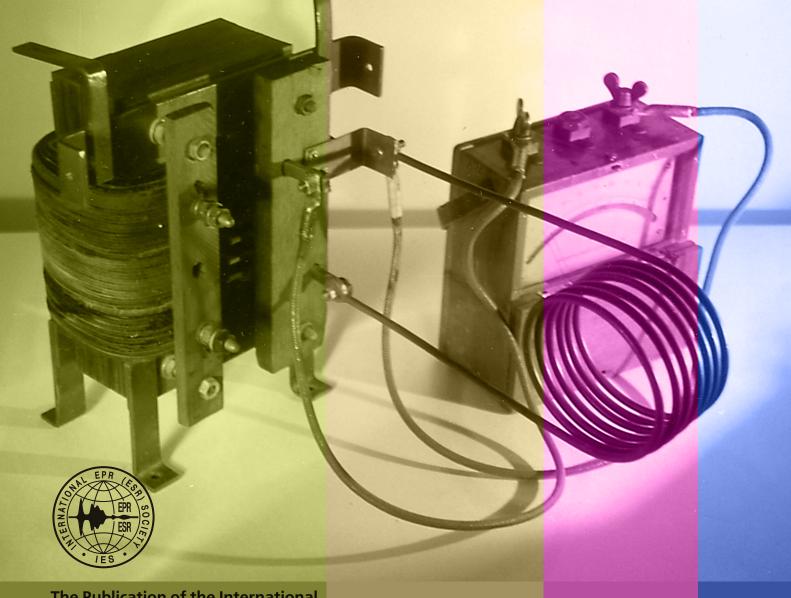
2014 volume 24 number 3





The Publication of the International EPR (ESR) Society



### Officers of the International EPR (ESR) Society

#### ACTING PRESIDENTS

Hitoshi Ohta October 1, 2012 until June 30, 2013 Lawrence Berliner July 1, 2013 until March 31, 2014 Klaus Möbius April 1, 2014 until December 31, 2014 Past President Late Seigo Yamauchi January – September 2012

#### VICE PRESIDENTS Americas

Lawrence Berliner Department of Chemistry and Biochemistry, University of Denver, 2090 E. Iliff Ave, Denver, CO, OR 80208 USA phone: 303-871-7476, fax: 303-871-2254 e-mail: berliner@du.edu web: www.du.edu/chemistry/Faculty/Iberliner.html

#### Asia-Pacific

Hitoshi Ohta Molecular Photoscience Research Center, Kobe University, 1-1 Rokkodai, Nada, Kobe 657-8501, Japan phone: +81-78-803-5646, fax: +81-78-803-5770 e-mail: hohta@kobe-u.ac.jp

#### Europe

Klaus Möbius Department of Physics, Free University Berlin, Arnimallee 14, Berlin 14195, Germany phone: 49-30-838-52770 e-mail: moebius@physik.fu-berlin.de

### Fellows of the International EPR (ESR) Society

Anatole Abragam (1914–2011) John Michael Baker Brebis Bleaney (1915–2006) James R. Bolton Harvey A. Buckmaster Anders Ehrenberg Gareth R. Eaton Sandra S. Eaton George Feher George Fraenkel Erwin Hahn Karl Hausser (1919-2001) Noboru Hirota Wayne Hubbell Clyde A. Hutchison, Jr. (1913-2005) James S. Hyde Lowell Kispert Daniel Kivelson (1929–2003) Melvin P. Klein (1921–2000) Harry Kurreck August H. Maki (1930-2008) Harden McConnell (1927-2014) Bruce R. McGarvey

#### SECRETARY

until August 31, 2014 Sushil K. Misra Concordia University, 1455 de Maisonneuve Boulevard West, Montreal (Quebec), H3G 1M8, Canada phone: 514-848-2424 ext. 3278, fax: 514-848-2828 e-mail: skmisra@alcor.concordia.ca

from October 1, 2014 Aharon Blank Technion – Israel Institute of Technology, Haifa 32000, Israel, phone: +972-4-829-3679, fax: +972-4-829-5948 e-mail: ab359@tx.technion.ac.il

#### TREASURER

Tatyana I. Smirnova North Carolina State University, Department of Chemistry, Campus Box 8204, Raleigh, NC 27695-8204, USA phone: (919) 513-4375, fax: (919) 513-7353 e-mail: tatyana\_smirnova@ncsu.edu

#### IMMEDIATE PAST PRESIDENT

Jack H. Freed Department of Chemistry and Chemical Biology, Director of ACERT, B52 Baker Laboratory, Cornell University, Ithaca, NY 14853, USA phone: 607-255-3647, fax: 607-255-0595 e-mail: jhf3@cornell.edu

#### FOUNDER PRESIDENT

Harold M. Swartz Dartmouth Medical School, Department of Radiology & EPR Center, 7785 Vail Room 702, Hanover, NH 03755-3863, USA phone: 1-603-650-1955, fax: 1-603-650-1717 e-mail: harold.swartz@dartmouth.edu

Keith A. McLauchlan Klaus Möbius Yuriy N. Molin James R. Norris John R. Pilbrow Charles P. Poole, Jr. Aleksandr M. Prokhorov (1916-2002) Kev M. Salikhov Tengiz I. Sanadze (1930-2011) Arthur Schweiger (1946-2006) Charles P. Slichter Leslie H. Sutcliffe Harold M. Swartz Martyn C. R. Symons (1925-2002) Wolfgang E. Trommer Yuri D. Tsvetkov Joan H. van der Waals George D. Watkins John A. Weil (1929-2010) Samuel I. Weissman (1912-2007) David Whiffen (1922-2002) Hans C. Wolf



#### www.epr-newsletter.ethz.ch

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

#### EDITOR

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

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

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

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

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

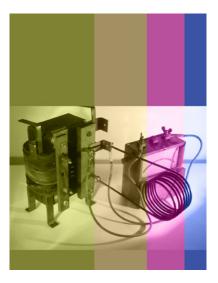
Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

The *EPR newsletter* is published quarterly by the International EPR (ESR) Society and is available in electronic and printed form to all members of the Society. The deadlines for submission of news for upcoming issues: Spring March, 15; Summer June, 15; Fall September, 15; Winter December, 15.

ISSN 1094-5571



**PRINTING:** LaPlume and Sons Printing, Inc. One Farley Street, Lawrence MA 01843 USA phone: (978) 683-1009, fax: (978) 683-4594



The cover picture shows the welding transformer with solenoid and ammeter, a component of the E. K. Zavoisky experimental setup of 1944, when he discovered the phenomenon of electron paramagnetic resonance (see also Igor I. Silkin "The Discovery of Electron Paramagnetic Resonance by E. K. Zavoisky", *EPR newsletter*, 14/4, pp. 12, 13 (2005)).







The Publication of the International EPR (ESR) Society

## volume 24 number 3 2014

#### 2 Editorial

by Laila Mosina

- 3 Bruker ESR Thesis Prize, Bruker Award 2014 to J. Wrachtrup, JEOL Prize 2014 to D. Klose, and Voevodsky Prize 2014 to K. M. Salikhov
- 4 Interview with Jörg Wrachtrup on the Occasion of His Bruker Award 2014
- 5 Interview with Periannan Kuppusamy on the Occasion of His Piette Award 2014
- 6 IES Poster Award to Agnieszka Adamska-Venkatesh

#### 7 History of ESR Research in Japan: Physics by Hitoshi Ohta

EPR newsletter anecdotes

**Present meets future** 

In memoriam

Awards

- **10 Double Interview with Jennifer Mathies and Edgar Groenen** *edited by Sabine Van Doorslaer*
- 12 Haim Levanon (1938–2014) by Gerd Kothe, Alexander Berg and Aharon Blank
- John Stewart Waugh (1929–2014)
   by Robert G. Griffin
- 16 Harden M. McConnell (1927–2014) by Larry Berliner

20

- 47th Royal Society of Chemistry International EPR Meeting
- by Graham Smith
  21 EUROMAR 2014
  by Gunnar Jeschke
- 24 International Symposium on Catalytic Systems for Energy Conversion by Edward Reijerse
- 23, 27Notices of meetings27Market place

## Editorial

#### Dear colleagues,

I wonder if the cover picture of this issue looks familiar to you. You may have started to remember when and where you saw this piece of equipment. For sure, those who visited the Zavoisky Museum at the Kazan Federal University or read the article by Igor I. Silkin, curator of the Zavoisky Museum, "The Discovery of Electron Paramagnetic Resonance by E. K. Zavoisky" in the EPR newsletter, 14/4, pp. 12, 13 (2005) must have immediately recognized the welding transformer with solenoid and ammeter as a component of the Zavoisky experimental setup. Yes, it was on January 21, 1944 that E. K Zavoisky observed an EPR signal for the first time. A wonderful touch of varying colors adds the magic of the New Year atmosphere to this picture.

2014 marked the 70th anniversary of the discovery of EPR and in the forthcoming issue of the *EPR newsletter* 24/4 (2015) you will find a report about the relevant conference "Magnetic resonance: fundamental research and pioneering applications" (MR-70) in Kazan. This was also the meeting point for four IES Presidents, Larry Berliner, Hitoshi Ohta,

Klaus Möbius, and Wolfgang Lubitz. They kindly shared with the *EPR newsletter* their ideas about the future development of EPR so please look forward to the forthcoming issue.

The future of EPR is the young generation of the EPR researchers and the new "Present Meets Future" column edited by Sabine Van Doorslaer features Jennifer Mathies and Edgar Groenen confronting the views and experiences of an early stage researcher in EPR with those of her mentor (pp. 10, 11). Interviews of Jõrg Wrachtrup (p. 4) and Periannan Kuppusamy (p. 5), and the IES Poster Award report by Agnieszka Adamska-Venkatesh (p. 6) also make interesting counterpoints.

We never forget about our roots (see, e.g., recent 24/1-2, pp. 18, 19; 21/1, pp. 8-12, etc.). The article, "History of ESR Research in Japan: Physics" by Hitoshi Ohta, in the "EPR newsletter Anecdotes" and edited by John Pilbrow (pp. 7–9) gives a comprehensive account about the origin of the success of the Japanese EPR researchers.

To make your mouth water, I also open to you some details about the future issues of the *EPR newsletter*. In the forthcoming issues you will find the report of the IES Annual General Meeting 2014 (Nara, Japan) with the success stories of Stephen Hill and

S

 $\mathbf{R}_{\mathbf{S}}$ 

EPR | ENDOR | NMR etc.

**Research Specialties** 

1030 S. Main St, Cedar Grove, WI 53013

920-668-9905 Phone / Fax

James R. Anderson

E-mail: Janderson36@wi.rr.com

Specializing in Scientific Instrumentation Design | Manufacture | Upgrades | Repair

Varian / Bruker - accessories - parts - service

Hans van Tol, Tomoaki Miura, and Nicholas Cox, IES Awardees. Also the reports about the research performed by Jackie Esquiaqui, Noah Horwitz, Alex Marchanka, and Zhelin Yu, recent IES Poster Awardees. Sabine Van Doorslaer will continue her "Present Meets Future" column featuring Heinz-Jürgen Steinhoff and his PhD student Daniel Klose. Daniel will also tell about his JEOL Prize research. The "Guest of the Issue" column, edited by Wolfgang Lubitz, will host Howard Halpern with his exciting story about oxygen imaging with pulse spin lattice relaxation EPR. The concepts of effective spin and fictitious angular momentum will be considered by Sushil K. Misra and Czeslaw Z. Rudowicz in the "Tips and Techniques" column edited by Keith Earle. And many more to go!

Happy New Year to all of you and your dear ones! On behalf of my colleagues from the Editorial Board of the *EPR newsletter*, Candice Klug, Hitoshi Ohta, Sabine Van Doorslaer and Sergei Akhmin, I wish you, our dear readers, all the best! You are always welcome with your opinions and ideas to make our publication even more attractive and instructive!

**Since 1978** 

Laila Mosina







The Bruker Prize of the Royal Society of Chemistry for 2014 was awarded to Prof. Jörg Wrachtrup, University of Stuttgart at the 47th Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry in Dundee. The picture shows (from left to right): Prof. Jörg Wrachtrup, Dr. Graham Smith (University of St. Andrews) and Peter Höfer (Bruker BioSpin GmbH).



JEOL Prize winner Daniel Klose (University of Osnabrück) with Peter Meadows (JEOL UK; centre) and Graham Smith (left).





#### Bruker ESR Thesis Prize

The ESR Group of the Royal Society of Chemistry and Bruker Corporation are pleased to announce the inaugural Bruker ESR Thesis Prize – a 5,000 euro award and a prize lecture at the ESR Group Meeting in April 2015, set up to recognize outstanding work by PhD students in the field of ESR Spectroscopy. Further information is here:

http://www.esr-group.org/ conferences/2014-conferencesouthampton/bruker-prizes/

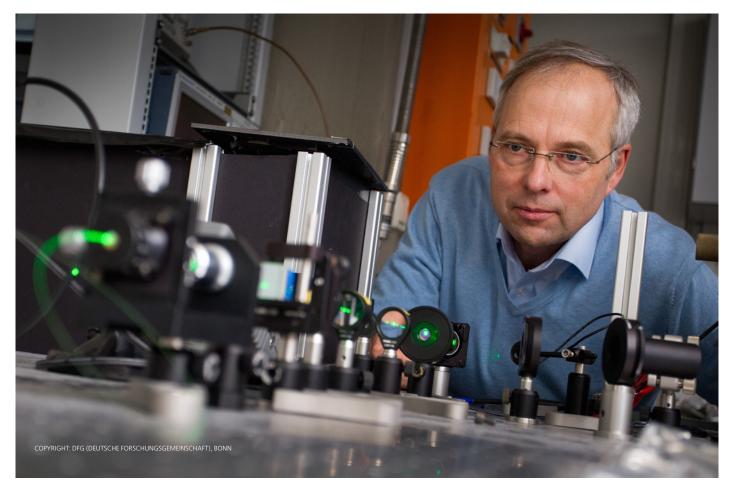
#### The rules of the competition are:

1 To be eligible for the Bruker ESR Thesis Prize, the thesis viva voce examination must have taken place within 730 days of the deadline.

Applications should be submitted by the thesis author and must include a one-page summary, as well as letters of support from the thesis supervisor and one of the external examiners.

Submissions will be shortlisted by the RSC ESR Group Committee. Each of the shortlisted works will be sent to an expert reviewer, appointed by the Committee, for comments on quality, importance and impact. The Committee will then collate reviewer comments and make an award decision.

The Voevodsky Prize 2014 was awarded to full member of the Russian Academy of Sciences Kev M. Salikhov, Zavoisky Physical-Technical Institute, Kazan for his outstanding contribution to the development of the theoretical fundamentals of spin chemistry and chemical radiospectroscopy. The Voevodsky Award 2014 was presented by Renad Z. Sagdeev, Chairman of the Selection Committee, full member of the Russian Academy of Sciences, at the III School for young scientists "Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics" in Novosibirsk. The picture shows (from left to right): Kev M. Salikhov and Prof. Viktor Bagryansky (Institute of Chemical Kinetics and Combustion, Novosibirsk).



