspire to reach 2000+ followers!

The IES Twitter activities are strictly on point to help the mission of the IES. We tweet and retweet newest EPR publications of Members (members can request a tweet through <https://ieprs.org>) to help increase the visibility of EPR (ESR) publications, we help spread the word for conferences featuring EPR (ESR) research and connect with our friends of the European Federation of EPR @european_epr, the Royal Society of Chemistry EPR group @RSC_ESR and other societies.

We recently launched a Twitter membership drive #joinIES and an EPR (ESR) community building campaign with the hashtag #sharEPR by encouraging students to share a photo of their favorite EPR instruments and a sneak peek at what EPR can do. This campaign has already taken off. Ask your students to join!

Of course, we continue our support via traditional and proven avenues that sometimes are simply the best methods. The IES will support EPR (ESR) researchers at all major conferences featuring EPR (ESR) through the sponsorship of Poster Awards. In 2021, we have so far offered support in the form of Poster Awards to the Royal Society of Chemistry EPR spectroscopy meeting, Rocky Mountain Conference EPR meeting, Asia Pacific ESR meeting, International Society of Magnetic Resonance and Asia Pacific NMR combined conference and the Modern Development of Magnetic Resonance conference in Kazan. The list can increase, so let us know if you need our support.

The IES designates every year one international conference at the IES designated main meeting. We negotiate a deal with the conference organizers to register their participants in EPR (ESR) sessions as IES members for free, offer additional monetary sponsorship and earn the right to hold its Annual General Meeting (AGM) after one of the main EPR (ESR) sessions open to IES members and the general public. The IES is very pleased to designate the ISMAR-APNMR as the IES conference with the mutual support agreement in place. This means all participants of the ISMAR-APNMR meeting who will choose one of the 4 EPR (ESR) sessions/topics will obtain the IES membership for free for a whole year! Take advantage of it, we need you!

When COVID-19 hit, we all had to pause and rethink our business as usual, both in our private lives and our research conducts. The IES immediately recognized the positive energy and ingenuity of student researchers of EPR (ESR) who launched a virtual EPR Zoom meeting series, and decided to jump at this chance and support them. The IES wanted to help put a structure in place, such that such meetings that help connect researchers worldwide can become a sustainable online activity in the future. Now, it is called the IES Virtual EPR meeting (IVEM), run by wonderful young researchers in two time zones of Europe/Americas and Asia/Pacific. Their past and upcoming talks are advertised on the IES webpage with the help of the IES secretary Aharon Blank (see <https://ieprs.org/on-line-activities/>). Please continue to come to the IVEMs, agree to give talks and encourage your students to participate.

The third sequel of the Best Paper Award competition was announced (due date was April 5th, 2021). The IES looks forward to highlighting exciting advances and breakthrough development in the broad area of

EPR and ESR. This award will be given to up two publications per year, and the first author recognized with this award. The expectation is that the first author is a young scientist. Nomination can be made by any ACTIVE IES member (dues must be paid for 2021), faculty or student. If self-nomination is made, it can be made only by the first author or the corresponding author. Nomination by first author should be accompanied by letter from the corresponding author explaining the role of the first author.

I hope you are convinced at this point that it is worthwhile to support the IES. Help us do all of these activities by becoming a paying member, and encourage your students to become paying members. Remember that a larger membership makes our Society also attractive for our sponsors. If you are a sponsor, please support the IES. We will return your support by helping you advertise EPR supplies, services and instruments through all channels and avenues available to the IES.

I hope very much, that together with all the other Officers of the IES, I will help keep our Society attractive for all of you, succeed in attracting new members and continue to make our society visible and respectable to other scientific communities. I am sure there are many more things that the IES society can do. If you have any suggestions and wishes, do not hesitate to contact me directly via email (songihan@ucsb.edu) or talk to me at conferences in the future – I cannot wait to see many of you in person again!

Till then, remember the IES *needs you* and *wants you*. Join us: <https://ieprs.org/registration/>

With best regards and on behalf of the whole Executive Officer Board (see above) of our Society.

Songi Han
President of the IES

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Michael R. Wasielewski,
IES Vice-President Americas

Michael R. Wasielewski, Professor of Chemistry, Northwestern University, obtained his BSc (1971), MSc (1972) and PhD (1975) degrees from University of Chicago. He has applied modern time-resolved EPR spectroscopy and magnetic field effects to chemistry and related fields, and has contributed to understanding electron transfer reactions in problems ranging from biomimetic models for the photosynthetic reaction centre to fundamental approaches in molecular electronics and spintronics. He developed the first molecular systems to successfully mimic many of the key spin properties of photo-generated paramagnetic states in photosynthetic reaction centres, and he has shown how covalent donor-acceptor systems can be used to understand spin-correlated radical ion pairs and the triplet states that result from their recombination. His pioneering work in the field of molecular spintronics has used these phenomena to develop molecular systems which provide fundamental insights into the multi-spin interactions necessary to manipulate some aspects of quantum information.



Yasuhiro Kobori,
IES Vice-President Asia-Pacific

Yasuhiro Kobori graduated from Tokyo Institute of Technology, Japan, in 1992. He received his M. S. degree in chemistry from Tokyo Institute of Technology, Japan, in 1994 and received his Ph.D. in Chemistry in 1998 from Tokyo Institute of Technology. In 1996, he joined a group of reaction dynamics (Professor Shozo Tero-Kubota's group) as an Assistant Professor at Tohoku University, Japan until 2002. Then, he moved to an EPR research group (Prof. James R. Norris Jr.) of the department of chemistry, The University of Chicago as a Postdoctoral Research Associate, and as a JSPS Overseas Research Fellow. In 2006, he moved to the department of chemistry, Shizuoka University as an Associate Professor until 2013. Then, he moved to the Graduate School of Science, Kobe University, as a full Professor. Since 2017, he has been a Professor of Molecular Photoscience Research Center, Kobe University. He was a recipient of 2006 Young Investigator Award of the Society of Electron Spin Science and Technology (SEST) in Japan. He received The Japanese Photochemistry Association Award and International Investigator Awards of the Japan Society for Molecular

Science in 2019. His current research interest includes vibronic effects in photochemistry for the light-energy conversion systems by his developments of electron spin polarization imaging analysis based upon the transient EPR measurements to characterize geometries and motions of the paramagnetic species.



Maxie Roessler,
IES Vice-President Europe

Maxie Roessler is a Principal Investigator at Imperial College London. She completed her DPhil at Oxford University under the supervision of Professor Fraser Armstrong FRS in 2012, whilst being affiliated with the Centre of Advanced Electron Spin Resonance (CAESR) and working closely with Dr. Jeffrey Harmer. She received the Margaret K B Day scholarship and DPhil thesis commendation for her doctoral work on EPR investigations of iron-sulfur cluster relays in enzymes and was a runner up for the Jeol Prize. She started her independent career at Queen Mary University of London in 2013, where she received an Outstanding Contribution to Teaching Award, and moved to Imperial College to 2019 where she is now

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New IES Executives

building up PEPR (Centre of Pulse EPR spectroscopy) after securing a major grant from the Engineering and Physical Sciences Research Council.

She leads a diverse and multidisciplinary research group that combines pulse EPR, electrochemistry and biochemical methods. Her current research focus is on mechanistic investigations of complex redox-active enzymes in respiration and photosynthesis, primarily making use of 'intrinsic' unpaired electrons. Her group is also developing novel methodology that combines (protein) film electrochemistry and EPR spectroscopy to gain new insights into redox-active catalysts, including enzymes.



