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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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WESTPORT
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The cover picture illustrates aspects of the research of Patrice Bertet, recipient of the IES medal in Physics/Materials Science 2025. It shows an electron spin (red arrow), relaxing from up to down states while emitting a microwave photon towards a superconducting single-microwave photon detector (device schematics on the right).The graphical design studio "Idées fraîches" who did the cover picture is gratefully acknowledged.

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Editorial

Dear colleagues,

I presume PhD students and their supervisors were very excited to learn about the new initiative of the IES to establish travel grants for PhD students to attend IES sponsored conferences (35/1-2, p. 4). The first winners are Yannik Limbach and Marvin Lenjer to attend EUROMAR 2025, and Ehsan Shirdel Tazehkand and Trent McHenry for the EFEPR Summer School 2025. The IES Travel Grant winners should prepare a short article on their experiences of the conference for our publication. Marvin's contribution is published in this issue (p. 15) and Yannik's contribution will be published in the forthcoming issue. No doubt that happy smile on Marvin's face activates a flow of young researchers eager to participate in a competition for this grant and results in the increase of the visibility of our society.

It was a brilliant idea of Songi Han to introduce a new column in the *EPR newsletter*, Meet Our Sponsor. The first contributor to this column was Eric Bryerton, Virginia Diodes (31/3, pp. 6, 7) followed by Yu He, CIQTEK (32/3-4, pp. 7, 8), Eugeny Kryukov, Cryogenic Ltd, (32/3-4, pp. 9, 10), and Jack H. Freed, ACERT (33/1-2, pp. 4, 5). It was great to add a personal touch and to get an answer to the curiosity about what story lies behind the hardware and software we use in our research.

In this issue, we welcome our new major sponsor, LINEV Systems, Inc. and give the floor to its Founder and CEO, Vladimir Linev (pp. 3, 4). In fact, it would have been better to say we welcome back our major sponsor, because LINEV Systems is formerly known as ADANI Systems, and the latter supported the IES for more than five years in past.

Interviews with Olav Schiemann and Patrice Bertet, IES Medals 2025 Awardees, also add a personal touch to their science. The same could be said for articles by supervisors Marina Di Valentin, Kiminori Maeda, Claudia Tait, and Marina Bennati on the successes of their students Daniele Panariti, Akihiro Tateno, Maximilian Mayländer, Lorenzo Catini, and Annemarie Kehl, respectively (pp. 5–14).

Special thanks go to Gunnar Jeschke for his continuing collaboration with our publication (pp. 16, 17).

I guess you were looking forward to the report of the IES AGM 2025 which was held at the 58th Annual International Meeting of the ESR Group of the RSC, London, UK. Not to worry, you will find that and many other interesting things in the forthcoming issue of the *EPR newsletter*.

Laila Mosina

Interview with Dr. Vladimir Linev, Founder and CEO of LINEV Systems, Inc.

EPR newsletter: *Dear Dr. Linev, the IES greatly appreciates the support of LINEV Systems, a company with a decades-long track record in compact, application-oriented technologies, which contributes to the EPR community by generating products of importance to our community. We are most appreciative that you agreed to share with us the origin and evolution of the SPINSCAN spectrometer and to answer the questions of this interview. What motivated you to create a compact ESR spectrometer?*

We saw a clear gap between the potential of ESR and its accessibility. The technology was powerful but confined to specialized laboratories. Our goal was to bring ESR into broader use, to make it practical, compact, and aligned with real-world needs. We were pioneers in developing benchtop ESR spectrometers, releasing our first version over 40 years ago. That innovation initiated an entirely new direction in ESR instrumentation. Others followed, but the system architecture and logic were originally defined by our approach. As technology evolved, so did our instruments. A notable milestone was the CMS 84000, with over 200 units installed in the U.S. and more than 300 worldwide, many of which remain in active use across academic and industrial laboratories. Today, SPINSCAN carries this legacy forward with enhanced capabilities, modern usability, and proven long-term reliability.

How does SPINSCAN differ from other benchtop ESR systems now on the market?

SPINSCAN is not a scaled-down adaptation. It is a purpose-built platform grounded in original, patented engineering. We developed proprietary microwave modules, resonators, and a detection chain that are optimized for compact architecture. We were also the first to integrate a complete set of high-value features into a benchtop format, including: alanine dosimetry, variable temperature control, photochemical stimulation with in-situ illumination, multi-orientation and angular control, automated sample handling, and software-driven acquisition and analysis. These were not add-ons – they were designed into the system from the beginning. SPINSCAN remains plug-and-play, upgradeable, and dependable, delivering full-scale ESR performance in a compact footprint.

Who are your typical users, and what are the key applications for SPINSCAN?

Our user base includes universities, contract labs, radiation facilities, and aerospace organizations. One of the most advanced applications is alanine-based dosimetry, where our Spinscan XDS is used in high-reliability radiation verification settings. We also support cross-disciplinary teams in chemistry, biology, and materials science who need precision, flexibility, and simplified operation without compromising data quality.

Your company works across digital X-Ray imaging for security, and NDT. How do these areas relate to ESR?

They are all built on a shared foundation: turning invisible phenomena into actionable data. Whether we are imaging cargo or tracking radicals, the challenges are similar: clean signals, smart filtering, and accurate interpretation. This synergy means technologies developed in one field often enhance another. The engineering mindset behind SPINSCAN was informed by decades of cross-sector innovation.

SPINSCAN seems designed with long-term usability in mind. How does that affect user experience?

That is essential. From stable calibration and fast setup to modular upgrades and automation, every detail is made for real labs with real constraints. Researchers get more time for science, less time troubleshooting. The result is a system that adapts to evolving needs and integrates smoothly into diverse workflows.

LINEV Systems US is based in the United States. What role does it play in your global strategy?

As CEO, I see our U.S. division, which is established in 2006, as a strategic hub for North and Latin America. It ensures local support, regulatory alignment, and access to our global R&D pipeline. Proximity to users and responsive service are just as

critical as innovation. This dual presence – global reach, local delivery – is part of what makes LINEV Systems different.

Your company refers to itself as a system innovator. What does that mean in practical terms?

We do not just build devices – we build solutions. Innovation for us starts with understanding user challenges, not with adding features. Every part of SPINSCAN is there to serve a defined function. We believe in purposeful engineering: do not design for features – design for function. That mindset has shaped everything we have created.

What is your message to researchers thinking about adding ESR to their capabilities?

The technical barrier is no longer a limitation. With SPINSCAN, you do not need a specialized room, extensive training, or complex calibration. You just need curiosity and a problem worth solving. ESR is now accessible, powerful, and compact. Compact does not mean compromised – it means engineered for purpose. If you are in radiation science, materials research, or life sciences, this is a tool that will expand what you can see and understand.

LINEV Systems US: Compact Innovation for Real-World ESR

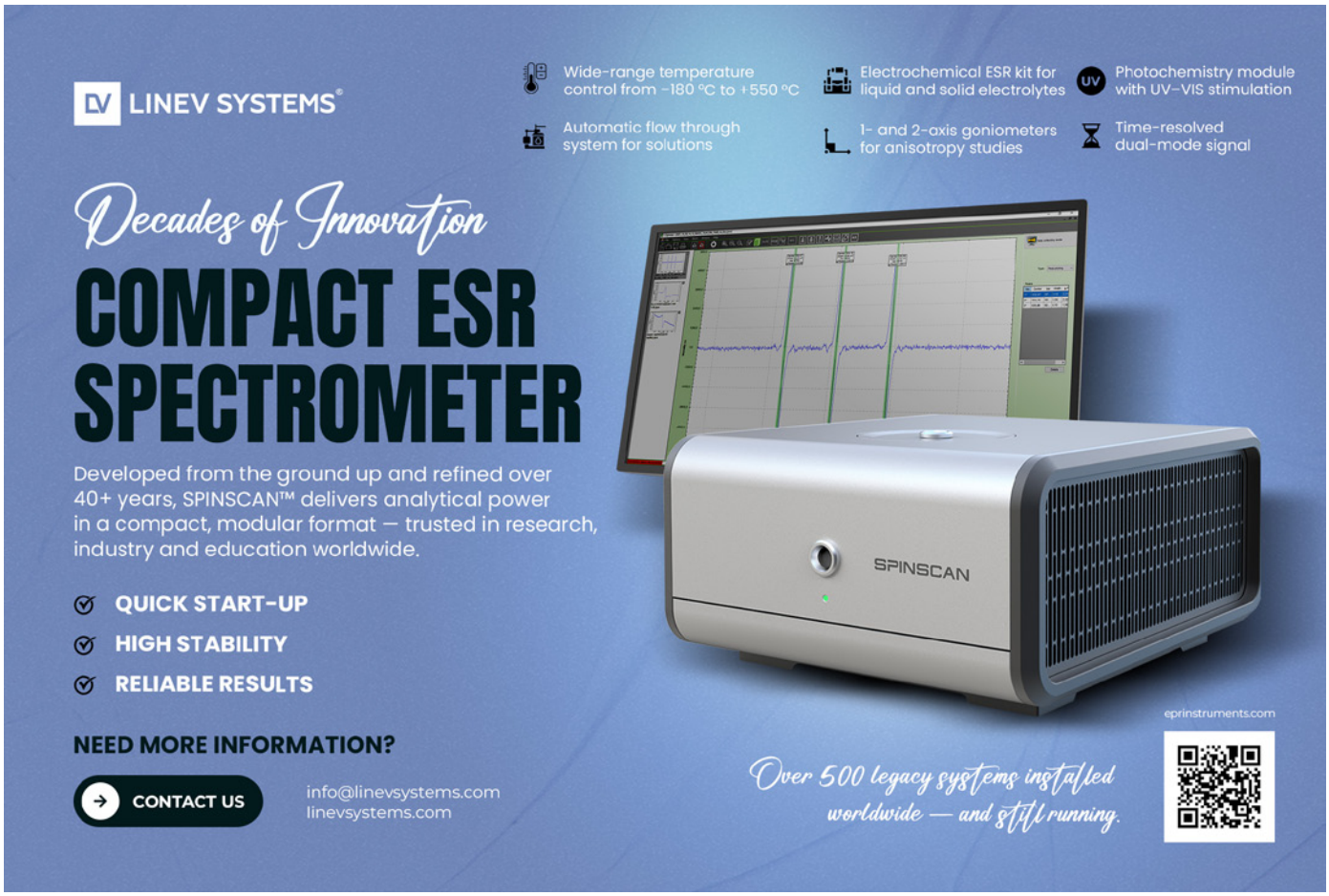
LINEV Systems US is part of the global LINEV Group, known for pioneering innovations in scientific instrumentation and X-ray imaging. With over 30 years of engineering experience and thousands of systems deployed worldwide, the company focuses on developing compact, intelligent, and purpose-built tools for real-world applications.