## Interview with Jörg Wrachtrup on the Occasion of His Bruker Award 2014

**EPR newsletter:** Dear Professor Wrachtrup, on behalf of the readers of the EPR newsletter we congratulate you on your Bruker Award 2014. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?

I started studying physics at the Free University in Berlin in 1983. I was always fascinated by physics and studying that subject was a clear choice to me from my school days on.

#### Who introduced you into magnetic resonance?

Berlin had (and has) a strong magnetic resonance community. When it was time to choose a subject for my diploma thesis I had a choice between two groups doing EPR at the FU physics department. I did my diploma with Klaus Möbius (on triplet state EPR) who introduced me to the technique. For my PhD I joined the research group of Dietmar Stehlik and Christian von Borczyskowski. In a collaboration with a French research group lead by Michel Orrit we did the first electron spin resonance experiments (ODMR) on single molecules. Most importantly we also did coherent spin driving and did see the first Rabi oscillations as well as single spin echos.

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

I mostly enjoy our work in quantum physics and its application in sensing. We try to generate complex interacting spin systems by nanotechnology, generate entanglement and do complex spin control on such systems. This work combines the fun and knowledge we have on spin physics with quantum optics.

Things like quantum non-demolition measurements and feedback control are not known to classical spin resonance and extend the range of application quite considerably. We use this knowledge for precision nanoscale sensing and entirely new realm of EPR.

#### What is the driving force for you in your research?

I'm entirely motivated by curiosity. Our work does allow me to deeply look into quantum mechanics and explore its possibilities. I learn a lot from quantum optics and atom physics which is great fun.

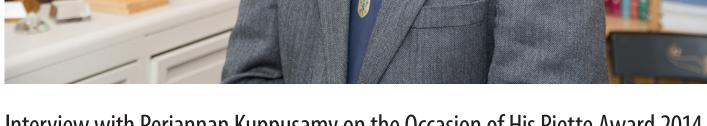
## The 70th anniversary of the EPR discovery is celebrated in 2014. What is your idea about the future of EPR?

Modern EPR technology has an increasing share in bioanalytics. In addition, I do see multiple fascinating opportunities for EPR in my area of research. As quantum nanoscience matures spins in solid will become a key playground.

I'm absolutely certain that magnetic resonance and its coherent control techniques will become a vital part of future quantum technology. Diamond spin quantum sensors do have the option of getting a wide-spread alternative detection technique for EPR and NMR with the potential to image and do spectroscopy down to the single electron and nuclear spin level.

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

There is plenty of opportunity of EPR in physics!



### Interview with Periannan Kuppusamy on the Occasion of His Piette Award 2014

**EPR newsletter:** Dear Professor Kuppusamy, on behalf of the readers of the EPR newsletter we congratulate you on your Piette Award 2014. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?

I come from a very humble background where none of my family members were formally educated. When I completed a master's program in chemistry with distinction (#1 among state universities) I realized I had the potential to do things differently and do it in a way to stand out from the rest. I suppose that confidence pushed me towards choosing a career in scientific research, which I thought would provide opportunity to explore and be the first to seek new knowledge.



Who introduced you into magnetic resonance?

Undoubtedly, it was my graduate adviser, Prof. P. T. Manoharan. He gives impressive lectures, and it was one of his lectures on magnetic resonance (EPR) during my college days that introduced me to this field.

#### What is the driving force for you in your research?

The very idea that whatever I am doing is new and that no one else has done it before is exciting to me. Particularly attractive to me is the research in academic institutions where one has the freedom to the research of interest. The driving force in my research is my satisfaction and recognition I get from my peers and the impact of my research to the society.

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

I have been passionate about developing EPR oximetry and bringing the EPR technology for clinical use. I am very happy to tell you that we (at Dartmouth) will soon be starting the first clinical trial using EPR measuremnts. However, the dearest to my heart is the research to understand the biological effect of oxygen, the elixir of life. We have found very intriguing data on the use of oxygen itself as a therapeutic agent for cancer and cardiovascular diseases. I am looking forward to the emergence of a new field – oxygenomics.

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

There is a perception of pessimism among young researchers that opportunities in magnetic resonance is becoming limited; MRI field is saturated and EPR has only limited scope. This is not true. We all know that the first manuscript on MRI was rejected although it became a Nobel prize-winning work later. We also recognize Larry Piette's pioneering EPR measurement in the seventies that has led to the development of in vivo EPR technology including capability for human applications. Success in science is all about being optimistic, believing, and pursuing what you're passionate about.

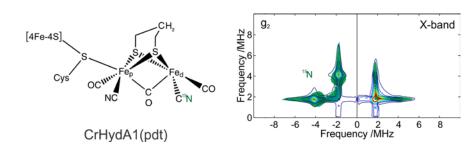


I would like to thank for the opportunity to write about my research topic: [FeFe] hydrogenases. Below I discuss some of the results which were presented recently at the International Symposium: Catalytic Systems for Chemical Energy Conversion which was organized on the occasion of 65th birthday of Prof. Wolfgang Lubitz, where my poster was awarded a prize from the International EPR Society.

Hydrogenases are enzymes which catalyze the oxidation of H<sub>2</sub> as well as the reduction of protons to form H<sub>2</sub> and are of growing interest in the light of renewable energy technologies development. The active site of [FeFe] hydrogenase is referred to as the "Hcluster" and consists of a "classical" [4Fe-4S] cluster connected via a protein cysteine side group to a unique [2Fe]<sub>H</sub> sub-cluster. The low oxidation state of the iron atoms in the binuclear sub-cluster are stabilized by CN- and CO-ligands. In addition, a bidentate dithiol ligand bridges the two iron centers. We could show that various biomimetic complexes of the diiron sub-cluster can be inserted with the help of the maturation protein HydF [1] or even directly [2] into apo-protein of [FeFe] hydrogenase, which contains only the [4Fe-4S] part of the H-cluster. This finding has caused great enthusiasm in the community as it opens

the possibility to build better enzymes using synthetic components. In such an attempt in a recent study we showed that [FeFe] hydrogenase from Chlamydomonas reinhardtii (CrHydA1) can be maturated with the biomimic complex  $[Fe_2(pdt)(CO)_4(CN)_2]^{2-}(pdt^{2-} = propan$ edithiolate) (referred as "pdt complex") containing a CH<sub>2</sub> group in the dithiolate bridge. While it results in an almost inactive hybrid enzyme CrHydA1(pdt) it can be stabilized in two redox states (oxidized and reduced) [3]. Importantly, FTIR and EPR studies showed that the oxidized form of CrHydA1(pdt) is almost identical to the native H<sub>ox</sub> state but much easier to obtain in pure redox state. Based on our studies we could conclude that the [2Fe]<sub>H</sub> sub-cluster (Fe<sup>I</sup>Fe<sup>II</sup>) is in the mixed valence configuration, while the [4Fe-4S]<sub>H</sub> sub-cluster is oxidized (2+) [4]. Since it is a promising structural and electronic model system for the native  $\boldsymbol{H}_{\mathrm{ox}}$  state we therefore decided to study it in more detail.

Taking advantage of the variant with <sup>15</sup>N and <sup>13</sup>C isotope labeled CN-ligands we performed advanced pulsed EPR studies on this hybrid protein using hyperfine sublevel correlation spectroscopy (HYSCORE) and electron nuclear double resonance (ENDOR) at different operation mw frequencies. Two



Agnieszka Adamska-Venkatesh receives the IES Poster Award from Klaus Möbius, IES President, at the International Symposium: Catalytic Systems for Chemical Energy Conversion in Mülheim an der Ruhr, Germany.

<sup>13</sup>C hyperfine couplings were observed and assigned to CN-ligands bound to terminal and proximal irons. Only one <sup>15</sup>N coupling was detected and assigned to the CN-ligand bound to the terminal iron. Also the <sup>1</sup>H ENDOR and <sup>14</sup>N HYSCORE spectra of oxidized CrHydA1(pdt) are very similar to those of native  $H_{ox}$  [4]. This confirms the previously proposed model of the electronic structure of the H-cluster in which the spin density is delocalized over the two iron atoms of the bi-nuclear sub-cluster. In addition, high resolution data allowed determination of the relative orientation of the obtained hyperfine tensors and the relative orientation of the distal CN-ligand in the g-axis frame. The obtained results are consistent with available crystal structures assuming that the g-tensor orientation follows the local symmetry of the binuclear sub-cluster in which the Fe-Fe bond represents one of the g- principal axes. The results and their implications are discussed in the detail in the paper that we recently submitted to the Physical Chemistry Chemical Physics.

These results could not be obtained without close collaboration between synthetic chemists, biochemists and spectroscopists and in this place I would like to thank for great collaboration research groups of Prof. Mark Fontecave from CEA and Prof. Thomas Happe from Ruhr University in Bochum. I would also like to acknowledge Prof. Wolfgang Lubitz and Dr. Edward Reijerse for creating wonderful working environment in our MPI institute.

- J. Esselborn, C. Lambertz, A. Adamska-Venkatesh, T. Simmons, G. Berggren, J. Nothl, J. Siebel, A. Hemschemeier, V. Artero, E. Reijerse, M. Fontecave, W. Lubitz, T. Happe: Spontaneous activation of [FeFe]-hydrogenases by an inorganic [2Fe] active site mimic, Nature Chemical Biology 2013, 9 (10), 607–609.
- A. Adamska-Venkatesh, D. Krawietz, J. Siebel, K. Weber, T. Happe, E. Reijerse, W. Lubitz: Artificially maturated [FeFe] hydrogenase reveals new redox states (in preparation)
- A. Silakov, B. Wenk, E. Reijerse, W. Lubitz: <sup>14</sup>N HYSCORE investigation of the H-cluster of [FeFe] hydrogenase: evidence for a nitrogen in the dithiol bridge, Physical Chemistry Chemical Physics 2009, 11 (31), 6592–6599.

G. Berggren, A. Adamska, C. Lambertz, T. Simmons, J. Esselborn, M. Atta, S. Gambarelli, J. Mouesca, E. Reijerse, W. Lubitz, T. Happe, V. Artero, M. Fontecave: Biomimetic assembly and activation of [FeFe]hydrogenases, Nature 2013, 499 (7456), 66–69.

## History of ESR Research in Japan: Physics

## Hitoshi Ohta

Molecular Photoscience Research Center, Kobe University e-mail:hohta@kobe-u.ac.jp

Evolution of magnetic resonance, which Started during World War II, reached Japan when General Headquarters (GHQ) of USA brought scientific journals and books to American Centers and major Japanese universities in 1948. Taking this opportunity Junkichi Itoh of Osaka University started ESR, FMR and NMR researches (Fig. 1). Although Itoh's interests shifted eventually to NMR, ESR results began to emerge from his Lab around 1950 through work by Minoru Fujimoto, who later became a Professor in Canada. Meantime Toshihiko Okamura of Tohoku University started to present FMR results, and Hiroo Kumagaya and his group at the Institute of Science and Technology, University of Tokyo (later Chiba University)

started to present ESR results. Although Okamura passed away at a relatively young age, his ESR research was taken over by Muneyuki Date who moved from Okamura's Lab. to Osaka University in 1960. This coincided with the installation of a Helium liquefier at Osaka University. However, Kumagaya himself went back to the nuclear physics research and the ESR research was taken over by Hidetaro Abe who moved to Institute of Solid State Physics (ISSP) at the University of Tokyo in 1958 [1, 2]. Parallel pumping experiments and studies of relaxation processed in antiferomagnets were carried out in Abe's Lab. Hitoshi Yamazaki moved from Abe's Lab. to Okayama University in 1972. After the direct observation of density of states of spin waves in low dimensional magnets, Yamazaki studied chaos phenomena involving magnons under strong microwave excitation. This work was continued by Michinobu Mino. In Okayama, Kokichi Oshima and Takashi Kambe studied organic systems by ESR.

Kazuo Morigaki, who joined ISSP in 1966 after previously working in Itoh's Lab and at Sony, studied metal-insulator transitions and impurity conductivity in semiconductors using ESR [3].

Asako Kawamori, who received her Doctors. degree in Itoh's Lab with an NMR study of NaClO<sub>3</sub>, moved to Kwansei Gakuin University in 1962. At that time the second X-band ESR system produced by JEOL was installed at Kwansei Gakuin University (Fig. 2). It was here that Kawamori began EPR studies of paramagnetic ions doped in both organic semiconductor and NH<sub>4</sub>Cl together with NMR studies. In 1979 she visited van der Waals in Leiden and Norris and Feher in the USA during her sabbatical, and her interest started to shift to photosynthetic systems. In 1981 a new Varian ESR system was installed in Kawamori's Lab making it possible to observe the signal from Mn<sub>4</sub> in PSII of photosynthesis system from 1984. Moreover, first pulsed ESR system in Japan made by Bruker was installed in Kawamori's Lab. in 1989 with funds provided to encourage private universities. In cooperation with Dzuba and Astashkin, who stayed at Kawamori's Lab. at the time, ELDOR



Fig. 1. Group photo of staffs related to condensed matter physics in School of Engineering Science around 1973. It was established at Osaka University in 1961. Front row from left, Professors Kiritani, Asayama, Takeo Nagamiya, Fujita, Junkichi Itoh, Haseda, Narita and Nishida. Second row from right, the second is Kazuko Motizuki, who provided this photo. She was an Associate Professor working with Prof. Nagamiya at the time.

measurements of photosynthesis systems were performed. After Kawamori's retirement, the study of photosynthetic systems using pulsed ESR was taken over by Hiroyuki Mino at Nagoya University.

Here I would like to discuss briefly developments in the theory of ESR in Japan. The Kubo-Tomita theory [4] became a standard theory in EPR, and it has been world wide for more than a half century. This theory also played an important role in constructing linear response theory, and it is also a starting point for most later ESR theories. Mori and Kawasaki also formulated a theory to interpret the behavior of ESR linewidths near phase transition in ferromagnets and antiferromagnets. On the other hand, Kanamori and Tachiki formulated a theory to interpret the ESR shift, and it was used in Nagata-Tazuke theory for low dimensional antiferromagnets, which will be discussed later. Japanese contributions to ESR theory was not limited to EPR but also included antiferromagnetic resonance (AFMR). AFMR theory was developed by Takeo Nagamiya (Fig. 1) et al., and they succeeded in interpreting the very detailed AFMR results in  $CuCl_2 \cdot 2H_2O$  for the first time [5]. The appearance of Nagamiya-Yoshida-Kubo theory surprised many scientists around the scientists have been significant, for instance, ESR theory for S = 1/2 one dimensional antiferromagnet using quantum field theory by Oshikawa (ISSP) and quantum numerical calculations of ESR by Miyashita (University of Tokyo).