Aharon Blank, IES Secretary

Aharon Blank is an associate Prof. at the Schiluch Faculty of Chemistry, Technion – Israel Institute of Technology. Born in 1972, graduated from the Hebrew University of Jerusalem in 1992 with degrees in Mathematics, Physics and Chemistry; Completed his Master degree at Tel Aviv University in 1997 in electrical engineering – Physical electronics under the supervision of Prof. Raphael

Kastner and finished his PhD in 2002 at the Hebrew University of Jerusalem in Physical Chemistry – Electron Spin Resonance (ESR), under the supervision of the late Prof. Haim Levanon. During this time he served 9 years in the IAF as a Scientific Officer and also as a CTO in a medical device company, developing miniature intravascular MRI. Following his PhD he spent 3 years at Cornell University as a Post Doc at the group of Prof. Jack Freed (on a Rothschild post-doctoral fellowship), developing the subject of ESR microscopy, and since 2005 he is a Faculty member at the Technion. Aharon main interests today are development and applications of new methodologies in the field of magnetic resonance. His group works on miniature sensitive ESR resonators; small, self contained NMR and ESR medical tools; ESR probes for micro and nano imaging; and ESR and NMR approaches to quantum technology.




Peter Z. Qin, IES Treasurer

Peter Z. Qin received his B.S. degree in Physics from Peking University in China in 1991. He carried out his graduate study on RNA folding and catalysis under the men-

torship of Professor Anna Marie Pyle at Columbia University in the City of New York, and received his Ph.D. degree in 1999. From 1999 to 2002, Dr. Qin carried out postdoctoral research work with Professor Wayne L. Hubbell at University of California, Los Angeles, developing methods of Site-Directed Spin Labeling to study RNA. In 2002, Dr. Qin joined the faculty of the Department of Chemistry, University of Southern California, at which he was promoted through the rank and current holds a tenured full professor appointment. Dr. Qin's research focuses on understanding mechanisms of nucleic acid recognition by studying the relationship between structure, dynamics, and function of nucleic acids and protein/nucleic acid complexes. The Qin group develops and applies Site-Directed Spin Labeling techniques, both in bulk and at the single-molecule level, to monitor structure and dynamics of nucleic acids and protein-nucleic acid complexes under physiological conditions. Current projects in the Qin group focus on using spin-labeling in conjunction with other techniques to investigate mechanisms of target recognition by the programmable CRISPR nucleases that are revolutionizing genome engineering.

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:
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Zavoisky Award 2020

Scrolling through the domains of EPR

Klaus-Peter Dinse

When I was informed that I would be honored by receiving the Zavoisky Award, I was looking at the list with previous Awardees, most of them accompanying me during my scientific life. I set down feeling much honored being part of the group. As experimental physicist I tried to define a short summary, indicating how this could happen. I settled down drawing a magic triangle, consisting of the words: “people, instrumentation, and topics”. This can also be phrased as being initially guided by an exceptional mentor, being allowed building a special instrument attracting outstanding scientists from all over the world, who are bringing exceptional probes. This combination proved fruitful during my scientific life. In the following I will briefly sketch a few examples.

My early interest in RF technology was the starting point to develop liquid state ENDOR under the guidance of Klaus Möbius, designing a custom built multi kW transmitter, whose power was dissipated in a water-cooled rf loop inside a water cooled microwave cavity. This brute force design was very successful, opening the way to perform liquid state ENDOR over a wide temperature range. This triggered the interest of Harry Kurreck from the Chemistry department, whose PhD student Wolfgang Lubitz loved to take spectra from isotopically labeled organic compounds. The interpretation was done in “project style”, involving Martin Plato and Reinhard Biehl. Together with Reinhard, TRIPLE resonance in solution was also established. The capability of these machines attracted various people, only to mention Arnold Hoff, bringing Bacteriochlorophyll samples.

Another example of such a magic triangle was given in the Max-Planck Institute in Heidelberg in the group of Karl Hauser. Being aware of the multi-pulse playground in NMR, I tried to establish similar experiments exclusively in the optical domain. Here the perfect scientific surrounding was given, with Ulrich Haeberlen, the co-developer of high resolution NMR in solids and Herbert Zimmermann, synthesizing doped crystals for echo spectroscopy. Again it was important to set

up a special Laser system allowing performing multi pulse experiments with relative spectral resolution of 10^9 .

The combination of cutting edge technology, outstanding persons, and interesting topics turned out to be also effective when starting pulsed EPR, a technique now possible by using fast digitizer and high microwave power technology, now accessing the ns time domain. With this set-up, we could investigate highly mobile spins in 1D conductors, synthesized by Dieter Schweitzer at the same institute in Heidelberg. Michael Mehring had done pioneering work at Dortmund, probing solids with echo experiments, and I had the chance to inherit part of his spectrometer, when moving to Dortmund to my first independent position as associate professor. With my PhD student Thomas Prisner we set out for highest time resolution and it was exciting to perform for the first time FT-EPR in solution with ultimate resolution and to present it as promising method for the study of free radicals. Now the stage was set to combine the method with pulsed Laser excitation, exploring charge transfer reactions with ns time resolution together with Hans van Willigen.

The method could also be used to probe field distributions in type II superconductors and deriving information about the temperature dependence of the critical length in these compounds. This work was continued in a sabbatical at the ANU in Canberra (Australia) together with Richard Bramley. Again, it turned out to benefit from the combination of exceptional samples, outstanding people and an outlook into new fields of physics.

Having had so much fun in the time domain, it was tempting to try similar experiments in the optical domain. Having learned from Bernhard Blümich that missing high power can be compensated by using stochastic excitation, I tested this idea in the lab of J. L. Hall (later Nobel laureate) during a sabbatical in Boulder (US). Using their cw Laser set up having excellent frequency stability, it was possible to perform true multiplex spectroscopy on Iodine gas.

I finally moved to Darmstadt as full professor in the chemistry department, were DFG funding allowed me to obtain one of the first BRUKER W-band spectrometer. In combina-



The “old” high power ENDOR cavity received from Klaus Möbius in Hirschegg 2003 on occasion of my 60th birthday.

tion with the home-built FT-Xband machine we were well set for probing chemical reactions in the time domain in cooperation with Dieter Beckert (Univ. Leipzig). Using a 2D pulse protocol optimized for the study of chemical exchange, a proton abstraction reaction after Laser excitation could be observed with microsecond time resolution “live on stage”.

The multi-frequency EPR machines could also be used for the study of various Carbon-based materials like C60 and Carbon nanotubes. These new compounds with their amazing symmetry attracted the interests of dedicated students. With Björn Corzilius and Jens van Slageren (TU Stuttgart) we started exploring charge and spin mobility in metallic nanotubes, searching for the predicted superconductivity, samples prepared in outstanding quality by Kenji Hata (Tsukuba). Clearly also atoms in fullerene cages were in the center of experiments, being helped by Wolfgang Harneit, Klaus Lips, and Björn Pietzak in the group of Alois Weidinger (Helmholtz-Zentrum Berlin) preparing N@C60.

Since 1998 I was co-organizer of the DFG funded special research program: “High Field EPR in Biology, Chemistry and Physics” together with Klaus Möbius, giving me a close insight into developments in the field. In 2002 Jürgen Roedel from the material science

Awards

department at the TU Darmstadt initiated a special DFG program investigating antiferromagnetic materials (SFB 595). The properties of these compounds are controlled by defects and vacancies, whose presence can be studied by EPR. If the available frequency and field range was not sufficient to characterize these paramagnetic centers, visits to the National High Magnetic Field Lab (NHMFL, Tallahassee) were fruitful and gave me opportunity to cooperate with Johan van Tol and Andrew Ozarowski.

