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

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The cover picture illustrates aspects of research carried out by Michael Wasielewski, recipient of the IES Silver Medal in Chemistry 2018. It shows an electron donor-acceptor molecule that has proven valuable for studying quantum coherences in photo-generated radical pairs.







The Publication of the International EPR (ESR) Society

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Editorial

Dear colleagues,

In this issue, we part with the fifth President of the International EPR Society, IES Fellow Yuri Tsyetkov. The heartfelt farewell words of his colleagues and friends (pp. 8, 9) express deep grief and high appreciation of his achievements and contribution to the development of magnetic resonance. As Yuri told in his interview on the occasion of his Zavoisky Award 2013 (24/1-2, pp. 15, 16), the driving force for his research was curiosity and doubt, desire to understand, why this happens in this way and not otherwise in his field of science. This was an eternal chase for truth, not attainable in its absolute meaning. His message to the younger generation of the EPR researchers: "EPR is a powerful tool for the studies with a sound theoretical and experimental basis. It should be used for solving the diverse topical problems in physics, chemistry and biology. My experience showed that this is one of most interesting occupations in science. Let you search for and find new applications of EPR, develop the theory and methods of the experiment. I am sure that you will get deep satisfaction

on this way and be filled with the desire to learn more and more. I wish you success!" sounds as his scientific testament. We will miss Yuri and our grateful memory will keep him alive for the years to come.

The report about the IES Annual General Meeting (pp. 3–5) summarizes the diverse activities of the IES in 2018 and presents the plans for the future. This meeting took place at the third joint conference of the International Asia-Pacific EPR/ESR Society and the International EPR/ESR Society (pp. 11, 12). Special emphasis was made on the necessity to increase the IES membership in order to enhance the impact of the IES on the field and attract sponsors. Please note one of the recent initiatives of the IES – the establishment of a new IES Publication Award for the IES members.

As usual, it is a pleasure to thank our enthusiastic *EPR newsletter* team and collaborators for the help and support and inspiring contribution to the development of our publication: CEOs of the IES; Associate Editors Candice Klug (Americas) (who is never tired to find new EPR Faculty to be featured in her column), Hitoshi Ohta (Asia-Pacific), and Sabine Van Doorslaer (Europe) (whose the Present Meets Present column provides a look into the fruitful mentor-student collaboration); Keith Earle and Stefan Stoll (who keep search for new tips and techniques, and software for their relevant columns), Wolfgang Lubitz (the guests of the issue featured in his column open new horizons for our readers), and John Pilbrow (the entertaining and instructive EPR newsletter Anecdotes column); Sergei Akhmin, our creative technical editor; Yevhen Polyhach, our highly responsible webmaster; and last but not least, Scott Morton of LaPlume Printing, our long-term reliable and extremely efficient printer.

To keep you updated: starting in 2019, David Britt agreed to succeed Wolfgang Lubitz as editor of the EPR: Hot Topics column.

On the threshold of the thirty years of the International EPR/ESR Society, the *EPR newsletter* team is full of vigor and enthusiasm to keep the high standards of our publication.

Dear colleagues, welcome to our future issues and remember, it is you who produce news! Laila Mosina





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IES ANNUAL GENERAL MEETING 2018

Minutes of the Annual General Meeting of the International EPR/ESR Society for 2018, held during the Third Joint Conference of the Asia-Pacific EPR/ESR Society and the International EPR(ESR) Society, The University of Queensland, St. Lucia, Brisbane, Australia, September 26, 2018.

Agenda:

- 1. Introduction (T. Prisner)
- 2. Welcome of new IES members (H. Hirata) 3. Short Report of the 2017 AGM at ISMAR
- (H. Ohta) 4. Secretary Report (A. Blank)
- 5. Treasurer Financial Report 2017-18 (T. Smirnova)
- 6. *EPR newsletter* Editor Report (L. Mosina presented by T. Prisner)
- 7. Planned IES Activities in 2019:
 - Annual General Meeting: EFEPR Meeting Bratislava (T. Prisner)
 - Poster Awards in 2019 (T. Prisner)
 - Awards of IES in 2018/2019 (T. Prisner)
 - EPR Summer Schools USA & Europe (S. Han)
 - Social Media (S. Han)
- 8. Other Topics (T. Prisner)

1. Introduction by Prof. Thomas Prisner

Dear Colleagues,

On behalf of the IES Executive Board I wish to welcome all participants to the Third Joint Conference of the Asia-Pacific EPR/ESR Society and the International EPR(ESR) Society, The University of Queensland, St. Lucia, Brisbane, Australia, September 26, 2018.

I would like to express my gratitude to the conference organizers of this meeting, especially to Jeffrey Harmer, Steven Bottle, Nick Cox, and for allowing our General Meeting to take place during this Conference.

2. Welcome of new IES executives (2018-2020) by Prof. H. Hirata

President: Thomas Prisner Vice President Asia Pacific: Hiroshi Hirata Vice President Americas: Songi Han Vice President Europe: Gunnar Jeschke Secretary: Aharon Blank Treasurer: Tatyana Smirnova Immediate Past President: Hitoshi Ohta *EPR newsletter* Editor: Laila Mosina

3. Short Report of the previous AGM at ISMAR 2017 on July 27, 2017 Quebec City, Canada by Hitoshi Ohta

See *EPR newsletter* 27/4 (2017) pp.3–5

4. Secretary's Report, Aharon Blank

The Secretary is responsible for the day-to-day operations of the Society, and ensures efficient functioning of the Society, e.g.:

1. The Secretary shall maintain all the records of the Society shall keep the minutes of Society meetings, and be responsible for the distribution of all essential information to members.

2. Sending out invoices to the sponsors (in consultation with the Treasurer).

3. Informing members (and sponsors) of the various items of interest, e.g. announcements of conferences, workshops, publication of new issues of *EPR newsletter*.

4. Organization of material for awards given by the IES: medals, certificates and citations.

5. Overlooking financial status and membership of the Society (in consultation with the Treasurer).

6. Website: maintenance and upgrades, adds and positions. We are looking for interesting photos, papers, links – please send them out.

- 7. Answering any enquiries.
- 8. Organizing AGM.

