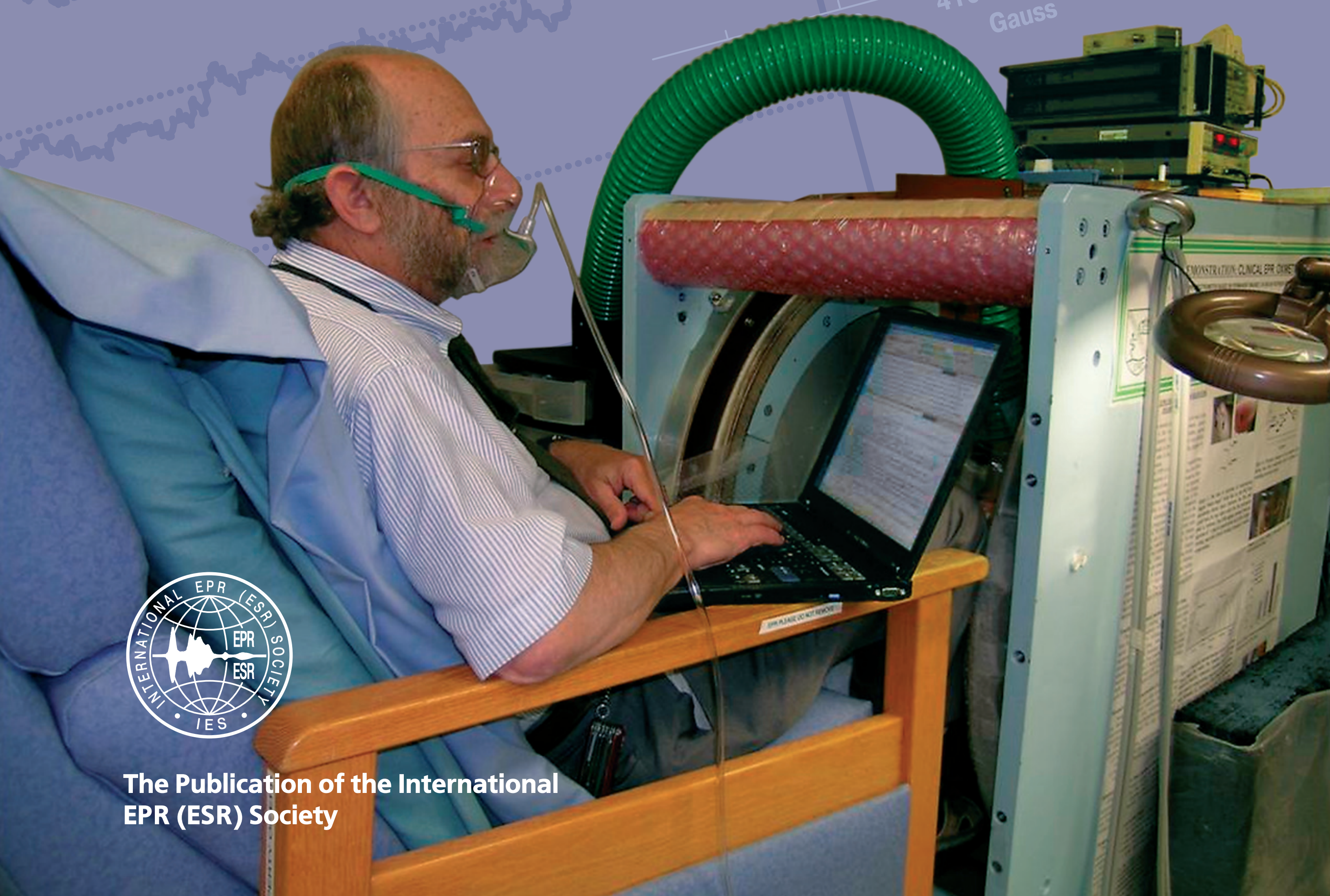
# epr newsletter

2007
volume 16 number 4



The Publication of the International EPR (ESR) Society

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

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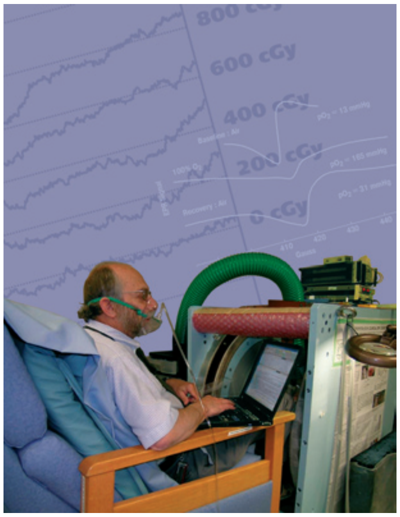


**The cover picture** highlights the development of clinical in vivo EPR spectroscopy being pursued at the EPR Center at Dartmouth Medical School led by Harold M. Swartz, recipient of the 2005 Zavoisky Award. Shown in the foreground is an image taken during a tissue oximetry measurement session where Dr. Swartz was the volunteer (and multi-tasking as usual). In this measurement the partial pressure of oxygen in subcutaneous tissue of the foot is being measured at L-band using the unique whole-body clinical EPR spectrometer. Clinical EPR oximetry is performed using India ink, which is an accepted marker for use in humans and whose line broadens deterministically with increasing $pO_2$. Data from a similar study in a patient where $pO_2$ was measured within a melanoma tumor are shown in the background just above the right-hand side of the spectrometer. These were the first EPR spectra recorded from India ink injected in human tumor tissue in vivo. These spectra demonstrate an increase in intratumoral $pO_2$ observed when the patient breathed 100% $O_2$, relative to room air. Intratumoral $pO_2$ is a critical factor in the efficacy of radiation therapy, and it is hoped that data such as these could be used by clinicians to ▶




Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

improve cancer treatment. Additional data presented in the background highlight the development of in vivo EPR techniques for retrospective radiation dosimetry using paramagnetic centers generated in tooth enamel. The density of these centers is proportional to the absorbed radiation dose and the centers are stable for durations long enough to enable archeological dating. The unique characteristics of EPR tooth dosimetry make it an attractive approach for performing triage in the general population following radiation accidents or deliberate attacks by terrorists or war.




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www.epr-newsletter.ethz.ch/corporate_sponsors.html


# Editorial

Dear colleagues,

I am happy to share with you an e-mail message from George Feher, which I have received recently. To quote, "I very much enjoyed your special ENDOR issue of the EPR newsletter and felt honored and tickled to have not only the technique but also its developer remembered. Often after 50 years an idea becomes public property and the originator forgotten (e.g. who of you thinks of Abragam and Pryce when using a Spin Hamiltonian?). Thanks for remembering and the terrific job you did." What a great compliment from a great man to all contributors to the previous issue! Dear George, thank you for your kind words!

Various aspects of the life of the EPR community are reflected in the minutes of the Annual Meeting of the IES hosted by the EPR Symposium in Breckenridge, Colorado (p. 3). One of the important points was concern about the state of finances. It is vital to have members paying their membership dues regularly. By the way, have you paid yours?

In summer 2006 Jack Freed kindly invited me to visit the five-year old National Biomedical Center for Advanced ESR Technology (ACERT) at Cornell University. I was greatly impressed by their activities and thought it would be good to have an extended presentation of this center in the newsletter. The current issue has several ACERT-oriented columns. The article about the 5th anniversary of ACERT describing the philosophy and perspectives of ACERT and new technologies they are disseminating to the biomedical community (p. 10), the brief overview of the software for simulation and analysis of EPR spectra developed at ACERT (p. 19) and the fascinating story about the magic of singing (p. 17) give you a better understanding of how one of the leading EPR centers functions, demonstrate its achievements and disclose a passion for singing of one of its collaborators. Also look forward to the 'Pro&Contra' column in the forthcoming issue featuring Jack Freed's article on dipolar spectroscopy.

To mark the 55th anniversary of Felix Bloch's Nobel Prize in Physics, we offer our readers "Felix Bloch Reminiscences" of Erwin Hahn in the '*EPR newsletter* Anecdotes' column (p. 15). Erwin is an enthusiastic contributor to the newsletter (see also 15/1, p. 14 and 16/2-3, pp. 10–12). I enjoy our collaboration tremendously. Shame on me, I learned only recently that last year Erwin celebrated his 85th birthday. I am sorry we missed an opportunity to publish a relevant article featuring a great scientist and a great personality in the 'Anniversaries' column. Dear Erwin, our belated but very heartfelt congratulations and best wishes! For the future, I have made a note about your birth date in my files.

Not to forget, you may remember the article "Composing Music: Josef Peter Heinzer" (13/3, pp. 9–11). In this interview, Josef mentioned difficulties in finding an orchestra to play his music. Since this article, he had the opportunity to record two orchestra works: Baie Mahault for violin, cello, piano and orchestra as well as the Symphony Nr. 4. Both orchestra works are available at www.swisspan.ch; if somebody is interested he may contact Josef Heinzer directly at web.mac.com/josefheinzer.

Sad news: Brebis Bleaney, Fellow of the IES and one of founding-fathers of EPR, passed away on November 4, 2006. Anatole Abragam and Michael Baker say their last farewells to him in the 'In Memoriam' column (p. 17). My personal meeting with Brebis and Betty Bleaney led me to know that they were a very loving couple caring tenderly about each other. Dear Betty, we all send you our condolences.

Laila Mosina

**If you have recently become a new faculty member in EPR spectroscopy, or know someone who has, please contact an Associate Editor for inclusion in future *newsletters*. Thank you!**
***Candice Klug***

# IES Annual Meeting 2006

Held at the 26th International EPR Symposium, Breckenridge, USA on 26 July 2006.
The meeting was opened and chaired by the President of the Society, Professor Wolfgang Lubitz and opened at 17-00.

### 1 Attendance (19)

**Members:** G. Eaton, P. Fajer, G. Gerfen, L. Mosina, S. Misra, J. Enemark, S. Eaton, R. Morse, E. Reijerse, B. Gaffney, G. Hanson, W. Lubitz, L. Kispert, B. Hoffman, G. Jeschke, G. Malovichko and C. Felix.

Apologies were received from B. Kalyanaraman, S. Tero-Kubota, C. Corvaja, S. Fairhurst and Yu. Tsvetkov.

### 2 The Minutes of the 2005 General Meeting

held on the 2nd of August 2005 were presented and Sandra Eaton moved that they be accepted as a true record of the previous meeting. Reef Morse seconded the motion which was agreed to unanimously. There were no matters arising from the 2005 General Meeting report.

### 3 Secretary's Report

• ***IES Awards 2006.*** Wolfgang Lubitz presented Prof. John Pilbrow with his Fellowship of the Society at a special ceremony in the Physics Department at Monash University after attending the ANZMAG meeting held in Murramarang National park in NSW. Prof. Kálmán Hideg received the Silver Medal for Chemistry in recognition of his contribution to the design and synthesis of nitroxide compounds and their impact on the development of site-directed spin labeling. The Silver Medal for Biology/Medicine was awarded jointly to Professors Periannan Kuppusamy and Jay Zweier for recognition of their work in modern EPR imaging and *in vivo* EPR.

The Young Investigator Award (2005) and the Silver Medal for Instrumentation (2005) will be presented to Dr. Eric McInnes (Manchester) and Mr Jos Disselhorst (Leiden) at the 6th European Federation of EPR Groups Meeting being held in Madrid in September this year.

• ***IES Awards 2007: Call for Nominations.*** Nominations are invited for the following awards: Silver Medal Physics/Materials Science, Young Investigator Award and Fellow of the Society.

For details of how to submit nominations please visit the web site: ieprs.org for the full constitution and by-laws of the Society. All nominations must be accompanied by a 100-150 word citation in support of the nomination. No nomination can be considered without a citation. Additional supporting material may be included. Please send your nomination to the President by the closing date: 15th November 2006.

### 4 President's Report

On behalf of the IES Executive Committee, Prof. Wolfgang Lubitz welcomed all participants to the 2006 General Meeting of the IES and the 29th International EPR Symposium. He expressed his gratitude to Professors Sandra and Gareth Eaton for again allowing our General Meeting to take place during this Symposium and for providing time in the program to present the 2006 Silver Medals for Chemistry and Biology/Medicine to Prof. Hideg and Prof. Kuppusamy.

Sadly, Prof. Arthur Schweiger died suddenly earlier this year. He generously set up and hosted the newsletter website, contributed a regular column and prepared a CD containing the newsletter archive. Arthur was a Gold Medal winner of the Society (1998), a former IES Secretary (1993–1996), a great scientist and a friend to many of us. The President asked the attendees to stand for one minute's silence in recognition of Arthur Schweiger.

In October Wolfgang Lubitz took over the presidency from Yuri Tsvetkov at the EU COST Working Group 15 EPR Meeting in Budapest. He also represented the Society at the ANZMAG meeting in February 2006 in Australia, at the RSC EPR group meeting in April in Edinburgh, UK and at the 29th ▶



# The 5th General Meeting of the Asia-Pacific EPR/ESR Society (APES)

## Novosibirsk, Russia August 26, 2006

The 5th General Meeting of the Asia-Pacific EPR/ESR Society (APES) was held during the Asia-Pacific EPR/ESR Symposium (APES'06) (see p. X). Sixty nine APES members attended the General Meeting.

The following researchers were elected as the APES Council Members for 2006–2008 as the Office Bearers during the meeting:

President:
Prof. Hitoshi Ohta (Japan)
Vice-President:
Prof. Graeme R. Hanson (Australia)
Vice-President:
Prof. Sergei A. Dzuba (Russia)
Founder President:
Prof. Czeslaw Rudowicz (Poland, formerly Hong Kong)
Secretary/Treasurer:
Prof. Toshikazu Nakamura (Japan)

Country Representatives:
Australia/New Zealand:
Prof. Graeme R. Hanson
Japan: Prof. Seigo Yamauchi
People's Republic of China: Prof. Yong Li
India: Prof. P. Sambasiva Rao
Republic of Korea: Prof. Sa-Ouk Kang
Vietnam: *to be appointed*
Russia (Far East):
Prof. Elena G. Bagryanskaya
Advisory Council Member:
Prof. Kaushala P. Mishra

The next General Meeting of APES will be held during APES'08 in Australia.

