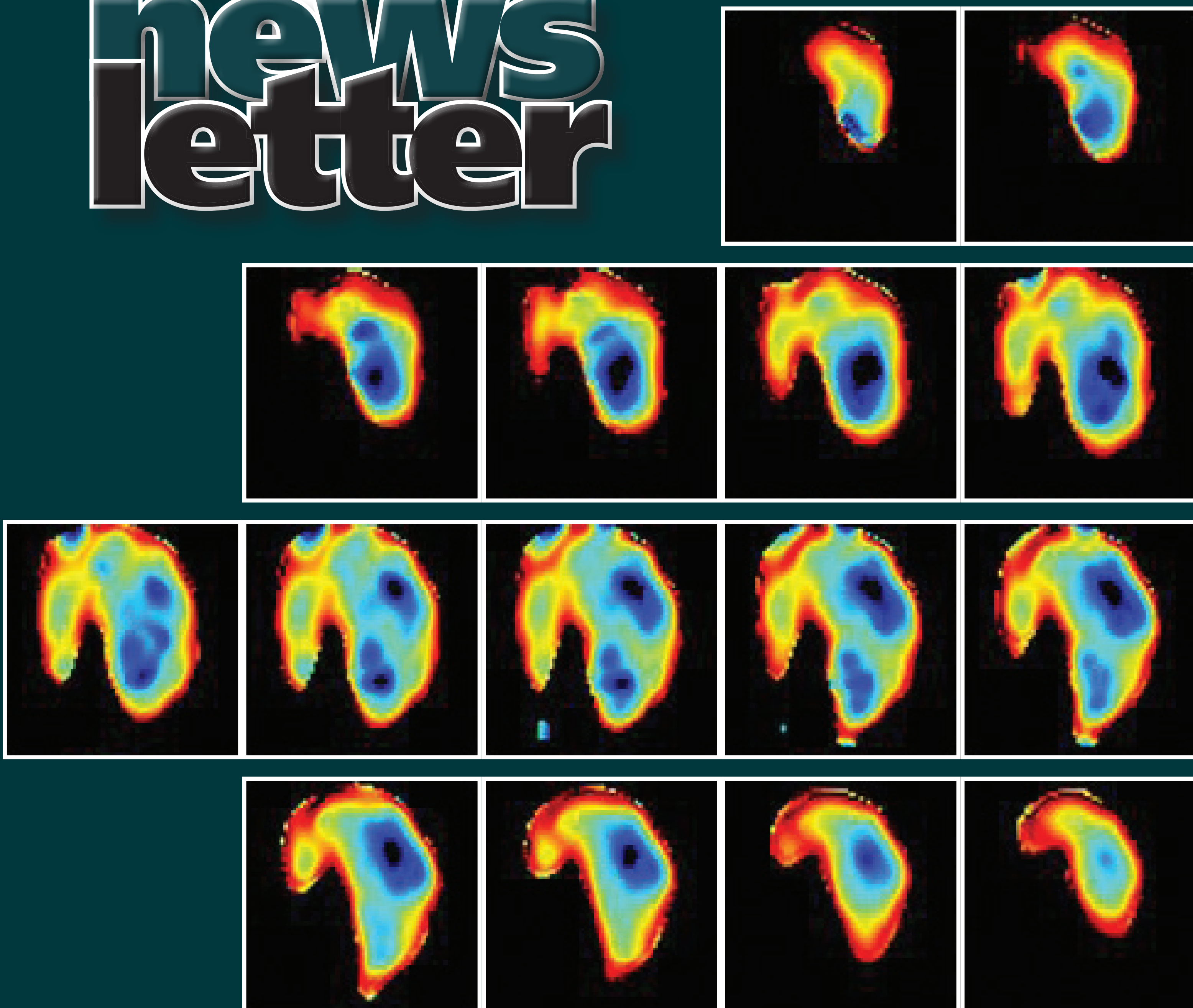
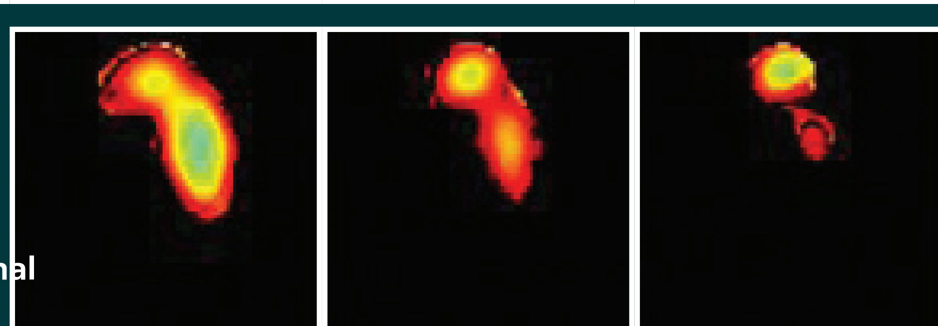
# epr newsletter

2020
volume 30 number 4





The Publication of the International EPR (ESR) Society

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Gareth R. Eaton
Sandra S. Eaton
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George Fraenkel (1921–2009)
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Samuel I. Weissman (1912–2007)
David Whiffen (1922–2002)
Hans C. Wolf


**epr newsletter**

https://ieprs.org/newsletterpage/

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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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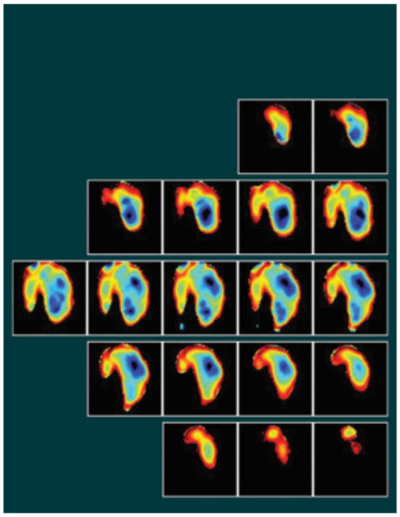
TECHNION | PRINTING UNIT



**The cover picture illustrates** aspects of research carried out by Sankaran Subramanian, Fellow of the IES, recipient of the IES Silver Medal (Instrumentation) 2000. It shows relaxation-weighted *in vivo* FT-EPR Oxygen images (1 mm sagittal slices) of normal (left) and SCC tumor-bearing (right) legs of a C3H mouse infused with the trityl radical (Oxo63) using 3D single point imaging with phase-encoding in all 3 dimensions. The hypoxic regions are deep blue in colour. See also his article “My love for Magnetic Resonance” (*EPR newsletter*, 30/3, 11–17).

# epr newsletter

The Publication of the International EPR (ESR) Society

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# Editorial

Dear colleagues,

Frankly, I could not remember any other year than 2020 that I have been so eager to say farewell to. It was a very unusual year. It showed us only too well that life is fragile and unpredictable. This leap year 2020 cut off our personal contacts, put masks on us and made us practice social distancing. However, the corona virus has failed to stop the internet which has given us an almost limitless transfer of thought over distances.

You must have already received an email message from Thomas Prisner with his Letter of the President and his drawing (p. 3) but this letter is really worth rereading and should be kept in print for the coming generations of magnetic resonance researchers to know what we felt and how we lived and survived in the covid pandemic. The report of the IES Annual General meeting 2020 (pp. 4–6) shows that in the final year of Thomas Prisner's team as IES officers the IES not only survived, but the activities of the IES were as vibrant and diverse as in the pre-pandemic era. Presumably all of us contributed to the next executive board by actively voting and the forthcoming issue 31/1 of the *EPR newsletter* will introduce the IES team for the years 2021–2023.

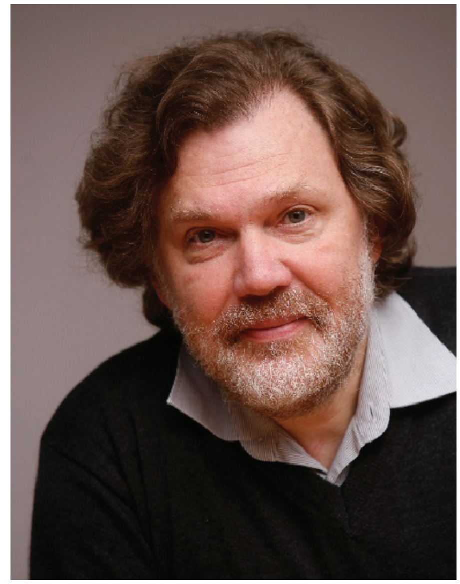
2020 was a challenge for the *EPR newsletter* as well and it was such a delight that we did it! You had already enjoyed previous issues of 2020, 30/1-2 and 30/3, and all in full color! Some hints to the current issue: as usual, Wolfgang Lubitz invited an outstanding scientist, Pavel Baranov, to his Guest of the Issue column, and Pavel told us an exciting story about optically detected magnetic resonance in semiconductors (pp. 7–9). All are welcome to congratulate David Collison, Eric McInnes, Fei Kong and Jason Sidabras on their awards (pp. 12–15) and Elka Georgieva on her new EPR Faculty position (p. 20)! Once again Kalina Ranguelova and Ralph Weber, who were stimulated by Peter Höfer, breathed life into the Tips and Techniques column with their report about the analysis of polymers using EPR (pp. 16, 17). It is a special pleasure to attract your attention to the special issue of *Applied Magnetic Resonance* on the occasion of the 85th anniversary of Yakov Lebedev, a famous scientist who had a major impact in the field of magnetic resonance (p. 18).

Last but not least: I just cannot resist quoting Eric McInnes' message to the young generation of magnetic resonance researchers (pp. 12, 13) "This has been a very difficult time for young researchers, particular through the long period of being unable to work in the lab, and the surrounding uncertainty. However, we will come through it eventually and there will always be opportunities for talented young people in magnetic resonance: it is so central to so many areas of physical and biological science. I'd also emphasise that, more than ever, we are stronger as a community if we support each other. Community initiatives such as the IES virtual seminar series, organised by Nino Wili in Zurich, give me faith in the future and tell you everything you need to know about the talent coming through." Well said, Eric! I couldn't agree with you more!

A very big thank you to all contributors to the *EPR newsletter*! Meet you in 2021!

Laila Mosina

# Letter of the President



What a strange year it has been! When I visited Beijing in January (fortunately still unaware of the break-out of the Coronavirus), I did of course not know that this would be the only journey outside Germany this year. All conferences, workshops and schools were cancelled or shifted to next year. Holiday reservations were useless due to flight cancellations. Restrictions, lock-downs, home-office, shops and cultural events closed almost everywhere in the world. We could see that science (virology and epidemiology in this case) was suddenly a headline in the media. But we also saw that it is still en vogue to ignore facts (not only in the case of the Coronavirus pandemic) and to deny scientific evidence. Something that would not have been possible in Germany 30 years ago! I think that we as scientists have to fight more actively against this bad habit of 'alternative facts'. It was also frustrating to see how much the pandemic uncovered selfish behavior; on an individual and national level. While Italy (and shortly later Spain and France) was extremely hit by the pandemic, countries in Europe closed their internal borders.