Its flagship product, **SPINSCAN**, is a benchtop ESR spectrometer designed from the ground up not as a scaled-down system, but as a fundamentally new platform. It integrates original patented microwave architecture, AI-assisted optimization, and modular options for alanine dosimetry, photochemistry, and temperature control.

Used in academic, medical, industrial, and aerospace settings, **SPINSCAN** enables high-precision ESR analysis with minimal infrastructure. The US, UK and EU divisions provides technical support, compliance services, and user training.

LINEV's mission is to make advanced scientific technologies more accessible, scalable, and adaptable bringing ESR to those who need it most, without compromise.

Learn more at www.linevsystems.com



Interview with Professor Olav Schiemann on the Occasion of His IES Medal in Biology/Medicine 2025

EPR newsletter: *Dear Professor Schiemann, on behalf of the readers of the EPR newsletter we congratulate you on your IES Medal in Biology/Medicine 2025. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

From a fairly young age, I was fascinated by fossils and dinosaurs. Then I came across a "Schüler Duden Biologie", I opened it, and there was this colorful DNA double helix with an obvious explanation of how it functions. This looked at the same time so simple and beautiful that I thought this is what I want to work on. School being a horror for me, I went with the help of my mother to the University of my hometown, Lübeck, and was able to get several practicals, including two fantastic ones with Bernhard Irrgang (now director of R&D at Weleda) in an organic chemistry lab. They were so supportive, inclusive, and encouraging. Even after having tipped over a bowl with a liquid they synthesized over a month, I was just told: "Shit happens, keep on going".

Considering my marks at school, it was still a tough decision whether I should study, but an uncle of mine said that if I failed, I could still become an apprentice (gardening was high on the list), which convinced me. Whether Biology or Chemistry as a subject was settled after I talked with two guys from biochemical companies at the Hannover Messe, who both recommended chemistry as the basis on which I could build biochemistry. And, Chemistry had no Numerus Clausus.

In 1989, I started my studies in Chemistry at the University of Marburg. I loved the freedom, all the possibilities, and the lab courses. To my delight, my marks improved (admittedly, I failed the first Thermodynamics exam), and my enthusiasm for Chemistry kept growing.

Who introduced you into magnetic resonance?

For the Diploma thesis and the PhD, I needed to decide whether to do Bioinorganic Chemistry or Organometallics. Again, I thought it would be better to get a solid grip on inorganics first and then add the biology bit. So I joined the group of Christoph Elschenbroich, working with many methods, including continuous wave EPR spectroscopy, on exchange-coupled open-shell organometallic systems (Eric knows which ones). For his group members, Christoph gave a lecture on EPR spectroscopy from an inorganic chemistry perspective, but also including theory. I thought, this is a highly exciting method.

For my Postdoc, I had the idea to find a connection between the exchange coupling constant J and the rate of the electron transfer rate k_{et}. Christoph, knowing this, put one day an article from Jacqueline Barton (Caltech) on charge transfer in DNA, a highly controversially discussed topic at that time, on my desk. I just thought, wow, that's where I want to go. Christoph, being humble, said: "She will never take you, and if she does, you will only get a space in the corner of the dark distillery room, but try". So I sent her an e-mail (yes, we already had e-mail). After two weeks, she wrote back asking what I wanted to work on. I wrote her about my idea, and she asked me to come the same evening. The cw EPR spectrometer at Caltech was not in good shape and we were eager to get data, so Jackie sent me to Scripps and then to NASA's Jet Propulsion Laboratory (what an adventure: I was only allowed to move in there in the presence of an armed soldier and was locked in the lab). Finally, she sent me to Nick Turro at Columbia (he was a marvelous guy), where I got the light-excitation experiments on DNA in the EPR cavity to work. When I came back to Pasadena, Jackie asked how I liked New York. I replied that I don't know, I was just in the lab. I think that impressed her, and she sent me a second time, fully paid, telling me I should also look around New York, which I then did. Working in such a controversial field was extremely exciting, and I knew that I wanted to stay in science and pursue a Habilitation.

For my Habilitation, I thought to work with NMR and EPR on my topic in Frankfurt. I first asked Christoph Elschenbroich and Friedrich Hensel in Marburg whether they would support this. Instead of a reply, Hensel picked up the phone and called Rüterjans in Frankfurt. He invited me to come to Frankfurt and said that I should also talk with Thomas Prisner (a new guy in Frankfurt), who does EPR. Thomas spent a lot of his time, and we talked and talked and talked. In the end, he asked whether I would like to join his group instead of Rüterjans', and I immediately said yes. In that way, I started to move into pulsed EPR (Thomas drew me to the dark side). I was particularly interested in PELDOR/DEER, which I wanted to use at first to measure weak exchange coupling constants in DNA, but then moved slowly into the field of structure-dynamics-function relationships in nucleic acid complexes.

While the habilitation as such was quick, getting a professorship wasn't, even with the support of Maria-Elisabeth Michel-Beyerle and Wolfgang Lubitz. After three terms as acting professor at the Technical University in Munich, Thomas urged me to move abroad, and Graham Smith tried to convince me to move to St. Andrews. So I decided I would give St. Andrews a try if they offered me the advertised RCUK fellowship and applied. My plan B was that if it doesn't work out or if I don't like it there, I would become a gardener (there it was again). But it turned out to be one of my best decisions and one of Thomas' best advices. Already at the interview in St. Andrews, I felt very welcome. Moving there was fantastic; all of a sudden, everything I did was recognized as something that I did, and it was also formally acknowledged as such in no time. On top, we were a great team: Malcolm White, Jim Naismith, Graham and his group, and the whole St. Andrews/Dundee magnetic resonance gang. But St. Andrews is small and remote, and my wife with our two little ones stayed in Germany, because she works in international banking, meaning we commuted St. Andrews-Frankfurt for three years. In 2011, I took up the professorship in Bonn and moved there with my family. However, the Scottish flag is still on the wall in my office. So, in the end, all was good!

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

Discussing science. Supporting young scientists on their way. Travelling around the world and talking with people. For example, I am very grateful to Daniella Goldfarb for the Weston Visiting Professorship at the Weizmann Institute and for the friendship with Raanan Carmieli, also at the Weizmann Institute, because people and friendship matter. And Research can open paths beyond science, e.g., demonstrating with Raanan in Tel Aviv, reminding Nethanjahu and his lot to care about the hostages still held today by Hamas and to "Bring Them Home, Now".

Doing science, talking politics, and drinking wine with Benjamin Kaupp (with him and Helmut Grubmüller, we got the time-resolved PELDOR to work).

What is your idea of a team work in science?

Hosting and working together with people from different areas of science, nationalities, and religions. Working at different places. Sharing new ideas, compounds, and instrumentation. Acknowledging the work of other people. Supporting other people/scientists.

What is your opinion about the future of EPR and the development of its applications and methods?

I think there can be a bright future for in cellulo and in operando/in situ EPR. But we have to bring EPR across the experts' border and broaden it into the non-expert fields: biologists, material scientists etc. This requires simpler and especially cheaper instrumentation and timely repair/support of it. Nobody will buy a pulsed EPR spectrometer for €2Mio to learn something about the first coordination sphere of a metal ion or to get one distance.

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

Follow your heart and do what you really want to do, not just because it is fashionable at the moment. For example, when I started my habilitation, I was working on a niche system with a niche method (EPR on oligonucleotides). Take risks. Don't give up too quickly. Talk to people and decide based on knowledge. Find people whom you trust and at least listen to (maybe not always follow) their advice.

In the end, I would like to thank all of my past and current group members for their knowledge, enthusiasm, and enjoyable atmosphere in the lab. Without them none of the work awarded would have been possible.

Interview with Professor Patrice Bertet on the Occasion of His IES Medal in Physics/Materials Science 2025

EPR newsletter: *Dear Professor Bertet, on behalf of the readers of the EPR newsletter we congratulate you on your IES Medal in Physics/Materials Science 2025. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

Many professors during my school years provided various levels of guidance. I also remember reading Feynman lectures in physics passionately. I found quantum physics particularly interesting, and I therefore chose quantum optics and atomic physics for my Master's degree, and later my PhD.