Hitoshi Ohta, APES President


**Profs. Kálmán Hideg and Wolfgang Lubitz**

EPR Symposium in Breckenridge, CO, USA. He will try to also represent the Society at several of the forthcoming EPR meetings in 2006/2007.

The Fellowship of the Society was presented to John Pilbrow in a small ceremony at Monash University, Melbourne, Australia in February by the President (see *EPR newsletter* 16/1, p. 5). The 2006 Silver Medals to K. Hideg and P. Kuppusamy were presented here in Breckenridge – and the 2005 Silver Medal for Instrumentation to J. Disselhorst and the 2005 Young Investigator Medal to E. McInnes will be presented at the European EPR meeting in September this year in Madrid by the President.

We will continue to report on all these events in the newsletter of the Society. I want to thank all the members of the Medal Committees for their excellent work for the Society and the former President and the Vice Presidents for their very much appreciated support and help!

### 5 Treasurer's Report

There was concern about the state of the finances, which are a result of members not having paid their membership dues. There needed to be a push for the payment of membership fees, with a suggestion from S. Misra and R. Morse that e-mail message be sent out to remind people who have not paid. Additionally, J. Enemark suggested that an e-mail be sent out in December requesting members to pay their dues for the following year. There was also a suggestion that the Society should approach companies for more sponsorship income.

**2005 Full Year Accounts** ($) (unaudited)

| | |
|---|---|
| Balance January 1, 2005 | 7073.38 |
| Income: | |
| Membership Fees | 6959.00 |
| Total Income | 14032.38 |
| Expenses: | |
| Bank & credit card fees | 712.54 |
| Web design & fees | 330.20 |
| Newsletter | 10913.00 |
| Awards | 150.00 |
| State of Illinois | 8.00 |
| Total Expences | 12113.74 |
| Balance December, 30, 2005 | 1918.64 |

• ***Society (official) Website.*** A series of screen shots was shown (see *EPR newsletter* article on using the IES website members' pages) on how to login to the Society's website (www.ieprs.org) allowing members to check whether their membership was current, pay for past and future years and also change their personal details.

A motion was moved that ALL reports be accepted by S. Eaton and was seconded by R. Morse. The motion was unanimously supported.

### 6 Newsletter Editor's Report

Laila Mosina presented the *EPR newsletter* Quiz prize (see *EPR newsletter* 16/1, p. 6) to Gareth Eaton and summarized the contents of the issues (15/3, 15/4 and 16/1) since the last IES Annual General Meeting. Their cover pictures illustrate research of recipients of the Bruker Prize 2005 (Dinse), Zavoisky Award 2004 (Salikhov & Stehlik) and the IES Gold Medal 2005 (Lubitz). On behalf of the Editorial Board, she thanked most heartily all contributors to the *EPR newsletter* with special thanks going to the CEOs of the IES and editors of the columns in the *EPR newsletter*: Shirley Fairhurst, John Pilbrow, and Thomas Prisner, and also to Stefan Stoll, our web-master and Sergei Akhmin, our Technical Editor. Laila is most appreciative of the support from Bruker BioSpin, and Sandy and Gareth Eaton, which provided her with the opportunity to participate in this symposium.

Laila Mosina gratefully acknowledged collaboration with Graham Timmins and Takeji Takui, Associate Editors, who "pass on their batons" in 2006 to Candice Klug and Hitoshi Ohta, respectively. We are deeply saddened by the untimely demise of Arthur Schweiger, who contributed a lot to the development and success of the *EPR newsletter*.

She also presented a preview of the latest issue 16/2-3, a double issue dedicated to the 50th anniversary of the discovery of ENDOR by George Feher.

Wolfgang Lubitz thanked Laila Mosina for her excellent work on the Societies newsletter.

### 7 Thanks

The IES thanks the following Corporate Sponsors for their contributions in 2005–2006.

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*GMW Associates*
*Elsevier*
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*Update Instruments Inc.*
*Scientific Software Services*
*Norell Inc.*

The IES thanks the following for their contributions in 2005–2006.

Newsletter Editor: Laila Mosina

Associate Editors 2003–2006: Graham Timmins, Thomas Prisner and Takeji Takui.

Associate Editors 2006: Thomas Prisner, Candice Klug and Hitoshi Ohta.

All paid up members.

### 8 Any Other Business

• ***Internationalization of the IES Annual Meeting.*** The president suggested that we should internationalize the Society's Annual Meeting by holding it at different locations associated with different EPR meetings around the world. This would enable international members to attend at least one IES meeting every couple of years as it was difficult to attend all EPR meetings. He suggested that the next meeting be held in conjunction with the RSC EPR meeting in Oxford on 25–29 March, 2007. The members approved this ▶

idea and it will be held in Oxford next year.

• ***EPR Mentor Prize in Honour of Larry Kevan.*** Reef Morse suggested that the Society create a mentor Prize in honour of Larry Kevan. Larry was a great mentor to his students and believed that educating students in theory and application of EPR spectroscopy is extremely important for the discipline. A new Mentor Prize would allow the society to recognized good mentors. Whilst there was general agreement about this a mechanism for its implementation was not put forward and the matter was passed onto the IES committee for further discussion.

• ***The 2007 International EPR Symposium.*** Lowell Kispert asked about the date for the 2007 symposium. Sandra Eaton responded that the dates for the meeting were listed in the Vendors information Guide (The dates are: 49th Rocky Mountain Conference on Analytical Chemistry, 22–26 July 2007) and that next year's meeting would also be held in Breckenridge to test the viability of the location. She also commented that this year the symposium was organized by a number of people and that this would also be the case for future meetings. Both Gareth and Sandra have put in place an organizational structure whereby the Vice Chair for the meeting in 2007 will become the Chair in 2008. This will ensure the long-term continuity of the conference.


**Profs. Periannan Kuppusamy and Wolfgang Lubitz**

The Chairman and Secretary thank Graeme Hanson for taking the minutes of the meeting. The meeting closed 18:39.

Awards

## IES Young Investigator Award 2007

**Leonid Kulik**

Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia

*in recognition of his development of novel pulse EPR methods, their application to chemical and biological systems, and his excellent contributions to unravelling the electronic structure of the water splitting complex in oxygenic photosynthesis.*

## Fellow of the IES 2007

**Professor Leslie H. Sutcliffe**

Institute of Food Research, Norwich, United Kingdom

## The 2007 Wolf Prize

**George Feher**

University of California, San Diego, USA

*in recognition of his research on photosynthesis, "revealing the basic principles of light energy conversion in biology".*

# The Zavoisky Award 2006 to Jan Schmidt

The 2006 Zavoisky Award in Electron Paramagnetic Resonance Spectroscopy was awarded to Professor Jan Schmidt, Huygens Laboratory, Leiden, The Netherlands) in a ceremony marking his outstanding contribution to high-field and high-frequency pulsed EPR and ENDOR techniques applied to semiconductor nanomaterials.

The ceremony was preceded by the Annual Workshop "Modern Development of Magnetic Resonance", 27–29 September 2006.

The Zavoisky Award was presented on September 29, 2006 in Kazan, the capital city of the Republic of Tatarstan (Russia). It was there that academician E. K. Zavoisky discovered EPR in 1944. The Zavoisky Award consists of a Diploma, a Medal and one thousand US dollars.

The Zavoisky Award was established by the Zavoisky Physical-Technical Institute of the Russian Academy of Sciences with support from the Kazan State University, the Springer-Verlag Publishing House, the Republic of Tatarstan, the Tatarstan Academy of Sciences, the AMPERE Society and the International EPR Society. The Award Selection Committee consisted of well-known experts in EPR: Professors G. Feher (La Jolla), D. Gatteschi (Florence), H. M. McConnell (Stanford), K. A. McLauchlan (Oxford), K. Möbius (Berlin), and the Chairman, K. M. Salikhov (Kazan). The selection of the Awardee was made after consultations with the Advisory Award Committee which comprises B. Bleaney (Oxford), Yu. N. Molin (Novosibirsk), and Yu. D. Tsvetkov (Novosibirsk).

Previous winners of the Zavoisky Award were: W. B. Mims (1991), B. Bleaney (1992), A. Schweiger (1993), J. R. Norris, Ya. S. Lebedev and K. Möbius (1994), J. S. Hyde (1995), G. Feher (1996), K. A. Valiev (1997), J. H. Freed (1998), J. H. van der Waals (1999), H. M. McConnell and Bruker Analytik GmbH (2000), K. A. McLauchlan (2001), W. Lubitz (2002), W. L. Hubbell (2003), K. M. Salikhov and D. Stehlik (2004), and H. M. Swartz (2005).

The selection of Professor Jan Schmidt was made from many nominations solicited from international experts in EPR.

The Award Ceremony starting in the afternoon of September 29 was attended by about 200 people, among them were the scientists who had participated in the preceding Workshop.

The ceremony was chaired by Professor K. M. Salikhov. He, as the Chairman of the Award Committee, announced the decision of the Zavoisky Award Committee. The presentation was made by the Deputy Prime Minister of the Republic of Tatarstan, Minister of Culture Z. R. Valeeva. The Vice-Rector of the Kazan State University, Professor N. K. Zamov, the Vice-Chairman of the Presidium of the Kazan Scientific Center of the Russian Academy of Sciences, Professor O. G. Sinyashin, and the President of the Tatarstan Academy of Sciences, Professor A. M. Mazgarov warmly congratulated the laureate. Letters of congratulations from Professor B. H. Meier, President of the AMPERE Society, Professor W. Lubitz, President of the International EPR Society, and Professor A. Bax, President of ISMAR, were handed to Professor Jan Schmidt.

J. Schmidt gave his Zavoisky Award lecture in which he told about four decades in the footsteps of the pioneers in EPR spectroscopy. A concert by a string quartet preceded and followed the ceremony. The event was concluded with a Banquet in honor of Professor J. Schmidt and his outstanding contributions to EPR. During their stay in Kazan the laureate and his spouse visited the Kazan State University, the places of historical and cultural interest in Kazan, and the Raifa monastery.

The Organizing Committee owes special thanks to the Russian Academy of Sciences, Russian Foundation for Basic Research, and the NIOKR Fund of the Republic of Tatarstan.

# The Order-of-Merit "Verdienstkreuz 1. Klasse" to Klaus Möbius

The order-of-merit "Verdienstkreuz 1. Klasse" of the Federal Republic of Germany has been bestowed on Klaus Möbius by the Federal President Horst Köhler on May 23, 2006 in recognition of outstanding scientific achievements in molecular and biophysics and of having established sustaining international cooperations with scientists in East and West.

This order was handed over to Klaus Möbius by State Secretary Hans-Gerhard Husung from the Senat of Berlin in a special colloquium of the Physics Department of the Free University Berlin on November 24, 2006. University and Institute staff members and students, many foreign guests from Russia, Israel, Poland, Italy, Holland and United States, and a large number of Klaus' friends and co-workers were present at the ceremony. Klaus Möbius does not need any presentation to the readers of the *EPR newsletter* (see also 16/2-3, pp. 12–13) but this is certainly an occasion to stress once more his high standing in the international scientific scenario.

Congratulations to Klaus Möbius from the international EPR community!

Giovanni Giacometti

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

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**Web:** www.molspec.com

Contributor to the International EPR Society

# Quadrivial Pursuit*

Keith Earle

My life has been greatly enriched, in very different ways, from my career in science and by the opportunities I've had in musical performance. I've been interested in both since earliest childhood. As many readers of this newsletter know, one of my chief scientific interests is in instrumentation development for pulse and cw high field ESR. The goal of my research is to bring the benefits of high field ESR to bear on fundamental questions of structure and dynamics in a variety of systems. Along the way, I've become quite adept at recognizing and exploiting useful techniques in the microwave and optical domains for solving instrumentation-related issues. I often feel that the intuition I've developed for recognizing elegant solutions to problems in instrumentation design has been fostered by 'aesthetic cross-training' in music.

During my childhood, I grew up in a home where music was a constant but casual influence. Over the years I dabbled in playing piano, trumpet, and a variety of recorders. All of this early exposure to instrumental music gave me a very solid background in basic music theory and allowed me to develop the ability to read and learn music quickly. Those skills have been very helpful to me over the years, particularly as a full-time professional scientist with precious little time for practicing or rehearsing.

When I was in junior high school at the age of 14 or 15, I was recruited into my home church's choir. My voice had already changed, and since I could read bass clef, due to my piano studies, I was placed in the bass section. In high school, I joined the school choir and started to participate in regional choirs. Except for general advice on vocal technique from the choir directors with whom I worked, I didn't have formal voice training at that time.

After my junior year in high school, at age 17, I auditioned for and was accepted into the Boston University Tanglewood Institute Young Vocalists Program. Tanglewood, as many readers of this newsletter will know, is the summer home of the Boston Symphony Orchestra. It was incredibly stimulating to be in such an atmosphere. We had daily voice lessons, small ensemble and large ensemble rehearsals, solfège and Dalcroze eurhythmics classes. I realized during the course of my stay at Tanglewood that I didn't have the single-minded drive necessary to become a professional musician, but the training I got reinforced my basic musicianship skills to the point that I've been able to hold my own in just about any musical ensemble with which I've been associated.

In college, in addition to my course work in physics, I took harmonic analysis and voice lessons and sang in several ensembles. The early music movement was really taking off when I was an undergrad, and there was a keen interest in singers with an analytical turn of mind, as well as supple technique, who were adventurous enough to help interpret and perform exciting but unfamiliar music being heard for the first time, in some cases, in centuries.