Fortunately, also the opposite was and is happening (at least after the first shock). This summer I was happily surprised to notice the beautiful blue sky above Frankfurt, usually criss-crossed by condensation trails of many airplanes heading to or leaving Frankfurt. That indeed reminded me of how it used to be half a century ago in Germany. Of course, we as scientists are privileged in the sense that we can work from home easily (at least for some time) and the laboratories were after all the safest places to be this year. Fortunately, many online seminars and lectures stepped into the vacuum of cancelled conferences and meetings. It is of course convenient to listen to a scientific talk from home without traveling, but many of us realized that this alternative cannot fully replace real conferences. As a speaker, I want to see the reaction of the audience and as a listener, I like the opportunity to casually talk to the speaker sometime later in a coffee break or at a joint evening dinner. And, of course, you don't get distracted so easily. On the other hand, scientists who hardly ever came to conferences can now attend these online meetings, and it is easier to gather a group of scientists for discussions and work meetings if you can do it online.

I hope very much that next year we will have the opportunity to meet in person again at conferences and workshops, but I also believe that this pandemic year will change our traditional habits of scientific communication. I think that especially for young scientists (at a master, PhD or Postdoc level) this year has been very difficult. At this early stage it is very motivating and important to attend workshops, schools and conferences. To present the first (unpublished) results on a poster and discuss them with experienced older scientists and to get connected with other young scientists working on similar topics is such an important part of a scientific path. I hope very much that the people who have missed out on these opportunities this year will get their chance to present their research again in the upcoming year! It was good to see that some online events have already been created which allowed people to present their work – for example, the PhD students organized EPR online meetings (first initiated in Europe by Nino Wili from ETH Zürich and now also with an Asia version) or the two day online EUROMAR meeting organized by Óscar Millet. And it was impressive to see that the traditional Kazan EPR conference indeed took place partly in-person this autumn. IES was very happy to support these initiatives with prizes for young scientists. I am also very happy that Songi Han, as American Vice President of IES and Aharon Blank, as the IES secretary, initiated an IES Twitter page, which serves as fast up-to-date information and news exchange for the whole EPR community.

The end of this year marks also the end of my time as president of the society. There were so many things I wanted to do but was unable to – but I am very thankful that I had such a supportive and active executive board, which helped so much to get things done! Many thanks to the former president Hitoshi Ohta and to the three Vice presidents, Hiroshi Hirata, Gunnar Jeschke and Song-I Han, for their very active participation, for many helpful suggestions, advices and comments. Special thanks go of course to Laila Mosina; without her, the flagship of IES – the EPR Newsletter – would not be what it is now! Thanks to Peter Qin, for taking over the responsibility as treasurer for the society, and of course, last but not least, to the secretary of IES Aharon Blank, who takes care of everything from webpage design and maintenances, to printing and shipping of the Newsletter, membership fees, announcements, deadlines, and much more. Many thanks to all of them! The next important step for all of us will be to elect the new executive board for the years 2021-2023. I would very much appreciate if you all would contribute to the next executive board with active voting. There are many things to be done to keep our EPR/ESR society active and attractive. An active vote of all of us will be a strong support and encouragement for the new board to serve our society the upcoming years.

Finally, I wish all of you healthy and peaceful holidays and a very good start of the New Year 2021. I hope very much to see many of you again in person at some occasion!

Best regards,
Thomas

# IES ANNUAL GENERAL MEETING 2020

Minutes of the Annual General Meeting of the International EPR/ESR Society for 2020 held online on November 4 and 5, 2020 (Held via Zoom). Two AGMs recording can be found in: https://youtu.be/ExuXaIhrfpo and https://youtu.be/9hE2wj8w39A.

**Agenda:**

1. Introduction (Thomas Prisner)
2. Presentation of the IES Fellowship to Daniella Goldfarb (Thomas Prisner)
3. Presentation of the IES Gold Medal to Jörg Wrachtrup (Thomas Prisner)
4. Report of IES activities 2019-2020 (Thomas Prisner)
5. Secretary's Report (Aharon Blank)
6. Treasurer's Financial Report 2018-2019 (Peter Qin)
7. EPR newsletter Editor's Report (Laila Mosina)
8. Discussion and Voting on Amending IES Bylaws (Aharon Blank)
9. Call for Nominations of New Executive (2021-2023) (Thomas Prisner)
10. Planned IES Activities in 2021 (Thomas Prisner)
11. Discussion and Suggestions (Thomas Prisner)

**1. Introduction (Thomas Prisner)**

Dear Colleagues,

On behalf of the IES Executive Board I wish to welcome all participants of the online IES Annual General Meeting 2020.

I first want to introduce IES executives (2018–2020)

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

**2. Presentation of the IES Fellowship**
to Daniella Goldfarb (Thomas Prisner)
Award lecture by Daniella Goldfarb

**3. Presentation of the IES Gold Medal**
to Jörg Wrachtrup (Thomas Prisner)
Award lecture by Jörg Wrachtrup

**4. Report of IES activities 2019–2020**
(Thomas Prisner)

Short Report of the previous Annual General Meeting at the XIth Conference of the European Federation of EPR Groups (EFEPR 2019), Bratislava 1–5 September 2019. Participants ~120. Organizer: Michal Zalibera. See *EPR newsletter* 29/4 (2019) pp. 3–5.

**Silver Medals for 2019**

*Silver Medal Biology/Medicine 2019*
Hassane Mchaourab, Vanderbuilt University
*Silver Medal Physics/Materials Sciences 2019*
Robert Bittl, Free University of Berlin

30 years of IES at Rocky Mountain Conference, Denver 2019.

During the Rocky Mountain Conference we had a special session of short presentations of the development in the last 30 years in the fields:

*Physics/Materials Sciences* (Christoph Boehme)
*Biology/Medicine* (Harold Swartz)
*Chemistry & Instrumentation* (Gareth Eaton)
Moderator: (Thomas Prisner)

Special Session dedicated to 30th anniversary of IES at the International Conference (EPR-75), Kazan 2019.

**Poster Prizes 2019**

– Royal Society Meeting Glasgow 2019:
Luis Fabregas Ibanez (ETH Zürich)
Benjamin Tucker (Oxford)
– EFEPR Meeting Bratislava 2019:
Kwinten Maes (Gent)
Tomás Hajdu (Bratislava)

EPR School Denver 2019

First EPR School in US, 17–21 July, Denver. Initiated and co-sponsored by IES and Shared EPR. 40 Students (200 Applications). 4 days with lectures, tutorials and practical courses.

Support of 8th EFEPR School in Brno 2019
Organizer Petr Neugebauer (Brno)
Teaching EPR to young PhD students
Creating young EPR scientists network

**Fellows of IES 2020**

David Britt, UC Davis
Daniella Goldfarb, Weizmann Inst. Rehovot

**Gold Medal 2020**

Jörg Wrachtrup, University Stuttgart

**John Weil Young Investigator Award 2020**

Sabine Richerts, University Freiburg

**Best Paper Award 2019/2020**

Fei Kong, Univ. Science and Technology China: *Kilohertz electron paramagnetic resonance spectroscopy of single nitrogen centers at zero magnetic field*, Science Advances 2020, 6, eaaz8244

Jason W. Sidabras, MPI CEC Muelheim: *Extending electron paramagnetic resonance to nanoliter volume protein single crystals using a self-resonant microhelix*, Science Advances 2019, 6, eaay1394

**Poster Prizes 2020**

EPR Meeting MDMR 2020 Kazan:
George Andreev (Kazan)
Andrey Petrov (Kazan)
2 Poster Prizes at online EUROMAR December 2020

IES Support for Virtual EPR Meeting (IVEM)
https://ieprs.org/on-line-activities
IVEM Organization
Coordinator: Nino Wili, ETH Zurich & International Committee Asia/Pacific Edition:
Hiroki Nagashima, Saitama University
Fei Kong, University of Science and Technology of China
Martyna Judd, Australian National University in Canberra
Julien Langley, Australian National University in Canberra

**5. 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, ads and positions. We are looking for interesting photos, papers, links (see next) – 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.

***Major tasks over the last year:***

1. Launching a new web site
2. Re-negotiating sponsorship agreement with Bruker
3. "Recruiting" volunteers for Bruker Webinars
4. Handling Awards, fellowships and the "Best paper Award" new initiative
5. Updating the IES twitter page (with Songi Han and Thomas Casey)
6. Changing print house and mailing out of the *EPR newsletter* (with Niv Yaakobi)

Presentation of the IES Tweeter page and its features.

Presentation of the web site and its features:
– Conforms with accessibly standards
– Compatible with browsers and smartphones
– Hosted on Technion Servers (Free)
– Includes all the *EPR newsletter* database

New print house and "self" *EPR newsletter* mailing:
– Enables to mail out full color hard copies of the *EPR newsletter*
– Saves on mailing and handling expenses

### 6. Treasurer's Report (Aharon Blank, Peter Qin)

2019 Financial Report ($)

| | |
|---|---|
| **Balance January 1, 2019** | **54,359.85** |
| ***Deposits*:** | |
| Membership | 4,774.97 |
| Sponsor Contributions | 12,402.00 |
| Misc (Transfer from JW Fund for 2018 award paid from main account) | 1,004.99 |
| TOTAL deposits | 18,181.96 |
| ***Expenditures*:** | |
| Internet Commerce & Merchant Services, Banking | 864.63 |
| IES Community Support (Conferences, Training, Poster Awards) | 4,079.39 |
| IES Operation (Web, Printing, Editorial) | 15,902.58 |
| Misc (Registration, Postage, etc.) | 195.60 |
| TOTAL expenditures | 21,042.20 |
| **Balance December 31, 2019** | **51,499.61** |

2020 January-September Financial Report ($)

| | |
|---|---|
| **Balance January 1, 2020** | **51,499.61** |
| ***Deposits*:** | |
| Membership | 2,274.00 |
| Sponsorship | 23,750.00 |
| TOTAL deposits | 26,024.00 |
| ***Expenditures*:** | |
| Financial Service Fees (Merchant, Services, Banking) | 477.59 |
| IES Community Support (Virtual Gp Mtg) | 919.98 |
| IES Operation (Web, Printing, Editorial) | 12,159.73 |
| Misc (Registration) | 10.00 |
| TOTAL expenditures | 13,567.30 |
| **Balance September 30, 2020** | **63,956.31** |

**John Weil Fund**

Established in 2010 in memory of Prof. John Weil by family, friends, and colleagues to support John Weil Young Investigator Award.

| | |
|---|---|
| **Starting Balance ($) on 01/01/2019** | **23,492.94** |
| Interest Income | 137.87 |
| Distributions in 2019 (for 2018 John Weil Young Investigator Award) | 1,004.99 |
| **Ending Balance (as of 12/31/2019)** | **22,625.82** |

No actual YIA expense incurred in 2019.

