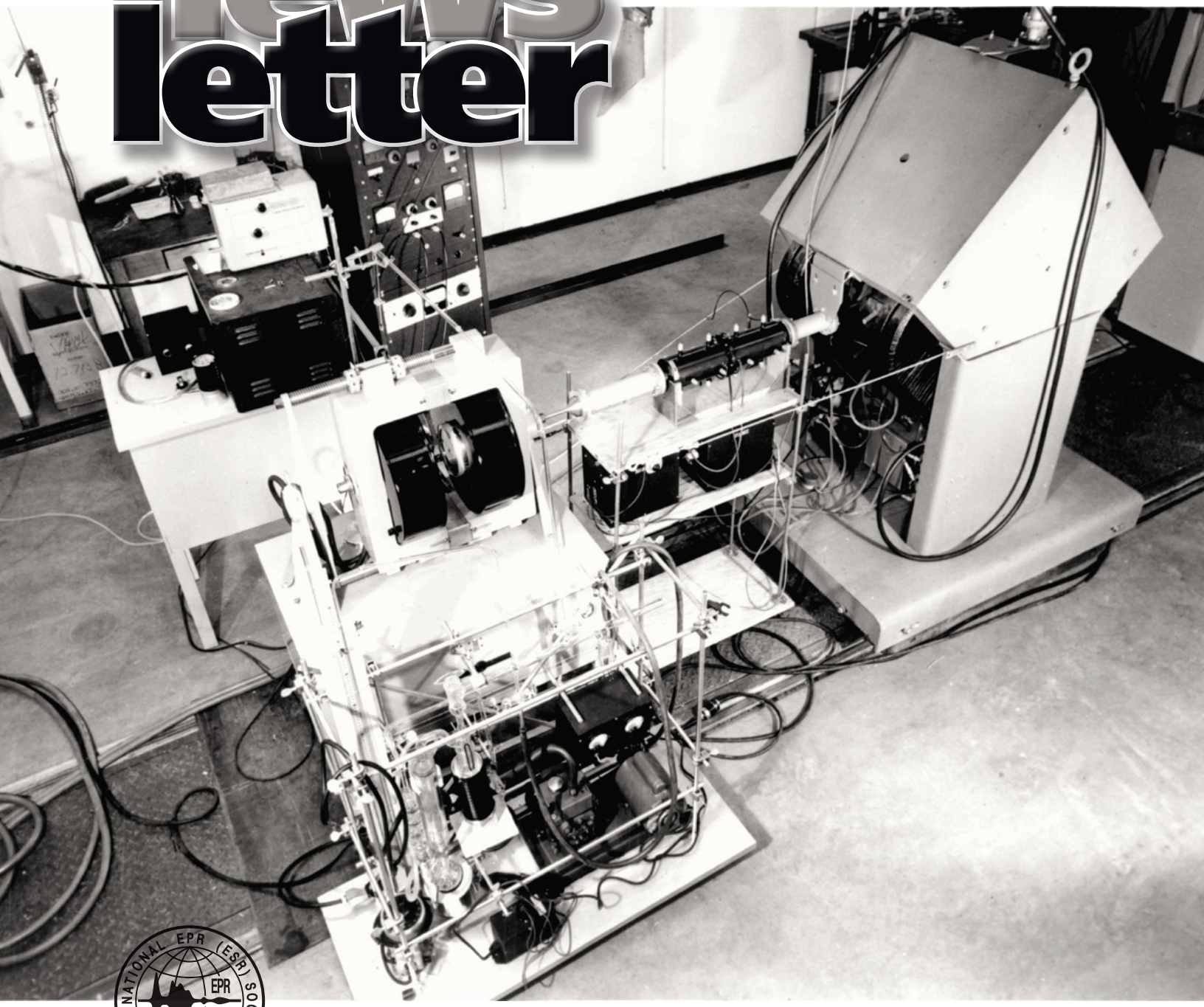
epr newsletter

2013
volume 23 number 3



The Publication of the International
EPR (ESR) Society

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July 1, 2013 until March 31, 2014

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www.epr-newsletter.ethz.ch

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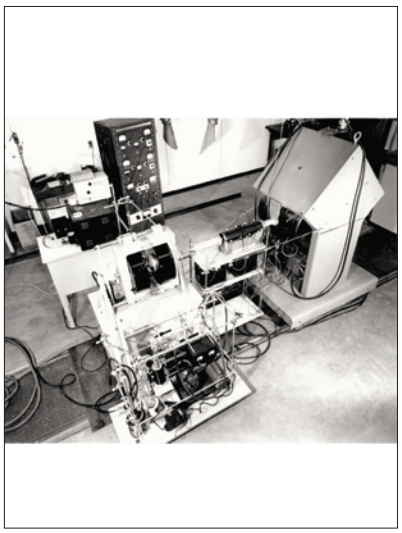


The cover picture illustrates aspects of research carried out by Richard Fessenden, recipient of the Zavoisky Award 2012. It shows the experimental arrangement for the early work at Mellon Institute (1960–1970) involving electron beam irradiation of liquid hydrocarbons. The ESR magnet is at center, with the Varian ESR bridge above, and the vacuum line for transferring the volatile hydrocarbon to the cavity below. The large magnet at the right bends the electron beam from vertical to horizontal. The 3 MeV Van de Graaff accelerator is on the floor above. This year represents the 50th anniversary of the publication by Fessenden and Schuler of the initial extensive paper on liquid hydrocarbons (J. Chem. Phys. **39**, 2147 (1963); doi: 10.1063/1.1701415. This paper (at 49 pages) is the longest in Journal of Chemical Physics history.

epr newsletter

The Publication of the International EPR (ESR) Society

volume 23 number 3 2013

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Editorial

Dear colleagues,

It is good to realize that the "hot science" initiative of Graeme Hanson was greatly appreciated by our readership. Graeme continues with a nice collection of contributions in which EPR spectroscopy and imaging were crucial for the molecular characterization of the complex biological systems (pp. 14, 15). To keep this column running would satisfy the desire of our readership to be updated about hot topics in EPR. And, dear readers, you are welcome to contact Graeme with your contributions.

You must have noticed that usually the third issue of each volume includes a report about IES Annual General Meetings. Please do not worry, your expectations are not disappointed. In this issue you find the report about the IES Annual General Meeting 2013 (Crete, Greece) on pp. 3–5. This time the AGM report is an authentic reproduction of the PPT presentation given by Sushil Misra at this meeting so all of you will experience the effect of being there when reading it.

The EPR Symposium at the 55th Annual Rocky Mountain Conference on Magnetic Resonance held in Denver (see the relevant report on p. 17) was a meeting where an initiative of the IES Executive Committee to increase membership and reach out to the younger EPR scientists, by establishing two poster awards, was implemented for the first time. To give you an idea about their research, the first IES Poster Awardees, Thomas M. Casey and K. S. Bhagyashree, are given floor on pp. 10–12. They are preceded by Dane McCamey, the recipient of the IES Young Investigator Award 2013 (pp. 8, 9). We are happy that we can congratulate Dane, Thomas and K. S. Bhagyashree with their well-deserved awards, which should stimulate their future research. For sure, they will keep in their minds the words of David Cafiso, recipient of the Piette Award 2013 (p. 7), not to be discouraged by a result they do not expect or by a result that does not fit their theory. Our heartfelt congratulations to you, David!

Special congratulations to Jack Freed on his 75th birthday (p. 16) and for his Joel Henry Hildebrand Award 2014 (p. 7)!

The end of the year is a good time to look forward for problems to solve, the delight of overcoming difficulties, the new exciting results of research and fruitful discussions with colleagues and many other things that constitute a life of a researcher. As to the *EPR newsletter*, in the forthcoming issue 23/4 (2014) you will find an interview with Takeji Takui, Bruker Prize 2013 winner. Wolfgang Lubitz will tell you about the Lindau Nobel Laureates Meetings, Jan Henrik Ardenkjær-Larsen will report about the 4th DNP Symposium and the Eatons et al. will describe the rapid-scan EPR techniques, etc. It is never too much to thank again and again everybody who made our newsletter possible this year. Hopefully their support continues. We are always open to new contributors and please feel free to share with us your opinions and ideas.

Happy New Year to all of you and your dear ones! On behalf of my colleagues from the Editorial Board of the *EPR newsletter*, Candice Klug, Hitoshi Ohta, Thomas Prisner and Sergei Akhmin, I wish you, our dear readers, the best of everything!

Laila Mosina

International EPR/ESR Society
Annual General Meeting 2013
Held in conjunction with EUROMAR 2013, Crete, Greece
4th July 2013

The AGM began at 1:30 PM, and was conducted by Sushil Misra, Secretary, IES

All IES members and non-members were welcome to attend and participate in the meeting.
(- Let us know your views!)

International EPR (ESR) Society Executive
Vice President Asia Pacific: Hitoshi Ohta
(Acting President: October 4, 2012 – June 30, 2013)
Vice President Americas: Lawrence Berliner
(Acting President: July 1, 2013 – March 31, 2014)
Vice President Europe: Klaus Moebius
(Acting President: April 1, 2014 – December 31, 2014)
Secretary: Sushil Misra
Treasurer: Tatyana Smirnova
Past President: Jack Freed
Founder President: Harold Swartz

AGENDA
1. Acceptance of Report of the AGM– August 2012
2. President's Report, Awards, & Conferences 2012/2013
3. Secretary's Report
   a) Awards 2014; Call for Nominations
   b) Other Activities & Web Pages
4. Treasurer's Report: Financial Report 2012–2013
5. Newsletter Editor's Report
6. Thanks
7. Other business

An attendance Sheet was circulated (see attached file for names)
Mykhailo Azarkh, Anne-Laure Barra, Marina Bennati, Aharon Blank, Bela Bode, Liliya Bui, Eduardo Di Mauro, Jack H. Freed, Angeliki Giannoulis, Daniella Goldfarb, Pär Hakensson, Stephen Hill, Gunnar Jeschke, Marina Ilacovac-Kveder, Daniel Klose, Thomas Lohmiller, Andriy Marko, Johannes McKay, Sushil Misra, Thomas Nick, Petr Neugebauer, Hitoshi Ohta, Vasili Petrouleus, Graham Smith, Igor Tkach, Silvia Valera, Sabine Van Doorslaer, Maurice van Gastel, Maxim Yulikov.