I think it's important to note that although I've had years of vocal training, it's always been outside of a conventional conservatory environment. Over the years, I've performed in various ensembles, done solo recital work, taken leading roles in opera, operetta and musical theater, all without official endorsement from an accredited music degree granting program, with the exception of my time at Tanglewood. This has led to some big gaps in my knowledge of the standard repertoire for my voice type: bass-baritone. On the other hand, I know a lot of unconventional repertoire that would be inaccessible or unknown to singers with a conventional background.

Throughout college and graduate school I kept up my interests in languages and literature which has been very helpful as I explored French mélodie, German Lied as well as art songs from other traditions. I should men-

* (From wikipedia.org) In medieval educational theory, the *quadrivium* consisted of arithmetic, geometry, music, and astronomy. These followed the preparatory work of the trivium, made up of grammar, logic (or dialectic), and rhetoric. In turn, the *quadrivium* was considered preparatory work for the serious study of philosophy and theology.

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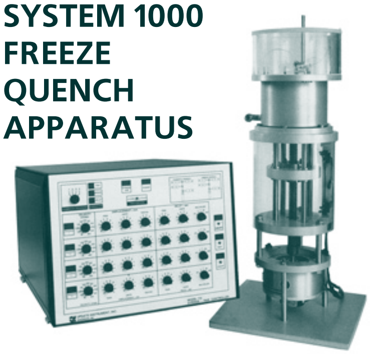

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tion that there are a number of wonderful Russian songs for low voice which encouraged me to learn (some) Russian. Some of my colleagues at ACERT are continuing my education in Russian culture by teaching me *русский мат*. To protect the guilty, I won't say who they are.

Over the years I've had some opportunities to combine scientific meetings with music-making opportunities. When I was in Klaus Möbius' lab in Berlin, for example, I joined the *Lindenkirchekantorei* for a performance of Britten's *War Requiem* with performances in Berlin, Moscow and St. Petersburg. I took advantage of the performances in Russia to arrange visits to Yakov Lebedev's lab in Moscow and Kev Salikhov's institute in Kazan.

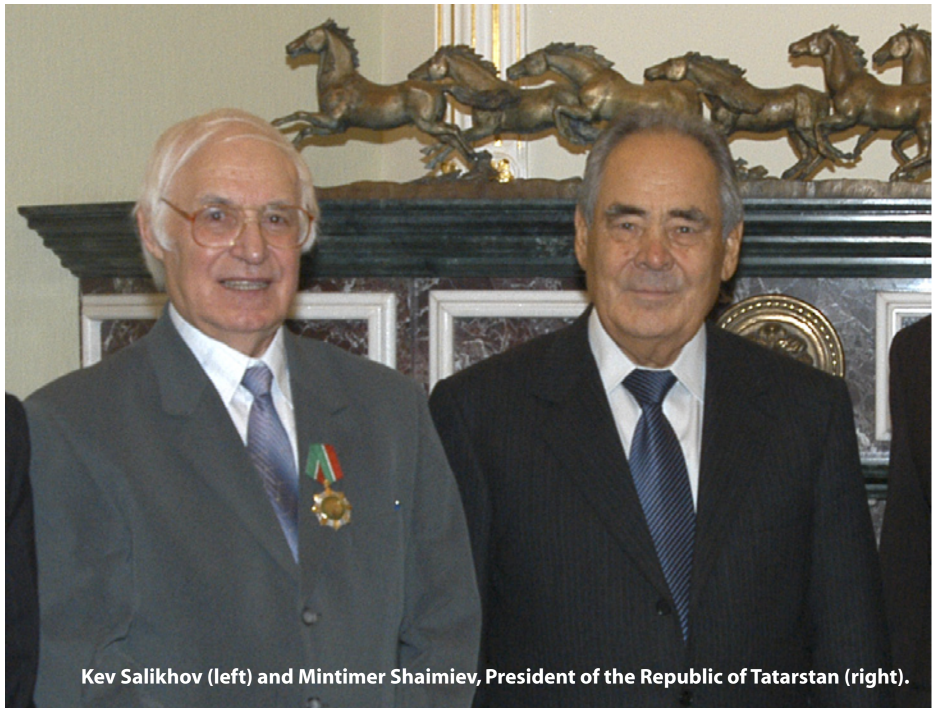
In recent years, I've been exploring my family's Scottish heritage, which has meant, among other things, learning *Gàidhlig* (Scots Gaelic) and how to play the bagpipe. I've also become interested in *Gàidhlig* song and its influence on piping and fiddling. In my lectures at the University at Albany, I've sometimes used my bagpipe to demonstrate standing waves and difference tones. It sometimes comes as a surprise to my students, as it does to some pipers, sadly, that the bagpipe can in fact be tuned. It's interesting to me that the bagpipe scale has been shifting from a set of intervals that are well-known to musicians in the early music movement to a scale based on equal temperament, such as the piano has, that is more familiar to mainstream musicians. My interests and training have placed me in a unique position to appreciate the aesthetic and technical reasons for these changes.

I'm certain that music will continue to enrich my life, as well as, I hope, for those for whom I perform. Music-making has also been a practical laboratory for understanding important physical concepts. I've tried to pass on those insights to my students in my lectures on introductory physics. On a purely visceral level, singing, particularly in a choir, and especially in the bass section has been a source of great pleasure for me over the years. I recommend the experience to anyone who can match and sustain pitch.

As an example of the kind of ensemble singing that I most enjoy, I've acquired permission for readers of this newsletter to listen to a cut from a CD entitled "Aural Borealis". The piece is *O magnum mysterium* by Giovanni Gabrieli (1557–1612). It's a motet based on the liturgy for the feast day celebrated on January 1st in the catholic tradition. As such, it seemed to me to be a seasonally appropriate choice. I sang in the bass section for this recording with a hand-picked choir assembled from all over upstate New York. It's illustrative of the very best ensemble singing with which I've been associated. One feature of the recording might be of particular interest to readers of this newsletter. The engineers placed a colleague and me close to an 'accent microphone' to enhance the bass contribution to the recorded sound. This is one of the common tricks of the trade in making recordings. If you listen carefully to the lower voices in the choir, you can pick us out, or at least I can, but then, I know what I'm listening for! Readers who may be interested in acquiring the CD, which contains Baroque instrumental music as well as music for instruments and voices, should contact the director, Tom Folan: www.naz.edu/dept/music/faculty/FolanT.html.

Music-making has also been a great way to relieve pressure when problems in the lab have weighed heavily on me. The break provided by music-making has often allowed me to return to a problem refreshed and open to recognizing the solution when it pops up.

I'm grateful that music has played such an important role in my life. I'm also grateful that I recognized early on that music should play a secondary role in my life. Perhaps the most important contribution music has made to my life is the balance it has helped me to achieve between my work and outside interests.



Kev Salikhov (left) and Mintimer Shaimiev, President of the Republic of Tatarstan (right).

# 70th Birthday of Kev M. Salikhov

Kev Salikhov graduated from the Physical-Mathematical Faculty of the Kazan State University and obtained his PhD in 1963 at the Institute of High-Molecular Compounds of the Academy of Sciences of the USSR in Leningrad. In the end of 1964 he moved to Akademgorodok in Novosibirsk and started working in the Institute of Chemical Kinetics and Combustion of the Siberian Branch of the Academy of Sciences of the USSR in the laboratory of Professor V. V. Voevodsky. In 1988, Kev Salikhov was elected the Director of the Zavoisky Physical-Technical Institute in Kazan. As a director he demonstrated that he is not only a gifted scientist but also a talented science manager. The Zavoisky Physical-Technical Institute not only maintained but also strengthened its positions as one of the leading centers of radiospectroscopy despite of the hardships of Russian science due to Salikhov's radiating energy and his devotion to science. In 1989, he initiated the establishment of a Chair of Chemical Physics at the Kazan State University. Kev Salikhov is the Editor-in-Chief of "Applied Magnetic Resonance".

As a theoretical physicist, Kev Salikhov contributed tremendously to the realization of essential scientific programs in the study of spin exchange, the development of the pulse methods of EPR and spin chemistry.

He made a decisive contribution to the theory of Heisenberg spin exchange in diluted paramagnets. He proposed kinetic equations to describe spin exchange during the collision of paramagnetic particles in solutions and used them to calculate the spin exchange cross sections for free radicals, paramagnetic complexes, triplet excitons, and also the exchange conversion cross section for positronium by paramagnetic particles. He predicted a new mechanism for the shift of EPR lines due to the exchange interaction (Yu. Molin, K. M. Salikhov, L. I. Zamaraev *Spin Exchange. Principles and Applications in Chemistry and Biology*, Springer, Berlin 1980).

Kev Salikhov laid the theoretical foundations for pulse EPR methods. He theoretically showed the possibility to observe the modulation of the electron spin echo signal in amorphous substances. For the first time he studied the role of the selectivity of the excitation of an electron spin system by microwave pulses forming the electron spin echo signals. He developed the theory of the phase relaxation of electron spins in solid paramagnets due to the spin-spin dipole-dipole interaction between paramagnetic centers. The monograph of K. M. Salikhov, A. G. Semenov and Yu. D. Tsvetkov *Electron Spin Echo and Its Application* (Nauka, Moscow 1976), was the first in the literature on pulse EPR methods.

Theoretical results obtained by K. M. Salikhov essentially influenced the formation and development of a new field of science, spin chemistry. He formulated the general formalism of the theory of magnetic-spin effects in radical reactions and with its help developed the theory of the influence of external magnetic fields on radical reactions, the theory of the magnetic isotope effect, and the theory of chemical polarization of nuclear and electron spins during chemical reactions. He theoretically predicted the extremal character of the field dependence of the recombination probability of radical pairs. He established the main regularities of the chemical polarization of nuclear spins in weak magnetic fields and theoretically predicted the effect of the mutual influence of nuclei on their polarization. He established the basic principles of the stimulated polarization of nuclear spins (K. M. Salikhov, Yu. N. Molin, R. Z. Sagdeev, A. L. Buchachenko *Spin Polarization and Magnetic Effects in Radical Reactions*, Elsevier, Amsterdam 1984; K. M. Salikhov *Magnetic Isotope Effect in Radical Reactions*, Springer, Wien 1996). He proposed theoretically a new mechanism of electron spin polarization in triplet states due to spin-selective mutual annihilation of excited triplet states.

Kev Salikhov contributed significantly to the theory of time-resolved EPR spectra and the theory of EPR spectra of electron-hole pairs formed in the singlet state in photosynthetic reaction centers: he predicted quantum beats of the EPR line intensity, the anomalous phase of the primary spin echo signal, and double-quantum transitions.

Besides the IES Gold Medal (1996) and the Zavoisky Award (2004), Kev Salikhov has been honored with several prizes and awards. For his research on magnetic field and spin effects in chemical reactions he received the prestigious Lenin Prize (1986). He was elected Fellow of the Institute for Advanced Study (Wissenschaftskolleg zu Berlin) in the 1992/93 academic year. He was awarded the title "Eminent Scientist of RIKEN" (Japan 1996) and received the State Award of the Republic of Tatarstan (1998), Lecturer of the Society of Magnetic Resonance of Australia and New Zealand (2000), and the Humboldt Research Award (2001). On November 3, 2006, he was awarded the Order of Merit of the Republic of Tatarstan (see photo).

We wish Kev further success in his research and good health for the years to come.

Yuri Molin
Yuri Tsvetkov

# Fifth Anniversary of ACERT

**Jack H. Freed**
Cornell University, Ithaca,
New York, U.S.A.

I am very pleased to be writing this article in celebration of the fifth anniversary of our National Biomedical Center for Advanced ESR Technology (ACERT) at Cornell University. It was launched in September, 2001, and we have been fortunate to have received renewed funding from the National Center for Research Resources (NCRR) of the National Institutes of Health (NIH) for another five years.

ACERT is an outgrowth of the long and extensive developments of methods, both experimental and theoretical, of modern ESR at Cornell. At ACERT we are disseminating these new technologies to the biomedical community in order that its impact will transcend beyond the ESR community. ACERT therefore welcomes collaborations with researchers in the U.S.A. and elsewhere. Our collaborations cover a wide range of biomedical research areas, for which our modern ESR methods are well-suited. The activities at ACERT are greatly facilitated by the extensive range of modern state-of-the-art ESR spectrometers that we have developed and continue to develop. It is my belief that we are now in a watershed period for the ESR field, something like the period of one or two decades ago in NMR, when the latter emerged to its present prominence in biomedical research. The ESR field is currently in a similar period, and those of us at ACERT feel that we are contributing to this.

#### Philosophy and Perspectives of ACERT

It is perhaps appropriate at this juncture to describe the philosophy and perspectives of ACERT. We believe that there are many compelling reasons to invest in the development of modern ESR methods for applications in biophysical and biomedical research. The potential of ESR may best be evaluated by considering (1) its absolute sensitivity, (2) its spectral resolution, (3) its sensitivity to different types of molecular motion, including translation, rotation, and intermolecular relative diffusion, (4) its ability to measure both short and long distances in biomolecules as well as distance distributions, (5) its ability to measure the spatial distribution of probe molecules with micron resolution, (6) the limited degree to which the measurement perturbs the "native" system, and (7) the convenience of the measurement. Methods that excel according to one or more of these criteria have found widespread use in biomedical research, for example nuclear magnetic resonance (NMR) including NMR microscopy, electron microscopy, and fluorescent or radioactive tracer molecule labeling. Although these methods may individually surpass ESR in one of these capabilities, in many ways ESR provides an optimal combination of all of these features. ESR provides good spectral and spatial resolution as does NMR, but with much higher absolute sensitivity per spin, a timescale more appropriate for examining molecular dynamics, the ability to measure longer distances, and the ability to achieve finer spatial resolution on smaller numbers of spins.