Returning to experiments. Muneyuki Date, who moved to Osaka University in 1960, extended the Nagamiya-Yoshida-Kubo AFMR theory and, at the same time, extended the frequency-magnetic field region of AFMR experimenst. Frequencies were extended to the millimeter wave region from conventional X-band, and the field region was extended to 6 T using a pulsed magnetic field with a 10 mm bore mini-coil immersed in liquid Helium. This was a high magnetic field at the time when there were no superconducting magnest. Using this system, Date succeeded in observing impurity resonance and spin cluster resonance [7]. Later the pulsed magnetic field was extended to 50 T and submillimeter wave ESR was achieved with the combination of a far infrared laser. This submiliimeter wave ESR was developed by Mitsuhiro Motokawa at Date's Lab. and non-linear g-values [8] were studied by Shin-ichi Kuroda, who is now performing double resonance experiments at Nagoya University after staying at

sity is continued by Hitoshi Ohta following Motokawa's move to the Institute for Material Research (IMR), Tohoku University in 1994. At Tohoku University submillimeter wave ESR was applied to the spin gap studies of the spin-Peierls system, CuGeO<sub>3</sub>, and the orthogonal dimer system  $SrCu_2(BO_3)_2$  [9]. The research activity at IMR is continued by Hiroyuki Nojiri following the retirement of Motokawa. Activity at Osaka University was continued by Koichi Kindo (now at ISSP, Univ. Tokyo) and Masayuki Hagiwara (who moved from Riken in 2004) at the Center for Quantum Science and Technology under Extreme Conditions, Osaka University after the retirement of Date.

Duirng the late 1980's, Koichi Katsumata at Riken studied Haldane systems extensively. This focused particularly on ESR results on NENP doped with Cu that supported the valence bond solid model proposed for Haldane systems. This research activity and high frequency ESR studies using a vector network analyzer are continued by Hagiwara at Osaka University following the retirement of Katsumata.

In 1972 Kazukiyo Nagata, who moved to the Banno group at ISSP as assistant professor from Date's group, proposed the Nagata-



world during the 1950's, illustrating the high level of Japanese researches in magnetism [6]. As can be seen from these results, the basic formulations of ESR theory were established over the decade from 1950 to1960 mainly in Japan. Recently basic research on ESR theory became an active field again due to developments in statistical mechanics and computational methods. Contributions by Japanese the University of Alabama AIST (National Institute of Advanced Industrial Science and Technology). Mistuhiro Motokawa became a Professor at Kobe University in 1986, and studied the magnetic field induced phase transition system CsCuCl<sub>3</sub> and triangular antiferromagnets such as the singlet ground state system CsFeCl<sub>3</sub> using submillimeter waves [9]. Research activity at Kobe Univer**Fig. 2.** X-band ESR system produced by JEOL was installed at Kwansei Gakuin University in 1962. Asako Kawamori can be seen in the center.

Tazuke theory which explains the g-shift observed in the ESR of one-dimensional antiferromagnets [10]. After moving to the Tokyo Institute of Technology in 1974, Nagata developed fundamental ESR theories for low dimensional antiferromagnets, such as the typical ESR line shape coming from the long time tail, the magic angle, and the side band absorption which corresponds to g = 4. The research activity at the Tokyo Institute of Technology is continued by Hidekazu Tanaka, who studied the AFMR of triangular antiferromagnets by high frequency ESR, following the retirement of Nagata.

Yoshitami Ajiro studied one-dimensional antiferromagnets and two-dimensional triangular lattice antiferromagnets during his career in Hirota's group at Kyoto University (which will be discussed in the forthcoming ESR history in chemistry), Fukui University and Kyushyu University. The details of his ESR studies of these systems can be found in reference [11]. Of particular importance is his theory explaining the anomalous behavior of ESR linewidths observed in delafossites,  $ACrO_2$  (A = H, Li), which are model examples of Heisenberg triangular lattice antiferromagnest, by the spin fluctuation related to Z<sub>2</sub>-vortex excitations. This has attracted attention related to the recent studies of highly frustrated spin systems.

Kazumi Horai, who started ESR studies of magnetic impurity centers in Matsumura's group in Kyushyu University, moved to Nagoya University after a period in Date's group at Osaka University. In the 1970's he began ENDOR experiments and studied the hyperfine interaction of magnetic ions in ligand fields. These hyperfine interaction studies began first with Masanori Arakawa. Hideo Takeuchi (now at the Toyota Technological Institute) joined later. Horai began conduction electron ESR by the transmission technique with Sanshiro Sako at Mie University. After moving to Fukuoka University, Horai continued the study with Akihiko Nishida. Then Arakawa who moved to the Nagoya Institute of Technology, continued the EPR studies of magnetic impurity centers together with ENDOR and developed methods to analyze these centers with Hiroshi Ebisu and Takeuchi.

Motoji Ikeya, who became an assistant professor in the Faculty of Engineering, Nagoya University in 1967 during the middle of his doctoral studies at the Faculty of Engineering, Osaka University, started ESR experiments on color centers in alkali halides. After joining the group of J. Crawford at North Carolina University, who was well-known for studies of point defects, Ikeya moved to Yamaguchi University in 1973. Since the appearance of his famous paper in Nature in 1975 [12], whose cover is the photo of calcareous cave, Ikeya developed the fundamentals of dating and dosimetry using ESR. It is established that ESR dating lead to dates beyond several tens of thousand years, which is the limit of conventional radiocarbon dating, and it led to important discoveries in geology and anthropology. In 1987, Ikeya moved to Osaka University as a Professor. There he developed also the ESR microscope and extended the studies of ESR dosimetry. Some of this work is continued by Chihiro Yamanaka and Shin Toyoda.

Junichi Isoya, who gained his PhD at the University of Tokyo in 1972, retired from Tsukuba University in 2011. Isoya's main field was ESR studies of semiconductor, including pulsed ESR studies on diamond and silicon carbide, and fundamental studies of solid state quantum computing using ESR in collaboration with Kohei Itoh of Keio University.

The Institute of Molecular Science in Okazaki has a variety of ESR systems which are made available to many scientists. These facilities include an early Varian X-band ESR, a Bruker ESP300E (X-band) installed in 1992, while Bruker E500 (X-band) and E680 Wband have been in operation since 1999. At the moment Toshikazu Nakamura is responsible for these spectrometers in succession to Tatsuhisa Kato who is now at Kyoto University.

Finally I would like to thank Prof. A. Kawamori, Late Prof. K. Nagata, Prof. T. Nakamura, Prof. H. Mino, Prof. M. Mino, Prof. M. Motokawa, Prof. M. Oshikawa, Prof. H. Takeuchi, Prof. H. Tanaka, Prof. C.

#### **EPR newsletter Anecdotes**

Yamanaka, Prof. H. Yamazaki for comments on or photos for this article. Without their helps it would have been impossible to complete this article. I would also like to thank my aunt late Kazuko Motizuki for providing the photo (Fig. 1). She was the first woman to gain PhD in theoretical physics at National University in Japan and was the first woman Full Professor at Osaka University, who showed my way into physics research. Finally I would like to thank Laila Mosina who encouraged me to translate this article into English. It was originally written for the tenth anniversary of The Society of Electron Spin Science and Technology (SEST, http://www.sest.gr.jp/en) in Japanese [13], and translated into English for the EPR newsletter.

#### References

- Abstract book of Japanese Physical Society Spring Meeting (1995) (in Japanese).
- 2. J. Itoh, Butsuri 50 (1995) 491 (in Japanese).
- 3. K. Morigaki, Buseiken Dayori 47 (2007) 38 (in Japanese).
- 4. R. Kubo and K. Tomita, J. Phys. Soc. Jpn. 9 (1954) 888.
- 5. T. Nagamiya, K. Yoshida and R. Kubo, Advance in Phys. 4 (1955) 1.
- 6. J. Kanamori, Butsuri 61 (2006) 640 (in Japanese).
- M. Date and M. Motokawa, Phys. Rev. Letters 15 (1965) 854.
- S. Kuroda, M. Motokawa and M. Date, J. Phys. Soc. Jpn. 44 (1978) 1797.
- M. Motokawa, Denshi Spin Science Vol.3 (Spring) (2005) 4 (in Japanese).
- K. Nagata and Y. Tazuke, J. Phys. Soc. Jpn. 32 (1972) 337.
- Y. Ajiro, Denshi Spin Science Vol.8 (Spring) (2010) 4 (in Japanese).
- 12. M. Ikeya, Nature 255 (1975) 48.
- H. Ohta, Denshi Spin Science Vol.9 (Autumn) (2011) 100 (in Japanese).

Are you interested to become a member of the International EPR (ESR) Society? Please find the registration/ information form for new/continuing members of the IES and non-credit-card payment instructions for individual members on this Web site: www.epr-newsletter.ethz.ch/contact.html





# **PRESENT MEETS FUTURE**Edited by Sabine Van Doorslaer

The European Union administration uses the term early stage researchers (ESR) for young scientists. For our field, this acronym could not be more appropriate, because the future of EPR/ESR lies in the hands of the young researchers, building on the achievements of their predecessors. But how do the young researchers see their own future and the future of EPR in general? Are their dreams different than those of their predecessors? Is being a young scientist in 2014 more difficult than it was for their mentors in the past? And what about these mentors, do they feel that they have realized their early scientific dreams and goals?

In this 'Present meets future' feature, I will be confronting the views and experiences of an early stage researcher in EPR (PhD student or young postdoc) with those of one of his/ her mentors. The first double interview is with Dr. Jennifer Mathies (currently postdoc at MIT, Boston) and her 'PhD father' Prof. Dr. Edgar Groenen (University of Leiden). As it can be understood from their CVs (see inset), both came to EPR via a detour.

#### How and when did you start your career? Was it a childhoods dream to become a scientist, or was it a consequence of fortuitous choices? What attracted you in EPR?

**Edgar**: At high school I had fascinating teachers for chemistry and mathematics, and the same applies to the professor who introduced me to theoretical chemistry in my second year at the university. They were at the basis of my career, which I owe to the inspiring supervisors and colleagues in later years. During my masters study I got already interested in magnetic resonance, but my thesis supervisor convinced me that applying electric fields can be fun as well. After my research on the Stark effect in condensed matter, I joined

an industrial laboratory. In those days spectroscopy, solid-state NMR and Fourier transform IR, played a minor role in my research. I performed my first EPR experiment only at the age of 35. I still love EPR because there is no other experimental tool that brings us closer to the molecular wave function, which forms the heart of the quantum description of matter. The spin Hamiltonian is a beautiful concept and invaluable in EPR, but one should not forget that the real information is hidden in the tensors.

Jennifer: I wanted to study physics after high school, because I thought it would be interesting and challenging. During my studies and later on during my PhD it turned out that I was particularly good at running complex experiments. And I always found quantum mechanics very exciting. Hence, spectroscopy is a good fit.

## What accomplishment in your (short or long) scientific career are you very proud of?

Jennifer: During my PhD I spent a lot of time and energy figuring out how to do CW EPR at 275 GHz with a sensitivity high enough to detect high-spin transition-metal sites in proteins and enzymes. We just submitted a manuscript in which we report for the first time distinct zero-field splitting parameters for the high-spin Fe<sup>3+</sup> ions bound to either of the two homologous lobes of human serum transferrin. In addition, from the small variations we observed in the zero-field splitting parameters, we were able to deduce that the structure of the iron site in one lobe is affected by the conformation of the other lobe, but not vice versa. I am very proud that we were able to realize our ideas regarding the spectrometer, and that we could also take the next step and address a biological question.

**Edgar**: I am proud of the fact that my cooperation with students and colleagues has been scientifically productive and personally rewarding.



Jennifer Mathies (°1981) studied Experimental Physics at Leiden University (The Netherlands). During her master phase she worked on scanning tunneling microscopy (STM) and later on single molecule spectroscopy during a research internship at UCLA. After a detour into atmospheric chemistry and physics and a job in IT she returned to Leiden University at the end of 2007 to become a PhD student in the group of Edgar Groenen, working, among other topics, on high-frequency EPR on high-spin transition-metal sites. After defending her thesis in March 2012, she has taken on a postdoc position in the group of Bob Griffin (MIT, USA), crossing the bridge between EPR and NMR by working on DNP, in particular on pulsed DNP and radical development for cross-effect DNP.

Edgar Groenen (°1949) studied Chemistry at Leiden University (NL) with a major in Theoretical Organic Chemistry and minors in Theoretical Physics and Applied Mathematics. He continued to obtain a PhD with a thesis on "Charge transfer transitions in organic molecules". After working 8 years as a researcher at the Royal Shell Laboratory in Amsterdam, he moved back to Leiden University, first as a lecturer in the department of Physics and Astronomy, then senior lecture and since 2003, he is a full professor in Experimental Physics. He has a long-standing career in EPR and optics, and is/was a mentor to many. In 2003, the IES awarded him the Silver Medal for Physics and Material Science. During 5 years (2008-2013), he was also vice-dean and responsible for education in the Faculty of Mathematics and Natural Sciences of Leiden University.



Can you describe one of the most enjoyable moments in your (short or long) scientific career?

**Edgar**: My most enjoyable moments in science are those at which an analysis or suggestion from my side helps to find the solution of a problem that has kept me and my colleagues busy for quite some time. To mention a few early ones: (i) the realization, after months of fighting with beautiful ESEEM data, that pyridine in the lowest triplet state adopts a boat conformation, and (ii) the insight, which came in a memorable Easter weekend, that the triplet excitation of a single crystal of  $C_{60}$  is delocalized over a pair or a chain of  $C_{60}$  molecules. Not the big things, but the small victories.

Jennifer: I've always very much appreciated close collaboration, although it can be challenging to establish mutual trust and make interests coincide. Also, there have been several "eureka" moments. For example, the moment I realized that in a newly discovered radical in RNR class III the exchangeable proton had to be one of the beta-protons of cysteine, or when I identified a mode characteristic to the 13,14 cis configuration of spheroidene, which helped us to show that this second configuration only occurs in the reaction center of the R26 mutant of *Rhodobacter spheroides*.

#### Choosing a scientific career is not always an easy road to go. What were the problems that you met (or are still having) in pursuing your scientific career and your EPR dream?

Jennifer: Especially when you are just starting your PhD you are vulnerable. You don't know how to do science on your own yet, so a bad advisor or a type of research that doesn't fit your interests could make you abondon science altogether. I was lucky enough that I got a chance to start over, I'm very grateful for that.

**Edgar**: I returned to academia after a period in industry because I wanted to combine research and education. It was the right decision, which I enjoy till today, although the boundaries set by the money available for research are sometimes frustrating.

#### Jennifer, what expectations and plans do you have for your further career? Do you want to continue in academia?

Jennifer: Yes, I would like to, very much. I enjoy what I do, and I would like to continue doing it. It would be great to run my own lab and follow up on my own research interests.

Edgar, are there specific expectations that you cherished as a young researcher that have come true? Or did your career take turns that you never anticipated at the start, but that have been fulfilling nevertheless? Is there an old scientific dream that you still want realize?

Edgar: I had no big dreams when I started in EPR, but always had clear goals in mind for say five years ahead. At the moment we develop temperature-cycle EPR at high microwave frequencies for kinetic and mechanistic studies of biochemical reactions.

## How do you see the future of EPR and your role in this?

Jennifer: Here at MIT, there are a lot of people who ask me to contribute to their projects being an "EPR expert" and in this sense I have more work than I can handle. However, I also get the impression that most of these people think of EPR as a saturated field of research and are therefore reluctant to invest time to really grasp it. I don't think these people are right, there is still a lot unexplored, both in method development and in application. I would see new developments coming from cross-pollination with other areas of research and other spectroscopic techniques.

