epr newsletter

2015
volume 25 number 3-4

The Publication of the International
EPR (ESR) Society

Officers of the International EPR (ESR) Society

PRESIDENT

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

VICE PRESIDENTS

Americas

Stephen Hill
EMR Program Director,
NationalHigh Magnetic Field Laboratory,
1800 E. Paul Dirac Drive, Tallahassee, FL 23310 USA
phone: 1-850-644-1647
e-mail: shill@magnet.fsu.edu

Asia-Pacific

January 1, 2015 until Febryary 25, 2015

Graeme Hanson
The University of Queensland,
Queensland, 4072, Australia
phone: +61-7-3365-3242
e-mail: graeme.hanson@cmr.uq.edu.au

from Febryary 26, 2015

Elena Bagryanskaya
Vorozhtsov Institut of Organic Chemistry
Russian Academy of Sciences,
pr. Lavrentieva 9, Novosibirsk, 630090 Russia
phone: 7-383-330-88-50
e-mail: egbagryanskaya@nioch.nsc.ru

Europe

Graham Smith
Scool of Physics & Astronomy, University of St. Andrews,
NorthHaugh, St. Andrews KY 16 9SS, Scotland, UK
phone: 44(0) 1334-46-2669
e-mail: gms@st-andrews.ac.uk

SECRETARY

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

TREASURER

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

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

July 1, 2016 until December 31, 2017

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

FOUNDER PRESIDENT

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

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

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

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

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

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

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

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

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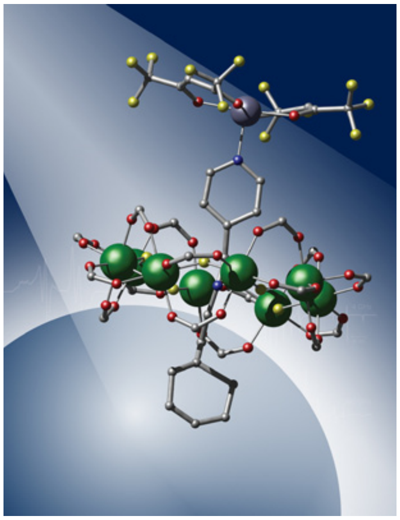
volume 25 number 3-4 2015



The cover picture illustrates aspects of research carried out by Eric McInnes, recipient of the IES Silver Medal for Chemistry 2015. It shows a supramolecular complex of a transition metal cluster and a copper ion where EPR can measure the weak exchange interaction between them.

IES business

Awards

Guest of the issue

Software

New books and journals

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Editorial

Dear colleagues,

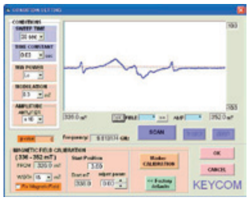
Are you pleasantly surprised that as a New Year present you get a double issue of the *EPR newsletter* and not a single one?! Sure you did not expect it and perhaps you keep wondering what underflows led to this result. Sorry to disappoint you, nothing romantic or mysterious, only the most pragmatic reason. Historically, starting from 2004, issue no. 4 of a volume was the first issue of the year and in a way it was an oxymoron (hope I use this word correctly). So sooner or later this problem had to be solved. Therefore finally here we are with the double issue of the *EPR newsletter* 25/3–4 (2015) and the first issue of 2016 will be 26/1. Enjoy! Let you surf the pages of the newsletter as you please and dwell on columns you like most.

It was talking to Gary Gerfen at the EPR Symposium of the Rocky Mountain Conference in Snowbird, Utah when I realized what one of the most important features of our newsletter is. Gary and I recalled the story of the publication of Bill Mims' reminiscences on the first days of electron spin echo spectroscopy in biology (*EPR newsletter* 17/1, pp. 10–12 and 17/2–3, pp. 17–20). To say it in big words, this publication saved Bill Mims' notes for eternity. It was a light-bulb moment for me: in fact, *EPR newsletter* is not a collection of short-lived news. This news belongs to many years to come. It is an encyclopedia of the life of the EPR community containing a lot of interesting information that is known to a very limited number of colleagues if any. Please believe me, surfing back issues may be quite enlightening and breathtaking.

Happy New Year to all of you and your dear ones! On behalf of my colleagues from the Editorial Board of the *EPR newsletter*, Candice Klug, Hitoshi Ohta, Sabine Van Doorslaer and Sergei Akhmin, I wish you, our dear readers, all the best. Please feel free to contribute your news to our publication. Your inputs are always welcome.

Laila Mosina

PS To open just one little secret concerning the forthcoming issue 26/1 (2016): you will find the "Present Meets Future" column edited by Sabine Van Doorslaer featuring Elena Bagryanskaya and Olesya Krumkacheva, a mentor and a young researcher, respectively.



ANNUAL GENERAL MEETING 2015

Minutes of the Annual General Meeting of the International EPR(ESR) Society for 2015, held during the Rocky Mountain Conference on July 29, 2015, in Snowbird, Utah.

AGENDA

1. Introductory notes by Prof. Hitoshi Ohta
2. President's Report
3. Secretary's Report
4. Treasurer's Report (Financial Report 2014–15)
5. *EPR newsletter* Editor's Report
6. Thanks
7. IES Awards Ceremony

1. Introductory notes by Prof. Hitoshi Ohta

Dear Colleagues,

On behalf of the IES Executive Board I wish to welcome all participants to the 26th General Meeting of the IES at the Rocky Mountain Conference in Snowbird.

I would like to express my gratitude to the conference organizers of this meeting, especially to Prof. Kurt Warncke, Chair of EPR Symposium, and Prof. John Morton, Co-Chair of EPR Symposium, for allowing our General Meeting to take place during this Conference.

International EPR (ESR) Society Executives: IES Executives (2015–2017) have been elected following the IES Constitution: President: Hitoshi Ohta; Vice President Asia Pacific: Graeme Hanson / Elena Bagryanskaya (Since March, 2015); Vice President Americas: Stephen Hill; Vice President Europe: Graham Smith; Secretary: Aharon Blank; Treasurer: Tatyana Smirnova; Immediate Past President: Lawrence Berliner (first 1.5 years) Klaus Möbius (subsequent 1.5 years); Founder President: Harold Swartz

2. President's Report

I start my report with very sad news. Vice President Graeme Hanson passed away on February 25, 2015. It was only 2 months after he started as the Vice 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.

2.1. Brief report of the previous AGM – Nara, Nov 2014, see *EPR newsletter* 24/4.

2.2. The importance of IES and its activities.

For basic science and applied research, EPR/ESR spectroscopy is continuing to become 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 within the wide magnetic resonance community.

We'll be making a renewed effort to expand our membership. We 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 attractiveness 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 example of IES participation in International EPR conferences: APES-IES-SEST 2014, Nara, Nov 12–16, 2014 (Specially reduced registration fee for IES members).

Second example: EPR BioDose 2015 and the 2nd IES Symposium, Hanover, Oct 4–8, 2015.

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 to grow and flourish.

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 (see below).

2.3. IES Awards for 2015

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 to Silver Medals in various specialized areas of EPR, Young Investigator Awards and IES Fellowships. Please visit www.ieprs.org for full details on IES constitution and by-laws relating to Awards.

2015 IES awards the following distinctions: Silver Medal for Biology/Medicine, Silver Medal for Chemistry, Young Investigator Award (IES), IES Fellowships and IES Poster Awards (eight in 2014 and ten scheduled in 2015).

2015 Silver Medal for Biology/Medicine: Murali Krishna Cherukuri (USA) / Derek Marsh (Germany)

2015 Silver Medal for Chemistry: Eric McInnes (UK)

2015 Young Investigator Award (IES): Ilia Kaminker (USA)

2015 IES Fellowships: Dante Gatteschi (Italy), Robert Griffin (USA), Edgar Groenen (Netherland), Brian Hoffman (USA), Sankaran Subramanian(USA)

IES Poster Awards

The IES sponsors student awards for the best posters at select EPR-related meetings each year. Eligible candidates are graduate students and post docs (not later than 3 years after their PhD). Certificate + US$200 award + 1 year membership of IES.

IES Poster Awards for 2015: The 3rd Awaji International Workshop on Electron Spin Science & Technology: Biological and Materials Science Oriented Applications (AWEST 2015), Jun 14–17, 2015, Awaji Island, Japan; EUROMAR 2015, Jul 5–10, 2015, Prague Congress Centre, Prague, Czech Republic; Rocky Mountain Conference on Magnetic Resonance, Jul 26–30, 2015, Snowbird, Utah, USA (Annual General Meeting of IES 2015); EPR BioDose 2015 and the 2nd IES Symposium, Oct 4–8, 2015, Hanover, New Hampshire, USA; 2015 International Chemical Congress of Pacific Basin Societies (PACIFICHEM 2015); Nitroxide Radicals: Synthesis and Functional Bio-/Nanomaterials Symposium #309 Dec 15–20, 2015, Honolulu, Hawaii, USA (Asia-Pacific).

We want to thank all the members of the Awards and Fellowship Committees for their excellent work for the Society.

Hitoshi Ohta

Call for IES Award Nominations 2016: Nominations are invited for: Silver Medal Physics/Materials; John-Weil Young Investigator Award; Fellowship of the Society.

Nominations, accompanied by curriculum vitae, are due by 1 November 2015. For more information, see our www.ieprs.org at the "Awards" page.

3. Secretary's Report: Sushil Misra (up to August 31, 2014), Aharon Blank (from October 1, 2014)

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

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

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

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

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

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

f. Website (revamping). Please, visit web site www.ieprs.org. New for 2015: "Position/Equipment" page, "IES Poster Awards" list.

g. Answering any enquiries.

h. Organizing AGM.

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

We want to thank Sushil Misra and Aharon Blank for their excellent work as Secretaries of the Society.

Hitoshi Ohta

4. Treasurer's Report: Tatyana Smirnova (Financial Report 2014–15)

2014 Financial Report ($) (self-audited)

Balance January 1, 2014	17,110.58
Deposits:	
Membership	7,018.16
Sponsors	8,556.00
Bruker contribution to printing	2,226.00
Total Income	17,800.16
Expenses:	
Credit card fees, internet commerce and merchant services	739.48
Web design / maintenance & fees	1,133.82
Newsletter printing (including 2,226.00 paid by Bruker)	4,785.10
Newsletter Editorial	3,242.00
State of Illinois+misc	18.80
Awards and medals	2,187.40
Total Expences	12,106.60
Balance December 31, 2014	22,804.14

Comments from the Treasurer:

We have balanced the budget in 2014!

In 2014-15 the Society gained the sponsorships of:

Oxford Instruments NanoScience. – Sponsor ($1,500/year)

Elva-1 Microwave Handelsbolag – Supporter ($750/year)

Active Spectrum – Major Sponsor ($2,500/year)

Thank you, members and sponsors, for your support!

Eric McInnes (left) and Hitoshi Ohta (right).

2015 (January-June)
Financial Report ($) (self-audited)

Balance January 1, 2015	22,804.14
Deposits:	
Membership	2,900.09
Sponsors	8,786.50
Conference funds APES2014, IES and SEST2014	5,780.83
Total Income	17,467.42
Expenses:	
Credit card fees, internet commerce and merchant services	344.29
Web design / maintenance & fees	493.00
Newsletter printing	2,475.00
Incorporation fee	13.00
Awards and medals	1,107.29
Total Expences	4,432.58
Balance June 30, 2015	35,838.98

Thank you, sponsors:
Bruker BioSpin, Corp
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Wilmad-LabGlass
Scientific Software Services
Research Specialties
Molecular Specialties
KeyCom Corp
Norell, Inc
GMW Associates

Status of membership as of July 1, 2015	
Membership: paid for 2012	221
Membership: paid for 2013	237
Membership: paid for 2014	260
Membership: paid for 2015	169
out of which:	
Full members	169
Emeritus	18
Students	54
Postdoctoral members	18
Complementary/sponsored	50

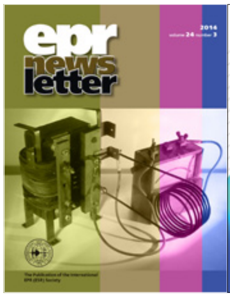
Members represent 30 countries:
Japan 85, Germany 21, Russia 23, USA 67.

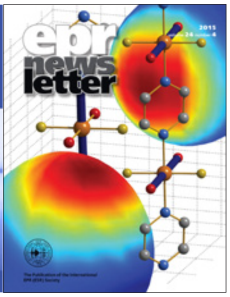
We want to thank Tatyana Smirnova for her excellent work as Treasurer of the Society.

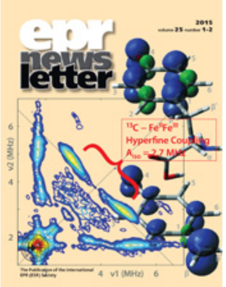
Hitoshi Ohta

5. *EPR newsletter* Editor's Report: Laila Mosina

Since the previous Annual Meeting of the IES in 2014 in Nara (Japan) we published two single issues, 24/3, 24/4, and prepared a double issue 25/1-2. The latter is displayed at the conference. We hope you had a look at 24/3 and 24/4 on the newsletter website and got relevant copies.







Now we start with the preparation of the forthcoming issue 25/3. To remind you, we present the columns of the newsletter:

Columns of the *EPR newsletter* 25/3 (2015)

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

In 24/3, Sabine Van Doorslaer started the "Present Meets Future" column.

Starting from 25/3, Wolfgang Lubitz succeeds the late Graeme Hanson in editing the "EPR → Hot Science" sub-column.

Dear colleagues, please feel free to submit your material to all columns. It is you who produce the news, we just present it in the *EPR newsletter*. 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, Wolfgang Lubitz, Stefan Stoll, Keith Earle and David Budil, Sabine Van Doorslaer, and also to Yevhen Polyhach, our web-master, and Sergei Akhmin, our Technical Editor. I gratefully acknowledge collaboration with Associate Editors Candice Klug, Hitoshi Ohta and Sabine Van Doorslaer.

6. Thanks

The IES thanks the following Corporate Sponsors for their contributions in 2012–2014:
Adani Systems
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Resonance Instruments
Scientific Software Services
Wilmad-LabGlass

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All paid up members
Newsletter Editor: Laila Mosina
Technical Editor: Sergei Akhmin
Associate Editors: Thomas Prisner, Candice Klug, Hitoshi Ohta, and Sabine Van Doorslaer

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Vice President Americas: Stephen Hill
Vice President Europe: Graham Smith
Vice President Asia Pacific: Elena Bagryanskaya
Secretary: Sushil Misra / Aharon Blank (since Oct 1, 2014)
Treasurer: Tatyana Smirnova
Immediate Past President: Lawrence Berliner
Founder President: Harold Swartz

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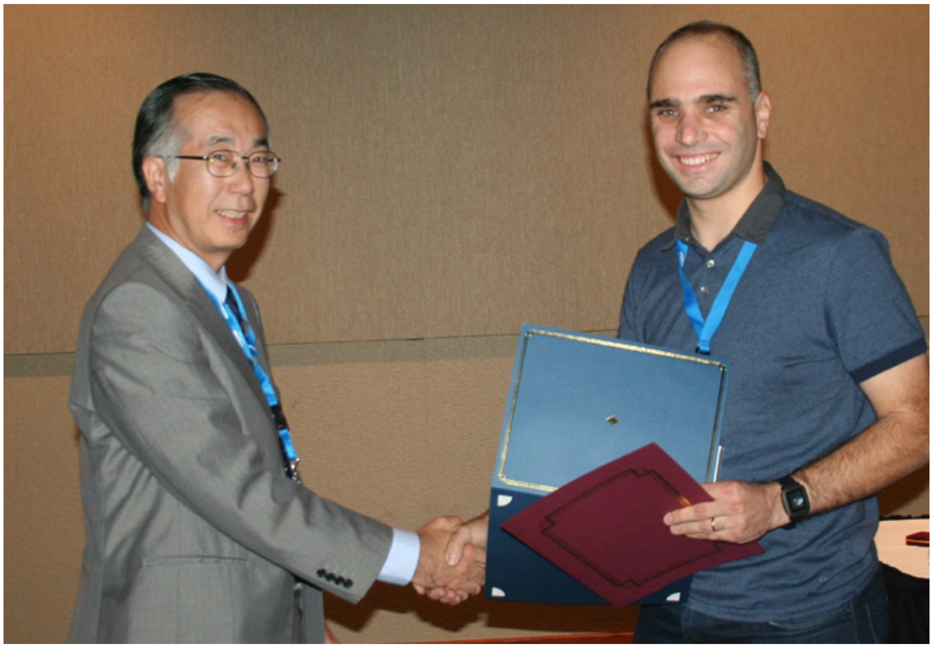

Hitoshi Ohta (left) and Ilia Kaminker (right).

IES Silver Medal in Biology/Medicine 2015 to Murali Krishna Cherukuri

Prof. Hitoshi Ohta presents Dr. Murali Krishna Cherukuri with the IES Silver Medal in Biology/Medicine at SEST2015, November 2 at Niigata, Japan.