Who introduced you into magnetic resonance?

I entered magnetic resonance only recently ! My PhD, which I obtained in 2002 at the Ecole Normale Supérieure in Paris, was about fundamental quantum physics with atoms and photons. Under the supervision of Jean-Michel Raimond, Michel Brune, and Serge Haroche, I discovered cavity quantum electrodynamics, which studies the interaction of individual atoms excited in Rydberg states with individual microwave photons stored in a superconducting high-Q cavity. I found fascinating the idea that the cavity was able to dramatically enhance the spontaneous emission rate of the Rydberg atoms and completely alter their dynamics, by concentrating spectrally and spatially the vacuum fluctuations of the microwave field. This insight inspired some of our recent developments in magnetic resonance.

I then did a postdoc in the Netherlands, in TU Delft, in the group of Hans Mooij. There, I discovered the field of superconducting qubits, which are superconducting electrical circuits containing Josephson junctions. When cooled at 10mK into their ground state, these quantum non-linear resonators behave as "artificial spin-1/2". They can be used as quantum bits for quantum computing, which was the main goal of Hans Mooij's group, as well as many others in the world. More recently, we have used these circuits for microwave photon counting and single spin detection.

Because these circuits are macroscopic quantum objects, their quantum state is very fragile, making their measurement challenging. In 2004, the teams of R. Schoelkopf and M. Devoret at Yale used on-chip superconducting microwave resonators, fabricated by patterning thin-films using standard lithography techniques, to measure superconducting qubits by microwave reflectometry at millikelvin temperatures. Their experiments were a major source of inspiration for my later research, for at least reasons. First, these on-chip resonators have a high quality factor but also ultra-small mode volumes, many orders of magnitude smaller than a cubic wavelength, which makes them ideal for high-sensitivity EPR spectroscopy, as I realized several years later. Second, we learned from the Yale team how to perform microwave measurements on a chip at millikelvin temperatures and at the quantum limit, using a combination of low-noise and low-temperature microwave amplifiers, including superconducting ones.

In 2006 I joined the Quantronics group at CEA Saclay as a permanent researcher, to develop qubit research for quantum computing, working with D. Vion and D. Esteve.

At that time, superconducting qubits had really short coherence times, in the microsecond range, which drastically limited their possible application in computing. We had the idea to use electron spins in solids as a quantum memory for superconducting qubits, able to store their quantum state over much longer times than the qubit coherence time. Indeed, at low temperatures and in well-chosen matrices, it was well-known that spin coherence times could be longer than milliseconds.

This is how I finally started working with spins!

I met several brilliant researchers who kindly introduced me to spin physics and magnetic resonance: Vincent Jacques and Jean-François Roch for NV centers in diamond; John Morton and Jarryd Pla for donors in silicon, Philippe Goldner, Thierry Chaneliere, Sylvain Bertaina for rare-earth-ions. John has moreover always been particularly supportive and instrumental in introducing our work to the EPR community, through various invitation to conferences.

I am immensely grateful to all of them for their precious collaboration and support throughout the years. I am also grateful to the EPR community, which has always been extremely welcoming, with special thanks to Sun Un, Gunnar Jeschke, Daniella Goldfarb, and many others.

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

Upon conducting experiments where spins were considered as quantum memory for superconducting circuits, I started wondering, around 2013, whether it might be interesting to use the superconducting circuits for ultra-sensitive spin detection instead. I quickly realized that single-spin sensitivity was, in principle within reach, by combining ultra-small mode volume resonators, and microwave detection at the quantum limit of sensitivity. This insight has been very fruitful and has guided my research since that time.

Towards that goal, we consistently applied to spins in solids the concepts and ideas from quantum physics and optics that I learned during my early researcher years. One highlight was the observation in 2016 of the spin Purcell effect by Audrey Bienfait, who was then PhD student in our group. Audrey observed a dramatic enhancement of the energy relaxation of donors in silicon coupled to a high-Q superconducting planar cavity of small magnetic mode volume, when their Larmor frequency was resonant with the cavity. This constituted the first observation of spin dynamics being altered by quantum fluctuations of the microwave field, as predicted by Purcell in 1946. This was very exciting to me, as a first hint that we could possibly apply cavity quantum electrodynamics to spins!

Another idea came from discussions with my colleague Emmanuel Flurin, in 2018. Together, we realized that counting the microwave photons emitted by spins when they relax radiatively should out-perform standard inductive detection in terms of sensitivity, because photon counting is not sensitive to vacuum

field fluctuations, contrary to quadrature detection. Within a few months, Emmanuel invented and demonstrated a state-of-the-art microwave photon counter based on a superconducting qubit. We rapidly applied it to spin detection, and reached single-spin sensitivity in 2022 with our PhD student Zhiren Wang. Since then, we have used this method to observe real-time quantum jumps of individual nuclear spins, demonstrate single-atom DNP, and high-resolution ENDOR spectroscopy of individual nuclear spins.

I hope that single spin detection by microwave photon counting will make an impact in magnetic resonance, and will be considered, one day, as a general-purpose spectroscopy method.

What is your idea of a team work in science?

Science is by nature a collaborative effort. Our research involves a lot of varied technical and scientific expertise, in many different areas – low temperatures, microwave measurements, nanofabrication, superconducting qubits circuit design, materials science, chemistry, ... I am very fortunate to be part of the Quantronics group in the Service de Physique de l'Etat Condensé (SPEC) at CEA Saclay, a fantastic team without which this research would have been impossible. I would particularly like to acknowledge the key contributions of my colleagues Emmanuel Flurin, with whom I've had the immense chance to team up since 7 years, and of James O'Sullivan who joined the group more recently. And most importantly, I would like to thank the PhD students, postdocs, and technicians who contributed to our work over the years.

What is your opinion about the future of EPR and the development of its applications and methods?

Being still relatively new to EPR, I am lacking the perspective to make relevant statements about the future of EPR, so I'd like to restrict the question to single spin EPR.

The potential of single spin EPR for high resolution magnetic imaging and spectroscopy has been demonstrated by many beautiful experiments conducted with single NV centers in diamond, a paramagnetic center whose spin can be optically detected at the individual defect level. I find particularly inspiring recent experiments using a single NV as a nano-antenna to perform high-resolution spectroscopy and atomic-scale imaging of individual ^{13}C nuclear spins inside the diamond matrix surrounding the NV (see for instance the work of J. Wrachtrup in Suttgart, T. Taminiau in Delft, C. Degen in Zurich, and many others). Single-spin EPR detected by spin-polarized STM is also rapidly developing, although with a lower spectral resolution so far.

These experiments suggest a natural question: is single-spin NMR spectroscopy and imaging also possible in individual molecules? I hope we will be able to contribute to this question in the future, using single electron spin detection by microwave photon counting. I am grateful to the European Research Council to support this research with the project ONESPIN.

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

As a relatively newcomer to the field, I am amazed by the beauty and power of magnetic resonance spectroscopy. I still find incredible how much detailed information at the atomic scale can be obtained, in a completely non-invasive manner, and at such low energies. I think we can expect in the future many exciting developments, in particular on nano-scale magnetic resonance spectroscopy. Therefore, I encourage the young researcher generation to be bold, creative, and ambitious in their scientific goals!

IES Poster Prize at the 2024 Spin Chemistry Meeting

Daniele Panariti:

First, I would like to begin by expressing my sincere gratitude to the International EPR (ESR) Society for recognizing my poster presentation at the Spin Chemistry Meeting 2024 in Kobe. Sharing my research findings with the EPR community at the conference was a truly rewarding experience, and I am grateful for the chance to do so again in the IES newsletter.

Among the projects I worked on during my PhD, one major area of focus was understanding how long-lived electron spin polarization is generated and transferred in weakly-coupled peptide bridged chromophore-radical conjugates. Photochemically generated systems often result in spin states whose populations strongly deviate from those expected at thermal equilibrium. This phenomenon has attracted considerable interest, particularly in light-induced triplet-doublet systems, which are promising candidates for unraveling the mechanisms behind spin communication in molecular materials, with potential applications in quantum information technology and light-induced dynamic nuclear polarization [1].

A new electron spin polarization transfer mechanism was recently observed in a weakly-coupled triplet-doublet spin-system, where the triplet state precursor and the radical are fixed 2.4 nm apart in a mutant of a human neuroglobin [2]. The transfer of net polarization from the photoexcited Zn(II)-protoporphyrin IX to the radical probe was ascribed to the interplay between the dynamic Jahn-Teller effect and the electron-electron dipolar coupling [3]. The non-Boltzmann distribution of the spin sublevel populations is generally separated into two different components: multiplet and net polarization. While multiplet polarization corresponds to the part of the enhanced polarization in which states with equal and opposite values of the spin magnetic quantum number are equally populated, net polarization accounts for any population imbalance between these paired sublevels.

To delve deeper into this new electron spin polarization transfer mechanism, we engineered a rigid bis-labeled α-helical model peptide to connect the nitroxide radical, the artificial amino acid TOAC, to either a free-base (H_2P) or a zinc (ZnP) tetraphenyl porphyrin chromophore, over distances ranging from 1.4 nm to 4.2 nm. The chromophores ZnP and H_2P were selected due to their distinct symmetries, which dictate the activity of the dynamic Jahn-Teller effect. The results presented at the conference demonstrate that net absorptive polarization, driven by the dynamic Jahn-Teller effect in the triplet state of ZnP, can be transferred to a stable radical and that the magnitude of the polarized radical scales with the inter-spin distance as r^{-3}, aligning with the expected behavior in the weak-coupling regime. The findings also reveal that the polarization of the radical lifetime can be sustained as long as the triplet remains polarized, which is approximately two orders of magnitude longer than its spin-lattice relaxation. This extended lifetime allows for more time to manipulate and transfer the polarization to remote spins.