Taking a sabbatical at the Molecular Science Institute in Okazaki (Japan), I investigated metallo-endofullerenes together with Tatsuhisa Kato, with whom I collaborated also recently, and together with Robert Bittl we were probing the mobility of the NO radical encased by a modified C60 cage.

After retiring I had the chance to move with equipment to the Free University Berlin (group of Robert Bittl), and became part of ongoing catalysis research in the UniCat Center of Excellence. Again it proved fruitful to use the full EPR toolbox for the investigation of paramagnetic centers in catalysts, also completing for missing facilities in Berlin by visits to the NHFL spectrometers. Here again it was

essential to combine exceptional samples provided by the groups of Robert Schlögl (Fritz-Haber Institute) and Reinhard Schomäcker (TU Berlin), working with outstanding students Carlos Carrero, Till Wolfram, Wiebke Riedel, and my son Arne, using state-of-the-art EPR methods.

To my surprise, I recently had the chance to accompany the progress of EPR on a chip (EPRoC), by which the old idea of the Pound oscillator is revived by Jens Anders (TU Stuttgart) in the mw domain. He is using advanced chip technology for the construction of a miniature EPR spectrometer, whose topologies can be designed working at frequencies up to 700 GHz. This set-up utilizes near field detection, and apart from measuring tiny samples in conventional cw mode, it enables rapid scan with scan rates of more than 400 THz/s as well as stochastic excitation. Thus the old dream of true multiplexing stochastic EPR as an alternative for FTEPR might be revived. This again is an example, how the combination of excellent people, ground breaking technology, and focus on special samples, in this case important for solar energy research in the group of Klaus Lips (Helmholtz-Zentrum Berlin), is essential for scientific progress. ●



2021 IES Silver Medal for Chemistry

The IES Silver Medal in Chemistry for 2021 is awarded to Professor Elena Bagryanskaya in recognition of her many outstanding and fundamental contributions to the application of EPR involving the interactions and reactions of groups containing electron spins. She has led the development of novel spin labels based on sterically hindered nitroxides, hy-

drophilic trityl radicals, photoactive porphyrins and new conjugation chemistries. These new labels provide enhanced spectral and relaxation properties for EPR applications. She used these new labels to make pioneering distance measurements in biomolecules at room temperature by pulse dipolar spectroscopy, and has applied them to proteins, nucleic acids and a very complex biomolecular nanomachine – the ribosome. Professor Bagryanskaya's work on spin-dependent interactions between molecules produced novel breathing crystals. Reversible changes in the crystal morphology (breathing) result from magnetostructural transitions controlled by electron spin interactions. She also developed living polymerization reactions using nitroxide radicals based on her studies of dynamic nuclear polarization and free radical reactions. Collectively, her contributions to the field of EPR have expanded our understanding of the role of electron spin in chemistry and has increased our ability to study the properties of macromolecular assemblies. Professor Bagryanskaya is the author of over 200 publications and is highly active in the EPR community. She is a member of the editorial board of Applied Magnetic Resonance, a member of the ISMAR committee, the former Vice-President of the International EPR Society (IES), President of the Pacific EPR Society (APES), and President of the Russian EPR Society. She works at the N. N. Voroztsov Institute of Organic Chemistry SB RAS as Head of Magnetic Resonance laboratory and Director.



2021 IES Silver Medal for Instrumentation and Methods

Professor Stefan Stoll is hereby recognized for his seminal contributions to computational EPR spectroscopy and analysis. As a graduate student, Professor Stoll conceived of and initiated the development of the first generally applicable package for simulating and fitting EPR data. The result, EasySpin, enjoys continued expansion and is now a mainstay of the field of EPR and an essential tool used by virtually all modern EPR laboratories around the world. Remarkably, Professor Stoll has invested significant effort and resources into making EasySpin a freely available and accessible tool, while he continues to contribute to dissemination of this important software tool through ►



regular and ongoing training workshops for spectroscopists of all backgrounds, as well as regular and continued upgrades to the software packet. Professor Stoll continues to make new and innovative contributions to the field of EPR methods. Recently, he developed new theoretical tools based on Bayesian statistics for bringing rigor to the analysis of DEER experiments. Professor Stoll's ongoing research, along with his development of EasySpin, set a standard of high-quality science and leadership fully befitting the IES Silver Medal.



2021 IES Fellowship

Professor Klaus-Peter Dinse is renowned and respected member of the international EPR community. He has made outstanding contributions through the use of EPR to the study of photochemical electron transfer reactions, photochemical reaction intermediates, endohedral fullerenes and catalytically active metal centers. Professor Dinse helped advance the use of Electron Nuclear Double Resonance

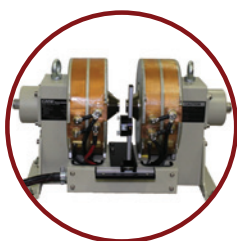
(ENDOR) spectroscopy, optically detected magnetic resonance (ODMR), and optical nuclear double resonance (ONDR). As an established researcher, he extended his scope of research into coherent optical spectroscopy where he made brilliant use of photon echo modulation effects for high-resolution optical spectroscopy. Professor Dinse was also an early adopter of state-of-the-art pulsed EPR techniques, as well as advanced the use of multi-frequency and high-resolution EPR spectroscopy to solve important research questions. He has furthermore fostered the field of EPR as an academic teacher and as a highly respected reviewer and advisor to international funding agencies, as well as magnetic resonance research consortia and institutions. Prof. Dinse has more than 180 publications and is a recent recipient of the Zavoisky Award 2020. The International EPR (ESR) Society is proud to honor Professor Klaus-Peter Dinse for his distinguished contributions to EPR by naming him as a Fellow of the Society.

2021 IES Young Investigator John Weil Award

The John-Weil Young Investigator Award for 2021 is awarded to Dr. Thomas Schmidt for his contributions to the field of isotope labeling of proteins for distance measurements by pulsed Double Electron Electron Resonance (DEER). He has published an original publication on phase memory time, T_m , edited DEER methodology that allows for transverse relaxation aided distance assignment of pulsed DEER data by relying on a localized chemical environment-dependent relaxation of spin labels via amino acid specific protonation of methyl groups in an otherwise deuterated background. The implementation



of this novel technique in conjunction with two-dimensional singular value decomposition analysis allowed for the differentiation and assignment of dipolar distances in proteins. This approach promises to be generally applicable to help address important challenges of DEER based distance measurements of protein complexes. Dr. Thomas Schmidt has also characterized the HIV-1 reverse transcriptase maturation pathway and its conformational changes using advanced structure calculations and EPR methods. The outstanding research contributions of Dr. Thomas Schmidt to the field of EPR is evidenced by multiple original research contributions to the field of EPR to advance protein structure studies and to biomedical science in general. As a junior scientist, he is already a vital contributor to a vibrant, new scientific field, and his careful and persistent research has led, and is likely to continue to lead, to meaningful advances in addressing pivotal questions in biology and medical science, as evidenced by more than 500 citations of his work.



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- Metrolab PT2026 Pulsed-wave NMR Teslometer for precision measurements with overall accuracy to 5ppm and 33Hz measurement speed, suitable for high-stability closed-loop magnet control.
- Additional measurement equipment includes: Fluxgate Magnetometers (room temperature and cryogenic), 1-axis and 3-axis precision Hall Probes, Fast Digital Voltage Integrators, and precision Current Transducers & Electromagnet Power Supplies.