*We want to thank Peter Qin for his excellent work as Treasurer of the Society.*

### 7. EPR newsletter Editor's Report (Laila Mosina)

Since the previous Annual Meeting of the IES in 2019 in Bratislava (Slovakia), we published single issues 29/3 and 29/4, and a double issue 30/1-2. We hope you had a look at 29/3, 29/4 and 30/1-2 on the newsletter website and got their copies.

Now we finalized 30/3 and work on the forthcoming issue 30/4. 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!

It was a pleasant surprise for you to find color in printed copies of the *EPR newsletter* 30/1-2. This metamorphosis is due to the activities of Aharon Blank on searching means to reduce mailing costs of the newsletter. As a result, he found not only an option to mail copies worldwide from Israel (mailing costs from Israel are lower than those from the States) but also an option to move printing from the States and


print the newsletter in full color at Printing Unit of Technion in Haifa.

2020 opens a new era of the *EPR newsletter* production. The previous transformation occurred in 2003, when we printed 13/1-2, the first issue of our publication with a color hard cover, at LaPlume and Sons Printing. The cover, originally printed in color only on the front and back, is paid for by Bruker. Our printers introduced full color on the entire cover and switched to better paper at no additional cost for the IES.

For seventeen years we enjoyed collaboration with Scott Morton and his highly professional team and now we say a big thank-you to all of them.

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, Sabine Van Doorslaer, and also to Yevhen Polyhach (for the taking care of 29/3 and 29/4), Sergei Akhmin, our Technical Editor, and Scott Morton, LaPlume and Sons Printing (for printing 29/3 and 29/4).

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.*

### 8. Discussion and Voting on Amending IES Bylaws (Aharon Blank)

Currently, IES bylaws include a tri-annually silver medal Award for "Instrumentation"

We are requesting the amendment of this Award to "IES silver medal for instrumentation and methods (including theory and software) developments"

It is also requested that the Award will be given in 2021 instead of 2020 (just for one occasion), and then continue with the usual cycle (2023, etc.).

*The change in the Bylaws is approved by the attendees of the meeting.*

### 9. Call for Nominations of new Executive 2021–2023 (Thomas Prisner)

From IES Board proposed new Executive Officers (2021–2023)

**President** Song-I Han, UC Santa Barbara
**Vice-Presidents**
*Europe* Maxie Roessler, Imperial London
*Americas* Michael Wasielewski, Northwestern Univ.
*Asia-Pacific* Yasuhiro Kobori, Kobe Univ.
**Secretary** Aharon Blank, Technion
**Treasurer** Peter Qin USC
**Immediate Past President**
Thomas Prisner
**Editor EPR newsletter** Laila Mosina, Kazan Physical-Technical Institute

### 10. Planned IES Activities in 2021 (Thomas Prisner)

Silver Medal for Chemistry and Instrumentation/methods
Fellows of IES
John Weil Young Investigator Award
- Nominations by active IES members
- 100–150 word citation
- CV
- Publication List
- pdf of 2 recent publications

EPR Publication Award (for young scientists)
- Self nomination
- First author with support letter from corresponding author/supervisor which explains the contribution of first author

### 11. Discussion and Suggestions (Thomas Prisner)

Create more visibility of the Society
Also for young researchers!
– Invite young scientists (YIA/Poster Prize winners) to the IES Board Meeting – *at real meetings …*
– Create an interactive Communication Platform on our Webpage – Twitter …
– Put links to tutorials, special articles on our new Webpage
– Create a directory of EPR groups
– Host EPR database - first for Dipolar EPR Data

### Thanks

The IES thanks the following Corporate Sponsors for their contributions in 2020:
- Adani Systems, Inc
- Applied Magnetic Resonance (Springer)
- Bruker BioSpin Corp
- GMW Associates
- JEOL RESONANCE, Inc
- L & M EPR Supplies
- Rotunda
- Virginia Diodes, Inc

Special thanks go to the Zavoisky Physical-Technical Institute, Kazan for supporting the Newsletter, and to:
- All paid up members
- Newsletter Editor: Laila Mosina
- Technical Editor: Sergei Akhmin
- Associate Editors: Candice Klug, Hitoshi Ohta, and Sabine Van Doorslaer

**Attendance list** (some names are given below)

Natasha Arellano
Elena Bagryanskaya
Aharon Blank
Pierre Dorlet
Asif Equbal
Akiva Feintuch
Yasmin Ben Ishay
Betty Gaffney
Angeliki Giannoulis
Daniella Goldfarb
Songi Han
Joshua Harbort
Robert Hayes
Stephen Hill
Hiroshi Hirata
Gunnar Jeschke
Müge Kasanmascheff
Olesya Krumkacheva
Andriy Marco
Dane McCamey
Fraser McMillan
Laila Mosina
Toshikazu Nakamura
Petr Neugebauer
Hitoshi Ohta
Thomas Prisner
Mario Ranges
Ashley Redman
Sharon Ruthstein
Peter Qin
Vinicius Santana
Alexander Schnegg
Stefan Stoll
Claudia Tait
Markus Teucher
Francesco Torricella
Nino Wili
Jörg Wrachtrup

# A fantastic scenario for ODMR in semiconductors: from spin ensembles to single spins, from boiling helium to boiling water temperatures


## Pavel G. Baranov

Ioffe Institute, Saint Petersburg, Russia


*"Quantum bits: Better than excellent"*
D. DiVincenzo
Nat. Mater, 2010

Modern technology development demands enhanced power efficiency, miniaturization, and speed but these enhancements have their limits. Dominating technology scenarios developed for the semiconductor industry imply that the number of electrons needed to switch a transistor should fall to just one single electron. Any device with nanoscale features inevitably displays some type of quantum behavior and the main task is to exploit quantum-based ideas, to seek a radical technology, with completely novel quantum components operating alongside existing silicon and optical technologies. Spin is a pure quantum object and spin properties begin to play an important and, in some cases, a decisive role in the operation of nanoscale devices. Quantum science seems to transform 21st century technologies.

Electron paramagnetic resonance (EPR) is a tool to manipulate electron spins in solids. Because of the limited sensitivity of conventional EPR, optically detected and electrically detected EPR is favored to detect small numbers of spins. In both approaches, the spin state information is transferred to a photon or charge state, respectively. In spin-dependent optical emission or photoconductivity, the spin-to-photon or spin-to-charge transfer, respectively, is typically achieved via a spin-dependent recombination process involving paramagnetic states of recombining partners. In optically detected magnetic resonance (ODMR), a microwave-induced repopulation of Zeeman sublevels is detected optically, i.e., there is a giant gain in sensitivity since the energy of an optical quantum is by several orders of magnitude higher than a microwave one. Thus, it becomes possible to detect a very small number of spins down to a single spin! [1, 2].

Until recently, the practical applications of semiconductors involved the use of charge- and spin-carrier ensembles. The capability to efficiently control spin states is the key question of semiconductor spintronics. The unique quantum properties of nitrogen-vacancy (NV) color centers in diamond, which represent a vacancy in the nearest environment of a carbon atom which is replaced by nitrogen [3], have opened a new era in spintronics: it has become possible to manipulate the spin states of a single atomic-size center at room temperature using ODMR. The optical detection of magnetic resonance of a single spin has become possible because of the existence of a unique cycle of optical alignment of the spin sublevel population in the NV center ground state. The prospect of room-temperature quantum information processors now sounds not like science fiction any more. The diamond age of quantum electronics could be just around the corner as has been recently declared by D. D. Awschalom, R. J. Epstein, and R. Hanson, in their article "The Diamond Age of Spintronics", *Scientific American* 297, 84 (2007).

The unique quantum properties of NV center in diamond have motivated efforts to find defects with similar properties in silicon carbide (SiC), which can extend the functionality of such systems [4–8]. "Quantum bits: Better than excellent" is how D. DiVincenzo titled his article [*Nat. Mater*. 2010]: "excellent" is diamond, "better" is SiC. The NV center, is in many ways the ideal qubit, but diamond is neither cheap nor easily processed into new sophisticated devices. There is a Russian proverb "It's not a tsar's business", the diamond-brilliant is too expensive, and not well suited to compete with the existing silicon-based electronics. SiC, which can be regarded as an artificial superlattice, is taking on a new role as a flexible and practical platform for harnessing the new quantum technologies. SiC is a technologically friendly material, used in various devices (LED, MOSFETS, MEMS). A special feature of SiC is the existence of its different polytypes, and for each of the polytypes, the properties of spin color centers are unique; furthermore, even in one polytype, the center may be located in different nonequivalent positions in the lattice. This allows choosing the center with parameters (for instance, optical and microwave ranges) suited for a specific problem. Atomic-scale color centers in bulk and nanocrystalline SiC are considered as a material platform for spintronics, photonics compatible with fiber optics, quantum information processing and sensing at ambient conditions. Their spin state can be initialized, manipulated and read out by means of ODMR, via level anticrossing (LAC) and cross-relaxation (CR) [9–19]. A convincing point with SiC is that, similar to diamond, the stable spinless nuclear isotopes guarantee long dephasing times. Finally, coherent manipulation of spin states has been performed at room temperature and even at temperatures higher than room temperature by hundreds of degrees. It has been shown that there are at least two families of color centers in SiC with $S = 1$ and $S = 3/2$, which have the property of optical alignment of the spin levels and allow a spin manipulation. The spin-1 center is a SiC divacancy of the neighboring positions with covalent molecular bond. The spin-3/2 center is a negatively charged silicon vacancy $V_{Si}^{-}$ in the paramagnetic state, that is noncovalently bonded to the neutral carbon vacancy $V_C^0$ in the non-paramagnetic state, located on the adjacent site along the SiC symmetry c axis. These centers are usually referred to as the corresponding zero-phonon lines (ZFLs). For the $S = 3/2$ family, the ground state and the excited state were demonstrated to have spin $S = 3/2$ and a population inversion in the ground state can be generated using opti-