President's Report (H. Ohta):

Dear Colleagues,

On behalf of the IES Executive Committee, I wish to welcome all participants to the 24th General Meeting of the IES and the EUROMAR 2013. I would like to express my gratitude to the conference organizers of this meeting, especially to Prof. *Georgios Papavassiliou, chairman of the Conference and the Organizing Committee Members* for allowing our General Meeting to take place during this Conference.

Now I have to report a very sad news. Prof. Seigo Yamauchi passed away suddenly on Sept. 26, 2012. It was only 9 months after he started as the President of IES. It was a great loss for our society. However, his will to expand and strengthen the society remains forever inside our hearts. Then the society faced the situation to decide a new President. After the discussion among the Executive Members of IES, it was decided that three Vice-Presidents will act as the acting President equally during the remaining term as follows:

Hitoshi Ohta	2012.10.04-2013.06.30
Lawrence Berliner	2013.07.01-2014.03.31
Klaus Moebius	2014.04.01-2014.12.31

For basic science and applied research, EPR/ESR spectroscopy is becoming an increasingly important tool in a wide range of fields, from physics and chemistry to geology, biology, and medicine. The International EPR (ESR) Society will continue working to promote EPR and to foster scientific collaboration.

We'll be making a renewed effort to expand our membership. I believe that the IES has a lot more room to grow in terms of due-paying members. To achieve this, we need to increase the visibility and appeal of the Society.

New functions to increase the visibility of the Society were discussed among the Executives. One of the ideas was to have joint IES symposium with other related EPR (ESR) conferences.

First joint symposium will be the following:
Joint Conference of APES2014, IES and SEST2014
(APES-IES-SEST2014)
Date: Nov. 12–16, 2014
Place: Todaiji Cultural Center, Nara, Japan
http://apes-ies-sest.org/
As the reduced registration fee is scheduled for IES members, we expect to attract present and new members of IES.

Attracting present and new members will be one of central focus of IES, and we welcome ideas from current members. We look forward to hearing from you and working together to help the Society grow.

We need to communicate and collaborate with scientists both inside and outside of the EPR field. The *EPR Newsletter* is intended to help mediate the exchange of information about excellent laboratories and scientific meetings.

A major function of the IES is to honor distinguished contributors to EPR/ESR.

The awards were initiated in 1992 with the Gold Medal and extended in various specialized areas of EPR. This year we award prizes of the Silver Medals in Physics/Materials Science, the Young Investigator Award and IES Fellowship.

Silver Medal: Physics/Materials Science
2007 Thomas Prisner
2010 Naresh S. Dalal
2013 No award given

Young Investigator Award
2007 Leonid Kulik
2009 Stefan Stoll
2011 Enrica Bordignon (regular)
2011 Alexey Silakov (John Weil)
2012 Laxman Mainali (John Weil)
2013 Dane Robert McCamey (regular)

IES Award 2013

Young Investigator Award
Dr. Dane Robert McCamey, School of Physics, University of Sydney, NSW 2006, Australia
In recognition of his contributions to electrical detection of spin resonance in both organic and inorganic semiconductor materials and devices, particularly his contributions to the development of pulsed techniques, and the development of pulsed electrically detected spin resonance at high magnetic fields

IES Fellows of the Society
2010 James R. Norris, Yuri D. Tsvetkov
2011 Michael Baker, Lowell Kispert, Klaus Moebius
2013 Prof. Dr. Wolfgang Trommer,Faculty of Chemistry, Technische UniversitΔt Kaiserslautern, 67663 Kaiserslautern, Germany. In recognition of his life's work in the fields of EPR spin labeling

I want to thank all the members of the Silver Medal, Young Investigator Awards and Fellowship Committees for their excellent works for the Society.

H. Ohta

(End of President's report)

Secretary's Report (Sushil Misra):

Unfortunately nine months after being the President, Seigo Yamauchi passed away. We had to fill the gap. A solution was found in that the three vice presidents were appointed as acting presidents for 9-month terms each, with the first term beginning on October 4, 2013, in the order of Hitoshi Ohta, Larry Berliner, and Klaus Moebius. We are grateful to them for accepting these responsibilities.

IES Awards 2014
Nominations are invited for the following awards:

Gold Medal
Instrumentation
*John-Weil Young Investigator Award **
Fellows of the Society
**The awards alternate between regular and JW awards.*

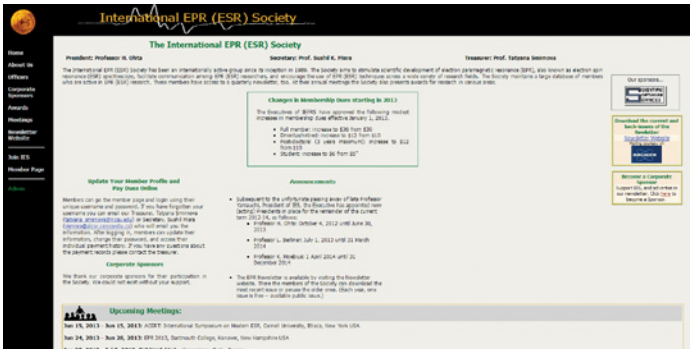
Please visit http://www.ieprs.org for full details on constitution and the by-laws relating to awards.

Please send nominations to the IES President.

Closing date: 15th November 2013

IES Activities
The Secretary is responsible for the day-to-day operations of the Society, and ensures efficient functioning of the Society, e.g.
1. Sending out invoices to the sponsors;
2. Informing members of the various items of interest to them, e.g. announcements of conferences, workshops, publication of new issue of EPR Newsletter;
3. Organization of awards given by the IES: medals, certificates and citations;
4. Overlooking financial status and membership of the Society;
5. Website (revamping);
6. Answering any enquiries;
7. Election Notices;
8. Organizing AGM;
9. Liaisons with the President, Treasurer, Editor of the EPR newsletter, and the members of the IES Executive.

IES Web Site:
It has been recently revamped. A sample representative page follows. One can navigate to items of interest from there, including paying membership dues.



http://www.ieprs.org
Thank you.

(End of Secretary's report)

Treasurer's Report (Tatyana Smirnova - read by Sushil Misra in her absence)

2012 Financial Report (self-audited)

Deposits:

Membership	$ 3,606.39
Sponsors	$ 7,450.00
Bruker printing co-payment	$ 3,710.00
Transfer from Australian account	$ 1,075.79
	$ 15,842.18

Expenses:

Credit card fees, internet commerce and merchant services	$ 541.33
Web design/maintenance & fees	$ 549.88
Newsletter printing	$ 9,325.00
Newsletter Editorial	$ 3,242.00
State of Illinois + misc	$ 35.88
	$ 13,693.41
Balance December 31, 2012	$ 11,192.25

Comments from the Treasurer:
– We have balanced the budget in 2012!!!!
– In 2012/2013 the Society gained the sponsorships of:
Adani Systems - Major Sponsor
Magnettech GmbH - Major Supporter
Cryogenic Ltd – Contributor

– The membership dues were modestly raised in 2013 by 20% or less in 2013 to the nearest dollar in various categories.

Thank you, members and sponsors, for your support!

Status of membership as of June 1, 2013

Complementary	43
Membership: paid for 2012 or 2011	288
Full members	203
Emeritus	24
Students	32
Postdoctoral members	26

Members represent 30 countries:
- Japan 33
- Germany 22
- Russia 33
- USA 100

(End of Treasurer's report)

Newsletter Editor's Report (Laila Mosina - Read by Sushil Misra in her absence)

Since the previous Annual Meeting of the IES in 2012 in Copper Mountain CO (USA) we published four single issues, 22/2, 22/3, 22/4 and 23/1 (the latter is just finalized). We hope all of you had a look at these issues on the newsletter website and got copies of 22/2, 22/3 and 22/4.

Now we start with the preparation of the forthcoming issue 23/2. To remind you, we present the columns of the newsletter.
Columns of the EPR newsletter 23/2 (2013):

– Editorial
– IES business
– Awards
– IES Young Investigator Award Revisited
– Another Passion
– Anniversaries
– EPR newsletter Anecdotes
– In Memoriam
– Pro & Contra
– Software
– Tips and Techniques
– Notices of Meetings
– Conference Reports
– New EPR Faculty
– New Books and Journals
– Market Place
– Reader's Corner
– Guest of the Issue

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

On behalf of the Editorial Board, I thank most heartily all contributors to the EPR newsletter with special thanks going to the CEOs of the IES and editors of the columns in the EPR newsletter: John Pilbrow, Candice Klug, Thomas Prisner, Stefan Stoll, Keith Earle and David Budil, and also to Yevhen Polyhach, our web-master, and Sergei Akhmin, our Technical Editor. I gratefully acknowledge collaboration with Associate Editors Candice Klug, Hitoshi Ohta and Thomas Prisner.

(End of Newsletter Editor's report)

THANKS (Sushil Misra)
The IES thanks the following Corporate Sponsors for their contributions in 2012-2013:

Adani Systems
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L&M EPR Supplies
Magnettech GmbH
Molecular Specialties
Norell
Research Specialties
Resonance Instruments
Scientific Software Services
Wilmad-LabGlass

Special thanks go to ETH Zurich for hosting the Newsletter website and the Zavoisky Physical-Technical Institute, Kazan for supporting the Newsletter, and to
All paid up members
Newsletter Editor: Laila Mosina
Technical Editor: Sergei Akhmin
Associate Editors: Thomas Prisner,
Candice Klug and Hitoshi Ohta

Thank You for Attending

A report of this meeting will appear in a future IES Newsletter.