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70 Years of the Groupement AMPERE

Seventy years ago, the Groupement AMPERE was founded in France. This is a time to remember and to look forward. With reference to its history as reviewed on the occasion of the Society's 65 anniversary [www.ampere-society.org] a few memories are recalled, and activities of the last years setting the stage for the future are outlined.

The Groupement AMPERE started as an association of scientists engaged in the study of molecules with radio waves. Its mission gave rise to the acronym *AMPERE* meaning *Atomes et Molécules Par Études Radio-Électriques*. Five years later the Society was incorporated in Switzerland. Given the complex state of Europe in those days, a key function of the Society was to maintain links between Western and Eastern Europe. In these days without internet the *Bulletin du Groupement AMPERE* and the main event of the Groupement AMPERE, the *Congress AMPERE*, were the central communication channels between the different international member laboratories.

The Congress AMPERE, the British Radiofrequency Spectroscopy Group, and the

European Experimental NMR Conference merged in 2005 under the umbrella of the Groupement AMPERE to form *EUROMAR*, the largest of many activities of the Society today. A remarkable Congress AMPERE was the one in September 1961, just a few weeks after the infamous division of EUROPE with the establishment of the iron curtain. It took place in Leipzig, East Germany, with attendees from East and West, proving that science is stronger than politics.

With time, specialized colloquia and schools were organized and new divisions established. The AMPERE homepage www.ampere-society.org is an informative source on the Society's activities and history. Landmark discoveries were discussed at these meetings. For example, N. Bloembergen reported on *Cross-Relaxation Effects in Magnetic Resonance* 1960 in Pisa, A. Abragam on *Polarisation dynamiques des noyaux* 1961 in Leipzig, E. R. Andrew on *Nuclear Magnetic Resonance in Rapidly Rotated Solids*, E. L. Hahn on *Developments in Nuclear Magnetic Double Resonance*, I. Solomon on *Magnetic Resonance of Conduction Electrons*

1966 in Ljubljana, K. M. Salikhov et al. on *Modulation phenomena in Electron Spin-Echo* 1968 in Grenoble, R. Blinc on *Nuclear Double Resonance Studies of Order-Disorder Ferroelectrics*, A. Lösche on *Some NMR investigations of Liquid Crystals*, and J. S. Waugh, M. G. Gibby, S. Kaplan, A. Pines on *Proton-Enhanced NMR of Dilute Spins in Solids* 1972 in Turku, P. C. Lauterbur et al. on *Magnetic Resonance Zeugmatography* and P. Mansfield, P. K. Grannell, A. A. Maudsley on *Diffraction Microscopy in Solids and Liquids by NMR* 1974 in Nottingham, R. R. Ernst et al. on *Application of Two-Dimensional Spectroscopy to Problems of Physical, Chemical and Biological Relevance* 1978 in Tallin, A. Pines on *NMR with Lots of Protons and no Magnetic Fields* 1986 in Rome, H. W. Spiess on *2D and 3D Solid State NMR of Polymers* 1992 in Athens, P. T. Callaghan on *Microimaging Studies of Flow and Diffusion* 1996 in Canterbury, and A. Schweiger on *Dances with Electron and Nuclear Spins* 1998 in Berlin. Other key lectures remain in the books of abstracts, including the famous lecture by Jean Jeener proposing 2D NMR



Figure 1. The AMPERE tree. The stem and the branches of the crown represent the different activities of the Groupement AMPERE. New branches grown in the last 10 years are marked in green. In 2019, the publication division of the Groupement AMPERE has launched the non-profit, open-access journal 'Magnetic Resonance' (<https://www.magnetic-resonance-ampere.net/>).

spectroscopy at the AMPERE Summer School in Basko Polje, 1971.

Since the fall of the iron curtain and with the formation of a unified Europe, the Groupement AMPERE continues to serve its mission in the spirit of its founders, *Se Connaître, S'Entendre, S'Entraider*, i.e., to get to know each other, to listen to each other, to aid one another. Today it is an umbrella organization for different divisions and a wide range of magnetic resonance activities in Europe. Its function is represented by the AMPERE tree (Fig. 1), a living organism, which keeps on growing. Within the last decade it has grown the new branches of the European School on Biological Solid-State NMR, the Hyperpolarized-Magnetic-Resonance Division, and the Publication Division. The Publication Division has launched the open-access journal 'Magnetic Resonance' (<https://www.magnetic-resonance-ampere.net/>), which is published non-profit by Copernicus Publications, with the mission to provide affordable open access with high-quality contributions through interactive public peer reviewing. A developing bud of the AMPERE tree is the Alpine Conference on Magnetic Resonance in Solids.

The Groupement AMPERE maintains and expands its services for the whole community engaged in Magnetic Resonance and Related Phenomena in Europe and worldwide. It aims at accommodating new developments in new areas which are progressively opened by the evolution of science. To maintain the vigor of the Groupement, its statutes, i.e., its constitution, have been revised in 2016. The revision maintains the historical structure of the organization (Fig. 2), where the *General Assembly* elects the *AMPERE Committee* to which it delegates most of its power. The committee strives to represent all European countries and magnetic resonance disciplines in a balanced way including attention to gender. The Committee decides on the general policy of the association and elects the members of the *Bureau AMPERE* to handle the day-to-day business in between meetings at the EUROMAR conference each year. In addition to replacing the *Congress AMPERE* conference by the *EUROMAR* conference, the major change in the constitution is that the time of service in the AMPERE Committee has been limited to four years with one reelection possible. This assures periodic rejuvenation of the Committee and Bureau members. To enable limited term service of Committee members, many distinguished personalities have gracefully vacated their long-term Committee positions.

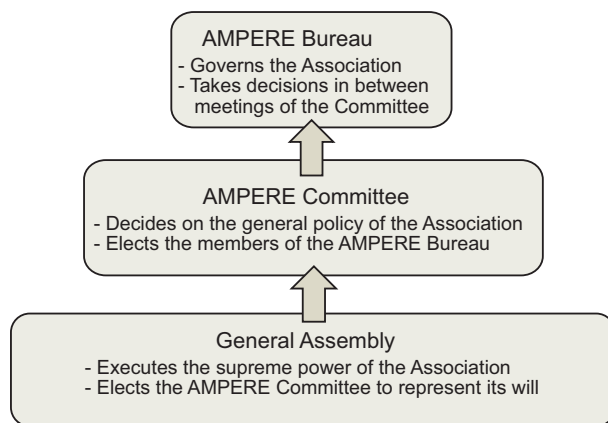


Figure 2. Structure of the Groupement AMPERE.

Other operational changes were introduced to facilitate the functioning of the Society. One was to increase the visibility of the Groupement AMPERE in an effort to foster its acceptance in the scientific community and better communicate its mission 'to contribute to the progress of Radio Spectroscopy, Magnetic Resonance and Related Phenomena.' The AMPERE tree (Fig. 1), a new AMPERE logo, and posters at AMPERE Conferences explaining the Society and its mission resulted from it. Moreover, the guidelines to organize AMPERE events were updated to assist the members of our Society in organizing conferences and avoiding mistakes as most of us are amateurs in this business. With the registration fee to any AMPERE event, the participant becomes a member of the Groupement AMPERE for one year and as such is eligible for reduced fees at other AMPERE events. Also, each member is entitled to participate and vote in the General Assembly at the annual EUROMAR conference. The budget of the Groupement AMPERE is generated from the membership fees and conference surplus, which is split between the Division treasury and the AMPERE treasury. From the income of the AMPERE umbrella society, its operating costs are covered, awards, and as of recent, also stipends for young scientists to attend AMPERE events. Up to 2016, the distinguished *AMPERE Prize* was supported by Bruker, when the company decided to diverge the support to the Ernst Prize at the EUROMAR Conference. Since then, the AMPERE Prize is awarded biannually from the budget of the Groupement AMPERE to an early-stage independent researcher. Since 2002 the Raymond Andrew Prize is awarded by the Groupement AMPERE to a young scientist for an outstanding PhD thesis in magnetic resonance during the opening and prize session of the EUROMAR congress. Its resources are covered by a donation of the Andrew family, which is administered by the Groupement AMPERE.