As the dynamic Jahn-Teller effect is not essential for the generation of net polarization in photoexcited chromophores, triplet states with strong zero-field splitting interactions can also be employed in the electron spin polarization transfer to weakly-coupled radicals. To explore this scenario and expand the range of suitable chromophores for radical polarization, a BODIPY derivative and an erythrosin B chromophore were inserted in two additional peptide-based model compounds. Our findings show that the solid-state triplet mechanism, occurring during intersystem crossing, leads to the rapid generation of emissive net polarization in the photoexcited triplet states of both chromophores, which can then be transferred to the weakly-coupled radical.

In conclusion, we provided key insights into the role of electron-electron dipolar coupling and net polarization in triplet states, both of which are crucial for the proposed mechanism and should be considered in the design of similar triplet-doublet systems. Importantly, the source of net polarization was found to be irrelevant if it originates in the photoexcited triplet state and the dipolar coupling conditions are met.

Lastly, I would like to thank my supervisor, Marilena Di Valentin, for her invaluable guidance, as well as to everyone who has contributed to this project.

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2. M. G. Dal Farra, C. Martin, E. Bergantino, Y. E. Kandrashkin, A. van der Est, M. Di Valentin,

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3. Y. E. Kandrashkin, M. Di Valentin, A. van der Est, *J Chem Phys* **2020**, 153, 1–11.

Marilena Di Valentin:

In line with the Italian tradition, Daniele completed all of his academic training, from his bachelor's degree to his doctoral studies at the University of Padova. I feel fortunate that he chose Physical Chemistry as his main subject as it allowed me to spark his passion for spectroscopy through the course I taught. As a result, I have had the pleasure of mentoring him throughout all the stages of his career. It has been a true privilege to share my knowledge of light-induced EPR spectroscopy with him and most importantly one of the projects I consider among the most innovative, but at the same time highly complex and risky, that I have proposed to a student. The focus of his PhD thesis was on the generation and transfer of long-lived electron spin polarization from a porphyrin triplet state to a nitroxide radical, separated by distances reaching the limit of 5 nm, in model peptide rulers, We have faced frustrations together, but Daniele persevered even when the results were ambiguous, gradually achieving breakthrough achievements.

Now that few months are left before he starts a new journey, I already miss this special student of mine. Daniele's many qualities derive primarily from his dedication to science with a scrupulous and at the same time creative approach, which encompasses an innate ability to translate that deep theoretical understanding into solid interpretation of the experimental data. His talents are accompanied by persistence, hard work and an appreciable generosity in sharing his knowledge with other students of the group. He is a young scientist who embodies the values of Science.

He has already received numerous awards for his accomplishments. Last but not least, the recent prestigious IES poster prize at the Spin Chemistry Meeting 2024 is a well-deserved recognition of his merits.

I am confident Daniele will have a brilliant research career in academia or wherever his talents take him next. Watching his achievements has been and will continue to be rewarding because training young scientists like him is among the most fulfilling aspects of my (our) work at University.

IES Poster Award at APES 2024

Akihiro Tateno:

At first, I would like to thank the IES committee for selecting me for the IES Poster Award at APES2024. I was interested in controlling the reaction of radical pairs with AWG and developed a transient absorption detection type AWG-RYDMR system.

The control of radical pair (RP) reaction is an important subject applied to the improvement of luminescence efficiency of organic light emitting diodes (OLEDs), isotope enrichment and the elucidation of quantum mechanical mechanisms underlying reactions in living organisms. The method of observing the yield change of reaction products of radical pairs in a magnetic field with the application of an oscillating magnetic field (RF) is called reaction yield detected magnetic resonance (RYDMR), and a single-color RF has been used for RYDMR. However general RPs have multiple nuclear spins, it is difficult to induce transitions in all nuclear spin configurations with a single-color RF, and there are also limitations such as spin locking when trying to cover the frequency with RF intensity. To overcome this problem, we have developed a method to control RP by irradiating waveforms based on the local optimization theory from an arbitrary waveform generator (AWG) [1–3]. Here we report the experimental results of RYDMR with arbitrary waveforms for the BSA-AQDS system in the created system.

The details are given in [4], but here we extract and explain some of the important results. For the evaluation of RYDMR effects (ΔMFE), the magnetic field effects of transient absorption (ΔA) during RF irradiation (MFE_{on}) and during non-irradiation (MFE_{off}) were defined as follows:

$$MFE_{on/off}\,(\%) = 100 \times \frac{\int_{t_{st}}^{t_{en}} \Delta A(B, B_1^{on/off}, t) - \Delta A(0, B_1^{off}, t)\,dt}{\int_{t_{st}}^{t_{en}} \Delta A(0, B_1^{off}, t)\,dt}$$

$$\Delta MFE\,(\%) = MFE_{on} - MFE_{off}$$

The arguments of ΔA correspond to the applied static magnetic field B, the oscillating magnetic field B_1 on/off, and time t, respectively. Fig. 2 (c) of [4] shows the B_1 spectrum in a resonance field (5.17 mT) of single-color RF (145 MHz). ΔMFE decreases with increasing B_1, but the signal is inverted around B_1 = 0.4 mT. This is due to spin locking and confirms that there is a limit to ΔMFE in single-color RYDMR. Fig. 4 (a) of [4] shows the field sweep RYDMR spectra of single-color RF (B_1 = 0.34 mT) and periodic chirp RF (145±15 MHz FM frequency 10 MHz). In case of chirp RF, |ΔMFE| near resonance field is larger than that by single-color RF. This means that the reaction yield is boosted by AWG. This phenomenon can be explained by the coverage of hyperfine structures by chirp RF and the reduction of spin-locking effects by FM.

With the use of AWG, we were able to achieve yield changes that were not possible with single-color RF. In the future, we plan to further improve the yield by irradiating the designed waveforms.

Recently, I was also interested in RF-induced reaction yield change by RF at lower magnetic fields and performed single-color RYDMR experiment. RYDMR measurements were performed such that the peak of the low field effect is the resonant field in systems exhibiting low field effects (Xanthone-DABCO in SDS micelle). The lower limit of yield change that can be achieved by static magnetic field is the low field effect, and if spin mixing by RF can exceed this efficiency, reaction yields that cannot be achieved by the static magnetic field effect will be possible. The results obtained so far show that the combination of the peak magnetic field and single-color RF can outperform the low magnetic field effect caused by a static magnetic field. The next step is to further enhance the low field effect by using arbitrary waveforms.

Finally, I would like to thank again the IES committee for selecting me, the members of my laboratory for their support in my daily research life, and the Motizuki Fund of Yukawa Memorial Foundation for supporting my presentation at APES 2024.

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2. K. Masuzawa, M. Sato, M. Sugawara, and K. Maeda: *J. Chem. Phys.* **152**, 014301 (2020)
3. A. Tateno, K. Masuzawa, H. Nagashima, and K. Maeda: *Int. J. Mol. Sci.* **24(11)**, 9700 (2023)
4. A. Tateno, H. Nagashima, and K. Maeda, *Chem. Phys. Lett.* 864 (2025)

Kiminori Maeda:

Dr. Akihiro Tateno conducted interesting research in the Maeda Laboratory at Saitama University until March 2025. His research focused on the theoretical and experimental control of radical pairs using magnetic resonance phenomena induced by an arbitrary waveform generator (AWG).

He started his work with theoretical modelling to explore coherent and anisotropic control mechanisms for radical pairs. Based on these findings, he developed the world's first low-magnetic-field AWG-RYDMR system by integrating an AWG and a radio frequency amplifier. This innovative setup demonstrated enhanced radical pair recombination without inducing spin locking. Dr. Tateno also investigated the relationship between this phenomenon and magnetic field effects in low-field regimes.

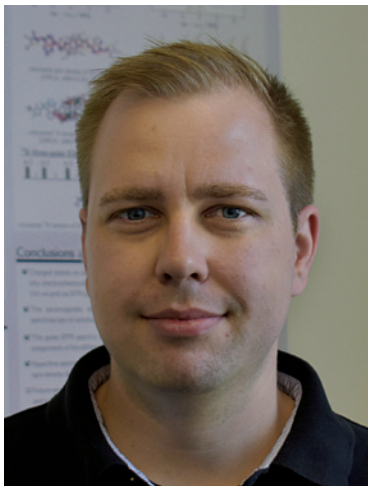
I believe it was his exceptional self-learning ability that led to these achievements. In the laboratory, he started by reading books on quantum mechanics and spin dynamics, quickly applying what he had learnt to his research. He designed RF coils for experimental applications using a simulation program for electrical circuits, carrying out most of the programming and device fabrication himself – a testament to his impressive versatility and technical skill.

During his time in our laboratory, he participated in many national and international conferences, where his work was recognized with several awards, including this IES Poster Award at the Asia-Pacific EPR Conference and the RSC Poster Awards at the Spin Chemistry Meeting 2024 in Kobe.

From spring 2025 onwards, Dr. Tateno is embarking on a new research project in a laboratory specializing in ultrafast phenomena at the nanoscale. While we are sad to see him graduate from Saitama University and leave our group, we look forward to future collaborations, particularly in the field of spectroscopy.