Other Business

Aharon Blank and Daniella Goldfarb made the suggestion that the amount of ~$8,000* (*see footnote below*) for printing EPR Newsletter can be freed, and used towards supporting student activities and summer schools. EPRNL can be made available electronically. Sushil Misra replied that this matter will be discussed by the Executive. Graham Smith wondered how Laila Mosina would react to this suggestion. He asked if these summer schools will be exclusively organized by IES, or done jointly with other organization. That way one can move the work around. Sushil Misra replied that it can be combined with schools conducted by other organizations, and rotated geographically. He added that IES has already decided to give poster awards to student participants.

Footnote:
** A subsequent breakdown by the Treasurer revealed that the actual cost for printing is rather ~ $4,500.*

Adjournment

The meeting adjourned at 2:10 PM.

Virginia Diodes, Inc.
virginiadiodes.com

Transmit and Receive Systems Covering the 70-3000GHz Spectrum

VDI offers a wide variety of transmit and receive systems covering the 70-3000GHz spectrum. These systems incorporate VDI's frequency extension and mixer components coupled with commercially available microwave oscillators and amplifiers.

For transmit systems, we can configure them with or without a source. A VDI Amplifier / Multiplier Chain (AMC) requires a customer low frequency source (typically <20GHz, 10dBm nominal). A VDI Transmitter (Tx) integrates a source (oscillator or synthesizer) with the VDI AMC. Similarly for receive systems, we can configure them with or without a source. A VDI Mixer / Amplifier / Multiplier Chain (MixAMC) requires a customer low frequency local oscillator. A VDI Receiver (Rx) integrates the LO with the MixAMC.

Standard AMCs and MixAMCs have been developed to provide high performance frequency multiplication and downconversion for full waveguide band coverage. These systems can be used to extend traditional spectrum analyzer and signal generators into the THz and mm-wave ranges. VDI's standard AMC and MixAMCs offer various modes of operation. VDI AMCs can be operated in standard frequency mode (<20GHz, 10dBm nominal) or high frequency mode (<45GHz, 0dBm nominal). VDI MixAMCs can also operate in standard and high frequency modes. Customers also have the option to operate MixAMCs for block-down conversion or as a spectrum analyzer extender. Standard AMCs and MixAMCs are available from WR15 (50-75GHz) to WR1.0 (750-1100GHz).

VDI offers both narrow-band high-power and broadband low-power systems. High-power systems use VDI's D-series X2 multipliers to achieve maximum multiplier efficiency and power handling. VDI has developed many high power systems for special customer applications, such as a novel multiplier based source with output power of 100mW at 200GHz.

Reconfigurable / modular AMCs are also available upon request. See www.vadiodes.com for more details, or contact us at vdirfq@vadiodes.com for advice on system configuration.

Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids 2014 to Jack H. Freed

The American Chemical Society has announced that Jack H. Freed is the 2014 recipient of the Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids sponsored by ExxonMobil Research and Engineering Co. This national award recognizes distinguished contributions to the understanding of the chemistry and physics of liquids. Professor Freed will be presented the award at the Society's 247th ACS National Meeting in Dallas, TX on Tuesday, March 18, 2014. The 2014 ACS National Award Recipients were reported in the September 9 issue of Chemical & Engineering News. His award citation is "For his development of electron spin resonance into a powerful methodology and his applications of it to problems of the dynamics and structure of liquids."

Jack H. Freed is well-known to many readers of the EPR Newsletter. He is the Frank and Robert Laughlin Professor of Physical Chemistry and Director of the National Biomedical Center for Advanced ESR Technology (ACERT) at Cornell University. He is a world-renowned leader in the electron-spin-resonance (ESR) field. His fundamental theories of spin relaxation, and their experimental verification, have become the gold-standard used by many in ESR. He is the past president of the IES, a Fellow of the American Academy of Arts and Sciences, Royal Society of Chemistry (FRSC), American Physical Society, and Inaugural Fellow, International Society of Magnetic Resonance. He has been the recipient of other notable awards, including the Buck-Whitney Award, American Chemical Society (1981) for his contributions to ESR; Bruker Award, Royal Society of Chemistry (1990); Gold Medal, International ESR Society (1994); Irving Langmuir Prize in Chemical Physics, American Physical Society (1997); Zavoisky Award, Russian Academy of Science (1998); E. Bright Wilson Award in Spectroscopy, American Chemical Society (2008); and, the ISMAR Prize, International Society of Magnetic Resonance (2013).

The Joel Henry Hildebrand Award was established in 1980. The ExxonMobil Research and Engineering Co. has sponsored the award since 1992.

Interview with David Cafiso on the Occasion of His Piette Award 2013

EPR newsletter: *Dear Professor Cafiso, on behalf of the readers of the EPR newsletter we congratulate you on your Piette Award 2013. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I have always been interested in how things work. When I was young, I took apart door locks, radios and televisions – and later automobiles – because I was interested in how things worked. Science seemed like a natural fit. What could be better than a career where one tried to figure out how the world worked?

Who introduced you into magnetic resonance?

I was introduced to magnetic resonance by Wayne Hubbell while I was a graduate student at UC Berkeley. We started by designing spin labels that could detect membrane potentials, and I was fascinated by the idea that we could use magnetic resonance to do things that could not be done with microelectrodes. This work got me thinking about interfacial potentials and internal membrane potentials that control protein structure and modulate function.

What is the driving force for you in your research?

My research has always been focused on biological membranes and membrane proteins, and I have always been interested in trying to understand the fundamental physical principles that govern the function of these systems. Relatively simple physical concepts such as surface potentials and double-layer theory can give rise to more complicated cellular phenomena, and I have always found it very satisfying to understand these systems in a quantitative manner.

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

There are many aspects of our research that have captured my attention over the years, but I am currently fascinated by the use of magnetic resonance methods to investigate conformational equilibria in membrane proteins. We now have a set of tools, for example using spin labels and EPR, that allow us to characterize discrete structural states that are sampled by proteins. We now recognize that these states are often not seen by crystallography but play an important role in protein function.

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

Well, there are many messages that are useful. But, I think it is very important for any scientist to not be discouraged by a result that they do not expect or by a result that does not fit their theory. If the experiment is correctly designed, it is telling you something about the way things work, and if the result does not fit your expectations, you now have the opportunity to learn something.

IES Young Investigator Award 2013 to Dane R. McCamey

I was honored to receive the International EPR/ESR Society Young Investigator Award for 2013 at the 55th Rocky Mountain Conference on Magnetic Resonance in July. The award was presented by the (Acting) President of the International EPR/ESR Society, Prof. Lawrence Berliner, and I thank him and the Board of the Society for this Award.

I was introduced to spin resonance during my PhD in the Centre for Quantum Computation at the University of New South Wales, Australia. My project was initially aimed at investigating, in the context of quantum information processing, defects at the silicon/silicon dioxide interface. This interface has been an area of particular interest in ESR for many years, due to its importance for conventional electronics. One of the major challenges we faced was that we were interested in investigating the impact of these defects on a single phosphorus donor, so conventional approaches to detecting ESR were not very useful. Electrically detected magnetic resonance (EDMR), where ESR is detected using the resonant change in the conductivity of a material, provided a way to resolve this difficulty. My PhD supervisor at the time, Prof. Bob Clark, sent me to Munich to learn how to do this in the group of Prof. Martin Brandt. Using a series of nanoscale electrical devices fabricated by electron beam lithography, we were able to electrically detect the spin resonance of as few as 50 phosphorus donors in a 50 nm × 50 nm device. This represented an increase in sensitivity of over 7 orders of magnitude when compared with conventional ESR approaches. Subsequent collaborative work involving researchers from UNSW and Munich resulted in a number of useful technological advances in this area, including incorporating spin manipulation hardware onto devices compatible with operation at millikelvin temperatures and fast readout of EDMR using RF engineering approaches, and which are now gaining more widespread use.

Following my PhD I took up a postdoctoral appointment in Christoph Boehme's group at the University of Utah. During my three years there I worked in two main areas – improving the sensitivity of pulsed EDMR of donors in silicon, and applying pEDMR techniques to organic devices.

Usually, signal intensity in EDMR is insensitive to spin polarization. However, there are a number of cases where very large spin polarization leads to increased signal strength (in particular when the thermal polarization exceeds the dynamic polarization caused by spin-dependent recombination rates). Unfortunately, this usually requires either very low temperatures or very high magnetic fields. Fortunately, Hans van Tol and colleagues at the National High Magnetic Field Laboratory have spent significant effort developing a wonderful pulsed spectrometer that operates at 8 or 12 Tesla (240 or 330 GHz), which provided the polarizations we required as well as the ability to do multipulse ESR experiments. By modifying this spectrometer to make it suitable for pEDMR experiments on donors in silicon, a number of results were able to be obtained. We measured what was at the time the longest electrically detected electron spin phase coherence time, in excess of 100 μs. We also showed that information (both classical ▶

and quantum) could be written to the electron spin, transferred to the nuclear spin, and stored there for times in excess of 6 minutes (classical) and 3 ms (quantum) before being read out electrically. As well as the scientific outcomes which they produced, the pEDMR capabilities developed at the NHMFL are now available to other researchers using that facility.

