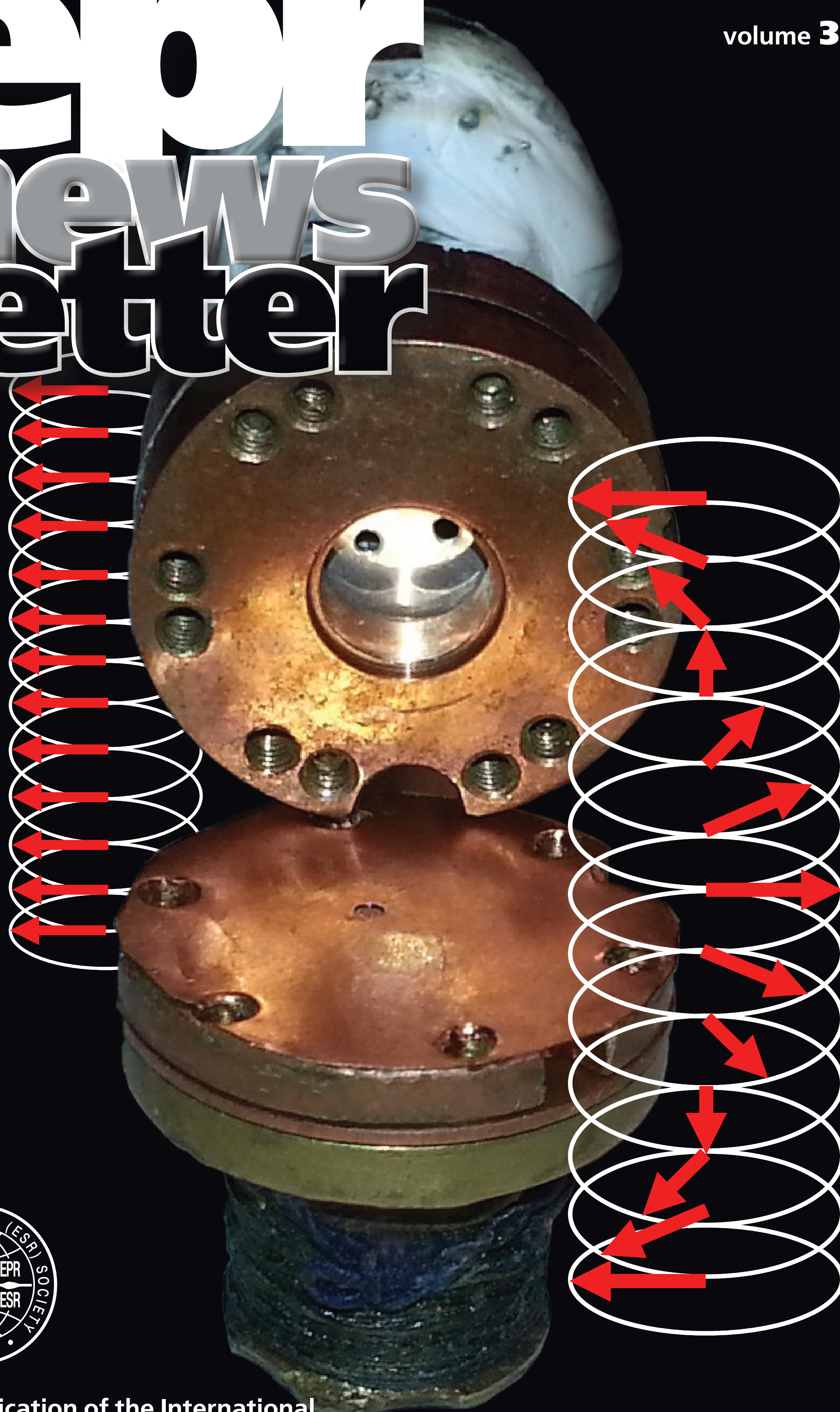
epr newsletter

2021
volume 31 number 4



The Publication of the International
EPR (ESR) Society

epr newsletter

https://ieprs.org/newsletterpage/

The official publication of the International EPR (ESR) Society is supported by the Society, by corporate and other donors, and the Zavoisky Physical-Technical Institute of the Russian Academy of Sciences, Kazan, Russian Federation.

EDITOR
Laila V. Mosina
Zavoisky Physical-Technical Institute
Russian Academy of Sciences
Kazan, Russian Federation
mosina@kfti.knc.ru

ASSOCIATE EDITORS
Candice S. Klug
Medical College of Wisconsin
Milwaukee, WI, USA
candice@mcw.edu
Hitoshi Ohta
Molecular Photoscience Research Center,
Kobe University, Kobe, Japan
hohta@kobe-u.ac.jp
Sabine Van Doorslaer
University of Antwerp, Antwerp, Belgium
sabine.vandoorslaer@uantwerpen.be

TECHNICAL EDITOR
Sergei M. Akhmin
Zavoisky Physical-Technical Institute
Russian Academy of Sciences
Kazan, Russian Federation
akhmin@inbox.ru

FOUNDING EDITOR
R. Linn Belford
Illinois Research Center, University of Illinois
at Urbana, Urbana, IL, USA
rbelford@uiuc.edu

EDITORIAL OFFICE
Zavoisky Physical-Technical Institute
Russian Academy of Sciences
Sibirsky trakt 10/7, Kazan 420029
Russian Federation
phone: 7-843-2319096
fax: 7-843-2725075

Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.
The *EPR newsletter* is published quarterly by the International EPR (ESR) Society and is available in electronic and printed form to all members of the Society. The deadlines for submission of news for upcoming issues: Spring March, 15; Summer June, 15; Fall September, 15; Winter December, 15.

ISSN 1094-5571

TECHNION | PRINTING UNIT

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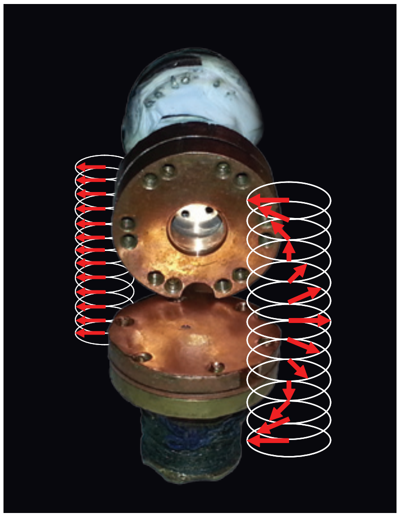


The cover picture illustrates aspects of research carried out by Sergei Demishev, recipient of the Zavoisky Award 2021. It shows the cavity used in the high-frequency EPR spectrometer developed at the Prokhorov General Physics Institute of the Russian Academy of Sciences (Moscow) for the investigation of quantum materials and quantum critical systems, in particular, magnetic metals with the spiral magnetic structure.

КАЗАНСКИЙ ФИЗИКО-ТЕХНИЧЕСКИЙ ИНСТИТУТ

Editorial

Dear colleagues,

By now most of you might have already heard sad news Nobel laureate, Richard Ernst who contributed to the development of the methodology of high resolution NMR, died recently. It is a great loss for the magnetic resonance community.

The *EPR newsletter* enjoyed fruitful collaboration with Richard Ernst on several occasions, to start with our special issue devoted to Nobel Laureates in Magnetic Resonance (vol. 14/1-2). In this issue, we published Richard Ernst's article about Tibetan thangkas (vol. 14/1-2, p. 15–18). It is interesting to note that between 1985 and 1992, Richard Ernst published a series of papers, together with Arthur Schweiger and other members of his research group, which were devoted to subjects like phase cycling in EPR, new ESEEM approaches and pulsed ENDOR schemes, reduction of deadtime problems and longitudinal detection, to mention a few. Richard Ernst also wrote an article for the *EPR newsletter* on 150 years of ETH Zürich (vol. 15/1, pp. 12,13). In 2010, we were privileged to be able to reproduce his article on follies of citation lists and academic ranking lists published in *Chimia* (20/1, pp. 10,11). I am sure his article found a response in the soul of every researcher, it suffices to quote any citation from this article, e.g., "The present hype of bibliometry made it plainly obvious that judging the quality of science publications and science projects by bibliometric measures alone is inadequate, and reflects the inadequacy of science management regimes staffed by non-scientific administrators or by pseudo-scientists who failed to develop their own personal judgment". Does it not sound like an echo of our own thoughts?!

Kristina Comiotto (ETH Zürich) kindly attracted my attention to several obituaries to Richard Ernst, and in this issue you find an obituary to Richard Ernst written by Alexander Wokaun. We are grateful to him for the permission to reproduce this obituary in the *EPR newsletter*, the same goes to Fabio Bergamin (ETH Zürich) and Denise Schmid (Hier und Jetzt Verlag, Zürich).

In this issue, we also say farewell to Sergei Orlinskii who left us only too early in the prime of his creativity. His death was a great shock to everyone who knew him. An outstanding experimental physicist, an expert in the field of EPR spectroscopy, an active IES member, a true representative of the EPR school at the Kazan Federal University, Sergei is missed terribly. Our grateful memory will keep Richard Ernst and Sergei Orlinskii alive for the years to come.

The research in the field of EPR continues in spite of the coronavirus pandemic as is clearly demonstrated in this issue by Letter of the IES President by Songi Han, success story of Sergei Demishev, Zavoisky Awardee 2021, interviews with Thomas Schmidt, John Weil Young Investigator Award 2021, and Nandita Abhyankar, IES Best Paper Award 2020/2021, Rapid Scan EPR story by Boris Dzikovski, Ralph Weber and Kalina Ranguelova, ISMAR-APNMR-NMRSJ-SEST2021 conference report by Ikuko Akimoto and Hitoshi Ohta, and the overview of the special issue of *Applied Magnetic Resonance* on THz Spectroscopy by Hitoshi Ohta and Tôru Sakai.

On behalf of the Editorial Board, I thank most heartily all contributors to the *EPR newsletter* with special thanks going to the CEOs of the IES and editors of the columns in the *EPR newsletter*: John Pilbrow, Candice Klug, Wolfgang Lubitz, Stefan Stoll, and Sergei Akhmin, our Technical Editor. I gratefully acknowledge collaboration with Associate Editors Candice Klug, Hitoshi Ohta and Sabine Van Doorslaer.

In the New Year 2022, I wish you all good health and further discoveries in EPR, this fascinating field of science. Let the *EPR newsletter* have an increasing flow of contributions and enhanced feedback from our dear readers!

Laila Mosina

Letter of the President

Dear friends, colleagues and students of the international EPR/ESR society (IES),

The year 2021 is coming to an end. At the end of 2020, we all thought 2021 will be the year of revival and the year of finding our way back to the "good old days" of conducting research, connecting with collaborators and meeting new science friends, and yet it was not. 2021 was the year that tested our resilience, challenged our familiar routines and forced us to invent new ways of connecting with scientists and managing our lives. We lost loved ones and respected scientists. We had to learn to become stronger and more flexible. The International EPR Society did its small part to support our community, almost entirely virtually. We have learned the hard way how much in person interactions mean to us, and are yearning for our scientific reunions!