We would like to extend our heartfelt thanks to Professor Masanobu Wakasa for generously providing access to high-performance AWG equipment, which was instrumental to this project. We wish Dr. Tateno continued success in his scientific endeavors.

IES Poster Award at the 2025 joint ENC-ISMAR



Maximilian Mayländer:

Photoinduced and electrochemically induced charged paramagnetic states in organic semiconductors probed by EPR

First, I want to thank the International EPR (ESR) Society for awarding me an IES Poster Prize at the ENC-ISMAR conference 2025 and for the opportunity to share part of my research in the EPR newsletter.

Our group is investigating spins and spin dependent processes in materials and devices for energy applications using EPR spectroscopy. In this context, we are interested in paramagnetic ionic states of organic donor polymers and acceptor molecules, as these species play a key role in the fundamental processes underlying organic electronic devices, for example organic photovoltaics [1]. Spin and charge delocalisation in these radical ions are thought to influence device efficiency by affecting charge separation and recombination dynamics and charge mobility.

We investigate the radical cations and anions of organic semiconductors in various chemical environments, such as in solution or thin films, by EPR spectroelectrochemistry. Combined with hyperfine spectroscopic techniques, this approach offers detailed insight into the spin and charge density distribution. Interpretation of these experimental results is supported by DFT calculations, which help us correlate observed EPR parameters with molecular structure and the surrounding environment.

In the work described on the poster, we electrochemically generated the paramagnetic ionic states of materials used in organic photovoltaics: PTB7-Th acting as an electron donor, and EH-IDTBR serving as an electron acceptor. Using an adapted three-electrode setup within an EPR tube [2–4] combined with chronoamperometry, we can control and monitor the redox processes in situ. This allows us to characterise the radical ions via cw EPR and UV-vis absorption spectroscopy under electrochemical control. We then flash-freeze the samples to trap these short-lived species, enabling us to apply pulsed hyperfine techniques such as Q-band ^{1}H Davies ENDOR, ^{14}N ESEEM, and HYSCORE for more detailed characterisation.

For a better understanding of how the chemical environment influences the spin properties of the anions and cations, we compare the electrochemically generated species with those observed under photoexcitation in donor:acceptor blends. By illuminating a PTB7-Th:EH-IDTBR blend and probing it with EPR, we obtain spectra that reflect the steady-state populations of photoinduced charge carriers. The EPR spectra of the electrochemically generated species serve as reference points, allowing us to assign features in the overlapping EPR spectrum of the blend. Furthermore, the ^{1}H Davies ENDOR spectra reveal variations in spin density distribution, especially in the case of EH-IDTBR, suggesting that the molecular environment influences the charge delocalisation.

To complete the picture, we are currently conducting spectroelectrochemical EPR measurements on neat films of the semiconductor materials.

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Claudia Tait:

Max joined my group in June 2024 as a postdoctoral researcher supported by a DAAD PRIME fellowship. He had previously completed his PhD at the University of Freiburg in Sabine Richert's group, investigating the spin dynamics of photoexcited chromophore-radical systems. With an interest in further developing his skills in pulse EPR techniques and in methodological work, he was drawn to a project on EPR spectroelectrochemistry aimed at exploring paramagnetic states in materials relevant to organic photovoltaics and organic electronics more broadly.

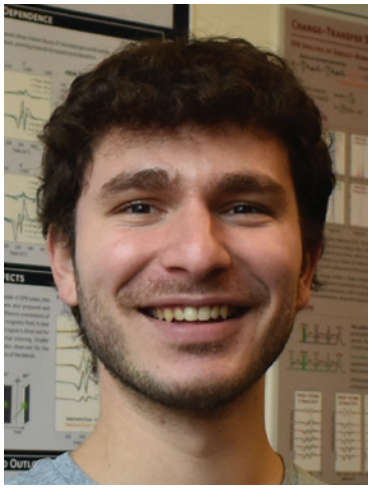
The goal Max set out to achieve was to develop a setup that would allow the generation of charged states on a variety of organic semiconducting molecules, both in solution as well as in films, and their characterisation using a combination of continuous-wave EPR

and pulse EPR at X- and Q-band frequencies. The primary focus is to quantify charge delocalisation and its dependence on the molecular environment through a combination of hyperfine EPR techniques and DFT calculations.

Now, just over a year into his time in the group, Max has made remarkable progress toward this goal. With extraordinary dedication and ingenuity – and often supported by his trusted 3D printer – he designed and built a series of EPR electrochemical cells tailored to different types of measurements. These custom cells enable investigations of both solution and film samples, at room temperature for continuous-wave EPR and under cryogenic conditions for pulsed EPR at X- and Q-band. His successful measurements on donor and acceptor molecules for organic photovoltaics were presented on his poster, and he is actively extending this work to include further materials and a more detailed characterisation.

I am grateful Max's hard work has been recognised with an IES poster prize at the 2025 joint ENC-ISMAR conference in Asilomar.

CIQTEK Poster Prize at the 2025 RSC ESR meeting



Lorenzo Catini:

Insights into recombination processes in organic solar cells through electrically detected magnetic resonance

Organic solar cells have recently seen a sharp rise in efficiency, now exceeding 20%, however, the fundamental mechanisms underlying current generation are still not fully understood. ESR and Electrically Detected Magnetic Resonance (EDMR) can provide new insights since states with unpaired electron spins play a crucial role in the photovoltaic mechanism: light absorption in a blend of organic electron donor and acceptor molecules leads to formation of a singlet exciton, followed by charge separation if the exciton reaches the donor:acceptor interface. The generated charges then travel towards the electrodes, supplying electricity to an external circuit. The desired charge transport by hopping and any charge recombination following re-encounter of opposite charges are spin- dependent processes, as their rates depend on the relative spin configuration of charge pairs, and can be probed by EDMR [1, 2].

At the annual ESR meeting in London, I presented a poster on my research, using EDMR to investigate four different donor:acceptor blends used for organic solar cells: two blends with a fullerene acceptor (PBDB-T:PCBM and PM6:PCBM both with an efficiency of ~7%) and two with a non-fullerene acceptor (PBDB-T:ITIC and PM6:Y6 with efficiencies of ~12 and 15%, respectively). The goal was to unveil any differences in their photo- and spin physics through EDMR and correlate them to their differences in efficiency. To perform EDMR experiments, I fabricate fully working, miniaturized devices, which I then investigate on a traditional EPR spectrometer integrated with a custom-built transimpedance amplifier for EDMR detection. I spent the first part of my PhD developing a fabrication method for the miniaturized solar cells and optimizing the EDMR set up. Once these two were ready, I wanted to identify and characterise the species involved in charge recombination. To do so, I performed a pulse EDMR experiment monitoring device current as a function of field and time after application of a microwave π pulse and, in combination with EasySpin simulations, I was able to identify both the donor and acceptor molecules contributing to the overall EDMR signal. To further investigate the nature of the spin-dependent process and role of different spin states, I performed Rabi nutation experiments. This is particularly useful as it enables to clearly identify weakly coupled spin pairs and triplet excitons based on their nutation frequency. With these experiments, I was able to identify spin locking features at field positions corresponding to spectral overlap of donor and acceptor EPR signatures, indicating the presence of weakly coupled charge pairs involved in processes directly affecting device current. I am now working on understanding how differences observed between the blends I am investigating explain their performance and identify strategies for increasing current generation efficiency.

I am extremely grateful to have received the CIQTEK Poster Prize at the 2025 RSC ESR meeting and I would like to sincerely thank the committee for awarding me this prize. I'm also very honoured to be able to share my research with the international ESR community through the IES newsletter.

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2. A. Schnegg, J. Behrends, M. Fehr, K. Lips, *Phys. Chem. Chem. Phys.*, 14, 14403–14712, **2012**.

Claudia Tait:

I am delighted Lorenzo has been awarded a poster prize at the 2025 RSC EPR meeting in London for his work on exploring spin-dependent processes in organic photovoltaics by electrically detected magnetic resonance (EDMR).

Lorenzo joined my group at the University of Oxford in October 2022 with a Sir David and Lady Clary Graduate Scholarship from Magdalen College. His project involved the challenging task of setting up and performing EDMR spectroscopy on a series of donor:acceptor blends for organic photovoltaics, complementing our parallel studies investigating the different photoinduced spin states in the same materials by transient and pulse EPR.

Lorenzo embraced this challenge and dove into his first major task: the design and fabrication of functioning organic photovoltaic devices small enough to fit into an EPR resonator. He overcame initial hurdles with determination and a consistently positive attitude, and developed a protocol for the reliable fabrication of miniature devices that reproducibly yield high photocurrents.

This progress then allowed him to focus on determining the optimal measurement conditions and experiments to investigate spin-dependent processes in organic photovoltaics based on different donor:acceptor systems by pulse EDMR. By combining re-

sults from pEDMR, echo-detected pEDMR and pEDMR-detected Rabi experiments, Lorenzo gained a series of insights into spin-dependent recombination in the investigated devices, described on his poster, and revealed interesting differences between various types of donor:acceptor blends.

This is however only the beginning, and Lorenzo is now expanding both the types of EDMR experiments performed and the devices under investigation, driven by the desire to fully understand the role of different spin states and correlate the spin-dependent behaviours observed via EDMR with device performance.