9. Liaisons with the President, Treasurer, Editor of the *EPR newsletter*, and the members of the IES Executive.

Presentation of the web site and its features by the secretary.

5. Treasurer's Report, Tatyana Smirnova (Financial Reports)

Comments from the Treasurer: Thank you, members and sponsors, for your support! Bruker BioSpin Corp. JEOL RESONANCE Inc. Oxford Instruments NanoScience Virginia Diodes, Inc. Elva-1 Microwave Handelsbolag Magnettech GmbH L&M EPR Supplies **Research Specialties** Molecular Specialties **KEYCOM** Corporation **GMW** Associates Adani Systems, Inc. Norell, Inc.

2017 Financial Report (\$)

Balance January 1, 2017	34,347.74
Deposits:	
Membership	5,619.11
Sponsors	8,228.51
Bruker contribution to	
printing	2,226.00
Contribution for Newsletter	
distribution	23,727.28
SEMRC for students awards	200.00
Donations for Conferences	1,500.00
TOTAL deposits:	41,500.90
Expenditures:	
Internet commerce and	
merchant services	671.58
Web design/maintenance	
& fees	419.73
Newsletter printing	7,801.00
(including 2,226.00 paid	
by Bruker)	
Newsletter distribution	18,330.54
Newsletter Editorial	3,242.00
State of Illinois	13.00
Conference support	4,000.00
Awards and medals	3,061.20
TOTAL expenditures:	37,539.05
Balance December 31, 2017	38,309.59

2018 January-June Financial Report (\$)

Balance January 1, 2018	
38,309.59	
Deposits:	
Membership	2,400.10
Bruker contribution to	
printing	742.00
Sponsors	14,600.00
Travel grant from Bruker	1,176.40
Refund from bank	10.00
TOTAL deposits	18,928.50
Expenditures:	
Credit card fees, Internet	
commerce and merchant	
services	409.78
Newsletter printing	1,865.00
State of Illinois + Miss	13.84
Conference support	
(APES 2018)	3,000.00
Awards and medals	608.20
Website support	255.25
TOTAL expenditures	6,152.07
Balance June 30, 2018	51,086.02

John Weil Fund. Established in 2010 in memory of Prof. John Weil by family, friends, and colleagues to support John Weil Young Investigator Award. No distributions in 2017. Balance 23,492.94

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Annual General Meeting 2018



From left to right: Thomas Prisner and Michael Wasielewski.

We want to thank Tatyana Smirnova for her excellent work as Treasurer of the Society.

6. EPR newsletter Editor's Report, Laila Mosina

Since the previous Annual Meeting of the IES in 2017 in Quebec (Canada), we published single issues 27/3 and 27/4, and a double issue 28/1-2. We hope you had a look at 27/3, 27/4 and 28/1-2 on the newsletter website and got their copies.

Now we finalized 28/3 and work on the forthcoming issue 28/4. To remind you, we present the columns of the newsletter:

- Editorial
- IES business
- Awards
- IES Young Investigator Award Revisited
- Another Passion
- Anniversaries
- EPR newsletter Anecdotes
- In Memoriam
- Present Meets Future
- Software
- Tips and Techniques
- Notices of Meetings
- Conference Reports
- New EPR Faculty
- New Books and Journals (including EPR Hot Science)
- Market Place
- Reader's Corner
- Guest of the Issue

Please feel free to submit YOUR material, dear colleagues!!!

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, Keith Earle and David Budil, Sabine Van Doorslaer, and also to Yevhen Polyhach, our web-master, and Sergei Akhmin, our Technical Editor.

I gratefully acknowledge collaboration with Associate Editors Candice Klug, Hitoshi Ohta and Sabine Van Doorslaer.

We want to thank Laila Mosina and her editorial team for their excellent work for the EPR newsletter of the Society.

7. Planned IES Activities in 2019

• In order to increase our impact on the field and attract sponsors, we need a large number of IES members of about 1,000 (at the moment we have only ~200 paid members). Our budget is mainly supported by the sponsors! Proposal after AGM in Torino 2016 by Bruno Guigliarelli was to add affiliation of members from the national societies (examples: France 100, Japan 200 etc.). We plan to pursue this avenue with an initiative for the 30 year anniversary of IES and offer 1 year free associate membership for members of national EPR societies!

• Annual General Meeting is planned during the EFEPR Meeting Bratislava, September 1–5, 2019. The organizers of the meeting have offered us the following advantages:

- Have Board and General Meeting at the conference
- Presentation of IES Prizes
- Collect IES Member Fees with the registration fees

We plan to provide financial support for the conference organizers.

• Poster Awards for EPR students in 2019.

- Certificate and 200 \$

- Create visibility for young EPR researchers on conferences
- Display at IES webpage and in *EPR newsletter*
- Attract young students to become IES member

Poster Awards are planned at the following conferences: Royal Society EPR Meeting Glasgow; Rocky Mountain Conference Denver; ISMAR/EUROMAR Meeting Berlin; EFEPR Meeting Bratislava.

- Awards of IES in 2018/2019.
- Silver Medal in Physics/Material Sciences
- Silver Medal in Biology/Medicine
- Fellows of IES

– John Weil Young Investigator Award Required: Nominations by active IES members (100-150 word citation) + pdf of 2 recent publications (for John Weil).

Deadline for Nominations is 15th November 2018!

- NEW EPR Publication Award for members of IES.
- Self nomination
- Corresponding author or
- First author with support letter from corresponding author

Deadline 15th March 2019!

• We plan to help organize and support EPR Summer Schools USA and Europe. This introduces EPR spectroscopy to young scientists, creates active networks between young researchers in EPR. Future plans: have the material of such schools on our webpage.

- EPR Winter Schools in Czech 2019
- EFEPR Groups organizes such EPR Schools in Europe regularly (every 2-3 years) since 1999 in Caorle, Italy:

One week of lectures, tutorials and practical courses; 100 participating students; 10-15



From left to right: Aharon Blank, Thomas Prisner, Sunshuke Furuya and Hitoshi Ohta.

Annual General Meeting 2018

teachers; Learn state-of-the-art methods; Get together with leading experts; Present own work on poster; Create own network (we are not alone!).