Let's celebrate the small ways in which our EPR/ESR community has built connections, recognized talents of both new and established researchers and is continuing to work on building a meaningful platform that evolves with our dynamic community.

The IES has given 9 Poster Award in 2021 to talented students across continents. The IES congratulates Fabian Hecker and Luis Ibanez Fabregas for winning Poster awards at the 54th RSC EPR conference, taking place virtually from Cardiff University, Annemarie Kehl and Matthias Brettschneider for winning Poster awards at the 17th Euromar, as well as Akane Yato, Ririko Nakaoka, Jasleen Kaur Bindra for winning Poster awards at the ISMAR-APNMR-SEST conference. We regret not being able to mingle in Slovenia, Japan and the U.K., but the 2021 Modern Development of Magnetic Resonance (MDMR) brought scientists together for a much needed in person conference in Kazan at which Arina Tarasova and Bogdan Rodin won Poster awards!

The IES also awarded medals and prizes to the trail blazers of our field! The 2021 Silver medal in Chemistry was awarded to Elena Bagryanskaya, whose long-standing contributions to our field was featured at the ISMAR-APNMR-SEST conference. The 2020 Young Investigator awardee (YIA) Sabine Richert was featured at the 54th RSC-EPR meeting and the 2021 YIA awardee Thomas Schmidt featured at the 17th Euromar meeting. The 2021 Silver medal in Instrumentation and Methods was awarded to Stefan Stoll for his impactful development of powerful and widely accessible EPR software and tools. We congratulate the 2020 IES Fellow David Britt and 2021 IES Fellow Klaus-Peter Dinse, and cannot wait to read their laudatios at future conferences. You can find all IES awardees featured in the *EPR newsletter*, delivered to you.

The IES best paper Award has been running on "pilot" for the last 3 years, and we will for next year formalize this procedure by setting it up in the IES bylaws. The 2021 IES Best Paper awards went to Luis Fábregas Ibáñez, Michal Kern and Nandita Abhankar. All awardees shared their work with the broader EPR community through the IES Virtual EPR Meetings (IVEM) and publications in the *EPR newsletter*!

In fact, the resilience of our community is best reflected in the student-led IVEMs. We are already into the second generation of organizers of the IVEM committee, led with dedication by Zhongyu Yang and Thomas Schmidt together with Annalisa Pierro, Zhijie Li, Jana Eisermann, Jaideep Singh, Jing Jin, Julien Langley and Li Feng Li, and Nir Dayan. You are welcome to sign up to listen to and present at IVEMs, here: https://forms.gle/Usv8sbj3LUr7QvcE8. ALL IVEM speakers get the opportunity to submit synopsis and their photo to the *EPR newsletter* to be highlighted by Laila Mosina, Editor of the publication.

And congratulation to 30 authors and experts in dipolar EPR around the world for publishing a community paper on DEER/PELDOR in J. Am. Chem. Soc. volume 143 this year. What an incredible service to the community!

I should not forget to emphasize that the many activities of the IES would not be possible without your valued Membership and our Corporate Sponsors and Patrons. Thank you.

Cheers to all of you and see you soon!

Songi Han

Zavoisky Award 2021

Sergei V. Demishev

Receiving the Zavoisky Award in 2021 was a great honor for me, but also a big surprise. Looking at my scientific carrier as an experimentalist, it is hardly possible to call me a pure EPR man from the very beginning. In student times at Low Temperatures and Cryogenic Engineering Department of Moscow State University, my topic was so-called pressure spectroscopy of impurity states in semiconductors. In 1984, after finishing my doctoral course and getting PhD degree, I took a position at General Physics Institute, a new research institute of the Russian Academy of Sciences, which was founded a year earlier by Nobel laureate Alexander Prokhorov. Those who know the history of quantum electronics might think that it was the right chance to get connected with EPR because of the special role in the maser invention of Prokhorov's research in paramagnetic resonance. However, this was not true, and for about a decade I was still in the field of electron transport in amorphous semiconductors, which finally bring me a Doctor of Sciences degree (the second degree, which is higher than PhD in my country). Fortunately, my boss at GPI Professor Yuri Kosichkin gave me the tasks in microwave spectroscopy, so learning of the new to me experimental technique was on the way. In the nineties of the past century, our lab started a collaboration with John Singleton's group from the University of Oxford, who needed our expertise in microwave measurements in the strong magnetic fields at low temperatures. For that reason, I became involved in studying the magneto-optical response of degenerate 2D electrons in organic conductors including the cyclotron and magnetic resonances. Simultaneously at GPI, we moved to an investigation of various strongly correlated materials, especially metals. As a result, my topic "EPR and strongly correlated and quantum materials" was formed and lasts up to now. So it turned out that EPR became the main part of my scientific life finally.

Typically in strongly correlated materials, you have a concentrated magnetic system, consisting of localized magnetic moments in every unit cell interacting with each other and with itinerant electrons if any. Quantum material is the solid, which macroscopic properties are driven by quantum mechanical regulations. Apart from the superconductors, some popular examples are quantum spin chains, spin nematics (solid-state analogs of liquid crystals), and topological insulators. A related topic is quantum phase transitions, which occur at absolute zero but affect physical properties at finite temperatures. Amazing, that just EPR technique provides in many aspects the best tool to study these complicated objects.

Indeed, in most cases, the EPR is a phenomenon related to the magneto-optical response of a system consisting of isolated magnetic ions. In the diluted case, this is the microwave radiation-induced transitions between Zeeman levels of the individual spin in the crystal matrix. This problem may be described theoretically more or less easily. On the experimental level, the considered case is handled by commercially available and effective EPR spectrometers, nowadays covering a wide frequency range. For that reason, the standard EPR technique has widespread applications from chemical and biochemical reactions to the dating and the food industry. In contrast, a strongly correlated material belongs to the case of a concentrated magnetic system, where the theoretical situation is much more difficult since the collective spin dynamics in a magnetic field is not easy to compute. Moreover, the EPR in a strongly correlated magnetic metal provides an additional challenge for experimentalists. First of all, it is necessary to get rid of the edge effect and influence of the macroscopic gradient of the magnetic field in the sample. Secondly, the correct theoretical evaluation of the EPR line shape accounting skin effect is a must. The situation is complicated by the fact that the EPR spectrum of strongly correlated or quantum material is noticeably broadened by spin fluctuations. It took time for us to solve all these problems. Thanks to my colleague and close collaborator Dr. Alexey Semeno; his creativity and fantastic expertise in microwave measurements allowed us to succeed.

For strongly correlated materials and quantum solids, it is essential to move to relatively high frequencies at least 60–100 GHz due to the fact that in these solids EPR lines are broad. For that reason, our own microwave spectrometer with the 8 T superconducting magnet was built using BWO tunable sources in the beginning and nowadays using network vector analyzer. An original experimental geometry for cavity measurements was developed and a new method, which provides etalon-free absolute calibration of cavity absorption in the units of magnetic permeability and implies data analysis schema allowing obtaining the full set of spectroscopic parameters including the g-factor (gyromagnetic ratio), line width (relaxation parameter) and oscillating magnetization. The latter quantity is not often if ever obtained from EPR data. In contrast to the "pure EPR" technique, the resonance measurements in our ansatz must be accompanied by magnetoresistance and magnetization measurement.

New experimental and theoretical possibilities allowed us to be effective with the EPR study of quantum phase transitions in magnets with spiral magnetic structure and quantum spin chains. It turns out to be possible to establish the existence of a quantum critical point, despite the impossibility of conducting experiments in a quantum critical system at zero temperature. In our group we discovered electron paramagnetic resonance and spin nematic effect in a strongly correlated metal – cerium hexaboride. This material is so unusual that is called "exception to exception" in the literature. For the first time, we were able to detect and study localized magnetic moments on the surface of a highly correlated topological insulator – samarium hexaboride, which appears as a result of low-temperature self-organization of topological surface at helium temperatures. As long as EPR line shape analysis provides direct information about spin fluctuations in strongly correlated systems and quantum materials it became possible to find new phenomena in the field of magnetism. These are so-called spin fluctuation transitions, corresponding to a change in the characteristics of spin fluctuations under the influence of control parameters (for example, temperature or material composition), which is not associated with the formation of phases with long-range magnetic order. Nevertheless, although we have achieved considerable progress in experimental studies and there are several breakthroughs and very valuable theoretical results, the ESR research on metals with strong electronic correlations is still awaiting Columbus, who will map the new beautiful islands of scientific knowledge. Just the EPR method either indicates the necessity for clarification or deep revision of the prevailing paradigm.

In concluding words, I may say that it is never late to change your field of research and turn to beautiful EPR physics. Your expertise in another area will help, for example, my background in low temperature condensed matter physics was very useful for a harmless switch to EPR in quantum solids. However, the background is not solely your knowledge; it is also your origin and surrounding. I will always be grateful to my mentors at Moscow State University – Professors Nickolay Brandt and Victor Moshchalkov, who taught me to love the physics of condensed matter. Here I would like to thank my colleagues at GPI Dr. Alexey Semeno, Dr. Nickolay Sluchanko, and Prof. Vladimir Glushkov for many years of joint work shaping my understanding of EPR area of research. Special gratitude should be passed to my colleague and friend Prof. Hitoshi Ohta from Kobe University and his group members for many years of collaboration and joint studies of various strongly correlated materials with the help of electron paramagnetic resonance.

Interview with Dr. Thomas Schmidt on the Occasion of His John Weil Young Investigator Award 2021

EPR newsletter: *Dear Dr. Schmidt, on behalf of the readers of the EPR newsletter we congratulate you on your John Weil Young Investigator Award 2021. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I suppose part of the question is how I was introduced to science? I grew up in a small village in East Germany just after unification and as one can imagine there was a relative variety of turmoil and uncertainty. My family owned a chunk of land that we used to grow crops (largely potatoes and grains) in addition to working on the fields, I worked out of the garage fixing up mopeds and other small motorcycles to make some additional pocket money (of course tax free). During my entire childhood I harbored a big love for monster movies which I maintained till today. This included the giant squid in '20000 leaks under the sea', 'Godzilla' and of course Dinosaurs which I suppose one could credit with a fond love for the unknown. Anyway, during my schooling I went to the gymnasium which prepped me to go to college, however there was a fair amount of certainty that I would not be able to go and would remain in agriculture or become a mechanic (not that there's anything wrong with it), however that turned out something that I did not want and hence I dropped out of Highschool. In the end I took a flight ticket to Las Vegas and figured I can get rich there… I don't think I was sure how though. Anyway, upon arrival I found very soon that instead of gold on the street I would have to find rather a shelter at a church in Pharump, NV. I spent a lot of time in prayers and bible studies with a variety of folks while helping the church with manual labor. At one point our pastor Glen advised me to obtain my GED, which subsequently permitted me to go to college in the USA… which spurred my next move to Santa Barbara (the heaven on earth) where I was able to enroll into the Community college and begin my studies. Now to the question of what made me study science. To be honest I am not sure, it appears that it just fell into place and my fascination was engaged after attending classes (even though it was initially zoology).