**Edgar**: The future of EPR is in its applications in diverse fields as one of the indispensable methods to determine (electronic) structure. For the foreseeable future an EPR community remains necessary to further develop the method in relation to its relevance for studies in biological and material science. Besides, we need big advances in ab-initio quantum chemistry, and if I were young ...

#### Are there matters that you think the EPR community should pay more attention too?

Jennifer: I think it is important to keep an eye out to other disciplines and techniques and to be open to collaboration.

**Edgar**: Besides our own "offspring", we should pay attention to the training of people that just want to use EPR. In this respect, in Europe the EFEPR schools could play a role, but in their present form they concentrate on the education of specialists. In my opinion, we should look for ways to strengthen our international co-operation. We have a wonderful community and we should benefit more from it.



## Haim Levanon (1938–2014)

It was a deep shock for me to hear that Haim Levanon passed away on March 5, 2014 at the age of 76. In recent years, when overseas travels became more difficult for him, we regularly talked on the phone several times a year. It is very sad to conceive that one cannot talk with him anymore.

Haim graduated at the Hebrew University of Jerusalem and received his Ph.D. in Physical Chemistry in 1969. Immediately after his doctorate, he moved to St. Louis/USA where he worked for three years at the Washington University in the laboratory of Sam Weissman, one of the pioneers of electron paramagnetic resonance. In 1972, Haim returned to Israel and became Lecturer, Associate Professor and finally Full Professor in the Department of Physical Chemistry at the Hebrew University of Jerusalem. From 1990 to 1999, he was Director of the Farkas Center for Light-Induced Processes.

Haim and I met for the first time at Argonne National Laboratory/USA where he spent a Sabbatical Leave in the Photosynthesis Group of Marion Thurnauer and Jim Norris. Haim liked these extended research stays abroad which included a Sabbatical Leave in the Radiation Laboratory at the University of Notre Dame/ USA, a Fellowship of the Japanese Society for the Promotion of Science at the Tohoku University in Sendai/Japan and a Humboldt Award at the Free University of Berlin/Germany and the University of Freiburg/Germany.

In the years 1997–2006, Haim and his coworkers and students were regular visitors of Freiburg, performing carefully designed EPR experiments on photo-generated triplet states and radical pairs using our time-resolved EPR spectrometers. On extended research stays, Haim was always accompanied by his wife Hedva. They lived either in a private apartment near the old city of Freiburg or in the guest-house of the University. It was a great pleasure for me and my wife Sigi to introduce our guests to the Black Forest and the Alsass visiting scenic and historic sites on both sides of the River Rhein.

Haim was a true patriot who sincerely loved his country. It was a matter of the heart for him to show his friends the beauty of the Holy Land. We remember with pleasure a trip to the Galilee which he offered to us in 2005. The first stop after a long drive through the West Bank was Bet She'an with its most impressive Roman Theatre. Then, we visited Christian Shrines at the Sea of Galilee. After a wonderful picnic in the Northern Galilee, we crossed the Jordan River to the Golan Heights. In the late afternoon, we stopped near Bet She'an, where one of Haim's sons was running a fish farm. On the way back, Haim took again the West Bank route and we arrived in Jerusalem at 10 o'clock at night. What a fascinating trip! Three thousand years of the varied history of the Holy Land in just one day.

In Haim's scientific activities, there are two major subjects: The study of the light-induced processes which lead to the formation of transient paramagnetic species and the characterization of these species by time-resolved multi-frequency EPR. Using liquid crystals as anisotropic solvents, Haim and his team gained deep insight into the formation of electron spin polarization in the triplet states of organic macrocycles and metal complexes. In addition, he was interested in the light-induced spin chemistry of photosynthetic systems. Applying high time and spectral resolution EPR, Haim and his cooperation partners were able to obtain novel information on the primary electron transfer steps of natural and artificial photosynthesis.

Apart from excellent research activities, the life's work of Haim Levanon is distinguished by an exceptional commitment to the scientific community. For 20 years, he served as Editorin-Chief of the Israel Journal of Chemistry. Moreover, he organized as Chairman or Cochairperson various international conferences in Jerusalem such as the 50th Anniversary of the Israel Chemical Society, the Advanced Study Institute of the Hebrew University on the Primary Events of Photosynthesis, the International Conference on Magnetic Resonance of Biological Systems, the Joint U.S.-Israel Symposium on New Developments in Primary Photosynthesis, the International Symposium on Fullerene Chemistry and the International Meeting on Spin Chemistry.

During these conferences, Haim took great care of the comfort and safety of the participants. I shall never forget an incident that occurred in 2002 at the time of the second intifada. Together with Sigi, I attended an International Meeting organized by the Israel Chemical Society. The Meeting took place in a traditional Jewish Hotel in Jerusalem. For the safety of the participants, there were guards in front of the Hotel and probably also in the Hotel. Since Sigi had not been to the Old City before, we planned a visit in connection with the Meeting. First, Haim strictly opposed this visit, but finally he agreed. So, one morning, Sigi and I took a taxi to the Jaffa Gate and entered the largely "deserted" Old City. As a result of the second intifada, the number of tourists visiting Israel had drastically decreased. Without the "guiding" stream of tourists, it was difficult to find one's way. Yet, at the end of the day, we succeeded to visit most of the highlights of the Old City.

However, departing from Haim's advice, we did not leave the Old City for lunch, but stopped at the Roof Café in the Jewish Quarter. As far as I can remember, we were the only guests. Crossing through the Jaffa Gate in the afternoon, we noticed numerous police cars in front of the Gate. As suggested by Haim, we went over to the King David Hotel and took a taxi back to the conference venue. There, we met Haim and Hedva in deep concern. Around noon, a female suicide bomber had attacked visitors on Ben Jehuda.

Haim Levanon was a well-known international scientist of high reputation. He had numerous co-operations with leading groups from different countries all over the world including the United States (Argonne National Laboratory, Northwestern University, University of Notre Dame), Germany (Free University of Berlin, University of Freiburg, University of Cologne) and Japan (Tohoku University, Sendai). His innovative and topical work in the field of electron spin science was recognized by several national and international honors and awards. He was President of the Israel Chemical Society for the years 1984 to 1987. In 1992, Haim received the Max Planck Research Award together with Klaus Möbius. In 2002, Haim Levanon was the recipient of a Humboldt Award in recognition of his accomplishments in research and teaching. Since 2004, he was President of the Israeli Humboldt Club.

With Haim Levanon, the scientific community has lost an outstanding international scientist in the field of electron spin science. In addition, I have lost a sincere and warmhearted friend.

> Gerd Kothe Department of Physical Chemistry University of Freiburg

I first met Haim in the end of 1993 when I visited his laboratory aiming to find a job after my immigration to Israel from the former Soviet Union. Previously, I had worked on the steady-state EPR of spin-labeled biological systems, including photosynthetic ones to reveal principles of their functioning. Of course, I had been impressed by Haim's papers on time-resolved EPR investigations of the photoinduced processes in various artificial donor-acceptor ensembles to mimic primary events in photosynthesis. The state-of-the art techniques used in these experiments opened new horizons in the field and were available only in a few laboratories in the world. Thus, without any doubts, I accepted Haim's offer to join his group.

One can imagine my situation at that time: to start a new life at 42 with poor spoken English, practically nil Hebrew, and daily routine of a two child family in a new society – all these things did not make my adaptation at the lab easier. However, despite his hot-headed nature, Haim patiently tried to facilitate my life – he spoke with me, both in English and Hebrew, went deep into my problems and efficiently helped to solve them.

After a new coworkers' "accommodation" at the lab, Haim began to send us to the prominent scientists in Europe and US to extend our collaboration with their laboratories, employing modern experimental techniques studying novel supramolecular systems. Yet, looking back, I understand how Ham's boost was important to all of us.

In the last years of his life, Haim was seriously ill, but in spite of getting progressively worse, he came to the laboratory and tried to be useful for his group.

Haim Levanon was widely recognized as one of the pioneers and leaders in time-resolved EPR studying photophysical and photochemical processes in various photosynthetic model systems, embedded in anisotropic liquid crystalline media. The high orientation degree of the chromophores embedded in magnetically aligned liquid crystals significantly facilitated a detailed determination of their magnetic parameters. Employment of the nematic liquid crystals as a solvent combined with selective laser light excitation of supramolecular entities allowed us to identify short-lived intermediates and reveal their origin and fate in photoinduced electron transfer reactions in different donor-acceptor systems mimicking processes and states occurring in the native photosynthetic apparatus. He was recipient (with Prof. K. Möbius of FUB, Germany) of 1992 Max-Planck Research Award, 1994 Willstätter Lecturer, Germany, and Recipient of 2002 Humboldt Award.

Haim Levanon will certainly be missed by his colleagues and the EPR community as a whole. Alexander Berg, Institute of Chemistry, The Hebrew University of Jerusalem

My first encounter with Haim was during my undergraduate studies at the Hebrew University of Jerusalem, where I have attended his course on the subject of Magnetic

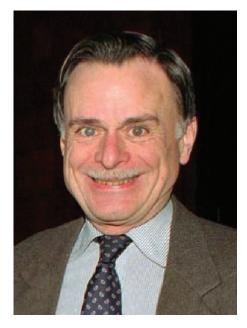


From left to right: Yehuda Heimlich, former PhD student, now a director at Israel Port Authority, Alexander Berg, Haim Levanon, and Aharon Blank.

Resonance. I found this course very interesting and it was one of the main reasons for me choosing to work on this subject further on. Later, during my mandatory military service I was working on some ideas for developing materials which would efficiently absorb electromagnetic radiation, based on some magnetic resonance phenomenon. This brought me again to Haim, whom I met in Tel Aviv following one of his meetings in the board of Israel Chemicals. In view of this meeting I have decided to further pursue this subject and thus, although my Master studies were conducted at Tel Aviv University in electrical engineering, I was co-advised also by Haim and performed some of the experiments in his lab. It did not take long time after I finished my MSc to decide to continue on my PhD work with Haim. Shortly before I started the actual lab work with him, Haim invited me to a Spin Chemistry conference he organized in Jerusalem attended by the finest scientists in the field (e.g., Feher, Pines, Freed). In general Haim was an excellent conference organizer and due to his great local patriotism he always insisted that they will be held in Jerusalem (which was home town for his family for at least 7 generations). For example, when the ISMAR meeting that was supposed to be in Israel was relocated to Rhodes, he became very upset about it and did not want to attend it.

During the 4+ years I spent in Haim's lab (1998-2002) I have learned a lot about experimental scientific work, writing papers and proposals and many other issues required from modern scientists. Haim provided me a lot of scientific space to freely operate around and promote subjects that were of my interest. He was always very dedicated to his work, maybe even too much... to the verge of affecting his health. Before I went to a post-doc in Cornell he helped me a lot in recommendations and in establishing contact with Prof. Freed. In 2009 I thought it should be a good time to organize a special 70th birthday meeting, which were attended by many of his friends and colleagues from Israel and abroad. I believe Haim enjoyed this meeting a lot, with his health being still quite OK at the time. Haim will be missed by his many former students, colleagues, and family. I am sure we can all reconcile by the fact that he lived a full life, achieving significant scientific and professional success, raised a great family, and educated many students, which are currently in the forefront of academic and industrial life in Israel and abroad.

Aharon Blank Technion – Israel Institute of Technology



## John Stewart Waugh (1929–2014)

Our good friend, mentor and colleague, John Stewart Waugh, a physical chemist who is recognized as the founding father of the field of high resolution NMR in solids, died in Lincoln, MA on 22 August 2014 at the age of 85.

John was born on April 25, 1929 in Willimantic, Connecticut where his father, an economist and statistician, was a professor at the University of Connecticut in Storrs. He attended Dartmouth College, graduating in 1949 with highest distinction in chemistry. Subsequently, he performed his graduate research at Cal Tech where in 1953 he completed a thesis entitled "Line Profiles in Nuclear Magnetic Resonance Absorption", supervised by Prof. Donald M. Yost. As a grad student at Caltech, and about 4 years after the discovery of NMR, Waugh built the first of the many NMR spectrometers that he and his colleagues designed and assembled. He used a borrowed magnet and some World War II surplus electronics, and the instrument enabled his Ph.D. research which consisted of studies of the structure of the bifluoride ion,  $HF_2$ , in solids. In 1953 Waugh accepted a position as Instructor in the Chemistry Department at MIT and, using lab space and a magnet furnished by Francis Bitter, initiated a research program on molecular motion and phase transitions. In 1955 John was promoted to Assistant Professor, and he rose through the ranks, becoming A.A. Noyes Professor, and in 1989 Institute Professor, the highest honor

that MIT can bestow on one of its faculty. A year earlier, in 1988, John was awarded the James S. Killian Faculty Achievement Award, an honor bestowed by MIT in recognition of extraordinary professional accomplishments and service to the Institute. He became an emeritus Professor in 1997 but continued as an invaluable member of the MIT community until his death, a total of 61 years.

John's research during the period 1953–1968 focused on many interesting problems in chemistry and physics characteristic of the early days of nuclear and paramagnetic resonance. For example, he provided the first coherent explanation of ring current shifts in <sup>1</sup>H NMR spectra of aromatic molecules<sup>1</sup>, coupling in strongly coupled spin systems<sup>2,3</sup>, relaxation in liquids and gases<sup>4</sup> and theoretical treatments of relaxation<sup>5</sup>. In 1968 he published a paper on measurements of spin-lattice relaxation in complex spin systems using Fourier transform spectroscopy that is now known as the "inversion recovery" method<sup>6</sup>. It remains the most common approach to measuring spin-lattice relaxation rates in gases, liquids, and solids.

In 1966, while working as a consultant for the small company Magnion, Waugh and his friend Edward Ostroff made the serendipitous discovery that the length of a free induction decay in a solid is extended by application of a train of intense radio frequency (rf) pulses to the spin system<sup>7</sup>. This germinated three seminal papers published in 1968 that laid the foundations of high resolution NMR in solids<sup>8–10</sup>. The initial publications were devoted to suppressing homonuclear dipolar interactions in solids and observing the underlying chemical shifts and their spatial anisotropy<sup>11</sup>, the feature that renders NMR spectra so important to chemistry, physics, biology and medicine. In addition and no less important, Waugh and Ulrich Haeberlen introduced a theoretical framework to understand the experiments, average Hamiltonian theory (AHT)<sup>8,10</sup>, an especially powerful form of time-dependent perturbation theory. In the same papers, an analysis of multiple pulse experiments indicated that certain sequences allow the homonuclear dipolar Hamiltonian to be refocused<sup>8</sup>. This calculation resulted in a demonstration of time reversal in homogeneously broadened spin systems, something that was thought impossible at the time<sup>12</sup>. Eventually, AHT provided the intellectual underpinnings for magic angle spinning (MAS), spin decoupling, dipolar recoupling and many other stimulating ideas in magnetic resonance, and it stands today as probably the most important theoretical idea in the field.