 First IES/SharedEPR Summer School on EPR Spectroscopy

Location: University of Denver (DU)

Dates: July 19, 2019 evening – July 23, 2019 morning

Capacity: 40 students (mostly US, with a group of slots for international students)

Accommodation: DU student housing Lecturers: will be selected and contacted once

program is finalized

Practicals: in Eaton lab at DU, supplemented with loan spectrometers from Bruker Curriculum principles:

The school is targeted to students that don't have experience with EPR. It consists of lectures with tutorials for all students, and of practicals (both in the EPR lab and in the classroom) for small groups. Each lecture is immediately followed by a tutorial, where students work through worksheet to help them practice the concepts of the preceding lecture. Practicals start only after all fundamental lectures/tutorials are done. This assures that any student can take any of the practicals already in the first practical session

EPR Summer School will be advertised by Peter Höfer at Bruker (to those who bought EPRNano) and David Rockcliffe (NSF program officer, to Dept chairs)

- Membership Campaign
- EPR is a vibrant method with many applications – but that has to be reflected by a strong Society with many members!
- Companies are willing to sponsor our Society if they see a larger number of active members!

- We have to teach EPR to young students and to other scientists, a strong Society can support and initiate such activities!
- We should support EPR faculty in their career promotion with prizes.
- How to increase Membership? It has to be of self-interest to stay an IES member.
- Give out non-monetary recognitions for EPR papers published and list on IES webpage? Recognitions could be "IES Prize Paper". Need to be member to enter the contest.
- Need to be member to receive any prize or scholarship. Its okay to ask recipient after nomination to become member.
- Social Media
- Benefits for young researchers to become IES member?
- Be part of a network.
- Generate an @IES Twitter account and "New EPR papers" rubric to tweet EPR papers. Obtaining tweets increase the Altmetric of papers.
- Mendeley users should download the EPR papers.

8. Prizes Awarded in 2018

- Silver Medal in Chemistry: Michael Wasielewski (see photo)
- John Weil Young Investigator Award: Sunshuke Furuya (see photo)
- Fellow: Hideo Utsumi
- Poster Prize Winners: *RSC ESR Meeting London* Kaltum Abdiaziz (Queen Mary, London) Nino Wili (ETH Zürich) *Rocky Mountain Conference* Donald Mannikko (Washington Univ.) Stephan Pribitzer (ETH Zürich) *EUROMAR Nantes* Angeliki Giannoulis (Weizmann) Paola Guaraccini (Padua)



From left to right: Aharon Blank, Yuta Koizumi, Sugyeong Hong and Thomas Prisner.

APES Meeting Brisbane (see photo below) Yuta Koizumi (Fukui) Sugyeong Hong (KBSI Seoul)

9. Thanks

The IES thanks the following Corporate Sponsors for their contributions in 2018: Bruker BioSpin Corp JEOL RESONANCE Inc Oxford Instruments NanoScience Virginia Diodes, Inc Elva-1 Microwave Handelsbolag Magnettech GmbH L & M EPR Supplies Research Specialties Molecular Specialties KEYCOM Corporation GMW Associates Adani Systems, Inc Norell

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All paid up members

Newsletter Editor: Laila Mosina Technical Editor: Sergei Akhmin Associate Editors: Candice Klug, Hitoshi Ohta, and Sabine Van Doorslaer

Attendance list

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Interview with Professor Betty Gaffney on the Occasion of Her IES Fellowship 2017



EPR newsletter: Dear Professor Gaffney, on behalf of the readers of the EPR newsletter we congratulate you on your IES Fellowship 2017. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?

I was encouraged to observe nature by parents and grandparents who had studied various aspects of biology. I remember my first "philosophic moment" at age ~3-4 when I observed that a solid crayon left for some time in the hot summer sun becomes a liquid. My scientific window on the world became focused later by encouragement from chemistry faculty when I was an undergraduate at Stanford, and one summer at UCLA. Overall, I was drawn to scientific puzzles to be solved.

Who introduced you into magnetic resonance?

For a chemistry major at Stanford, 1957-1961, practically every class did. The person who first explained details of his own experiments to me was Professor Richard A. Ogg. He had reported the proton NMR spectra of liquid ammonia, with and without traces of water, and related experiments, in 1954. I accepted manifestations of spin exchange as a means of studying chemical equilibria and dynamics as common knowledge after his enthusiastic explanation. I also was introduced, by Ogg, to discussions about paramagnetic broadening of the proton NMR signals in solutions of lithium in liquid ammonia. Shortly after, I did undergraduate research with Harry S. Mosher, who was determining the complex chemical structure of tetrodotoxin by NMR methods. In retrospect, walking into these labs and asking to know more was a most amazing opportunity for an undergraduate.

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

I look at my research as a progression of experiments to bring EPR methods to bear on biology and to address why nature makes so many, apparently redundant, lipids. I have regarded every "most recent" research result as the "best one yet". One reason for that outlook is that technology opportunities, in both instrumentation and biology, have continually opened new doors. EPR has allowed me to focus in on unique questions about the lipid oxidizing enzyme, lipoxygenase, over many years. I do admit a particular fondness for EPR spectra of S > 1/2 species, though. They provide fun puzzles.

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

To paraphrase a response Linus Pauling is reported to have made, when asked how he had so many good ideas, he is said to have replied you have to have many ideas. So I echo that response: think of the big puzzle you would like to solve and then generate ideas to accomplish the steps along the way. If it can't be done yet, overcome the obstacles. Tell me about your ideas in your manuscript introductions. If the results change your ideas, that's wonderful too.

IES Silver Medal for Instrumentation 2017

G. Jeschke

PR spectroscopy has always relied on tech-Lnology developed for radar applications. In fact, my own way to EPR was influenced by work with radar electronics and by programming a radar simulator during military service. In the second semester of my chemistry studies at Technical University Dresden I joined the NMR group of Gisbert Grossmann, where experience with radar and programming allowed me to contribute to research rather soon. My first acquaintance with arbitrary waveform generators (AWGs) dates back to doctoral studies in the group of Arthur Schweiger at ETH Zürich. By interfacing a 200 MSa/s AWG with 8 bit vertical resolution to a home-built pulsed EPR spectrometer, I could perform ENDOR experiments with radiofrequency chirp pulses.