Several heroes of magnetic resonance have left our community in the last years. Many of them were members or associate members of the Groupement AMPERE. We are commemorating Raymond Andrew (2014), John S. Waugh (2014), Endel Lippmaa (2015), Erwin Hahn (2016), Peter Mansfield (2017), George Feher (2017), Nicholas Bloembergen (2018), Charles P. Slichter (2018), Zeev Luz (2018), Stefano Caldarelli (2018), Sir Rex Richards (2019), Alfred Redfield (2019), Yoji Arata (2019), Dieter Michel (2020), and Konstantin Ivanov (2021). We miss their presence at the AMPERE meetings, but their spirits

and their achievements stay with us.

For many years up to 2018, Gunnar Jeschke was the Secretary General of the Society, who carries the major workload. He reformed the AMPERE webpage and converted the Bulletin AMPERE into a more attractive newsletter, which is now disseminated by email. It not only contains the minutes of the meetings of the AMPERE General Assembly, the Committee and the Bureau, but also conference and meeting announcements, reports of recent conferences, award lectures, and a portrait of a distinguished scientist in each of its four annual issues. In 2018 Matthias Ernst succeeded Gunnar Jeschke and enthusiastically serves the Society as the current Secretary General. As the Covid-19 virus attempts to paralyze our treasured lifestyle and many conferences had to be cancelled in 2020, the Groupement AMPERE is confronting the new challenges. Online platforms and are being explored for common use by all AMPERE Divisions. EUROMAR 2020 has courageously been turned into a very successful online conference by Óscar Millet and his team following a new format with short five-minute talks of young investigators framed by the award lectures for the Richard Ernst Prize, the Raymond Andrew Prize, and the AMPERE Prize. EUROMAR 2021 was planned to be a hybrid conference with online participation and physical attendance in Portorož but had to be revised to be essentially just online. New ideas about how the Groupement AMPERE can better serve the magnetic resonance community are being discussed exploring the wider acceptance of online media. Last but not least it is each of us who defines our Society by her and his interactions and contributions including submissions to the new AMPERE journal *Magnetic Resonance*.

Se Connaître, S'Entendre, S'Entraider!

Stay well and let us meet again soon,

Bernhard Blümich
(President)

DeerLab, new flavor in dipolar EPR data analysis

Luis Fábregas Ibáñez

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DeerLab is a new open-source, free software package for analyzing dipolar EPR spectroscopy experiments such as DEER, RIDME, DQC, etc. It is distributed as a package for Python, an open-source programming language. DeerLab can be downloaded from its GitHub repository (github.com/JeschkeLab/DeerLab).

History and motivation

The development of DeerLab started as part of my graduate studies at Gunnar Jeschke's lab at ETH Zurich, where I had been exploring and working on new approaches to regularization of DEER and TRIER data. The Jeschke lab was home to the well-known DeerAnalysis software, which had become a standard in our community. New developments in dipolar EPR data analysis and the limitations of DeerAnalysis culminated in the commitment to develop a successor. The original plan was to rewrite the backend of DeerAnalysis to incorporate some of these new developments. This new software would be a joint effort between two labs: the Jeschke lab and Stoll lab at the University of Washington.

During the summer of 2019, I visited and stayed at the group of Stefan Stoll in Seattle.

There, Stefan and I started working on this new Matlab-based project we nicknamed DeerAnalysis 2.0 (as some early users might recall). By the end of the summer, the first working pre-releases were published. At that point, we realized that the software's scope and potential had outgrown the original ideas of DeerAnalysis. We decided then to baptize our work with a new name: DeerLab. Back in Zurich, thanks to a small yet growing user base, we continued developing DeerLab, incorporating as much feedback as we could.

In early 2020, the COVID pandemic resulted in a paradigm shift in everyday life for all of us. The switch to isolation and telecommuting ironically provided the opportunity to develop DeerLab intensively. In August 2020, the program (now written in Python) had reached a robustness level, which led to the first paper about DeerLab in the new open-access Magnetic Resonance (MR), making the introduction of DeerLab official.

Features

Despite being actively developed, DeerLab has already grown into a large software suite for dipolar EPR data analysis. Figure 1 summarizes some of the most relevant features of DeerLab as of v0.12.2. DeerLab provides a flexible framework for modeling dipolar signals and fitting them robustly and efficiently to the data.

DeerLab incorporates theoretical and methodological advancements such as full-model fitting,

global fitting of arbitrary models, bootstrapped uncertainty analysis, etc. DeerLab can model the underlying distance distributions either as a parametric model (e.g., Gaussians, sphere/shell models, disordered physical models, etc.) or as a non-parametric model (e.g., obtained via Tikhonov regularization such as DeerAnalysis or Long-Distances). Dipolar signals can be accurately analyzed by, e.g., modulation pathways to model arbitrary multi-pulse DEER experiments or high-harmonic pathways to model RIDME or SIFTER experiments.

Independently of choice, the model can always be fitted to an arbitrary number of signals in a "one-step" analysis without modifying them (i.e., without background-correction, artifact removals, etc.). A variety of algorithms implemented in DeerLab, all based on the least-squares principle, facilitate such an analysis for an arbitrary number of signals.

Before interpretation, a measure of the uncertainty in the results is necessary. DeerLab's uncertainty quantification framework permits the estimation of the uncertainty of any fitted or calculated quantity. Current versions of DeerLab offer two uncertainty estimation methods. On one hand, the asymptotic method provides an approximate but very fast estimation of the uncertainty. This way, an estimate of uncertainty is always available without added effort. On the other hand, the bootstrapping method provides some of the most accurate uncertainty estimates, albeit at the cost of a slower calculation.

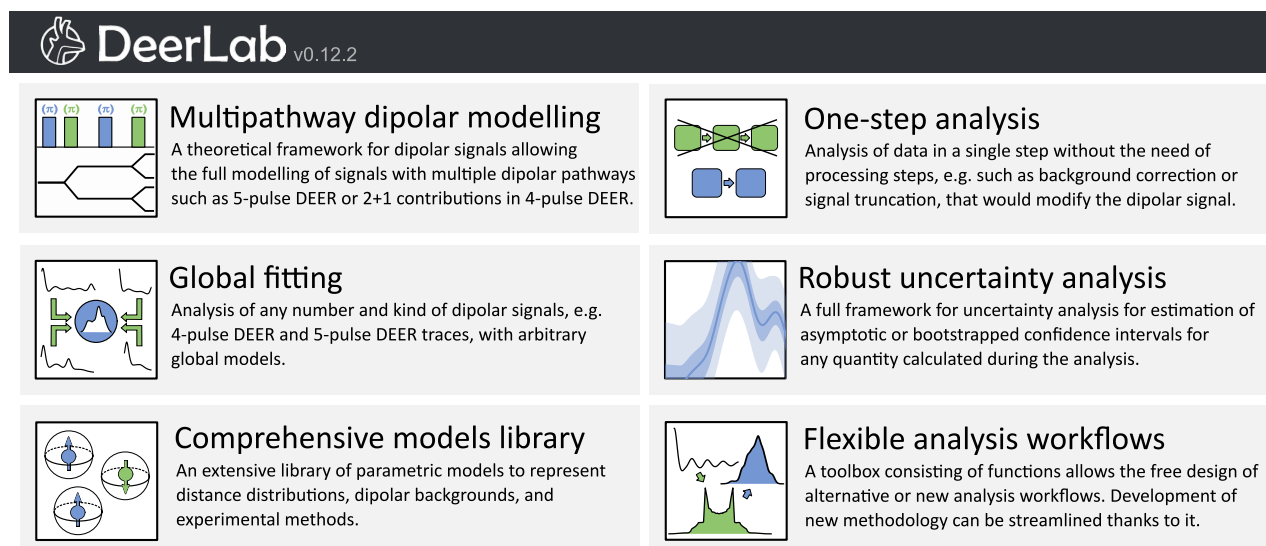


Figure 1. Key features of the DeerLab software package.