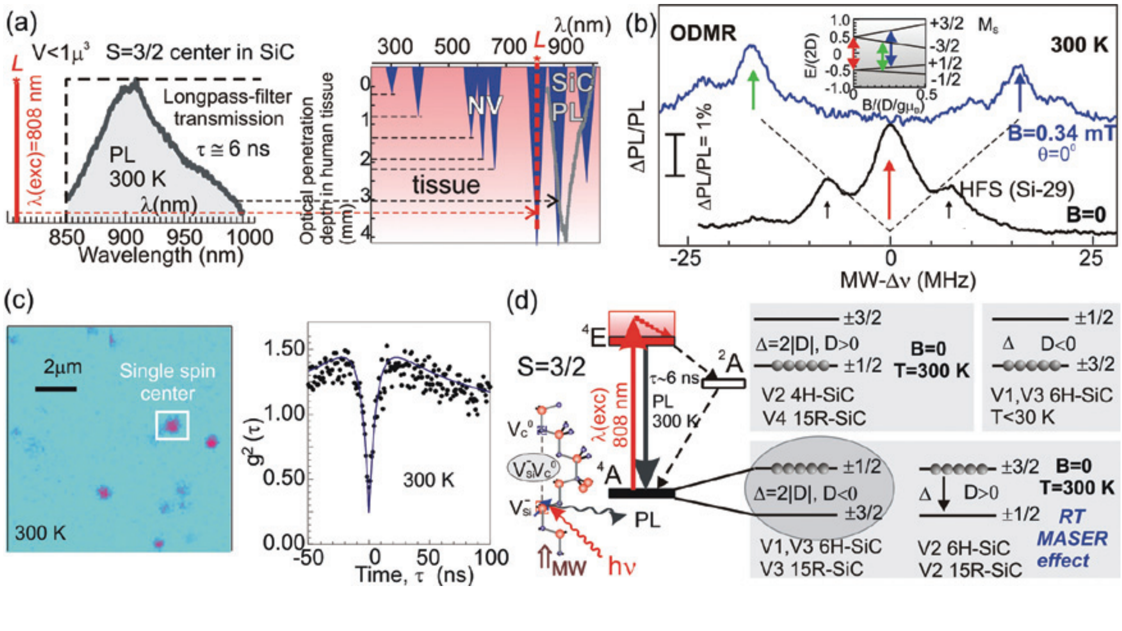



Fig. 1. a) An example of the room temperature photoluminescence (PL) spectra of spin-3/2 centers in SiC (left); the depth of light penetration (in the form of blue peaks) into biological tissues for different wavelengths of light (right). b) A typical ODMR signal of the spin-3/2 centers in SiC in zero and $B$ = 0.34 mT magnetic fields. A hyperfine structure (HFS) with twelve Si atoms of the next nearest-neighbor (NNN) shell is shown. c) Confocal raster scan of single color center photoluminescence (PL) in SiC and a correlation function of the color center. d) The schemes of optically induced alignment of spin level populations for spin-3/2 centers and possible configurations of spin-3/2 center. For more information see ref. [20].

cal pumping, leading to stimulated microwave emission even at room temperature and above.

Spin-1 and spin-3/2 centers in SiC emit in the near-IR, that is, in the vicinity of fiber-optic transparency band. As a result, one could do quantum manipulation at room temperature in the materials which are used for electronics at telecommunications frequencies. Jörg Wrachtrup, who pioneered the manipulation of single-defect spin states in diamond [3], sees potential applications for SiC defects beyond quantum computing [see *Physics Today*, 2011]. “I could envision using tiny silicon carbide crystals to do micro- or nanoscale magnetic resonance imaging on cells and other biological systems. It really could open up a whole new world of scientific applications”.

In line with this statement, Figure 1a shows an example of the room temperature photoluminescence (PL) spectra of spin-3/2 centers in SiC. The right-hand picture shows the depth of light penetration into biological tissues for different wavelengths of light. It can be seen that the spectral range for centres in SiC is more favorable compared to the optical characteristics of NV centres in diamond according to K. Kalka, H. Merk, H. Mukhtar (*J. Am. Acad. Dermatol.* 42, 389, 2000).

Figure 1b presents a typical experimental microwave (MW) dependence of the ODMR signal of the spin-3/2 centers in SiC, $\Delta\nu$ is the zero-field splitting (ZFS). The ODMR signal is detected under laser excitation $\lambda$ = 808 nm in zero and $B$ = 0.34 mT magnetic fields. The vertical bar indicates the ODMR contrast. A hyperfine structure (HFS) due to the interaction with $^{29}$Si nuclei for twelve Si atoms in the next nearest-neighbour (NNN) shell of the Si vacancy is shown by arrows. The inset shows the energy level diagram and corresponding resonance transitions. Figure 1c shows a confocal raster scan of the single-colour center PL at 300 K in 4H-SiC; bright spots indicate V2 emitters (left) and the right hand picture shows the intensity time correlation function of colour center in the square, showing photon antibunching at zero delay, proving that the studied colour center is a single one. The schemes of optically induced alignment of spin level populations in a zero magnetic field at room temperature for spin-3/2 centers (possible configuration is depicted) in different SiC polytypes are shown in Fig. 1d.

Figure 2a, as an example, shows signals of room temperature ODMR and level anti-crossing (LAC) of the V2 spin centers in a 4H-SiC crystal. The signals were recorded by lock-in detection of the change in the PL in the near-IR range with application of a constant magnetic field and an oscillating low-frequency magnetic field. The energy of the corresponding spin levels is shown at the top. The LAC in the absence of the MW field (MW “off”), denoted as LAC1 and LAC2; for LAC1 $B = D$ and for LAC2 $B = 2D$, where ZFS $\Delta = 2|D|$, and two ODMR signals recorded at the MW field on 40 and 45 MHz are shown. The choice of frequencies was due to the fact that when the ODMR signal approaches the LAC1 signal, the ODMR signal increases several times and approaches the LAC1 signal intensity. The ODMR line shift $\Delta B$ at frequencies of 40 and 45 MHz is shown demonstrating the principle of measuring magnetic fields by the ODMR method. The point of the LAC1 weakly depends on the orientation of the crystal in a magnetic field, and therefore it can be used for measuring magnetic fields (and temperatures with LAC1 for excited state) in powder materials. It is assumed that if the ODMR signal coincides with the LAC, polarization of the surrounding silicon $^{29}$Si and $^{13}$C carbon nuclei with long relaxation times is possible through hyperfine interactions. Circles indicate areas of reduction of the signals with a certain polarization of $^{29}$Si, which are present in the signals of the ODMR in the form of satellites. We assume that optical registration of nuclear magnetic resonance on polarized nuclei $^{29}$Si and $^{13}$C of spin centers in SiC will find a number applications (quantum computing, NMR imaging, gyroscopes, etc). In Fig. 2b the PL zero-phonon lines (ZPLs) in 15R-SiC of the corresponding spin-3/2 centers (top) and X-band direct-detected (DD) EPR spectra induced with ZFLs V2, V3 and V4 (bottom) are demonstrated. In Fig. 2c (bottom) optically induced ESE spectra measured in 15R-SiC are shown; the light-induced inverse population of the spin sublevels of V2 centers is depicted in the inset. Figure 2c (top) shows the ENDOR spectra measured for the low field (lf) and high-field (hf) transitions indicated in the ESE spectra [16].

Observed Rabi nutations in SiC persist for about 0.1 ms at RT and there is evidence that the probed spin ensemble can be prepared in a coherent superposition of the spin states. The electron spin of the spin-3/2 centers can be manipulated by a low-energy microwave field of 1–300 MHz which is compatible with NMR imaging. The color centers in SiC are optically active in the near infrared spectral

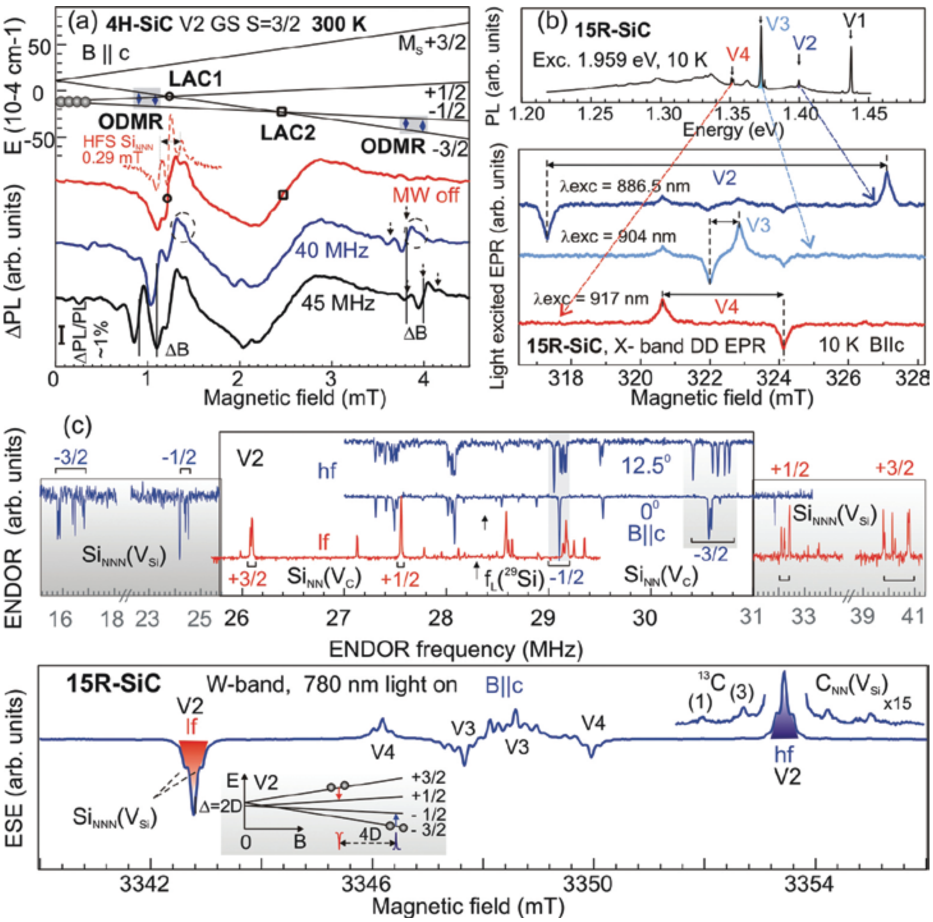



Fig. 2. a) Room-temperature detection of the change in PL of spin-3/2 centers in a 4H-SiC: the level anti-crossing (LAC) signals (MW off) and ODMR. ODMR line shift Δ*B* in a magnetic field for two frequencies demonstrates the principle of measuring magnetic fields. b) (top) The PL ZPLs in 15R-SiC of the corresponding spin-3/2 centers. (bottom) X-band direct-detected (DD) EPR spectra induced with ZFLs V2, V3 and V4. (c) (bottom) Optically induced ESE spectra measured in 15R-SiC. (top) ENDOR spectra measured for the lf and hf transitions indicated in the ESE spectra. For more information see ref. [16].

region, which is preferential for potential in vivo biological applications due to the deepest tissue penetration and which is compatible with fiber optics. The concept of sensing is based on variants of the ODMR technique with sensitivity down to a single-spin [4, 13, 14]. Demonstrated spin properties of the color centers in SiC and related nanostructures open up new avenues for quantum computing, quantum sensing, bio-labeling, for future single-particle and single defect quantum devices and related biomedical sensors. The optically induced population inversion of spin states at RT leads to stimulated microwave emission, which can be used to implement solid-state masers and extraordinarily sensitive radiofrequency amplifiers.