In the outlook section of my doctoral thesis I suggested microwave pulse shaping with the 1 GSa/s AWGs that were state of the art at the time. However, this idea was premature, given the price of these instruments in 1997 and the only modest bandwidth improvement expected at this sampling rate.

When I was appointed professor in Konstanz in 2006, I reconsidered such pulse shaping. Meanwhile, the bandwidth of AWGs had become appealing, driven by their development for radar applications. However, cost of an at-



tractive state-of-the-art AWG exceeded what was left of my startup grant after buying the pulsed EPR spectrometer required for becoming operational at all. At startup in Zürich in 2008, I decided to direct initial instrumentation efforts to optimization of an existing home-built high-power pulsed Q-band spectrometer for DEER distance distribution measurements. We also adapted resonators for this purpose. This work, carried out largely by Yevhen Polyhach and René Tschaggelar, improved DEER sensitivity by more than an order of magnitude compared to standard X-band technology (DOI: 10.1039/c2cp41520h).

In 2011, the first AWGs appeared on the market whose bandwidth exceeded the limitations imposed by other components of a pulsed EPR spectrometer, even disregarding resonator limitations, at a price affordable with my remaining startup money. By coincidence, Andrin Doll, who had written a master thesis on an Overhauser DNP setup the year before, was available for a doctoral project. An ETHinternal grant made it possible to hire him from January 2012 for constructing a newgeneration pulsed EPR spectrometer. The new architecture is based on the idea of replacing the console by only three devices - an AWG with integrated sequencer, a fast digitizer, and a field controller. At 12 GSa/s, we had more than sufficient waveform bandwidth and could afford to place the intermediate frequency outside the excitation band (DOI: 10.1016/j. jmr.2013.01.002). The resulting spectral purity allows for applying long and strong frequencyswept pulses. Andrin demonstrated this by enhancing the central transition of high-spin species by a sweep through the satellite transitions (DOI: 10.1039/c4cp05893c). A DEER experiment on Gd(III)-Gd(III) spin pairs with such a pre-polarization step used several excitation bands that covered a total width of 2.5 GHz, strongly exceeding resonator bandwidth. Such ultra-wideband excitation well beyond resonator specifications is possible by adapting the frequency modulation function of pulses to the resonator mode profile, provided that high power is available and can be applied over a long time.

The AWG, run at 8 GSa/s, and an affordable 2 GSa/s digitizer can be synchronized with very low jitter via a common high-frequency clock (8 GHz). Since detection bandwidth is resonator-limited, this sampling rate of the digitizer was sufficient, except for the requirement of setting the intermediate frequency well outside the detection band. Andrin solved this problem by subsampling. The coherent setup based on these principles achieved a detection bandwidth of 800 MHz (DOI: 10.1016/j. jmr.2014.06.016).

Our ultra-wideband spectrometer project aimed at enhancing sensitivity with respect to the best spectrometers available in our lab. This implied that experiments with monochromatic rectangular pulses would provide the same signal-to-noise ratio as a current commercial X-band pulsed EPR spectrometer and our high-power upgraded commercial Qband pulsed EPR spectrometer or better. We succeeded in X band, but not yet in Q band. For our single-stage upconversion concept we could not find filters at Q-band frequencies that would provide sufficient image rejection during downconversion (DOI: 10.1016/j. jmr.2017.01.004). Still, Q-band sensitivity is suitable for both method development and some of our application work. We are currently designing and building a second spectrometer of this type, which will eventually solve the remaining problem.

As a second important design specification, we required that the spectrometer would run in routine operation (ideally 24 hours a day/7 days a week) in the absence of its creator. Andrin Doll has left our lab in summer 2016. The spectrometer is happily humming along. New experiments, such as the two-dimensional distance correlation experiment TRIER (DOI: 10.1016/j.jmr.2017.07.012), and chirp-echo EPR spectroscopy (CHEESY) after hole burning (DOI: 10.1016/j.jmr.2018.02.001) have been demonstrated in his absence.

Beyond ultra-wideband excitation and detection, the AWG-based spectrometer provides much more flexibility than spectrometers of the previous generation. Any phase increment of microwave pulses is possible, and since the spectrometer has only a single microwave channel, channel balance is no longer a problem for phase cycling schemes. The built-in sequencer allows for specifying, in a convenient way, coupled parameter variations and realizing them without reprogramming overhead during experiment execution. Non-uniform sampling schemes can be easily realized in indirect dimensions. Pulse amplitude can be varied during an experiment. Fast communication between the control computer and the digitizer allows

for downloading the whole transient without overhead, even in single-shot mode. This, in turn, provides access to more sophisticated digital signal processing, thus further improving sensitivity. For instance, digital filtering and echo integration with a window function matching the echo shape become possible.

The potential of the AWG-based spectrometer architecture is not yet fully used. For instance, ultra-wideband operation calls for adapted resonator designs. Building on the Hyde-Sidabras concept of multi-loopmulti-gap structures, René Tschaggelar and Frauke Breitgoff could demonstrate, for 1.6 mm outer diameter sample tubes in Q band, a microwave field strength exceeding 40 MHz throughout a 1 GHz band (DOI: 10.1007/ s00723-017-0956-z). Such resonators also provide better microwave field homogeneity than earlier designs, thus improving the precision of spin control.

Recently, even faster digitizers have become affordable that will allow us to eliminate subsampling. That way another analog filter is replaced by better digital signal processing. We expect that the combination of new resonators and a faster digitizer will push detection bandwidth beyond 1 GHz at Q-band frequencies.

The next challenge is a user-friendly interface. The spectrometer is currently operated via Matlab scripts. While method developers in our group are content with this, easier setup of standard experiments via a graphical user interface is required for application work. In the long run, measurement, signal processing, simulation and fitting should be integrated into one set of software modules that communicate with each other at ease. Only after this has been achieved, the new spectrometer generation can be considered mature.