Who introduced you into magnetic resonance?

My first introduction to magnetic resonance was given to me during my undergraduate degree when I did research with Dr. Karin Crowhurst at the California State University, Northridge. Of course back then it was still a solution state NMR with the focus on proteins, however that being said I became intrigued by the idea of eluting minut secrets pertained in molecular machines called proteins. Later on, thanks to Dr Crowhurst, I pursued my PhD specifically in protein NMR under the guidance of Dr Tobias Ulmer on membrane proteins. During that time I truly started to understand the beautiful dance performed by the spins to the orchestra of pulses. After 5 fruitful years, I decided to continue my journey in the field of NMR and approached Marius Clore to take me in as an postdoctoral fellow. I perceived that the NIH would be the right place to widen my perspective on NMR, but little did I know that I will find a new love from my failure. The initial pursuit was to determine the conformational exchange of HIV reverse transcriptase, but the protein kept on aggregating, therefore I decided to give EPR (DEER) a try due to its ability to freeze proteins in time. Luckily for me my PI did very much support me on that endeavour and we soon saw the great potential in this technique. It was at that moment that we realized that one could build on top of NMR techniques and use isotope labeling to a wider extent pertain relaxation information induced by the local chemical environment.

How did you accomplish anything with two kids?

Towards the last year of my PhD, I became the student president for the graduate student organization of the medical campus at USC, fortunate to me I was chosen to give the graduation speech, which was a rather big honor (especially as an international student). While giving my speech most of the attendees did not realize that besides being busy in the laboratory trying to balance the grad student life, I also became a father with my son Otto. Of course that was a rather large motivation to finish my PhD and move on towards a larger pay scale balanced with the idea of succeeding in research. Well, like most other folks, I was unaware what a large barrier that would represent towards the scientific endeavor and how one's life would split into family and professional life. The ability to come in on the weekend or stay for late night experiments was shortened or plain simply diminished. Therefore it was necessary to arrive early in the laboratory to accomplish anything at all. Furthermore, I would try to leave early in the evening to make it home for dinner to permit time with the family which did not permit group outing at the closest "watering well". However there were many moments on the weekend that Otto would join me in the laboratory enjoying splashes of liquid nitrogen to the joy of many of my coworkers who happily shared their secret chocolate reserves with him. Maybe a funny story, Otto was around 3 years old and with me in the EPR room while setting up experiments.

While turning my back on him he was enabled by a faustian thought to push several glowing buttons around the magnet which surely ended the day's experiment, therefore a quick advice: besides not permitting pacemakers close to your magnets, also avoid toddlers. Life became exponentially more interesting when baby number two arrived, as with two kids everything had to be planned from the morning hours with brushing the teeth to the evening as no spare minute could be wasted, however once mastered one could truly enjoy science and family values. I truly suggest bringing your laptop and a set of papers with you wherever you go, you never know when you have a spare minute to finish that next paper, for example one of my papers was largely finished during a camping trip to Jamestown while the kids were busy playing and therefore exhausted in the evening. Another side fact, while having the interview we had two emergencies back to back, Felix split his chin and Otto broke his arm which both required a visit to the ER. Those kinds of events certainly add to your stress levels besides the normal failed experiments. However, please keep in mind we are not the first or last ones to have a family and enjoy our place in the scientific community so all can be dealt with.

What are your main interests of work in magnetic resonance?

Recently the biomolecular EPR field has seen enormous advances comprised by the development of cryogenic probes that reduce thermal noise, non-uniform sampling and associated processing algorithms; and last but not least the development of a vast array of sophisticated EPR experiments that permit the rich information contained in electron spins to be extracted and exploited in unambiguous ways. However, my particular interest is in the application of DEER in conjunction with isotope labeling techniques that has already shown great promise in gains of accessible distances, but more importantly it permits to distinguish and subsequently assign distances to their molecular origin. The real question then remains: what new roles will Isotope-directed EPR play in biology? Which outstanding fundamental questions in molecular biophysics will become tractable by Isotope-directed EPR? Recent developments of rapid freeze quench techniques permit capturing molecular processes at µs to ms intervals, such as enzymatic reactions, protein folding and subtraction recognition events. Isotope-directed EPR of proteins is uniquely equipped to answer questions in regards to conformational exchange to address binding induced folding and subsequent quantitative kinetics and structural characterization of minor populated states. Current projects target the substrate binding pathways of calmodulin to M13; using isotope labeling techniques calmodulin was deuterated to permit long evolution times, however its substrate remained protonated, therefore inducing side specific proton relaxation enhancement of the paramagnetic tag upon interaction. This technique in conjunction with rapid freeze quench permits the temporal resolution of intermediates along the binding pathways towards the final Calmodulin/M13 complex. A rather recent target of interest is the monitoring of the effect of directional forces on protein folding and subsequent molecular dynamics. Mechanical forces have shown to play important roles in protein folding; it should become feasible to study this biophysical property by EPR spectroscopy. Specifically, one would attach a molecular spring to two sites of a protein and thereby apply a directional force between the two attachment sites. In the context of the previous example, together with segmental isotope labeling strategies, one would envision the spring to be placed onto calmodulin hence regulating the transition into its compact complex with M13, or in case of M13 increasing the energy barrier to form its helical fold upon interaction with calmodulin, as present in the final complex. Those sorts of studies would draw this class of studies into the EPR-feasible arena and open the gate to never ending possibilities.

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

When I started my PhD training in NMR, I initially believed that this was the technique which I will be loyal to, however during my postdoctoral training in NMR, I started to develop a devotion towards EPR which developed into a full fledged affair. What drew me in were the open field of experimentation and the supporting community behind this method embodied by the international EPR society. Overall I am very happy that I did the switch and am able to source both techniques for my future gains. I believe that conjoined endeavours between various biophysical tools and analysis softwares produce the most meaningful studies, therefore I truly enjoy forging methods together to produce a joined outcome. Therefore I believe for the coming generation it is essential to know/learn other spectroscopic methods, such as NMR, and subsequently conjoin them in their studies. In regards to EPR, I feel that we have a strong community that is truly accepting of a fast range of ideas and applications and allows young scientists to thrive. In the words of Carl Sagan: "Imagination will often carry us to worlds that never were. But without it we go nowhere", we need to have space to imagine experimental applications through a strong support system. I believe we are further attaining it as through the IVEM online seminars hosted by the IES. One last word of encouragement: EPR is ripe to address a plethora of fundamental questions, however the problem that remains for you is the number of hands needed to attain the answers.

Interview with Dr. Nandita Abhyankar on the Occasion of Her IES Best Paper Award 2020/2021

EPR newsletter: *Dear Dr. Abhyankar, on behalf of the readers of the EPR newsletter we congratulate you on your IES Best paper Award 2020/2021. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I wanted to be a scientist from quite a young age. One of the reasons was to understand how the world works. I felt that science provides a way to translate the abstractness of the world into tangible ideas. The other reason was simply that I thought scientists were really cool and I wanted to be one of them or at least be able to talk to them in their language.

Who introduced you into magnetic resonance?

I was introduced to EPR spectroscopy in my doctoral work. I found it quite engaging because it directly applies concepts of quantum mechanics, which was introduced to me by a brilliant professor, Prof. Shridhar Gadre, when I was getting my Master's degree at Pune University, India.

What are your main interests of work in magnetic resonance?

I am currently interested in exploring microwave-matter interactions at the nanoscale: firstly, how microwaves can be manipulated over deep-subwavelength scales using metamaterials and secondly, how these metamaterials can be used to obtain strong coupling between microwaves and different types of samples.

What are you trying to be better at?

There are many things I need to work on and one of these is how to reach out and start conversations with other scientists in the field. Great ideas rarely emerge in isolation so I'm trying to learn how to exchange ideas productively.

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

Don't be afraid to take a risk, either in the question you're asking or the answer you're proposing. Also don't be afraid to ask for help. 'Decoherence' shows the ability to interact with the environment and ultimately to regain alignment with the field.

Veronika Szalai:

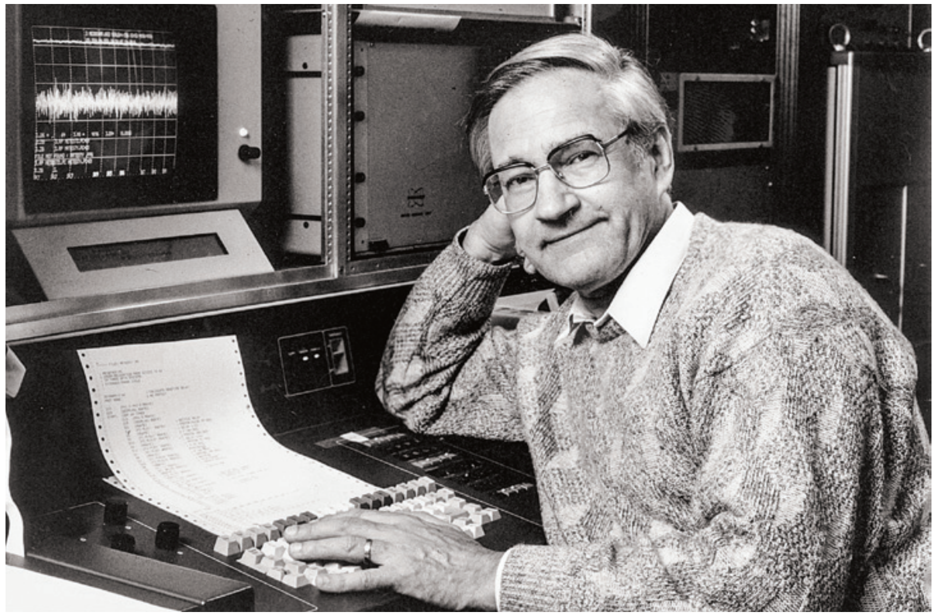
It is my pleasure to highlight Dr. Nandita Abhyankar and the work for which she won the Best Paper Award from the IES[1]. The words I use most often to describe Nandita are persistent and positive. When she first inquired about a post-doctoral position, my advice was that she needed to shift the distribution of "in preparation" vs. "submitted/published" manuscripts in her CV. Now that I know Nandita well, her ability to respond to this mentoring advice is not surprising; at the time, however, I was surprised when she sent me her updated application not long afterward with this issue fully addressed. Her finitiative (finishing what one initiates) convinced me that she could succeed at the challenging post-doctoral project she proposed. She started her project to design, fabricate, and implement the novel microresonator design she presented in her talk with limited background in multiphysics modeling, instrumentation design, and nanofabrication. The steep learning curve did not intimidate her: no matter the research challenges, she carried on and found a way forward. As an example, the reviews for the Science Advances paper were returned to us in early spring 2020, just as COVID-19 shut down lab access. Obtaining experimental evidence to address a reviewer comment became impossible. Rather than being stymied by this setback, she used her – by then – well-developed skill in multiphysics simulations to provide a reasonable estimate of the spatial extent of the sensing region in her device. The associate editor accepted the manuscript after inclusion of this additional information.