Organic electronics are particularly amenable to investigation using pulsed electrically and optically detected magnetic resonance techniques. First, spin plays an important role in a large number of electronic processes which directly impact device performance. Second, their thin film nature makes conventional ESR approaches challenging. A collaborative effort between the research groups of Boehme and John Lupton was instigated to apply pulsed EDMR techniques to organic devices, resulting in a quite productive research project. Direct measurements of the phase coherence times of polarons in organic materials under operating conditions were performed. Phase coherence times approaching a microsecond at room temperature were seen, and this now holds some promise for developing room temperature quantum systems. Direct measurement of the local (nm) variation of the Overhauser fields in a polymer were measured, showing that EMDR can provide qualitatively different information due the observable being spin pair permutation symmetry, rather that net ensemble polarization. This work also demonstrated similarities between the spin physics which occurs in organic semiconductors and in engineered quantum bits in gallium arsenide, providing a way to engineer the spin environment by appropriate chemical synthesis of deuterated materials.

Following a move to the University of Sydney, I continued to work in this area. For example, combining work by two students – Tom Keevers' theoretical modeling at Sydney and William Baker's experimental work at Utah – enabled us to use coherence measurements to determine transport properties of intermediate pairs in organic materials. Use of more complex quantum control and error correction approaches (such as dynamic decoupling) may provide even greater abilities in this area.

ESR is enjoying a renaissance, not just in its use and breadth of application, but also through the development of completely innovative techniques based on advances in quantum science and progress in electrical engineering. As a community, I believe we should make every effort to embrace and integrate these approaches into mainstream ESR to maintain its relevance for future research challenges. To this end, I am currently developing a pulsed ESR facility at the University of New South Wales, where I am now a faculty member. I hope that by encouraging the use of complex quantum control techniques and by developing new experimental approaches, investigators in broader areas such as materials science and biology will continue to find new uses for ESR.

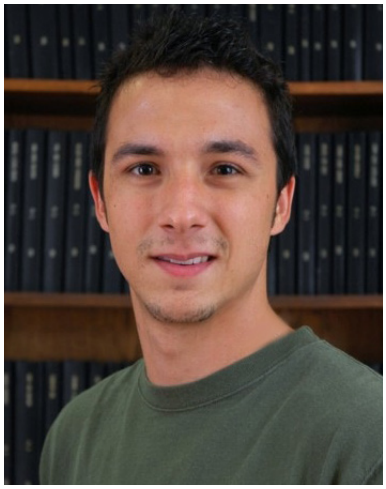
Finally, I would like to take this opportunity to acknowledge the effort and major contributions of all the students, postdoctoral researchers and faculty members with whom I have worked, particularly Prof. Robert Clark, AO and Prof. Alex Hamilton, my PhD supervisors; Dr Andrew Ferguson, for initially pointing me in the direction of EDMR; Prof. Martin Brandt and Dr Hans Huebl, who taught me much of what I know about EDMR; Prof. Christoph Boehme for providing a stimulating and productive scientific environment in Utah; and Dr Hans van Tol and Dr Gavin Morley at the NHMFL for providing both a wonderful User Facility and an excellent collaborative research team.

From left to right: Thomas M. Casey, Hitoshi Ohta and Bhagyashree K. S.

IES Poster Awards

As an initiative to increase membership and reach out to the younger EPR scientists, the IES Executive Committee decided to commit $500 towards two poster awards at relevant meetings. We began this year, starting with the 2013 Rocky Mountain Conference (articles by Thomas M. Casey, Michigan State University, East Lansing, MI, USA and K. S. Bhagyashree, Indian Institute of Science, Bangalore, India and photos in another story in the newsletter) and will continue at the 2014 APES Conference in Nara, Japan. The posters were judged by a blue ribbon international committee and the event was well received. We are, of course, quite interested in obtaining a sponsor for this award in the future.

Lawrence J. Berliner, President



Thomas M. Casey:

I would like to thank the organizers of the 2013 International EPR Symposium and Rocky Mountain Conference on Magnetic Resonance for the opportunity to share my work in an environment dense with pioneers and leaders in the field. I would also like to acknowledge Dr. John McCracken at Michigan State University for his support and guidance throughout my graduate career as well as Drs. Robert Hausinger, Piotr Grzyska, and William Kittleman for their invaluable collaborative contributions to our efforts. I have since moved on to a postdoctoral position at the University of Florida with Dr. Gail Fanucci where I am excited to have the opportunity to continue contributing to the magnetic resonance community.

My presentation at the symposium involved the use of Electron Paramagnetic Resonance (EPR) Spectroscopy to investigate the active site structures of two non-heme Fe(II)/α-ketoglutarate (α-KG) dependent enzymes: taurine/α-KG dioxygenase (TauD) and xanthine/α-KG dioxygenase (XanA). TauD catalyzes the hydroxylation of taurine, leading to liberation of sulfite for providing a sulfur source in *Escherichia Coli* [1]. XanA is believed to be homologous to TauD [2] but has not yet been structurally characterized. This enzyme catalyzes the hydroxylation of xanthine as part of a purine degradation pathway in certain fungi. Other enzymes in this class catalyze a diverse set of reactions involved in antibiotic and small molecule synthesis, oxygen sensing, biodegradation, DNA repair, and epigenetic regulation [3]. However, certain aspects of the active site structures and key steps in the mechanisms are believed to be generally conserved. These enzymes use a common 2-His 1-carboxylate Fe(II) coordination motif known as the "facial triad" where one face of the octahedral Fe(II) coordination sphere is occupied by 2 histidine ligands and 1 carboxylate ligand that can be supplied by either a aspartic acid or glutamate residue. The cofactor, α-KG, chelates the Fe(II) center in an orientation relative to the "facial triad" ligands that is critical for proper function of these enzymes. One of the most important conserved steps in the mechanisms is the oxidative decarboxylation of α-KG that leads to the formation of a reactive Fe(IV)=O intermediate. Interestingly, certain members of this class can bind α-KG in different spacial positions and maintain expected catalytic behavior. While the involvement of α-KG in the mechanism has been studied [4], the factors that influence its spacial positioning in the complex have not been directly addressed. Much of what is known about the mechanisms used by these enzymes has been derived from studies of TauD. However, these studies have been supported by limited structural information, namely, relatively low resolution crystal structures where the placement of a small molecule such as taurine is subject to considerable error.

First, using Electron Spin Echo Envelope Modulation (ESEEM) Spectroscopy we measured the position and orientation of taurine in TauD's active site. TauD solutions containing Fe(II), α-KG, and natural abundance taurine or specifically deuterated taurine were prepared and treated with nitric oxide (NO) to make an $S = 3/2$ $\{FeNO\}^7$ complex that is amenable to robust analysis with EPR spectroscopy. Using ratios of ESEEM spectra collected for TauD samples having natural abundance taurine or deuterated taurine, interactions with specific deuterons on taurine could be studied separately. The Hamiltonian parameters used to calculate the amplitudes and line shapes of frequency spectra containing isolated deu-

terium ESEEM were obtained with global optimization algorithms. The position and orientation of taurine that was obtained by translating the Hamiltonian parameters to effective dipolar distances and spacial coordinates was found to support the currently accepted model for taurine's involvement in the mechanism. This not only lends to the understanding of the mechanism used by TauD but suggests these methods for characterization of other, less well understood, enzymes in this class. The results and a full discussion of their implications were published in September 2013 in the ACS Journal of Physical Chemistry B. (Volume 117, Issue 36, Pages 10384–10394. DOI: 10.1021/jp404743d).

Next, we used Hyperfine Sub-level Correlation (HYSCORE) to measure the orientations of the ligands directly coordinated to Fe(II) in TauD. HYSCORE spectra were collected for the samples described above and signatures of ^{1}H and ^{14}N nuclei of the directly coordinated histidine ligands and ^{1}H nuclei on taurine were identified and quantitatively analyzed using simulations. The results of our analyses support the previous ESEEM study as well as the currently accepted structural model for the directly coordinated ligands. Comparison of this data with corresponding spectra collected for additional samples prepared either without taurine or without α-KG revealed the behavior of the directly coordinated ligands as a function of α-KG and taurine. This can provide a means for determining the factors that influence the proper ligand orientations in the functioning active site complex. In addition, we demonstrated a simple method for analyzing congested, orientation selective, HYSCORE spectra. A detailed report of the results and their implications is currently being prepared for publication.

Applying these methods to the study of XanA has produced interesting results. While some similarities in the data are observed, the differences raise questions about the validity of the proposed homology to TauD. For example, initial analyses may suggest that XanA exhibits different α-KG binding behavior. This study will represent the first structural characterization of XanA. Look for a report of this work in the near future as well.

The various data simulations were done using the EasySpin software package [5]. Thank you to all who have shown an interest in our work and to those who have encouraged me as a young scientist. Please feel free to contact me with any questions or comments at: tcasey3@chem.ufl.edu.

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Bhagyashree K. S.:

I was surprised and delighted at the same time to receive the award. It was my first EPR conference and I enjoyed the interaction I had through the conference. The conference helped me gain deeper understanding of EPR and its applications. I would like to thank my co-author and advisor Prof. S. V. Bhat, without his guidance and support this research would not have been possible. I would also like to thank the organizers of the conference.

FMR Evidence for Temperature Dependent Sign Reversal of Magnetocrystalline Anisotropy in Bulk and Nanoparticles of $La_{0.85}Sr_{0.15}MnO_3$

K. S. Bhagyashree and S. V. Bhat

Department of Physics, Indian Institute of Science, Bangalore-560012, India *

Ferromagnetic resonance (FMR) provides a unique technique to study magnetocrystalline anisotropy (MA). While torque magnetometry, the standard technique of investigating MA, requires single crystal samples, with FMR even polycrystalline materials can be used to understand the nature of MA. We have carried out ferromagnetic resonance studies of magnetocrystalline anisotropy in bulk and nanoparticles of $La_{0.85}Sr_{0.15}MnO_3$ and $La_{0.875}Sr_{0.125}MnO_3$ as a function of temperature in the range 4–300 K. We observe a rare occurrence of temperature dependent switch in the sign of MA from negative to positive as the temperature is increased in both bulk and nanosamples of $La_{0.85}Sr_{0.15}MnO_3$ while $La_{0.875}Sr_{0.125}MnO_3$ samples do not show any sign reversal.