Despite these significant advantages, ESR had been lagging far behind NMR in its application to biomedical research. The reasons for this were mainly technical: the much larger magnetic moment of the electron requires higher frequencies and faster timescales, where the technology had been less developed. But the technological gap between NMR and ESR has dramatically narrowed in recent years, and it has been feasible to implement many new methods in ESR.

In recent years there has been a resurgence in the use of ESR for biomedical studies spurred by strides in understanding protein structure and functional dynamics through site-directed spin labeling (SDSL) of proteins [1–11]. In particular, doubly labeled SDSL has emerged as a powerful approach [4, 5, 10, 12–18]. New instrumentation developments greatly enhance these capabilities and allow ESR to be successfully applied to the complex structural and dynamical aspects of membranes and proteins. In addition, the theoretical methodologies for the interpretation of such experiments have been successfully developed. Many of these instrumental and theoretical advances were made in our laboratory prior to ACERT and have continued at ACERT.

The relevant developments of ESR instrumental technology have been in three main areas [10, 19]. The first is the extension of standard continuous-wave ESR (cw-ESR) to high fields/high frequencies, (HF). The second is time-domain ESR, including pulsed 2D and Fourier Transform ESR as well as double quantum coherence (DQC)-ESR. These developments have involved harnessing and adapting new and emerging technologies in microwave and millimeter wave electronics. The third is in the development of ESR microscopy both cw and pulsed. This has involved miniaturizing the technology for ESR imaging.

#### High Frequency ESR at ACERT

The extension of ESR to high frequencies (in the millimeter-wave end of the far-infrared region), with corresponding high magnetic fields, has been one of the most important instrumental advances [20, 21]. The primary advantages in going from gigahertz to subterahertz frequencies include increased signal-to-noise ratio (SNR) and improved spectral resolution in many cases [10, 19, 22]. Less obvious but equally important, are two other virtues. First, higher frequency ESR acts as a faster 'snapshot' of the motional dynamics [10, 19, 23, 24]. That is, for a given diffusional rate the spin label motion appears to become slower as one utilizes higher frequencies. Thus, for example, for the same motional rate, at low or conventional frequencies (e.g. 9 GHz) one may observe motionally narrowed spectra, whereas at high frequencies (e.g. 250 GHz) the spectra may display very slow motion, almost at the rigid limit. This behavior is a consequence of the increased importance of the *g*-tensor as the magnetic field is increased. This 'snapshot' feature has led us to a multi-frequency ESR approach for studying the complex modes of motion of proteins [11, 25, 26] DNA [27] other polymers [28] as well as membranes [29]. That is, at higher frequency, ESR spectra can 'freeze-out' the slow tumbling motions of the macromolecules, or the slow restricted overall motion of lipids in membranes, leaving only the faster internal modes of motion. ESR performed at lower frequency is then used to study the slower motions, e.g. the overall tumbling. The availability of a wide range of frequencies at ACERT, e.g. 9, 35, 95, 170, 250 GHz now enables a powerful multifrequency approach to study complex dynamics [26]. (One may contrast this with solution NMR, where all modes are usually in the fast motional limit and contribute only to $T_1$ and $T_2$.)

A second feature is the great improvement, over conventional cw-ESR, in orientational resolution of the nitroxide spectrum, due to the dominant role of the *g*-tensor [19, 20, 30]. For rigid limit spectra at 250 GHz, one can clearly distinguish the well-separated spectral regions corresponding to those nitroxide spin labels with their *x*-axes parallel to $B_0$, their *y*-axes parallel to $B_0$, and their *z*-axes parallel to $B_0$. Then as motion is introduced (e.g. by warming the sample) one can discern the axis (or axes) about which the motion occurs. Because of this enhanced resolution, the 95–250 GHz slow-motional spectra are much more sensitive to the details of the motional dynamics than are those at microwave frequencies [30]. In current work at ACERT we are benefiting from this feature of the high-frequency ESR spectra. For example, in studies of a peptide in an aligned membrane we can 'read off' from the spectrum the changing structural alignment of the peptide as a function of temperature [26, 31].

Another key application of HF-ESR is to the study of transition-metal ions found in metallo-enzymes [20, 32, 33]. Here for spins greater than 1/2 the spectrum is significantly affected by the zero-field splitting (zfs), which can be much larger than the Zeeman splitting at conventional ESR frequencies [22]. In general, transition metal ions have substantial *g*-tensors, which can yield substantial *g*-tensor broadening in disordered solids that tend to obscure the other spectral features. At ACERT, we have shown in several cases that the use of single crystals in HF-ESR is able to dramatically suppress this source of broadening [34–36].

Whereas early development and application of HF-cw-ESR at 150 GHz (2 mm) by Lebedev's group in Moscow utilized microwave technology [37], sub-millimeter-wave quasi-optical technology was required to gain entrance to the far-infrared regime, as we originally showed by developing a 9 T, 250 GHz (1.2 mm) spectrometer [38]. With its transmission mode design, a quasi-optical lens train was used by us to propagate the beam from the source to the Fabry-Perot resonator and then on to the detector. Subsequent improvements of this transmission mode design led to a very high sensitivity 250 GHz ESR spectrometer that can detect as little as $1{\cdot}10^8$ spins per Gauss of linewidth [22]. More recently, quasi-optical reflection and induction bridges were developed, promising even greater SNR improvements [10, 21, 22, 26, 39–41]. At ACERT, we have constructed two production-line spectrometers operating at 95 GHz and at 170/240 GHz which are based on such state-of-the-art quasi-optical technology. High sensitivity is achieved even in aqueous biological samples using specially designed quasi-optical Fabry Perot resonators.

## Pulsed ESR at ACERT

Time-domain ESR represents a second highlight of ESR development at ACERT. Of particular significance has been the development of pulsed ESR techniques in two dimensions (2D) [10, 19]. 2D-ESR has many analogies to 2D-NMR which has frequently been applied to the study of spin-relaxation and dynamics. In the case of NMR spectroscopy, the molecular motion in liquids leads to nearly complete averaging of the motion-dependent terms in the spin Hamiltonian, and their residual effects are then reflected only in the relaxation times $T_1$ and $T_2$ as already noted. These motional effects may be accounted for by second order perturbation theory, commonly referred to as Redfield theory. However, the equivalent terms for ESR are much larger, so they frequently lead to effects too dramatic to be addressed by perturbation theory. Instead they require a powerful approach, based on the stochastic Liouville equation, known as slow-motional theory. This theory showed that the dramatic lineshape changes are particularly sensitive to the microscopic details of the dynamics [42–44].

Unfortunately, cw-ESR spectra, especially at conventional frequencies, have only a limited resolution to the dynamics. The foremost challenge is to distinguish between the homogeneous (hb) and the inhomogeneous broadening (ib). The needed discrimination may be accomplished with the aid of electron spin echoes. But it was first necessary to develop a pulse spectrometer with very short dead-times in order to respond rapidly enough for the short relaxation times typical of ESR spectra from nitroxide spin labels in fluid media. Even more powerful are the 2D-Fourier transform (2D-FT) techniques, which required a pulse spectrometer that supplies wide spectral bandwidths in addition to very short dead-times [19, 45–48]. The availability of the second spectral dimension simultaneously provides the hb and the spin-relaxation processes, as well as elucidating the sources of the ib.

These virtues of 2D-FT-ESR, in particular 2D-ELDOR (for electron-electron double resonance), provide the capability to address both dynamics and local ordering, as we have demonstrated in several studies on membrane vesicles [10, 19, 47, 49, 50], and on lipid/protein interactions [10, 19, 48, 51]. That is, the extent of local ordering is reflected in the inhomogeneous broadening, whereas the dynamics is readily studied through the homogeneous linewidths and the evolution of the cross-peaks with time. In general, 2D-ELDOR spectra exhibit more dramatic variation as membrane properties are changed, as compared to cw-ESR, often making it possible to provide simple qualitative distinctions of the membrane properties [10, 19, 47, 48]. Our latest work at ACERT addresses the application of 2D-ELDOR to biological membranes [52].

Given the virtues of time-domain ESR, including the direct determination of relaxation rates and differentiation between hb and ib, vs. the virtues of HF-cw-ESR, including enhanced orientational sensitivity and greater sensitivity to the details of the molecular dynamics, it has been an important objective at ACERT to extend pulse techniques to higher frequencies. The challenge here was to develop a coherent pulsed high-power source at mm-wave frequencies. This is because spin-labeled biomolecules in fluid media have even shorter transverse decay times due to increased hb and ib. Thus, very short pulses of sufficient intensity are required. Furthermore, the spectral bandwidth of the slow-motional spectra increase with frequency, and this also requires intense short pulses if one is to irradiate the whole spectrum in 2D-FT-ESR experiments. At ACERT we have developed a coherent pulsed high-power spectrometer at 95 GHz which produces kW pulses that yield $\pi/2$ pulses as short as 3–5 ns [26, 53]. This has led to the extension of 2D-ELDOR to high frequency as we have demonstrated on nitroxide samples in aqueous solution and spin labeled peptides and lipids in membranes at or near room temperature [26, 53].

The fast time scales of FT-ESR will enable us to address important biophysical questions relating to the functional dynamics of proteins. Nanosecond resolution is achievable in following the time evolution of a (small) region of the spectrum, and 0.1–1 microsecond resolution is possible for the entire nitroxide spectrum that is collected by a FID. For comparison, studies by conventional cw-ESR of the transient behavior of bilabeled bacteriorhodopsin following light activation have been able to resolve key distance changes occurring on the 1 ms to 1 s time scale [13].

Another example is protein folding and unfolding, which constitute fundamental processes in living organisms. They can be studied by rapid mixing techniques. Time resolution as short as 100 μs has been achieved using cw-ESR in a kinetic-type experiment [54]. FT-ESR clearly can provide excellent resolution on this time-scale. 2D-FT-ESR experiments, which are based on performing a series of FID's, would also afford excellent time-resolution. But they would require coordinating the more sophisticated pulse sequences and time stepping of, e.g. 2D-ELDOR with the flow experiments. ACERT plans to develop the needed technology for such experiments.

The ability to doubly SDSL has made ESR an important method for the determination of intramolecular distances in biomolecules [17]. Double quantum coherence (DQC) is a powerful application of pulsed ESR with short and intense pulses, permitting distances between interacting spins to be measured in frozen media for separations ranging from about 10 to 80 Å [10, 17, 55–58]. In our development of DQC at ACERT we have shown that a sufficiently high microwave magnetic field, $B_1$, with a large resonator bandwidth is needed in order to irradiate nearly all the electron spins and to suppress unwanted signals and other artifacts, thereby providing good SNR. The virtue of DQC pulse sequences is that they permit detection of only the weak dipolar interaction between the two nitroxides in the ESR signal. In favorable cases, one may obtain the distance simply from the oscillations in echo amplitude vs. echo time that are due to just this dipolar interaction. More generally, our newer methods for inversion of the dipolar signal yield directly the distance distribution [59, 60]. The excellent SNR currently available at ACERT at 17 GHz makes it possible to obtain good results on 4 μM solutions (corresponding to just 50 pmoles) of bilabeled sample. Planned improvements will enable us to reduce this concentration to as small as 1 μM of bilabeled proteins. In addition, at ACERT we have established the more familiar technique of DEER, at 17 GHz [60, 61]. It is a very good complement to DQC. Although its sensitivity is less than DQC for low concentration samples, it is better optimized for high concentration samples. As we extend DQC and DEER to higher frequencies (e.g. 35 and 95 GHz) using our high-power pulsed spectrometers, we anticipate further increases in sensitivity enabling the study of even smaller amounts of bilabeled proteins. Measurements of longer distances are most effective in providing constraints on the structures of large, complex proteins [17, 57, 60–64]. Pulsed ESR has several key advantages when compared to fluorescence energy transfer: there is no orientational $\kappa^2$ problem, since the electron-spin dipole moments are aligned by the magnetic field; the same spin label is used at both sites rather than a distinct donor and acceptor; spin labels are generally smaller than most flourophore labels; and the distribution in distances can be directly measured.

### ESR Microscopy at ACERT

A very new development in ESR instrumentation at ACERT has been in ESR microscopy. When heterogeneous samples are considered, ordinary magnetic resonance spectroscopy often lacks the capability to properly resolve the various spectral features originating from different parts of the sample. The obvious solution to this problem is to obtain spatially resolved spectral information by means of magnetic resonance imaging. NMR has been doing just that for years, not only with large subjects at mm-scale resolution (as in medical MRI), but also with microscopic samples at micron-scale resolution (termed NMR microscopy [65]). Commercial NMR microscopes and imaging probes are available from several vendors and are used for the characterization of tissues, non-invasive tracing of unicellular organisms, investigation of transport phenomena, histological-like applications and much more, with practical resolution limits of ~10–20 microns [3, 66–70]. Two primary factors limiting the resolution in NMR microscopy are the weak signal from a small imaged voxel, and the diffusion of the spin-bearing molecules over the long time-scale of NMR (e.g. $T_2$'s ~ ms) [69, 71, 72].

ESR imaging had been less developed with respect to microscopy, and, prior to our recent efforts was mainly concentrated on the observation of large biological subjects [73–76] with mm-scale resolution. We have developed an ESR microscope (ESRM) that is already on a par with the most advanced and mature NMR microscopy techniques [77–79]. Developments in ESR resonator technology, magnetic field gradient coils, and fast current drivers at ACERT have enabled us to obtain three dimensional ESRM images with resolution as good as ~3×3×8 microns with test samples. The current ESR microscopes at ACERT, operating at 9 and 16 GHz, can image both solid and liquid samples, in both cw and pulse mode.