JEOL Prize 2025

Annemarie Kehl:

To my great pleasure I had the opportunity to present our work on the effects of nuclear dipolar couplings in ^{19}F-ENDOR spectroscopy at the 58th RSC conference in London and to be awarded the JEOL prize for my presentation. It is a great honor for me and an encouragement for my future work to receive this prize. I would like to express my gratitude to JEOL for providing this opportunity, to the committee for the selection and the IES for the chance to introduce my work in this newsletter. I am also very grateful to Marina Bennati as my Ph.D. supervisor for all the support throughout this project, during my studies and my time at the Max Planck Institute for Multidisciplinary Sciences in Göttingen.

^{19}F-ENDOR spectroscopy is emerging as a method of choice to determine distances in the angstrom to nanometer range by measuring the hyperfine interaction between an electron spin and ^{19}F nuclear spins [1]. I have started working in the field of ^{19}F-ENDOR by implementing the measurements at our 263 GHz spectrometer. Due to the combination of the high magnetic field, the small hyperfine coupling size in the range of kHz and the strong anisotropy (compared to protons) of the chemical shielding this work has for the first time resolved the effects of the chemical shielding in ENDOR spectra [2]. This already demonstrated that, apart from the opportunity to determine distances, ^{19}F-ENDOR spectra also have the potential to reveal previously hidden interactions. While interactions like the chemical shielding could be neglected so far, they now need to be investigated and considered in the data analysis.

Distance measurements in biomolecules provide many possible applications for ^{19}F-ENDOR. Often the structure of biomolecules is flexible and thus a distribution of distances is present, resulting in multiple spin-dipolar couplings. This correlates to a broadening of the line width in frequency domain ENDOR spectra [3]. However, other line broadening mechanisms in ^{19}F-ENDOR spectra can obscure the distance information, thus limiting both the resolution and the accessible distance range.

To disentangle this ambiguity and thereby enhance the applicability of ^{19}F-ENDOR we started an investigation of the different line broadening mechanisms. For this a combination of rational molecular design, frequency and time domain ENDOR methods as well as quantum mechanical spin dynamics simulations were applied [4].

The observation of the chemical shielding has already shown that small effects usually only observed in NMR are now resolved in ENDOR as well. Similarly, it is also possible to see the effect of the nuclear dipolar couplings between fluorine and protons in the ENDOR spectra. The couplings to protons in the close vicinity of up to 14 kHz were identified as a major source of spectral broadening. The effect could be simulated with spin dynamics simulations and removed experimentally by H/D exchange, resulting in reduction of the spectral width to 9 kHz.

With these findings we were able to move on to more challenging biomolecular model systems and applied the identified strategies to the analysis of ENDOR spectra of a spin labelled RNA duplex. There, the spectral ENDOR line width could be predicted, which in turn enabled the extraction of a distance distribution, representing a first step towards a quantitative determination of distance distributions in biomolecules from ^{19}F-ENDOR.

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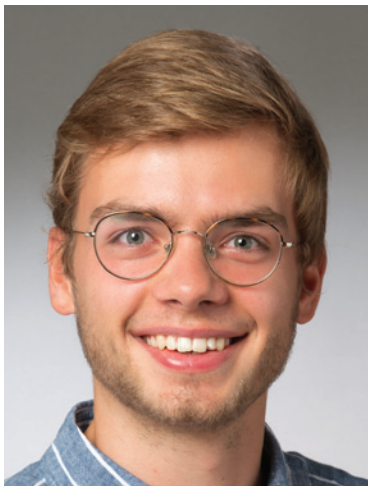
2. A. Kehl, M. Hiller, F. Hecker, I. Tkach, S. Dechert, M. Bennati, A. Meyer, *JMR*, **2021**, 333, 107091.
3. L. Remmel, A. Meyer, K. Ackermann, G. Hageluecken, M. Bennati, B. E. Bode, *Angew. Chem. Int. Ed.* **2024**, 63, e202411241.
4. A. Kehl, L. Sielaff, L. Remmel, M. L. Rämisch, M. Bennati, A. Meyer, *PCCP*, **2025**, 27, 1415–1425.

Marina Bennati:

I was excited that Annemarie received the JEOL Student Lecture Competition Award at the 58th RSC conference in London. I have known her for the time of her Bachelor studies, when she got interested in electron spin resonance (EPR) spectroscopy and performed her Bachelor as well as her Master thesis in my group. During these initial research stages, she had already learned several EPR spectroscopic methods to characterize radical intermediates in enzymes as well as spin labelled proteins. During her PhD, she was able to push boundaries in several aspects of our research. In a first stage, she performed ^{19}F electron-nuclear double resonance (ENDOR) at a Larmor frequency of 263 GHz. Her results revealed nuclear spin interactions such as chemical shift anisotropy, which were not observed so far in the EPR literature. This turned out to be a key aspect in the analysis of ^{19}F ENDOR spectra for molecular distance determination. In a second stage, as part of a research consortium with the Department of Mathematics in Göttingen, she investigated spin dynamics in novel type of ENDOR experiments, specifically cross-polarization and time domain ENDOR. For this, she developed a spectral simulation code for spin dynamics *SimDyn*, which included many features so far not accessible in other open software. This allows to predict individual spectral contributions in ENDOR, as well as to design new experiments. The work led to advances in ^{19}F ENDOR spectroscopy, particularly paved the way for determination of distance distributions in biomolecules, complementing other magnetic resonance and biophysical methods. I'm very pleased that Annemarie decided to continue her academic career in EPR joining the group of G. Jeschke and receiving an ETH postdoctoral Fellowship. I would like to congratulate her for all her achievements and the well-deserved award.

IES Travel Grant at EUROMAR 2025



Marvin Lenjer:

I am a third year PhD student in the research group of Prof. Marina Bennati at the Max Planck Institute for Multidisciplinary Sciences in Göttingen, Germany. At the EUROMAR 2025 conference, I had the opportunity to present our research on 94 GHz chirp and phase-modulated EPR experiments for spin dynamics analysis and ENDOR spectroscopy.

Over the last decade, shaped microwave (MW) pulses have evolved into valuable tools for EPR spectroscopy. They have been used to improve existing experiments by providing tuneable broadband or band-selective frequency profiles as well as to design new experimental approaches. However, most applications were performed at low EPR frequencies (X- or Q-band) where high MW powers is available, with only rare examples at W-band (94 GHz) or higher frequencies.

Our work is focused on the implementation of chirp and phase modulated pulses at a commercial Bruker E680 W-band (94 GHz) EPR spectrometer using a SpinJet arbitrary waveform generator. Despite hardware constraints including a limited resonator bandwidth (140 MHz) and comparably low Rabi frequency (≤20 MHz), using shape pulses turned out to be, in many instances, beneficial also at our setup. In particular, we applied frequency chirped MW pulses for Fourier transform EPR spectroscopy and phase modulated pulses for performing echo experiments during spin locking. In my contribution to the EUROMAR 2025, I presented our results using these experiments for the analysis of spin dynamics during microwave irradiation and for hyperfine spectroscopy.

Microwave arbitrary waveform generators become more and more abundant in both commercial and home-build state-of-the-art EPR spectrometers. As a consequence, there were multiple contributions about instrumentation and application of shaped pulses in EPR at this EUROMAR conference. Generally, I have the feeling that the interest in this topic is growing, which made it even more fun to present our results.

I would like to thank the International EPR Society for awarding me a travel award to attend the EUROMAR 2025 conference. I am very grateful that I could present my research at this conference, hear many interesting presentations on other topics of magnetic resonance and meet new people and friends from the magnetic resonance community.

mmmx.info

The x in MMMx

Gunnar Jeschke

After starting at ETH Zurich in April 2008, I suddenly found myself with a lot of free time before my new coworkers arrived in September. With a teaching break until mid-November after lecturing nine contact hours per week at my previous institution, I decided to start a pet project. This project, which I called MMM, was intended to create a convenient graphical user interface (GUI) and visualization tool for simulating distance distributions from spin-label rotamer libraries – a concept we had introduced the previous year in a study on a membrane transporter [1].

My next-door colleague thought it was crazy that I would program something so basic and established as protein visualization, but at the time, this was the price to pay for having your own customizable software package. The full name "Multiscale Modeling of Macromolecules" was a nod to a concept that was popular in polymer science, though I never fully implemented that vision. Secretly, the MMM acronym also referenced a childhood competition in East Germany for small hands-on projects, called "Messe der Meister von Morgen".

After Zhenia (Yevhen Polyhach) and Enrica Bordignon joined my group in September, Zhenia took over rotamer library modeling while Enrica gave me feedback on program features. Even before our first technical publication on the rotamer library, MMM had already gained a small user base.

In August 2010, our manuscript on the rotamer library approach was harshly rejected by the *Journal of Physical Chemistry B*. Our appeal was unsuccessful, but after a few tweaks, the same paper received glowing reviews elsewhere and was eventually published [2]. Later, computational biophysicists adopted our approach [3].

Over the years, I grew dissatisfied with the 2008 decisions on data structure and implementation. The integration of MMM functions with the GUI had become overly complicated, making it difficult to implement ensemble modelling for intrinsically disordered proteins. It was time for a fresh start.

Coincidentally, the team behind the popular protein visualization package Chimera had just done the same, adding a capital X to create ChimeraX. As my team was much smaller, I could only afford a small x – and so MMMx was born in 2020. This was a fortuitous development, as I suddenly had ample time to program after my lab was abruptly closed due to the pandemic.

At the same time, my colleague Laura Esteban Hofer was also homebound for the same reason, and began contemplating ensemble modelling of the RNA-binding protein SRSF1 based on her DEER results (Figure 1). This marked the start of a highly fruitful collaboration, as Laura provided valuable feature suggestions and helped debug my code [4].