For details, see the forthcoming issue of the *EPR newsletter*

The International Zavoisky Award 2015

Professor **Vadim A. Atsarkin** (Kotel'nikov Institute for Radio Engineering and Electronics, Russian Academy of Sciences,Moscow, Russian Federation)

The Award is presented in recognition of a lifetime's work in magnetic resonance and, in particular, the laureate's contribution to the development of spin thermodynamics and to studying the dynamic nuclear polarization phenomenon.

Professor **Dante Gatteschi** (University of Florence, Florence, Italy)

The Award is presented in recognition of a lifetime's work in magnetic resonance and, in particular, the laureate's contribution to the understanding of the nature of the single molecule magnets.

For details, see the forthcoming issue of the *EPR newsletter*

IES Silver Medal for Chemistry 2015

Eric McInnes:

I first met EPR spectroscopy as a chemistry undergraduate at Edinburgh University, during my final year research project with Lesley Yellowlees. She was expert in spectroelectrochemistry methods with optical spectroscopy, but I focused on their application in EPR. I stayed in Lesley's group for my PhD, modeling the charge transfer properties of di-immine platinum group complexes that have been studied as solar dyes. Lesley and I taught each other EPR over that period, and I remember the papers of August Maki and of Phil Rieger being particularly educational. In 1995 I took a post-doctoral position at Manchester University with Frank Mabbs and David Collison. This was when the Manchester UK EPR Facility, funded by the UK Engineering and Physical Sciences Research Council (EPSRC), was started and I was the first post-doc employed in that centre. When I arrived I did my first single crystal EPR experiment (I think this was an initiation ceremony in Frank's group) on a Cr(V)-oxo complex doped in an Os(VI)-nitrido host – I am still waiting for Frank and David to write the paper! Not long after we took delivery of a Bruker ESP system with L-, S-, X-, K- and Q-band bridges so I received a swift education in the merits of multi-frequency EPR. I undertook a number of different projects, but the most influential for the rest of my career was in collaboration with Richard Winpenny's group back in Edinburgh. It was Richard that got me interested in molecular magnetism, and I learned a lot from our early work together on transition metal clusters, first on simple Cu(II) dimers, but then on high-nuclearity and large spin ground state Cr(III) species. This work prompted my first use of high-field/frequency methods, with Graham Smith at St Andrews who was busy revolutionizing the design of such spectrometers. In 1999 I took a second post-doctoral position, at the University of East Anglia with Andrew Thomson and Annie Powell. I was there for one year, doing my first synthetic chemistry for a few years, and also using magnetic circular dichroism (MCD) spectroscopy to probe the molecular memory effect in the famous Mn$_{12}$ cluster.

I started a lectureship back in Manchester in January 2000, replacing the retiring Frank Mabbs. I was very fortunate that Richard Winpenny was appointed as the Chair of Inorganic Chemistry later that year, and we have collaborated closely ever since. I was also lucky to have a very talented first group of PhD students, including Stergios Piligkos (now on the faculty at Copenhagen University), Gopalan Rajaraman (now at the Indian Institute of Technology Bombay) and David Low, and my first post-doc, Rebecca Laye, was also hugely important in establishing the group. Together we started spectroscopic, theory, modeling and synthetic projects in molecular magnetism. I have always enjoyed the close collaboration between chemistry and physics in this field, and this led us to several unexpected areas of study, for example the discovery of large magnetocaloric effects in molecular systems. EPR was one of the most powerful tools for probing the electronic structure in these complicated exchange-coupled species, hence helping to explain their often weird macroscopic magnetic behaviour.

One project focused on a new class of materials prepared in Richard's group; a family of heterometallic ring-like structures, the first of which were based on a Cr(III)$_7$M(II) core. The physics and chemistry of these molecules has proved to be a lot of fun. For example, the antiferromagnetic exchange coupling in Cr$_7$M leads to a low, but non-zero, ground state spin. Because M can be almost any divalent metal ion, the nature of the ground state can be changed at will within an isostructural family; this allowed us to systematically probe problems such as the limits of the giant spin approximation commonly used for transition ion clusters. We are still studying these systems as the chemistry has been developed with a view to functional materials, leading to extraordinary supra-molecular structures including multi-rotaxanes, and we can use pulsed EPR techniques to probe the weak interactions between the molecular components. This work, and work on understanding spin relaxation effects in large clusters, has included a close collaboration with Arzhang Ardavan at Oxford.

One common theme through the years has been the use of EPR to probe electronic exchange interactions. EPR has an enormous amount to contribute in this area (for example, see Bencini and Gatteschi's textbook), and there are many examples where it allows determination of exchange interactions that

▶

are too weak or too strong to be measured by conventional magnetometry methods. It can also give insight into less familiar but important phenomena such as antisymmetric exchange and spin frustration effects. In recent years we have used EPR, and complementary techniques including inelastic neutron scattering, to probe the nature of exchange between metal ions with large magnetic anisotropy (due to orbital effects), including 3d, 4d, 4f and 5f-ions and the consequences for, e.g. the cluster anisotropy and relaxation effects.

As co-Director of the EPSRC UK EPR Facility I am lucky to have the opportunity to work with people in many different scientific areas, and I have always enjoyed the push this gives me to learn new things. A recent example is the close collaboration we have developed with Stephen Liddle (who has recently moved to Manchester from Nottingham), who has been making fantastic developments in actinide chemistry. We are now doing extensive work to understand the electronic structure of such systems, where crystal-field and spin-orbit interactions can be of comparable magnitude, and where the extent of covalency effects is still being debated. EPR has a lot to contribute to such problems.

I feel enormously flattered to receive the Silver Medal for Chemistry and am very grateful to the International EPR Society for this honour. Of course, the work on which this is based is the result of many people. There are far too many undergraduate, postgraduate and postdoctoral researchers, colleagues and collaborators to name them all but, in addition to the people named above, I must thank Floriana Tuna (Manchester) for her enormous contribution in many of these projects. I am also grateful to the EPSRC, the EC, The Leverhulme Trust, Bruker BioSpin, the ILL, and The University of Manchester for funding.

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Interview with Tadeusz Sarna on the Occasion of His Piette Lecture 2015

EPR newsletter: *Dear Professor Sarna, on behalf of the readers of the EPR newsletter we congratulate you on your Piette Lecture 2015. We are most appreciative that you agreed to answer the questions of this interview. Why did you start towards your career in science?*

I was always fascinated by unusual physical phenomena that could be directly observed, deduced from results of sophisticated experiments or postulated on the basis of a novel theory. As a kid, I read science fiction and dreamed about being a scientist. Actually, during the Sputnik era, to become a physical scientist was quite fashionable, at least in Poland and in the former Soviet Union, and not restricted just to nerds. In high school, I was fortunate to have a very good mathematics teacher, who stimulated my interest in natural science. During my University study, the fascination with physics was extended to biology and I became a biophysicist.

Who introduced you into magnetic resonance?

I was introduced to electron paramagnetic resonance, at least theoretically, by Professor Lev A. Blumenfeld, a great scientist and teacher who taught physical chemistry to biophysics students at the Faculty of Physics, Moscow State University (MGU), where I spent my final three years as an exchange student. However, hands-on experience with EPR spectroscopy I gained during my MS research in the Department of Biophysics, MGU, being trained by Eno Ruuge and Alexander Vanin, who are among pioneers of biomedical EPR applications. Sasha was actually my MS Thesis supervisor. During my postdoctoral fellowship, which I spent in Medical College of Wisconsin during the time that the National Biomedical EPR Center was being established, I had the opportunity to collaborate with such distinguished scientists and experts in the field of EPR and related techniques as James S. Hyde, Harold M. Swartz and Brian M. Hoffman from Northwestern University.

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

If I am to select just one research topic that is particularly dear to me, I would have to name the biophysics of melanin. I have been involved in melanin study for many years and it still remains of interest to me. Melanin pigments exhibit unusual properties for biological material; they show electric conductivity, ion and electron exchange ability, antioxidant and photoprotective action, and they are paramagnetic, which makes EPR spectroscopy suitable for their detection and characterization in different biological systems. Although melanins seem very stable, and the preservation of a melanin in Jurassic cephalopod ink sac was recently reported, we have demonstrated using EPR spectroscopy (as well as chemical analysis) that human retinal pigment epithelial melanin undergoes in situ photochemical oxidation, resulting in age-dependent modifications of its key physicochemical properties, which can compromise biological functions of the melanin. In my opinion, this mostly overlooked and neglected issue is of importance for it may shed new light on structure-function relationship of this unique biological pigment.

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

My message to the young generation of magnetic resonance researchers is simple and perhaps predictable: take advantage of the spectacular development of various advanced techniques that are now available for specialized measurements in solid state physics, chemistry, biophysics and biomedical sciences. Do not hesitate to contact colleagues with complementary expertise or specialized equipment that may be located far away from your home laboratory. These days visiting places practically all of the world is quite easy and the scientific collaboration that may develop as a result of such visits is priceless.

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Bruker ESR Thesis Prize 2015

Joshua R. Biller:

I would like to thank the organizers of the 2015 Royal Society of Chemistry Meeting and Bruker Biospin for the inaugural international thesis prize in EPR. I was grateful for the opportunity to share my thesis work with the wider EPR community at the associated lecture during the 48th annual RSC EPR meeting in Southampton. I also wish to express my very deep gratitude to Dr. Gareth Eaton, Dr. Sandra Eaton, Dr. George Rinard, Richard Quine (at the University of Denver) and Dr. Mark Tseytlin (now as West Virginia University). Each of these five mentors expended considerable time and energy teaching me the theory and application of EPR.

The first part of my presentation at the RSC conference involved study of the relaxation times (T_1, T_2) of a wide variety of nitroxide radicals and their frequency and line width dependence in aqueous solution at room temperature (295 K). Measurement of T_1 was done primarily with inversion recovery experiments at low (< 0.5 mM) concentrations. A subset of nitroxide T_1 was also measured with saturation recovery, and there was good agreement between the techniques under these experimental conditions. Many thanks go to Dr. Hanan Elajaili, who exerted considerable time and effort into making the very difficult saturation recovery measurements. Measurement of T_2 was done through two pulsed echo decay experiments.

Under these conditions, T_1 is equal to, or slightly longer than T_2. Tumbling correlation times spanned a small region from ca. 9 to 50 ps, in viscosity regimes of 1–20 cP. The importance of this regime, aside from its proximity to *in vivo* conditions, is that it corresponds to a "crossing point" between two relaxation mechanisms, spin rotation and the modulation of A-anisotropy through the electron-nuclear-dipole (END) mechanism [1, 2]. Small changes in radical structure related to hyperfine coupling, or changes in tumbling correlation time, can have a large impact on T_1 and T_2. By measuring relaxation times from 34 GHz to 250 MHz, we found $1/T_1$ increased from X-band to 1.5 GHz, and then decreased from 1.5 GHz to 250 MHz. This was successfully accounted for with a third, thermally activated process [3–5].

The wide variety of ntiroxides measured allowed us to observe that both removal of the gem-dimethyl groups and the identity ($^{14}N/^{15}N$) of the nitrogen isotope in the radical structure had an effect on the magnitude of the thermally activated process. Even when immobilized, the nitrogen-oxygen fragment is subject to an out of plane bending of 10–20 degrees [6]. This "soft" structural parameter could be modulated by rotational motion of the gem-dimethyl groups. Recently the temperature dependence of this thermally activated process was investigated by a different laboratory in ionic liquids and organic solvents, with the authors concluding "…expression of the thermally activated process to describe the temperature dependence in liquid solutions has been vindicated" [7].

The relaxation studies yielded a "road map" for organic chemists on how to build nitroxides which should give T_1 and T_2 values 4–10x larger than what is currently observed (ca. 500 ns). Since drawing a target structure on a piece of paper is orders of magnitudes faster than synthesis in a flask, it's also good to work with what you have at hand. The second part of the presentation highlighted some of my work developing the new rapid scan EPR for *in vivo* imaging at 250 MHz. We were able to show great improvement in imaging nitroxide radicals at 250 MHz with RS over CW in terms of acquisition time and spatial resolution [8]. Since then we have also been able to show rapid scan has superior sensitivity [9] at 250 MHz, similar to results which have been observed at X-band [10]. The rapid scan technique generates field sweeps of 5–10 mT in fractions of a millisecond, and since publication of my thesis, the door has been opened to fast full spectrum imaging of pH sensitive trityl molecules [11, 12], redox sensitive dinitroxides [13] and hydroxide radical trapped with BMPO [9].

Currently I am a National Research Council (NRC) post-doctoral associate at the National Institute of Standards and Technology in Boulder, CO. Working with Dr. John Moreland, I am constructing a low field DNP spectrometer to investigate dynamic nuclear polarization enhancements in fluid solution and in the very low field "hyperfine dominant" region. I am very excited to continue my career in magnetic resonance, and to continue to interact with and learn from the greater EPR community. I welcome any questions or comments at: joshua.biller@nist.gov

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IES Poster Award 2014

Alexey Alfonsov:

First of all I would like to express my gratitude to the organizers of the APES-IES-SEST 2014 conference for the opportunity to share my work among the scientists working in the field of Electron Spin (Paramagnetic) Resonance. I would also like to acknowledge Dr. Vladislav Kataev and Prof. Bernd Buechner at the IFW Dresden for the great support and guidance throughout my research career. I am very grateful to Prof. Hitoshi Ohta at the Kobe University, who offered me a possibility to conduct my investigation of the magnetic properties of halfmetallic Heusler compounds using a novel torque-detected electron spin resonance technique, developed in his laboratory.

During the last couple of years of my research, I have been studying Heusler compounds using a nuclear magnetic resonance (NMR) technique. Heusler compounds are very promising materials for spintronics application due to their unique properties. Theory predicts that they are halfmetallic ferromagnets [1], which is one of the most important criteria for realizing a spin transfer torque device. The half-metallic Heusler compounds have some properties, which are extremely important for spintronics, and can be accessed only by the high field and multifrequency electron spin resonance (HF-ESR) technique. In particular such properties are magneto-crystalline anisotropy, responsible for stability of the magnetization, and Gilbert damping, which determines how fast one can switch the magnetization. Unfortunately it is not always possible to use conventional ways of detecting ESR signal in the case of metallic and ferromagnetic samples. However, in the laboratory of Prof. H. Ohta, at the Kobe University, there is a unique torque detected ESR setup [2], which seemed to be a very promising technique for ferromagnetic resonance study of thin Heusler films. This kind of experiments were not performed before, but thanks to the colleagues in the Prof. H. Ohta laboratory, especially to Dr. E. Ohmichi, Dr. S. Okubo and Dr. T. Sakurai, it was possible to perform the measurements, and moreover, to obtain the results, which also helped me to win a 2014 IES Poster Award at the APES-IES-SEST 2014 meeting in Nara.

During my research at the Kobe University I have measured at a low temperature frequency and angular dependences of FMR signals of a set of $Co_2FeAl_{0.5}Si_{0.5}$ films with different thickness. To perform these measurements, firstly, I have modified the existing measurement setup in order to increase the sensitivity, which was necessary to detect ferromagnetic resonance signal from thin films with thicknesses down to 20 nm. One of the most important experiments was a measurement of the FMR response from the 84 nm $Co_2FeAl_{0.5}Si_{0.5}$ film, detected at room temperature simultaneously by standard Bruker X-band spectrometer and by the deflection of a cantilever. As can be seen in Figure (a), the signal to noise ratio is comparable in these measurements. My following study at high frequencies (40–160 GHz) showed that all the investigated samples exhibit a relatively strong FMR response detected through the cantilever deflection (Figure (b)). This FMR response shares some qualitative similarities, namely, at higher frequencies (above 80 GHz) the FMR signal splits into two lines, the linewidths of both lines are rather broad, reaching value of 1 T. In addition, the linear fit of the frequency dependences yields a rather high g-factor values, of the order of 6. All these findings are nontrivial and need to be further investigated in detail, namely it is important to understand the origin of the second line, which exhibits an inverse angular dependence. It is also important to find the reason for such a large linewidth and the high slope of the frequency vs resonance field dependence. Notably, even a preliminary quantitative analysis of the data yields an important information on anisotropic and dynamic magnetic properties of the studied materials. For instance, the analysis of the linewidth as a function of the frequency dependences showed that the 84 nm film with the highest structural order (amount of $L2_1$ type order reaches record 81% [3]) has the lowest damping. This facts suggests a strong correlation between the chemical ordering and the damping in Heusler alloys. Based on the band model, the Gilbert damping constant is roughly proportional to the total density of states (DOS) at the Fermi level [4, 5]. The transition from B2 to $L2_1$ type of order induces a decrease of DOS for minority spins and, therefore, is expected to reduce the damping.

This research was supported by a DFG international research grant, project numbers AL 1771/1-1 and AL 1771/2-1.