Obviously, I received the IES Silver Medal 2017 for instrumentation only on behalf of my group. I am very grateful to Christian Bauer (MPI for Polymer Research Mainz), Enrica Bordignon, Frauke Breitgoff, Andrin Doll, Luis Fábregaz Ibáñez, Jörg Forrer, Inés García Rubio, Katharina Keller, Daniel Klose, Yevhen Polyhach, Stephan Pribitzer, Nino Wili, and Maxim Yulikov. Model compounds from the group of Adelheid Godt at Bielefeld University were indispensable for testing and improving our instruments and pulse sequences.





Yuri D. Tsvetkov (1933–2018)

It is with great sadness to hear that Prof. Yuri D. Tsvetkov, member of the RAS and for many years head of the Institute of Chemical Kinetics and Combustion in Novosibirsk, died. Yuri Tsvetkov headed one of the pioneering institutes for the development of modern pulsed EPR methods. So many famous scientists, working in this field of spectroscopy are related to this institute and worked together with Prof. Yuri Tsvetkov over decades. They were at the forefront of technological development of pulsed EPR spectroscopy in the 1960s, explored in much detail the hyperfine oscillations, which arise in solid samples after excitation with strong microwave pulses and other dynamical effects related to spin relaxation. Both of these features of pulsed EPR time traces are nowadays used regularly in many laboratories worldwide for quantitative analysis of paramagnetic molecules. In the 1980s the Novosibirsk EPR group pioneered another very important field by pulsed EPR: Pulsed Electron-Electron Double Resonance (PELDOR), which is momentarily one of the most active areas of EPR spectroscopy. It describes the dipolar interaction between two (or more) radicals in a solid powder sample, which can be used to extract intermolecular distances in the nanometer range with high precision. The publication in Chemical Physical Letters from 1984 is 300 times cited and created a new field of applications for pulsed EPR spectroscopy: the determination of structural distance restraints in disordered macromolecules. This method, renamed to Double Electron-Electron Resonance (DEER) in 1993 and later-on extended to a 4-pulse sequence, is at the moment probably the most widely used application of pulsed EPR methods. The Novosibirsk group of scientists around Yuri Tsvetkov explored the methodology and potential application fields in much detail and should get much credit for the discovery and invention of this powerful application. Prof. Yuri Tsvetkov received many awards for his scientific contributions. Just to name a few: the Silver Medal in Chemistry from the IES in 1999 (and July 9, 2018 Page 2 of 2 Fellow of IES since 2010), the Bruker Lecture of the Royal Society of Chemistry EPR group in 2006 and the Zavoisky Award in 2013. He also served as president for the IES from 2002–2005. As sad as it is to hear, that one of the pioneers of pulsed EPR spectroscopy died, it is good to see that so many excellent scientists out of his laboratory emerged and continue working in this spirit. All my regards and compassion to his family and to his scientific family

Thomas Prisner President of the International EPR Society

* * *

I met Yuri Tsvetkov for the first time in July 1951, when we passed the entrance exams to the Physics and Technology Faculty of Moscow State University. The faculty was transformed into an independent educational institution - the Moscow Institute of Physics and Technology (MIPT) already in September. Since then, our life and scientific paths were parallel courses. Five and a half years in a student hostel, several years of work in Moscow at the famous Institute of Chemical Physics, and finally, the move to Novosibirsk (1961), where the first large scientific center in Siberia was organized.

After the WWII, schoolchildren dreamed of becoming secret nuclear physicists, and Yuri and I were no exception. The most difficult entrance examinations were at the Faculty of Physics and Technology, and probably that is why we were sure – that is what we need. Alas, in the third year we were told that a hydrogen bomb had already been tested and other specialists were needed. We had to choose other professions.

Once Yuri mentioned that our new lecturer on chemical kinetics started an interesting research. This man was Vladislav Voevodsky, an active and talented researcher, a disciple of the future Nobel laureate Nikolai Semenov. This new area was chemical EPR spectroscopy. From this moment, the fate of Yuri, like mine, was associated with Voevodsky until his untimely death (1967).

Yuri was a great enthusiast and skilled at creating complex experimental setups. I remember that even in our student years, together, we assembled an efficient EPR spectrometer from the handy elements, and Voevodsky demonstrated it (together with us) to the high visitors. In parallel, during the diploma practice at the Institute of Chemical Physics, we assembled a more sophisticated superheterodyne spectrometer using the advice of specialists. The first results obtained on this homebuilt spectrometer were included in our joint publications with Yuri.

After moving to Novosibirsk, my scientific interests changed many times, although they returned to magnetic resonance in one form or another. Yuri remained faithful to EPR spectroscopy all his life. The most fruitful stage of his scientific work associated with the development of pulsed EPR spectroscopy began in Siberia. He becomes a pioneer and a recognized leader in the field of chemical applications of this method. Here he formed his scientific school. His students successfully work not only in Russia, but also abroad. His students and experts will tell about all this much better.

Yuriy Molin Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Novosibirsk, Russia

It was the deep regret that we learnt about sad demise of Professor, Academician Yuri Dmitrievich Tsvetkov who died suddenly at the age of 85 on July 7 2018.

On behave of all APES community we express our heart-felt condolence on this sad occasion. His death is a great loss for all EPR community. Yu. D. Tsvetkov and his school created the foundations of a new trend in radio spectroscopy-EPR Fourier spectroscopy, which has a high resolution. He and his team developed for the first time, pulsed EPR spectroscopy of dipole interactions (PELDOR), which makes it possible to measure distances between paramagnetic particles in the nanometer range. Recently, the methods developed by him have been increasingly used in studying the structure and dynamics of complex biological objects. In particular, team of Yu. D. Tsvetkov discovered and thoroughly studied the universal libration type of molecular

^{* * *}

motion in biomembranes, studied the conformational structure and aggregation of spin-labeled membrane-modifying proteins.

He was the head of the thesis of 16 PhD and 4 Habilitation. Yuri Tsvetkov was the author and co-author of more than 300 scientific papers, including 6 monographs, member of the editorial boards of the journals "Structural Chemistry", "Chemical Physics".

During three years he was President of the International Society for Paramagnetic Resonance, scientific councils and editorial boards of a number of domestic and foreign journals.

He was laureate of the State Prize of the USSR, winner of the Bruker Prize for Chemical Radiospectroscopy and the International Zavoisky Award and a Silver Medal of the International EPR Society.