Scripting

The main novelty of DeerLab is perhaps its format. Unlike similar packages for dipolar EPR analysis, DeerLab is not distributed as a graphical user interface but rather as a package of scriptable functions (akin to the Easyspin and Spinach packages). As a result of being a scripted program, DeerLab comes with a series of advantages.

While scripting might appear intimidating to non-programmers, DeerLab takes everyone's programming skills into account and adjusts its user-interface accordingly. DeerLab is designed such that its use for routine work requires minimal programming and theoretical skills while still providing a full and robust analysis. The most notable function is the `fitmodel` function, which acts as the core DeerLab function for routine analysis. Figure 2 shows an example of a simple script to analyze two 4-pulse DEER traces. A few script lines can achieve a full analysis, including confidence intervals of the distance distribution, background, parameters, etc. DeerLab also offers a selection of examples to use for alternative types of analysis or as templates for new workflows.

Nonetheless, DeerLab offers complete access to every single feature of its framework for more advanced users. Those who want to develop new or more complex workflows can profit from the vast collection of functions to virtually design any desired workflow.

Automation of routine workflows becomes straightforward with scripts. For example, running a new analysis method over thousands of datasets requires minimal changes to a script. When dealing with workflows requiring long times (days or weeks), the script-format facilitates running them, e.g., in computation clusters, to speed up the analysis and reduce the wait (to mere hours or days). Furthermore, scripts can be easily shared with other people, facilitating collaboration. Most importantly, scripts can be published along with data, ensuring that anyone can reproduce published results.

Code Language

DeerLab is entirely written in Python and thus free software. However, the development of DeerLab began in Matlab, the first pre-releases (v.0.9 and older) still were based on Matlab. In contrast to Python, Matlab is a non-free commercial product. In July 2020, we opened an internal debate on whether to migrate all DeerLab's source code to an open-source language such as Python or Julia. While Julia is a rising star in scientific programming,

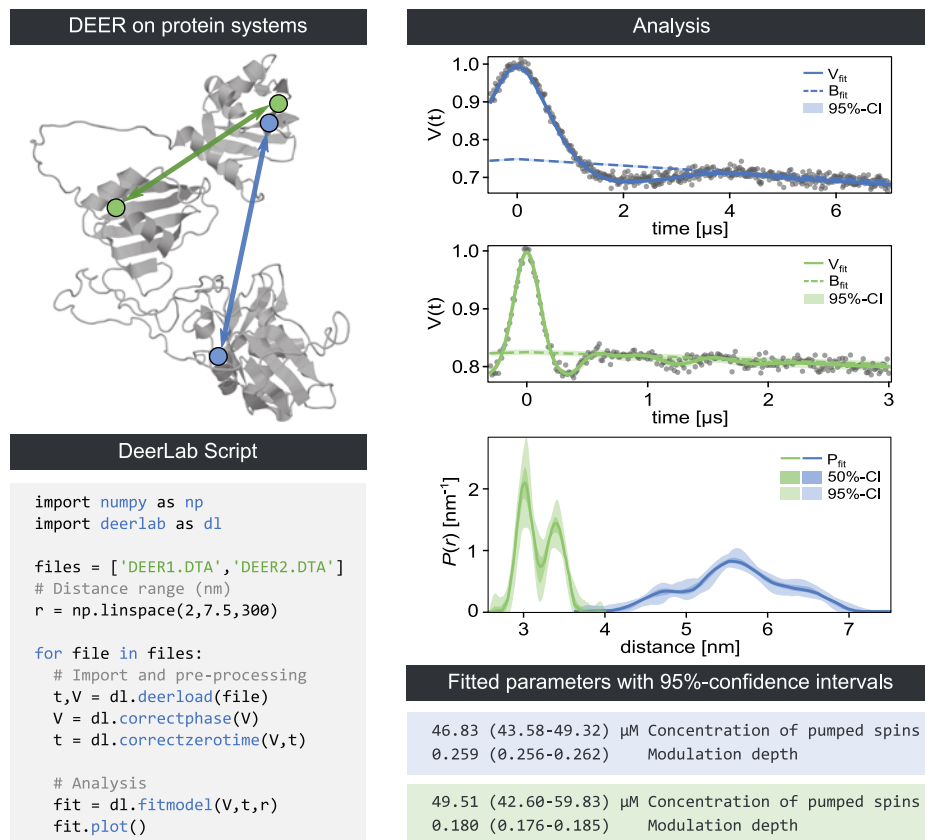


Figure 2. A simple script for routine analysis of multiple 4-pulse DEER signals.

it was still too young to be robustly introduced into our community.

Thus, the choice was between Matlab or Python. We investigated and benchmarked DeerLab under both languages for several weeks to ensure we took the best decision. All technical arguments (performance, scripting styles, development frameworks) were on equal terms for Matlab and Python. On one side, the most used packages in EPR spectroscopy (e.g., Easyspin, Spinach, DeerAnalysis, GLADD/DD, MMM, Defit, etc.) are based on Matlab. Consequently, our community has deep roots in Matlab. On the other side, Python has the invaluable advantage of being free and open-source, yet it has not found widespread usage in our community. Another significant benefit is the easier integration of tools like DeerLab with the many Python-based biostructural tools. The decision was now: remain in the commercial yet familiar Matlab or migrate to the open-source Python at the risk of a potential accessibility barrier for our community. In the interest of the open-source initiative during a Zoom call between Gunnar, Stefan, and me, we unanimously voted to take a leap of faith towards Python and released DeerLab v.0.10.0, fully migrated to Python.

After one and a half years, it is encouraging to see (based on feedback thus far) that DeerLab users (especially those who had already been working with the Matlab version) have appreciated the decision. Many users seem to support the open-source characteristics despite the associated varying efforts to adapt to a different scripting language.

Robust development

DeerLab has grown into an extensive package with multiple functionalities. Manually testing the whole package before releasing a new version is impractical and prone to end up with a broken program. DeerLab's development has always been test-driven via small unit tests that check individual functionalities of the program. As of early 2021, DeerLab has a test suite consisting of over 400 tests covering over 85% of the source code. An automated system blocks the release of any new version of DeerLab if a single unit test fails, preventing the presence of any broken functionality.

We developed DeerLab such that anyone who wants to contribute can do so. DeerLab has used the git version control system from the very beginning to manage the source code. Version control grants access to every state of

Software

the software at any point in development, ensuring reproducibility of results even when using non-released versions.

In combination with testing, it ensures that DeerLab is production-ready at any point in development and upon release. It also serves as an archive of historical changes to the software, letting anyone go back in time and understand why and how a developer introduced a change.