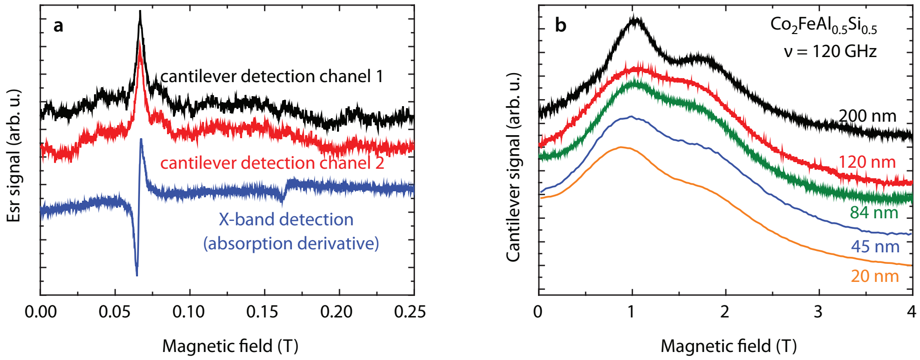

Figure: a) Comparison of the FMR signal from 84 nm film of $Co_2FeAl_{0.5}Si_{0.5}$ measured at room temperature by the commercial X-Band spectrometer from Bruker (bottom line) and by custom made setup with piezocantilever being a detector (two top lines). The measurements were carried out simultaneously; b) Cantilever detected FMR signal from $Co_2FeAl_{0.5}Si_{0.5}$ thin films with different thicknesses, measured at the frequency of 120 GHz, with the magnetic field parallel to the film plane and at the temperature of 8 K.

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IES Poster Award 2014

Fumitoshi Ema:

I would like to thank the International EPR/ESR Society (IES) and the organizers of the joint conference of Asia-Pacific EPR Society (APES)-IES-Society of Electron Spin Science and Technology (SEST) in 2014 (APES-IES-SEST 2014) for providing me the opportunity to introduce our research. I was honored to get the Student Poster Award from the IES at the conference. At the conference, I had valuable experiences to discuss our research, receiving a lot of advises at my poster. Furthermore, it was nice to get lots of scientific information from the presentations by many distinguished researchers there.

I encountered an attracting molecule of hexaphyrin from Prof. Atsuhiro Osuka at Kyoto University. This molecule has a twisted Möbius topology consisting of the π-electrons. I started my research applying an EPR spectroscopy to the hexaphyrins under supervision of Prof. Yasuhiro Kobori at Kobe University collaborating with Prof. Atsuhiro Osuka, Prof. Kazunobu Sato (Osaka City University) and Prof. Takeji Takui (Osaka City University). In my poster presentation, I presented our research on the time-resolved EPR (TREPR) study of the electronic structure in the excited triplet state of [26]- and [28]hexaphyrin. Hexaphyrin is one of the expanded porphyrins with larger macrocyclic structure composed of expanded π-conjugated systems and are known to have unique characters in photochemical, magnetic, and electrochemical properties, those of which are not seen in the well-known porphyrins [1, 2]. In addition, hexaphyrins possess different redox states, namely, 26π and 28π electronic systems. Especially, [28]hexaphyrins exist as an equilibrium between twisted Möbius conformations and planar rectangular conformations in solution. At low temperature, however, rapid interconversions are inhibited to give the twisted Möbius conformation. Then, the connection between the molecular structures and the photophysical properties in the twisted Möbius topology have become of great interest. Aromaticity and antiaromaticity of the hexaphyrins were experimentally revealed in recent years in the ground states [3–5]. However, the electronic structure of the excited triplet states of molecules with the twisted Möbius topology has not been clarified yet [6]. Furthermore, the relationship between the electronic states and the aromaticity or the antiaromaticity has not well been investigated in the excited states. Thus, we observed the excited triplet states of the planar rectangular [26]hexaphyrins and the twisted [28]hexaphyrins using an X-band TREPR method, which has been the powerful to characterize the electronic character in the excited triplet states, as pioneered by Prof. Seigo Yamauchi [7].

TREPR spectra obtained from [26]- and [28]hexaphyrns at 77 K showed the typical splitting widths derived from the spin-spin dipolar coupling, and thus are assigned to the excited triplet states. In addition, magnetophotoselection effects were clearly observed for the EPR spectra depending on the polarization direction of the excitation light. Then, I performed theoretical analyses of the TREPR spectral using a homemade MATLAB code based on the line-shape theory [8, 9]. For [28]hexaphyrins, especially, the zero field splitting (ZFS) parameters D, E and the value of $|E/D|$ were different from those of the planar porphyrins like tetraphenylporphyrins (TPP), indicating that the excited state of twisted Möbius [28]hexaphyrins has the unique electronic structure. Moreover, the ZFS parameters were coincident with those obtained via theoretical calculations using spin density distributions obtained by a molecular orbital calculation with a CIS/cc-pVDZ method. From the ZFS parameters, it has been revealed that the spin density of the excited triplet state is not uniformly delocalized in the twisted [28]hexaphyrin macrocycle, while the unpaired electrons are highly delocalized in the π-conjugated system of the [26]hexaphyrin. These results clearly showed that the excited states of the molecules with the twisted Möbius topology have the characteristic electronic structures.

Now, I am aiming for revealing the relationship between aromaticity and the electronic structures in the excited triplet states. This relationship would pave the way for modulating the photochemical properties of the highly conjugated systems for several applications of novel molecular photo-electronic devices consisting of molecular-wires and molecular-diodes. Furthermore, I am glad to know that Prof. Klaus Möbius got interested in the excited triplet state character of a molecule with Möbius topology such as hexaphyrins [10].

I would like to greatly acknowledge collaborators: Dr. Shohei Saito (Nagoya University), Prof. Atsuhiro Osuka (Kyoto University), Dr. Mana Tanabe, Prof. Seigo Yamauchi (Tohoku University), Dr. Kenji Sugisaki, Prof. Kazunobu Sato, Prof. Takeji Takui (Osaka City University), Prof. Takashi Tachikawa (Kobe University) and the laboratory members. I am happy to engage in the curious research like this and to investigate with them. And I especially would like to appreciate Dr. Zhebin Fu (Tokyo Institute of Technology), Dr. Tomoaki Miura (Niigata University), Prof. Hisao Murai (Shizuoka University), and Prof. Yasuhiro Kobori (Kobe University) who have been supported me since I was an undergraduate student and I encountered the EPR instrument in Shizuoka University before moving to Kobe University. I thank editorial staffs for providing me an opportunity to write a report for the *EPR newsletter*.

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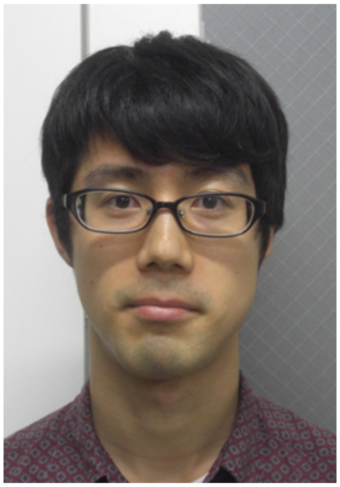
IES Poster Award 2015



Takeshi Yamane:

First of all, I would like to thank the organizers of the 3rd Awaji Island Conference (3rd AWEST 2015) for the IES poster award and express my gratitude for giving me such an opportunity to write about my recent work. Our research is on electron spin resonance (ESR) spectroscopy of metallocomplexes with proton-electron synchronized transfer. The synchronized motion between protons and electrons is an important event in chemistry and recognized as a key step in certain biological molecular systems, in which ATP syntheses take place by using active proton pumps as well as through the conduction of electrons by cytochrome *c* in living matter [1–3]. In such biological systems, the driving mechanism of the synchronized motion has not been well understood, and thus relevant dynamics has been the focus of current topics in both biological and materials science. Quantum cooperative phenomena associated with the proton and electron transfer have attracted considerable attention from a view point of multifunctionality. Biimidazolate metal complexes can afford various types of coordination networks in which "complementary" hydrogen bonds between the biimidazolate ligands are involved. Relevant investigations so far documented have been done in solution whereas very few examples are found in the solid state [4]. Mixed-valence metallocomplexes with functional ligands could be candidate materials which reveal the proton-electron synchronized transfer in the solid state. Previously, Tadokoro and coworkers reported a mixed-valence rhenium binuclear complex with two hydrogen bonds between biimidazolate ligands which shows the synchronized motion between protons and electrons [5]. The aims of this work are to study the electronic structure of the rhenium complex in the crystal and the mechanism of unusual ferroelectric property seen in single-crystal experiments at low temperature.

In this contribution, our research focused on rhenium mononuclear complex [Re(III)Cl$_2$(P^{n}Pr$_3$)$_2$(Hbim)], [Re(IV)Cl$_2$(P^{n}Pr$_3$)$_2$(bim)] and a binuclear complexes [Re(III)X$_2$(P^{n}Pr$_3$)$_2$(Hbim)][Re(IV)X$_2$(P^{n}Pr$_3$)$_2$(bim)] (H$_2$bim = 2,2'-biimidazolate; X = Cl or Br). We have carried out magnetic susceptibility measurements, ESR spectroscopy and quantum chemical calculations. The structure of the binuclear complex is different from the one previously reported, in which one hydrogen bond is involved. The magnetic susceptibility measurements of tetravalent and trivalent rhenium mononuclear and mixed-state binuclear complexes showed obvious difference of the magnetization between the trivalent and tetravalent rhenium centers. The results are in good harmony with the ESR spectroscopy: Only Re(IV) is ESR-detectable (S = 3/2) and Re(III) ESR-silent (S = 0).

X-ray crystallographic data revealed that the Re(IV) mononuclear complex has two different orientations in a unit cell, and the Re(III)-Re(IV) binuclear complex a single orientation with an inversion center at the middle of the hydrogen bonds. Two sets of six hyperfine lines due to the rhenium nuclear spin (I = 5/2) were observed for all the single-crystal-line samples. For the Re(IV) mononuclear complex, the distinguishable hyperfine spectra are due to the site splitting according to the crystal symmetry. For the binuclear complexes, however, ESR hyperfine splittings observed at helium temperatures indicated the occurrence of a spectral superposition of the two complexes arising from magnetically non-equivalent rhenium centers, suggesting that the binuclear complex is in the mixed-valence state composed of Re(III) and Re(IV). The angular dependence of the single-crystal ESR spectra can be interpreted by incorporating the contribution from the large zero-field splitting parameter. The experiment, in which the oscillating magnetic field is parallel to the static field, allowed us to observe hyperfine "forbidden" transitions ($\Delta|M| = \pm1, \pm2$). The intensity distribution of the forbidden transitions implied nuclear-Zeeman dominant patterns [6].

The ESR spectra of the binuclear complexes were subject to line broadening with increasing temperature, and the distinct ESR signals merged into one hyperfine structure at certain temperatures. The temperature dependence of the spectra was reversible. We analyzed the temperature dependence of the linewidth by using an Arrhenius equation and estimated the activation energy between the two proton-localized states, Re(III)-Re(IV) and Re(IV)-Re(III).

Accurate determination of the fine-structure tensors requires high-field/high-frequency ESR spectroscopy at low temperature as well as Zeeman perturbation approaches from both the theoretical and experimental sides. We also have carried out quantum chemical calculations of the g-, fine-structure and hyperfine structure tensors for the complexes, comparing the calculated values with the experimentally derived ones.

I would like to acknowledge Prof. Tadokoro and coworkers for providing all the samples. I also would like to thank my supervisors Prof. Sato and Prof. Takui and all the laboratory members for their stimulating discussions and advice.

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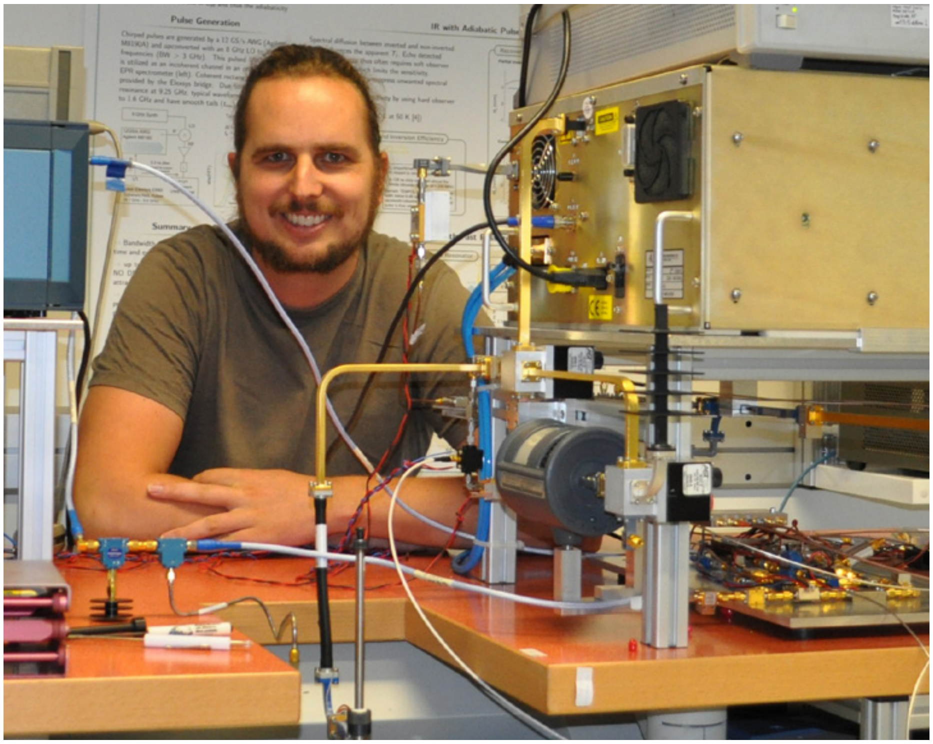
JEOL Prize 2015



Andrin Doll:

The RSC meeting in Southampton was full of interesting and inspiring contributions. I enjoyed the atmosphere at the conference very much and thank the local committee for the organization. I was deeply honored that my presentation on Gd-Gd distance measurements with frequency-swept pulses was awarded the JEOL prize. The work I presented there [1] represents one of two major branches of my almost-finished PhD thesis. These two branches are (i) improving DEER/PELDOR distance measurements and (ii) Fourier-transform (FT) techniques with frequency-swept pulses. These kind of pulses are well established in the field of nuclear magnetic resonance, but could only be applied recently at microwave frequencies for electron spin excitation thanks to fast arbitrary waveform generators (AWG).

At the beginning of my PhD thesis from January 2012 on, I therefore studied how well frequency-swept inversion pulses perform on ordinary EPR instrumentation at X-band. It was of particular interest whether we can extend the inversion bandwidth beyond 500 MHz into the ultra-wideband regime. As a key outcome of this initial work [2], we found a way to compensate the pulses for the frequency dependence of the B_1 field amplitudes due to the bandwidth of the microwave resonator. Moreover, we used a frequency-swept pulse as pump pulse in four-pulse DEER and as an inversion pulse in inversion recovery measurements. The inversion recovery experiments gave evidence that we inverted the entire nitroxide spectrum. From the DEER experiments, we learned that the optimum pump pulse on a broad spectrum such as Cu(II) is not necessarily a perfect π pulse.

After these initial investigations, I stopped EPR experiments for almost 6 months in order to build a first prototype of an X-band spectrometer fully controlled by a 12 GSa/s AWG. This spectrometer then allowed for FT EPR with frequency-swept pulses with up to 700 MHz excitation bandwidth [3]. The resonator compensation developed previously was crucial for these experiments. As a result, we outlined important aspects of solid-state FT EPR with frequency-swept excitation pulses. From an instrumentation point of view, the resonator bandwidth remains important because it cannot be compensated during detection. When taking into consideration the spin dynamics, it should be noted that refocusing with frequency-swept pulses imposes different evolution times for different parts of the spectrum. As a consequence, FT EPR spectra encode nuclear modulation along the frequency axis. This effect turned out to be important when correlating FT EPR spectra of nitroxides to inversion recovery. In particular, nuclear modulation corresponds to admixture of remote frequencies in a FT EPR spectrum. Since longitudinal relaxation in glassy frozen solutions of nitroxides depends strongly on orientation, we observed an influence of nuclear modulation on apparent T_1 times extracted from FT EPR spectra.

The home-built AWG spectrometer turned out to enable several other experiments that would not have been possible with an extended commercial spectrometer. In particular, we could excite and observe very fast nuclear modulation frequencies up to 200 MHz in oriented Cu(II) centers related to the Cu nucleus [4]. This could turn out as an appealing technique for multi-nuclear metal centers. Moreover, the flexibility in pulse sequence programming allowed for a critical comparison between experiment and theory [5]. In particular, we found experimental agreement between inver-

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sion efficiencies of frequency-swept pulses and the Landau-Zener formula. These experiments further required a spatially homogeneous B_1 field and long coherence times. The Landau-Zener formula allows to calculate the nominal flip angle of a frequency-swept excitation pulse, which eases the treatment of spin dynamics considerably. Furthermore, the implications of spatial B_1 inhomogeneity and of short coherence times improved our understanding on refocusing with frequency-swept pulses.