Preparation and characterization.

The nanoparticles of both the compositions were prepared by standard sol-gel technique and sintered at 600 °C for 12 hours. The bulk samples were prepared by sintering the nanoparticles at 1400 °C for 12 hours.These samples were characterised by powder X-ray diffraction (XRD) and energy dispersive X-ray analysis (EDAX). The particle size of the nanoparticles was measured using transmission electron microscopy (TEM).

Rietveld refinement done on the XRD pattern of nanoparticles of $La_{0.85}Sr_{0.15}MnO_3$ gives a best fit with cubic structure with the space group Pm-3m and the bulk of the same crystalizes in rhombohedral structure, analysed using hexagonal space group R-3cH. For the nanoparticles of $La_{0.875}Sr_{0.125}MnO_3$ the Rietveld refinement shows that the structure is rhombohedral with the space group R-3cH and for the bulk it is orthorhombic with space group Pbnm. EDAX confirms the stoichiometric ratios of these compounds. TEM is done on the nanoparticles of both $La_{0.85}Sr_{0.15}MnO_3$ and $La_{0.875}Sr_{0.125}MnO_3$ samples. The histograms show that the average particle size in both the samples is ~27 nm.

VSM measurement has been done on these samples in order to observe the ferromagnetic transition. It showed that the nanoparticles of $La_{0.85}Sr_{0.15}MnO_3$ underwent a ferromagnetic transition at ~280 K whereas the bulk did so at ~240 K. The nanoparticles of $La_{0.875}Sr_{0.125}MnO_3$ underwent ferromagnetic transition at ~250 K and the bulk sample at ~210 K. These are in accordance with the earlier reports.

* A summary of the poster no. 201 at the 55th Annual Rocky Mountain Conference on Magnetic Resonance presented by K. S. Bhagyashree

FMR measurements.
The ferromagnetic resonance signals were recorded with a Bruker EMX EPR spectrometer between the temperatures 4–300 K. We make use of the fact that FMR signal shape is a definitive indicator of the nature and sign of magnetocrystalline anisotropy of the sample [1].

The lineshape of signals from $La_{0.85}Sr_{0.15}MnO_3$ bulk and nanoparticles at the lowest temperature used is indicative of negative uniaxial anisotropy. As the temperature is increased the lineshape gradually changes to the one corresponding to positive uniaxial anisotropy [1]. These FMR signals were analysed using the simulation program 'ROKI' [2] and the required parameters were extracted. These parameters were used to plot the uniaxial anisotropy field (H_a) and uniaxial anisotropy constant (K_u). The graph shows a switch from negative to positive in H_a and K_u at ~205 K for the bulk and at ~240 K for the nanopartilces with increasing temperature.

The sign change in MA is usually associated with a structural change. According to the phase diagram [3], bulk $La_{0.85}Sr_{0.15}MnO_3$ undergoes a cooperative Jahn-Teller (JT) transition around 200 K, which is below its T_c and where the switch in MA from negative to positive has been observed. It is possible that the cooperative JT transition is driving the sign reversal of MA observed in bulk $La_{0.85}Sr_{0.15}MnO_3$. For the nano sample we can interpret that the cooperative JT transition must have been shifted to slightly higher temperature since the sign reversal has been observed at ~240 K.

In order to confirm that this sign reversal in MA from negative to positive occurs only in $La_{0.85}Sr_{0.15}MnO_3$ due to cooperative JT transition occurring below T_c we did the FMR measurement of $La_{0.875}Sr_{0.125}MnO_3$ in which the cooperative JT transition is above T_c. FMR done on bulk $La_{0.875}Sr_{0.125}MnO_3$ shows that at very low temperatures the FMR signals are broad and asymmetric and indicative of negative uniaxial anisotropy. This asymmetry disappears at ~220 K (T_c ~ 220 K) and a symmetric signal is seen till 300 K. But we do not see any switch in the anisotropy from negative to positive unlike in the bulk and nano $La_{0.85}Sr_{0.15}MnO_3$.

FMR done on nanoparticles of $La_{0.875}Sr_{0.125}MnO_3$ also indicates negative uniaxial anisotropy at lowest temperatures which persists till 220 K. At 230 K the signal becomes symmetric. At 240 K we observe a broad low field signal (T_c ~ 250 K) which persists till room temperature. But the broad signal bifurcates from the low field signal and moves further to the lower field with increasing temperature. So it can be concluded that this is the signature of the so called Griffith's phase [4] and not of positive anisotropy unlike in the $La_{0.85}Sr_{0.15}MnO_3$ sample.

To conclude, our FMR studies show [5] that in the $La_{0.85}Sr_{0.15}MnO_3$ samples, where there is a co-operative Jahn-Teller transition within the ferromagnetic phase the magnetocrystalline anisotropy switches sign around the transition temperature. However, samples of $La_{0.875}Sr_{0.125}MnO_3$ which do not have any cooperative JT transition in the FM phase do not show any change in the sign of MA.

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5. K. S. Bhagyashree and S. V. Bhat: to be published.

New Books & Journals

EPR => Hot Science

The second edition of this column introduces new research utilising EPR spectroscopy in the areas of metalloenzyme biochemistry (photosynthesis and hydrogenase), the development of new spin probes for EPR imaging and the application of EPR imaging in elucidating the dual role of the p53 gene, which, depending on oxygenation, can elicit apoptotic death signals or NOS3-mediated survival signals in the infarct heart. Importantly, in all of these studies EPR spectroscopy (continuous wave and pulsed techniques) and imaging was crucial for the molecular characterisation of the complex biological systems.

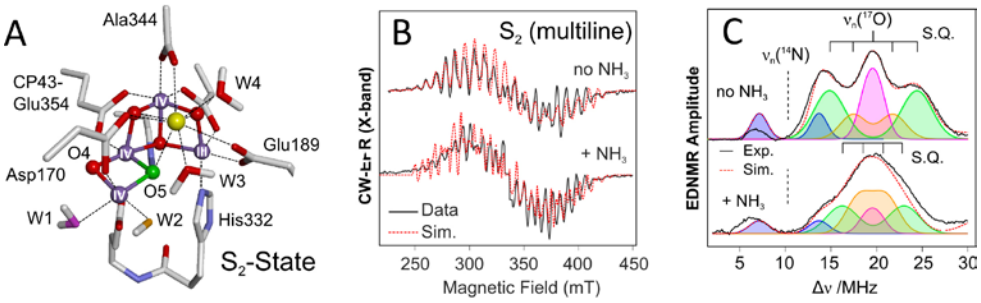
I look forward to receiving contributions that showcase the very best research carried out primarily by IES members and has been published in high impact journals, typically the best journals in the appropriate field of research. IES members are invited and encouraged to contribute general summaries (word document) of no more than 200 words, together with a colour image to Graeme Hanson (Graeme.Hanson@cai.uq.edu.au).

Graeme Hanson
Centre for Advanced Imaging
The University of Queensland
Australia

^{17}O ELDOR-Detected NMR Study of the Oxygen Evolving Complex of Photosynthesis 5

The oxygen evolving complex (OEC) of Photosystem II (PSII) consists of an inorganic tetramaganese-calcium cluster linked together by five oxygen bridges. Recently W-band ELDOR-detected NMR (EDNMR) has been applied to this system to identify the two substrate water sites of the cluster [1]. As these two sites exchange rapidly with bulk water, the substrate oxygen atom can be labeled with ^{17}O ($I = 5/2$). Interestingly, one of the μ-oxo bridges of the complex could be labeled with ^{17}O supporting the notion that this unique oxygen bridge likely represents one of the substrate water sites of the water splitting reaction, as described in our recent review [2].

The identity of the exchangeable bridge was obtained in the most recent work published in PNAS (Pérez Navarro, M.; Ames, W. M.; Nilsson, H.; Lohmiller, T.; Pantazis, D. A.; Rapatskiy, L.; Nowaczyk, M.; Neese, F.; Boussac, A.; Messinger, J.; Lubitz, W.; Cox, N. *Proc. Natl. Acad. Sci. USA*, **2013**, 110, 15561–15566). This study represents a collaboration between the Mülheim laboratory (Germany) and research groups in France, Germany and Sweden. In this study the binding of ammonia (NH_3), a water analogue, to the OEC was used as a probe to locate the μ-oxo bridge. This limits the number of possible O-O bond formation reaction pathways to two, which represent either an i) nucleophilic attack or ii) radical coupling of the exchangeable μ-oxo bridge.

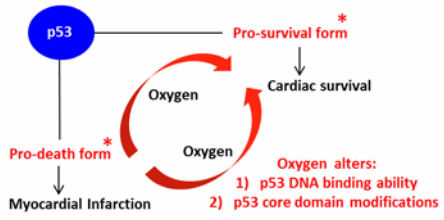


Structure of the OEC (A); X-band EPR spectrum (B) and ^{17}O EDNMR spectrum (W-band; S.Q. = sinmTgle quantum transitions) of the OEC without and with NH3 addition (C).

1. Rapatskiy, L.; Cox, N.; Savitsky, A.; Ames, W. M.; Sander, J.; Nowaczyk, M.; Rögner, M.; Boussac, A.; Neese, F.; Messinger, J.; Lubitz, W. *J. Am. Chem. Soc.* **2012**, 134, 16619–16634.
2. Cox, N.; Pantazis, D. A.; Neese, F.; Lubitz, W. *Acc. Chem. Res.* **2013** 46, 1588–1596.