In the early 1970's Waugh and two graduate students, Alexander Pines and Michael Gibby, demonstrated that high resolution experiments could be extended to observation of <sup>13</sup>C, <sup>15</sup>N, <sup>31</sup>P, etc. spectra; i.e., to low abundance, weakly-coupled spin systems<sup>13,14</sup>. The problem of the long  $T_1$  of these nuclei was addressed by transferring polarization from abundant spins, namely <sup>1</sup>H, using the proton enhanced cross polarization (CP) method. A third feature was the incorporation of <sup>1</sup>H decoupling to ensure high resolution<sup>15</sup>. Today this seminal approach to solid state NMR is employed on a routine basis in hundreds of labs around the world. It permitted observation of high resolution dipolar couplings in single crystals<sup>16</sup> and was combined with multiple pulse NMR in a manner that reintroduced dipole couplings into NMR spectra, a separated local field (SLF) experiment<sup>17</sup>, that allowed measurement of internuclear distances in a manner consistent with the goal of high resolution. Finally, integration of MAS into this approach<sup>18,19</sup> lead to the precursor of what are today known as dipole recoupling methods, which permit the determination of structures of proteins in membranes and amyloid fibrils. These are all methods that enable studies on systems that are not easily examined with diffraction or solution NMR, the two primary tools of structural biology.

Although he rarely discussed instrumentation in his public lectures, Waugh was a master architect of NMR spectrometers and the accessories necessary to implement his experiments<sup>20</sup>. His contributions to spectrometer design include methods for the control of the phase, amplitude and frequency of rf pulses, heterodyne detection, computerized pulse programmers, quadrature phase detectors and multiple tuned rf coils<sup>21</sup> in low temperature NMR probes<sup>22</sup>. His ability to conceive and implement these features allowed him to execute experiments that were impossible in other laboratories and permitted him and his colleagues to move forward in areas not accessible to labs with commercial spectrometers. They are features that are found in virtually every NMR instrument in operation today.

As recognition of his considerable intellectual accomplishments Waugh received many awards and prizes. He was a fellow of the American Academy of Arts and Sciences, a member of the National Academy of Sciences, and chair of the Division of Chemical Physics of the American Physical Society. His prizes and awards include the Langmuir Award, the Wolf Prize, and most recently the Welch Prize, given for basic research that benefits humankind. He also received Caltech's Distinguished Alumnus Award and an honorary doctorate from Dartmouth College.

Finally all of us will remember fondly John's well developed sense of humor which was manifest in a sharp wit that was often focused on himself, his colleagues or what he considered the pompous of the moment. Thus, he referred to the method outlined in his seminal paper on multiple pulse NMR by the authors Waugh, Huber and Haeberlen<sup>9</sup> as the WAHUHA experiment. In addition, in the early 70's when the "cycle/second" was abandoned in favor of the "Hertz", he came to the rescue of the "radian/second", the unit of preference in all magnetic resonance cal-

- Waugh, J. S.; Fessenden, R. W. Nuclear Resonance Spectra of Hydrocarbons: The Free Electron Model J. Am. Chem. Soc. 1957, 79, 846–849.
- Fessenden, R. W.; Waugh, J. S. Strong Coupling in Nuclear Resonance Spectra I. The Five-Spin System of trans-Propenylbenzene J. Chem. Phys. 1959, 30, 944–949.
- Fessenden, R. W.; Waugh, J. S. Strong Coupling in Nuclear Resonance Spectra II. Field Dependence of Some Unsymmetrical Three-Spin Systems J. Chem. Phys. 1959, 31, 996–1001.
- Johnson, C. S., J.; Waugh, J. S.; Pinkerton, J. N. On the Mechanism of Nuclear Relaxation in Gaseous and Liquid CHF3 J. Chem. Phys. 1961, 35, 1128–1129.
- Deutch, J. M.; Waugh, J. S. Correlation Functions in Nuclear Relaxation. I. Analysis of Random Motions from Field-Dependence of Relaxation Times J. Chem. Phys. 1965, 43, 1914–1918.
- Vold, R. L.; Waugh, J. S.; Klein, M. P.; Phelps, D. E. Measurement of Spin Relaxation in Complex Systems J. Chem. Phys. 1968, 48, 3831–3832.
- Ostroff, E. D.; Waugh, J. S. Multiple Spin Echoes and Spin-Locking in Solids Phys. Rev. Letters 1966, 16, 1097–1098.

culations. In particular in a 1968 paper he defined a new unit the "As" so that 1 Hz =  $2\pi$  As<sup>23</sup>. The As is used by the afficionados of magnetic resonance to denote angular velocity in inverse seconds, or an "Avis". His summary comment was that despite the new definition of the As, "Hertz is still #1"

Waugh moved to Lincoln, MA in 1965 and resided there until his death. He was an avid sailor and the owner of many sail boats including one appropriately named the "Magic Angle" and serviced by a dingy the "Spin Echo". He is survived by his wife of 31 years, Susan, with whom he spent many happy seasons sailing the coast of Maine, traveling, and raising a succession of beloved Labrador

- 8. Waugh, J. S.; Wang, C. H.; Huber, L. M.; Vold, R. R. Multiple-Pulse NMR Experiments J. Chem. Phys. 1968, 48, 662–6670.
- Waugh, J. S.; Huber, L. M.; Haeberlen, U. Approach to High-Resolution NMR in Solids Phys. Rev. Letters 1968, 20, 180–182.
- Haeberlen, U.; Waugh, J. S. Coherent Averaging Effects in Magnetic Resonance Phys. Rev. 1968, 175,, 453–467.
- Mehring, M.; Griffin, R. G.; Waugh, J. S. Direct Measurement of Chemical Shielding Anisotropies: Fluoranil J. Am. Chem. Soc. 1970, 92, 7222–7223.
- Rhim, W.-K.; Pines, A.; Waugh, J. S. Violation of the Spin Temperature Hypothesis Phys. Rev. Letters 1970, 25, 218–220.
- Pines, A.; Gibby, M. G.; Waugh, J. S. Proton Enhanced Nuclear Induction Spectroscopy J. Chem. Physics 1972, 56, 1776.
- Pines, A.; Gibby, M. G.; Waugh, J. S. Proton-Enhanced NMR of Dilute Spins in Solids J. Chem. Phys. 1973, 59, 569–590.
- Mehring, M.; Pines, A.; Rhim, W.-K.; Waugh, J. S. Spin-Decoupling in the Resolution of Chemical Shifts in Solids by Pulsed NMR J. Chem. Phys. 1971, 54, 3239–3240.

retrievers. He is also survived by a son and daughter, Frederick and Alice, as well as by five grandchildren.

John Waugh was a towering figure in NMR and EPR and his intellect, achievements, and wonderful sense of humor was an inspiration to everyone who knew and worked with him. He will be sorely missed by all of us in the magnetic resonance community.

> Robert G. Griffin Department of Chemistry and Francis Bitter Magnet Laboratory Massachusetts Institute of Technology Cambridge, MA 02139, USA

- Griffin, R. G.; Pines, A.; Waugh, J. S. Observation of 13C-14N Dipolar Coupling in Single Crystals of Glycine J. Chem. Phys. 1975, 63, 3676–3677.
- Hester, R. K.; Ackerman, J. L.; Cross, V. R.; Waugh, J. S. Resolved Dipolar Coupling Spectra of Dilute Nuclear Spins in Solids Phys. Rev. Letters 1975, 34, 993–995.
- Stejskal, E. O.; Schaefer, J.; Waugh, J. S. Magic-Angle Spinning and Polarization Transfer in Proton-Enhanced NMR J. Magn. Res. 1977, 28, 105.
- 19. Maricq, M. M.; Waugh, J. S. NMR in Rotating Solids J. Chem. Phys. 1979, 70, 3300.
- Ellett, J. D.; Gibby, M. G.; Haeberlen, U.; Huber, L. M.; Mehring, M.; Pines, A.; Waugh, J. S. Spectrometers for Multiple-Pulse NMR Advances in Magnetic Resonance 1971, 5, 117–176.
- Cross, V. R.; Hester, R. K.; Waugh, J. S. Single Coil Probe with Transmission-Line Tuning for Nuclear Magnetic Double Resonance Rev. Sci. Instrum. 1976, 47, 1486–1488.
- Griffin, R. G.; Ellett, J. D.; Mehring, M.; Bullitt, J. G.; Waugh, J. S. Single Crystal Study of the 19F Shielding Tensors of a Trifluoromethyl Group J. Chem Physics 1972, 57, 2147–2155.
- 23. Ellett, J. D.; Waugh, J. S. The Chemical Shift Concertina J. Chem. Phys. 1969, 51, 2851–2858.



Is your company involved in magnetic resonance in any way? If so, consider advertising in the *EPR newsletter*. Your company will have its own advertising and information box in each issue. It will be seen by a targeted audience of thousands of specially selected scientists worldwide. Information on sponsoring the Society and advertising is shown on this Web site: www.epr-newsletter.ethz.ch/corporate\_sponsors.html

#### CRYOGENIC Cryogen Free Technologies

## Superconducting EPR magnets in cryogen free cryostats

- Up to 12T vertical or 7T horizontal with 89mm bore
- Compact 7T vertical or 3.5T horizontal, 40mm bore
- Variable temperature cryostat for standard resistive magnets & probes. Temperature range 2–300 K

Cryogenic Limited, Units 29/30, Acton Park Industrial Estate, The Vale, Acton, London W3 7QE, UK. Tel: +44 (0)20 8743 6049 Fax: +44 (0)20 8749 5315 E-mail: <u>sales@cryogenic.co.uk</u>

### L&M EPR Supplies, Inc.

4152 W. Lisbon Ave., Milwaukee, WI 53208 Phone: (414) 324-1052; Fax: (262) 889-2368 www.lmepr.com sales@lmepr.com

ິ	TPX Capillaries	EPR Sampling Tubes
ш- С	Quantity	Price/Part (\$US)
Ξ	1–19	60.00
Ê	20–99	50.00
₽.	100+	40.00
-		



## Harden M. McConnell (1927–2014)

Tarden Marsden McConnell passed away HOctober 8, 2014 after a struggle with cancer. He was born in Richmond, Virgina on July 8, 1927. He had an early fascination with science when one could purchase chemicals without the worry of government regulations and oversight. His parents were not intrusive, even after he destroyed two laundry tubs in their Washington, D.C. basement. He found his high school education in chemistry not very challenging, but the mathematics teachers were more inspiring. He obtained a scholarship in 1947 from George Washington University and earned a B.S. in chemistry in just three years. Afterwards, he attended the California Institute of Technology (Caltech) working with Norman Davidson for his Ph.D., graduating in 1951. After Caltech he was a National Research Council Fellow at the University of Chicago under Robert S. Mulliken where he worked on the catalysis of *cis-trans* isomerization in ethylene by paramagnetic substances, attributed to spin exchange interactions between the triplet state of twisted ethylene and the paramagnetic catalyst.

He then spent a relatively short, but highly productive, period with Shell Development Company, Emeryville, CA from 1952–1956, which had just purchased a Varian NMR spectrometer, an instrument which then was out of the financial reach of many academic institutions. This was where he first established himself as a leader in magnetic resonance. At Shell, he published a version of group theory for NMR spectra and spent lots of time on magnetic resonance problems, including relating molecular orbital theory to the nuclear spin-spin splittings seen in high-resolution NMR<sup>1</sup>. He became aware of the fact that proton nuclear hyperfine splitting was being observed in the EPR of aromatic free radicals, where the "odd electron" and its spin were believed to be confined to  $\pi$ -molecular orbitals. Since these protons lie in the molecular plane, the observed isotropic proton hyperfine splitting should be due to the Fermi contact hyperfine interaction, requiring a finite spin density at the proton. This fundamental discrepancy between experiment and theory, neglecting electron spin correlations, prompted him to write a paper accounting for the proton hyperfine splitting in these aromatic free radicals. Also while at Shell McConnell conceived the phenomenon of electron spin polarization in a  $\pi$ -molecular orbital (aromatic radical) through exchange coupling that can produce appreciable electron spin polarization in s-atomic orbitals at the aromatic protons. From this work, the famous McConnell equation was derived,  $A = Q \cdot \rho$ , which relates the proportional dependence of the hyperfine splitting constant on the spin in compounds such as benzene radical anion.<sup>2</sup>

This seminal McConnell equation paper was published just about the time when he accepted a position in the Department of Chemistry at CalTech (1957), where his longstanding academic career began. One project initiated at this time was to measure and verify negative spin density and this was, in fact, the first time that a negative spin density in a free radical was demonstrated.<sup>3</sup> He also made many contributions to understanding NMR. In the famous McConnell equations, he combined equations for a simple two-state chemical exchange process with the Bloch equations (first described by Gutowsky) for a classical description of nuclear spins in a magnetic field. This provided a useful starting point for the analysis of slow, intermediate and fast chemical exchange.<sup>4</sup> Another important contribution to our understanding of organic radicals involved the concept of odd alternate aromatic radicals where the spin density alternates in sign from one atom to the next.<sup>5</sup> McConnell theorized that if a

3D array of these radicals was stacked on top of one another so that each negative spin was paired with a neighbor positive spin, they could arrange themselves in such a way that the state of lowest energy would have the largest spin resulting in, i.e., potential molecular "ferromagnetism".<sup>6</sup> This suggestion stimulated a great deal of experimental work (but unfortunately not yet any significant practical applications) and was confirmed theoretically in important papers by other researchers in the field.<sup>7</sup>

The field of triplet excitons also became a major interest in McConnell's group, stimulated by the EPR observation of the triplet state naphthalene by Hutchison in 1957.<sup>9</sup> This stimulated McConnell to question what would be the nature of triplet naphthalene molecules in pure naphthalene? He made theoretical calculations of the expected resonances of a propagating triplet state, ie. and conceived the triplet exciton<sup>9</sup>. This resulted in a flurry of experimental and theoretical work eventually at Stanford. One project involved observing triplet excitons in charge-transfer crystals under very high hydrostatic pressure.<sup>10</sup>

Very shortly after the Stanford move in 1964, the McConnell group began studies of EPR applications to labeled macromolecular systems. While most scientists equate spin labels to the ill-named 'nitroxide' or aminoxyl radicals, the first spin labeling experiments were, in fact, demonstrated with a 'real' natural drug, the cation radical of the antidepressant, chlorpromazine radical, which was shown to intercalate the major groove of DNA. In this very clever experiment, DNA fibers/strands flowed through a very narrow capillary placed in a modified K-band cavity so that the direction of flow was either parallel or perpendicular to the applied magnetic field direction. The resulting 'oriented' spectra displayed the major axes of the hyperfine interaction for this nitrogen centered radical, confirming geometrically, intercalation into the DNA.<sup>11</sup>

While the pioneering chlorpromazine radical DNA experiment was truly seminal, its general versatility was probably limited to nucleic acids where intercalation was possible. Hence a more general approach, particularly for enzymes and proteins, was needed. Two organic chemists in the group, Tom Stone and Trent Buckman, synthesized an isocyanate analog of a pyrrolidinyl aminoxyl radical (nitroxide) that covalently labeled the amino group in poly-L-lysine, a synthetic polypeptide that could adopt an  $\alpha$ -helical or random coil conformation, depending on the pH since the terminal ε-amino group was protonated at pH values below pH 10 or 11. The late Pier Luigi Nordio worked out the lineshape theory with McConnell. Even though the 'tether' to the aminoxyl radical ring was more than four single bonds of rotation, the motional information from the spectra were uniquely sensitive to the state of the polypeptide backbone, the  $\alpha$ -helical conformer being more rigid than the random coil.<sup>12</sup> Hayes Griffith synthesized an analog of the ubiquitous protein modification agent, N-ethyl maleimide in the lab, which alkylates cysteine thiol groups in proteins and several proteins and enzymes were modified with this spin label to first demonstrate protein spin labeling.<sup>13</sup> Several important pioneering papers resulted from these first studies on several enzymes and proteins. One project involved synthesizing a spin labeled substrate analog of the proteolytic enzyme, a-chymotrypsin, that could probe the dynamics and orientation of the substrate at the active site during catalysis.<sup>14</sup> There was an intense interest in studying hemoglobin, an allosteric protein, for which the xray crystal structure was reported. Several labeling experiments were done with the maleimide and iodoacetamide spin labels that reacted with the  $\beta$ -93 cysteine thiol group; others were analogs of allosteric effectors of hemoglobin.5-16 This was truly a golden era where many of the applications of spin labeling and nitroxides (aminoxyl radicals) that are used today were conceived.