In parallel to the efforts at X-band with the home-built spectrometer, I extended a commercial Q-band spectrometer by our AWG. The experiments performed on this spectrometer were mostly dedicated to optimization of Gd-Gd distance measurements. First of all, I rearranged the equilibrium populations on the energy levels of the $S = 7/2$ Gd(III) spin to enhance the echo signal [6]. The frequency-swept pulses for population transfer had inversion bandwidths above 1 GHz and long durations of 2 µs. As a result, the net excitation bandwidth was an order of magnitude beyond the bandwidth of the microwave resonator. From a technical point of view, this implied rather clean pulse formation and handling of heating effects. Even with these large inversion bandwidths, only a fraction of the entire Gd(III) spectrum could be covered. As a consequence, best enhancement to almost three times the equilibrium signal was achieved for a Gd(III)-DOTA complex, which had the narrowest EPR spectrum amongst the investigated complexes. An important complex for us was Gd(III)-PyMTA, because our collaborators Mian Qi and Prof. Adelheid Godt at the Bielefeld university synthesized a number of well-defined distance rulers with Gd(III)-PyMTA labels. For this complex, the enhancement of the DEER echo signal was 85%.

As follow-up to the population transfer techniques, I investigated further on frequency-swept pump pulses in Gd-Gd DEER [1]. Due to the high-spin state of Gd(III), sensitivity optimization required a critical balance between modulation depth and loss of echo intensity due to the pump pulse. For this, a very simple and fast procedure to optimize pulse parameters based on two data-points of the DEER signal did the trick. Further sensitivity optimization was achieved by using two consecutive pump pulses that pump the Gd(III) spectrum on both sides. Modulation depths were as high as 20%, whereas the associated loss of echo intensity was less pronounced with the consecutive pump pulses than with a single pump pulse. Understanding the behavior of the echo intensity with consecutive pulses was an interesting question to be addressed with spin dynamics simulations. Here, I found two mechanisms that explain why consecutive pulses achieved better sensitivity. The first mechanism is related to coherence transfer within the energy levels of the $S = 7/2$ observer spin. The second mechanism is related to inhomogeneous Bloch-Siegert phase shifts due to spatial B_1 inhomogeneity, which are largely refocused with the consecutive pulses. Given the interest in Gd(III) spin labeling for distance measurements, I am very curious in further developments of related techniques.

Currently, I am finishing my PhD project, which involves both writing my thesis and bringing the developed hardware and software to the next level. The home-built AWG spectrometer just got an upgrade and can now be operated either at X- or at Q-band. A complementary setup at W-band is also under construction.

I am very thankful to Gunnar Jeschke for supervision of my PhD project. He gave me the very generous opportunity of a PhD project tailored to my skills as electrical engineer and my interest in physics. Among other things, this extraordinary deployment was possible because I got in touch with him one year ahead of my PhD project during my master thesis on dynamic nuclear polarization [7].

Moreover, I need to thank a number of other people with whom I directly worked together during my project. Spin dynamics simulations were always very important for understanding and interpreting the experiments, such that I am grateful for all interactions with Stephan Pribitzer, who is the core developer of SPIn DYnamics ANalysis (SPIDYAN) which can be downloaded from our website (www.epr.ethz.ch). Furthermore, I thank Takuya Segawa for his fruitful work on hyperfine spectroscopy, which I consider to be a very interesting technique. During my project, I also got to explore a number of interesting sub-projects during semester and master theses. Here I am grateful to the work of several eager students, namely Bettina Basel, Nino Wili, Andreas Dounas, Janne Soetbeer and Stephan Pribitzer. Finally, I am very grateful for the series of Gd-rulers synthesized by Mian Qi in the group of Prof. Adelheid Godt. Without these rulers, the optimization of Gd-Gd distance measurements would not have been possible.

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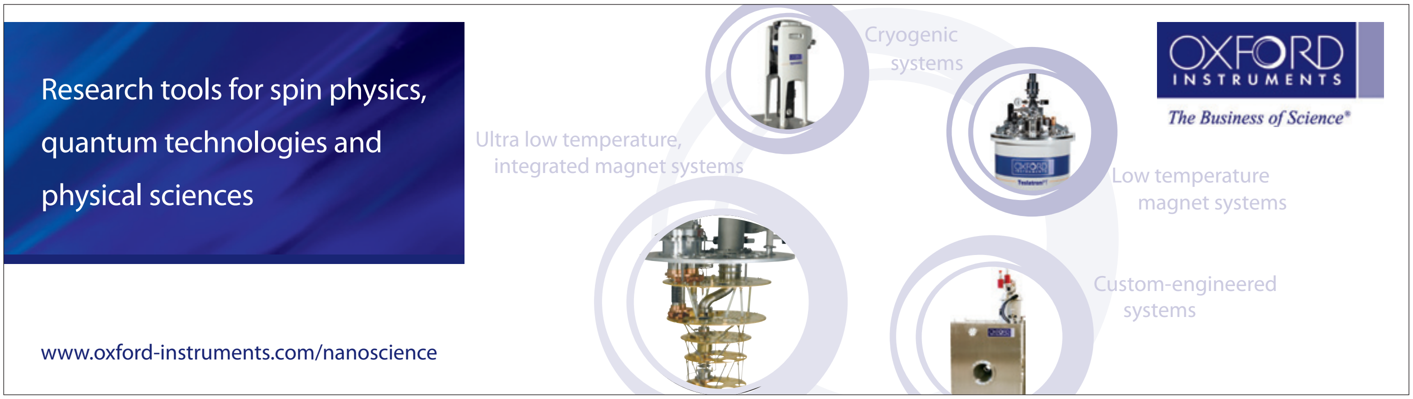
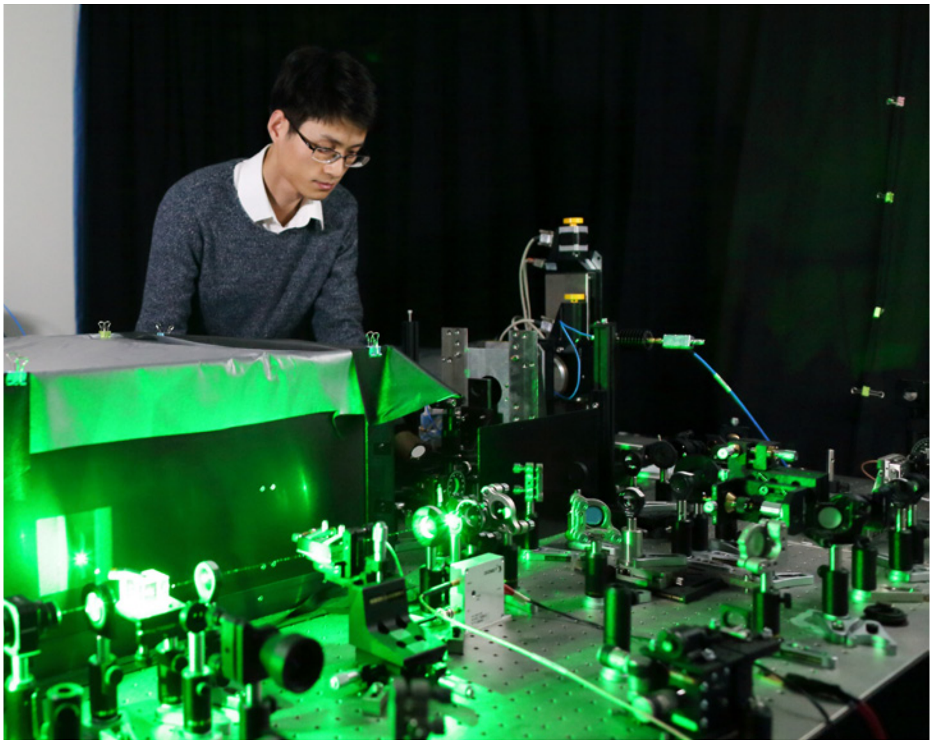


APES Young Scientist Award 2014



Fazhan Shi[*]:

Nanoscale magnetic resonance with single electron spin sensor under ambient conditions

I would like to thank the organizers of the 2014 Asia-Pacific EPR/ESR Symposium, International EPR (ESR) Society Symposium and the 53th SEST annual meeting for the opportunity to share my work in an environment dense with pioneers and leaders in the field. Then I would like to thank all my collaborators. These experiments could no be done without their help. Specially, I would also like to acknowledge Prof. Jiangfeng Du at University of Science and Technology of China for his great support and guidance throughout my graduate career. Here I also give thanks to Prof. Jörg Wrachtrup and Dr. Friedemann Reinhard. I visited Wrachtrup's group in University of Stuttgart and stayed there for one year. I learned a lot and broadened my horizon.

My presentation at this symposium involves nanoscale Nuclear Magnetic Resonance technique based on nitrogen-vacancy (NV) defects in diamond. As one of the most important technologies in modern science, the magnetic resonance technology is capable of obtaining information of material composition and structure in an accurate, rapid and non-destructive way. As one of the most popular technologies, magnetic resonance is widely used in science and medicine. Conventional spin-magnetic resonance spectrometers are based on the principle of ensemble detection and the test object is an ensemble sample containing billions of identical spins. Applications of magnetic resonance spectroscopy to nanoscale samples remains an elusive goal, especially at room temperature. The scientific goal becomes within reach by using NV as the sensitive magnetic probe, due to the amazing features of NV and the rapidly development of quantum controls on it. The single NV spin can be easily polarized and detected with a confocal microscope. Such electron spin has ultra-long coherence time even at room temperature, and this property enables the spin to be ultra-sensitive to external magnetic noise with characteristic frequency. Instead of traditional detection manner, weak magnetic signal generated by the nanoscale spin system is mapped to the phase of superposition of the NV electron spin, so as to realize high sensitivity signal detection.

Firstly, we designed and constructed the Optically Detected Magnetic Resonance (ODMR) spectrometers to meet the requirement of the quantum manipulation on a single NV spin at room temperature. A typical homebuilt setup includes optics, microwave and electronic parts. The confocal microscopy is used to address, initialize and readout the single spin, the microwave bridge is used to manipulate the spin, and electronic parts is employed for synchronizing the whole setup. On the home-built setup, we have experimentally realized atomic-scale structure analysis of single nuclear-spin clusters [1]. Through decoherence measurement of nitrogen vacancy centers under dynamical decoupling control, the sensing of single ^{13}C at nanascale has been realized by J. Wrachtrup's, M. Lukin's and R. Hanson's groups, independently. A step towards the grand goal of structure analysis of single molecules would be direct measurement of the interactions within single nuclear spin clusters. In this work, we sensed a single ^{13}C-^{13}C nuclear spin dimer located about 1 nm from the NV center and characterized the interaction (~690 Hz) between the two nuclear spins. This was achieved by measuring NV center spin decoherence under various orders of dynamical decoupling control at room temperature. From the measured interaction we derived the spatial configuration of the dimer with atomic-scale resolution.

Secondly, we demonstrated the detection of nuclear magnetic resonance signals from a (5 nm)^3 voxel of various fluid and solid organic samples under ambient conditions [2], in J. Wrachtrup's group. We employed very shallow NVs, embedded approximately 7 nm below the surface of a bulk diamond to record NMR spectra of various samples placed on the diamond surface. We find that its detection volume consists of only 10,000 nuclear

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[*] University of Science and Technology of China.

spins. It's a "first step toward molecular-scale magnetic resonance imaging", reviewed by Prof. P. Hemmer.

Besides nano-NMR, we also detected a single electron spin by combining dynamical decoupling controls together with double electron-electron resonance sequenses. We study a single dark (named by 'N2') electron spin defect in diamond which is magnetically coupled to a nearby NV center. Moreover, we show that the NV center's spin polarization can be transferred to the electron spin by combining two decoupling control-NOT gates. The two results imply that the NV center's two key advantages, namely optical spin polarization and detection, could be extended to any electron spin in its vicinity. This enables dark electron spins to be used as local quantum registers and engineerable memories. It could also be treated as a mediate amplifier to detect nuclear spins far away from NVs. Recently, we succeed in recording the electron spin resonance spectra of single proteins [4] and deriving the dynamic information of the proteins.

These researches, together with many other excellent reports on nano-MR, indicate that the NV under dynamical decoupling control is a useful probe for magnetic resonance spectroscopy and imaging. They provide new methods for nanoscale science, including physics, life science and chemistry.

Thank you to all who have shown 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 via: fzshi@ustc.edu.cn

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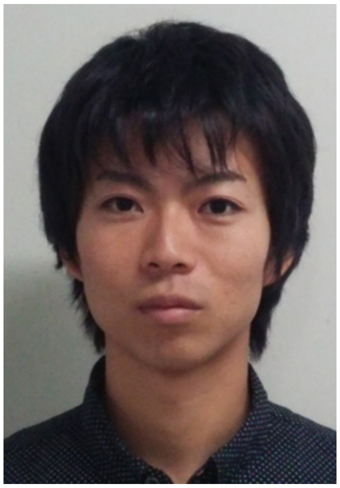
APES Poster Award 2014



Tsubasa Okamoto:

First, I would like to thank all organizers of the joint conference of APES-IES-SEST2014 for giving me the opportunity to discuss my study with many researchers. I could make some good discussions and got some opinions to further develop my study. I would also like to thank Prof. Hitoshi Ohta and Assoc. Prof. Eiji Ohmichi at Kobe University for their supports to my work. In this letter, I would like to make an acknowledgement for awarding me APES Poster Award and introduce our research to all IES members.

Electron spin resonance (ESR) is widely used in various research fields such as chemistry, physics, and biology in order to probe local spin properties from g-factor analysis. Conventionally, ESR measurements are performed using a commercial X-band (~ 10 GHz) spectrometer. Its sensitivity is very high, typically on the order of $\sim 10^9$ spins/gauss. On the other hand, high-frequency ESR (HFESR) technique is useful to investigate microscopic properties of spin systems. In particular, high g-factor resolution and observations of broad ESR lines are unique features of HFESR. Moreover, multi-frequency ESR measurements allow detailed THz spectroscopy of spin systems. However, because of the lack of intense light sources beyond 100 GHz, spin sensitivity of HFESR measurement is not generally high. So its application to low-spin-concentration sample such as biomaterial is quite difficult and extremely large sample amount, on the order of 10 mg, is needed.

To solve this problem, our group has developed an ultrasensitive ESR technique in high frequency range beyond 100 GHz using a microcantilever for small-volume sample [1–3]. So far a spin sensitivity as high as 10^9 spins/gauss is achieved and multi-frequency ESR of μg-order sample was possible in the THz range of up to 370 GHz.

Here, I explain details of our cantilever-detected ESR technique. A tiny piece of ng- or μg-order sample is mounted on the end of a microcantilever, and an electromagnetic wave is irradiated via over-sized waveguide while a static magnetic field is applied. Magnetization change associated with ESR absorption is sensitively detected as magnetic torque or field-gradient force acting on the sample. Recently, we have developed a new ESR detection system based upon fiber-optic interferometer [4]. This technique is extremely sensitive and we succeeded in ESR detection of hyperfine splitting of Mn^{2+} impurities in MgO (Mn^{2+} concentration is <0.2 %).

In this system, Fabry-Perot cavity is formed between the cantilever surface and the optical fiber end. Cantilever deflection is sensitively detected as a change of interference amplitude. In our system, a fiber-coupled tunable laser is used to make the cavity length in the optimal condition. The sample holder is inserted into a cryostat and is cooled down to 4.2 K. An electromagnetic wave is introduced via a polished stainless tube and is focused by a brass horn at the end of the light pipe. The electromagnetic-wave intensity is modulated, and its synchronized signal is detected with a lock-in amplifier as a reference. In order to detect a field-gradient force, a hollow cylindrical piece of ferrite magnet is placed below the sample-mounted cantilever. The field gradient force is given by the product of magnetization M_z component along magnetic field and magnetic field gradient dB/dz, which is typically 50–100 T/m in this study.

In my study, I try to apply our cantilever technique for metal protein for the first time. Metal proteins contain metal ions in the unit, which play important roles in biological reactions as an active center. Most famous metal protein is hemoglobin, which contains four Fe ions in the unit. It is well known that ESR technique is useful to study metal proteins since ESR is sensitive to the local electronic structure of metal ions such as valence state and ligand configurations. In addition, as mentioned above, HFESR is able to observe the zero-field gap directly. Compared to conventional HFESR technique, our cantilever technique needs less sample volume by four orders of magnitude, and therefore would be promising for small-volume analysis of metal proteins.

In my poster presentation at this conference, I showed the first attempt to detect HFESR signals of biological systems using a microcantilever. Myoglobin was chosen as test sample in this study, since the sample can be easily obtained and there are a lot of literatures. I made some improvements to our apparatus, and successfully increased the detection sensitivity, though ESR signal from myoglobin was not detected. After this conference, continuous efforts have been made for the detection and further experiments are now undertaken. In the near future, I hopefully apply this technique to many kinds of metal protein.