Around the same time the manuscript was published, Nandita's technical accomplishment was featured on the NIST website[2]. In addition to the paper, a non-provisional patent application for this technology was filed in September 2021 and a material transfer agreement and a cooperative research & development agreement have been put in place with other institutions. She also has been awarded the Physical Measurement Laboratory's Distinguished Associate Award and the NIST Post-doc and Early Career Associates in Research - Technical Achievement Award. As her mentor, I'm thrilled at her success and eagerly look forward to her next steps!

[1] https://advances.sciencemag.org/content/6/44/eabb0620.

[2] https://www.nist.gov/news-events/news/2020/11/new-twist-measuring-spin-nist-develops-microresonator-study-electron-spin.

Richard Ernst * (1933–2021)



Richard Ernst in his laboratory at ETH Zurich in 1991. (Image: Private archive Richard Ernst.)

It was with great regret and deep sadness that I learned of the death of Richard Ernst. Richard was more than just a doctoral supervisor to me; he was my mentor and fatherly advisor. His pioneering research into nuclear magnetic resonance laid the foundation for the later development of magnetic resonance imaging (MRI). Far beyond the world of analytical chemistry and structural research, his findings thus live on every single day in hospitals and radiology practices around the world.

I first met Richard when I was studying chemistry at ETH Zurich. At the time, I was attending, as he had done before, lectures by professors of physical chemistry such as Hans Heinrich Günthard and Hans Primas. I was so impressed by Richard's own lectures on the principles of physical measurement and the fundamentals of nuclear magnetic resonance, by the lively and spirited manner in which he delivered them, and by his personality that I approached him in the spring of 1974 about a topic for my thesis.

That autumn, I was granted the opportunity to join Richard's group as a doctoral student. In his passionate commitment and absolute dedication to science, he set the highest of standards for himself, making him a role model for everyone in the group without asking too much of them. It would often happen that, after an afternoon spent in discussing a scientific problem, Richard would come back the next morning with a solution formulated in his neat handwriting, having worked on it late into the evening or even during the night. Our Monday group seminar was another example – if one of the doctoral students was unable to attend and present, Richard would step in and himself give an exposé on the topic foreseen.

Those years between 1974 and 1978 were incredibly exciting. It was during this time that the fundamental advances were achieved that would allow two-dimensional spectroscopy to acquire the pre-eminent position it now enjoys in chemistry, biology, and medicine. In neighbouring laboratories, my fellow postgraduates from the group were working on increasing the sensitivity of MRI techniques. While writing my own thesis on a different aspect of multidimensional spectroscopy, I was able to witness expectations and breakthroughs in imaging technology first hand. Successfully defending my thesis to complete the project marked a key milestone in my life.

And it was on Richard's advice – another testament to his excellent mentoring skills – that I devoted my attention to a different field of experimental methodology during my postdoctoral stay in the United States. This is how I became involved in laser spectroscopy, which then also formed the basis of my habilitation in another team at ETH Zurich between 1982 and 1986. A book we were writing together meant that Richard and I remained in touch during this period as well.

In 1991, when I was teaching at the University of Bayreuth, the news that Richard had won the Nobel Prize in Chemistry brought great joy to the research community, not least to me. I also have fond memories of a seminar week in Ticino some time afterwards, when Richard invited all his former doctoral students and colleagues to join him for a review of the developments that had taken place over those key years. As we reflected, it was remarkable to see the many different career paths the graduates of the group had chosen – another sign of the solid and diversified knowledge base Richard had given us to prepare us for our professional careers. He, too, branched out into other areas, including classical music and especially Tibetan art – a field in which he became a great connoisseur of the mythology and symbolism behind the Tibetan paintings on cloth known as thangkas.

The Nobel prize marked the beginning of a new era in Richard's work. After everything he had achieved, he was more than deserving of the accolade, yet he regarded it as more of a calling to use the influence it brought to advocate a subject that had always been close to his heart. With boundless energy, he devoted articles and lectures to scientists' social responsibility, and to how important it was for them to reflect on the meaning and consequences of their work. Testing the limits of his physical endurance, he travelled widely to present these ideas at international conferences and as a guest speaker at research institutes on all continents. Richard lobbied fervently to keep the administrative burden on Swiss university staff low and to preserve academics' freedom to develop new, creative ideas.

At the same time, he took his responsibilities in university administration and as an advisor on numerous committees very seriously, fulfilling them with the same diligence as he did his scientific work. After his retirement, Richard continued to pursue his interest in the history of arts. He could now devote more of his time to analysing the pigments used in the thangkas, narrowing down the place and time of their creation, and developing his restoration skills to the point that he was able to restore age-dulled and damaged paintings to their original radiance.

With Richard's passing, we have lost a dedicated polymath, a man to whom ETH Zurich, science, and society owe a huge debt. His passion for chemistry and its meaningful application for the benefit of society is a shining example that will continue to serve as a model for us all.

Alexander Wokaun

* This text is an abridged and edited version of the epilogue to the book Richard R. Ernst. Nobelpreisträger aus Winterthur. Autobiografie. Hier und Jetzt Verlag, Zürich 2020. Reprinted with permission of the publisher. English translation of the book: https://www.routledge.com/Searching-and-Researching-An-Autobiography-of-a-Nobel-Laureate/Ernst-Meili/p/book/9789814877923

Sergei B. Orlinskii (1962–2021)

On September 25, 2021, an outstanding experimental physicist, an expert in the field of EPR spectroscopy, Associate Professor of the Kazan Federal University Dr. Sergei B. Orlinskii passed away.

Sergei Orlinskii was born on May 1, 1962. In 1984 he graduated from the Faculty of Physics of the Kazan State University with a degree in radiophysics. His Diploma thesis was of such a high level that he was offered a research position in the Laboratory of Magnetic Radiospectroscopy and Quantum Electronics at the university. In 1989, he successfully defended his Ph.D. thesis "Experimental study of inorganic phosphate glasses activated by rare-earth ions by the electron spin echo method" supervised by Dr. Andrey Antipin. In the period from 2000 to 2006, he worked at the Huygens Laboratory at Leiden University (The Netherlands), where he was engaged in the improvement of existing and development of new methods of high-frequency EPR and ENDOR spectroscopy. He participated in the creation of the first pulsed EPR spectrometer with an operating frequency of 275 GHz. Sergei Orlinskii carried out a number of pioneering works on the study of nanostructures using high-frequency EPR/ENDOR methods. From 2006 until recently, he remained active in both teaching students and being engaged in scientific research at the Kazan University.

Sergei Orlinskii was a world-class scientist, a recognised specialist in the field of magnetic resonance in condensed matter. He has received recognition as the author of over one hundred scientific articles in high-rated international physics scientific journals and as a reviewer of the international journals articles; as chairman, organizer and speaker at some of the most prestigious international conferences and various forums.

Sergei Orlinskii was a true representative of the EPR school at the Kazan Federal University and carried on its traditions in education and research. He was loved by students, respected by his colleagues. He brought together scientists from many fields with whom complex interdisciplinary research was carried out. Sergei Orlinskii was the ideological inspirer and the PI of grants for the Russian Foundation for Basic Research and the Russian Science Foundation. Sergei Orlinskii was an outstanding scientific advisor, communicating techniques and research style, helping to see and appreciate the true beauty of the experiment. He supervised three Ph.D. theses (by M. Volodin, B. Yavkin and Y. Kutin) and initiated the creation of a joint postgraduate study at the Kazan Federal University and the University of Antwerp (Belgium).

Since September 2006, Sergei has been actively involved in the work of the Federal Center for Collective Use at the Kazan Federal University. He took an active part in the launch of the newest high-frequency EPR, Elexsys-680, and its subsequent modernization. Sergei Orlinskii had extensive experience in teaching. It began with lectures on all aspects of the general physics course at the Kazan Institute of Chemistry and Technology; in recent years, he passed on his extensive knowledge in the field of EPR spectroscopy to the Master's degree students of the Kazan Federal University. He was one of the authors of the textbooks "High-field, pulsed, and double resonance studies of crude oils and their derivatives" and "Nanoparticles: Workhorses of Nanoscience" devoted to EPR spectroscopy.

Sergei Orlinskii remains an example of boundless devotion to science, a real model of a modern scientist: boldly going forward, opening new horizons for humanity. At all times, even those difficult for the development of science, he remained confident in the correctness of his life choice, was a man full of optimism and kindness, openness and friendliness, and faith in the future of our scientific school. He knew how to inspire colleagues, support and lead them, generously share scientific ideas, be a reliable friend and an honest scientist. The memory of him is forever in our hearts.

A. Aganov, E. Alakshin, G. Andreev, V. Atsarkin, E. Baibekov, P. Baranov, T. Biktagirov, A. Bogaychuk, Yu. Bunkov, G. Dolgorukov, A. Dooglav, A. Egorov, I. Garifullin, O. Gnezdilov, E. Groenen, I. Gromov, I. Motygullin, B. Gabbasov, M. Gafurov, E. Goovaerts, M. Eremin, B. Epel, D. Kan, A. Klochkov, F. Khamidullin, B. Kochelaev, Yu. Kochneva, E. Kondratyeva, A. Konkin, I. Kurkin, Y. Kutin, V. Kuzmin, A. Makarchenko, G. Mamin, L. Mosina, F. Murzakhanov, V. Naletov, S. Nikitin, E. Pavlova, A. Parfishina, Yu. Proshin, R. Rakhmatullin, A. Rodionov, I. Romanova, T. Safin, K. Safiullin, K. Salikhov, M. Salakhov, V. Semashko, J. Schmidt, D. Shurtakova, V. Skirda, V. Soltamov, L. Tagirov, M. Tagirov, Yu. Talanov, D. Tayurskii, G. Teitelbaum, S. Van Doorslaer, M. Volodin, I. Volodina, V. Voronkova, I. Vlasov, B. Yavkin, R. Yusupov, D. Zverev

The Rapid Scan accessory comprises the following components :

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

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- Compatible with all variable temperature accessories

EPR

Innovation with Integrity

Rapid Scan EPR: on the way to superior time resolution for kinetic studies

Boris Dzikovski, Ralph Weber and Kalina Ranguelova

Kinetics studies by EPR can be challenging – continuous wave EPR (CW-EPR) often does not have the required time resolution. Pulsed EPR has superior time resolution but often suffers from low sensitivity and bandwidth limitations. Rapid Scan EPR (RS-EPR) offers better sensitivity compared to CW and pulse EPR combined with superior time resolution compared to CW-EPR. In addition, RS-EPR can simultaneously monitor kinetics of multiple species. In this report we demonstrate the potential of the Bruker (RS-EPR) accessory: https://www.bruker.com/en/products-and-solutions/mr/epr-instruments/rapidscan.html for kinetic studies.