The MMMx program offers much of the functionality of its predecessor, MMM, including handy in silico spin labeling and distance distribution calculations – all with the added convenience of programmatic access. Plus, users can still leverage the slick(?) GUI of MMM for visualization.

But the real purpose of MMMx is ensemble modeling. It can incorporate distance distributions, small-angle scattering data, and NMR paramagnetic relaxation enhancement (PRE) restraints to build and analyze ensemble models of those pesky, heterogeneously structured proteins [5].

The program goes well beyond EPR – it can import data from the Protein Ensemble

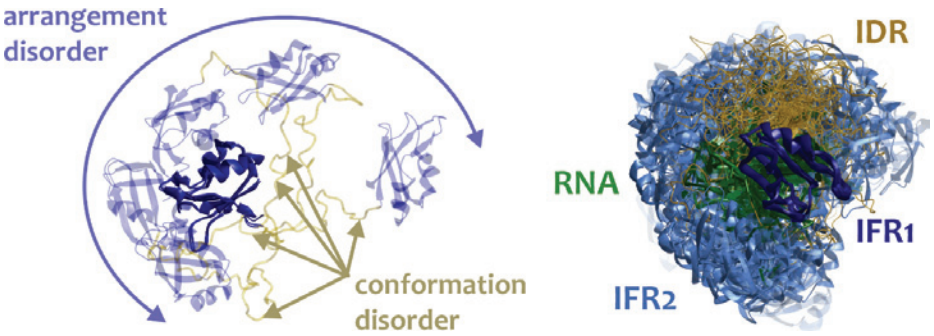


Figure 1. This is how most eukaryotic proteins really look like. The left panel shows the five most diverse conformers of free SRSF1 (PED00497, ensemble generated with MMMx). RNA-recognition motif 2 (RRM2, transparent blue) displays arrangement disorder with respect to RRM1 (dark blue), because the intrinsically disordered linker between these two IFRs exhibits conformation disorder. The right panel shows an ensemble model, based on DEER and PRE data, of the same protein after binding RNA 5'-UCAUUGGAU-3' (green). IFR2 has the same size as IFR1, it is just not always in the same place. Visualized by MMMx/MMM.

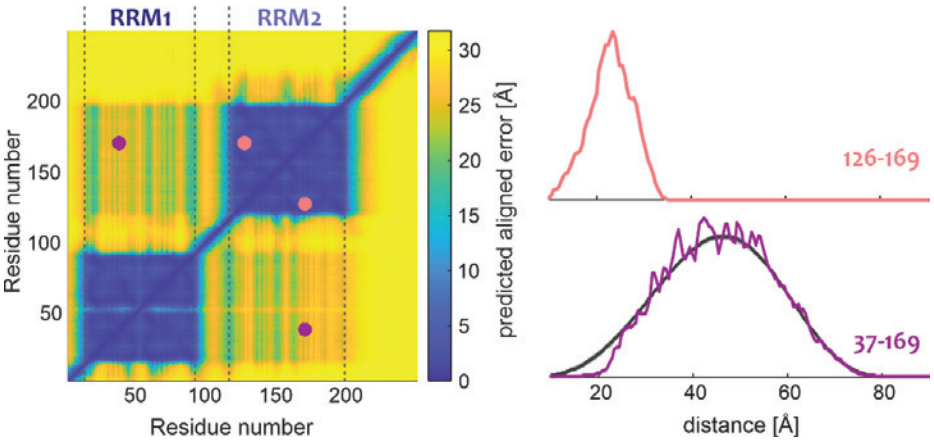


Figure 2. AlphaFold knows about non-folding. The left panel shows the predicted aligned error (PAE) matrix that AlphaFold puts out for free SRSF1. Two site pairs are marked, one within the same IFR (126-169 in RRM2, pink) and one with residues in different IFRs (37-169, violet). In the former case, one expects a narrow distance distribution (top right panel) that is dominated by rotamer disorder of the two spin labels. In the latter case (bottom right panel) distribution width is dominated by arrangement disorder. The black curve with grey uncertainty band in the bottom right panel is an experimental distance distribution. The colored curves in the right panel are simulated from the ensemble PED00497. Visualized by MMMx/MMM.

Database (PED) and AlphaFold output, identify intrinsically folded regions (IFRs) and disordered ones (IDRs), and detect whether those IDRs are behaving like random coils or not [6, 7].

In fact, when we scanned the entire human proteome in the AlphaFold Protein Structure Database using MMMx, we found that most proteins contain a mix of IFRs and IDRs [5]. Looks like an ensemble approach is an absolute necessity these days. Who would've thought?

DEER distance distributions are pretty much the only way we can currently quantify the arrangement disorder between IFRs and link IDR conformations to IFRs (Figure 2). This is great news for EPR spectroscopy. MMMx might be the go-to tool for this work – feel free to borrow it for your own projects.

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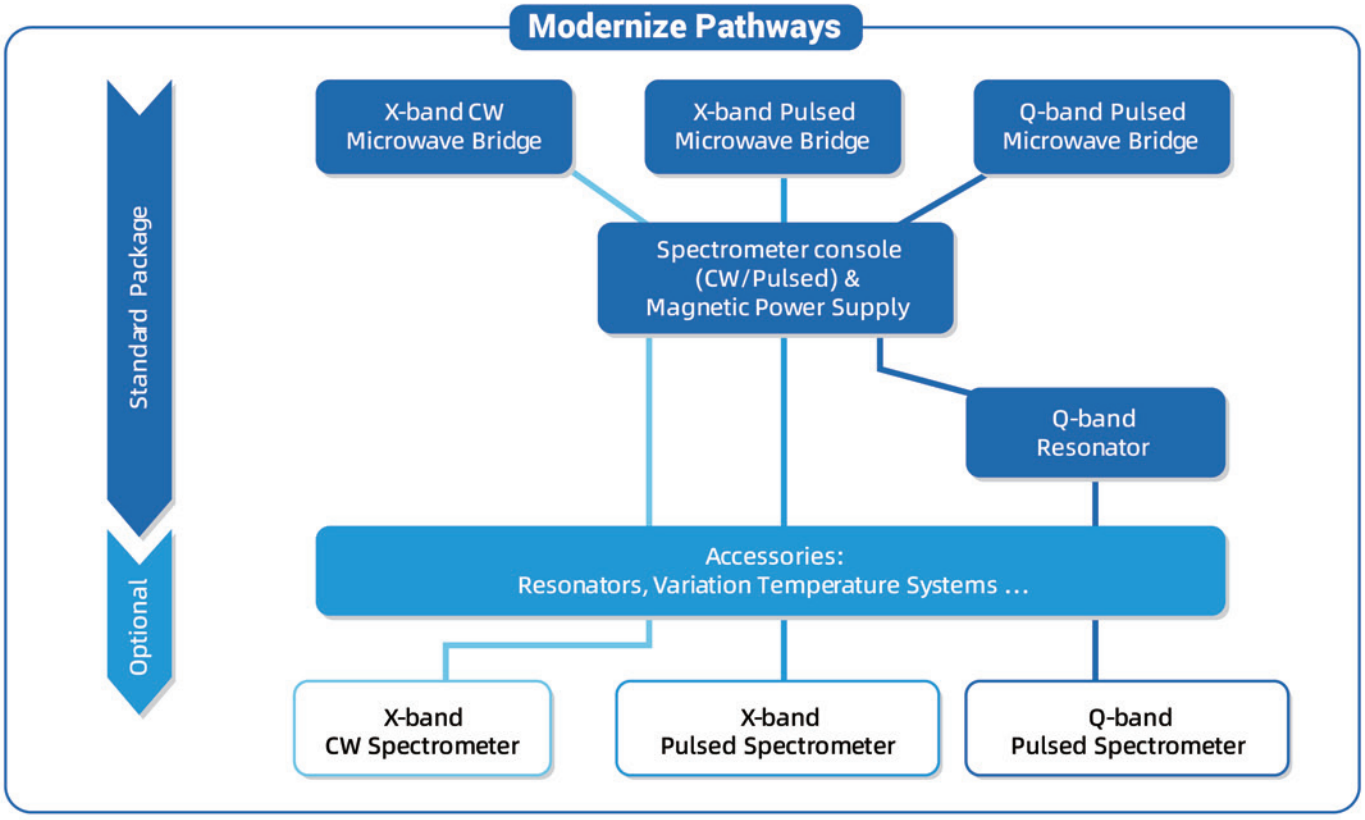

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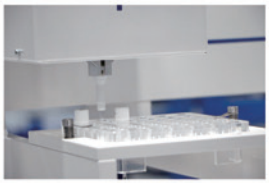