In the 1960s, little or nothing was known about the "fluidity" of cell membranes. In some groundbreaking experiments in 1968-1969 with Wayne Hubbell, he concluded that cell membranes were in a bilayer fluid-like state. In fact, the spin labeling approach was apparently the first biophysical technique applied to study the dynamic structural properties of membranes and bilayers.<sup>17-19</sup> The Mc-Connell group determined how to measure lateral and transverse diffusion properties of phospholipids in lipid bilayer membranes as well as work that demonstrated how lipid spin labels could probe of membrane structure, flexibility, 'flip-flop', bent fatty acid chains as well as phospholipid lateral diffusion in bilayer membranes.<sup>20–23</sup>

McConnell's group also made important demonstrations of the power of utilizing NMR proton relaxation enhancements of spin labeled proteins in order to both 'map' the protein structure and explore the dynam-



Harden's Birthday– a surprise conjured up by three members of the group. The entire lab went for the trip, but half were on the deck slouching from seasickness! Harden's theory was that the angular momentum vectors for the "seasick" folks were not aligned with that of the boat!

ics of the structure as well, which was one of the early studies that stimulated many other researchers to pursue this approach later on and is now a fixture in the armament of NMR protein structure methods.<sup>24</sup>

Harden McConnell became interested in the field of immunology when many labs had been trying, unsuccessfully, to show that major histocompatibility complex (MHC) peptide complexes could stimulate specific T cells. Together with graduate student, Tania Watts, he demonstrated for the first time binding of specific antigenic particles to the appropriate MHC in liposomes and supported bilayers and that specific peptides and specific MHCs in lipid membranes were sufficient to trigger a biological response from a specific T-cell. This resulted in a series of important papers on the role of MHC against virus molecules in defense.<sup>25</sup>

The McConnell group also expanded into the commercial world. He was part of a joint company, SynVar, that was a joint venture between Syntex and Varian, both of which had close ties to Stanford. Their products were specific spin label reagents and diagnostics. The most successful venture was in 1983, when he founded Molecular Devices Corporation with three former Stanford postdocs, Gillian Humphries, J, Wallace Parce and Dean Hafeman and a talented engineer, Calvin Chow. Sometime later a 4th former postdoc, Jack Owicki, joined the company. A great commercial success was the very efficient multiplate reader. It was eventually sold to a Canadian firm, MDS, Inc., which is still in business.

Needless to say, Harden McConnell received many accolades for his groundbreaking work over the decades, certainly too many to discuss here in detail. A major recognition was in 1965, when he was elected to the U.S. National Academy of Sciences at the age of thirtyeight. He won many other awards including the 1983 Wolf Prize in Chemistry, 1989 U.S. National Medal of Science for Chemistry and the 1988 U.S. National Academy of Sciences Award in Chemical Sciences. With relevance to the International EPR(ESR) Society, he was chosen for the Gold Medal (with an emphasis in Biology and Medicine) in 1997 and in 2014 he was elected a Fellow of the IES. He was also the 1995 Bruker Awardee of the Royal Society of Chemistry and the 2000 Zavoisky Award recipient. The American Chemical Society recognized him several times with the 1962 National ACS Award in Pure Chemistry, 1968 Harrison Howe Award, 1972 Irving Langmuir Award in Chemical Physics, and the 1990 Peter Debye Award in

#### In Memoriam

Physical Chemistry. Harden McConnell was certainly nominated for the Nobel Prize in Chemistry (and possibly other areas as well), but was never chosen as a finalist.

The impact of an individual on the earth can be measured only by what he/she left behind and contributed to society. Of course family is the most important and Harden's wonderful wife Sophia and three children Trevor, Hunter and Jane have carried on with the tradition of giving back to society. In addition, Harden had many scientific 'children' in the people that he trained, mentored and taught as graduate students, postdoctorates and visiting scientists, which number almost 200. Most of these people went on to prestigious, productive academic careers or influential, productive research re-

- 1. Analysis of spin-spin multiplets in nuclear magnetic resonance spectra, H.M. McConnell, A.D. McLean and C.A. Reilly, J. Chem. Phys., 23, 1152-1159 (1955)
- 2. Indirect hyperfine interactions in the paramagnetic resonance spectra of aromatic free radicals, H.M. McConnell, J. Chem. Phys., 24, 764-766 (1956)
- 3. Radiation damage in organic crystals. I. CH(COOH)<sub>2</sub> in malonic acid, H.M. McConnell, C. Heller, T. Cole and R.W. Fessenden, J. Amer. Chem. Soc., 82,766-775 (1960)
- 4. Reaction rate by nuclear magnetic resonance, H.M. McConnell, J. Chem. Phys., 28, 430-431 (1958)
- 5. Spin densities in several odd alternant radicals, H.H. Dearman and H.M. McConnell, J. Chem. Phys., 33, 1877-1878 (1960)
- 6. Ferromagnetism in solid free radicals, H.M. Mc-Connell, J. Chem. Phys., 39, 1910 (1963)
- 7. Molecular design and model experiments of ferromagnetic intermolecular interaction in the assembly of high-spin organic molecules. Generation and characterization of the spin states of isomeric bis(phenylmethylenyl)[2.2]paracyclophanes, A. Izuoka, S. Murata, T. Sugawara, H. Iwamura, J. Am. Chem. Soc., 109 (9), 2631-2639 (1987)
- 8. Paramagnetic resonance absorption in naphthalene in its phosphorescent state, C.A. Hutchison Jr., B.W. Mangum, J. Chem. Phys., 29, 952-953 (1958)
- 9. Paramagnetic excitons in molecular crystals, H. Sternlicht and H.M. McConnell, J. Chem. Phys.,

lated positions in industry and government. This is a legacy that must be highly admired that, unfortunately, not all academic scientists can claim.

The author had the honor and privilege of being mentored by McConnell and to work in the company of several students who went on to major research careers with high accolades. Lastly, Harden McConnell was a superb teacher, mentor and friend who influenced the lives of many of his students and postdoctorates. His legacy will live on and the lessons and principles that he taught his coworkers will continue to bear fruit.

Larry Berliner

- 35, 1793-1800 (1961); Paramagnetic excitons in solid free radicals, H.M. McConnell and R. Lynden-Bell, J. Chem. Phys., 36, 2393-2397 (1962)
- 10. Pressure induced phase transitions in triplet exciton crystals, A.W. Merkl, R.C. Hughes, L.J. Berliner and H.M. McConnell, J. Chem. Phys., 43, 953-957 (1965)
- 11. Interaction of the radical ion of chlorpromazine with deoxyribonucleic acid, S.I. Ohnishi and H.M. Mc-Connell, J. Amer. Chem. Soc., 87, 2293 (1965)
- 12. Spin-labeled biomolecules, T.J. Stone, T. Buckman, P.L. Nordio and H.M. McConnell, Proc. Natl. Acad. Sci., 54, 1010-1017 (1965)
- 13. A nitroxide-maleimide spin label, O.H. Griffith, H.M. McConnell, Proc. Natl. Acad. Sci., 55, 8-11 (1966)
- 14. A spin-labeled substrate for alpha-chymotrypsin, L.J. Berliner and H.M. McConnell, Proc. Natl. Acad. Sci., 55, 708-712 (1966)
- 15. Spin-label study of hemoglobin conformations in solution, S. Ogawa and H.M. McConnell, Proc. Natl. Acad. Sci., 58, 19-26 (1967)
- 16. States of hemoglobin in solution, R.T. Ogata and H.M. McConnell, Biochemistry, 11, 4792-4799 (1972)
- 17. Spin-label studies of the excitable membranes of nerve and muscle, W.L. Hubbell and H.M. McConnell, Proc. Natl. Acad. Sci., 61, 12-16 (1968)
- 18. Motion of steroid spin labels in membranes, W.L. Hubbell and H.M. McConnell, Proc. Natl. Acad. Sci., 63, 16-22 (1969)

PS The background for this article would never have been as accurate without the help of my mentor, Harden McConnell, who with the encouragement of O. Hayes Griffith and Alvin Kwiram, decided to write his memoirs for the benefit of his past students and postdocs. They were officially published (launched) on March 1, 2014 as hardenmcconnell.org, which was also the source for the article in the EPR newsletter, 2014, vol. 24, no. 1-2 pp. 18-19 entitled "Research Studies of Harden M. Mc-Connell: Together with Graduate Students, Postdocs and Colleagues." The article in this issue is actually an excerpt from a detailed biography by the author (L. J. Berliner, "Harden M. McConnell - the life of a giant in magnetic resonance: a biography and personal account" to be published 2015).

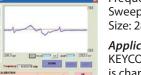
- 19. Molecular motion in biological membranes, H.M. McConnell, in The Neurosciences; 2nd Study Program, F.O. Schmitt (ed.), The Rockefeller University Press, New York, pp. 697-706 (1970)
- 20. Lateral diffusion in spin-labeled phosphatidylcholine multilayers, P. Devaux and H.M. McConnell, J. Amer. Chem. Soc., 94, 4475-4481 (1972)
- 21. Lateral diffusion of phospholipids in a vesicle membrane, R.D. Kornberg and H.M. McConnell, Proc. Natl. Acad. Sci., 68, 2564-2568 (1971)
- 22. Inside-outside transitions of phospholipids in vesicle membranes, R.D. Kornberg and H.M. McConnell, Biochemistry, 10, 1111-1120 (1971)
- 23. The flexibility gradient in biological membranes, H.M. McConnell and B.G. McFarland, Ann. N.Y. Acad. Sci., 195, 207-217 (1972)
- 24. Spin label induced nuclear relaxation: Distances between bound saccharides, histidine-15, and tryptophan-123 on lysozyme in solution, R.W. Wien, J.D. Morrisett and H.M. McConnell, Biochemistry, 11, 3707-3716 (1972)
- 25. Antigen presentation by supported planar membranes containing affinity purified I-Ad, T. Watts, A.A. Brian, J.W. Kappler, P. Marrack, H.M. McConnell, Proc. Natl. Acad. Sci., 81, 7564-7568 (1984)
- 26. High affinity fluorescent peptide binding to I-Ad in lipid membranes (supported planar membranes/ antigen presentation/T cell), T.H. Watts and H.M. McConnell, Proc. Natl. Acad. Sci., 83, 9660-9664 (1986)

## Characteristic Technologies

#### http//www.keycom.co.jp/ info@keycom.co.jp







#### Specification:

Sensitivity: S/N  $\ge$  10 at 4 mW, 1  $\mu$ M TEMPOL water solution Better at 80 mW

Sweep magnetic field: 15 mT (applicable to customize) Size: 28(W)×26(D)×35(H), 27 kg

#### Applications:

KEYCOM desktop electric spin resonance ESR-X10SB is characterized by its simple system with only one box. It is light and compact. Truly portable! Sweep magnetic field and frequency can be custom designed according to your specific purpose.

Frequency: 9.6 GHz (applicable to customize)

#### INSTRUMENT FOR ROUTINE AND RESEARCH APPLICATIONS

# **CMS 8400**



Bench - Top Electron Spin Resonance (ESR) Spectrometer

Affordable compact unit with accuracy of large systems and high sensitivity

 Easy integration with optional equipment and accessories for X-band range

**ADANI Systems, Inc** 5731 NW 151 st. Miami Lakes, FL 33014 Office: (703) 528-0035 Fax: (703) 528-0045

E-mail: info@adanisystems.com www.adanisystems.com



CMS 8400



## A new design of microwave unit.

Much better sensitivity using 'High Sensitivity Mode'

the next generation in electron spin resonance

JES-X3 Series,





RESONANCE

JEOI

 Manufacturer : JEOL RESONANCE Inc.

 1-2 Musashino 3-chome Akishima Tokyo 196-8558 Japan
 Sales Division
 ☎ +82-42-526-5226
 sales@j-resonance.com

JEOL Ltd. http://www.jeol.com/ 1-2 Musashino 3-Chome Akishima Tokyo 196-8558 Japan Sales Division Telephone:+81-42-528-3381 Facsimile:+81-42-528-3386



#### **Conference reports**

#### 47th Royal Society of Chemistry International EPR Meeting Dundee, Scotland, April 6–10, 2014

The 47th Royal Society of Chemistry annual International EPR meeting was held in April in in the Ballroom of the Invercarse hotel, Dundee, Scotland. This venue offered spectacular views over the River Tay, which is the longest river in Scotland and the largest in the UK, whilst being virtually next to Dundee Botanical Gardens. The venue had the presentation area, the dining area and the bar, integrated in one large room, which proved a very successful combination.

The RSC meeting is the longest continuously running annual EPR conference in the

One of the highlights of the RSC meeting is the annual award of the prestigious Bruker Prize, followed by the Bruker lecture. Professor Jörg Wrachtrup from Stuttagrt became the 30th winner of this award for his ground-breaking work on EPR via optical detection in diamonds that has made made room temperature single spin detection a practical reality and has opened up many new applications. This work has inspired a whole new field and resulted in numerous Science and Nature papers. The Bruker Prize is awarded by the RSC committee after an extensive nomination process and is strongly informed by the views of past winners, and Prof. Jörg Wrachtrup joins an extremely distinguished group of scientists



Poster prize winner Michael Stevens (Dundee University) with Graham Smith (left).



world and is well known both for its very high quality and friendly, informative and engaging atmosphere. The committee and local organisers work hard to keep costs down and the event is one of the least expensive major meetings in the EPR calendar with the relatively modest registration fee covering accommodation, food, three evening drinks receptions, trips, and the banquet.

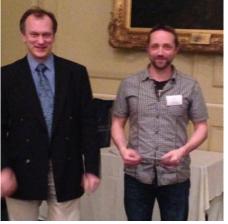
The quality of the meeting can be judged by the invited speakers and there were wonderful talks from David Britt, Christoph Boehme, Stephen Lyon, Gail Fanucci, David Cafiso, Gunnar Jeschke, Sabine van Doorslaer, Tom-Owen Hughes and Mark Newton, who not only contributed great scientific talks but made them accessible to an audience that came from a broad range of scientific disciplines. whose work has illuminated the field over the last three decades.