Quantum technologies based on coherent control of the spins of color centers in diamond and silicon carbide have developed fantastically over the past two decades. The combination of supersensitive optical techniques for high-resolution image detection and reliable coherent control using magnetic resonance are key components in the development of the first quantum devices based on these materials. The possibility of highly accurate scaling of color centers and achieving long coherence times opens up new prospects for so-called hybrid quantum processes, in which color centers are associated with different types of qubits. There is no doubt that this area of research will develop rapidly in the near future and, as can be expected, will lead to the emergence of new quantum technologies.

Support by the Russian Science Foundation (RSF) was extremely important in writing the Springer book "Magnetic Resonance of Semiconductors and Their Nanostructures: Basic and Advanced Applications" [4]. We would like to thank K. M. Salikhov and L. V. Mosina for the offer to write this book. It became possible to carry out a number of works on spin centers in SiC with financial support from the RSF, Project No. 20-12-00216.

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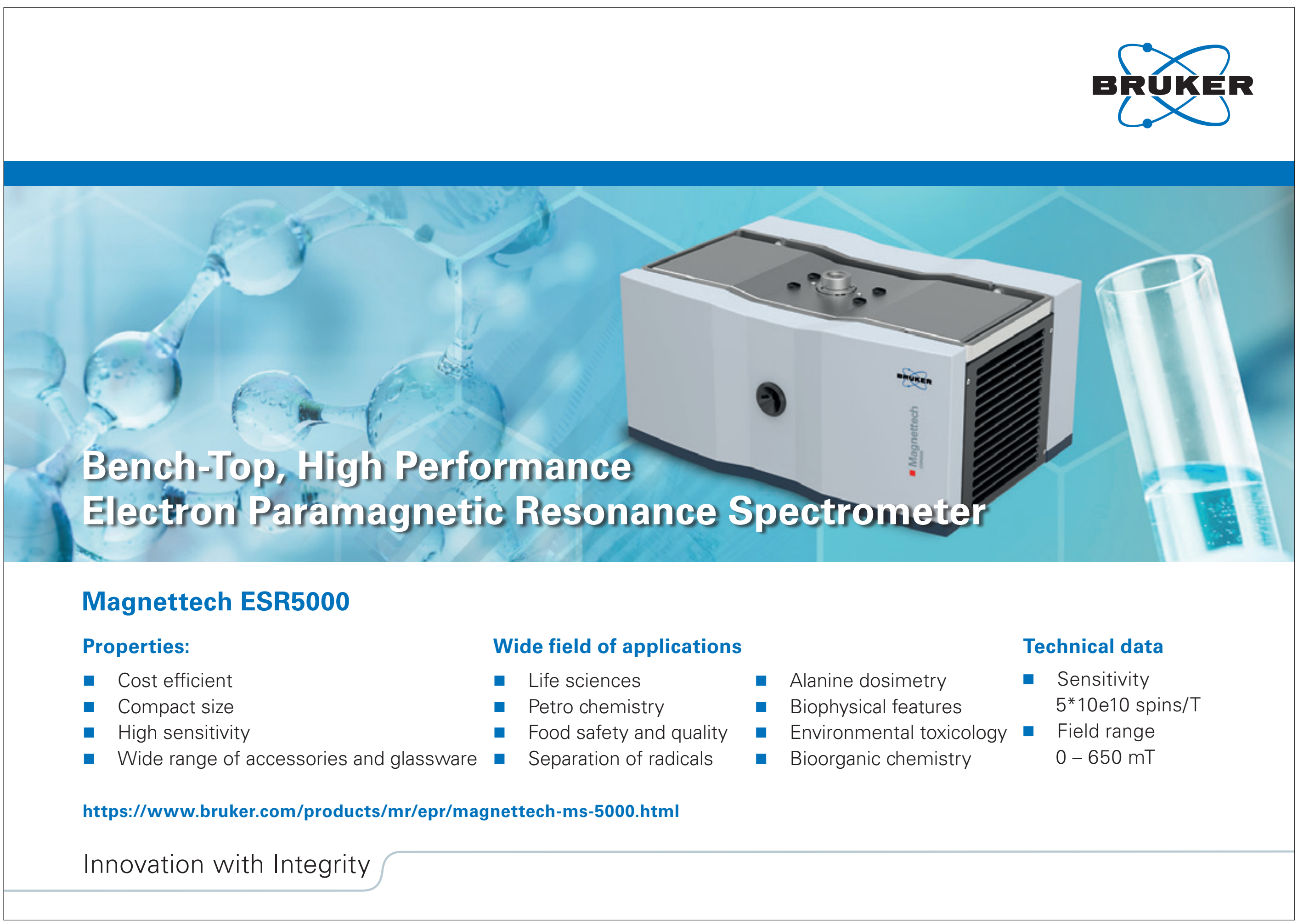
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Innovation with Integrity

# Bruker Prize 2020 winner: David Collison

Since 1986 Bruker BioSpin has generously sponsored an annual lectureship and prize, given to a scientist who has made a major contribution to the application of EPR/ESR spectroscopy in chemical or biological systems. Last year, the ESR Spectroscopy Group of the Royal Society of Chemistry were delighted to announce that the recipient of the Bruker Prize 2020 was Prof. David Collison of The University of Manchester. The nominations emphasised David's seminal contributions to experimental and theoretical fundamentals of transition metal EPR, from bioinorganic chemistry to molecular materials, including his authoritative textbook.[1] Some aspects of David's work over the years were highlighted in a recent article in this newsletter celebrating his 65th birthday.[2] Crucially, the nominations also stressed his important and selfless work in developing, supporting and nurturing the EPR community throughout his career. As co-founder and director of the successful EPSRC UK National EPR Facility, he has fostered collaboration not only between EPR spectroscopists, but also between the EPR and wider science communities. This has had significant impact in widening the application base and popularising applications of EPR across the scientific spectrum. David was due to deliver his 2020 Bruker lecture, entitled "The attraction of unpaired electrons", at the 53rd Annual International Meeting of the RSC ESR Group in March/April of 2020. Unfortunately, this conference had to be cancelled due to the Covid19 pandemic. Instead, David will be invited to present his lecture and formally receive the prize, at a future meeting.

The list of previous Bruker Prize winners is available at the group website.[3]


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3. http://www.esr-group.org/bruker-lectures/


# Interview with Professor Eric McInnes on the Occasion of His Tilden Prize 2019

**EPR newsletter:** *Dear Professor McInnes, on behalf of the readers of the EPR newsletter we congratulate you on your Tilden Prize 2019. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I enjoyed science at high school, and that fed through to studying chemistry at university. I didn't have any grand plan at that stage, I just followed what interested me.

*In your success story on the occasion of your IES Silver Medal for Chemistry2015 (EPR newsletter, 25/3-4, pp. 7, 8) you described your way in magnetic resonance from the first steps to becoming co-Director of the EPSRC-funded National EPR Facility for EPR at Manchester. What projects are under way and how do you meet the challenges of the coronavirus outbreak?*

The Covid19 situation has been enormously difficult for everyone, and I hope all our EPR friends and colleagues across the world are keeping safe and well. The University of Manchester shut down in March and it wasn't until July that we were able to partially reopen the labs. At present we are still working under social distancing rules which restrict us to four people in the EPR labs at any time, so we are operating on a rota with weekly shifts between defined teams. It has been a real team effort to make this work, and I am grateful to everyone in the EPR group for the way they've pulled together. I am particularly indebted to my colleague Adam Brookfield, our technician, who has been immense in getting everything back up-and-running and making the lab work in a safe and sensible manner. Of course, there have also been an awful lot of Zoom meetings...

As I write this a second national lockdown has started, although universities remain open.

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

I don't have a favourite project - they are all my favourites! At the moment we have significant efforts in areas ranging from molecular magnetism and supramolecular chemistry, to f-element chemistry, to porous materials. I'm very lucky to have many colleagues in Manchester who have interesting problems involving paramagnets, and I have always hugely enjoyed that collaborative aspect of science.

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

This has been a very difficult time for young researchers, particularly through the long period of being unable to work in the lab, and the surrounding uncertainty. However, we will come through it eventually and there will always be opportunities for talented young people in magnetic resonance: it is so central to so many areas of physical and biological science. I'd also emphasise that, more than ever, we are stronger as a community if we support each other. Community initiatives such as the IES virtual seminar series, organised by Nino Wili in Zurich, give me faith in the future and tell you everything you need to know about the talent coming through.

# The IES Best Paper Award 2019/2020

## Fei Kong:

I am honoured to have received the IES Best Paper Prize 2020 for the Science Advances publication titled "Kilohertz electron paramagnetic resonance spectroscopy of single nitrogen centers at zero magnetic field" [1]. This research was part of my postdoctoral research focusing on microscale EPR with quantum sensors, jointly supervised by Professor Jiangfeng Du and Professor Fazhan Shi at University of Science and Technology of China (USTC). I would like to acknowledge the China Postdoctoral Science Foundation, the National Natural Science Foundation of China, and the National Key Research and Development Program of China, which funded this research.

The aim of this project is developing a methodology to improve both the spatial and spectral resolution of EPR. The conventional induction-based EPR spectrometer requires millions to billions of spins to obtain detectable signal, and thus has limited spatial resolution. Recently, the sensitivity has been promoted to single-spin level by using quantum sensors, such as nitrogen- vacancy (NV) centers in diamond [2, 3]. However, the current megahertz spectral resolution is still underwhelming.

The spectral resolution is mainly limited by the line broadening. In a previous work, we have shown that the line broadening of powder spectra can be completely removed by zero-field EPR [4]. More importantly, the NV center does not lose sensitivity at zero magnetic field. In this work, we address the magnetic noise-induced line broadening by utilizing a special transition at zero field that is naturally immune to noise. Actually, this kind of transition exists in many EPR species, such as some radicals, $Cu^{2+}$, $VO^{2+}$, $Nd^{3+}$, etc. [5, 6] All these species have a spin-half electron spin with hyperfine coupling with a spin half-integer nuclear spin. At zero field, there exists a group of zero-quantum states which have zero first-order dependence on magnetic field, and thus the transition between them is insensitive to the magnetic noise.