It was Yuri Tsvetkov who convinced me to move my scientific interest from spin chemistry to application of pulse Dipole EPR spectroscopy and introduced to Asia Pacific EPR Society as a member of APES committee and convinced APES committee to organize APES 2014 in Novosibirsk.

We participate together in several International EPR conferences in UK, Germany, Italy, etc.

He has a nice sense of humor and very optimistic character.

Elena Bagryanskaya President of the Asia-Pacific EPR Society

* * *

∕uri D. Tsvetkov was a giant in the field I of pulsed EPR and its chemical applications. He, the group he led at the V. V. Voevodsky Institute of Chemical Kinetics and Combustion, and the graduates of that group are a major force in the field from the late 1960s through today. He was a major driver in the development of pulsed EPR from a tool of solid state physics into an array of methods for investigating chemical, structural, dynamic and reactive properties in chemistry, biology and biophysics. The work of his group has always been characterized by a tight coupling of theoretical advances, instrumental innovation and experimental rigor. I always found that their work was carefully thought out and thoroughly planned so that the physical insights from their experiments revealed as much as possible about the systems they studied.

Yuri went to Akademgorodok at its founding in 1957 and had many roles in shaping his lab, his institute and the Siberian Branch of the Academy for six decades. When he retired, he returned to science full time and shaped the development of DEER/PELDOR spectroscopy into a significant research method for the structural and conformational characterization of biomacromolecules and soft matter.

I saw in Yuri a deep care for and sense of responsibility to his students. He trained them well, encouraged and promoted them through the good times and the bad. Today, people from his lab are in institutes and universities in Novosibirsk, in Russia, and throughout the world. These people, along with the science they made together, are a part of Yuri's legacy to science and to the world. I am proud that I knew him as a friend and mentor.

Michael K. Bowman University of Alabama, Tuscaloosa, USA

* * *

I twas indeed very sad to learn about the passing away of Academician Y. D. Tsvetkov. I recall many moments of fruitful scientific discussion with him during the APES meetings we attended. I especially remember his visit to Bangalore in 2004 to participate in the APES meeting organized here. We have lost a very eminent EPR spectroscopist in his passing away. On behalf of the EPR community in India and on my own behalf I offer heartfelt condolences.

S. V. Bhat, FNASc, FNA, FASc. President, Asia-Pacific EPR/ESR Society (2015–2016) NASI Senior Scientist Platinum Jubilee Fellow, Department of Physics, Indian Institute of Science, Bangalore-560012, India

* * *

Yuri Tsvetkov was respected worldwide as one of pioneers of electron spin echo (ESE) spectroscopy and its applications in chemistry and biology. His scientific activity was related with development of methodology of ESE and study of properties and structure of free radicals and spin probes. This work started in 1967, when a homemade ESE spectrometer was built in the Institute of Chemical Kinetics and Combustion of Russian Academy of Sciences, Novosibirsk. It was one of the first spectrometers in the world that is especially designed for chemical applications.

From that time, a lot of different fields were found where the ESE might be applied. One of the firsts was investigation of electronnuclear interactions in free radicals in solids. The approach has now been developed to a very powerful ESE envelope modulation (ESEEM) spectroscopy.

Another very important technique developed in his laboratory was pulsed electronelectron double resonance (PELDOR). Now it is widely used in different laboratories to study structure of biradicals, doubly spinlabeled and metal-containing biomolecules, and their aggregation.

ESE spectroscopy was also shown to be very useful in studying molecular motion of radicals. The first work in this field also was done in his laboratory (1981).

Yuri Tsvetkov has done a lot of administrative work – as a director of Institute of Chemical Kinetics and Combustion, a Chief Scientific Secretary of Siberian Brunch of USSR Academy of Sciences, a member of many editorial boards, President of the International EPR Society.

Under his supervision 16 Candidates of Science (equivalent to PhD) were defended. He got a prestigious USSR State prize – for development of EPR spectroscopy, silver medal of EPR society and three national medals. He also was a Full member of the Russian Academy of Sciences.

His close colleagues who worked with him for many years in his laboratory will remember him as a wise and gifted person, who was also prone for joking and ready to provide necessary assistance for everybody. We grieve over his unexpected demise.

On behave of his laboratory colleagues

Sergei Dzuba Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Novosibirsk, Russia

* * *

Please accept my sincere condolences on the death of Yuri. He was not only an eminent world class scientist but a person very helpful in development of our APE Society through his high-level and instrumental support as the IES President.

Czesław Rudowicz Institute of Physics, Faculty of Mechanical Engineering and Mechatronics, West Pomeranian University of Technology in Szczecin, Pacific EPR/ESR Society President, Polish EPR

Conference reports

59th Rocky Mountain Conference on Magnetic Resonance and 41st International EPR Symposium

July 22–27, 2018, Snowbird, Utah

The 41st International EPR Symposium at the 59th Rocky Mountain Conference on Magnetic Resonance (RMC) was held in the beautifully located ski resort Snowbird near Salt Lake City, Utah, United States, from Sunday July 22 to Friday July 27, 2018. After 2015, this is the second time the RMC was held as this venue outside of Colorado. This year, the RMC hosted parallel symposia on EPR and on solid-state NMR.

On Sunday, before the start of the scientific program of the EPR Symposium, Bruker gave a presentation on new and updated products and hosted an excellent dinner buffet. Besides Bruker, commercial sponsorship for the EPR symposium came from Virginia Diodes, Element 6, Cryogenic Ltd., and Signals GmbH.

The scientific program of the EPR Symposium extended from Monday morning to Thursday noon and was packed: It included 17 invited talks (25+5 minutes) and 43 contributed talks (12+3 minutes). The topics of the 14 sessions spanned a large range of topics, including biomacromolecules (structural biology, mostly DEER), spin centers in biology and chemistry (enzymology, catalysis), spin devices (with a significant number of talks using NV⁻ centers in diamond), materials, theory, instrumentation and other methodology, and EPR imaging. Two sessions were held jointly with the Solid-State NMR Symposium, with DNP as the overall topic. Invited talks in these session were given by Robert Griffin (MIT), Jean-Philippe Ansermet (EPFL, Lausanne), Björn Corzilius (Goethe University

Frankfurt), and Alex Smirnov (North Carolina State University). The after-dinner talk at the Wednesday conference banquet was given by Robert Griffin (MIT), who gave an entertaining overview of his early career.