Prof. Mark Newton from Warwick eloquently introduced the work, and Prof. Wrachtrup went on to present an outstanding lecture on "Shedding Light on Single Spins".

The RSC committee was also delighted, at the conference, to announce a brand new award sponsored by Bruker – the Bruker Thesis Prize. This will consist of a significant monetary prize and an invited lecture at the following RSC EPR Meeting. The first award will be open to all students, from anywhere in the world, who submitted their PhD after April 2013 with a submission deadline of end of September 2014. Further details can be found on the RSC website http://www. esr-group.org Michael Stevens from Dundee won the poster prize for his work characterising the rigidity of the RX spin label at various sites on  $\alpha$ -helices and  $\beta$ -sheets for Orientational PELDOR studies, and Marco Albertini and Matthew Dale from Warwick came joint second for their work on water mediated triplet triplet energy transfer and high pressure EPR instrumentation respectively.

The Jeol Prize for the best student talk featured eight extremely strong talks, all of which received strong recommendations from the judges but in the end Daniel Klose from Osnabruk came first for his highly accomplished talk entitled "Tracing the transient conformational signal in bacterial phototaxis using SDSL-EPR Spectroscopy" with Mika Tamskii from Warwick coming joint second





Poster prize runners up Marco Albertini (Padova; centre) and Matthew Dale (Warwick; right) with Graham Smith (left).

Jeol prize runner up Mika Tamski (University of Warwick) with Graham Smith (left).



for his work on "electrochemical EPR utilizing micro-electrodes and loop gap resonators".

The organisers also arranged a wide choice of trips that included a visit to Glamis Castle, a guided tour of St Andrews (including a visit to the labs), a guided tour of Dundee Botanical Gardens and a walk along the wind-swept white sands next to the Tenstmuir Forest Nature Reserve to see the local seal colony.

The conference banquet was held in historic Lower College Hall in St Andrews (the ancient capital of Scotland) and was followed by a Scottish Ceilidh (Country Dance) in Upper College Hall where a few showed off previously unheralded dancing skills, and where the many enthusiastically participated.

Many thanks go to the organisers Dr. David Keeble and Dr. David Norman from Dundee, and the rest of their team who did a spectacular job in organizing a splendid and highly enjoyable conference that received plaudits from all those who attended.

The 48th RSC conference in 2015 will be held in Southampton near the Easter Break and will be organized by Dr. Ilya Kuprov, with details appearing soon on the RSC EPR website.

> Graham Smith (Chair of the RSC Group)

#### EUROMAR 2014 ETH Zurich, Switzerland, June 29 — July 3, 2014

The EUROMAR 2014 meeting took place June 29th – July 3rd at ETH Zurich, Switzerland with almost 700 attendees. More than three quarters of the participants came from Europe. For the first time, Asia had almost caught up with America. The traditional tutorial lectures on early Sunday afternoon were given by Daniella Goldfarb (Hyperfine Spectroscopy), by James Keeler (Introduction to Relaxation Theory), and Rafael Brüschweiler (Synergies between NMR and MD to study protein motions). These lectures were followed by the Opening & Prize Session with addresses by Bernhard Blümich (President of Groupement AMPERE), Lucio Frydman (Chairman of the EUROMAR Board of Trustees), and Gunnar Jeschke (Conference Chairman). This session was chaired by the previous Chairman of the EUROMAR Board of Trustees, Geoffrey Bodenhausen with the prizes being awarded by Beat H. Meier, Chairman of the AMPERE Prize Committee. Olivier Duss received the Raymond Andrew Prize for an outstanding PhD thesis in the field of magnetic resonance that he had written in the laboratory of Frédéric Allain at ETH Zürich. His prize talk was entitled NMR and EPR as a Tool to Study the Assembly and Structure of a Large Protein-RNA Complex. The AMPERE Prize was awarded to Christian Griesinger (MPI for Biophysical Chemistry Göttingen, who gave an impressive prize lecture on New Methods for Measuring Protein Dynamics. The first day concluded with a Welcome Mixer offering a variety of local cheeses from Zürcher Oberland and with a Jam Session for the musically inclined.

The 13 plenary lectures, 48 invited parallel lectures, and 72 contributed parallel lectures were held Monday through Thursday. Their subjects covered a broad range of applications of NMR and EPR spectroscopy as well as of magnetic resonance imaging, method development, theory, and instrumentation. Biomacromolecules continue to dominate in application work, with more than a quarter of all scientific contributions falling into this category. The trend to addressing ever larger proteins and protein complexes by NMR continues. Work on sizeable membrane proteins with high-resolution or solid-state NMR techniques is no longer exotic, but still a field where work on every new protein is linked to development of new methodology. Even larger membrane proteins can be addressed in lipid



bilayer environments by EPR spin-labeling approaches, albeit at lower resolution. In-cell magnetic resonance is still in its pioneer days, but rapidly expanding. The advantage of magnetic resonance spectroscopies over crystallography in obtaining information on protein and nucleic acid dynamics is widely use, with impressive method development going on.

Despite the fact that a satellite meeting of the COST initiative TD1103 (*European Network for Hyperpolarization Physics and Methodology in NMR and MRI*) had taken place just in the two days before EUROMAR, sensitivity enhancement by hyperpolarization techniques was another major subject of the EUROMAR conference. In this field method development still dominates application work, although applications to surface science and catalysis have come of age. In method development, the combined use of hyperpolarization and long-lived states is certainly one of the main current trends. Techniques for fast acquisition of multi-dimensional data sets are also a popular subject and can also be combined with hyperpolarization. Metalloproteins, inorganic materials, and, last but not least, small molecules & pharmaceuticals were also prominent among the application talks. The 377 posters were displayed throughout the conference and presented during poster sessions on Monday and Wednesday afternoon. Finding a poster with a given number was perceived by some as an intelligence test, but according to observations by the organizing team, all poster locations attracted similar numbers of visitors. The poster sessions were very lively and, in addition, attendees were seen discussing posters during *Bruker's Hospitality Suites* on Monday evening and the *JEOL Reception* on Wednesday evening. Participation in the popular vote for the Poster Prizes was somewhat less impressive. After discussion



**ADANI Systems, Inc** 5731 NW 151st. Miami Lakes, FL 33014 Office: (703) 528-0035 Fax: (703) 528-0045

E-mail: info@adanisystems.com www.adanisystems.com

## ESR Spectrometer CMS-8400

Sensitivity	<b>5 - 10</b> <sup>14</sup>	spins/T	Sweep width	10 <sup>-4</sup> - 0,6	Т
Resolution	0,006	тT	Operating Frequency	9,1 - 9,5	GHz
Maximum magnetic field	0,7	Т	Microwave power to cavity	0,01 - 200	mW

- Portable, lightweight table-top unit

- Full computer controlled model with a new built-in magnetic field and frequency control systems

- g-value estimation
- Time resolving mode
- Operation as EPR analyzer with special applied methods

#### **Conference reports**

notices of Meetings

#### 7th Summer School of the European Federation of EPR groups on Advanced EPR

Berlin, Germany, August 24–31, 2015

http://www.helmholtz-berlin.de/events/efepr/index\_de.html

with the Poster Jury, the Prizes were awarded to Carlo Camilloni (University of Cambride), Monu Kaushik (Goethe-Universität Frankfurt/Main), and Marielle Aulikki Wälti (ETH Zürich). The *Swiss Chocolate* part of the prizes was given only to the two teams that were still represented at the Closing Session.

One of the highlights of the conference was the Richard R. Ernst Honorary Session on Tuesday evening during which Weston A. Anderson and Richard R. Ernst nicely complemented each other and provided a funny and at the same time serious account of the history of the 1991 Nobel Prize. This session opened a special view on science as a human endeavor and raised a chord in many participants. It was followed by an *Apéro Riche*, a Swiss-style reception that turned out to have a festive atmosphere.

Despite the fairly good weather and the attractions of Zürich, sessions were well attended throughout the conference. Somehow the protestant self-discipline of Zürich must have infected EUROMAR participants. As a reward, those who were still present for the *Conference Dinner* on Thursday evening could enjoy a beautiful evening Alp view. It was one of the rare dry and reasonably mild evenings in summer 2014, which made it possible to have the dinner *Biergarten* style in front of picturesque *Schützenhaus Albisgütli*.

Thanks are due to our sponsors and exhibitors, ETH administration, ETH technical staff, SV Service for catering the breaks and Apéro Riche, the EUROMAR Board of Trustees, the Scientific and Local Organizing Committees of EUROMAR 2014, speakers, session chairman, and poster presenters, our team of blue-shirt conference helpers, and to Matthias Ernst, Giorgia Zandomeneghi, and Kristina Comiotto for their immense contribution to organizing this conference. I hope that everybody enjoyed it as much as I did. Gunnar Jeschke

Chairman of EUROMAR 2014

The "7th Summer School of the European Federation of EPR groups on Advanced EPR" will be held from August 24th 2015 to 31st 2015 in Berlin, Germany. It will be organized by the member groups of the Berlin Joint EPR lab at the Free University Berlin and the Helmholtz Zentrum Berlin fr Materialien und Energie.

The advanced EPR School is an initiative of the European Federation of EPR groups (EFEPR) to ensure the continuation of the successful development of EPR techniques and their applications. Lectures and tutorials by top researchers in the field provide close coupling between theoretical background and the experimental techniques. Methodological aspects are closely linked to different fields of application ranging from biophysics to material sciences. Graduate students and post-docs with some basic background in magnetic resonance are the main target group of the advanced EPR School (but not only). Application for the school starts December 1st 2014 and will close March 31st. A number of grants are available for graduate students and post-docs. Grant applications can be submitted together with the general application on the school web site.

For further details about the school and the application process, please visit our website.

We are very much looking forward to receiving your application. If you need more information, please do not hesitate to contact us.

On behalf of the organizing committee Dr. Alexander Schnegg Helmholtz-Zentrum Berlin fr Materialien und Energie GmbH Institut fr Silizium-Photovoltaik Kekulé-str. 5 D-12489 Berlin, Germany phone: +49 30 8062 41373 fax: +49 30 8062 41333 e-mail: alexander.schnegg@helmholtz-berlin.de

#### 57th Annual Rocky Mountain Conference on Magnetic Resonance 2015 EPR Symposium

Snowbird, Utah, USA, July 26–30, 2015 http://www.rockychem.com

#### Piette Lecture: TBA Topics & Session Chairs: Spin Devices: Ania Bleszynski-Jayich (Uni-

versity of California, Santa Barbara) – Chair Materials: Christoph Boehme (University of Utah) – Chair Methods: Susumu Takahashi (University of Southern California) – Chair Biological Macromolecules: John McCracken (Michigan State University) – Chair Biological EPR, Including Advances in Spin Labeling: Fraser MacMillan (University of East Anglia) – Chair *In-Vivo EPR*: Boris Epel (University of Chicago) – Chair

#### Scientific Committee:

Kurt Warncke (Emory University) – Chair John Morton (University College London) – Co-Chair 2015, Chair 2016 Ania Bleszynski-Jayich (University of California, Santa Barbara) Christoph Boehme (University of Utah) Boris Epel (University of Chicago)

Fraser MacMillan (University of East Anglia) John McCracken (Michigan State University) Susumu Takahashi (University of Southern California)

## Serving the scientific community for special and one-of-a-kind jobs

We have experience in designing computer interfaces for older scientific instruments, spectral analysis and image reconstruction as well as mapping and graphic layouts. Contact us for your specific needs.

Installation services

 Parts replacement service contracts  Consulting and programming
 Consulting, training, and modification services

• Experience in a number of computer languages including C, C++, FORTRAN, BASIC and assembly EWWIN - EPRWare for Windows EPR data acquisition, manipulation and line shape analysis software for Windows. SpecMan4EPR

S<sup>3</sup> Products for Spectroscopists

Software for control of pulse spectrometers.

See what we can do for you, download trial versions of our software. Visit our website for details





International Symposium on Catalytic Systems for Energy Conversion Mülheim an der Ruhr, Germany, July 23–25, 2014

n the occasion of the 65th birthday of Wolfgang Lubitz a very special three day Symposium was organized at the Max Planck Institute for Chemical Energy Conversion in Mülheim an der Ruhr, Germany. Wolfgang Lubitz started his career at the Free University of Berlin where in 1977 he obtained his PhD in the group of Harry Kurreck and Klaus Möbius. After his habilitation he spend one year as postdoctoral fellow in the group of George Feher (UC San Diego). According to Wolfgang, this was a key experience for him (both scientific and private). Following short periods as associate Professor in Berlin and Stuttgart, he became full professor at the Max Volmer Institute of the Technical University in Berlin where he stayed for 10 years. In 2000 Wolfgang Lubitz became director (together with Professor Karl Wieghardt) at the MPI for Radiation Chemistry in Muelheim which was later renamed in MPI for Bioinorganic Chemistry. Very recently, following the appointments of Prof. Robert Schlögl and Prof. Frank Neese as directors, our institute reoriented its scientific mission and is now called "Max Planck Institute for chemical Energy Conversion". The main themes of Wolfgang Lubitz' research: Photosynthesis, Water Splitting, and bio-hydrogen production, perfectly fit also in the new mission of our institute and his "birthday symposium" covered many aspects of both bio-energy conversion as well



Front: Bärbel Friedrich and Wolfgang Lubitz.

as homogeneous and heterogeneous energy conversion catalysis. During his highly successful scientific career Wolfgang supervised many talented students who later became successful scientists and continued to collaborate with him. Wolfgang Lubitz loves to maintain good contacts with his former coworkers and other collaborators and can be regarded as a "champion of networking". It is therefore no surprise that among the more than 180 scientist who participated in his birthday symposium his former coworkers were strongly represented.

The Symposium was organized in the auditorium of our partner institute, the MPI for Coal Research and hosted a total of over 180 participants. 71 abstracts were submitted. 26 lectures and 45 posters covered a large variety of topics related to energy conversion and conservation.

The Symposium was opened by Robert Schlögl, the managing director of our "MPI-CEC" institute. Klaus Möbius with whom Wolfgang has a very long standing friendship and collaboration spoke the laudatio and he commemorated many interesting and amusing stories from Wolfgang's Berlin time (picture 1). All lecturers gave their personal touch and started their talk discussing special events and memories on their long standing (or sometimes recent) collaboration they shared with Wolfgang.



#### **Conference reports**



From left to right: Martin Plato, Wolfgang Lubitz, Friedhelm Lendzian, and Klaus Möbius.

The spectrum of topics covered during the symposium is too wide to discuss here in detail. Therefore I will limit myself to selected highlights and the more EPR oriented contributions.

New spectroscopy oriented methods were presented by Frank Neese (Theoretical Spectroscopy), Peter Hildebrand (Vibrational Spectroscopy), Stephen Cramer (Nuclear Resonance Vibration Spectroscopy), Alexander Schnegg (Electrical Detected Magnetic Resonance), Edgar Groenen (High Field EPR), and Thomas Prisner (PELDOR) as well as Hitoshi Otha (High Frequency, High Pressure EPR). Frank Neese discussed new approaches that go beyond the DFT method to calculate the zero-field splitting, which is a very important parameter in high spin paramagnetic systems.