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APES Poster Award 2014

Yung Szen Yap:

EPR experiments with arbitrary waveform pulses at millikelvin temperatures

In 2014, I had the chance to participate in a joint conference organized by Asia-Pacific EPR/ESR Society (APES), International EPR (ESR) Society (IES) and The Society of Electron Spin Science and Technology (SEST) in Nara, Japan. I truly enjoyed the conference and met with many distinguished EPR researchers and professors. I would like to take this chance to thank the organizers for their efforts and time for putting this wonderful conference together. I would also like to acknowledge the co-authors in this work: Dr. Yutaka Tabuchi, Dr. Makoto Negoro, Dr. Akinori Kagawa and my advisor, Prof. Dr. Masahiro Kitagawa. The work that was presented in that conference was carried out in Osaka University, Japan during my one-year research attachment, which ended on July 2015. Since then, I have resumed my academic position in Universiti Teknologi Malaysia (UTM), Malaysia.

During that conference, I presented our 17 GHz (Ku band) pulsed EPR spectrometer, which is capable of generating arbitrary waveform pulses for experiments at millikelvin temperatures [1]. At the core of the setup is an arbitrary waveform generator (AWG) and a dilution refrigerator equipped with a superconducting magnet. The AWG was used to generate arbitrary waveform pulses at 2.5 GHz (1.5 GHz bandwidth) which was up-converted to 17 GHz by mixing it with a c.a. 14 GHz signal generated from a local oscillator. The resulting pulse was then filtered using a high-pass filter and amplified using a travelling wave tube amplifier (TWTA) before it was directed into resonator located inside the dilution refrigerator. Due to the filter's cut-off frequency and the upper frequency limit of the TWTA waveguide output, our setup has an operating frequency range of 16.5–18.0 GHz. On the receiving side, the EPR signal was amplified using low-noise amplifiers and down-converted to 300 MHz before being sampled by an oscilloscope. The setup was designed for transmission measurements but it can be converted for reflection measurements as well. One may also carry out room temperature experiments by replacing the dilution refrigerator with a room temperature magnet [2].

Using this setup, we attempt to address two issues related to our target application area of molecular spin quantum computation: initialization and precise control of electron spin qubits. Initialization is the process where (almost) all of the qubits (in our case, electron spins) are prepared to a known state at the beginning of a quantum computation experiment [3]. For molecular spin quantum computation, this is done by polarizing electron spins to a near pure-state regime. A method to increase spin polarization is to cool the sample to very low temperatures, which necessitates the use of a dilution refrigerator. For example, the calculated thermal spin polarization for electron spins in a static magnetic field of 0.6 T at 100 mK is 99.94%. To demonstrate this, an inhomogeneously broadened sample was cooled down to 12.3 mK. By carrying out spin echo experiments at various temperatures from 1 K and by comparing the signal intensities, the thermal spin polarization was determined. In our experiment, we observed increasing signal intensities with decreasing temperatures, due to increasing thermal spin polarization. Using this method, we estimated an experimental spin polarization of at least 99% at 100 mK and below.

In regards to precise control of electron spin qubits, most pulsed EPR systems utilize rectangular pulses to excite electron spins. Unfortunately, rectangular pulses have poor frequency-selectivity and are prone to deformations, which leads to unwanted spin evolution. A well-known solution is to make use of advanced pulses e.g. composite pulses, shaped pulses, as well as numerically optimized pulses. The part responsible for generating such complex pulses is usually either a field-programmable gate array (FPGA) or, as in our case, an AWG. In our proposed setup, the combination of an AWG-based spectrometer with a dilution refrigerator permits us to apply advanced pulses to electron spins that are almost in the pure-state regime. As a demonstration, we applied a triple-frequency shaped pulse to selectively and coherently excite three different spin packets simultaneously, at 8 K, 1 K and finally at 14 mK. For a quantum computer with qubits addressed in the frequency space [4], multi-frequency pulses such as the one demonstrated in our work, plays a crucial role to selectively control specific qubits.

As thermal spin polarization depends on both the static magnetic field strength as well as the spin temperature, polarization above 99% is achievable at higher temperatures if a stronger static magnetic field is applied e.g. 99% spin polarization is attainable at 2 K for an EPR setup operating at 250 GHz (corresponding static magnetic field is 8.9 T). Unfortunately, at the present time, generating advanced pulses is technically challenging for frequencies above 50 GHz whereas lower frequency setups are based on mature technology with many techniques and components readily available. Inevitably, lower frequency setups would require lower temperatures to achieve similar polarization levels. Taking these factors into consideration, we have developed an arbitrary waveform pulsed EPR spectrometer at Ku band for millikelvin experiments and we look forward to carrying out more experiments in the near future.

Thank you to all who have shown an interest in our work. Please feel free to contact us with any questions or comments at:
yungszen@utm.my or
kitagawa@ee.es.osaka-u.ac.jp

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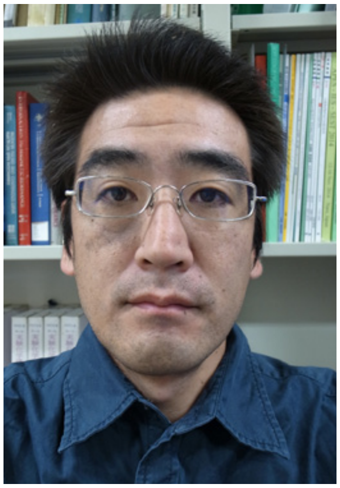
SEST Young Investigator Award 2014



Tomoaki Yago:

I was honored to receive the young investigator award from The Society of Electron Spin Science and Technology (SEST) for my time-resolved spectroscopic study on radical pairs and excited triplet states. This research is composed of time-resolved EPR study on the exchange interactions in radical ion pairs at the Tohoku University, time-resolved EPR study on light induced nuclear coherences in photo-excited triplet state at the University of Freiburg, and study of magnetic field effects on radical pairs in ionic liquids at the Saitama University. I started my scientific career at the Tohoku University in Sendai, Japan, where three EPR research groups (Azumi and Murai group, Tero group, and Yamauchi group) were active at 1998. In my PhD program, I belonged to the Tero group and studied the mechanism of exchange interactions (J) in radical ion pairs by observing chemically induced electron polarization (CIDEP) under the guidance of Prof. Kobori and Prof. Tero. In radical ion par systems including photosynthetic reaction centers, J is dominated by the charge transfer interaction generated by the electronic coupling between the cation and anion radicals. Since the electronic coupling also causes the charge recombination reactions, one can determine parameters of the charge recombination reaction from the observation of J through CIDEP. My research project was concerned with the determination of reorganization energies for charge recombination reactions in solvent-separated radical pairs in polar solvents. The reorganization energy is represented by a curvature of the Marcus parabola and determines the activation barrier of the electron transfer reaction. However, it was difficult to determine the exact value of the reorganization energy, which corresponds to the energy for the non-equilibrium state. On the basis of the J mechanism, I could determine the reorganization energies for several solvent-separated radical ion pairs. I found that the hydrogen bonding between solute and solvent increases the reorganization energy and affects electron transfer reaction rates. This finding offers new information to the understanding of the efficient ET reactions occurring in various biological systems, where the hydrogen bonding is ubiquitous.

After my PhD program, fortunately, I had the opportunity to continue the EPR study as a postdoc at the University of Freiburg in Germany. At the University of Freiburg, I studied light-induced spin coherences in photo-excited triplet states under the guidance of Prof. Kothe. In the Freiburg EPR group, the light-induced spin coherences in the spin-correlated radical pairs were studied on multi-frequency EPR spectrometers. The generation of such spin coherences is interpreted with the non-adiabatic change of the spin Hamiltonian during the fast photo-induced ET reactions. It was believed that the light-induced spin coherence phenomena are characteristic for the spin-correlated radical pairs, where the two electron spins interact weakly. My research project was concerned with the observation of the light-induced spin coherences in a photo-excited triplet state, where the electron spins in the molecule interact strongly. I could successfully observe oscillations of the EPR signals with respect to time from the photo-excited triplet state of pentacene by using X-band EPR spectroscopy. The oscillations originated from the nuclear coherences generated in the photo-excited triplet state. Even in the presence of the magnetic field, the photo-excited state is born at the virtually zero magnetic field since the spin-orbit coupling, which promotes the intersystem crossing from the singlet excited state to the triplet excited state, is independent of the external magnetic field. Then the photo-excited triplet state feels the external magnetic field and the spin Hamiltonian is suddenly switched from the zero-field spin Hamiltonian to the high-field spin Hamiltonian, This causes the non-adiabatic change of the spin Hamiltonian and generates the spin coherences in the photo-excited triplet state. The generated nuclear coherences were associated with the high electron polarizations created by the spin state selective intersystem crossing in the photo-excited triplet state. It is also predicted that the high nuclear polarizations are also created in the photo-excited triplet state even in the presence of the high magnetic field.

After the two year postdoc experience in Germany, I returned to Japan and was appointed as research associate at the Saitama University. At the Saitama University, I studied magnetic field effects on radical pairs in ionic liquids with Prof. Wakasa. Ionic liquids are liquids solely consisting of cation and anion. The combination of the cation and anion generally gives the crystals (salt) at room temperature due to the strong Coulomb interactions. In the ionic liquids, the crystallization is hindered by the delocalization of charges, the low symmetry of molecular shapes, and the large size of molecules. The ionic liquids are currently recognized as a new class of promising solvents in green chemistry, catalyst chemistry, and electrochemistry. However, the ionic liquids are known to have the complex liquid structures and the mechanisms of the chemical reactions in the ionic liquids are often unclear. The X-ray and neutron scattering studies and MD simulations have shown that nano-ordering structures are created in the ionic liquids. The magnetic field effects on the radical pairs were then studied by using laser flash photolysis to probe the diffusion motion of the radicals in the ionic liquids. We observed the large magnetic field effects on the yield of the escaped radicals (−25%-+220%). The detailed analysis showed that the diffusion motions of the radical pairs are restricted in the nanometer space, causing the large magnetic field effects in the ionic liquids. It was also found that the lifetimes of the radical pairs are prolonged to several hundred nanoseconds when the radicals have plus or minus charges in the ionic liquids.

These are my studies carried out in Japan and in Germany for more than ten years. Finally, I would like to acknowledge Prof. Kobori (Kobe University), Prof. Tero (Tohoku University), Prof. Kothe (Freiburg University), Prof. Lin (Washington University at St. Louis), and Prof. Wakasa (Saitama University) for their support and kind guidance. I also would like to thank my colleagues for their support, patience and encouragement.

SEST Young Investigator Award 2014

Yugo Oshima:

First of all, I would like to thank the Society of Electron Spin Science and Technology (SEST) and all the colleagues in Japan for giving me the Young Investigator Award, and I would like also to thank the International EPR Society for giving me the opportunity to report about our studies using the high-field ESR on molecular-based conductors and magnets.

Molecular-based conductors and magnets have attracted broad interests due to characteristic features such as the degree of freedom of the molecular design, flexibility, its wide variety of ground states and so on. In recent years, interesting phenomena such as the giant magnetoresistance or field-induced superconductivity have been observed in molecular conductors where conducting π-electrons interact with localized d-electrons. Moreover, nano-scaled magnets such as the single-molecule magnets (SMM) with unique magnetic network have been synthesized, and its peculiar magnetic properties have been revealed. High-frequency ESR is one of the important methods to clarify the ground states or the magnetic properties of such interesting molecular materials thanks to its high-sensitivity, high-resolution and accessibility to the high-magnetic field. For the past decade, we have developed a high-frequency ESR system optimized for molecular materials. Let me now introduce about three topics that we have achieved on molecular materials by the use of our high-frequency ESR system.

(1) *Studies on single-chain magnets and molecular conductors by use of the high-frequency ESR system* [1, 2]

SMM-based 'single-chain magnet' $[Mn_2(saltmen)_2Ni(pao)_2(py)_2](ClO_4)_2$ is a very good 1D magnetic system with strong uniaxial anisotropy and infinitesimal interchain couplings. Although many studies have been performed on SMMs, the low energy excitation of a 'single-chain magnet' has never been explored. Thanks to the high-frequency ESR, we have succeeded to observe ESR mode that is attributed to the spin wave excitation with strong magnetic anisotropy [1]. The uniaxial anisotropy constants and the exchange couplings have been also quantitatively deduced from our theoretical analysis.

Furthermore, ESR measurements of π-d molecular conductor β-$(BDA\text{-}TTP)_2FeCl_4$ were also performed [2]. Similar to its nonmagnetic analogue β-$(BDA\text{-}TTP)_2FeCl_4$, the π-electrons of β-$(BDA\text{-}TTP)_2FeCl_4$ is charge ordered and forms a singlet ground states at 113 K. On the other hand, the d-electrons are antiferromagnetically ordered at 5 K. From our detailed analysis using high-field ESR, we have found that the long-range order of d-electrons is achieved by the exchange, which is mediated through the fluctuating spin-singlets thanks to the strong π-d interaction.

(2) *Determination of the exchange energies in the nano-scaled molecular magnets by ESR* [3]

The magnetism of the polyoxometalate cluster $\{Mo_{75}V_{20}\}$, containing a saw-tooth ring of 10 corner-sharing triangles with 20 V^{4+} ($S = 1/2$), has remained debatable since it is masked by contribution from impurities as well as van Vleck paramagnetism. Here, we have demonstrated the usefulness of high-frequency ESR in such frustrated material by separating the contributions from the intrinsic molecules and magnetic impurities. Via the temperature dependence of the integrated intensity, we have determined the exchange parameters and also the low-energy spectrum [3]. Due to the high sensitivity of ESR, this method can be far more effective than the specific-heat measurements in characterizing the low-lying density of states.

(3) *Control of the electronic states by dynamical spin reversal* [4]

The molecular conductor λ-$(BETS)_2FeCl_4$ shows a superconductivity in the high magnetic field. This is due to the compensation effect between the external field and the internal field created by the localized d-electrons. In principle, the internal field can be alternated by the ESR transitions of d-electrons, and then, compensation effect might be broken. Thanks to the simultaneous ESR and transport measurements that we have developed, we have succeeded to destroy the field-induced superconductivity by ESR, namely, by dynamical spin reversals of d-electrons.

These studies have been done with the help of many collaborators from all around the world. Without their help, it was impossible to get awarded. I would like to give the credit to all my collaborators, especially to H. Nojiri H. Miyasaka, M. Yamashita (Tohoku Univ.), R. Kato, H.-B. Cui (RIKEN), S. Uji (NIMS), T. Sakai (JAERI), J. Yamada (Hyogo Univ.), H. and A. Kobayashi (Nihon Univ.), J. Schnack (Bielefeld Univ.), P. Kögerler (RWTH Aachen), S. A. Zvyagin (HZDR), M. Luban (Ames Lab.), T. Tokumoto (UAB), J. Krzystek, J. van Tol (NHMFL). And finally, I would like to express my sincere gratitude to Prof. J. S. Brooks (NHMFL) who passed away last year. The last topic was the one of the many collaborations with him. His ideas were always intuitive and interesting, and I've always admired his passions for science.

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SEST Excellent Presentation Award 2014

Hiroki Nagashima:

I would like to thank to the organizers of the joint conference of Asia-Pacific EPR/ESR symposium, International EPR (ESR) society Symposium and the 53th SEST annual meeting (APES-IES-SEST 2014) held on Nara for the opportunity to introduce my works to leaders and pioneers in the field. I would like to acknowledge Dr. Hiroyuki Mino for his many supports and supervision of my first career on the graduate school, Nagoya University. My presentation topic at the conference was about the structure and mechanisms of natural water oxidation catalyst, Mn cluster, using electron paramagnetic resonance (EPR) spectroscopy and electron nuclear double resonance (ENDOR) spectroscopy.

Mn cluster in photosystem II (PS II) oxidizes water molecules and produce O_2 in reactions of photosynthesis. Recent big step on the photosynthesis field is success of reveal the X-ray crystal structure of photosystem II with very high resolution (1.9 Å) [1]. The crystal structure clearly showed that the chemical formula of the Mn cluster is Mn_4CaO_5. Three Mn ions, Ca ion and four O ions compose the cubane structure and additional Mn ion and the O are located to the next of the cubane as a backrest of the chair. Four water molecules are ligated to the Mn ion and Ca ion. Water oxidation reaction is explained by Kok cycle model. The Mn cluster has five different redox states named S_n ($n = 0–4$). The crystal structure is revealed in the S_1 state that is the most stable state in the dark. The Mn cluster is oxidized by photo-induced charge separation in the reaction center and the S-state is advanced to the next state (S_n to S_{n+1}). The most oxidized state, S_4 state, is unstable intermediate state. S_4 state goes back to S_0 state rapidly with evolving O_2. In each S-state transition (except S_1 to S_2), one or two protons are released to out of the protein. Proton positions surrounding the Mn cluster are significant, however, the protons are not detected by the X-ray crystal structure. In the present study, we applied proton matrix ENDOR to the Mn cluster to detect protons surrounding Mn cluster.