To observe this line narrowing phenomenon, we also need to remove the line broadening contributed by the sensor itself, for instance, the short coherence time of the NV centers. Inspired by the correlation detection in NMR detections [7], we develop a similar pulse sequence that is compatible with zero-field EPR detection, and then the spectral resolution is limited to the sensor's lifetime, which is usually much longer than the coherence time. To demonstrate our method, we detect a single substitutional nitrogen center in diamond, which has an electron spin with coupling to a $^{15}N$ nuclear spin, by a nearby NV centers. The linewidth of the observed spectra is as narrow as 8.6 kHz, which is a 27-fold improvement compared with the ordinary spectrum.

This method will benefit many EPR studies. For example, the hyperfine constants can be measured with substantially improved precision, which can reflect more detailed local microenvironment information. In addition, our method is also applicable to measure the dipolar-dipolar coupling between dual spin targets, which offers interesting avenues for enhanced accuracy and detection range in distance measurement.

Our method is demonstrated on internal spin in diamond, while practical applications require target spins external to the diamond surface, where more challenges emerge. For example, the diffusion of external spin will also contribute to line broadening; the ubiquitous dangling bonds on the diamond surface will induce a strong magnetic noise that may exceed the noise-insensitive range; the detected spins may be bleached during the time-consuming measurement. My further research is to address these issues, and continuously pushing this technique to practical applications.

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### Fazhan Shi:

Fei Kong completed his PhD in Physics from University of Science and Technology of China (USTC) in 2018, and now is an outstanding postdoc at USTC.

As his PhD co-supervisor together with Professor Jiangfeng Du, I have worked with Fei for over eight years on a project of using NV center to develop high spatial and spectral resolution EPR technique, which is the subject of the paper for which he was awarded this prize. He is dedicated to science, highly intelligent, and works extremely hard. Less than one year after entering my group, he was responsible for building a microscopic magnetic resonance spectrometer, which has been running well so far, and has completed many excellent experimental work on this platform. During his PhD, he completed a series of scientific researches in quantum control and EPR spectroscopy [Phys. Rev. Lett. 115, 080501 (2015); Phys. Rev. Lett. 117, 060503 (2016); Nat. Commun. 9, 1563 (2018); Nat. Methods 15, 697 (2018)], and therefore won a series of honors and awards, such as the "Postdoctoral Innovative Talent Support Program", the "Outstanding Doctoral Thesis of the Chinese Academy of Sciences", and the "President's Award of the Chinese Academy of Sciences".

After the completion of his PhD, he continued the research in EPR spectroscopy as a postdoc in my group, and demonstrated some exciting applications in high-precision metrology [Sci. Adv. 6, eaaz8244 (2020); Phys. Rev. Lett. 124, 247701 (2020)]. Based on these works, he is dedicated to developing quantum sensing technology into a powerful EPR tool.

Overall, Fei has a solid foundation, a clear vision of the field he focused in, and the ability to open new research areas. He can independently conduct high-level research projects, and becoming a successful researcher. I wish him all the best for the next stage of his career.

# The IES Best Paper Award 2019/2020

### Jason W. Sidabras:

I am honored to have been awarded the 2019/2020 IES Best Paper Award for my work entitled "Extending electron paramagnetic resonance to nanoliter volume protein single crystals using a self-resonant microhelix", published in Science Advances [1]. This research was part of my PhD at the Max Planck Institute for Chemical Energy Conversion and Technical University Dortmund, under Profs. Wolfgang Lubitz and Dieter Suter. The ideas presented in this paper are one outcome from the successful submission and completion of an EU Horizon 2020 Marie Skłodowska-Curie Fellowship.

The major goal of this work was to study the orientation and magnitude of the g-tensor and hyperfine interaction tensors for the EPR active catalytic states of [FeFe]-hydrogenase in the same manner that [NiFe]-hydrogenase was studied [2, 3]. The orientations and magnitudes of the magnetic interactions of an enzyme are only available when single-crystal EPR is performed. However, unlike the [NiFe]-hydrogenase where crystal volumes are on the order of 1 µl, the [FeFe]-hydrogenase crystals volumes are less than 30 nl. The challenge was then to significantly enhance the absolute sensitivity to study crystals of limited volumes.

At X-band, this challenge was met by the design and fabrication of a micro-helix with an internal diameter of 0.4 mm, height of 1.2 mm, and 6.5 turns. Electromagnetic simulations guided the design and EPR experiment comparisons with standard samples showed that the micro-helix out-performs commercial resonators by a factor of 6 for continuous-wave experiments. With the increase in absolute sensitivity, a protein single-crystal of the [FeFe]-hydrogenase from *Clostridium pasteurianum* (CP1) with a sample volume of 3 nl (dimensions 0.3×0.1×0.1 $mm^3$) was able to be studied in the stable $H_{ox}$ state. Using pulse EPR, each signal was acquired in only 8 minutes and the resonator was rotated 180 degrees in order to record the orientationally dependent g-tensor. The whole set of rotational data was globally fit using EasySpin and a g-tensor (orientation and magnitude) was proposed. This work has gotten some traction outside of the EPR community with featured articles in the Royal Society of Chemistry magazine ChemistryWorld [4] and the basic science news aggregator Phys.org [5].

The micro-helix geometry boasts a large bandwidth (90 MHz) and high microwave magnetic field incident on the sample (3.2 $mT/W^{1/2}$) which allows advanced pulse EPR experiments to be performed with little incident microwave power. Therefore, hyperfine spectroscopy experiments, such as ESEEM and HYSCORE, can be performed without costly high-power amplifiers. This was demonstrated by collecting the angle dependent hyperfine interaction of the $^{14}N$ in the distal cyanide- and ADT-ligand to the distal iron using less than 2 W of power. Preliminary experimental data can be found in my PhD thesis [6]. However, the hyperfine fit and further analysis will be published in an upcoming manuscript.

I am very thankful to my collaborators that made this work possible. From the Prof. Happe group in Ruhr University Bochum, Drs. Jifu Duan and Martin Winkler grew the superb CP1 crystals. While Dr. Rana Hussein from Prof. Athina Zouni's group at Humboldt-University Berlin, grew PSII crystals which served as a standard to compare experimental methodologies using the micro-helix. Dr. Alexander Schnegg provided countless discussions and support during my tenure at the Max Planck Institute, which lead to this completed manuscript. I would like to give a special thanks to Dr. Edward Reijerse, who was integral in helping me with the interpretation of the data and the many conversations we have had about hydrogenases. Finally, I would like to thank Prof. Dieter Suter for his mentorship and patience throughout my doctorate and Prof. Wolfgang Lubitz for inviting me out to Germany to lead this fascinating and rewarding research.

Since completing my PhD, I have been hired as an assistant professor at the Medical College of Wisconsin's Department of Biophysics. I hope to continue my research with single-crystal EPR by increasing the sensitivity of the instrumentation and expanding the types of enzymes studied. It is my overall objective to study the structure and function of enzymes using advanced magnetic resonance techniques. This paper serves as a cornerstone to that research.


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## Wolfgang Lubitz:

In fall 2015 Jason Sidabras contacted me and asked for the possibility of a position in the EPR laboratory of our Max Planck Institute; he also expressed interest in doing his PhD in Germany. After obtaining his B.S. and M.S. in Electrical Engineering Jason had worked for many years very successfully in the laboratory of James Hyde at the Medical College of Wisconsin in Milwaukee, where he was involved in the development of many new microwave resonance structures for various EPR, MRI and related applications. After a discussion with the head of our EPR laboratory, Edward Reijerse, and consultation with Jim Hyde we offered Jason a position as a research engineer at the MPI in Mülheim. In March 2016 Jason and his wife Emily arrived in Germany; they got settled quickly in the new environment. Jason applied for a prestigious *EU Horizon 2020 Marie Skłodowska-Curie Actions Fellowship*. His excellent proposal was granted and formed the basis for his PhD work (2017–2019). This was supervised by Prof. Dieter Suter (Department of Physics, Technical University of Dortmund) and by myself (Biophysical Chemistry, Max Planck Institute for Chemical Energy Conversion).

Jason directly worked with Ed Reijerse in the excellent environment of the institute – and designed, constructed and tested several structures for microwave resonators for a wide frequency range for investigations of specific samples, e.g. thin films, surfaces or small volumes (single crystals, valuable materials). Next to many other remarkable results described in his thesis the most outstanding scientific work of Jason Sidabras was the successful design of a small self-resonant microhelix (i.d. 0.4 mm) for X-band frequencies by which, for samples of limited size, the absolute sensitivity could be greatly increased as compared to commercial cavity resonators. This offered the possibility to perform experiments on tiny samples of a few nanoliters, thus opening new vistas for EPR spectroscopy. The very large efficiency factor of the micro-helix also led to very low (external) power requirements and a smaller deadtime for pulse EPR experiments. The advantages of the microhelix design were nicely demonstrated by studying small single crystals of [FeFe] hydrogenase, an important enzyme in the field of energy research that reversibly converts protons to molecular hydrogen with very high efficiency. For the first time Jason could determine magnitude *and* orientation of the g tensor of a paramagnetic state in the enzyme's catalytic cycle and show that also hyperfine tensor information is accessible via pulse EPR experiments (ESEEM, HYSCORE). The approach can be easily used also for other small single crystals of paramagnetic macromolecules and is thus of general value for obtaining magnetic interaction tensors of such systems that are not available otherwise due to lack of sufficiently large single crystals. The results were published in *Science Advances* last year, for which he received the *Best Paper Award of the International ESR/EPR Society (IES) 2019/2020*. The work was also described in the media, e.g. by the Royal Society of Chemistry in the magazine *Chemistry World* (Nov. 2019). Furthermore, Jason presented his results on a large number of international conferences and symposia. His publication list is with over 30 papers very impressive.

Early in 2020 Jason defended his thesis at the TU Dortmund with very good results. Soon after his defense Jason was offered a position as Assistant Professor at the Biophysics Department of the Medical College of Wisconsin in Milwaukee. However, he could leave Germany only in November 2020 due to the COVID-19 pandemic. He stayed in our institute as postdoc for several months to work with Alexander Schnegg who is now responsible for the EPR laboratory after my retirement. During their time in Mülheim Jason and his wife Emily got two children, Juniper and Felix. I hope that they will look back with pleasant feelings at their stay in Germany where Jason finally got his doctoral degree in physics and founded a family. For all of us it was a pleasure to have him in the laboratory.

# Effectively Analyzing Polymers Using EPR Spectroscopy

Kalina Ranguelova and Ralph Weber
Bruker Biospin Corp., Billerica, USA

Free radicals in polymers are produced during synthesis, polymerization, photoinitiation, cross-linking, auto-oxidation, degradation, interaction with catalysts, stabilizers, fillers, etc. One of the most important developments in polymer science in the last 25 years is controlled radical polymerization. Another reason why radicals are so important is because most polymers, synthetic or biopolymers, undergo photo- and/or thermo-oxidative degradation. The mechanism of radical auto-oxidation in polymers established about 70 years ago is an autocatalytic radical chain process consisting of initiation, propagation, chain branching and termination reactions. It begins with the formation of initiating radicals when the polymer is exposed to elevated temperature, light, transition metal impurities (catalyst residues) or to high shear stress occurring during compounding and extrusion of polymers.