There were two evening poster sessions that featured a total of 72 posters. The poster sessions were well attended, and supported by the free drinks that the EPR Symposium was able to offer. A total of six student poster prizes were sponsored by the International EPR Society, Wiley, and Springer. The poster committee, comprised of invited speakers, awarded these to Stephan Pribitzer (ETH Zürich), Donald Mannikko (University of Washington), Graham Roseman (University of California Santa Cruz), Maxx Tessmer (Medical College of Wisconsin), Markus Teucher (Ruhr-Universität Bochum), and Yilin Shi (University of Denver).

The scientific committee of the EPR Symposium was comprised of Stefan Stoll (University of Washington, chair), Susumu Takahashi (University of Southern California, vice-chair), Ania Bleszynski-Jayich (University of California Santa Barbara), Christoph Boehme (University of Utah), Enrica Bordignon (Ruhr-Universität Bochum), Boris Epel (University of Chicago), Gail Fanucci (University of Florida), Songi Han (University of California Santa Barbara), Stephen Hill (Florida State University, National High Magnetic Field Lab), Dane McCamey (University of New South Wales), and John McCracken (Michigan State University). Committee members served as session chairs.

The number of registered attendees at the EPR Symposium was 147, the highest number since the beginning of recordings in 2000. Two thirds of the attendees were from the US, the other third from abroad. This shows that the



Poster award ceremony. From left to right: Susumu Takahashi, Gunnar Jeschke, Stephan Pribitzer, Donald Mannikko, Markus Teucher, Stefan Stoll, Graham Roseman, Maxx Tessmer, Yilin Shi.

EPR Symposium at the RMC continues to be one of the leading international conferences in EPR. A third of the attendees were students.

Immediately after the EPR Symposium, the NSF-funded SharedEPR network (led by Gary Gerfen, Albert Einstein College of Medicine) organized a workshop entitled "Software Tools for EPR Spectroscopy: Capabilities and Demonstrations" with presentations of 13 software packages. The workshop on Thursday afternoon and Friday morning drew a large crowd.

In 2019, the RMC will return to Colorado. The 60th RMC with the 42nd International EPR Symposium will be held at the Crowne Plaza Hotel in Denver, July 21–25, 2019. The chair for the 2019 EPR Symposium is Susumu Takahashi (University of Southern California).

> Stefan Stoll Chair, EPR Symposium 2018

SharedEPR workshop on EPR software July 26–27, 2018, Snowbird, Utah



The NSF-funded SharedEPR network organized a workshop entitled "Software Tools for EPR Spectroscopy: Capabilities and Demonstrations" that was held in Snowbird (Utah) on two half-days on July 26 and July 27, 2018, immediately after the conclusion of the 41st EPR Symposium and the 59th Rocky Mountain Conference on Magnetic Resonance at the same venue. The workshop had an attendance of about 90.

This was a unique workshop. For the first time, it brought together researchers and developers of almost all major EPR software packages that are currently in use in the EPR community. The 13 30-minute presentations and demonstrations covered software for spectral simulation and fitting, data analysis, and instrument control, thus providing a complete overview of the state of the art on how computers enable and facilitate EPR research.

The presenters were Gregor Hagelueken (University of Bonn; mtsslSuite with mtsslWizard), Gunnar Jeschke (ETH Zürich; DeerAnalysis and MMM), Stephan Rein (University of Freiburg; SpecProFi), Boris Epel (University of Chicago; SpecMan4EPR), David Budil (Northeastern University; NLSL), Eric Hustedt (Vanderbilt University; GLADDvu), Madhur

Conference reports



Srivastava (Cornell; wavelet denoising); Stefan Stoll (University of Washington; EasySpin), Kalina Rangueolva and Ralph Weber (Bruker; SpinFit and Anisotropic SpinFit), Ilya Kuprov (University of Southampton; Spinach), and Christian Altenbach (University of California Los Angeles; LongDistances and Short-

Distances). The program was put together by Stefan Stoll (University of Washington) and Gary Gerfen (Albert Einstein College of Medicine; lead investigator on the NSF SharedEPR grant).

Most software packages that were presented are available for free. Presenters encouraged

out from a 1930s, heritage-listed sandstone Cloister enclosing the Great Court.

It was the eleventh meeting of the APES society and the second time it has been held in Australia (Cairns 2008). There was 103 registered participants, 22 sessions and 72 presentations. Missing was Graeme Hanson, a giant of the Australian EPR community, who sadly passed away three years ago.

All APES countries were represented, presented their exciting research at the meeting which was a great showcase and demonstrates the strength of our expanding community. This APES community includes Russia, India, Japan, China, Australia, South Korea and the Philippines. This year we were joined by

the workshop attendees to contact them with issues and feature requests, to help improve the programs and to guide further development.

The workshop saw a lively discussion concerning methods for the analysis DEER data, a topic of broad concern and with significant ongoing research efforts. The two commonly used models to represent DEER distance distributions were presented and discussed: a parameter-free model that is fit to data using Tikhonov-regularized least-squares fitting, and a parameterized model consisting of several Gaussians that is fit to data using ordinary least-squares fitting. From the workshop, it appears that both methods are advancing, but that there is no complete consensus yet in the community about the relative merits of the two.