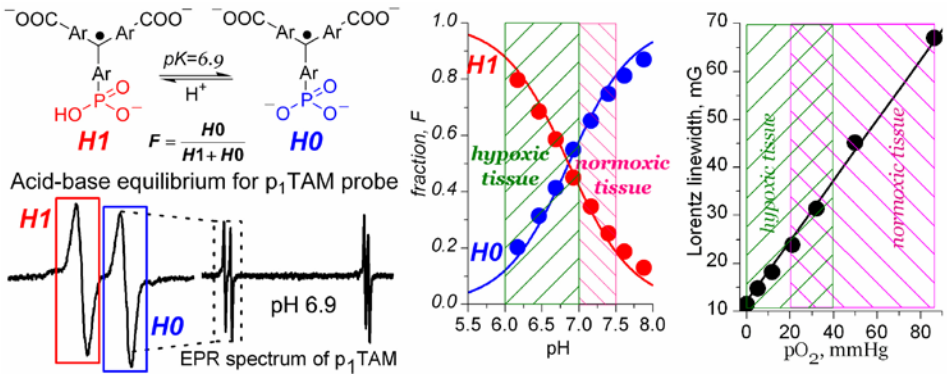
Oxygen Treatment Heart Attack: Take a Deep Breath & Relax 6

During a heart attack (also known as myocardial infarction, MI) when the flow of oxygen-rich blood to a section of the heart is interrupted and not quickly restored, heart muscle begins dying leading to progressive loss of heart function and congestive heart failure. Current therapies are not effective at limiting the progressive cell death. In this paper (Gogna, R.; Madan, E.; Khan, M.; Pati, U.; Kuppusamy, P. *EMBO Mol. Med.* **2013**, 5, 1662–1683), Kuppusamy et al. hypothesized a dual role for p53, which, depending on oxygenation, can elicit apoptotic death signals or NOS3-mediated survival signals in the infarct heart. They discovered that daily administration of a higher concentration of oxygen for a short period of time each day induced spikes in myocardial oxygen tension (as measured by EPR oximetry), which limited the progression of myocardial injury. "We all know that oxygen is crucial for survival, but it is intriguing to know that the same oxygen can be used like a drug to treat disease" – Kuppusamy wonders. The study further discovered that oxygenation altered the function of p53, a transcription factor that regulates cell cycle and triggers programmed cell death, from a death-inducing protein to promoting transcription of genes that help in survival of dying cardiac cells. Understanding this novel oxygen-mediated p53 survival pathway will open new avenues in cardioprotection molecular therapy.



Methods for Multifunctional Tissue Imaging, *In Vivo* 7

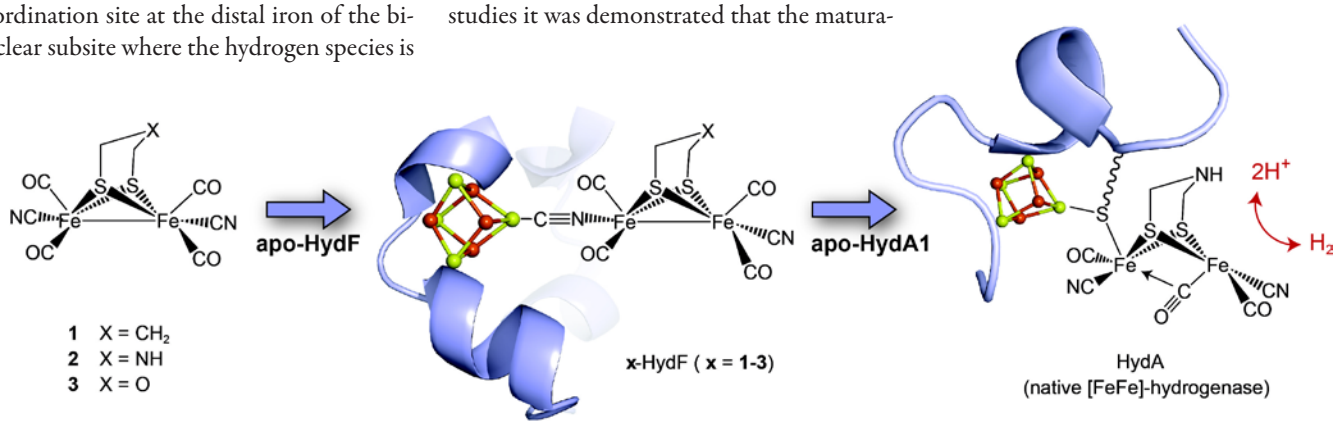
Numerous therapeutic effects and treatment strategies utilized in cell models *in vitro* cannot be reproduced in animal models or patients due to an inability to address tissue microenvironment (TME) contribution. For two leading causes of mortality in the world, cancer and ischemic heart disease, it is well documented that deviations in tissue oxygenation, pH, redox and glutathione homeostasis, as well as the crucial contributions of these factors within TME affect treatment efficiency and outcome. Therefore, recently developed EPR-based approaches for multifunctional monitoring of these TME parameters, *in vivo*, by an international team of collaborators involving researchers at The Ohio State University (Columbus, USA) and Institute of Organic Chemistry (Novosibirsk, Russia) provide important tools for drug screening, treatment optimization and outcome prediction in animal preclinical models. The developed trityl (Dhimitruka, I.; Bobko, A. A.; Eubank, T. D.; Komarov, D. A.; Khramstov, V. V. *J. Am. Chem. Soc.* **2013**, 135, 5904–5910) and nitroxide (Bobko, A. A.; Eubank, T. D.; Voorhees, J. L.; Efimova, O. V.; Kirilyuk, I. A.; Petryakov, S.; Trofimiov, D. G.; Marsh, C. B.; Zweier, J. L.; Grigor'ev, I. A.; Samouilov, A.; Khramtsov, V. V. *Mag. Res. Med.* **2012**, 67, 1827–1836) paramagnetic probes allow for non-invasive analysis of specific TME parameters, *in vivo*, when combined with low-field EPR or proton-electron double-resonance imaging, PEDRI. The dual functionality of the probes allows for the measurement of two parameters from the delivery of a single probe and a single spectrum thereby decreasing invasiveness for better correlation of these parameters independent of probe distributions.



Dual function trityl probe (Dhimitruka et al. J. Am. Chem. Soc., 2013, 135, 5904–5910)

Artificial Maturation of [FeFe]-hydrogenases: Biomimetic Chemistry and Biology in Synergy 8

Hydrogenase enzymes are champions in biohydrogen production. In view of the quest for renewable energy carriers there is great interest in the elucidation of the structure-function relationships of these ancient biocatalysts. The active site of [FeFe] hydrogenases, i.e. the "H-cluster", contains a binuclear Fe-Fe cluster coordinated by CO- and CN-ligands as well as a dithiolate bridging ligand containing a central amine. This di-iron subsite is connected through a bridging cysteine to a cubane cluster which is linked to the electron transport chain of the enzyme. It is generally assumed that the bridging amine moiety is responsible for shuttling protons to and from the open coordination site at the distal iron of the binuclear subsite where the hydrogen species is binding. Recently unequivocal evidence on the identity of this azadithiolate (ADT) bridge was provided in a collaboration between researchers from the Max Planck Institute in Muelheim and colleagues in Bochum and Grenoble (Berggren, G.; Adamska, A.; Lambertz, C.; Simmons, T. R.; Esselborn, J.; Atta, M.; Gambarelli, S.; Mouesca, J. M.; Reijerse, E.; Lubitz, W.; Happe, T.; Artero, V.; Fontecave M. *Nature* **2013**, 499, 66–69 and Esselborn, J.; Lambertz, C.; Adamska-Venkatesh, A.; Simmons, T.; Berggren, G.; Noth, J.; Siebel, J.; Hemschemeier, A.; Artero, V.; Reijerse, E.; Fontecave, M.; Lubitz, W.; Happe. T. *Nat. Chem. Biol.* **2013**, 9, 607–609). In these studies it was demonstrated that the maturation pathway of the H-cluster, which *in vivo* requires three helper proteins or "maturases" could be short-circuited by simply adding a synthetic analogue of the binuclear subsite to the apo-hydrogenase protein in which this part is lacking. Using FTIR and EPR it was shown that three bi-nuclear analogues containing a carbon, oxygen or nitrogen atom at the center of the dithiol bridge could be inserted into the apo-protein. But only the nitrogen containing analogue (ADT) afforded a fully active enzyme. This artificial maturation procedure is assumed to be functional for all [FeFe] hydrogenases.



Artificial maturation pathway for [FeFe] Hydrogenase using a single maturation factor HydF (Berggren et al., Nature, 2013, 499, 66-69).

Cornell Holds International Symposium on Modern ESR in Honor of Jack H. Freed on his Birthday and 50 Years at Cornell

Jack Freed's leadership and seminal contributions to ESR spectroscopy, in theory and technique development, are self-evident to our ESR community. Jack has won numerous national and international honors and awards from almost all of the prominent Scientific Societies; the latest honor being the award of the 2013 ISMAR Prize of the International Magnetic Resonance Society. Jack has been a Cornell faculty member since 1963, rising quickly to the rank of professor and now holds the Frank and Robert Laughlin Chair in the Department of Chemistry and Chemical Biology. As we know, Jack is the (founding) Director of the Advanced Center for ESR Research and Technology (ACERT) at Cornell. It was an opportunity for the ESR community and Cornell to recognize Jack's long-standing leadership and scholarly accomplishments. His former students and ACERT thus organized an International Symposium on Modern ESR Spectroscopy on the Cornell Campus, Ithaca, NY, on June 15, 2013 in honor of his 75th birthday and 50 years as a Professor of Chemistry at Cornell University. There were twelve speakers at the Symposium, eleven of them were former Freed graduate students and postdoctoral associates, now well-established in academia as well as national labs, and representing all corners of the United States and four different Continents. The symposium opened with the talk by Ron Mason, NIEHS, Triangle Park, NC. He summarized the latest advances and applications of spin trapping, with specific application to sulfite-derived free radicals and oxidation of Myloperoxidase to a free radical by activation of human neutrophils. This was followed by Eva Meirovitch of Bar–Ilan University, Tel Aviv, Israel. She summarized the latest developments on the "slowly relaxing local structure" (SRLS) approach as applied to NMR relaxation in proteins, techniques pioneered by Freed and coworkers for ESR studies. Yeon-Kyun Shin of Iowa State University, Ames, IA presented spin labeling and FRET approaches to study protein structure and dynamics. Antonino Polimeno, University of Padova, Padova, Italy, discussed his stochastic modeling of relaxation processes in biomacromolecules, a sophisticated approach requiring relatively modest computational time, and still enabling studies of coupled local and global motions. Sunil Saxena, a Freed graduate, now at University of Pittsburgh, Pittsburgh, PA presented novel pulsed and CW ESR studies of metal-ion coordination in aggregating peptides. Alexander Nevzorov, of North Carolina State University, Raleigh, NC presented his recent development of the Stochastic-Liouville approach in magic-angle spinning solid state NMR of oriented membrane proteins; again, Jack had earlier pioneered this methodology as currently used heavily in ESR spectroscopy. This was followed by a talk by Antonio Costa-Filho, University of Sao Paulo, Sao Paulo, Brazil, titled "On Spins, ESR, Freed, Proteins, Peptides: A South of the Equator Perspective" a highly illuminating discussion of the need for advanced ESR instrumentation in Brazil and other South American countries, and their advances in theoretical approaches. Then a breath-of-fresh air talk was presented by Aharon.