The first proton matrix ENDOR spectrum of the S_2 state Mn cluster has reported by Kawamori et al. [2]. Six pairs of ENDOR signals which arising from protons surrounding Mn cluster. We tried to assign the ENDOR signals respect to the high-resolution X-ray crystal structure. The number of ENDOR signals is relatively small than the numbers of protons, which expected to be detected. The small ENDOR signal width indicated that protons corresponding to the ENDOR signals have small distance distribution from the Mn cluster. It indicates that bulk water protons are hardly detected, however, some special water (ligated to the Mn cluster directly) protons are detectable by ENDOR. However, ambiguities of assignments were still remaining because some protons are located with similar distances from Mn cluster. Thus, we used oriented PS II membranes to clarify the positions of protons. Water molecules ligated to the Mn ion were distinguished using small orientation dependence of the ENDOR spectra. Additionally, the study of the S-state dependency (S_0 and S_1) of isotope exchange rates [3] and our ENDOR assignments indicated that one of water molecule ligated to the Mn ion is deprotonated in the transition of S_0 to S_1. Full ENDOR data and interpretations have already been published in June 2013 in Biochimica et Biophysica Acta (vol. 1827, pp. 1165–1173, DOI: 10.1016/j.bbabio.2013.06.001).

Next our study is the experimental validation of ENDOR assignments. The Ca^{2+}, which is one of the components of the Mn cluster, could be removed by biochemical treatment [4]. Ca^{2+} has a crucial role on the Mn cluster. Removal of Ca^{2+} occurs the inhibition of oxygen evolving activity. Reconstitution of Ca^{2+} to the Ca^{2+}-removed PS II evolves restoration of the oxygen evolving activity. Reconstitution of Sr^{2+} also recovers the oxygen evolving activity. Other metal ions cannot restore the activity. In the present study, we used Ca^{2+}-removed and Ca^{2+}-reconstituted PS II samples from spinach and Sr^{2+}-exchanged samples from *Thermosynechococcus vulcanus* that cultivated using only Sr^{2+}-containing medium culture. Biochemically Sr^{2+}-substituted PS II samples possibly contain some contaminations, however, cultivated *T. vulcanus* samples contain completely exchanged PS II. The ENDOR spectrum of Ca^{2+}-removed samples showed that one pair of peaks disappeared and the peaks were recovered by Ca^{2+}-reconstitution and Sr^{2+}-substitution. The peaks were previously assigned to the water molecule that is directly ligated to the Ca^{2+}. Sr^{2+}-substitution also affected to ENDOR peaks that assigned to water molecules ligated to the Ca^{2+}/Sr^{2+} ions, however, the structures of Ca-containing and Sr^{2+}-substituted are similar. The ENDOR results are interpreted as that Ca^{2+} has significant roles for the hydrogen bond between the Mn cluster and tyrosine residue, Y_Z, in order to efficient electron transfer and proton release. The ENDOR results of biochemically treated Mn cluster also supported our ENDOR assignments based on the crystal structure and orientation dependencies. Detailed report is going to be published in The Journal of Biological Chemistry (in press, DOI: 10.1074/jbc.M115.675496).

I appreciate to all who have shown an interest in our works. Please feel free to contact me if you have any questions or comments. E-mail address: hnagashima@bio.phys.nagoya-u.ac.jp.

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From Science and Ethics to Resolution Revolution in Optical Microscopy, from Atoms to Complexity in Surface Catalysis, from Global Warming to Science Education

The 65th Lindau Nobel Laureate Meeting
Lindau, Germany, 28 June – 3 July 2015

Klaus Möbius

Free University Berlin, Department of Physics
Max Planck Institute for Chemical Energy Conversion

About a year ago, Wolfgang Lubitz, as Guest of the Issue, had written an illuminating article in *EPR newsletter* (vol. 23, no. 4, 2014) about the remarkable conference series, "The Lindau Nobel Laureate Meetings", at the small island-town Lindau in Lake Constance in Germany. Once every year, some dozens of Nobel Laureates convene at Lindau to meet the next generation of leading young scientists: up to 650 undergraduates, PhD students, and post-doc researchers from all over the world. The defined goal of the Lindau Meetings is to foster the exchange among scientists of different generations, cultures, and disciplines.

In his article Wolfgang Lubitz detailed the general history as well as the scientific and social strategy of the Lindau Meetings. In summary this reads: Since their beginnings in 1951, the Lindau Meetings have evolved into a unique international forum for scientific exchange and humanistic responsibility. It was in 1949, only four years after World War II, that two German medical doctors, Franz K. Hein and Gustav W. Parade from Lindau, an island very close to the neighboring countries Austria and Switzerland, approached Count Lennart Bernadotte af Wisborg of nearby Mainau Island with a great idea: To jointly develop and implement the project of organizing a regular international conference of Nobel Laureates in Lindau in order to meet students from various countries. This was meant as a contribution to reconciliation after the horrors of the war. It marked the start of a long and continuing history. Only two years later, the first "European Meeting of Nobel Laureates" took place. It has developed into the highly esteemed institution of the annual Lindau Meetings which are jointly organized by two institutions – the "Council for the Lindau

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Federal President of Germany Joachim Gauck standing right to Countess Bettina Bernadotte in the middle of the Nobel Laureates during the Opening Ceremony of the 65th Lindau Nobel Laureate Meeting in Lindau, Germany, June 28, 2015.

Nobel Laureate Meetings" and the "Foundation Lindau Nobel Laureate Meetings". They act in concert to warrant the continuity of the meetings and to advance their constant development. But it needs the commitment of a multitude of supporters that hundreds of the best young scientists from around the world get the chance to participate in the Lindau Meetings year after year – and that the high standard and constant further development of these meetings can be warranted.

The commitment of Nobel Laureates to foster the exchange among scientists has been the mainstay of the Lindau Nobel Laureate Meetings ever since their beginnings in 1951. To this day, more than 350 recipients of the Nobel Prize have followed the annual invitation to meet the next generation of leading scientists at Lindau. The opportunity to join the annual gathering of Nobel Laureates at Lindau is provided exclusively to outstanding young scientists aged up to 35. In order to participate in a meeting, the young scientists have to pass a multi-step application and selection process. Every year, a scientific review panel, appointed by the Council for the Lindau Nobel Laureate Meetings, is responsible for evaluating the numerous applications by young scientist from all over the globe who aspire to participate in a Lindau Meeting. Those who ultimately attend have successfully passed a multi-stage selection procedure: a national process, followed by an international one. Taking into account the national selection procedures worldwide, in excess of 20,000 young researchers typically apply to attend each meeting.

The Selection Process is as follows: The national strategic partner with the Lindau Nobel Laureate Meetings, for example the national Research Council of a particular country, runs a national selection process whereby eligible institutions may nominate up to a fixed number of researchers at undergraduate, PhD and Post-doctoral stage. Those who succeed in this national selection process, which will be a fixed maximum of candidates for a given country, will then be nominated to the international selection process, which is conducted by the Lindau Review Panel. This panel makes the final selection from up to 1,500 profiles for every meeting before finally choosing the top 500 applicants (or more at special occasions) who will receive an invitation to Lindau. Nominees who are successful in the international selection process and who receive an invitation to the Lindau Meeting receive an Award which comprises their expenses for attending the meeting.

The stringent selection process by the scientific council members has resulted in a remarkable increase of the quality of the Lindau Meetings, which now bring together and intermix the best young talents worldwide with the Nobel Laureates. Quoting Wolfgang Lubitz: "This results in a fantastic scientific and personal atmosphere during the meetings, making the small island in Lake Constance for one week each year the scientific center of the world."

The Council and the Foundation feel committed to share the enthusiasm that characterizes the annual encounters between Nobel Laureates and young scientists with the general public. It is an integral part of the Lindau Meetings' mission to reach out beyond the meetings at Lindau and involve society in the dialogue on the importance of education, science and research. It is in this spirit that The Lindau Nobel Laureate Meetings have commented, by official statements and declarations, contemporary events of historical significance, for example:

– In 1955, fifteen Nobel laureates signed the "Mainau Manifest against Nuclear Weapons", which was co-signed by another 34 laureates by the end of the year.

– In 1961, Count Bernadotte introduced the topic of sustainability and environmental protection with his "Green Charta of Mainau".

– In 1973, the physics laureate Dennis Gabor, founding member of the "Club of Rome" (1968), addressed the world's limited energy supplies in his Lindau lecture, shortly before the first oil crisis.

– In 1993, medicine/physiology laureate Rita Levi-Montalcini placed science in the service of humanism. She introduced the "Charta of Human Duties" that was later signed by a large number of scientists.

– In 2015, the "Mainau Declaration 2015 on Climate Change" was proclaimed, up to now signed by 36 Nobel laureates participating in the 65th Lindau Meeting (see below).

A unique achievement of the Lindau Nobel Laureate Meetings is the firm intention – and realization – of intensive contacts and discussions between the Nobel Laureates and Young Scientists. In spite of the large number of participants – this year about 750, including laureates, young scientists and guests – the organizers succeeded in mixing them thoroughly with varying compositions, be it in Science Breakfasts, Plenary Lectures, Afternoon Discussions, Master Classes, Panel Discussions, Coffee Breaks, Academic Dinners, Get-Togethers, Concert, Public Lectures, French Evening, Bavarian Evening, Baden-Württemberg Boat Trip to and visit of the Isle of Mainau, Picnic on the Castle Meadow at Mainau. All these events gave ample opportunity to get further scientific and personal information, to meet and connect, to discuss and enjoy.

The 2015 jubilee meeting, the 65th Lindau Nobel Laureate Meeting (28 June – 3 July 2015), was dedicated to interdisciplinary scientific exchange between Young Scientists and Nobel Laureates from the fields of Physics, Chemistry and Medicine/Physiology. Appropriately, 65 Nobel Laureates from these fields participated in the jubilee meeting; in addition 2014 Nobel Peace Laureate Kailash Satyarthi from India and 1986 Nobel Literature Laureate Wole Soyinka from Nigeria enriched the Laureates' team. More than 650 young researchers from 88 countries discussed with the Laureates – and among themselves – about the future of science, society, global climate, and more. Kailash Satyarthi reported of concerted activities against slavish child labour in India and numerous other countries as well as on international movements to protect the rights of children for education and a safe childhood. Wole Soyinka is the first African to be honored in the literature Nobel category. His lecture was a flaming indictment against fundamentalistic barbarism in general – be it ethnically, politically or religiously motivated – and the terrorist group Boko Haram in particular. Boko Haram is an Islamistic extremist group based in northeastern Nigeria, but also active in Chad, Niger and northern Cameroon. Wole Soyinka emphatically denounced its murderous attacks against school children, notably kidnapping school girls. Boko Haram is systematically destroying educational institutions like schools and libraries in the villages; the Boko Haram terrorists have killed many thousands of people since 2009. Wole Soyinka's lecture was an aggrieving contrast to most of the other Nobel Laureates' lectures who reported on the award-earning fruits of higher education and creative thinking in science and humanities.

In the light of the increasingly interdisciplinary science sector, the program of the 65th Lindau Meeting addressed, among other issues, the question whether future breakthroughs in key areas can be expected from the interplay of different research branches. Accordingly, interdisciplinary research was among the hot topics of discussion at various stages of personal interactions during the Lindau Meeting. What started as taken-for-granted ("look into our laboratories", a Laureate said, "one thing is obvious: We are all working in multidisciplinary and multicultural research teams."). The immediate question was asked

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2014 Nobel Prize for Peace awardee Kailash Satyarthi from India. "I want to ignite the change in you," Satyarthi declared to the young scientists in Lindau. He enjoined them to act: "Don't stand on the fence and cheer. Jump in the ring."

1986 Nobel Prize for Literature awardee Wole Soyinka from Nigeria. Soyinka in Lindau: "How do I feel when I am invited to a congregation of scientists? I feel quite at home. When they break into their cultic scientific argot, I know when I'm not wanted and step out for a drink."

by a Young Scientist: "Is interdisciplinarity then a formula for gaining the Nobel Prize?" This was denied by all five Nobel laureates who took part in a Panel Discussion entitled "The Quest for Interdisciplinarity: Inspiration or Destruction?" at the 65th Lindau Nobel Laureate Meeting. Eric Betzig, Martin Chalfie, Steven Chu, Stefan Hell and William Moerner shared the experience that interdisciplinarity in the natural sciences was not a goal in itself, but a naturally developing concept determined by the specific field of research. As many scientific questions of the presence and future are too complex to be associated with a single scientific discipline, research will increasingly be based on interdisciplinary collaboration.

The discussions at Lindau clearly reveal the trend that young researchers are leaving the ivory towers of their disciplines to team up with colleagues from other disciplines and cultures – in order to find answers to the pressing questions of the future. "We need breakthroughs in medicine, energy generation and its social aspects, as well as climate change prevention", a Young Scientist said. "Most of these are closely coupled and need to be addressed in an interdisciplinary approach." "An important precondition for interdisciplinary research was that a free flow of communication was facilitated, just as unobstructed and lively like in cafeterias", as Nobel laureate Martin Chalfie put it. And Eric Betzig added "that the basis for exchange with colleagues of other disciplines was a substantial understanding of one's own discipline." "You have to be an expert in your own discipline," William Moerner voiced it. And Stefan Hell even perceived the chance that by interdisciplinary collaboration researchers would become aware of outdated dogmas in their own disciplines – and finally overcome them: "Those who remain trapped in paradigms will not succeed in changing things." And Steven Chu told the audience that not only the complexity of issues but also the excellence of his students had driven him to explore new fields: "This is how you can escape the competition and expand your knowledge."

Among the core themes of the 65th Lindau Nobel Laureate Meeting was Africa's perspectives. Accordingly, this year as many as 36 of the total 650 participating Young Scientists came from Africa – more than at any previous Lindau Meeting. They came from 15 of the 54 African countries: nine of them from South Africa, four each from Egypt and Cameroon, three each from Ghana and Mauritius, two each from Botswana, Nigeria and Zimbabwe, and one each from Ethiopia, Burkina Faso, Kenya, Madagascar, Rwanda, Sudan and Uganda. The participation of the Young Scientists from Africa was financed in part by the academic partners of the Lindau Meeting, like the German Academic Exchange Service (DAAD), the Department of Science and Technology of South Africa, and the World Academy of Science. Most of them, however, were invited due to a new initiative of the Lindau Nobel Laureate Meetings under the patronage of the former Federal President of Germany, Horst Köhler. The "Horst Köhler Fellowship Programme" is funded by the Robert Bosch Foundation.

When Africa is mentioned, one would think of a troubled continent, basically shattered by disasters, crises, wars, diseases. But this year's Lindau Meeting proved that this is at least an incomplete picture. When talking to these Young Scientists from Africa, one thing became evident: Many prejudices have to be revised, there is so much to learn from the African experiences! There is so much left to be done by the international science community!

In the past decade, the number of scientific publications from African scientists tripled. That sounds impressive, and indeed it is impressive. Nevertheless, according to the scientific journal Nature, the scientists from Africa published approximately as much as the researchers in the Netherlands. Meanwhile, about 1.5 per cent of all scientific publications come from Africa, a continent that is larger than the USA, China, India, Japan and Europe combined. The countries of Africa are extremely different from each other in their scientific and educational achievements. This was acknowledged by the Young Scientists from Africa as well as by the French 2008 Nobel Prize winner in Physiology or Medicine, Françoise Barré-Sinoussi: "You cannot simply define a research focus for the whole of Africa," she said, who conducts research in collaboration with colleagues from numerous African countries. There would not be the one right program for Africa. Even the AESA program (Alliance for Accelerating Excellence in Science in Africa), which was launched recently and supported predominantly by the Welcome Trust (London, UK), the UK Department for International Development and the Bill & Melinda Gates Foundation (Seattle, Washington, USA) should be aligned regionally. Special programs should be created for South, West, North and East Africa because only within each of these regions there are similar scientific challenges. Africa has a lot of talented young scientists, but there is a lack of opportunities for scientific research that is adequately funded and operational on an international level. The AESA program aims at improving the working conditions of scientists in Africa, putting the decision on research targets into local hands and curbing the brain drain. What is needed first is reliable power supply for the laboratories to properly cool perishable biological and medical samples. And then there is an urgent need for more competitive research infrastructure such as high-tech laboratories.

The research landscape in Africa is primarily focused on applied research in the fields of health and agriculture. But the Young Scientists from Africa and several Nobel Laureates made the point that it is also the basic research that African science needs – to lay the foundation for further scientific progress in the various disciplines that will ultimately lead to innovations "Made in Africa". This is one more reason that fair partnerships between African and European or American research institutions are being absolutely necessary. Cooperation on a par, as pursued by US Nobel Laureate Peter Agre, who does research on malaria in different African countries such as Zimbabwe, Zambia, Malawi, Congo and Mozambique, should be the normal situation.