Future

As of February 2021, DeerLab is still in its pre-release phase, actively developed in parallel to developing new techniques and theoretical

concepts. DeerLab's first stable version, v1.0.0, will be released as soon as the program reaches satisfactory robustness, quality, and usability levels. Furthermore, DeerLab will continue to grow to satisfy and adapt to the needs of our community. Potential future features would, e.g., account for high-spin systems, orientation selection, anisotropic g-values, multi-dimensional experiments, etc. I hope that over time DeerLab will grow into an invaluable tool for dipolar EPR spectroscopy.

Further details, as well as examples, can be found in the DeerLab documentation (jeschkelab.github.io/DeerLab).

Conference reports

The 59th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2020)

November 11–13, 2020, Online, Japan

The 59th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2020) was held online in November 11–13, 2020, Online, Japan. The meeting was originally planned to be organized at Kumamoto, Kyushu area. Due to the spread of covid-19 from the beginning of January 2020, the SEST decided in April to cancel the meeting at Kumamoto and to organize an online meeting as a replacement. In April–May, Japan had been in the 1st national state of emergency and so the activities in the universities and institutes had been much suppressed. Especially, the students in the 1st year in the graduate course had faced to the holding of activities in the laboratories and had spent frustrating time.

Under this circumstance, the SEST leadership decided to organize the meeting in online format by the commitment of all the SEST members. The most important motivation was that the stagnation of academic activities and breaks in the careers must be avoided or

minimized for young researchers and students who grow day by day.

Instead of the local organizer, the organizing committee was formed from many members from different institutes nationwide and so it was named as the “non-local organizing committee”. The vice-chair of the SEST was selected as the chairperson of the meeting accordingly.

The SEST had no experience of the online conference. To overcome the difficulties, many young researchers had joined as the session chairs, technical facilitators and others roles. The Institute for Materials Research, Tohoku University which is one of the hubs of the inter-university research collaboration offered generous support in technical and financial aspects including the use of ZOOM and REMO. With this support, we could make the participant fee of students free.

The total number of the participants was 194 including 74 students. There were 4 keynote talks, 38 general talks and 39 poster presentations.

The meeting started in the morning of November 13th. In the opening, the SEST chair Prof. Inanami expressed a greeting and explained about the process to the 1st online meeting.

The morning session consisted of four keynote talks from the representatives of chemistry, biology, physics and life-medical science. The participants enjoyed the excellent talks including the recent activities, trends and perspectives in the related fields. After the session, there was a lunch seminar by the Bruker Japan.

In the afternoon, the first session was the session of the SEST young researcher presentation award. Five nominated presenters gave the impressive presentation about their researches. The awarding committee selected two for the awards this year.

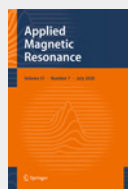
After the award session, there were two parallel sessions on the low-dimensional magnetic systems and materials sciences. The topics presented were the non-linear excitation in magnetic chains, quantum phase transitions, magnetism of radicals and electronic-spin state in complex materials. In the last part of the 1st day, there was a poster previewing with prepared presentation movies. In the evening, the SEST young researcher association had the meeting including a special lecture, an activity report and discussions.

The morning of the second day was devoted to the poster session. In one hour time frame, ten posters were presented in parallel by using a ZOOM breakout room function. The pre-



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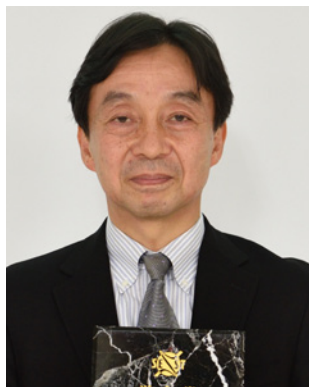
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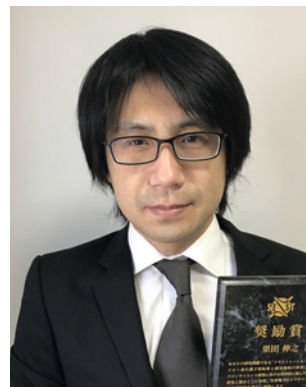
Prof. Kunihiko Tajima



Dr. Yuta Matsuoka



Dr. Ayano Enomoto



Dr. Nobuyuki Kurita

sensation was made by using a power point slide with a live question/comment. A small disadvantage was that the quick capturing of the presentation was difficult because of the absence of the large-size one page poster. The pre-distribution of the poster file in advance may help to complement this difficulty. After the two poster rounds, we have a second poster previewing, which was followed by the lunch seminar by JEOL.

The 1st session of the afternoon was the SEST annual meeting. There were reports about the SEST activities and current status in one hour.

In the last part, there is the report of the winners of the SEST society award and SEST young investigator award. This year, Prof. Kunihiko Tajima was awarded the SEST society prize for his outstanding contributions in chemistry. He has studied the molecular structure in varieties of materials and of substances and examined the generation/annihilation of short-lived paramagnetic species by using EPR and other techniques. It has covered a wide range of research areas and indicated the usefulness and the uniqueness of the EPR technique. Moreover, he has contributed to the development and education of related researchers and industrial applications.

The SEST young investigator award was given to three talented researchers, Dr. Nobuyuki Kurita (Physics), Dr. Ayano Enomoto (In-vivo and EPR instrumentation) and Dr. Yuta Matsuoka (Biology and pharmacy). The winners gave memorial talks about their researches.

The last part of the afternoon session was devoted to the two rounds of 2nd poster sessions. Real time discussions have been made in each break room.

In the evening, there was an exchange party event in the online REMO conference room. There were greeting from SEST chair and Prof. Anzai. Participants enjoyed the chatting in the meeting rooms. For the exchanges among participants, several slides of “my rec-

ommendation bottle” and my recommendation dish” were introduced. In the last part, winners of the SEST young presentation award and student poster award were presented. A few awards were given by the winners to the participants. In the last part, Prof. Akimoto introduced the SEST2021 which will be held as a joint meeting with ISMAR.

In the final day, there were two parallel session in the morning. One session was for chemistry and materials science including spintronics, photo chemistry and spin related materials science. The other session was biology, life science session including topics of cells, radicals and in-vivo. There was a report on the International EPR society annual general meeting in the lunch time.

In the afternoon, there were two parallel sessions on chemistry and interdisciplinary spin related science.

The topics were very diverse and covered fields from quantum computing to active oxygen in biology.

In the closing ceremony, the chairperson expressed the acknowledgement for participants, committee members, sponsors and supporting stuffs. With ending role of the all participants names involved, it was stated that a spin never stops the motion and the spin science will continue for our future. All the participants enjoyed the meeting despite many difficulties in organizing the 1st online SEST meeting.

Professor Hiroyuki Nojiri



EUROMAR 2020

EUROISMAR 2020 was supposed to be held in the Palacio Euskalduna (Bilbao) between the 5th and the 9th of July of 2020. It finally took the shape of an on-line meeting, during the 7th and 8th of December of 2020.

The meeting allowed celebrating the award ceremonies, and it was complemented by a plethora of flash presentations selected from the many abstracts submitted and where the young scientist's participation was promoted. Their participation was instrumental for the success of the on-line meeting.

Committees

International Scientific Committee: Inés García Rubio (ICMA, Zaragoza, Spain), Ana M. Gil (University of Aveiro, Aveiro, Portugal), Jesús Jiménez-Barbero (CIC bioGUNE, Derio, Spain), Arno Kentgens (Radboud University, Nijmegen, Netherlands), Antoine Loquet (IECB, Bordeaux, France), Oscar Millet (Chair, CIC bioGUNE, Derio, Spain), Miquel Pons (Universitat de Barcelona, Barcelona, Spain), Thomas Prisner (University of Frankfurt, Frankfurt, Germany), Christina Redfield (University of Oxford, Oxford, UK), Cristina M Thiele (Technische Universität Darmstadt, Darmstadt, Germany), Thomas

Vosegaard (Aarhus University, Aarhus, Denmark), Andrew G. Webb (Leiden University, Leiden, Netherlands).