RS-EPR is an alternative to CW and pulse techniques for obtaining EPR spectra. It was originally developed and promoted by the Eaton group at the University of Denver [1, 2].

In RS-EPR the magnetic field is swept repeatedly through the EPR transitions with a high sweep rate of 10–100 kHz, as shown in Fig. 1. This high sweep rate minimizes the effects of microwave power saturation. Since the time on resonance is short, higher microwave power can be used without saturating the spin system.

The ability to use higher microwave powers without saturation effects offers higher sensitivity. Figure 2 shows the dependence of the EPR signal intensity from the microwave power for a water solution of potassium nitrosodisulfonate (Frémy's salt). This inorganic nitroxide with known relaxation times is a common reference in saturation studies [3]. As seen in the figure, the higher MW power used for RS-EPR experiments results in a much stronger signal compared to CW-EPR. This advantage of RS-EPR is more pronounced for samples with very long relaxation times, e.g., defects in crystals, nitrogen centers in diamonds and various biological samples at very low temperature. For some of these samples, a signal-to-noise improvement up to two orders of magnitude is possible [2].

The Bruker RS Accessory operates at scan frequencies from 10 to 100 kHz, corresponding to a single scan time of 0.1 to 0.01 ms. This defines the best possible time resolution for very strong signals which give a good signal-to-noise ratio in a single scan. We were able to demonstrate good signals recorded with a time resolution of 1–10 ms with 10–100 averages, more than two orders of magnitude better than in conventional CW-EPR.

Figure 3 shows a sequence of EPR signals recorded during the free fall of a BDPA point sample (about 3×10^{17} spins) through the rapid scan resonator. This is a simple way to test and demonstrate the time-resolution capacity of the RS accessory. The rapid scan frequency was 20 kHz, each spectrum was recorded with 25 scans, resulting in a time resolution 1.25 ms.

As seen in Fig. 3, recording the series of full EPR spectra at this high sweep rate provides excellent signal-to-noise ratio. This corresponds to sub-millisecond resolution of RS-EPR for strong samples.

Many radical reactions include multiple radical species. Here an example of how RS-EPR provides insights into the chemical kinetics of the individual species is shown. Upon UV-irradiation of TiO_2 nanoparticles suspended in DMSO, two types of radicals are formed – superoxide ($O_2^{\bullet-}$) and hydroxyl radical ($^{\bullet}OH$). These radicals further react with DMSO to produce a methyl radical, resulting in three radical species [4]. The RS-EPR spectra of spin-trapping adducts of these

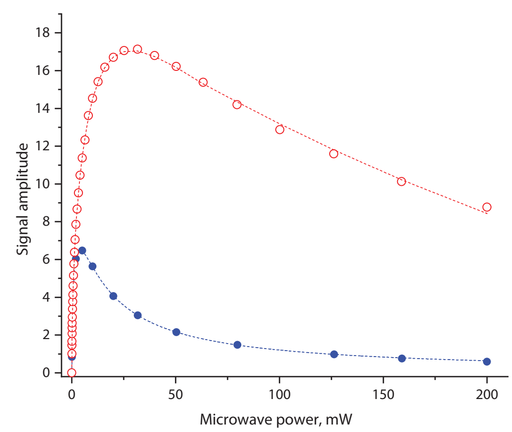


Figure 2. The dependence of signal intensity on the microwave power for the same sample of 0.9 mM of Frémy's salt in 50 mM K_2CO_3, CW-EPR (blue closed circles) and RS-EPR (red open circles). The RS-EPR frequency is 20 kHz. For RS the first derivative of the absorption signal was used.

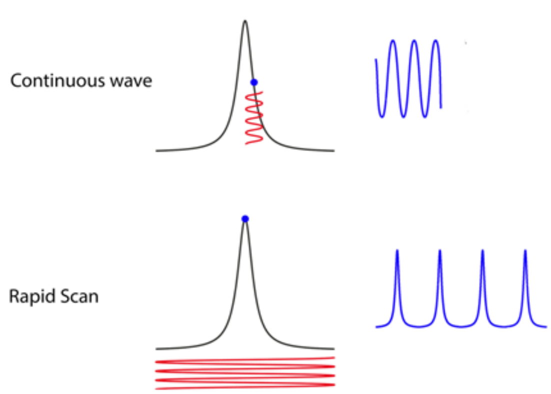


Figure 1. CW-EPR vs RS-EPR. In RS-EPR, the magnetic field is modulated over a range larger than the signal line width and the signal is directly observed via quadrature detection as absorptive line shapes. In CW-EPR the modulation is applied only to a small fraction of the spectrum, yielding a derivative line shape.

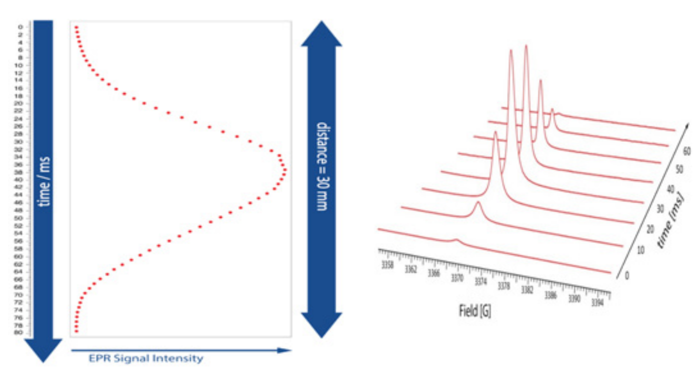


Figure 3. A BDPA sample free falling through the RS resonator. The spectra are recorded every 1.25 ms with 25 accumulations. The signal intensity vs the time after entering the resonator is shown on the left with the full EPR spectrum on the right (every 8th recorded spectrum shown).

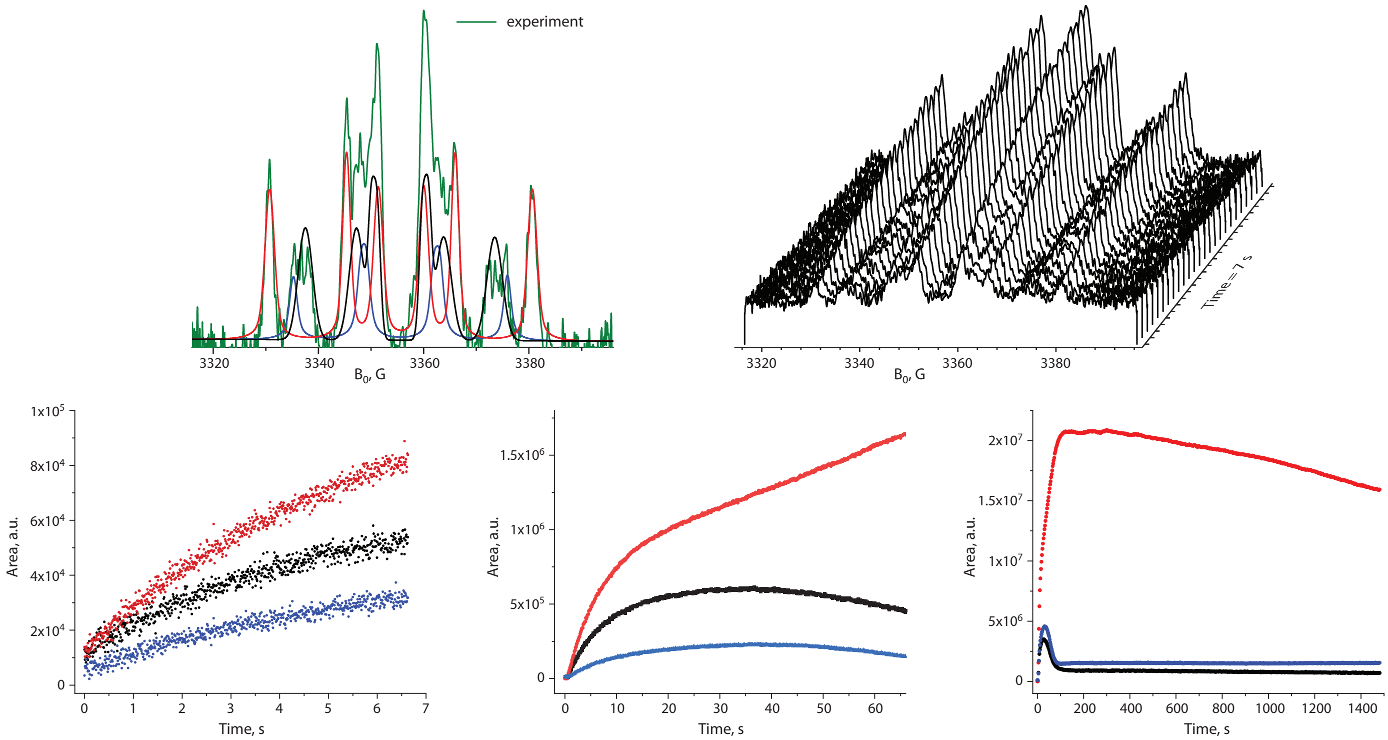


Figure 4. Top: RS-EPR spectra of DMPO spin trapping adducts for radicals emerging upon UV-irradiation of TiO_2 nanoparticles suspended in DMSO. The individual components corresponding to the DMPO adducts of superoxide (black), hydroxyl (blue) and methyl (red) are obtained using SpinFit. Bottom: the kinetics of the production/decay of these three adducts on three different time scales (see Table 1).

three radicals with the DMPO (5,5-dimethyl-pyrroline N-oxide) spin trap and their time evolution are shown in Fig. 4.

The minimum time resolution for acquiring the full EPR spectrum with conventional CW detection is here about 10 s, limiting its use only for long time scales. In Fig. 4 and Table 1 we see three different stages of the radical production and decay. The two faster time scales require RS-EPR, conventional CW-EPR would not have sufficient time resolution for these measurements.