ESR has inherently several potential virtues over NMR, which could make this technique more suitable for microscopic applications. For example, the signal per spin is much higher than in NMR [80], diffusion does not limit the resolution in the short time scales ($T_2$'s ~μs) of the ESR measurements [81–83], ESR micro-resonators detect with a quality factor ($Q$) of ~1000 compared to the $Q$~10 of the NMR micro-coils [65, 84], the ESR line-shape is more sensitive to dynamic effects--leading to richer information [10, 19] and finally there is the lower cost of ESR electromagnets. Since most samples do not contain unpaired electrons (e.g. stable free radicals), these paramagnetic species must be added in a manner similar to that of adding contrast agents in NMR or dyes in optics. This is a standard procedure, especially for microscopy. In addition, unlike NMR microscopy, ESRM is at its infancy and can still be significantly improved in many of its aspects. Future progress will include employing elevated frequencies to increase sensitivity, using pulsed field gradient techniques to directly measure and image the self diffusion coefficient, employing pulse techniques for the acquisition of full 3D spatial-1D spectral images, improved sample preparation techniques, and the use of combined optical-ESR imaging systems. Such future developments should enable routine ESRM measurements of bio-samples with a resolution better than 1 micron, which would enable one to obtain unique information about embedded radical distribution in live samples and other bio-related systems (e.g. controlled drug release [85]), $O_2$ concentration, reactive oxygen and nitrogen species in live cells, as well as self diffusion coefficients, molecular ordering parameters, and molecular dynamics.

### Spectral Simulation at ACERT

A major long-term activity of our research group, which continues at ACERT, has been to pioneer and develop methods for the rigorous interpretation of spin-labeled ESR spectra [42–44]. Unfortunately, the ESR spectra arising from many biological studies are complex and can be misinterpreted by superficial analysis. In our past work we demonstrated how detailed and accurate information regarding ordering and anisotropic rotational diffusion are obtained via ESR lineshape analysis over the whole motional range [42–44]. Our model of microscopic order with macroscopic disorder (MOMD) has proved of great value in analyzing studies on spin-labeled proteins [8, 86] or on lipid/protein interactions [58, 86–94]. Membrane vesicles offer a good example of this. Spin-labeled moieties in the different vesicle regions are oriented at all angles with respect to the magnetic field, thus providing a 'powder-like' spectrum with ib superimposed on the hb, and the degree of ib is determined by the extent of local (microscopic) ordering. This represents the first level of sophistication that we introduced into the analysis of ESR spectra from complex biological systems, and it has enabled a number of successful interpretations. Our theoretical methods of simulation have been developed for 2D-FT-ESR, in particular 2D-ELDOR [44, 95]. Since it is possible to distinguish in these experiments between hb and ib, it has been possible to clearly and unambiguously demonstrate the MOMD phenomenon [10, 19, 47, 48]. Very recently more advanced methods have been introduced in the analysis of 2D-ELDOR experiments which enable them to distinguish subtle changes in biological membranes (resulting from cellular activation) that cannot be discerned by conventional cw-ESR [52]. The very high resolution of 95 GHz 2D-ELDOR has posed new challenges to spectral computations, which we have recently addressed successfully at ACERT with the development of new computational algorithms.

Our more advanced dynamic model, known as the slowly relaxing local structure (SRLS) model, deals with the complexities of protein dynamics [23]. It simultaneously incorporates both the internal and overall modes of motion. This sophisticated model involves many dynamic and structural parameters, which necessarily require the multifrequency ESR approach described above in order to supply sufficient experimental data to fit them satisfactorily. The challenge of fitting ESR spectra at several frequencies simultaneously has been addressed at ACERT with a new software package utilizing the SRLS model [11]. Recent collaborative studies have shown that frequently two (or more) conformers with distinct spectra at each frequency are commonly found in the study of protein dynamics [11, 25]. The possibility of exchange between conformers is being addressed at ACERT in a new software package for multi-frequency ESR including SRLS.

### Concluding Remarks

Of course, this resurgence of interest in ESR is leading to emerging new ESR Centers world-wide. ACERT plans to interact with them with the goal of furthering the development of the modern field of ESR. Further information about ACERT, its activities and personnel, may be found at our website: www.ACERT.cornell.edu.

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# Felix Bloch Reminiscences*

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I am not inclined toward giving after dinner speeches. But, when Bill Little asked me to give a 'light speech' in memory of Felix Bloch, I had no alternative but to accept out of gratefulness to what I and many of us have gained from Felix. In recalling a few personal memories of Felix I don't claim to represent in my views everything about him, as you all knew him somewhat from different points of view. Nevertheless I will take the liberty to make a few generalizations about Felix from these memories.

When I first arrived as a postdoc at Stanford in 1950 I remember vividly my first contact with Felix Bloch. He was sitting on a lab stool in the basement of 'Old Physics Corner' hunched over a chart recorder inspecting NMR signals newly obtained by his students, huddled around him. That image of Felix epitomized his relationship toward experimentalists. He did theory for experimentalists, and liked to fancy himself also as an experimentalist. It was marvelous the way Felix could apply quantum mechanics with ingenuity and elegance directly to experiments. The clean lines of his physics reminds me of the music of Mozart – easy to read but demanding in its playing and interpretation.

Felix was in the habit of taking afternoon naps, and then would show up in the lab around four o'clock in the afternoon, ready and eager for activity, while the rest of us developed some fatigue toward the end of the day. I became aware of a tradition in force that adjusted to this habit of Felix. Everyday one or two of the NMR lab group, at least, were commissioned to remain in the lab to interact with Felix - something like guard duty in the military, riot that it was unpleasant, but just so make sure that by coincidence, not everybody might have gone home at the end of the day. Warren Proctor told me that this was a long practice at various times among Dharmatti, Packard, Rogers, Jeffries, West, Weaver, Anderson, Levinthal, Arnold, etc. Felix would, of course, make inquires as to how the research was going, and in turn, the group had the policy of preparing a question first in order to distract Felix from the fact that the group had nothing new to report for the day. In making up questions, they tried to steer clear of anything not in his expertise, but once they thought they fumbled completely and asked Felix about an electronic bug they couldn't eliminate. To their amazement, Felix went to the blackboard and wrote down seemingly irrelevant, impractical, formal Maxwell's equations. Finally he homed in on the final answer, pointing out the particular hardware that had caused the trouble.

This anecdote is just one out of many incidences which show the remarkable originality and self-reliance on fundamental principles which characterized Felix Bloch. In contrast, for example, I. I. Rabi, a highly intuitive physicist but with less finesse, on a similar occasion contributed his expertise on an experimental problem less directly as follows: Once he walked into his molecular beams lab at Columbia and was accosted by one of his students who complained about ground currents from the r.f. oscillator. Rabi instructed him by saying, "The solution is obvious. Put in the boundary conditions and solve Maxwell's equations!"

At Stanford Physics Colloquia, Felix demonstrated a remarkable reaction to physics he had never heard of before. The speaker would introduce a subject most people knew about, at least from the current literature, which Felix didn't read. For about the first half of the colloquium Felix would ask apparently dumb questions to bring himself up-to-date. Then for the rest of the colloquium, he would chime in and transcend the speaker by telling him where he might have gone wrong and what he or she should do improve his or her results. I like to contrast this kind of colloquium one-upmanship with that of Emilio Segre. Emilio usually appeared to be sleeping during a colloquium, but actually his audio reception was not switched off. He would wake up at the end of the talk and ask questions with the sharpness of a stiletto. On one famous occasion he interrupted his sleep by asking the speaker, "Tell me! Who supports your research?"

I once mentioned to Felix that the best one-upmanship at a physics talk I know of worked the other way. You all remember our one-time antiquarian Secretary of the American Physical Society (APS), K. K. Darrow, who, if he had lived a little longer, would have had the Bulletin of the APS printed in Latin. Darrow stood up in the rear of an auditorium when I. Lowe was giving a half-hour invited talk, and interrupted Lowe by intoning: "Dr. Lowe, would you kindly speak louder, enunciate clearly, and provide more perspicacity in your phraseology!" Lowe replied, "Sir, anyone who is interested in what I have to say is sitting up front!"

Felix was a wonderfully clear teacher. His fundamentalism was evident in his use of the original works of J. W. Gibbs as a text in his course in statistical mechanics. After his retirement Felix began the writing of a text on Statistical Mechanics based on his rigour of interpretation, which was unfinished at the time of his death. It was edited and extended subsequently by Professor J. D. Walecka. I learned only recently that Felix had a small hobby of doing this sort of thing in another vein. During short visits to Israel he resorted to the original Hebrew in carrying out translations of the Old Testament, which was so stated in his honorary degree Laudatio at Oxford University.

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The conventional label of Professors is that they should be absent minded, self involved, and somewhat remote at times. We all suffer a little bit from all of these things, but I must say that on social occasions Felix was quite a courtly, debonair host. Just for your amusement; may I give an account of the antithesis of Felix in the remote personality of Paul Dirac. Dirac at his college in Cambridge was asked by a Fellow of his college if he had a graduate student who could escort a young lady guest to a college dinner. Without hesitation, Dirac replied: "I had a graduate student once but he died!" There was another incidence relating to Dirac's late marriage in life, about which he was rather bashful. He was so shy about it that he introduced his wife to the Fellows of his Cambridge College, not as his new wife, but rather as Wigner's sister, which she was!

Felix had a down-to-earth appreciation of experimental physics which inclined him to have long discussions with experimentalists and with people like Russell Varian. Varian impressed Felix time and time again with the fact that his intuition was quite deep, not requiring any formalism whatsoever – something like that of a Michael Faraday. Most memorable were Felix's discussions, as you all remember, with Hans Staub, the Swiss experimentalist who was a close colleague of Felix. Handwaving arguments between those two were loud and ludicrous. First of all, Staub used the most eloquent and articulate profanity; and on numerous occasions the whole Physics Department would reverberate with the Schweitzer Deutsch Exclamations of "OOCH! YAH! OOCH! YAH!" The streams of Schweitzer Deutsch dialect from those two was no less weird than if two Martians had landed from outer space and had a conversation. A typical argument between Staub and Bloch would go as follows: When Bloch thought he had a good idea for an experiment Staub would shoot it down. Then Bloch would cuss at Staub good naturedly in Schweitzer Deutsch for ruining what he thought was a good idea.

Felix, of course, was highly amused by Staub's behavior, and Felix himself had a roguish sense of humor. I enjoyed his intellectual kind of satire. In those early days when his interests were more along the lines of single particle properties of spins and magnetic moments, the statistical aspects involving the chemistry of condensed matter did not initially excite him. I remember when Dick Norberg and I were telling him about our data in metals and liquids. Felix said, "Norberg, you should be a metallurgist... and Hahn, you should be a chemist!" Sometime later, Felix was trying to understand a paper by Al Redfield which dealt with the subject of spin-temperature. At first Felix was convinced that the paper was nonsense. Then after he read it again carefully, he finally understood it, was impressed by the paper, and asked me... "Tell me, Erwin, this guy Redfield, he must be Jewish?!" Then, after I read the paper, Felix asked me if I understood it. I said, ''Yes, about half of it, so I think Redfield must be half Jewish!" Actually, Al Redfield is a blue blooded thoroughbred New Englander Goy, who apropos to this story is now a Professor at Brandeis University. Speaking about nonsense reminds one of a pertinent Pauli story, one of many which Felix would tell, and then I want to make a connection between Bloch and Pauli. When Landau asked Pauli if he thought his theory of diamagnetism was nonsense, Pauli said, "Oh no! Far from it! What you said was so confusing, one could not tell if it was nonsense!"

In retrospect, having learned Pauli stories from Felix and others in the years following my short Stanford career, it appeared that Felix reflected a similar kind of Pauli humor with its cutting edges, but certainly not with the same cruelty. In a rather mild sense however, I believe Felix took on some of the pithy and sharp satirical humor of Pauli. It is well known that some of Oppenheimer's students took on certain behaviorisms of Oppenheimer. Certainly Felix did not go that far in behaving like Pauli. I came to this conclusion more so after having read the autobiography of Rudolf Peierls, entitled "The Bird of Passage". In fact the Pauli stories I have recounted are given in his autobiography. Peierls was a contemporary of Felix at Leipzig in 1927, and Felix was assistant to Pauli in 1928 and also in 1930 at the ETH in Zurich. For example, on more than one occasion I heard Felix say, probably influenced by Pauli, that he could get to know certain people better (those for example, who were candidates for a faculty position) by getting them drunk. Peierls, in his autobiography, gives an account of this very happening. Pauli invited Peierls to his house, got him drunk, found he was no more interesting than when he was sober, and abruptly sent Peierls home.

When it came to giving students advice, Felix always was ready with sympathetic fatherly counsel. This is where Bloch and Pauli certainly differed. A lot of us are acquainted with a Pauli 'one liner' in which he rejected a paper, as a referee for a publication, by saying "It's not even wrong!" That statement is the epitomy of the following real event, involving Bloch, Fokker, and Pauli. Pauli was teasing Bloch for making an error of a factor of 10000 in a calculation (actually, Bloch was only showing that in his calculation a certain effect was negligibly small). Then Pauli turned to Fokker and said, "This doesn't happen to you Fokker – your factors are correct." Fokker looked pleased. "Yes, you could write a paper with the least physical significance, but the factors would be correct." Fokker looked not so pleased.

Felix was not inclined temperamentally for the tasks of administration. As an Instructor at Stanford, I remember the occasion when a faculty meeting was called by Leonard Schiff. The meeting lasted only about twelve minutes because adjournment was moved and seconded by Felix, in violation of Robert's rules of order. It was a triumph of conciseness which nowadays would be impossible to impose.

I have touched only briefly on the character of Felix Bloch as a man who loved physics (with none of the same for administration), who made towering contributions to physics (deserving the Nobel Prize thrice over), who was imbued with good humor, culture and a deep concern about world affairs; and along with these things he was a devoted family man. The Bloch residence was a hospitable gathering place with Lore and the Bloch family coming together for numerous sessions of chamber music, often with Felix at the piano. He was an accurate and inspired performer. His style of playing exhibited a perfectionism, in constant awareness of nuances demanded by the composer.