Overall, the workshop was very timely, as EPR spectroscopist increasingly rely on software for their scientific work.

members of the international EPR society

from Germany, Israel, Poland, Switzerland,

the United Kingdom and the United States

Stefan Stoll and Gary Gerfen

The third joint conference of the Asia-Pacific **EPR/ESR Society and the International** EPR(ESR) Society

September 23–27, 2018, University of Queensland, Brisbane, Australia

The third joint conference of the Asia-Pacific EPR/ESR Society (APES) and the International EPR Society (IES) was held on the 23rd to 27th of September at the University of Queensland (UQ) in Brisbane, Australia. The conference venue, the University's main campus at St Lucia, is a leafy and green 114-hectare site bounded on three sides by the Brisbane River, seven kilometres from the centre of Brisbane city. The campus fans

of America. This was the third joint meeting of the two societies, further strengthening ties and fostering collaboration on a global scale. The conference was opened on Monday morning by Olav Schiemann (University of

Bonn) describing recent instrumental advances in freeze-quench technology coupled with PELDOR. We had two further plenary speakers on Tuesday and Thursday, Songi Han (University of California, Santa Barbra) and the recent Bruker prize winner Takeji Takui (Osaka City University), detailing treatises on DNP mechanisms and spin Hamilto-



Conference reports



nian approaches to high spin systems, respectively. We also had nine keynote lectures: Thomas Prisner, Subray Bhat, Graham Smith, Yoh Matsuki, Steve Hill, Sharon Ruthstein, Arzhang Ardavan and Matvey Fedin and thirty-six invited talks, covering diverse subjects from copper homeostasis to imaging to high field instrumentation and quantum computing.

Wednesday morning was devoted to two IES award presentations. Michael Wasielewski (Northwestern University) received the silver medal for chemistry for his significant contributions in the field of spin dynamics and quantum information science as studied by EPR. Shunsuke Furuya (RIKEN) received the John Weil Young Investigator award for his impressive theoretical work on low-dimensional quantum magnets. We also had three poster prizes awarded, two from the IES awarded to Sugyeong Hong (KBSI Seoul University) and Yuta Koizumi (Fukui University), and one from the Australian/ New Zealand magnetic resonance society (ANZMAG) awarded to Julien Langley (ANU). Further details from the meeting including the program and abstracts are available on the APES-IES2018 website (www.apes-ies2018.org).

A big thank you go to the sponsors of the meeting who include: University of Queensland (UQ), Bruker, Cryogenic, ClinEPR, Avanti and Magnettech. Without their support the meeting would not have happened.

And we would sincerely like to thank all participants for supporting the meeting and our two societies. The help we received from the APES and IES executive was greatly appreciated. We hope to see you again soon in Australia and wish the organizers of the next APES meeting in China success in 2020.

> Sincerely, Jeffrey Harmer, Steve Bottle, Nick Cox

new Books & Journals

Electron Spin Resonance Spectroscopy in Medicine

Editor: Ashutosh Kumar Shukla Publisher: Springer Singapore Number of Pages: XI, 221 Language: English Copyright: 2019 Copyright Holder: Springer Nature Singapore Pte Ltd. eBook ISBN: 978-981-13-2230-3 DOI: 10.1007/978-981-13-2230-3 Hardcover ISBN: 978-981-13-2229-7 Edition Number: 1, Number of Illustrations: 49 b/w illustra-

tions, 35 illustrations in colour

This book examines various applications of electron spin resonance spectroscopy (ESR) in medicine, covering topics such as interactions between blood and nanoparticles, physical intricacy of HbNO complexes, parasitic diseases, oxidative stress measurement, polymerization of resinous materials used in dentistry, tooth dosimetry and dermatological applications.



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cal details, it focuses on the applications and data interpretation of ESR as an emerging tool.

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notices of Meetings

EPR Summer School Denver 2019

University of Denver, July 17-21, 2019

The International EPR/ESR Society (IES) and the NSF-supported SharedEPR Network are co-organizing an EPR summer school to be held at the University of Denver immediately preceding the 2019 Rocky Mountain Conference on Magnetic Resonance. The school will concentrate on introductory material and thus will be appropriate for researchers with little or no experience in EPR who want to gain both an understanding of the underlying principles as well practical experience in EPR. Instructors for the courses will be internationally renowned experts in the field of EPR from both academia and industry and will be available for extended question and discussion sessions. Lectures, tutorials and practical training will cover the basics of continuous-wave EPR and pulse EPR, the analysis of EPR spectra, and principles of metal ion and nitroxide EPR.

Admission to the summer school will be free of charge and will include all course materials and supplies, accommodation in University of Denver dormitory housing for 4 nights, all meals, and an excursion to the Rocky Mountains. Applications will be accepted from all academic and professional levels but the school will be limited to under 50 participants. To apply for admission, please email a CV along with a brief (one page or less) description of your research and/or reason for your interest in EPR spectroscopy to Gary Gerfen at gary.gerfen@einstein.yu.edu. To ensure consideration of your application, please submit it on or before March 1, 2019. Selection of participants will be made by the executive boards of IES and SharedEPR. Notification of admission will be given by March 15, 2019. A limited number of travel stipends will be available to qualified participants. Further information will be made available at the websites of IES (www.ieprs.org) and SharedEPR (www.sharedepr.org). Questions can be emailed to Gary Gerfen.

The 52nd Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry

University of Glasgow, Glasgow, UK, April 7–11, 2019 Web: www.esr-group.org/ conferences/2019-conference-glasgow

The Meeting is the oldest EPR spectroscopy conference in the world, as well as the occasion on which Bruker Prizes are awarded to eminent EPR spectroscopists and talented PhD students, and the JEOL Student Prize is awarded for the best student research work. The lists of past winners of Bruker and JEOL Prizes are available here:

www.esr-group.org/bruker-lectures www.esr-group.org/bruker-thesis-prize www.esr-group.org/jeol-lectures

new EPR Faculty



Troy Stich became an Assistant Professor of Chemistry at Wake Forest University in July 2018. Troy earned his undergraduate degree in chemistry from Carnegie Mellon University in 2000 and studied with Mike Hendrich. He earned his PhD degree in physical chemistry at the University of Wisconsin – Madison in 2005 in the laboratory of Thomas Brunold where he studied the biosynthesis of vitamin B12 (cobalamin). Troy completed a postdoctoral fellowship in David Britt's lab at the University of California – Davis focusing on characterization of the tetra-manganese cluster in photosystem II. He was then promoted to Associate Research Specialist in 2011 after which he was actively involved in studies of biogeochemical manganese oxidation and radical SAM enzyme mechanisms. His current research focuses on exploring the plasticity of radical SAM and cobalamin-dependent enzymes by characterizing enzyme reaction intermediates using EPR spectroscopy and computational modeling.







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