Using RS-EPR is also essential because it records the overlapping spectra of all three species in a single sweep. Although CW-EPR can be successfully used for kinetics studies by setting the magnetic field at several values and following the time course of each component, this results in a lengthy experiment. In addition, identical samples for each of the time courses must be made. The overlap of the spectra from the different species also makes this approach problematic.

Table 1. Setup of the RS experiments for three different time scales shown in Fig. 4.

Time resolution	10 ms	100 ms	1 s
Experimental time	7 s	67 s	25 min
Number of points	670	670	670

Similarly, RS-EPR can be used to study evolution of fast physical processes. In this example, the partitioning of a radical between two immiscible phases, water and oil, is followed. Figure 5 shows a sam-

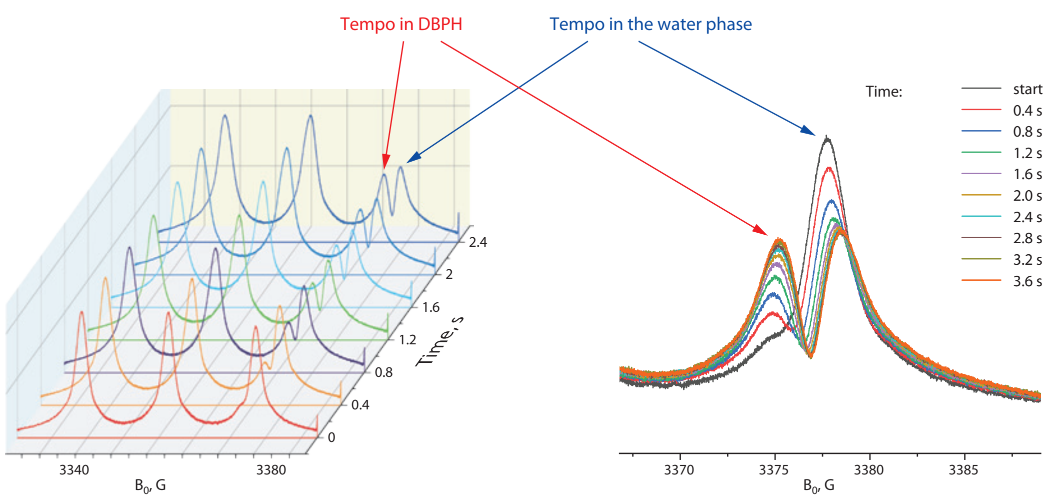


Figure 5. Kinetic of re-distribution of Tempo between water and oil (DBPh) phases after addition of DBPh to a 1 mM solution of Tempo in water/D_2O. The high field hyperfine component is magnified and shown separately on the right.

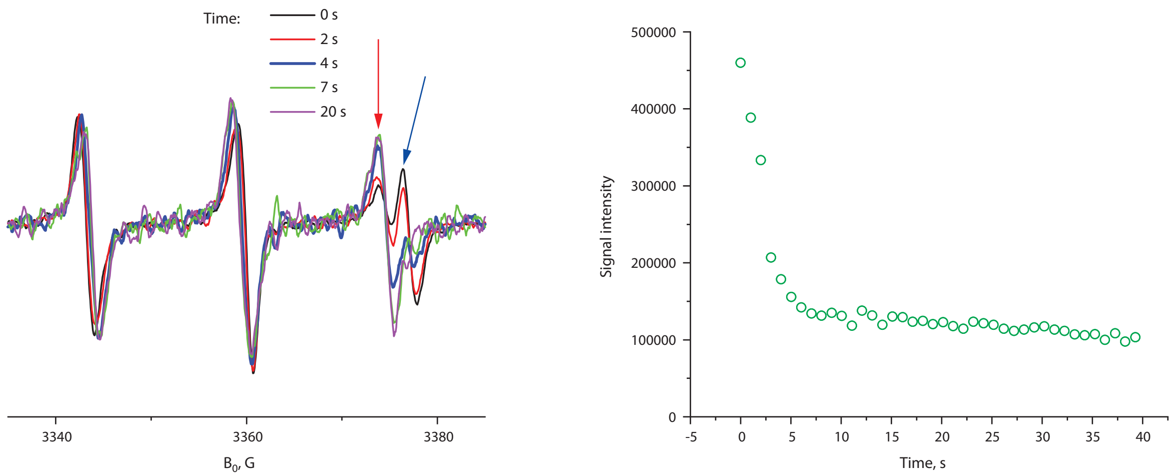


Figure 6. Kinetics of the reaction between Tempo in the paraffin (10% v)/water/SDS emulsion and dithionite. The total Tempo concentration is 100 μM. The left plot shows the first derivative of the RS-EPR spectra normalized by the signal intensity. Red and blue arrows point at the spectral components corresponding to Tempo molecules in the paraffin and oil phases respectively. The right side shows the change in the concentration of Tempo with time.

ple of 1 mM Tempo in water/D_2O into which a dibutyl phthalate (DBPh) phase was quickly mixed. The volume ratio of water and oil phases in the mixture was 15:1. The nitroxide partitions and diffuses into the DBPh droplets. The difference in the EPR spectra between the two phases allows observation of the partition kinetics of both species. The partition equilibrium settles within ~4 s. RS-EPR allows for observation of the partition process in real time.

Note that the spectral components corresponding to different non-mixing phases overlap and the spectrum extrema are shifting with the gradual emergence of the oil component. It underlines the benefit of recording the full spectrum at every time point using RS-EPR compared to the traditional CW technique of following the spectral intensity at a single field point.

Analyzing the spectra of individual species in a sequence of RS-EPR recordings can provide useful insights into the mechanism of the kinetics studied. Figure 6 shows Tempo in an emulsion of paraffin in water stabilized by sodium dodecyl sulfate (SDS) reacting with dithionite. Dithionite reduces the nitroxide and decreases the spectral intensity. Figure 6 shows the first derivative of the RS spectra which are normalized to the same intensity correcting for the signal decay when comparing the spectral shape at different times. Using the derivatives provides better visual resolution of the components and gives the spectrum a familiar appearance of conventional CW EPR.

As seen in the figure, the spectrum undergoes a quick change within the first four seconds, but its line shape remains mostly unchanged at longer reaction times. This time scale corresponds to a sharp break in the kinetic curve. During the fast initial stage of the reaction, dithionite reduces the Tempo molecules in the aqueous phase, causing almost complete disappearance of their EPR signal. Since dithionite cannot penetrate the hydrophobic paraffin interior of colloid particles no reaction occurs in this phase of the emulsion. Later in the time course the reaction is limited by the diffusion of Tempo molecules from the disperse organic phase into the aqueous phase where they are quickly reduced and show relatively little signal. Without the superior time resolution of RS-EPR the initial quick stage of the reaction could be completely missed.

Among promising biological application of RS-EPR is the study of lipid membranes, since many lipid rearrangements which can be monitored by EPR, such as viral fusion, membrane channel function and lipid/cholesterol exchange between membrane domains, occur on millisecond to second time scale. Recently, a paper on time-resolved monitoring of protein-membrane interaction was published by the Drescher group in the University of Konstanz, Germany [5]. It presents a study of spin-labeled human α-synuclein upon transfection into live cells using the Bruker RS-EPR unit.

In conclusion, we see that rapid scan EPR, in addition to increasing sensitivity for easily saturated samples, offers many advantages compared to CW EPR in studies of fast kinetics. It provides superior time resolution and facilitates simultaneous observation of multiple species.

1. G. R. Eaton and S. S. Eaton. Rapid Scan Electron Paramagnetic Resonance. Handbook of EPR Spectroscopy: Fundamentals and Methods, D. Goldfarb and S. Stoll, eds., John Wiley & Sons, 503–520 (2018).
2. D. G. Mitchell, M. Tseitlin, R. W. Quine, V. Meyer, M. E. Newton, A. Schnegg, B. George, S. S. Eaton & G. R. Eaton. X-band rapid-scan EPR of samples with long electron spin relaxation times: a comparison of continuous wave, pulse and rapid-scan EPR, Molecular Physics, 111: 2664–2673 (2013)
3. R. G. Kooser, W. V. Volland and J. H. Freed. ESR relaxation studies on orbitallt degenerate free radicals. I. Benzene anion and terphenyl. J. Chem. Phys. 50: 5243–5257 (1969)
4. D. Dvoranová, Z. Barbieriková and V. Brezová. Radical Intermediates in photoinduced reactions on TiO_2. (An EPR Spin Trapping Study). Molecules 19: 17279–17304 (2014)
5. T. S. Braun, J. Stehle, S. Kacprzak, P. Carl, P. Höfer, V. Subramaniam, M. Drescher. Intracellular Protein-Lipid Interactions Studied by Rapid-Scan Electron Paramagnetic Resonance Spectroscopy. J. Phys. Chem. Lett. 12: 2471–2475 (2021)

22nd International Society of Magnetic Resonance Conference (ISMAR) 9th Asia-Pacific NMR Symposium (APNMR) 60th Annual Meeting of the Nuclear Magnetic Resonance Society of Japan (NMRSJ) 60th Annual Meeting of the Society of Electron Spin Science and Technology (SEST) (ISMAR-APNMR-NMRSJ-SEST2021)

August 22–27, 2021, Osaka, Japan, Online

A joint meeting of the 22nd International Society of Magnetic Resonance Conference (ISMAR), the 9th Asia-Pacific NMR Symposium (APNMR), the 60th Annual Meeting of the Nuclear Magnetic Resonance Society of Japan (NMRSJ) and the 60th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2021) was held as an online virtual conference on August 22–27, 2021. This joint meeting was originally planned as an ordinary conference in Osaka, Japan. However, due to the spread of covid-19 and the worldwide ban on travel, ISMAR's local and international committees had decided in August 2020 to cancel the face-to-face meeting in Osaka and hold an online meeting. At that time, the local committee was still considering the possibility of foreign participants making presentation in Osaka. However, as the situation did not improve a year after the start of the covid-19, the committee finally decided to hold a full online meeting at the end of April 2021, taking account of the decision by the International Olympic Committee's (IOC) to host the postponed Tokyo 2020 Olympics / Paralympics without spectators. For SEST members, it was the second online meeting following last year.