May I close by expressing my thanks for the opportunity to recall memories of Felix Bloch, for the privilege of having interacted with him, and for the friendships acquired during those times at Stanford when he flourished.


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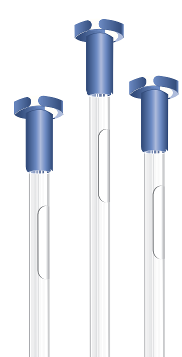
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# Brebis Bleaney (1915–2006)

Professor Brebis Bleaney, one of the founding fathers of EPR spectroscopy, died in Oxford on Saturday 4th November at the age of 91. He had a long association with Oxford, starting as an undergraduate at St. John's College in 1934. After completing his D.Phil. thesis in 1939, his work was interrupted by the war. He became the first Fellow and Tutor in Physics at St John's in 1947, where he remained until he transferred to Wadham College when he became the Dr. Lee's Professor of Experimental Philosophy and head of the Clarendon Laboratory in 1957. It was during that decade that he made his strongest contribution to EPR and was elected a Fellow of the Royal Society in 1950. After twenty years of administration, Brebis longed to get back to day to day involvement in research, so in 1977 he resigned the Dr. Lee's chair and started a new research career with a new research group on enhanced NMR, becoming a Warren Fellow of the Royal Society from 1977–80 and subsequently a Leverhulme Emeritus Fellow from 1980–82. He was awarded the Zavoisky Prize in 1992. He is survived by his wife Betty and their two children Michael and Heather.

The *EPR newsletter* published an article in 2005 celebrating Brebis's 90th birthday (on 6th June, 2005); about him, his work and his interaction with his students and collaborators.[1] As that article is so recent, this article will attempt to overlap with that as little as possible, but rather add to it a wider scientific perspective. To form a rounded picture one needs to read both articles.

From the brief chronology above, it is evident that there are four distinct phases to Brebis's contribution to science: from 1939–48 a wartime of development of microwave oscillators and circuitry for RADAR; from 1945–57, the period for which Brebis is best known for his invention and exploitation of EPR (simultaneously with its independent invention by Zavoisky in Russia); from 1957–77 mainly a heavy administrative load in charge of the Clarendon Laboratory, which comprised the major part of the Physics Department, but during which he still found time to write many single-author papers on innovative topics; and from 1977 until about 1995 a return to close involvement with research, possibly even closer, with a greater flurry of publications, than in the post-war period as there were no distractions by teaching and lecturing duties.

Brebis's principal exploitation of EPR was in dilute paramagnetic salts at low temperatures. One can trace the threads which led to this work from his earlier career: a D.Phil. thesis on the properties of matter at very low temperatures (a thermodynamic temperature scale using potassium chrome alum, the magnetic susceptibility of manganese ammonium sulphate, the vapour pressure of liquid helium II); the wartime work on microwave generation; a post-war measurement of the absorption of microwaves by gaseous ammonia. The milieu of Oxford also was right, with Simon, Mendelssohn, Kurti and Cooke working at very low temperatures using paramagnetic salts, and Griffiths and Bagguley working on different resonance topics. Brebis interacted strongly with other researchers: daily with his own research students, with other research groups in the Department as indicated by many joint publications, with researchers at other labs as shown by many visitors and his constructive comments at conferences, and very importantly with professional theorists like Pryce, Abragam, Stevens, Elliott and O'Brien. During this period, in addition to a flood of publications coming from his research group, he wrote a large number of single-author papers about a range of related topics, as well as some co-authored with other groups, which shows the great fruitfulness of his mind and the mutual influence between him and other research groups in the low temperature condensed matter field.

The strong interaction with professional theorists, also resulting in many joint papers, is an important feature of Brebis's contribution to the field, demonstrating how productive this could be by two-way mutual stimulation. For example, out of this interaction arose the concept of the spin Hamiltonian, used now by everyone for the analysis and understanding of experimental data.

***A Few Lines about Brebis***

*In the course of a long life it has been my good fortune to interact, collaborate and some time publish with a few great physicists. Without indulging in name-dropping, I think I can mention J. H. Van Vleck, E. M. Purcell, Felix Bloch, R. V. Pound, Jean Brossel and Alfred Kastler. I think that with none of all these, whom I admired and loved, was the contact closer and interaction fuller and friendlier than with Brebis Bleaney.*

*Let this be my last word about him.*

*Anatole Abragam*


TAKEN BY NINA ABRAGAM

[1] EPR newsletter 15/2, 7-8 (2005)

In the first decades, the frequencies of measurement of EPR were limited by available radiation sources and detectors and magnetic fields. Except for these limiting components, most of the spectrometers were home made. Possibly, the relative simplicity of the equipment and the ease of its duplication contributed to the rapid uptake of EPR, after Brebis's invention, by groups in other parts of the world. In the sixty years since its invention, the technique has become so widely used that commercially built spectrometers are now the norm. Also, in this early period, there was not the computing power now available; so, for example, complicated spin Hamiltonians were often solved using perturbation theory.

Bleaney's initial use of EPR to study d- and f-transition metal ions in solids, contributed to a firm understanding of the magnetic properties, optical spectra and interaction between the ions and their solid environment in paramagnetic salts and other crystalline solids. From this small beginning, by showing what could be achieved, this pioneering work stimulated an expansion of the use of the technique to the present usage over a wide range of topics involving unpaired electron spin by a wide range of scientists: chemists and biologists as well as physicists.

Hyperfine structure (HFS) became an important feature of Bleaney's early work, after its discovery in a diluted copper Tutton salt by R. P. Penrose, Brebis's his first co-worker on EPR. HFS is a thread which ran through much of his work, from measuring nuclear spins, to nuclear alignment and orientation to monitoring the distribution of unpaired electron spin around a paramagnetic ion or defect, to exploitation of ENDOR, to much of his later prolific career on enhanced NMR. The experimental realisation of enhanced NMR was made possible by collaboration with Neville Robinson, who designed and made the required high frequency spectrometer.

This renaissance of his personal research in his sixties and early seventies was quite remarkable, even allowing for the absence of teaching and lecturing duties. One wonders how many other ventures his fertile mind and great energy might have produced in the 20 years he devoted to administration.

Many of Brebis's early contributions, from around half a century ago, are now part of the folklore: his death is an occasion to remember his very large influence on the subject.

Michael Baker


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## *Advanced ESR Methods in Polymer Research*

Shulamith Schlick (Editor)

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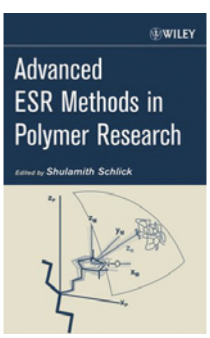


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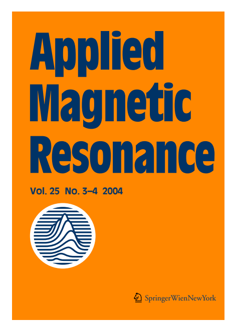


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Computer Corner

# Software Available from ACERT Web Site

Yun-Wei Chiang, Zhichun Liang, and J. H. Freed

There is extensive software available from the ACERT website for simulation and analysis of EPR spectra. Included are:

(1) Original versions of well-known programs described in the papers "Calculating Slow Motional Magnetic Resonance Spectra: A User's Guide" by D. J. Schneider and J. H. Freed [1] and "Nonlinear Least-Squares Analysis of Slow-Motional EPR Spectra in One and Two Dimensions Using a Modified Levenberg-Marquardt Algorithm" by D. E. Budil, S. Lee, S. Saxena and J. H. Freed [2] and their most recent updates: **EPRLL**, **PC**, **NLSL**, **PC.NEW**.

**EPRLL** – the basic simulation programs for CW spectrum calculation including the program EPRBL used to determine the truncated basis sets. A detailed description of the method and Version 1.0 of the program is given in the "User's guide" by Schneider and Freed (1989). See file UPDATE.DOC for cumulative changes through Version 1.6b that have been made in EPRLL and related programs since the publication of Version 1.0.

**PC** – the original PC version of the CW spectrum simulation programs (11/3/95).

**NLSL** – the least squares version of the above CW program described by Budil et al. (1996). See the subdirectory EXAMPLES for fitting examples to test.

**PC.NEW** – a version of the NLSL programs suitable for running on a PC with Windows 98/2000/NT/XP. Besides executables and calculation examples the folder contains files, which are necessary for Fortran Powerstation 4.0 to compile and link the source files from NLSL folder. See README.TXT in this directory.

(2) Original versions of well-known programs and recent updates for 2D-FT-ESR described in "Theory of Two-Dimensional Fourier Transform ESR for Ordered and Viscous Fluids" by S. Lee, D. E. Budil, and J. H. Freed [3], "Non-Linear Least Squares Analysis of Slow-Motion EPR Spectra in One and Two Dimensions Using a Modified Levenberg-Marquardt Algorithm" by D. E. Budil, S. Lee, S. Saxena and J. H. Freed [4], and "Two-Dimensional ELDOR in the Study of Model and Biological Membranes" by Y.-W. Chiang, A. J. Costa-Filho and J. H. Freed [5]: **NL2DC**, **NL2DR**, **NLSPMC**, **NLSPMC_ri**, **NLSPMC_qmr**.

**NL2DC** contains the two-dimensional Fourier Transform (2D-FT) version of the least squares program using the conjugate gradients matrix solution method. For 2D basis set pruning see the subdirectory BASIS in NL2DR.

**NL2DR** contains the 2D-FT version of the least squares program using the Rutishauser matrix solution method. For 2D basis set pruning see the subdirectory BASIS.

**NLSPMC** contains the 2D-FT version of the least-squares program using the conjugate-gradient method. This version is capable of simultaneously fitting multiple spectral components and multiple spectra of different mixing times. This is an upgraded version of the NL2DC. See "Lipid-Gramicidin Interactions: Dynamic Structure of the Boundary Lipid by 2D-ELDOR" by A. J. Costa-Filho, R. H. Crepeau, P. P. Borbat, M. Ge, and J. H. Freed [6].

**NLSPMC_ri** contains the full Sc- 2D-FT version of the least-squares program using the conjugate-gradient method. This version is modified from the NLSPMC. The fitting is performed in the full Sc- domain as described in "Two-Dimensional ELDOR in the Study of Model and Biological Membranes", by Y.-W. Chiang, A. J. Costa-Filho, and J. H. Freed [5].

**NLSPMC_qmr** contains the 2D-FT version of the least-squares program using the quasi-minimal residuals (QMR) method. This program was developed and optimized for fitting 2D-ELDOR spectra at high-frequencies in the very slow-motional regime. See "A New Lanczos-Based Algorithm for Calculating High-frequency Two-dimensional ELDOR Spectra in the Slow-Motional Regime" by Y.-W. Chiang and J. H. Freed [7].

The program source codes for the 2D-FT-ESR programs are designed for running under LINUX. They are stored in uncompressed format and may be obtained by ASCII ftp transfer. Tar files are provided for compressed data transfer and contain all files in the specific directories and subdirectories except the executables to save space.

READ.ME files are provided in each of the above directories giving further information on their contents and usage.

(3) Basic programs for CW spectral fitting using the SRLS model as described in "An Assessment of the Applicability of Multifrequency ESR to Study the Complex Dynamics of Biomolecules" by Z. Liang and J. H. Freed [8]: **NLSL.SRLS**, and its most recent update for dynamic exchange **NLSL.SRLS.EXCH**.

**NLSL.SLRS** contains the basic programs for CW spectral fitting using the SRLS model as described by Liang and J. H. Freed (1999). NLSL.SLRS is the fitting program, and ESRBS.SLRS is used to prune the basis set. LBSR.SLRS is for inputting all the parameters used in an ESRBS.SLRS calculation.

**NLSL.SLRS.EXCH** contains updates of NLSL.SRLS for dynamic exhange of the nitroxide between two conformers. NLSL.SRLS.EXCH can be used to perform spectral simulations. Basis set pruning and parameter inputing programs are the same as those listed in NLSL.SRLS.

(4) Software for Tikhonov regularization (TIKR) and maximum entropy (MEM) methods. The software was developed to extract pair distributions from pulsed ESR experiments. See: "The Determination of Pair Distance Distributions by Pulsed ESR Using Tikhonov Regularization" by Y.-W. Chiang, P. P. Borbat and J. H. Freed [9] and "A Complement to Tikhonov Regularization for Determination of Pair Distance Distributions by Pulsed ESR" ▶

by Y.-W. Chiang, P. P. Borbat and J. H. Freed [10]: **PD_Tikhonov**, **DPD_Pkg**.

**PD_Tikhonov** package includes all necessary functions required to extract the pair distributions from pulsed ESR experiments using the Tikhonov regularization method. MATLAB version 6.5 or higher is required to perform the task. PD_Tikhonov requires the use of the Regularization Toolbox package obtainable from the website: www2.imm.dtu.dk/~pch/Regutools/index.html. The toolbox is well documented with a detailed manual and illustrated with numerous examples. We strongly suggest users should first get acquainted with the Regularization Toolbox. After un-zipping the package, please read README.PDF file.

**DPD_pkg** package, includes all necessary functions required to perform TIKR and MEM methods and to extract the pair distributions from pulsed ESR experiments. DPD_pkg can be considered an upgraded version of PD_Tikhonov package since both TIKR and MEM are included in the package. MATLAB version 6.5 or higher is required to perform the task. DPD_pkg requires the use of the Regularization Toolbox package obtainable from the website: www2.imm.dtu.dk/~pch/Regutools/index.html and which is very well documented with a manual and illustrated with numerous examples. We strongly suggest users should first get acquainted with the Regularization Toolbox. After un-zipping the package, please read PD_DEMO.M file.

(!) The programs can be downloaded from: www.acert.cornell.edu/index_files/acert_ftp_links.htm.