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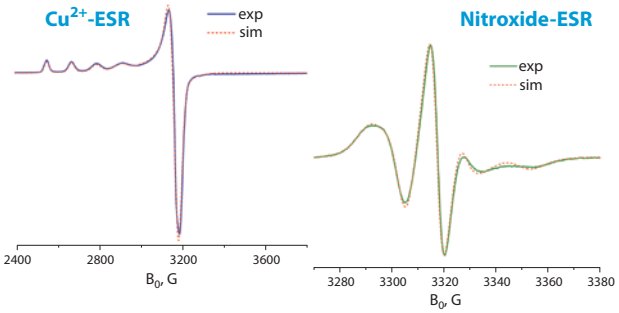
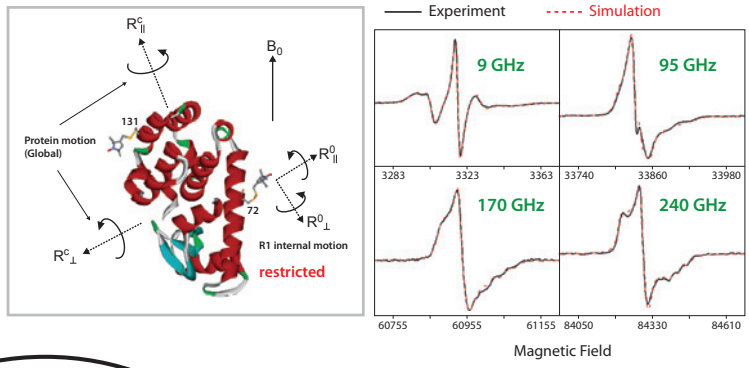
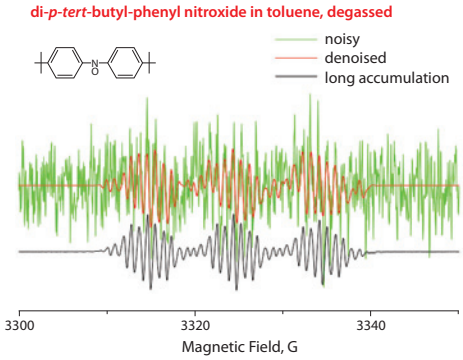


Multifrequency ESR

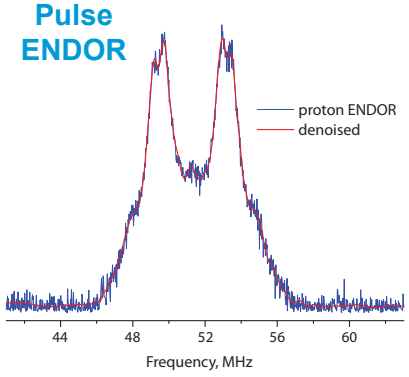


Denoising

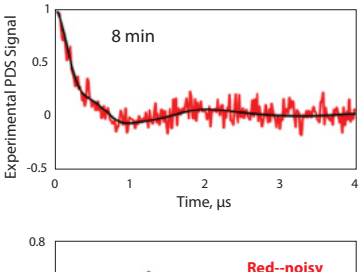


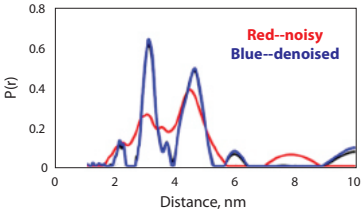
1) Perform
ESR Measurements
2) ESR Data Analysis
3) Advice on
ESR Experimental Design
4) Standard Samples
5) Contact Info Above

Pulse ENDOR

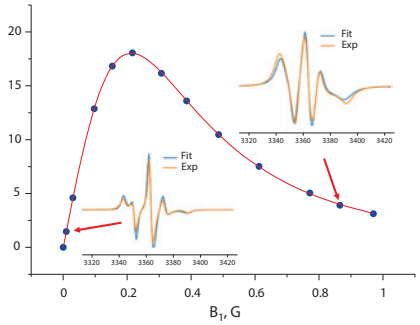


DEER & DQC



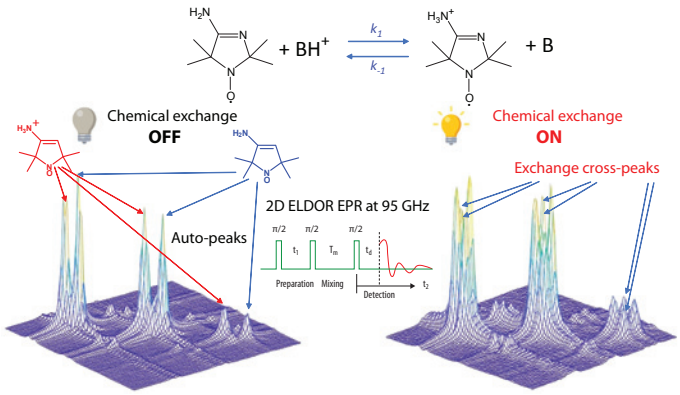


Simulation



Saturation Curve

2D ELDOR



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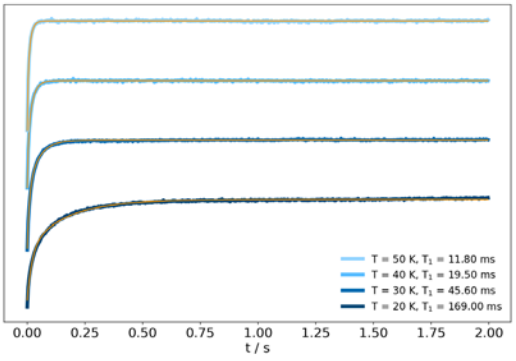

Left: The inversion recovery experiment on irradiated quartz at various temperatures.
Right: The new SpinJet-AWG II

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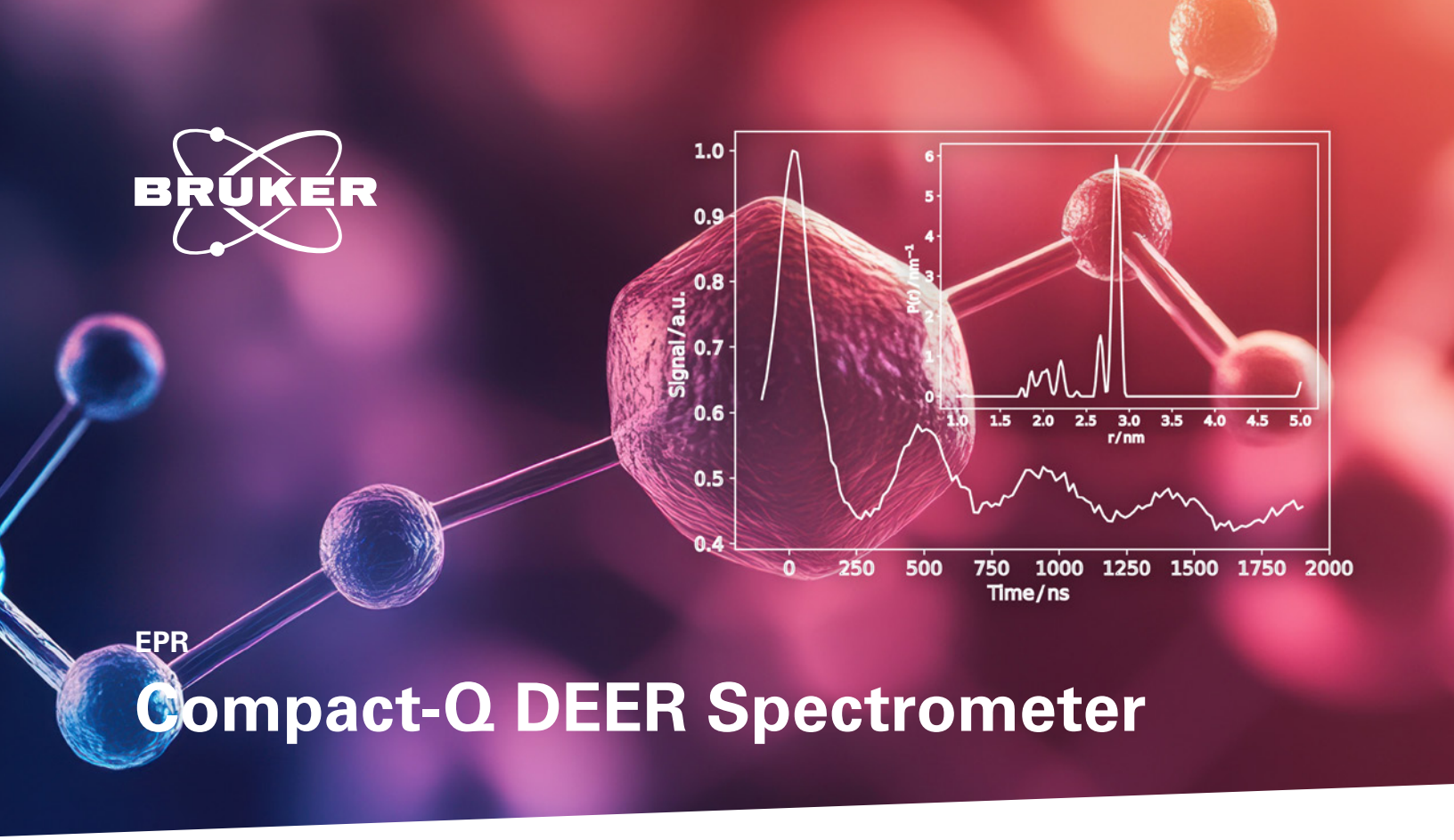

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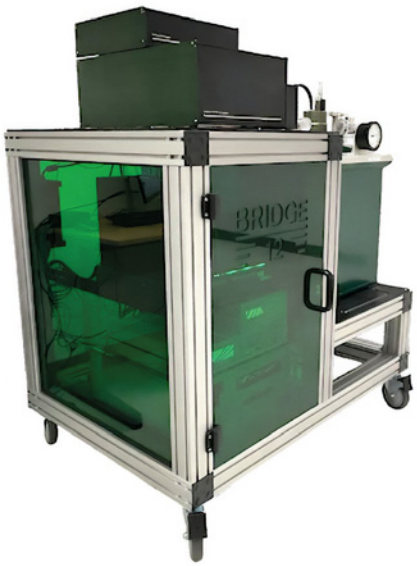

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