There are other industrially important polymer technologies and applications that are based on radical processes. Thus, millions of tons of unsaturated polyester resins, are cured (cross-linked) with radical initiators, predominantly peroxides. Drying of alkyd resins also proceeds via the radical mechanism – drying oils and alkyds are amongst the earliest types of thermoset coatings. They cross-link and solidify by reaction with atmospheric oxygen to produce hydroperoxides, which decompose to form O-centered radicals. Cross-linking occurs by radical combination reactions, resulting either in peroxide-, or carbon-carbon bonds. Photopolymerization of coatings, printing inks, adhesives, and microelectronic components is a multibillion dollar business and rapidly growing. Grafting is another example where modification of polymers by grafting of polar monomers is presented here.

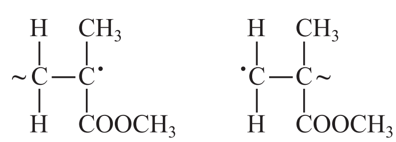
Gamma-irradiation and other sterilization methods can cause formation of long living radicals causing not only polymer degradation but alteration of the physico-chemical properties of the sterilized polymer and they may be a toxicological hazard. It is possible to investigate all these phenomena by using Electron Paramagnetic Resonance (EPR) spectroscopy. EPR spectroscopy is a non-invasive and non-destructive magnetic resonance technique for detection of paramagnetic species – free radicals, biradicals, triplet-state systems, transition metal ions, and point defects. The ubiquity of these paramagnetic species makes EPR an indispensable tool in polymer science among other mainstream analytical techniques. In this article, a few examples of effectively analyzing polymers using EPR are discussed.

## I. Polymer photodegradation

Degradation of polymers due to light exposure leads to discoloration and a decrease in the mechanical properties (elasticity, toughness, etc.). For example, polymethyl methacrylate (PMMA), also known as acrylic or acrylic glass, is a transparent and rigid thermoplastic material widely used as a shatterproof replacement for glass. It has many technical advantages, a few of them include excellent light transmission and high resistance to UV light and weathering. PMMA degrades due to light exposure forming two radical species (R1 and R2) identified by EPR (Figure 1). The figure in the middle shows a small amount of radicals prior to UV irradiation (the spectrum in black) and after exposure the red trace indicates the level of degradation in PMMA. To prevent this decomposition, hindered amine light stabilizers (HALS) are added to the polymer. When the polymer is exposed to UV-irradiation HALS suppresses radical damage in the polymer by forming a HALS-based nitroxyl radical. EPR detects the HALS radicals and by monitoring and quantifying the EPR signal, the effectiveness of HALS can be evaluated. This EPR application is successfully used to determine polymer photodegradation in both academic and industrial settings for research and quality control [1].

## II. Detecting defects in polymers

EPR spectroscopy has been successfully applied in studies of photodegradation reactions in material science with respect to products such as solar cells, fuel cells, batteries, etc. As a result, paramagnetic imperfections such as defects, vacancies, and free radicals affect the performance and properties of these materials. Therefore, it is crucial and mandatory to detect and characterize those species and with the EPR method one can gain insight into the stability 'soft spots' of the materials which is important for developing robust products. For example, Susarova et al. used EPR as a highly sensitive analytical technique for quality assessment of conjugated polymers and their performance in organic solar cells [2]. It has been shown that different batches of the same polymer reveal different photovoltaic performances correlating with the respective free radical concentrations. EPR data show that this is related to structural defects or impurities possessing unpaired electrons (Figure 2). These free radicals are believed to behave as deep traps for mobile charge carriers thus affecting the performance of the conjugated polymers in solar cells.




(R1) (R2)

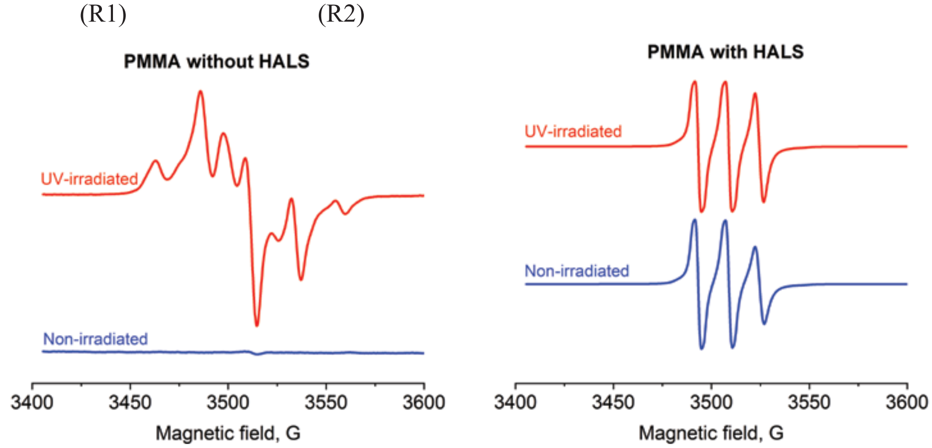
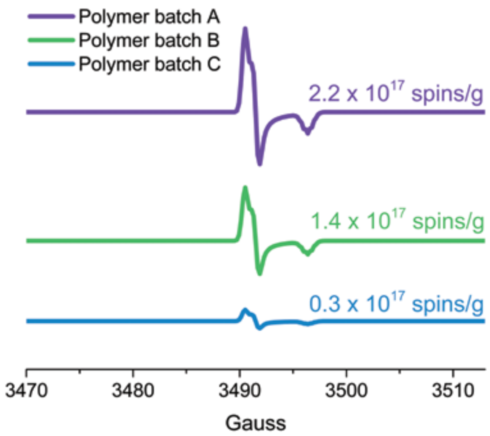



**Figure 1.** EPR signals generated in PMMA during UV-irradiation (left panel) is completely suppressed after addition of the HALS stabilizer where only the HALS EPR spectrum is observed (right panel).




| Polymer batch | Spin density Spins/g | Power Conversion Efficiency, % | Half Lifetime, hrs |
|---|---|---|---|
| A | 2.2e17 | 4.5 | 30 |
| B | 1.4e17 | 6.2 | 50 |
| C | 0.3e17 | 7.1 | 150 |

**Figure 2.** Quantitative EPR analysis of free radical defects presented as spins/g in conjugated polymers (used in solar cells). The number of defects correlates with the solar cell efficiency and stability (adopted from Ref. [2]).

pact the formation of humic substances and carbon sequestration. Free radicals in MPs can be detected with EPR, which can help in the development of measures to control their distribution and to aid in clean-up strategies.

Biodegradable polymers can be used to solve waste and plastic pollution environmental concerns. For example, the biodegradable biopolyester family is considered as an attractive alternative to the family of conventional petroleum-based polymers. Over two recent decades, temporal (dynamic) and spatial (structural) heterogeneity of biopolymers has been coherently investigated by EPR using nitroxide spin probes that are paramagnetic. Recent EPR studies showed the use of TEMPO as a spin probe loaded in homopolymers and nanofibers. From the rotation mobility of TEMPO-radicals the heterogeneity and crystallinity of biodegradable polymers was studied [5].

EPR is an excellent research method to analyze polymers because EPR spectroscopy can observe radicals under different experimental conditions such as chemical reactions, temperature variation and irradiation. In this article, we have reviewed some important EPR applications used in polymer science. The use of EPR for analysis of polymer degradation and other radical polymerization reactions is growing rapidly. The high sensitivity and versatility of EPR makes this technique a valuable tool in polymer research and further applications are expected to emerge in the future.

### III. Polymer sterilization

When it comes to polymer sterilization, gamma- and x-ray irradiation processes can effectively treat a wide variety of products of different materials, with varying densities, configurations and orientations. Some examples of products processed include packaging materials, medical devices, surgical products, cosmetics, etc. Gamma-rays and x-rays ionize insulators and polymers, resulting in radical reactions that are unique to irradiation. Some of the effects of ionizing radiation in polyolefins are: radical polymerization reactions (homolytic cleavage, dissociation), degradation, oxidation of polymers, graft copolymerization, cross-linking.

Radicals formed during sterilization of polymers cause degradation of the sterilized polymer and EPR can determine stability of the polymer after sterilization, characterize free radicals, identify their source and provide easy ‘go/no go’ decisions based on quantitative analysis for quality control and assurance.

For example, ultra-high molecular weight polyethylene (UHMWPE) is a semi-crystalline polymer that has been used for over four decades as a bearing surface in total joint replacements. It has been shown that UHMWPE is susceptible to oxidative free radical degradation following gamma radiation sterilization with subsequent loss of mechanical properties (wear-resistance). While contemporary UHMWPE sterilization methods have been developed to reduce or eliminate the free radical degradation, post irradiation thermal treatment of the polymer is required to ensure the oxidative stability of joint implants in the long term. EPR studies [3] from Harvard Medical School showed that: (i) annealing below the polymer melting point preserves the mechanical properties but the residual free radicals trapped in the crystalline regions are not eliminated, leading to oxidation in the long-term and (ii) annealing above the melting point (150°C) eliminates the free radicals but leads to a decrease in mechanical properties through loss of crystallinity during the melting process (Figure 3).

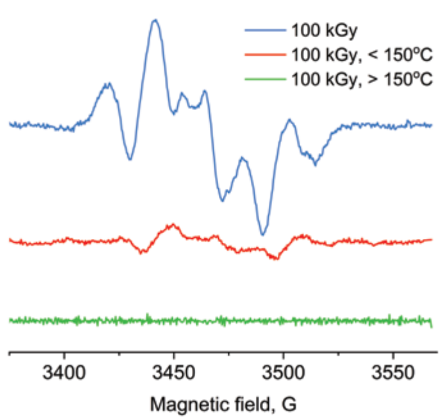



**Figure 3.** EPR spectra of 100 kGy irradiated, unmelted UHMWPE (blue trace), pressure treated (red trace), and melted at 150°C at ambient pressure (green trace) (adopted from Ref. [3]).