On Sunday, June 28, the 65th Lindau Nobel Laureate Meeting was officially opened by Countess Bettina Bernadotte af Wisborg, President of the Council. She gave a warm welcome to all the people attending the meeting and, specifically, to the President of the Federal Republic of Germany, Joachim Gauck, who gave the welcome address, and to the Young Scientists from around the world. President Gauck said that science needed such opportunities for "critical exchange, and as often as possible, cooperations that break boundaries – not least for funding scientific research." And Countess Bettina Bernadotte added "To inspire and motivate young scientists and researchers is the key concern of this Meeting." In her opening speech, she stressed that the dedicated and inquisitive young people were the main reason for the Nobel Laureates to be so exceedingly committed to the Lindau Meetings. Since the dialogue between cultures and societies is just as central to the Meeting as is the scientific dialogue, she was particularly pleased about the extremely strong international participation this year.

On Monday, June 29, the scientific program of the Lindau Meeting started with a plenary lecture on "Optical Microscopy: The Resolution Revolution" by German 2014 Nobel Laureate in Chemistry, Stefan Hell. He was awarded the Nobel Prize for the development of super-resolved fluorescence microscopy, sharing the Prize with two US scientists, William Moerner and Eric Betzig. All three of them held plenary lectures at the Lindau Meeting about their current and past research.

Stefan Hell is credited with having made tremendous improvements in the spatial resolution of nanoscopic images by by-passing the Abbe diffraction limit for illuminated samples. To this end, he and his team developed the STED (Stimulated Emission Depletion) microscope, which can resolve ultrafine details in the nanoscopic range with a wealth of structural information by means of emitted light from the sample. The key idea for going far beyond the Abbe limit is replacing passive illumination of the object by active light emission of fluorescent molecules.

After improving the spatial resolution, the next logical step was to stretch the temporal resolution to its limits. The greatest challenge was to achieve precise spatial resolution while at the same time recording random motions. If an object takes too long to visualize, the resulting image will be blurred. What is needed is therefore a means to capture a series of images. The Hell Laboratory appears to have achieved just that. Due to his discovery, light microscopy is back as one of the top techniques to discover hidden worlds in the living cell. The development of super-resolved fluorescence microscopy makes it possible "to map the innermost secrets of life", as the Royal Swedish Academy of Sciences puts it, "microscopy has become nanoscopy". In his lecture, Stefan Hell vividly described the path to success in opening these new dimensions – undoubtedly an encouraging account for young scientists and an advice to give unconventional methods a trial and to follow their curiosity. The applause of the audience in Lindau was correspondingly vivid.

During the following Tuesday and Wednesday, the plenary lectures of the Laureates took place in parallel at four different locations. Changing between the locations was not recommendable because of rather long distances between them. Here, only one example will be mentioned, the plenary lecture by Gerhard Ertl on "Catalysis at Surfaces: From Atoms to Complexity".

German physicist Gerhard Ertl received the 2007 Nobel Prize in Chemistry for his studies of surface chemistry – the fundamental molecular processes at the gas-solid interface. Surface catalysis is currently of extreme importance for technologies for renewable energy supply and environmental protection. Surface catalysis also explains such varied processes as why iron rusts, how fuel cells function, how artificial fertilizers are made and how catalytic converters in our cars work. When a gas or liquid molecule hits a solid surface the molecule may simply bounce back or be adsorbed. It can split into its constituent atoms, react with previously adsorbed molecules or even react directly with surface atoms. Surface chemistry can now even contribute to the understanding of the destruction of the ozone layer, as crucial reactions take place on the surface of ice crystals in the stratosphere.

2014 Nobel Prize for Chemistry awardee Stefan Hell from Germany.

2007 Nobel Prize for Chemistry awardee Gerhard Ertl from Germany.

Gerhard Ertl explored new techniques, such as tunnelling microscopes, to provide a complete picture of a surface reaction. He first determined the molecular mechanism of the Haber-Bosch process, in which iron is used to transform nitrogen from the air together with hydrogen to ammonia, which is the key compound for the production of artificial fertilizers. He went on to study the oxidation of carbon monoxide over palladium and platinum (catalytic converter) and discovered the phenomenon of oscillating changes in surface structure that occur during reaction.

His lecture addressed the question of spatial-temporal self-organization of matter which is so characteristic for living systems. It can also be verified with a simple inorganic reaction in which the observed phenomena of complexity can be traced back to properties of the atoms – and can be described by simple physical laws. This was illustrated with experiments with the catalytic oxidation of carbon monoxide on a platinum surface.

When visiting the various locations of the 65th Lindau Meeting, where the lectures, discussions, master classes or social events took place, one general impression was dominating – ▶

despite the versatility of issues covered: For most of the Young Scientists, pursuing their research careers is more than gaining knowledge for higher personal earnings. “Money is important”, they say, “but there is more to come than money.” Science should contribute to solving urgent problems of mankind. “We are trying to make the world a better place,” was agreed on by many Noble Laureates and Young Scientists. And many attendees unequivocally emphasized that Scientists should definitely have a stronger say in political and social debates. In particular, global warming and climate change are seen as the major challenge of the future. “Sufficient funds have to be allocated internationally to tackle key issues like green energy production, water security and technologies for cleaning of water on the large scale” one could often hear. Many young researchers stated that they would like to see new techniques applied to repel the effects of climate change. “It is the responsibility of scientists to find solutions for issues such as environment-friendly energy and food supply for the world population” was stressed specifically by Africa-born young chemists. The young people also pointed out that none of the established or new tools at hand is of any use, as long as our societies do not apply them to facilitate a sustainable and fair life for all people on the planet, for instance by supplying clean water and enough food. First and foremost, the industrialized nations have the responsibility to reduce carbon dioxide emissions and prevent further climate change. “The gravest problem of mankind at this time is the destruction of our beautiful planet. But the industrializing third-world countries with their 3-billion population tend to want things NOW no matter what the environmental costs are. This attitude they have adapted from the first-world countries where it was – and in many cases still is – the leading dogma of market-oriented uncontrolled capitalism. “But we seriously need to learn to think ahead”, a young physicist from India said, “for if we do not take lasting, long-term and concerted measures, it might be too late to revert the balances of nature back to its steady sustainable state.”

Mainau Declaration 2015 on Climate Change

We undersigned scientists, who have been awarded Nobel Prizes, have come to the shores of Lake Constance in southern Germany, to share insights with promising young researchers, who like us come from around the world. Nearly 60 years ago, here on Mainau, a similar gathering of Nobel Laureates in science issued a declaration of the dangers inherent in the newly found technology of nuclear weapons – a technology derived from advances in basic science. So far we have avoided nuclear war though the threat remains. We believe that our world today faces another threat of comparable magnitude.

Successive generations of scientists have helped create a more and more prosperous world. This prosperity has come at the cost of a rapid rise in the consumption of the world’s resources. If left unchecked, our ever-increasing demand for food, water, and energy will eventually overwhelm the Earth’s ability to satisfy humanity’s needs, and will lead to wholesale human tragedy. Already, scientists who study Earth’s climate are observing the impact of human activity.

In response to the possibility of human-induced climate change, the United Nations established the Intergovernmental Panel on Climate Change (IPCC) to provide the world’s leaders a summary of the current state of relevant scientific knowledge. While by no means perfect, we believe that the efforts that have led to the current IPCC Fifth Assessment Report represent the best source of information regarding the present state of knowledge on climate change. We say this not as experts in the field of climate change, but rather as a diverse group of scientists who have a deep respect for and understanding of the integrity of the scientific process.

Although there remains uncertainty as to the precise extent of climate change, the conclusions of the scientific community contained in the latest IPCC report are alarming, especially in the context of the identified risks of maintaining human prosperity in the face of greater than a 2°C rise in average global temperature. The report concludes that anthropogenic emissions of greenhouse gases are the likely cause of the current global warming of the Earth. Predictions from the range of climate models indicate that this warming will very likely increase the Earth’s temperature over the coming century by more than 2°C above its pre-industrial level unless dramatic reductions are made in anthropogenic emissions of greenhouse gases over the coming decades.

Based on the IPCC assessment, the world must make rapid progress towards lowering current and future greenhouse gas emissions to minimize the substantial risks of climate change. We believe that the nations of the world must take the opportunity at the United Nations Climate Change Conference in Paris in December 2015 to take decisive action to limit future global emissions. This endeavor will require the cooperation of all nations, whether developed or developing, and must be sustained into the future in accord with updated scientific assessment.

Signatories of the Mainau Declaration 2015:
Peter Agre, Michael Bishop, Elizabeth Blackburn, Martin Chalfie, Claude Cohen-Tannoudji, Steven Chu, James Cronin, Peter Doherty, Gerhard Ertl, Edmond Fischer, Walter Gilbert, Roy Glauber, David Gross, John Hall, Stefan Hell, Serge Haroche, Jules Hoffmann, Klaus von Klitzing, Harold Kroto, William Moerner, Ferid Murad, Ei-Ichi Negishi, Saul Perlmutter, William Phillips, Richard Roberts, Kailash Satyarthi, Brian Schmidt, Hamilton Smith, George Smoot, Jack Szostak, Roger Tsien, Harold Varmus, Robin Warren, Arieh Warshel, Robert Wilson, Torsten Wiesel.

The debate on the role of science in society and the responsibility of science for society, which President Joachim Gauck had called for so insistently in his speech at the Opening Ceremony on Sunday, was also in the focus of the Closing Panel Discussion on “Science Education” at Mainau Island on Friday, July 3. All the participants of the panel discussion, among them Lucia Godino, Postdoctoral Researcher from University Lausanne, Harold Kroto, Chemistry Nobel Laureate from Florida State University, Kailash Satyarthi, Peace Nobel Laureate from India, and Georg Schütte, State Secretary of the German Federal Ministry of Education and Research, agreed that “Science Education needs to be equitable and inclusive for All”. And that scientific knowledge, scientific methods, societal issues, personal needs, and career awareness are the main goals for science education. That science programs are primarily oriented towards accumulation of knowledge of the academic disciplines, their scientific facts, concepts, and principles that reflect the structure of systematic thinking and analyzing in science. But a really vivid, sometimes even controversial discussion flared up – partly including questions and comments from the large audience – only when “touchy” issues of how to change existing societal problems and grievances were addressed, for example poverty, illiteracy, and abuse of children worldwide.

All agreed that Science Education should enable students not only to understand the subject matter of science but also, even primarily, to develop inquiry abilities and critical thinking skills. Increasing interest in societal

Some of the Nobel Laureate signatories of the "Mainau Declaration 2015 on Climate Change" still on stage just after the signing procedure, July 3, 2015.

issues is evident in Science Education programs. Science teachers should be obliged to include these societal goals in their lecture programs to make them relevant to the concerns of all students. The goals for teaching science should put more emphasis on environmental concepts, world problems, decision making, and interdisciplinary studies – all areas related to the goal of teaching students how to deal with societal issues within their science frameworks.

The last day of the 65th Lindau Nobel Laureate Meeting was certainly a day that produced lasting memories for all who were involved. 36 attending Nobel Laureates congregated for an an emphatic appeal for global climate protection to the political leaders of the world – the "Mainau Declaration on Climate Change 2015". It states "that the nations of the world must take the opportunity at the United Nations Climate Change Conference in Paris in December 2015 to take decisive action to limit future global emissions."

The declaration can be found at:
http://www.lindau-nobel.org/wp-content/uploads/2015/07/Mainau-Declaration-2015-EN.pdf
and a few statements and comments at:
http://www.lindau-nobel.org/de/the-mainau-declaration-2015-on-climate-change/

Here are some statements by Nobel Laureates Brian P. Schmidt and George F. Smoot, signatories of the Mainau Declaration:

What is the key message of the Mainau Declaration?

B. P. Schmidt: The Message is that while there is uncertainty, the IPCC report on Climate change represents the best understanding of climate change today, and should be used as the basis of policy decisions by the world. The potential risks as outlined in this report are very high, and therefore action is required as part of the UNFCCC meeting in Paris.

G. F. Smoot: As scientists, we have learned the rigour of the science process and trust the results of the IPCC as a current summary of human?s best scientific results and projections on Climate Change. The evidence is very strong that the major portion of climate change is man made and that continuing business as usual presents great and increasing risk to humankind.

What would you like to achieve with this Mainau Declaration?

B. P. Schmidt: I would like to see the Nations of the world chart a course of Greenhouse gas emissions that provide a reasonable expectation that the total average temperature of the Earth will not rise more than 2 °C over the pre-industrial era.

G. F. Smoot: The primary goal is to draw the general public?s attention and add to the information they have been getting and then have that in term both directly and indirectly reach political leaders and convince them to do as much for the right reason of protecting the public and the world.

What will be the next steps? Do you want other scientists, especially young scientists to join?

B. P. Schmidt: We will make the document available for other science Nobel Laureates to sign, and will encourage the young scientists to become informed on the issue and act to ensure their communities are fully informed by the best possible information.

G. F. Smoot: The first is to show young scientists that this is an important issue and it is relevant to them and to show by the fact that Nobel Laureates are paying attention it is both relevant and important for them to also study and learn and tell their peers. We do expect much of the climate change science is done by your scientists and this helps give them credit, encouragement, and visibility.

Suggestions for further reading:
The lectures and panel discussion can be viewed in the Lindau Mediatheque that is found on the website www.lindau-nobel.org

Note added in proof:
On 7 December 2015, the Mainau Declaration 2015 on Climate Change, which in the meantime has been signed by 72 Nobel Laureates, was presented by the Nobel Laureates Serge Haroche and Claude Cohen-Tannoudji to President Francois Hollande, who hosts the 2015 Paris Climate Conference (30 November – 11 Dezember 2015) and chairs the UN Climate Talks COP21.

EasySpin: Past, Present, Future

Stefan Stoll
Department of Chemistry, University of Washington, Seattle, WA, USA

EasySpin is a free software package for the analysis, simulation and fitting of EPR spectra. It runs on Windows, Mac and Linux computers and is an extension of Matlab, a commercial technical computing platform that is widely used both in academia and in industry. EasySpin is available at http://easyspin.org.

History

EasySpin initially started when I was a graduate student in Arthur Schweiger's lab at ETH Zürich. At the time, I was acquiring solid-state CW and pulse EPR data on a series of cobalt complexes, and I needed a simulation program to extract the *g* and *A* values from the CW EPR spectra. Although the Schweiger lab had great software and expertise for simulating pulse EPR spectra (mostly based on the C++ library Gamma), as it turned out, there wasn't a good home-built program for the simulation of CW EPR spectra. So I set out to write one. In the process, I developed a series of new theoretical and algorithmic tricks to speed up powder simulations for general spin systems. Eventually, advancing the theory underlying spectral simulations in solid-state EPR became the topic of my Ph.D. thesis. After the adoption of EasySpin by others within the Schweiger lab, it slowly became known outside the lab and spread to other research groups.

Since the Zürich days, EasySpin has continued to grow and has followed me to my postdoc position with R. David Britt at UC Davis and to my faculty position at the University of Washington (since 2011). Today, EasySpin is used by many researchers in the worldwide EPR community. As of October 2015, the original 2006 paper about EasySpin in the Journal of Magnetic Resonance has been cited over 1360 times and is the 10th most cited article overall in that journal. When EasySpin 5 was released in July 2015, it was downloaded 1000 times within a month.

Of course, EasySpin was not developed in isolation. Many previously developed programs, such as John Weil's EPRNMR, Graeme Hanson's XSophe, MAGRES from the Nijmegen group, Bruker's SimFonia, Høgni Weihe's sim, and Jack Freed's EPRLL and NSLS, were both controls for testing purposes and inspiration for development and design. EasySpin owes a lot to the authors of these programs.

Functionality

Over time, more and more EPR functionality was added to EasySpin. Solid-state EPR and ENDOR capabilities existed from the initial version 0.9. Solution simulations were introduced in 2.1. Slow-motion simulations using the stochastic Liouville equation came in 2.5. Fitting capabilities first appeared in 2.7 and were expanded with every subsequent release. Pulse EPR simulations were introduced in 3.0. In 5.0, frequency-swept spectra and magnetometry were introduced. Figure 1 summarizes the key capabilities of EasySpin as of version 5.0. Aside from the high-level simulation functionality, EasySpin also includes many utility functions for spin physics, data import and export, and data analysis.

EasySpin's simulation functions have somewhat idiosyncratic names: `pepper`, `salt`, `garlic`, `chili`, `saffron`, `curry`. Many users ask where these names come from. The origin lies in the original purpose of EasySpin, the simulation of powder EPR spectra. In very early versions, the simulation function was named `pepr`, where the first `p` stands for "powder". Eventually, this morphed into `pepper`. When ENDOR was implemented, the corresponding simulation function was named `salt`. Subsequent names followed the food theme: `garlic` for liquid-state CW EPR spectra, `chili` for slow-motion CW EPR spectra, `saffron` for pulse EPR spectra, and `curry` for magnetometry.