Every effort has been made to ensure that these programs are correct and thoroughly tested. However, the programs are distributed 'AS IS', and all warranties, whether expressed or implied, as to correctness or fitness for any specific purpose are specifically disclaimed. In no event shall the authors be liable for any direct, consequential or incidental damages arising from the use of these programs. Free use and distribution of these programs is permitted with suitable reference to the original publication (see above) in any published work resulting from the use of these programs or programs derived from them. The programs may be copied and distributed, so long as, 1) due credit is given by retaining the comment lines at the beginning of each source file in all copies; and 2) all copies must be distributed free of charge.

Questions and comments may be directed to ACERT at acert@cornell.edu, which will forward the correspondence to the most appropriate person.

**Acknowledgement**

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# Notices of Meetings

## The 12th European Conference on the Spectroscopy of Biological Molecule (ECSBM 2007)

Bobigny (Paris region), France, September 1–6, 2007

www.ecsbm.eu

The conference covers all domains of biospectroscopy:

• Application of optical spectroscopy (UV, CD, Raman, SERS, IR, fluorescence, microfluorimetry) and imaging to different biosystems • Multidimensional spectroscopies • Biological systems analysed by neutron scattering and synchrotron radiation • Magnetic resonance (NMR, MRI and EPR) • Biomolecular dynamics within different time-scales • Single molecule and/or single cell spectroscopies • Theoretical approaches applied to biomolecular systems • Spectroscopic applications in medical (diagnosis), pharmaceutical and food domains • Applications in nanotechnology, micro-arrays, biosensors.

Alberto Mezzetti, member of the Organizing Committee of ECSBM 2007, LASIR Laboratory, University of Science and Technology of Lille, France
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## The 46th Annual (International) Meeting of the Society of Electron Spin Science and Technology (SEST 2007)

Shizuoka, Japan, November 6–9, 2007

SEST 2007 will be held at Shizuoka Gran-Ship in Shizuoka city, Japan, as an international symposium to celebrate the 5th anniversary of SEST. Shizuoka city is located in the middle part of Japan (near Mt. Fuji) and faces the Pacific Ocean. SEST 2007 is planning to invite about ten foreign distinguished scientists for the substantial and progressive discussion. Participants from all over the world are welcome. The details will be announced later.

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## The International Conference "Modern Development of Magnetic Resonance" (Zavoisky 100)

Kazan, Russian Federation, September 24–29, 2007

www.kfti.knc.ru/zavoisky100

The scope of the conference covers the following topics:

• Theory of magnetic resonance • Low-dimensional systems and nanosystems • Molecular magnets and liquid crystals • Strongly correlated electron systems • Chemical and biological systems • Medical physics • Other applications of magnetic resonance • Modern methods of magnetic resonance.

Participants of the conference are invited to submit their full original papers to be published in a special issue of *Applied Magnetic Resonance*. The papers should be prepared according to Instructions to Authors (www.springer.at/amr). The official language of the conference will be English.

Chairman of the conference
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Scientific secretary of the conference
Violeta K. Voronkova vio@kfti.knc.ru
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## The EPR Symposium at the Rocky Mountain Conference

Breckenridge, Colorado, July 23–27, 2006

During the Sunday afternoon preceding the conference there was a workshop on "Calculation of EPR Parameters and Spectra" with presentations by Saba Mattar, Sarah Larsen, Ralph Weber, and Graeme Hanson on theoretical calculations of EPR parameters and simulation methods. During the conference there were sessions on Distributions in Distances Between Spin Labels, Spin Label Dynamics and Spin Labels at High Fields, High Field EPR and NMR, EPR in Materials Science, and Metalloenzymes. The Lawrence Piette Memorial Lecture was presented by Wayne Hubbell. The Silver Medal in Biology/Medicine of the International EPR/ESR Society was presented to Periannan Kuppusamy and the Silver Medal in Chemistry was presented to Kalman Hideg. This was the first year that the conference was held in Breckenridge, which is in the mountains west of Denver. Based on the enthusiastic response of conference participants to the new location, the 2007 EPR Symposium will be held July 22–26, 2007 in the same location.

Sandra Eaton

## 35th Southeastern Magnetic Resonance Conference

Gainesville, Florida, USA, November 3-5, 2006

The 35th meeting of the Southeastern Magnetic Resonance Conference (SEMRC) was held November 3–5th, 2006 in Gainesville, FL. This meeting is held annually at various locations within the southeastern United States. The conference was hosted this year by the University of Florida, and Gail Fanucci and Joanna Long were the co-chairs of the meeting. Thirty two invited speakers presented work in the fields of EPR and NMR spectroscopy, with the plenary lecture given by Brian Hoffman of Northwestern University. In addition, more than fifty poster presentations were given, and students and postdoctoral fellows participated in both the talks and poster sessions. This regional magnetic resonance development and applications meeting will be hosted by the University of Alabama and chaired by Lowell Kispert in 2007

Candice Klug

## Asia-Pacific EPR/ESR Symposium APES'06

Novosibirsk, Russia, August 24–27, 2006

The symposium took place in Akademgorodok close to Novosibirsk. It was organized by the joint team of the Institute of Chemical Kinetics and Combustion and the International Tomography Center of the Siberian Branch of the Russian Academy of Sciences. The symposium continued the tradition of biannual meetings of APES.

The scope of the symposium ranged from theoretical and methodological aspects of EPR to its application in physics, chemistry and biology. Special sessions devoted to advanced EPR methods, spin labeling, free radicals, spin effects, photochemical systems and EPR investigation of novel materials. Many research reports were not limited by EPR methods but used the insights from other types of spectroscopy and analytical methods. This added a new dimension to the subjects of research and stimulated lively discussions.

The APES General Meeting was held during the symposium (also see p. 3).

Leading scientists not only from the Asia-Pacific region, but also from Europe and North America took part in APES'06. The symposium was attended by a total of 130 participants including 62 scientists outside Russia.

Leonid Kulik, Sergei Dzuba

## The 6th Meeting of the European Federation of EPR Groups

Madrid, Spain, September 5–8, 2006

During the meeting the whole range of EPR spectroscopy from biology to materials sciences was covered in the 42 talks and 88 poster presentations. Several sessions were also related to the COST P15 Action: Advanced Paramagnetic Resonance Methods in Molecular Biophysics.

Hyperfine and high-field EPR spectroscopy on metal centers and organic cofactor radicals in protein complexes was the major focus of the first two-days lecturing program. Several talks demonstrated the potential and accuracy that modern EPR spectroscopy, especially in conjunction with quantum chemical calculations, can achieve in the description of the electronic structure of such paramagnetic centers in biomacromolecules.

Thursday was dedicated to applications of EPR spectroscopy in materials science, ranging from surfaces, porous materials, inorganic solids to nanotubes and single molecules. Again, the combination of advanced EPR methods (as, for example, high-field EPR, pulse EPR and ENDOR) in combination with quantum theoretical calculations was most impressive. On Friday, quantum theoretical calculations of EPR parameters and new simulation strategies for EPR spectra were presented. In the afternoon two International EPR Society Awards for the year 2005 were given to Eric McInnnes (Young Investigator Award) and to Jos Disselhorst (Silver Medal Instrumentation) by the President of the IES Wolfgang Lubitz. The conference closed with a presentation of Gunnar Jeschke in memoriam to Arthur Schweiger. Two lively poster sessions accomplished the scientific part of the meeting, which was nicely embedded in social activities, such as an excursion to Segovia, a reception at the Madrid Town Hall and a conference dinner. The General Assembly of the EFEPR Groups thanked Carlos Sieiro and his Spanish organization team for the nicely organized meeting and decided to organize the 7th EFEPR Group Meeting in Antwerp in 2009.

Thomas Prisner

## The XXII International Conference on Magnetic Resonance in Biological Systems (ICMRBS)

Göttingen, Germany, August 20–25, 2006

I arrived on a sunny afternoon in Göttingen, Germany for the XXIInd ICMRBS meeting. This was my first ICMRBS meeting and thus, I did not quite know what to expect, although I had been able to take a quick look at the final program. This meeting has been an important forum for the field of protein and nucleic acid structure determination by multidimensional NMR techniques for a number of years. The program reflected the focus of the meeting and was therefore heavy on the NMR side. However, there were a number of people working in the field of EPR spectroscopy that attended the meeting and EPR spectroscopy was discussed in several sessions. The EPR talks spanned a variety of topics, for example, spin labeling, CW and pulsed methods for distance determination as well as the study of paramagnetic metal ions in biological setting.

The sessions were organized according to topic rather than technique. A few sessions had a strong EPR flavor, for example, the sessions on "Labeling Techniques" (talks by Sigurdsson and Steinhoff ), "Molecular Probes" (talks by Gaffney, Blank and Khramtsov) and

"Paramagnetic Proteins" (talks by Bennati, Lubitz and Un). EPR talks were also presented in other sessions: Langen described amyloid protein misfolding, Van Doorslaer discussed the use of high-field EPR to study high-spin ferric heme proteins, Freed talked about pulsed dipolar ESR spectroscopy and protein structure and Mchaourab presented his work on multidrug transporters. Out of eleven plenary talks, one was given by an EPR expert: Goldfarb described the application of high-field EPR/ENDOR to study protein-bound $Mn^{2+}$ in single crystals.

Since I have not attended many EPR conference, I enjoyed seeing the presentation of the people whose papers I had read but never seen in person. This included some of my EPR idols (who I will not list here!). Science-wise, I was impressed by the presentation by Bennati, in which she described how information about relative orientation of tyrosine radicals in ribonucleotide reductase was obtained using high-field EPR. The ability to access information about relative orientations of radical pairs is, in my opinion, an exciting frontier in the field of EPR spectroscopy.

The conference was very well organized and the venue at the University of Göttingen was well suited for the meeting. With a high-quality scientific program the meeting made for a very enjoyable experience and thus, I have my eyes set on the XXIIIrd ICMRBS meeting in San Diego at the end of August 2008.

Snorri Sigurdsson

## Workshop on Modern Electron Paramagnetic Resonance Spectroscopy

### Central Laboratory of Middle East Technical University Ankara, Turkey, November 6–10, 2006


**Group photo of the EPR Workshop in Ankara, Turkey.**

Recently, the Central Laboratory of Middle East Technical University (METU) held a workshop on electron paramagnetic resonance spectroscopy.

The METU Central Laboratory is a research and development center on advanced materials characterization and molecular biology-biotechnology. The objective for establishing the central laboratory is to supply state-of-the-art instrumentation for use by the researchers at METU in order to promote collaboration among the researchers and strengthen the research activities. METU Central Laboratory has X- and Q-band Bruker spectrometers in CW and pulse modes.

This workshop was organized due to the 50th anniversary of METU. The idea to organize such a workshop in Turkey was put front by the director of METU Central Lab. Prof. Çiğdem Erçelebi, EU-FP6 project coordinator Prof. Raşit Turan and Dr. Emre Erdem during the NANOMAT2006 meeting (Antalya, June 2006). After a short time, Dr. Rüdiger A. Eichel (Technical University of Darmstadt), Dr. Stefan Weber (Free University of Berlin) and Dr. Emre Erdem (Technical University of Darmstadt) proposed an intensive scientific program for this event. Nearly 60 scientists from different universities and institutions of Turkey attended the workshop.

The workshop consisted of two main parts. The first was an intensive and interactive practical course in the EPR laboratory in the morning. The practical course program concentrated mainly on the following modern experimental methods: CW EPR (X- and Q-band), basic pulse EPR, 2- and 3-pulse spin echo, inversion recovery, ESEEM, HYSCORE, WinEPR, and XSophe. The afternoon session of the event consisted of plenary seminars on topics that are important for EPR spectroscopy and included the basic theoretical background, experimental methods and examples of applications as follows:

• History of Magnetic Resonance (R. A. Eichel) • EPR spin Hamiltonian: electron and nuclear Zeeman interaction, fine structure and hyperfine interaction (E. Erdem) • CW EPR, Multifrequency aspects, pulsed EPR, ENDOR (S. Weber) • ESEEM, HYSCORE (R. A. Eichel) • EPR in life science (S. Weber) • EPR in materials science (R. A. Eichel) • EPR in nano science (E. Erdem)

On the last day of the event there was a discussion how to incorporate Turkish EPR scientists into the International EPR society. The first step to realize this idea was taken at the 6th EFEPR Meeting (Madrid, September 2006) where the membership of Turkey in the EFEPR groups has been approved by the vote of all delegates. According to the suggestion of Prof. E Goovaerts, Turkey will soon elect a representative person for the "Turkish EPR Discussion Group".

Finally, this workshop, no doubt, offered a real opportunity to the Turkish EPR scientists to discuss, share and exchange their ideas about the theoretical, experimental and computational aspects of modern EPR. Therefore, this activity certainly brought new perspectives, knowledge and collaborations to the Turkish EPR society.

Emre Erdem,
Technical University of
Darmstadt

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*Collected by Candice Klug*

**This is a new feature highlighting young investigators in the field of EPR spectroscopy who have recently became faculty members.**

## Keith Earle
University at Albany

Keith Earle became an Assistant Professor of Physics at the University at Albany (State University of New York) in January 2006. Keith received his PhD in Experimental Physics from Cornell University in the laboratory of Jack Freed. His thesis supervisor was David M. Lee. He continued his training in the design and construction of very high field EPR spectrometers (95–250 GHz) as a Research Associate at Cornell University followed by a position in 2001 as the Associate Director of ACERT (The Advanced Biomedical Research Center for Advanced ESR Technology). Keith's research currently continues in this field with a focus on the development and application of quasioptical techniques for very high frequency EPR spectrometers and the computational analysis of time-domain and multifrequency spectra. Keith continues his role as an Associate Director of ACERT.