### IV. Polymers and the environment

In the past decades, more and more plastic debris are produced and accumulated in the natural environment. They gradually become fragile and subsequently break down into small pieces due to chemical-, microbial-, or photo-aging. Plastic fragments with particle sizes less than 5 mm, defined as microplastics (MPs), are causing emerging concerns due to their adverse environmental impacts, especially in the ocean. When MPs are exposed to sunlight, a large amount of environmentally persistent free radicals (EPFRs) and reactive oxygen species (ROS) might be formed on the surface of MPs. Microplastics are easily ingested by organisms, including fish, invertebrates, and humans [4]. EPFRs play a role in the further generation of toxic compounds and are additionally involved in radical processes that impact the formation of humic substances and carbon sequestration.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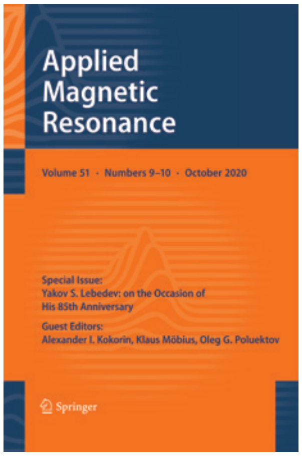


**Applied Magnetic Resonance 51/9-10 (2020)**
https://link.springer.com/journal/723/volumes-and-issues/51-9
**Yakov S. Lebedev:**
**on the Occasion of His 85th Anniversary**
**Co-Guest Editors:** Alexander Kokorin, Klaus Möbius, Oleg Poluektov

The Special Issue of *Applied Magnetic Resonance* in memory of late Prof. Yakov Lebedev has been published in autumn, 2020, on the occasion of his 85th birthday, thereby honouring an outstanding scientist who had a major impact in the field of magnetic resonance. The Special Issue contains 25 papers written by Prof. Lebedev's former collaborators as well as by scientists from all over the world who appreciate his scientific accomplishments and human personality. The papers describe applications and methodological developments in physical chemistry where Yakov Lebedev has left many distinctive footsteps. Over the years, Prof. Lebedev was mentor of numerous graduate students and postdocs, many of whom are still working as scientists at universities, industry and research institutions.

Prof. Lebedev focused most of his work in two main directions: elementary chemical processes in the condensed phase and new EPR methodology. Collaborating and interacting with him has always been a privilege, allowing for enjoyable discussions on issues of science, society and humanities.

Prof. Lebedev will be remembered for his excellent contributions to the field of EPR spectroscopy during his academic career as a scholar of great merit, efficient science manager, supervisor of numerous young researchers, and a highly respected human being.

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## International Conference "Modern Development of Magnetic Resonance" (MDMR2020)
### September 28 – October 2, 2020, Kazan, Russia

The annual International Conference "Modern Development of Magnetic Resonance" was held from September 28 to October 2, 2020 in Kazan. The conference was organized by the Kazan Zavoisky Physical-Technical Institute of the Federal Research Center "Kazan Scientific Center of the Russian Academy of Sciences" and the Kazan Federal University under the auspices of the AMPERE Society. The conference also included the ceremony of the International Zavoisky Award 2020 and the Workshop "Diamond-Based Quantum Systems for Sensing and Quantum Information". All events were organized in a mixed format: actual participation of scientists from Russia and online participation of scientists of other countries.

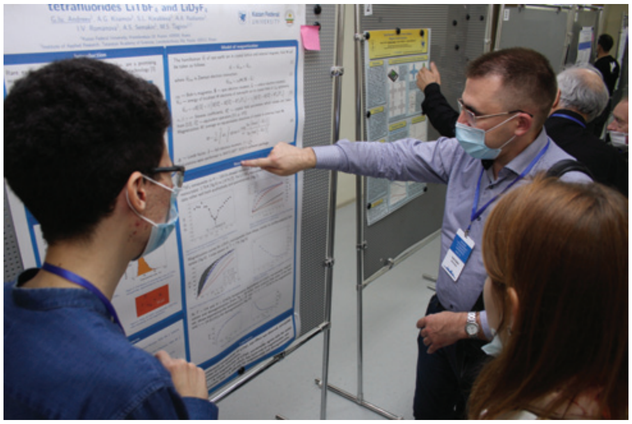
The conference topics were extremely diverse and included reports in the following fields:
– Chemical and Biological Systems
– Low-Dimensional, Nanosized and Strongly Correlated Electronic Systems
– Magnetic Resonance Instrumentation
– Electron Spin-Based Methods for Electronic and Spatial Structure Determination in Physics, Chemistry and Biology
– Modern Methods of Magnetic Resonance
– Molecular Magnets and Liquid Crystals
– Other Applications of Magnetic Resonance and Related Phenomena

The participants of the conference were leading scientists and experts in the field of magnetic resonance from Australia, China, Germany, Italy, Japan, Moldova, Russia, Scotland, Sweden, and USA. The total number of participants was 178, who presented 130 reports (12 plenary lectures, 62 oral talks, and 64 posters). The program of the conference and abstracts can be found at http://www.kfti.knc.ru/mdmr/2020/MDMR.2020.program.pdf and http://www.kfti.knc.ru/mdmr/2020/MDMR.2020.abstract.pdf, respectively.

From left to right: Kev Salikhov demonstrates the Zavoisky Award medal, and Alexey Kalachev holds the Zavoisky Award 2020 Diploma.

The opening ceremony and the first scientific session of the conference took place on September 28, 2020 and were chaired by Alexey Kalachev, Deputy Director of the Federal Research Center. Kev Salikhov, Chairman of the International Zavoisky Award Selection Committee, announced the name of the Zavoisky Awardee 2020: Professor Klaus-Peter Dinse (Free University of Berlin, Berlin, Germany). He was distinguished for his contributions to EPR spectroscopy of organic supramolecular systems and novel catalytic complexes. Leila Fazleeva, Deputy Prime Minister of the Republic of Tatarstan, and Oleg Sinyashin, Director of the Federal Research Center, congratulated heartily Klaus-Peter Dinse on his highly deserved award. Klaus-Peter Dinse also received congratulations from Thomas Prisner, IES President, Bernhard Blümich, President of the AMPERE Society, Robert Tycko, ISMAR President, and Christian Caron, Executive Publishing Editor, Springer-Verlag.

The first plenary session included the following plenary lectures: *From High Power to*



At the poster session.

From left to right: Kev Salikhov, and IES Student Poster Awardees at MDMR2020: George Andreev and Andrey Petrov.

*Low Power – Recipes for a Successful Scientific Life!* by Klaus-Peter Dinse, *DNP Enhanced Solid-State NMR Spectroscopy of Functional Materials* by Gerd Buntkowsky (Technical University Darmstadt, Darmstadt, Germany) and *New Paradigm of Spin Exchange* by Kev Salikhov (Zavoisky Physical-Technical Institute, Kazan, Russia).

A number of topical fundamental problems were discussed at the conference. These include: search for the element base of quantum computing and quantum informatics; synthesis and study of the properties of new materials with specified functional properties; problems of magnetism in solids; a new paradigm of spin exchange in dilute solutions of paramagnetic particles and its manifestation in EPR spectroscopy; etc.

New possibilities of NMR were featured in invited talks *Picoliter NMR Spectroscopy with Diamond NV Centers* by Victor Acosta (University of New Mexico, USA) and *Optically Hyperpolarized Nanodiamonds: Applications in Accelerated NMR and Sensing* by Ashok Ajoy (UC Berkeley, Berkeley, USA), which were presented at the Workshop "Diamond-Based Quantum Systems for Sensing and Quantum Information".

Two IES Student Poster Awards were granted at the MDMR2020. The IES Student Poster Award Selection Committee consisted of Kev Salikhov (Chairman) and members: Roman Babunts (Ioffe Physical-Technical Institute, St. Petersburg), Elena Bagryanskaya (Novosibirsk Institute of Organic Chemistry, Novosibirsk), Murat Tagirov (Kazan Federal University, Kazan) and Valery Tarasov (Zavoisky Physical-Technical Institute, Kazan). George Andreev and Andrey Petrov (both Kazan Federal University, Kazan) were chosen as the awardees.

The conference favored the exchange of ideas and recent achievements and its participants received a good impetus for their further research, which was especially important in the pandemic we all live through.

The organizers of the conference are sincerely grateful to the Government of the Republic of Tatarstan, Federal Research Center "Kazan Scientific Center of the Russian Academy of Sciences", and the Russian Foundation for Basic Research for the financial support.

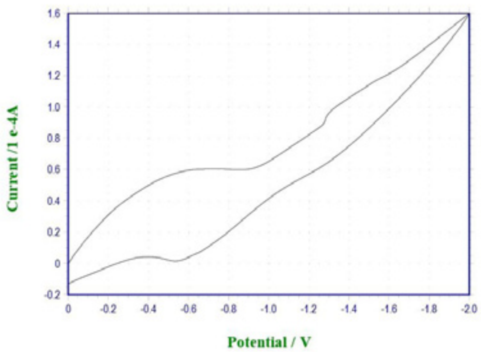
Kev Salikhov
Chairman of the Organizing Committee
MDMR2020
Violeta Voronkova
Scientific Secretary MDMR2020

## new EPR Faculty

### Elka Georgieva

Elka Georgieva became an Assistant Professor of Biochemistry in the Department of Chemistry and Biochemistry at Texas Tech University (USA) in September 2020. Dr. Georgieva received her MSc in Chemistry and Physics from Sofia University (Bulgaria) in 1998 and earned her PhD in 2005 in Chemistry from the Institute of Catalysis at the Bulgarian Academy of Sciences (Bulgaria) with Professor Nicola Yordanov. During her graduate career, she studied high-energy generated radicals in saccharides using EPR spectroscopy approaches. She then worked as a Visiting Postdoctoral Scientist in the Department of Biochemistry and Biophysics at Stockholm University (Sweden) with Professor Astrid Gräslund. In 2007, Dr. Georgieva became a postdoctoral fellow in the research group of Professor Jack Freed at the Center for Advanced ESR Technology in the Department of Chemistry and Chemical Biology at Cornell University (USA). In this position, Dr. Georgieva expanded her previous knowledge and experience in CW EPR spectroscopy and gained new knowledge in the state-of-the-art pulse EPR spectroscopy and its applications to protein structure and function. Thereafter, at Cornell University, she was promoted to Research Associate and Senior Research Associate. During her last two years at Cornell University, Elka Georgieva was working on an independent research program to study the structure and function of membrane proteins from human pathogens. She was the PI of an NIH R03 grant to study membrane transporters from *Mycobacterium tuberculosis*. As a faculty member and independent researcher at Texas Tech University, she will continue her studies on viral and bacterial proteins, and will also pursue new directions targeting human proteins linked to cancer. Dr. Georgieva will use EPR spectroscopy (CW and pulse) as one of the major techniques to tackle unsolved scientific problems related to protein systems with high biomedical relevance.

**Electrochemistry with EPR spectrometer:** Identify species and explore mechanisms in redox reactions




**Reduction of Benzoquinone**
**Top,** cyclical voltammetry curve.
**Bottom,** EPR spectrum at -2 V of the resultant benzosemiquinone radical anion.

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