Blank of Technion, Haifa, Israel, who discussed how to employ very small resonators (with very high filling factor) and induction detection to observe ESR signals from about 1000 spins, with a spatial resolution of about 500 nm. The last talk from a former Freed student was by Yun-Wei Chiang, National Tsing Hua University, Hsinchu, Taiwan, who summarized recent applications of CW and Pulse ESR spectroscopy to water-filled nanochannels, yielding a detailed understanding of interfacial water in biological channels of 2-7 nm pore diameter. The highlight was the pre-banquet talk by Klaus Möbius, Free University of Berlin, Berlin, Germany, a pioneer in ENDOR and high-frequency pulse and CW ESR spectroscopy. He discussed how ESR has been the most direct technique for understanding photosynthesis, since both paramagnetic metal ions and free radicals are directly involved in the electron transfer processes that are the basis of photosynthesis. He stressed that there is a very bright future and need for more sensitive high-frequency pulsed ESR techniques such as are being developed at ACERT. The Symposium ended with a gala banquet and several personal stories by senior colleagues, including a congratulatory letter from Nobelist Roald Hoffmann. The Cornell alumni related the fond memories of their young lives under Jack Freed's tutelage, described as hard but productive times. The Symposium ended with best wishes and singing of Happy Birthday to Jack, and an encore for such symposia. More details can be found at ACERT's homepage at www.acert.cornell.edu.

Naresh Dalal

55th Annual Rocky Mountain Conference on Analytical Chemistry: 36th EPR Symposium

Denver, Colorado, USA, July 28 – August 1, 2013

The "Return to Denver" as many called the 2013 Rocky Mountain (RMC) EPR Symposium was a great success! This was the first time in nearly 10 years (since 2005) that the EPR symposium was held in the city limits of Denver. The conference was held at the Crown Plaza Hotel, which is located near the 16th Street Mall with numerous choices for dining and socializing activities. This downtown location also provided for the opportunity to again visit the research labs of Gareth and Sandra Eaton and to hear talks and see demonstrations of the exciting advances they have been pioneering in the area of rapid-scan EPR. Bruker also held a workshop on Sunday evening on the Denver University's campus that highlighted new developments with applications to distance measurements, cryogen free data acquisition and tutorial modules. Participants in the workshop also experienced the new light rail system, which offered facile transportation between the hotel and Denver University.

The 2013 EPR symposium was also the second time the RMC meeting was "solo" for the EPR community; the first time being in 2011. We were quite pleased that there were ~130 registered attendees, which is a growth of nearly 30% from the previous "EPR only" RMC. The field of EPR spectroscopy is going strong with a sustainable group for "solo" conferences to continue in the future. The Denver location also allowed for a diverse gathering with international attendees coming from nearly all other continents including Europe, Asia, Africa, Australia, and South America!

For the first time at the RMC EPR Symposium, the International EPR Society (EIS) presented awards for the best student or post-doctoral research poster presentation. The IES hopes to provide this level of support for future meetings. Larry Berliner, current president of the IES, presented the young investigator award to Dame McCamey. Wolfgang Trommer was presented the IES Fellow Award and gave a plenary talk entitled "The Molten Globule State of Maltose Binding Protein: DEER Measurements at pH 3". The Piette lecture for 2013 was given by David S. Cafiso, entitled "Uncovering Secrets in Membrane Electrostatics, Cell-Signaling and Transport using EPR Spectroscopy".

The program for 2013 covered a vast span of areas of EPR research and spectroscopy, from spin-devices and quantum computing applications to dynamic nuclear polarization (DNP) and in vivo imaging. The conference hosted the following 8 sessions: EPR for Spin Devices, chaired by John Morton; Materials, chaired by Dane McCamey; Methods, chaired by Christoph Boehme; Biological Macromolecules, chaired by Kurt Warncke, Radical Radicals, chaired by Frederick Villamena; Frontiers in Spin Labeling, chaired by Fraser MacMillan; In Vivo EPR chaired by Boris Epel; Spin Labeling II, chaired by Howard Halpern.

During the meeting a group discussion was led by Gary Gerfen, who made an announcement describing the efforts of a group of EPR investigators (Gerfen, Fanucci, Lyon, Sherwin, Boehme) to establish a US based Network through the NSF funding opportunity, a Research Coordination Network proposal. A goal of the Network would be to establish a strong relationship with investigators currently participating in the German DFG funded Priority Program SPP1601 "New Frontiers in Sensitivity for EPR Spectroscopy: From Biological Cells to Nano Materials." Comments from the participants aided in the development of the NSF proposal, entitled "SHARED EPR Research – Supporting, Highlighting and Advancing REcent Developments in EPR Research" which is intended to be submitted this Fall.

Next year's chair is Mark Sherwin from the University of California Santa Barbara and the 2014 RMC EPR Symposium will be held together with the NMR community in Copper Mountain, Co. Kurt Warncke was chosen to be chair of the 2015 EPR Symposium and will act as co-chair for the 2014 meeting. The location of the 2015 meeting is still undecided, but discussions centered on holding the meeting either again in Denver or at a new location, such as Snow Bird, Utah.

Gail Fanucci

notices of Meetings

Oxygen Radicals from Detection to Disease
Ventura Beach Marriott, Ventura, CA USA
February 9-14, 2014
www.grc.org/programs.aspx?year=2014&program=oxygenrad

We are inviting you to apply for the upcoming Oxygen Radicals Gordon Research Conference, to be held February 9–14, 2014 at the Ventura Beach Marriott in Ventura, CA. Our outstanding scientific program with participation by leading as well as young investigators is one you won't want to miss.

The scientific program includes Keynote talks by Dr. Salvador Moncada (University College London, UK) and Dr. Sue Goo Rhee (Ewha Women's University, S. Korea) as well as exciting scientific sessions: Detection Methods: New and Improved; Protein Oxidative Modification And Turnover; Mitochondria: Redox Organelles; Free Radicals in Carcinogenesis; Oxidative Modifications in Aging and Age-Related Disease; Rates do Matter; Free Radical Metabolites in the Initiation of

Autoimmunity; A New Look at Dinitrosyl Iron Complexes in Cancer.

Additionally, a Gordon Research Seminar for young scientists will be held in conjunction with the above Oxygen Radicals Gordon Research Conference on February 8–9, 2014 (www.grc.org/programs.aspx?year=2014&program=grs_oxy).

Ronald Mason & Alicia Kowaltowski
Chairs
NIEHS/NIH
Laboratory of Toxicology & Pharmacology
Phone: (919) 541-3910
Web: www.niehs.nih.gov/research/atniehs/labs/ltp/freerad/index.cfm

International Conference "Magnetic resonance: fundamental research and pioneering applications" (MR-70)

Kazan Federal University, Kazan, Russia
June 23–27, 2014
http://mr70.kpfu.ru

The International Conference "Magnetic resonance: fundamental research and pioneering applications" (MR-70) is devoted to the 70th anniversary of the discovery of Electron Paramagnetic Resonance by E. K. Zavoiskii. The conference schedule will involve plenary talks (30 min), oral (20 min) and poster presentations. Scientists from all countries are invited to discuss the most significant results obtained with the use of magnetic resonance and magnetic relaxation measurements and theoretical models in condensed matter physics and modern applications of magnetic resonance techniques and methods.

The scope of the conference

State-of-the-art in application of magnetic resonance (EPR, NMR) in physics (strongly correlated systems, quantum magnets, molecular magnetism, nanoparticles and porous systems, phenomena in high magnetic fields, quantum technology materials, quantum computing, etc.), organic, bioorganic and physical chemistry, biology, medicine, geochemistry and geological prospecting, etc.

Chairman of the Organizing Committee
Albert Aganov,
Scientific Secretary of the Conference
Alex Dooglav
e-mail: Alexander.Dooglav@kpfu.ru

First Adriatic Symposium on Biophysical Approaches in Biomedical Studies

University of Split, Croatia, August 24–29, 2014

The very first Adriatic Symposium on Biophysics Approaches in Biomedical Studies will be held at the University of Split. The research presented at the symposium will focus on the structure, dynamics and function of membrane systems and proteins, the role of oxidative stress in human diseases, the detection and imaging of free radicals, and drug transport across membranes.

The organizers are: M. Raguz (University of Split, Croatia), B. Kalyanaraman (Medical College of Wisconsin, Milwaukee, USA), T. Sarna (Jagiellonian University, Krakow, Poland).

For more information contact Jane Thelaner at jthelane@mcw.edu.