Recent developments in Hydrogenase research were presented by Robert Bittl (EPR of Oxygen tolerant hydrogenases), Oliver Lenz (Metal clusters in oxygen tolerant Hydrogenases), Yoshiki Higuchi (X-ray structure of oxygen tolerant hydrogenases), Thomas Happe (Structure and Function in FeFe hydrogenases), Frazer Armstrong (Electrochemical experiments on oxygen tolerant Hydrogenases), and David Britt who gave a fascinating account of the investigation of the maturation mechanism of [FeFe] hydrogenases using advanced EPR spectroscopy on the isotope labeled active site (H-cluster). Using <sup>15</sup>N and <sup>13</sup>C labeled



tyrosine as substrate for the chain of maturases his group was able to establish a model for the synthetic pathway leading to formation of the CN and CO ligands to the H-cluster.

Intriguing stories from the field of photosynthesis and water splitting were told by Petra Fromme, Johannes Messinger, Leif Hammerström, Marc Brecht, and Jörg Matysik. In particular the new technique of femtosecond crystallography (a true "big science" project) employed by Petra Fromme and Johannes Messinger provides exciting new prospects to disentangle the individual steps in the water splitting reaction of Photo System II.

New insights in iron based bio-inorganic systems were covered by Sabine van Doorslaer and Maria-Eirini Pandelia who both used advanced magnetic resonance techniques (pulsed EPR and Mössbauer respectively) to elucidate the structure and function of enigmatic heam proteins (globins) and iron-sulfur proteins involved in biosynthetic processes.

Hydrogen oriented inorganic models were discussed by Brian Hoffman and Thomas Rauchfuss from different perspectives. As usual, the lecture by Brian Hoffman was highly entertaining and enlightening as he discussed the intricacies of metal bound  $H_2$  rotation in a "trigonal" bonding environment and its effect on <sup>1</sup>H ENDOR spectra. Thomas Rauchfuss led us through the intermediate steps involved in hydride stabilization in NiFe and FeFe hydrogenase model complexes.

One of the most powerful implementations of Chemical Energy Conversion is through (photo)electro-catalysis and (bio)electrochemistry. Wolfgang Schumann and Marc Fontecave provided thorough accounts of these processes as applied in oxygen reduction/evolution and CO<sub>2</sub> reduction.

The last talk of the symposium was given by Avigdor Scherz, who presented a fascinating journey from photosynthesis to photodynamic therapy in cancer treatment.

During the poster session the young scientists from our institute together with many invited colleagues from abroad could present their latest results. It was a great opportunity to discuss their research in a unique gathering of high ranked scientists from many disciplines.

Apart from science, the participants in the Symposium were entertained during two highly successful social events such as the summer "grill party" at the Institute's inner court with life music from our own house-band "The Energy Converters" as well as the open-air conference dinner which took place against the background of Muelheim's medieval castle "Schloss Broich". Edward Reijerse



Magnettech GmbH // Louis-Blériot-Str. 5 // D-12487 Berlin, Germany Phone: +49 30 6780 2526 // E-Mail: sales@magnettech.de // www.magnettech.de

### Bench-Top ESR Spectrometer MS5000

magnettech

High Performance Electron Paramagnetic Resonance Spectrometer



#### **Properties**

- Cost efficient
- Compact size
- High sensitivity
- Outstanding magnetic field stability
- Wide range of accessories and glassware

#### Wide field of applications

- Life sciences
- Petro chemistry
- Food safety and quality
- Separation of radicals
- Alanine dosimetry
- Biophysical features
- Environmental toxicology
- Bioinorganic chemistry and more

### **Magnetic Test and Measurement Equipment**

- Fluxgate Nanoteslameters for measurement of environmental fields with 1 nT (10 µG) resolution.
- Hall effect Teslameters for magnet field measurement and control with resolution to 0.1  $\mu$ T (1 mG)
- $\bullet$  NMR Teslameters with field measurement from as low as 1.4  $\mu T$  (14 mG) up to 23.4 T.
- Digital Voltage Integrators for flux change measurements.
- Precision Current Transducers and Electromagnet Power Supplies.
- Laboratory Electromagnet & Helmholtz Coil Systems for spectroscopy and imaging.



955 Industrial Road, San Carlos, CA 94070 Tel: (650) 802-8292 Fax: (650) 802-8298 E-mail: sales@gmw.com Web: www.gmw.com

## The 54th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2015)

Niigata, Japan, November 2–4, 2015 http://chem.sc.niigata-u.ac.jp/~sest2015/ index.html

The SEST annual meeting discusses science, application, methodology and theory of electron spins in various fields of materials science, chemical reactions, life sciences, environment issues and so on. Deadline for the registration and submission of abstracts is 23 August 2015. Contact Information:

Tadaaki Ikoma (Chair), Ko Furukawa (Vice Chair), Tomoaki Miura (Secretary) Department of Chemistry, Faculty of Science, Niigata University, 2-8050 Ikarashi, Nishi-ku, Niigata 950-2181, JAPAN.

#### POSITIONS

#### Associate Professor of Biophysics Medical College of Wisconsin

The Department of Biophysics at the Medical College of Wisconsin (MCW) is actively seeking applications for the position of a tenure track Associate Professor to become an integral member of the National Biomedical EPR Center. We seek faculty with experience in EPR instrumentation development and an interest in collaborating on biological applications of advanced EPR instrumentation. MCW offers a unique environment for EPR spectroscopy, with an array of state-of-the art research-driven, internally developed and commercial instrumentation from 0.5-140 GHz, a highly experienced team of specialized engineers working at the forefront of their field, and a diverse faculty carrying out biomedical EPR research. Candidates are expected to contribute to the ongoing innovation, development, and application of EPR

Phone & Fax: 81(25)2627738 Email: sest2015@chem.sc.niigata-u.ac.jp

#### Modern Electron Spin Resonance – New Methodologies and New Applications Technion, Haifa, Israel, February 4–5, 2015 http://mr-lab.technion.ac.il/Schulich\_Work-Shop/index.html

The meeting will bring together the research community that is focused on the development of new methodologies in the field of electron spin resonance (ESR) along with researchers that apply them to a wide range of scientific problems. It is also planned to be interlaced with the a meeting of the Israeli Magnetic Resonance club.

Relevant new methodological tools would include, for example:

instrumentation at MCW. We seek faculty with a physics, biophysics, or bioengineering background. Individuals with an interest in highly innovative EPR-related fields are also encouraged to apply. Experience in leading a team and obtaining extramural funds will strengthen the application. For consideration, send your statement of interest, CV, and the names of three references to Candice Klug, Professor of Biophysics (candice@mcw.edu). http://www.mcw.edu/EPRCenter.htm MCW is an AA/EOE.

#### Available: Used EPR Spectroscopist

Old, but well maintained EPR Spectroscopist, with wide application experience, seeks opportunity to support active research group. EPR-based publications over 5 decades, most recently 2011, mass spectrometry publications to 2014. Experience in the study of transient organic and organometallic free-radicals; transition metal complexes; spin-trapping; 1. Ultra high sensitivity ESR – few and single spin detection techniques

2. ESR with ultra-high spatial resolution

- 3. New pulsed techniques in ESR
- 4. New and alternative detection methods for ESR signal

Relevant new applications of these techniques include, for example:

 Detection and imaging of defects, impurities, and dopants in semiconductors
 Structure determination of large macromo-

lecular complexes

Spin-based quantum computing
 Efficient dynamic nuclear polarization

Important Dates:

Abstract Submission: Dec. 15th 2014 Organized by the Schulich Faculty of Chemsiry at the Technion Email: ab359@tx.technion.ac.il

#### **Market place**

spin probe; radical ions; matrix isolation and  $\gamma$ -radiolysis techniques; photocatalysis; polymer degradation and stabilisation etc. Has Bruker, Varian and JEOL operating experience, plus track record in NMR and mass spectrometry techniques. Would prefer to work in biochem/biological area, but would consider anything interesting. Opportunity arises due to restructure of Research Department in Australian steel company after 26 years faithful service. Excellent grant writing skills, 100% success rate. Speaks English, German and some French.

Please Contact: Phil Barker pba02985@ bigond.net.au or pbarker@uow.edu.au to receive user logbook and publications list.

#### Postdoctoral Associateships in Magnetics at NIST

We offer postdoctoral opportunities in magnetics at the National Institute of Standards and Technology in Boulder, Colorado, USA. Annual salary is \$65,600 plus benefits. Ap-

BRIDGE THE THZ GAP

Virginia Diodes, Inc. manufactures mm-wave and THz sources and detectors based on our planar Schottky diode technology. Our compact and mechanically robust devices operate at room temperature and are designed for turn-key operation. High power sources are available and can be tailored to meet your needs.

Contact VDI for more details!



#### VIRGINIA DIODES, INC.

434.297.3257 | vadiodes.com

#### **Market place**

pointments are for two years. Application deadlines are 1 February and 1 August annually (but inquire earlier).

The application process is competitive. Typical successful applicants have a strong research background and academic record. Letters of reference and an original research proposal are required.

U.S. citizenship and a background investigation are required (no exceptions). www.nist.gov/pml/electromagnetics/magnetics

#### Ohio State University – EPR Center Molecular Imaging Program

A postdoctoral position is available working on the synthesis of molecular probes utilizing stable radicals for biomedical spectroscopy and imaging.

Strong background in synthetic chemistry, compound purification and characterization required. Knowledge of radical chemistry and EPR spectroscopy desirable. Please send CV, select publications, and statement of research interests to Jay.Zweier@osumc.edu. OSU is an Equal Opportunity Employer.

#### Research Positions – Advanced EPR of Biochemical and Chemical Systems

Several research positions (doctoral and postdoc level) are presently available in the Biophysical Chemistry Department of the Max Planck Institute for Chemical Energy Conversion in Mülheim/Ruhr, Germany. We are looking for highly motivated young scientists in the field of Electron Paramagnetic Resonance who are interested in studying biochemical and chemical systems related to the topic of the institute. *In-house projects*:

- Photosynthetic systems (reaction centers, water oxidation);

- Hydrogenase enzymes and related model systems;

Radical enzymes and protein maquettes.
 *Collaborative projects*:

 – EPR instrumental developments dedicated to EPR studies of (single) protein micro crystals;
 – Advanced EPR investigation of highly reactive chemical intermediates and their weakly bound intermolecular complexes.

Our lab is equipped with 10 modern EPR spectrometers covering the frequency range from 2 to 244 GHz capable of the complete repertoire of CW EPR and pulse techniques (ENDOR/TRIPLE, ELDOR, ESEEM) in combination with laser excitation and freeze quench techniques. More details can be found on our website: www.cec.mpg.de.

Candidates should have project relevant knowledge and be trained in Magnetic Resonance Spectroscopy, preferably in EPR. Candidates with an interest in EPR instrumental development and microwave engineering are specifically encouraged to apply.

Please send your application including CV and the scope of scientific interests to: Prof. Wolfgang Lubitz

Max Planck Institute for Chemical Energy Conversion, Stiftstrasse 34-36, 45470 Mülheim an der Ruhr, Germany

e-mail: wolfgang.lubitz@cec.mpg.de

#### **Bruker BioSpin Corp**

Bruker BioSpin Corp is looking for a highly motivated individual to join our EPR Service team to install and support high technology EPR Spectrometer Systems in customer research labs. This individual will install and service our EPR Spectrometer Systems and train customers for basic operation of the equipment. A BS in electrical engineering, electronics or related fields or equivalent experience is required. Experience diagnosing and repairing electronic, electromechanical and/or mechanical equipment is required. General understanding of analog electronics, digital electronics, high voltage circuitry/ circuits, microwave technology, vacuum technology, cryogenics; strong technical skills on analytical instrumentation required.

Please send resume, cover letter and salary requirements to bruker.jobseprfse0620@ bruker-biospin.com

#### EQUIPMENT

#### EPR parts, electronics and hardware

Pulse generators, amplifiers, frequency counters, etc. We also offer X-band cavities, waveguide, klystrons, cells, etc. for Varian instruments.

Please contact techepr03@gmail.com for availability and pricing.

#### **Design and construction of EPR electronics**

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 kHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field-control units to voltagecontrolled scan operation. A 6-digit 1-ppm frequency counter is available in X-, C-, S-, L-band, or MHz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the University of Denver. **Please contact:** Richard W. Quine, e-mail: rquine@du.edu, phone: 1-303-871-2419

#### Available: Used Varian EPR equipment

(1) Varian E-104 EPR spectrometer with vertical style bridge and e-line fieldial. (2) Varian E-9 EPR spectrometer. Both available with warranty and continued service support. (3) Varian TM cavity with flat cell holders and flat cells. (4) Varian E-257 variable temperature controller with heater sensor and insert holder. (5) Varian E-272B field/frequency lock accessory.

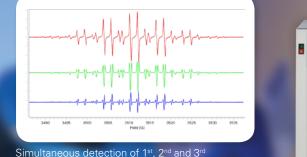
Please contact: James Anderson, Research Specialties, 1030 S. Main St., Cedar Grove, WI 53013, USA. phone/fax: 1-920-668-9905, e-mail: janderson36@wi.rr.com



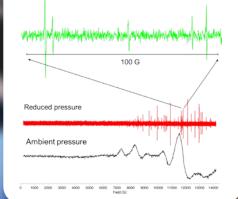
by Greater Magnettech GmbH // Louis-Blériot-Str. 5 // D-12487 Berlin, Germany // Phone: +49 30 6780 2526 // E-Mail: sales@magnettech.de // www.magnettech.de



## **CW-EPR Digital Upgrade**



harmonics of PNT sample.



High resolution, molecular oxygen Q-band EPR spectrum. Zoomed area shows the resolved individual EPR lines of the low pressure spectrum



-



## The latest digital technology for your ELEXSYS E500

Already well-known for exceptional CW-EPR performance, the ELEXSYS is evolving to provide you with the benefits of the latest digital technology and meet the demands of advanced EPR research. Update your ELEXSYS transputer/OS9 system with our Digital Upgrade Package:

- New field controller and Signal Processing Unit
- High dynamic range in both field and signal amplitude resolution
- Transient and rapid scan acquisition
- XEPR software for reference-free quantitative EPR and spin trapping data analysis

#### Discover new CW-EPR possibilities: www.bruker.com/epr

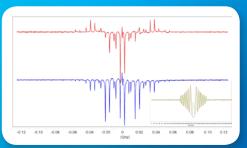
### Innovation with Integrity



## **FT-EPR Digital Upgrade**



2D experiments such as this HYSCORE spectrum can be completed in a fraction of the time with the SpecJet-II and PatternJet-II.



Shaped microwave pulses enable complete EPR spectrum inversion. Standard 13 ns square inversion pulse (top) and shaped 200 ns adiabatic inversion pulse (bottom).

Equip your ELEXSYS with the new Digital Upgrade Package, designed to meet the demands of cutting-edge pulse EPR research. Take your ELEXSYS transputer/OS9 system to the next level, joining the latest generation of FT-EPR spectrometers:

- Extensive MW pulse controls open up exciting new possibilities
- Unprecedented increase in efficiency and flexibility
- Direct phase cycling
- Simultaneous multiple slice acquisition

for your ELEXSYS E580

#### Unlock your spectrometer's potential: www.bruker.com/epr

Innovation with Integrity