## Akio Kawai
Tokyo Institute of Technology

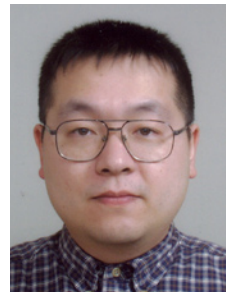
Akio Kawai became an Associate Professor of Chemistry at the Tokyo Institute of Technology, Japan, in April of 2006. He received his BS (1988), MS (1990) and PhD (1992) degrees from the Tokyo Institute of Technology under the supervision of Professor Kinichi Obi. His PhD thesis was concerned with studying dynamic electron spin polarization created in photo-excited triplet and doublet molecules by utilizing time-resolved EPR spectroscopy. He was a JSPS research fellow at the Tokyo Institute of Technology (1992) and a postdoctoral research fellow (1992–1993) at the University of California at Berkeley (Professor C. Bradley Moore) to learn laser spectroscopy of ultracold molecules in the gas phase. In 1994 he joined the Department of Chemistry at the Tokyo Institute of Technology as an assistant professor. From 1998–2001 he was a PRESTO JST researcher engaged in controlling a free radical molecular beam trajectry by an external magnetic field. His recent research interests lie in EPR spectroscopy of paramagnetic ionic liquids as well as electron spin dynamics of paramagnetic species such as nitroxides, triplet excited molcules and singlet oxygen generated in photochemical and photophysical processes.

## Kazuyuki Ishii
The University of Tokyo

Kazuyuki Ishii became an Associate Professor of Institute of Industrial Science at the University of Tokyo in the spring of 2006. Kazuyuki received his PhD in 1996 from Tohoku University where he studied the excited triplet state of porphyrin dimers by using time-resolved EPR (Advisor: Prof. Seigo Yamauchi). When he was a research associate in the laboratory of Prof. Nagao Kobayashi (April, 1996–March, 2006, Tohoku University), he had intensively studied phthalocyanines linked to nitroxide radicals in terms of the excited multiplet states consisting of the excited triplet chromophore and doublet nitroxides. Recently, Kazuyuki was selected by the Society of Electron Spin Science and Technology to receive the Young Investigator Award (2006).

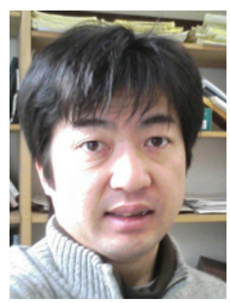
## Kazunobu Sato
Osaka City University

Kazunobu Sato was hired as a Professor of Chemistry and Materials Science in the Graduate School of Science at Osaka City University on April 1, 2006. He received his PhD from Osaka City University in 1994, and has studied organic high-spin molecules as models for purely organic magnets in terms of signle-crystal ESR/ENDOR spectroscopy under the supervision of Professors K. Itoh and T. Takui. He has developed pulse-ESR based two-dimensional electron spin transient nutation spectroscopy in order to identify molecular spin multiplicities of high-spin entities in a straightforward manner and to discriminate the high-spin species in mixed spin systems. His research focuses on an understanding of electronic structures and magnetic properties of exotic molecule-based magnetic materials and paramagnetic biological systems as well as paramagnetic metal complexes. He has developed the hybrid eigenfield method for ESR-based spectral simulation. Also, he has focused his great efforts on methodological developments of CW and pulsed electron-nuclear magnetic resonance spectroscopy, currently implementing developments of molecular-spin qantum computers and quantum information processing by invoking pulse-based electron and nuclear spin resonance technology.



## Hiroyuki Mino
Nagoya University

Hiroyuki Mino became an Associate Professor of Physics at the Nagoya University in the summer of 2005. He received his PhD in physics in 1995 from the Kwansei Gakuin University in the laboratory of Prof. Asako Kawamori where he studied the structure and physical properties of plant photosystem II. His undergraduate degree is in physics in Kwansei Gakuin University. He studied in the photosynthesis laboratory of Inoue Yorinao in RIKEN until 1999, and in the photobiology group of Ono Takaaki in RIKEN until 2001 as a postdoctoral fellowship. He collaborates with Itoh Shigeru who studies photosystem I at Nagoya University. He studies biophysical phenomena of proteins related to photosynthesis, spin label and metal complexes using EPR spectroscopy, and applications of new pulsed EPR techniques.



## Yasuhiro Kobori
Shizuoka University

Yasuhiro Kobori became an Associate Professor of Chemistry at Shizuoka University in April 2006. His training includes postdoctoral fellowships in transient EPR studies of electron transfer mechanism in artificial photosynthetic reaction centers and in protein-surfaces with James Norris at the University of Chicago and with Shozo Tero-Kubota at Tohoku University. He received his PhD in chemistry in 1998 from Tokyo Institute of Technology in the laboratory of Kinichi Obi where he studied the spin dynamics and exchange interaction in radical-triplet pair systems. His undergraduate degree is in chemistry from Tokyo Institute of Technology. Yasuhiro recently received the Young Investigator Award from the Society of Electron Spin Science and Technology in Japan for his study on electron transfer mechanism monitored by exchange interaction in charge-separated systems.

## POSITIONS

### Research Assistant Professor or Research Associate

Immediate openings (4) at Dartmouth Medical School in the Electron Paramagnetic Resonance (EPR) Center for the Study of Viable Systems for Research Assistant Professor (2) and Research Associate (2). For the Research Assistant Professor positions a PhD is required with expertise and experience in EPR instrumental development and/or microwave engineering. The selected individuals should be capable of independently carrying research developments that are consistent with the research directions of the EPR Center and eventually should be able to secure external funding for related research. For the Research Associate positions (requires MS or the equivalent in experience) the skills needed include expertise in at least one of the following: Tumor or Cell Biologist; EPR Instrumentalist; and microwave engineering skills. Submit complete curriculum vitae, statement of pertinent experience, and request three references be sent to: Harold M. Swartz, Dartmouth Medical School, 702 Vail, Hanover, NH 03755, fax: 603-650-1717, e-mail: harold.swartz@dartmouth.edu. *Dartmouth Medical School is an equal opportunity/affirmative employeer and encourages applications from women and members of minority groups.*

### Postdoctoral Positions Available at Davis Heart and Lung Research Institute, The Ohio State University

A position is available for a scientist with experience in magnetic resonance instrumentation development and application. The candidate should have experience in EPR/MR hardware or software development and applications to chemical or biological systems. Salary commensurate with experience. Please reference PA06 in your application.

A position is available for a scientist with experience in cardiac NMR spectroscopy or imaging research to perform isolated heart and in vivo studies of alterations in myocardial energetics and metabolism in the postischemic heart. Salary commensurate with experience. Please reference PA07 in your application.

*The Ohio State University is an equal opportunity/affirmative action employer. Qualified women, minorities, Vietnam era veterans and individuals with disabilities are encouraged to apply.* **Send CV to:**

Dr. Jay Zweier, 473 West 12th Avenue, Room 110, Columbus, Ohio 43210 or zweier-1@medctr.osu.edu.

### Postdoctoral Position Available at the Physics Department, National Dong Hwa University, Taiwan

A postdoctoral position is available in the laboratory of Prof. Shyue-Chu Ke at the Physics Department, National Dong Hwa University, Taiwan. The research will involve application of EPR and pulsed EPR spectroscopy to understand the fundamental questions related to adenosylcobalamin-dependent enzymatic reactions. Additional information about the laboratory is available at: www.phys.ndhu.edu.tw/teachers/ke/ke.htm.

Applicants should have experience in analytical techniques and continuous or pulsed EPR methods and data analysis. Experimental physical chemist with experience in cell culture or synthesis would be beneficial, but is not essential. The position is available this summer and appointments are for up to 3 years. If interested, please send a CV and summary of previous research experience to ke@mail.ndhu.edu.tw.

### The National Biomedical Research Center for AdvanCed ESR Technology (ACERT) at Cornell University invites applications for two Postdoctoral positions.

Applications are encouraged from individuals who can contribute strongly to areas of:

(1) **ESR Microscopy.** This position is for the further development of ESR-Microscopy to provide true micron resolution at very high spin sensitivity, and for its application to the study of small biological samples such as single cells. Recent references to ACERT research in this field include:

Blank A., Dunnam C.R., Borbat P.P., Freed J.H.: Appl. Phys. Lett. **85**, 5430–5432 (2004), www.acert.cornell.edu/PDFs/ApplPhysLett85_5430.pdf.

Blank A., Freed J.H., Kumar N.P., Wang C.-H.: J. Controll. Release **111**, 174–184 (2006), www.acert.cornell.edu/PDFs/JContRel_press.pdf.

(2) **Pulsed ESR and Molecular Dynamics.** This position is for the study of molecular motions of membranes and proteins by multi-frequency 2D-FT-ESR techniques at 9, 17, 35, and 95 GHz. Experience in pulsed ESR techniques and/or ESR spectral simulation is highly desirable. Recent references to ACERT work include:

Costa-Filho A.J., Crepeau R.H., Borbat P.P., Ge M., Freed J.H.: Biophys. J. **84**, 3364–3378 (2003), www.acert.cornell.edu/PDFs/BiophysJ84_3364.pdf.

Earle K.A., Hofbauer W., Dzikowski B., Moscicki J.K., Freed J.H.: Magn. Res. Chem. **43**, S256–S266 (2005), www.acert.cornell.edu/PDFs/MagnResChem43_S256.pdf.

Interested qualified candidates should direct their inquires to acert@cornell.edu.

Applicants should provide a cover letter and most recent CV. Two or three letters of recommendation are also required.

Additional information about the ACERT may be found at www.acert.cornell.edu.

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Gareth R. Eaton geaton@du.edu

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5. Varian E-272B field/frequency lock accessory.

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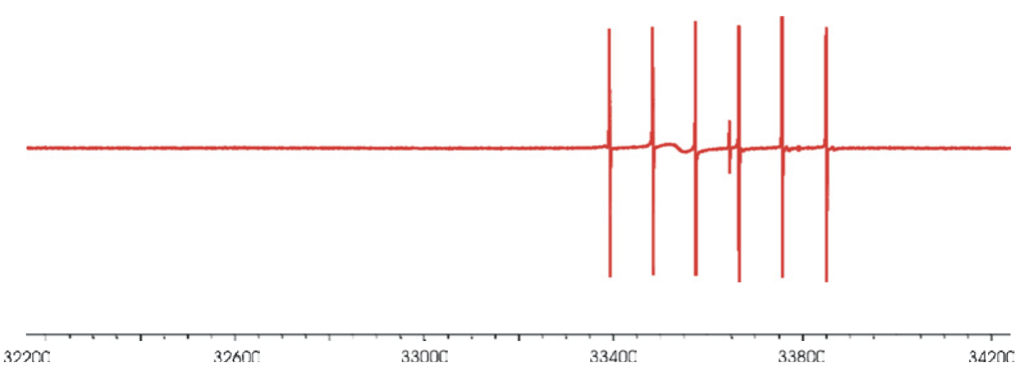


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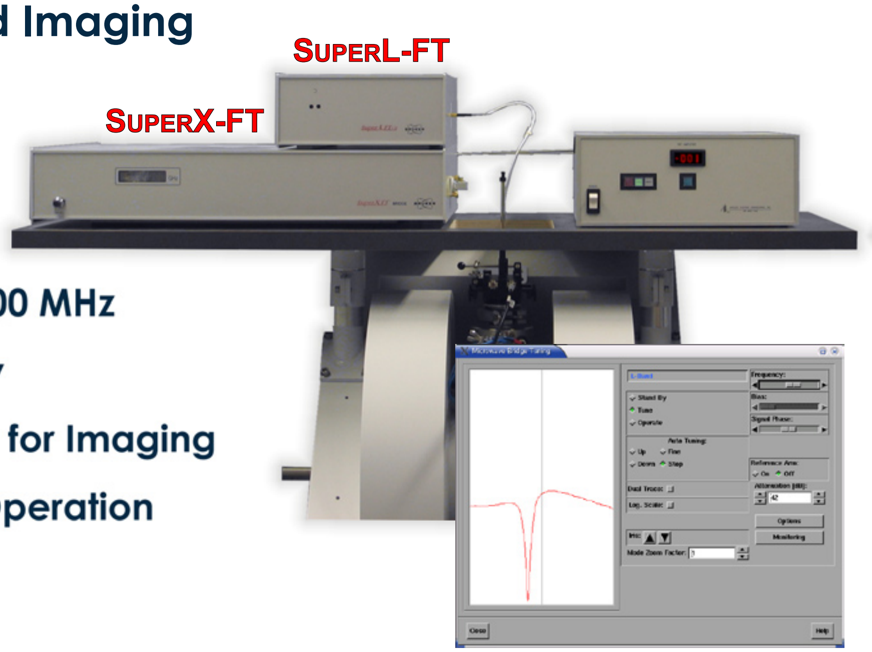


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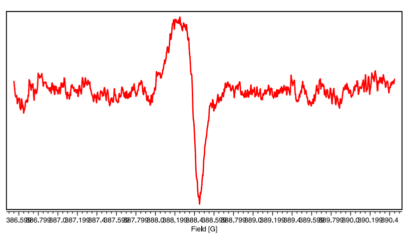
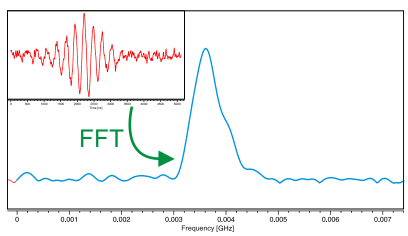
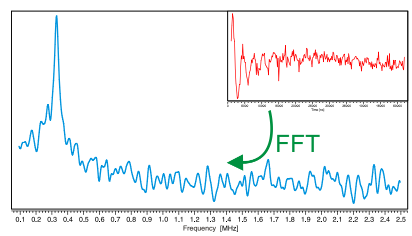
CW-EPR Spectrum




Pulse-EPR Echo




3-pulse ESEEM

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