POSITIONS

Postdoctoral Associateships in Magnetics at NIST

We offer postdoctoral opportunities in magnetics at the National Institute of Standards and Technology in Boulder, Colorado, USA. Annual salary is $65,600 plus benefits. Appointments are for two years. Application deadlines are 1 February and 1 August annually (but inquire earlier).

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

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

Ohio State University – EPR Center Molecular Imaging Program

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

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

Ohio State University – EPR Center

A position is open for an electrical engineer with experience in EPR equipment construction and repair. Ongoing projects include development and construction of in vivo EPR systems, EPR/NMR coimaging and PEDRI.

Strong background in electrical engineering, and RF/microwave electronics required. Knowledge of CW and pulsed EPR spectroscopy is desirable.

Please send CV, select publications, and statement of research interests to Jay.Zweier@osumc.edu. OSU is an Equal Opportunity Employer.

Post-doctoral position in structural studies of kinesins

A post-doctoral position is available immediately for a multi-disciplinary research project investigating the regulation of kinesin activity from the cellular to the molecular level. The group comprises the laboratories of Gary Gerfen, Ao Ma, David Sharp and Hernando Sosa in the Department of Physiology and Biophysics of the Albert Einstein College of Medicine, New York, USA. A strong interest in cell and structural biology is required for this position. A major component of the structure/function characterization will involve site directed spin label EPR (SDSL-EPR) spectroscopy, with contributions from Cryo-electron microscopy, X-ray crystallography, fluorescence spectroscopy and molecular modeling.

State of the art resources are available in each of the participating laboratories and in the core facilities of the Albert College of Medicine. These capabilities include EPR (PELDOR, high frequency, HYSCORE), several modalities of fluorescence microscopy (con-focal, epi, tirf, single-molecule polarization etc.), cryo-electron microscopy and state-of-the-art computer clusters for molecular simulations. All four laboratories in the group are located in the Albert Einstein College of Medicine in New York City, USA, which offers a vibrant scientific and social environment. Interested applicants should forward a CV and three reference letters to Gary Gerfen at gary.gerfen@einstein.yu.edu.

Yeshiva University is an equal opportunity employer committed to workforce diversity.

EPR Specialist Position at Johns Hopkins

Postdoctoral or specialist (staff) position is available immediately to study membrane proteins at the Johns Hopkins University School of Medicine in Baltimore, Maryland, USA. We study conserved membrane enzymes with implications for human health (see Nature Chem Biol 8:759, eLife 1:e00173, and Nature Rev Micro 7:411), and are generously funded by the National Institutes of Health (NIH) and the Howard Hughes Medical Institute (HHMI). The project uses site-directed spin labeling (SDSL) with nitroxide probes to study the dynamics, distance measurements, and saturation kinetics with CW-EPR methods. The applicant must have at least 3 years of prior experience in SDSL, EPR, spectrum simulations, and distance measurements as evidenced by publications. Experience with membrane proteins is preferred but not essential. Position will come with generous salary and benefits, depending on experience and record of achievement. Interested applicants please send detailed CV and contact information for 3 references to rosanna@jhmi.edu.

Research Positions – Advanced EPR of Biochemical and Chemical Systems

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

In-house projects:

- Photosynthetic systems (reaction centers, water oxidation);
- Hydrogenase enzymes and related model systems;
- Radical enzymes and protein maquettes.

Collaborative projects:

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

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

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

Please send your application including CV and the scope of scientific interests to:
Prof. Wolfgang Lubitz
Max Planck Institute for Chemical Energy Conversion, Stiftstrasse 34-36, 45470 Mülheim an der Ruhr, Germany
e-mail: wolfgang.lubitz@cec.mpg.de

Bruker BioSpin Corp

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

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

EQUIPMENT

EPR parts, electronics and hardware

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

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

For sale

Varian E-line spectrometer components as a system or individually: 9" magnet and power supply, 2 - consoles; 2 - E101 X-band bridges; 1 - E102 X-band bridge with GasFET & dispersion; TE102 and TE104 X-band cavities with ENDOR fittings and liq He Cryo Industries flow cryostat; 1 - E110 Q-band bridge with GasFET & dispersion; Q-band frequency counter; Q-band TE011 cavity components with pumped He Cryo Industries supervaritemp type cryostat; Dell computer and interface.

Contact Cindi Rohwer (email cindi.rohwer@unh.edu or via phone 1-603-862-1795) for further information.

For sale

Bruker ER 041 XK-H X-band microwave bridge and external controller.

Contact Cindi Rohwer (email cindi.rohwer@unh.edu or via phone 1-603-862-1795) for further information.

Design and construction of EPR electronics

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

For sale: Varian and ESR equipment

Resonance Instruments has available: (1) Replacement klystrons for Varian EPR bridges and some Bruker bridges (at reduced prices) and other klystrons; (2) Resonance Instrument's Model 8320A is a general purpose Hall-effect based magnetic field controller that provides direct control and precise regulation of the magnetic field between the pole pieces of an electromatnet. Its high resolution permits precise adjustment of the magnet's field either though the front panel keyboard or though an RS232 serial interface with your PC.

Please contact: Clarence Arnow, President, e-mail: 8400sales@resonanceinstruments.com, phone: 1-847-583-1000, fax: 1-847-583-1021.

Available: Used Varian EPR equipment

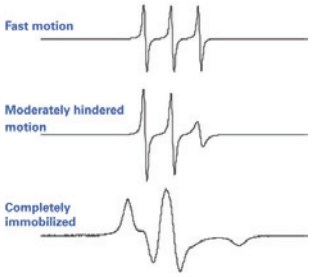
(1) Varian E-104 EPR spectrometer with vertical style bridge and e-line fieldial. (2) Varian E-9 EPR spectrometer. Both available with warranty and continued service support. (3) Varian TM cavity with flat cell holders and flat cells. (4) Varian E-257 variable temperature controller with heater sensor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

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

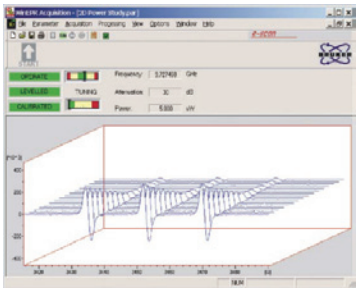
BRUKER

e-scan

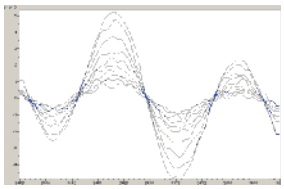
Probing protein mobility and membrane dynamics with spin labels



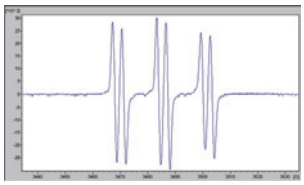
2D acquisition capability: microwave power saturation study



DPPH-Assay: Antioxidant activity



Spin-trapping of ROS



Application Areas:

- Free radicals
- Spin-labels and Spin-traps
- Reactive Oxygen Species (ROS)
- Reactive Nitrogen Species (RNS)
- Antioxidant-derived free radicals
- Transition metal complexes

The Table-Top EPR Research System

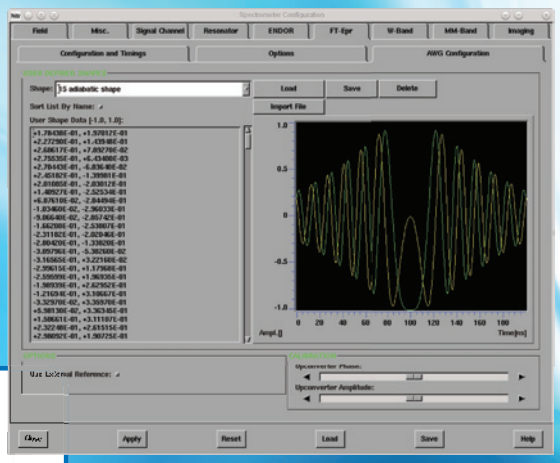
The X-Band research grade sensitivity and flexibility in a table-top system:

- Compact, easy to use and learn, table-top CW-EPR system
- The most direct tool for detection and characterization of free radicals and transition metal ions with g-values of ~ 2
- Automatic acquisition schemes (WinAcq), extensive data processing (WinEPR) and efficient spectral simulations (SimFonia) available on a Windows™ platform
- The e-scan is suitable for both research and teaching purposes

Contact us for more details: www.bruker-biospin.com/epr

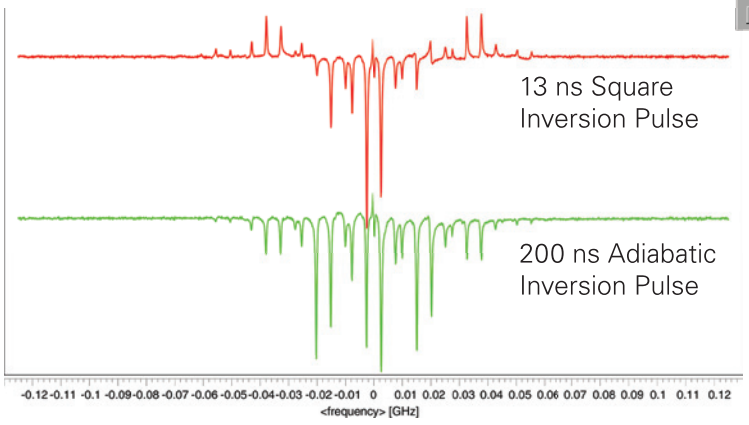
Optimum Pulse Control with SpinJet-AWG

Improved Results



Easy to Define Shapes

PNT Sample



Angew. Chem. , P. E. Spindler, S. J. Glaser, T. E. Skinner, T. F. Prisner, v52, p3425, 2013

User Optimization with SpinJet-AWG

User-defined pulse shapes within SpinJet-AWG allow a wide variety of experimental opportunities, for all available frequency bands from L-band to 263 GHz:

- Uniform spectrum inversion
- Optimized excitation
- Resonator compensation
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- Ramp up and down
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