Local Organizing Committee: Ignacio Alfonso (IQAC), Ana Ardá (CIC bioGUNE), Tammo Diercks (CIC bioGUNE), Nieves Embade (CIC bioGUNE), Marga Gairí (Universitat de Barcelona), M. Angeles Jiménez (IQFR), Jesús Jiménez-Barbero (CIC bioGUNE), Oscar Millet (Chair, CIC bioGUNE), Ana Poveda (CIC bioGUNE).

EUROMAR2020 and COVID-19

COVID-19 has resulted in a worldwide first order catastrophe that has affected the very fabric of our daily life, forcing us to constantly adapt to everchanging situations. As a result, EUROMAR 2020 was severely affected by the evolution of the COVID-19 pandemic. In an optimistic attempt of overcoming COVID-19 and after the first wave of the infection, it was decided to postpone the meeting from the original dates (5–9 July 2020) to the first week of December of the same year. I want to emphasize that the speakers were contacted and asked to reschedule, and the response was extremely positive and cooperative. Yet, in spite of the COVID-19 summer break, it was soon clear enough that a physical meeting at the end of the year would also be unrealistic. After careful deliberation between the committees and the organizing institutions it was finally decided to cancel the meeting as it was normally understood. Instead, we offered a minimalistic version of EUROMAR to render tribute to the prize awardees and also to allow the young scientist to actively participate in the format of poster submissions and flash presentations.

Promotion & Communication

Leading up to the EUROISMAR 2020 the conference website, <https://www.euromar2020.org>, was launched in October 2019, right after the Berlin EUROISMAR conference. Yet, the most effective communication channel was the twitter account. Each week, a tweet was sent to introduce a speaker or to distribute relevant information. In the end the effort

paid off and the EUROMAR twitter account increased the number of followers during the year to about four hundred.

The online conference Structure

Based on the COVID-19 pandemic escalation, the EUROMAR 2020 Organising Committee proposed to celebrate an on-line meeting version to cover the following goals: awarding ceremony of the prizes and short talks selected from the abstracts submitted by early-stage researchers. The platform chosen was Zoom. In addition, the same Zoom platform was also used to organize the customary meetings for the different committees in charge of the governance of EUROMAR and ISMAR. The conference was distributed over two days and arranged in a time-zone that favoured the attendance worldwide. The award lectures and introductions were held in Room 1 for all the attendees, while two parallel sessions (Room 1 and Room2) hosted the flash presentations from the selected abstracts. The topics for the parallel sessions were: Biomolecular NMR, Computation, EPR / ESR, Hyperpolarization, Instrumentation / hardware, In cell NMR, Materials, Metabolomics, MRI / In vivo, Small molecules & drug design, Solid-state NMR methods, Solid-state NMR applications, and Solution NMR methods. The attendance was free of charge but required previous registration. The sessions were recorded and a youtube channel was created to host all the lectures that were accepted to be made public. The links to the lecture channels are: <https://drive.google.com/drive/folders/1ldOfzailKB15Z2ED1sqyA3pkazYCo-Wn?usp=sharing> (7 Dec) and <https://drive.google.com/drive/folders/1MMbzN9KhTRsGzVZmxccIXioprb>

[ageWNn?usp=sharing](#) (8 Dec). A PDF with all the abstracts and the CV of the awardees was distributed among all the registered users.

Facts and Figures

4 Prize award events. 44 Poster presentations (5 min each). 170 Posters. 7 Best poster awards. 760 Unique e-mail addresses that participated. 1090 Registered e-mail addresses. 565 joint participants at the peak of the meeting.

Prizes

The prestigious Richard R. Ernst Prize to recognize recent beneficial applications of Magnetic Resonance was sponsored by Bruker. It was rightfully granted to honour the work of Clare Grey who currently is full Professor at the Department of Chemistry of Cambridge University. The Raymond Andrew Prize is awarded to a young scientist for his/her outstanding PhD thesis in magnetic resonance. On this occasion Christian Bengs got the award. Christian did his Ph. D. Thesis in the group of Prof. Malcolm Levitt at the University of Southampton. The also renowned AMPERE Prize was given to Thomas Theis who currently is Assistant Professor at the Department of Chemistry of the North Carolina State University. Finally, Paul Schanda was awarded the Varian Young Investigator Award. Paul will become Full Professor at the Institute of Science and Technology in Austria as of 2021.

On the other hand, the Journal of Magnetic Resonance, Elsevier, awarded 4 prizes to early-stage investigators in recognition of their excellent work. The “Magnetic Resonance in Chemistry Awards” were awarded to Dr. Kathrin Aebischer (ETH, Zurich), Lauriane Lecoq (University of Lyon), María Pía Lenza (CIC bioGUNE, Bilbao), Julien Manon (IIB, Gif-sur-Yvette). The awards were selected from the flash presentations by the Scientific Committee. Finally, the International EPR society also gave awards to the lecturers: Arnau Bertran (Oxford University), Yuri Kutin (Technical University Darmstadt) and Andreas Meyer (MPI Biophysics, Göttingen).

Professor Oscar Millet

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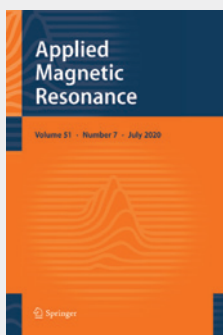
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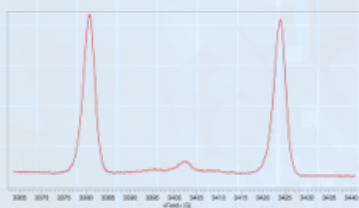
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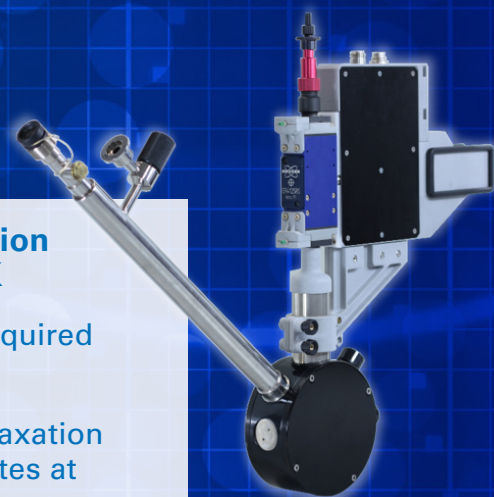
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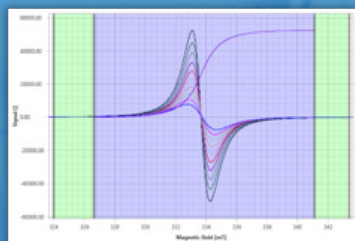
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SpinCount report

Date name	Height	Diameter	Volume	X start [mT]	X end [mT]	Spins	Spin conc. [M]
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.658e+019	9.367e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.658e+019	9.457e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.705e+019	9.533e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.731e+019	9.622e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.732e+019	9.638e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.720e+019	9.586e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.681e+019	9.446e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.637e+019	9.292e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.587e+019	9.117e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.490e+019	8.774e-001
Ultramarine_Ten	60	1	0.047	323.850	343.450	2.395e+019	8.438e-001

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