The scientific program was organized by the International Program Committee on behalf of ISMAR on the same scale as regular ISMAR conferences; 10 plenary talks, 101 invited talks, 111 oral talks promoted from poster, and 450 poster presentations. All presentations were categorized into Solution NMR (SOL), Solid state NMR (SS), Hyper polarization and emerging fields (HYP), Magnetic resonance imaging (MRI), and Electron paramagnetic resonance (EPR), according to the topics submitted. These sessions were scheduled in three time zones considering global attendees, typically in morning (7:00–10:00), afternoon (12:00–15:00), and evening (19:00–23:00) of Japan Standard Time (JST, UTC+9). Three parallel sessions ran at the same time, for a total of 54 parallel sessions over a five-day period, and there were three poster sessions. From a viewpoint of EPR field, 26% of all contributions had EPR topics, and 11 parallel sessions had been constructed with EPR topics named New Methods (1, 2, 3), DEER (1, 2, 3), Material Science (1, 2), In vivo ESR, Spintronics, Spin Manipulation. In these sessions, various targets such as in vivo/in vitro biological application, life science and medicine, geosciences, organic/inorganic semiconductors, low-dimensional materials, and magnetism were discussed.

As an online platform, Zoom Webinar was used for the plenary sessions, Zoom Meetings was used for the parallel sessions, and Remo was used for the poster sessions. The plenary/parallel session was organized by the session chair with the support of the session sub-chair to handle the interactions in Zoom. The mixing time, which is expected to be free discussions between presenter and audience, was set at the end of each time zone in the Zoom Meeting by setting Breakout Room for each talk, or on the REMO floor before and after the poster presentation period. This mixing time was fairly unique and was intended to facilitate discussions that were closer to a real meeting. All oral presentations were recorded by Zoom and made available for a month from University of Basel in Switzerland.

Timeline during the meeting was shared on Twitter, which were linked at the top page of the online-meeting site. Someone tweeted that he/she would move to the lab to give a presentation early in morning or late at night in the dark owing to the compromised schedule. By the way, who could have imagined the following situation? Despite the online conference, a distribution base was set up at a hotel in Osaka (Hotel Fukurashia Osaka Bay), and Japanese scientists and secretariat were in charge of the session during the conference. At the base, from early morning to late night in JST, people worked under strict infection-control regulations and slept in the hotel for quite a short time.

The following is a summary of day-to-day events related to participants in the EPR field. The meeting started on the evening of August 22. At the opening, Professor Toshimichi Fujiwara, the chair of ISMAR-APNMR-NMRSJ-SEST2021, gave a speech and explained the process of the online conference. Professor Robert Tycko, President of ISMAR, and Professor Akira Naito, Chair of APNMR, each said a few words at the beginning of the conference. Professor Takahisa Ikegami and Professor Takeji Takui celebrated the 60th meetings of NMRSJ and SEST from historic perspectives, respectively. Award-winning lectures were given by Professor Kamil Uğurbil, who received the ISMAR prize, Professor Alexander C. Forse and Professor Tuo Wang, who received the Abragam prize, and Professor Matthew S. Rosen, who received the Callaghan Lecture. At the Ernst Memorial Session, more than 10 related scientists spoke in honor of Professor Richard. R. Ernst, who passed away on June 4, 2021.

The first parallel session of the EPR field began on the evening of August 23 (JST). Two parallel sessions of the EPR field and the first poster session were held on August 24th (JST). After the night session, IES Annual General Meeting was held by the President Songi Han at the midnight (JST). This IES Annual General Meeting was recorded, and now you can view it at "On-Line Activities" of the IES website (https://ieprs.org). Three parallel sessions of the EPR field and the second poster session were held on August 25th (JST). The plenary lecture was given by Professor Thomas Prisner on the afternoon of August 25 (JST). Professor Elena Bagryanskaya received the IES silver medal for chemistry, the award lecture was given. Four parallel sessions of the EPR field and the third poster session were held on August 26. One parallel session of the EPR field was held at the morning on August 27. Corporate seminars were held by supporting companies, JEOL, Bruker, and Taiyo-Nippon-Sanso during the break time through the conference period.

At the closing session on the morning of August 27, the total number of the participants was announced to be 919 from 37 countries, including ca. 400 students and 40 from supported companies. Winners of poster presentation awards, IES Poster Award and SEST Excellent Presentation/ ▶

Poster Awards, JEOL/Taiyo-Nissan/AP-NMR Poster Awards were announced. By the way IES Poster Awards were given to Ms. Ririko Nakaoka (Hokkaido University, Japan), Dr. Jasleen Kaur Bindra (National Institute of Standards and Technology, USA), and Ms. Akane Yato (Saga University, Japan) after very competitive selections. Especially Ms. Ririko Nakaoka received also the SEST Excellent Presentation Award. The photos of IES Poster Prize winners are available on the IES website. The next meeting was announced by Professor Paul Gooley, the 23rd ISMAR on August 20–25, 2023 at Brisbane, Australia. Finally, Professor Stephan Grzesiek, the vise-president of ISMAR concluded the ISMAR-APNMR2021 conference.

On the afternoon August 27, after the closing of ISMAR-APNMR, the annual meetings of NMRSJ and SEST were continued as individual Japanese sessions. At the SEST meeting, there was a report on the activities and current status of SEST. The winners of the SEST award and the SEST young investigator award were announced, and the winners gave lectures. Professor Tadaaki Ikoma (Niigata University, Japan) received the SEST award for his outstanding contribution to chemistry and gave a lecture entitled "Magnetic structure and Spin Dynamics of Excited States in Molecular Materials". He is expected to make further scientific and social contributions to the field of spin science. Dr. Yusuke Wakikawa (Shizuoka Institute of Science and Technology, Japan) and Dr. Hiroki Nagashima (Saitama University, Japan) received the SEST young investigator award for their continuous research based on their doctoral dissertations. Dr. Wakikawa gave a lecture entitled "Spin Dynamics of Charge Carriers and Excitons in Organic Semiconductor Materials and Devices" and Dr. Nagashima gave a lecture entitled "Distance Measurements between Spins and Elucidation of Structures Surrounding Electron Spin by Electron Spin Resonance". In the last part, Professor Keizo Takeshita introduced the SEST2022 which will be held as in-person meeting at Kumamoto, Japan. Professor Osamu Inanami, President of SEST, concluded the SEST annual meeting.

We hope that all the participants enjoyed the meeting after overcoming many difficulties. Finally, we would like to thank for the support from IES. Thanks to this, EPR scientists who gave presentations at ISMAR-APNMR-NMRSJ-SEST2021 will receive a one-year IES membership in 2022.

Ikuko Akimoto
Hitoshi Ohta

IES Virtual EPR Meeting
September 22, 2021

Tailoring the EPR Excitation Field to Nanoscale Samples: an Overview of EPR Microresonators

Nandita Abhyankar
Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, USA
National Institute of Standards and Technology, Gaithersburg, USA

We describe the advantages of planar inverse anapole microresonators [1] for improving the sensitivity of inductive-detection EPR spectroscopy of mass-limited/volume-limited samples. Resonators with sub-microliter to sub-nanoliter active volumes are relevant to multiple application spaces, including EPR spectroscopy of precious bio-macromolecular samples, single microcrystals, and epitaxial layers [2, 3]; excitation/detection of spin qubits [4]; and miniaturization of EPR spectrometers.

The resonator lies at the heart of the EPR spectrometer and fulfils dual functions: first, it provides the EPR excitation field and second, it acts the detection element for inductive detection of EPR. The first role can be quantified in terms of the parameter η or the filling factor while the second role can be quantified as Q or the quality factor. The sensitivity of inductive detection is proportional to ηQ [5]. For volume-limited samples, shrinking the resonator provides a way to increase the filling factor up to its maximum value of 1. However, the decrease in resonator size inevitably deteriorates Q, offsetting the sensitivity gain from the increase in η.

To obtain maximum concentration sensitivity and absolute sensitivity for volume-limited samples, a high loaded Q must be maintained even as the active volume of the resonator is decreased. Additionally, for broad applicability, the resonator must: couple easily to a microwave feedline; have well-separated regions of B_1 and E_1 intensity where B_1 and E_1 are the magnetic and electric field components, respectively, of the incident microwave; and be scalable over a broad range of frequencies from 3 GHz to hundreds of GHz. Because volume-limited samples come in a variety of shapes & sizes (e.g., 'point' samples such as microcrystals are different from surface samples such as epitaxial films), B_1 must be confined and tailored to the sample type and application (e.g. CW vs. pulse EPR).

The planar inverse anapole is a design paradigm that fulfils all the requirements stated in the paragraph above [1]. It is a planar microresonator fabricated by depositing a thin metallic layer on a dielectric substrate using standard nanofabrication protocols. The anapole design diminishes radiative losses through destructive interference of the toroidal moment with the radiative electric dipole [6]. This cancellation results in improved Q at ambient temperatures, a notable advantage of the planar inverse anapole design. The large outer structure in the inverse anapole design converges on a small inner bridge around which the excitation field B_1 is concentrated. This small inner bridge forms the active surface of the resonator. The dimensions of the outer structure can be used to control the resonant frequency. Because the size and shape of the inner bridge can be varied independently of the outer structure, the B_1 'hotspot' can be optimized independently of the resonant frequency for specific sample sizes and types; e.g., a point-like bridge would be suited for a microcrystal sample while an extended interdigitated or multi-loop bridge would be suited for a thin-film sample. Decoupling the resonant frequency from the size and shape of the active surface makes the inverse anapole design scalable over a wide range of frequencies and customizable for varied samples.

Building on our previous report of room-temperature CW EPR measurements of single microparticles of dilute doped perovskite oxides [1], we report results obtained from the second generation of planar inverse anapole microresonators. This work demonstrates the applicability of and sensitivity of planar inverse anapole microresonators for room-temperature CW EPR measurements on solutions. In contrast to the first-generation design which used LSAT substrates, the present design uses inexpensive quartz substrates, reducing the material cost and making the resonator essentially disposable. We demonstrated the concentration sensitivity using sub-microliter volumes of a concentration series of aqueous solutions of 3-carboxy-proxyl radical. We successfully obtained CW EPR spectra from solutions with concentrations down to 1 μmol/L (conversion time: 1 s, 32-scan average, nominal modulation amplitude: 1 G). We plan to further improve the concentration sensitivity by decreasing the dimensions of the inner bridge structure from 5×1 μm to 0.1×0.1 μm.

Planar inverse anapole microresonators represent a new design paradigm that exploits a toroidal moment to improve the performance of EPR microresonators with nanoliter active volumes. The decoupling of resonant frequency and active volume results in exceptional scalability and customizability to varied samples, the demonstration of which will be the focus of our future work in this area.

Acknowledgments: This work was completed in the lab of Dr. Veronika Szalai at National Institute of Standards and Technology, Gaithersburg. Valuable guidance and collaboration were provided by Dr. Amit Agrawal, Dr, Robert D. McMichael, Dr. Jason Campbell and Dr. Pragya Shrestha. Nanofabrication was conducted at the Center for Nanoscale Science and Technology, NIST, Gaithersburg. This work was partially funded by NIGMS R21 Grant Award R21GM134406 and NIST MSE Grant Award 70NANB21H183 to the University of Maryland.

1. N. Abhyankar, A. Agrawal, P. Shrestha, R. Maier, R. D. McMichael, J. Campbell, V. Szalai: Scalable microresonators for room-temperature detection of electron spin resonance from dilute, sub-nanoliter volume solids. Sci. Adv. **6**, eabb0620 (2020)
2. J. W. Sidabras, J. Duan, M. Winkler, T. Happe, R. Hussein, A. Zouni, D. Suter, A. Schnegg, W. Lubitz, E. J. Reijerse: Extending electron paramagnetic resonance to nanoliter volume protein single crystals using a self-resonant microhelix. Sci. Adv. **5**, eaay1394 (2019)
3. J. C. Valdez-Lopez, S. T. Petr, M. P. Donohue, R. J. Bailey, M. Gebreeziabher, E. G. Cameron, J. B. Wolf, V. A. Szalai, P. R. Robinson: The C-terminus and third cytoplasmic loop cooperatively activate mouse melanopsin phototransduction. Biophys. J. **119**, 389–401 (2020)
4. P. Haikka, Y. Kubo, A. Bienfait, P. Bertet, K. Mølmer: Proposal for detecting a single electron spin in a microwave resonator. Phys. Rev. A 95, 022306 (2017)
5. D. I. Hoult, R. E. Richards: The signal-to-noise ratio of the nuclear magnetic resonance experiment. Journal of Magnetic Resonance (1969). 24, 71–85 (1976)
6. A. A. Basharin, V. Chuguevsky, N. Volsky, M. Kafesaki, E. N. Economou: Extremely high Q-factor metamaterials due to anapole excitation. Phys. Rev. B 95, 035104 (2017)

The 55th Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry
June 6–10, 2022, University of St. Andrews, St. Andrews, Scotland

https://www.esr-group.org/conferences/2022-conference-st-andrews

Featuring the 37th Bruker Lecture, the 8th Bruker Thesis Prize Lecture and the 26th JEOL prize talk competition.

Lead organiser: Dr Janet Lovett

The 61st Annual Rocky Mountain Conference on Magnetic Resonance
July 25–29, 2022, Copper Conference Center in Copper Mountain, Colorado

https://rockychem.com

In addition to invited papers, there will be contributed papers for posters and oral presentations, to be selected by the Organizing Committee from among the abstracts submitted.

Scientific Committee: Fraser MacMillan (University of East Anglia) – Chair, Dane McCamey (University of New South Wales) – Co-Chair 2022, Chair 2023, Aharon Blank (Israel Institute of Technology), Ania Bleszynski-Jayich (University of California Santa Barbara), Christoph Boehme (University of Utah), Gail Fanucci (University of Florida), Songi Han (University of California Santa Barbara), Stephen Hill (Florida State University, NHMFL), John McCracken (Michigan State University), Chandrasekhar Ramanathan (Dartmouth College).

E-mail: info@rockychem.com

17th International Symposium on Spin and Magnetic Field Effects in Chemistry Related Phenomena (Spin Chemistry Meeting 2022) (Including the IES AGM2022)
August 28 – September 1, 2022, Northwestern University, Evanston, IL

Spin Chemistry Meeting is a well-established forum to exchange knowledge and latest scientific results in the field of spin chemistry and related areas of research including applications in spintronics, material science and biology. The scientific program of the Conference will include plenary lectures, invited lectures, oral talks and poster sessions.

Previous Spin Chemistry Meetings were held in Tomakomai, Japan (1991); Konstanz, Germany (1992); Chicago, USA (1994); Novosibirsk, Russia (1996); Jerusalem, Israel (1997); Emmetten, Switzerland (1999); Tokyo, Japan (2001); Chapel Hill, USA (2003); Oxford, UK (2005); San Servolo, Italy (2007); St Catharines, Canada (2009); Noordwijk, The Netherlands (2011); Bad Hofgastein, Austria (2013); Kolkata, India (2015); Schluchsee, Germany (2017); St. Petersburg, Russia (2019).

Spin 2022 Organizers: Michael Wasielewski, Hosting Committee Chair
wasielewski-ofc@northwestern.edu
Melanie Sandberg, Program Coordinator
melanie.sandberg@northwestern.edu

Local Committee: Michael R. Wasielewski (Northwestern University), Malcolm D E Forbes (Bowling Green state University), Art van der Est (Brock University), Linda Shimizu (University of South Carolina), Emily A. Weiss (Northwestern University).

International Committee: Samita Basu (Saha Institute of Nuclear Physics), Jan Behrends (Free University, Berlin), Christoph Boehme (University of Utah), Art van der Est (Brock University), Malcolm D E Forbes (Bowling Green state University), Günter Grampp (TU Graz), Peter Hore (University of Oxford), Yasuhiro Kobori (Kobe University), Leonid Kulik (Novosibirsk State University), Jörg Matysik (University of Leipzig), Kiminori Maeda (Saitama University), Ron Naaman (Weizmann Institute), Marilena di Valentin (University of Padova), Michael R. Wasielewski (Northwestern University), Stefan Weber (University of Freiburg).

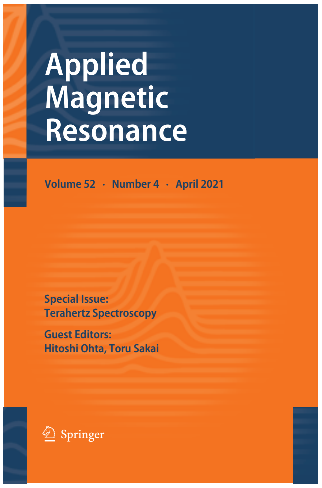
The Alpine Conference on Magnetic Resonance in Solids 2022
September 4, 2022 – September 8, 2022, Chamonix Mont-Blanc

http://www.alpine-conference.org

The Alpine conference is a high-level international forum for the discussion of recent developments and applications in the field of magnetic resonance in solids. The conference focuses on novel concepts, methods and instrumentation, as well as applications in fields including physics, chemistry, biology and materials science. Beyond its original and still core focus on solid-state NMR, the Alpine Conference welcomes contributions from EPR and MRI in solids.

Scientific Committee: Anja Böckmann (MMSB Lyon), Alexej Jerschow (NYU), Anne Lesage (CRMN Lyon).

The following speakers will give plenary lectures: Alexander Barnes (ETH), Marina Bennati (University of Göttingen, Max-Planck Institute for Biophysical Chemistry), Christian Degen (ETH), Lyndon Emsley (EPFL), Mei Hong (MIT), Michal Leskes (Weizmann Institute of Science), Rachel Martin (University of California, Irvine), Tatyana Polenova (University of Delaware), Kâmil Uğurbil (University of Minnesota).



Applied Magnetic Resonance 52/4 (2021)
https://link.springer.com/journal/723/volumes-and-issues/52-4
Terahertz Spectroscopy
Co-Guest Editors: Hitoshi Ohta, Tôru Sakai

This special issue of *Applied Magnetic Resonance* related to the Terahertz Spectroscopy (THz EPR) has been published in spring, 2021. The plan of this special issue started after the occasion of the International Zavoisky Award 2019, which was awarded to the guest editor HO as "Distinguished for his outstanding contributions to terahertz high-field EPR instrumentation and its applications in solid-state physics". In this special issue the definition of THz is from 0.1 THz to 10 THz, and the fixed THz frequency and the magnetic field sweep measurements combined with the multi-frequency THz sources will be considered as the THz EPR. The special issue contains 15 papers written by the world-wide experts working on THz EPR both experimentally and theoretically.

As the resonance field of EPR is proportional to the input frequency, THz EPR requires the high magnetic field produced by the superconducting magnet or the pulsed magnetic field. However, THz EPR has many advantages which will overcome the use of high magnetic field.

1) THz EPR will give the high spectral resolution because two resonances with slightly different g-values will be separated beyond their line-widths in the high frequency and the high magnetic field. This advantage will be especially useful for 3d-5d and 4f ion systems which have much larger line-width compared to that of radical molecules.

2) Related to above, THz EPR is required to detect EPR itself if the resonance has very large line-width such as several Tesla (T).

3) If the system has a large zero-field splitting, multi-frequencies comparable to the splitting and the high magnetic field are required to observe EPR because the conventional X-band EPR will give the EPR silent result. Moreover, the precise determination of the zero-field splitting by THz EPR will enable us to understand the system. Such zero-field splitting may come from the single magnetic ion anisotropy but also may come from the spin gap of the strongly correlated spin system or the antiferromagnetic gap in the magnetic order state of the antiferromagnet.

4) Strongly correlated spin systems show rich varieties of magnetic phase transitions under the magnetic field at low temperature. In order to understand such magnetic phases, multifrequency THz EPR under the high magnetic field enable us to tune the resonance into each magnetic phase and to understand the origin of magnetic phase transitions in the system.

Using above advantages, the applications of THz EPR to the quantum spin systems are discussed by several authors. Moreover, THz EPR instrumentations are recently extended to multi-extreme THz EPR together with above advantages. Therefore, the high pressure THz EPR, the highly sensitive mechanically detected THz EPR, and the ESR/NMR double-magnetic-resonance system for use at ultra-low temperatures or the surface coil for DNP-NMR are discussed. Finally recent theoretical approaches to understand the THz EPR experimental results are discussed.

The editors are very happy if this special issue will be considered as the mile-stone of THz EPR at the moment.

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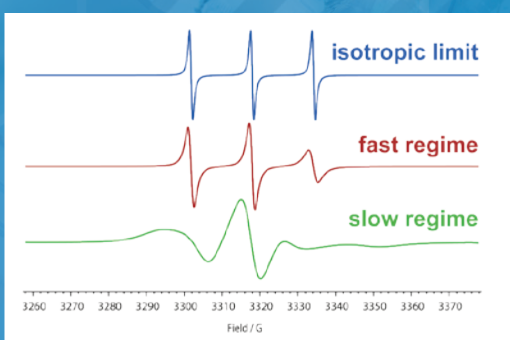
Nitroxide spectra under different motional dynamic regimes



Simulating and fitting of spectra of liquids samples

- An easy-to-use interface
- Automatic choice of dynamic regime
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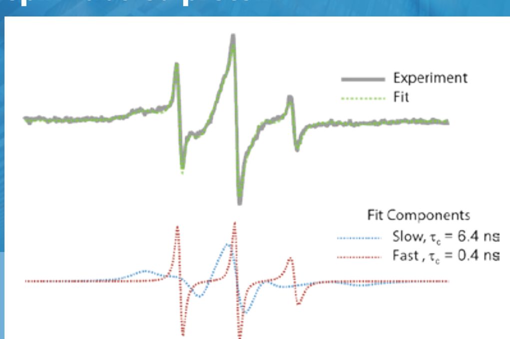
Two-component spectra of spin-labeled protein



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