Design Principles

The core design principle underlying EasySpin is an excellent usability and user experience for the broadest possible range of users, not just for users versed in spin physics. Therefore, the theoretical and algorithmic aspects of the simulation functions are hidden as much as possible, and the user input is kept at the minimum necessary to run simulations. For some simulation parameters, EasySpin tries to automatically determine best values. For example, it can automatically set appropriate sweep ranges for CW EPR spectra of simple spin systems. Also, EasySpin makes an effort to prevent the user from using certain theory levels (e.g. perturbation theory) beyond their scope of validity. However, since spin systems can vary over a wide range, this is not easy to do consistently for every case.

Occasionally, usability improvements introduce changes that are incompatible with older EasySpin versions. This happened, for example, in version 5.0 with the reorganization of coordinate frame definitions. Whereas we always make every effort to keep these incompatible changes at a minimum, we try to continuously innovate to make EasySpin easier to use. Bad design decisions in the past should not constrain possible usability improvements the future.

EasySpin 5.0

CW EPR - solid state
arbitrary spin systems
matrix diagonalization
perturbation theory
hybrid methods
efficient powder averages
overmodulation
phasing

CW EPR - slow-motion regime
arbitrary spin systems
stochastic Liouville equation
ordering potential
multiple solvers

CW EPR - isotropic
S = 1/2, no limits on nuclei
fast motional regime

Pulse EPR
solid-state
arbitrary *S*, no limits on nuclei
single-frequency rectangular pulses
arbitrary pulse sequences
highly efficient ESEEM & HYSCORE

ENDOR
arbitrary spin systems
excitation bandwidth selection
matrix diagonalization
perturbation theory

Least-squares fitting
many fitting algorithms
full GUI for multi-stage fitting
multiple objective functions
works with any type of simulation

Magnetism
arbitrary spin systems
SQUID magnetic moments
magnetic susceptibility

Spin physics
spin operators
spin Hamiltonians
spin coupling
Wigner 3j and 6j

Other tools
Euler angles
line shape functions
isotope data
import of experimental EPR data
from Bruker and other vendors
export to Bruker format

Figure 1: Overview of EasySpin capabilities.

Code Base

Most of EasySpin is written in Matlab, with a few performance-critical parts written in C. Matlab is a non-free commercial product. One might wonder why EasySpin is not built on free software such as Octave, Python or Julia. The reason is simple: Matlab is the best

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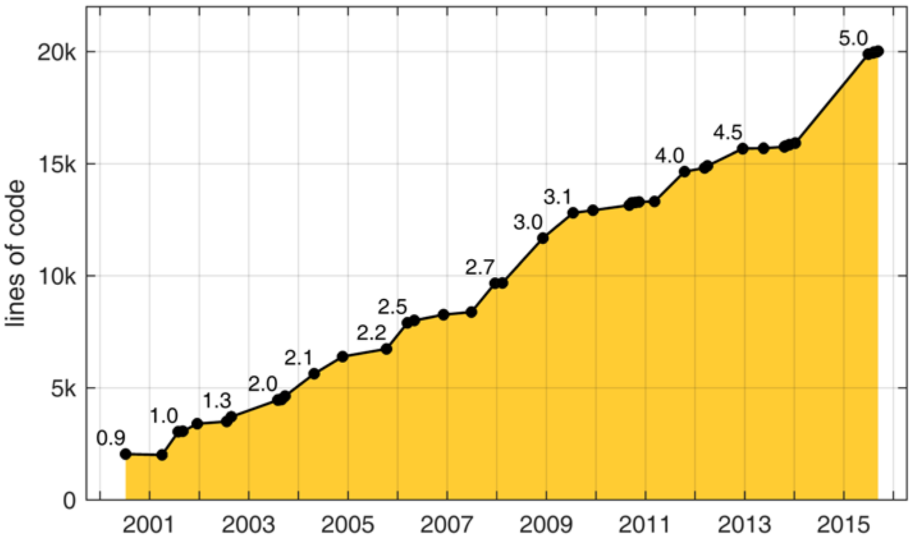

Figure 2: Lines of Matlab code for EasySpin versions, as a function of their release date.

technical computing software available. It is comprehensive, very efficient, bug-free, well maintained, has well integrated visualization, works smoothly on different platforms, and is easy to install even for researchers with little programming knowledge e.g. those in the biological and medical sciences. As both Matlab and the potential alternatives evolve, we will reexamine this choice. However, EasySpin will likely stay Matlab-based for the foreseeable future, since a conversion to another programming language will cost a lot of time.

For all its lifetime, EasySpin has been closed source. Users cannot see the Matlab code that runs the simulations. The reason behind the decision to keep the source closed is that it forces users to report bugs and wanted features. Open source lends itself to cloning and modifications. If there are bugs in a particular version of EasySpin, and a user fixes them in his/her own modified copy of EasySpin, then this bug most likely goes uncorrected in the official version which everybody else is using. Another reason for closed source is to encourage users to communicate the features they want, as opposed to implementing them only in their own local modified copies of EasySpin. As a result, all feedback from users worldwide goes directly into improving EasySpin, to the benefit of all.

Since its initial release, the code base of EasySpin has grown substantially. The graph in Fig. 2 shows the growth from about 2,000 lines of Matlab code – not counting comments – for version 0.9 (July 2000) to just over 20,000 lines as of version 5.0.10 (September 2015). This averages a growth by about 1,200 lines per year. To manage this large code base, EasySpin uses a modern software version control system (Mercurial) since version 4.0. Without this, keeping track of changes and staying organized would be impossible. EasySpin also has a semi-automated build system such that it takes minimal effort to test, package and publish a new release. With this, bug-fix releases can be pushed out on the day the bug is reported and fixed.

Testing

EasySpin is a package with a broad range of functionality, all of which needs to be tested thoroughly every time before a new version is released to the public. Manual testing is impossible. Since version 2.7, an automated test system is in place. It consists of a large number of EasySpin test calculations and simulations that are either verified by comparison to analytical expressions (direct tests) or by comparison to spectra obtained with earlier versions of EasySpin (regression tests). As of September 2015, the test suite comprises 519 tests with a total of 8,000 lines of code. Before it is released to the public, a new version must pass all tests of the test suite perfectly. When a test fails that previously passed, it is an indication that some recent changes broke old functionality and that this must be fixed. Additionally, whenever a serious bug is identified and reported by users, we fix it and add a test to the test suite to make sure this bug will never occur again. Without this and the automated testing, high-quality software development would not be possible. A key criterion for the quality of a test set is the coverage – what percentage of the code base is actually tested. As of September 2015, this is about 80% for the most used function `pepper`, 100% or close to it for most low-level functions (spin operators, spin Hamiltonian terms, etc.), and between 40% and 100% for most other functions.

Occasionally, EasySpin features are developed by writing the corresponding tests before writing the associated code. Initially, the tests will of course fail, since the feature is not implemented. Development then focuses on writing code so that all tests pass. At that point, the feature is considered implemented. In software engineering, this approach is called test-driven development. It helps to spell out the user interface of the new feature upfront and keeps development very focused.

Forum

Due to popular demand, in 2014 an online forum for EasySpin users was launched. A year later, over 100 people have posted on it. The forum has two benefits compared to email: The answers to user questions are visible to everybody on the forum, and other users can answer questions as well. Overall, the forum is a great platform for EasySpin users to interact and learn. It will be great to see more people on the forum actively participating in answering questions and thereby helping disseminate knowledge and expertise about EPR.

Future

For most of its existence, EasySpin was a one-person endeavor. With my transition into an independent career, time available for EasySpin development became much scarcer. As a result, development is now transitioning to a team. Currently, there are a handful of contributors, and I anticipate that this team will grow in the future.

EasySpin's development is driven by the needs in my lab and by needs from the user community. The list of user-suggested new features is very long. These include EDMR (electrically detected magnetic resonance), error statistics on fitting results, simulation of DEER (double electron electron resonance) and other multi-frequency pulse EPR experiments, pulse shaping, multi-core and multi-CPU parallelization, a graphical user interface for common experiments, interfacing with molecular dynamics software for the simulation of spectra in the slow-motional regime, Mössbauer spectroscopy, and many others. Over time, we plan to implement all these features. This will make EasySpin better and better at what it intends to be: a complete and robust platform for doing EPR on your computer, without the need to be an expert of the underlying spin physics. ●

EPR => Hot Science

The idea for this column came from Graeme Hanson, who to our dismay passed away so suddenly in February 2015. When Laila Mosina asked me at a conference in St. Petersburg to continue Graeme's column I agreed since I felt that it is important for the EPR community to know what is going on at the forefront of science in our field and how urgently EPR techniques are needed for the success of many difficult projects across the sciences.

The column will continue to showcase outstanding results primarily of IES members published in the best journals of the appropriate field of research. EPR spectroscopists are invited to contribute a general summary of their work (word file) of no more than 200 words together with an illustrative figure (with a caption if needed) and a few references to wolfgang.lubitz@cec.mpg.de.

Importantly, contributions should not violate publishers copyright!

In continuing the column, I have provided a few examples of excellent recent work from biophysical chemistry. I look forward to receiving many more exciting contributions from other laboratories for upcoming issues of the *EPR newsletter*.

Wolfgang Lubitz

Spinning on a cell – observing membrane protein conformation in the cellular environment 13

Title: Distance Measurement on an Endogenous Membrane Transporter in E. coli Cells and Native Membranes Using EPR Spectroscopy
Authors: Benesh Joseph, Arthur Sikora, Enrica Bordignon, Gunnar Jeschke, David Cafiso, Thomas F Prisner
Journal/Publication date: Angewandte Chemie International Edition 31 March 2015: Vol. 127, issue 21, pp. 6294–6297, DOI: 10.1002/ange.201501086

Membrane protein function encompasses local and global motions occurring over a wide range of time scales (from ps to ms), which all could be modulated by the surrounding environment [1]. However, determination of membrane protein structure and dynamics with high resolution in intact cells is very challenging and yet to be demonstrated. We applied continuous wave and pulsed EPR spectroscopy combined with molecular biology techniques to monitor dynamics and conformation of the outer membrane cobalamin transporter BtuB in intact *E. coli* cells. BtuB can be overexpressed in *E. coli* cells up to 105 copies per cell, comparable to the expression level of some endogenous outer membrane proteins. Overexpressed BtuB can be spin labelled and it can bind substrate and undergo conformational changes in live *E. coli* cells. Further, it is feasible to perform distance measurements using pulsed EPR on BtuB in whole *E. coli* cells and native outer membranes. This method opens up an opportunity for the first time to study structure, function and dynamics of outer membrane proteins in a native membrane and/or cellular environment.

1. Mchaourab, H.S., Steed, P.R., Kazmier, K. *Structure* **2011** 19: 1549–1561.
2. Polyhach, Y., Bordignon, E., Jeschke, G. *Phys. Chem. Chem. Phys.* **2011** 13: 2356–2366.

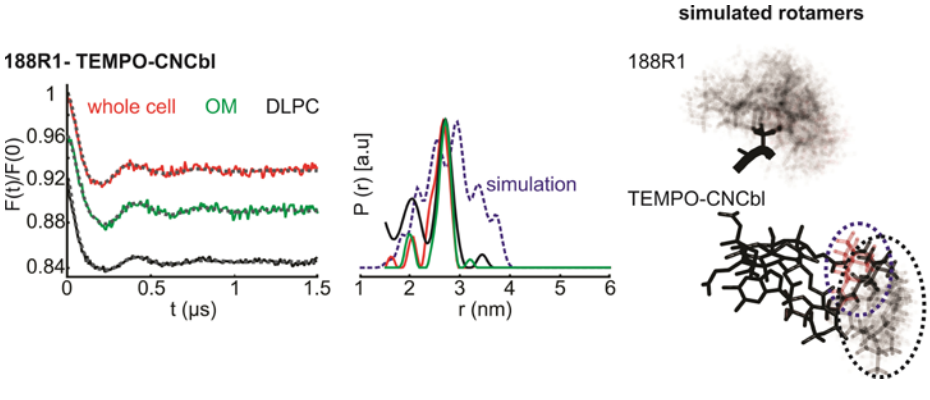

Figure: Distance measurement between BtuB spin labelled at position 188 and a spin labelled cyanocobalamin (TEMPO-CNCbl). The interspin distances were measured in whole cells, native outer membranes (OM) and synthetic DLPC vesicles, which all revealed similar results. Simulation (on PDB 1NQH, using MMM [2]) as well revealed similar distances (for TEMPO-CNCbl, contributed by the rotamers in red inside the blue circle) with the presence of additional distances in the range of 3-4 nm, contributed mostly by rotamers highlighted inside the black circle, which are unlikely populated in a membrane environment.

Pulse W-band EPR reveals the structure of nature's water splitting catalyst prior to O-O bond formation 14

Title: Electronic structure of the oxygen evolving complex in photosystem II prior to O-O bond formation
Authors: Nicholas Cox, Marius Retegan, Frank Neese, Dimitrios A Pantazis, Alain Boussac, Wolfgang Lubitz
Journal/Publication date: Science 15 August 2014: Vol. 345, no. 6198, pp. 804–808, DOI: 10.1126/science.1254910

Nature's water splitting catalyst consists of an inorganic tetramaganese-calcium cluster linked together by five oxygen bridges (Mn_4O_5Ca) [1, 2]. We have recently applied multifrequency-multiresonance pulse EPR spectroscopy to this system to reveal the structure of the catalyst in the last metastable state (S_3) of its reaction cycle, the state immediately prior to O-O bond formation.

We find that the structure of the catalyst evolves away from the X-ray crystal structure, with its stoichiometry changing. The catalyst gains an additional oxygen ligand (OH) such that it should now be described as a Mn_4O_6Ca complex. These results were obtained using ^{55}Mn-ELDOR-detected NMR. Careful analysis of the metal centered hyperfine coupling of the complex coupled to density functional

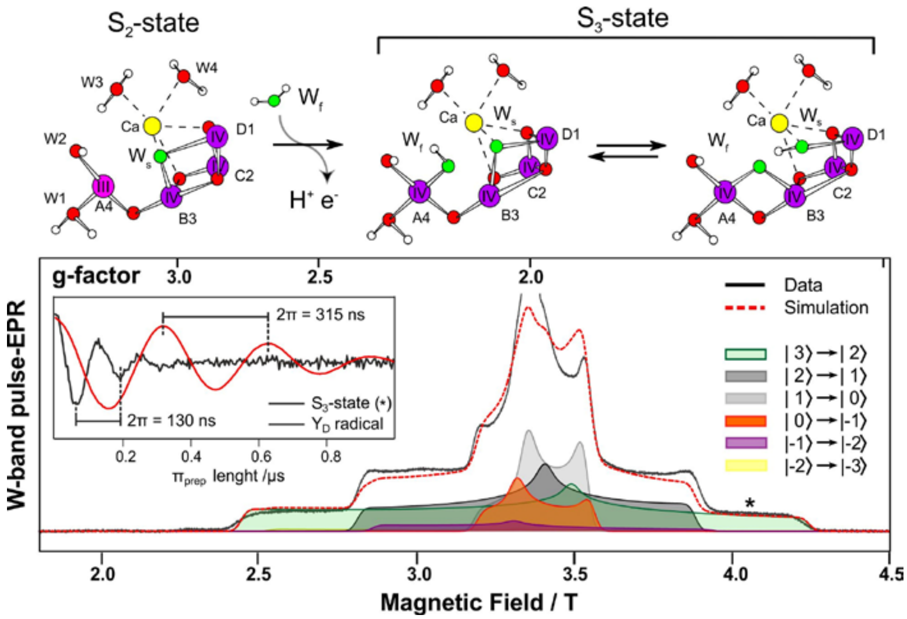

Figure: Pulse W-band EPR data of nature's water splitting catalyst poised in the S_3 state. The insert shows a microwave nutation curve measured for the S_3 state signal relative to a $S = ½$ standard. The models above show the evolution of the structure of the cofactor during the S_2 to S_3 transition.

theory calculations allowed the ligand field oxidation state of each Mn to be obtained – it represents an all Mn^{IV} complex where all Mn ions are six coordinate. The structure of the activated catalyst suggest the O-O bond forms between two adjacent, manganese bound oxygens, an oxo bridge and the new oxygen ligand introduced into the structure.

1. Umena, Y., Kawakami, K., Shen, J.R., Kamiya, N. *Nature* **2011** 473, 55–60.
2. Cox, N., Pantazis, D.A., Neese, F., Lubitz, W. *Acc. Chem. Res.* **2013** 46: 1588–1596.

Bioassembly of the catalytic site of [FeFe] hydrogenase studied by EPR techniques 15

Hydrogenase enzymes can play a useful role in sustainable energy programs by reducing protons to make hydrogen fuel. The [FeFe] hydrogenase can produce close to 10,000 hydrogen molecules a second at the catalytic H-cluster which consists of a [4Fe-4S] cluster linked to a unique binuclear Fe cluster with CO and CN ligands along with an azadithiolate bridge. How does nature make such a complex cofactor? David Britt's laboratory at UC Davis has been using EPR and other spectroscopies to study the bioassembly of the H-cluster, in collaboration with James Swartz at Stanford University and Steve Cramer at UC Davis. The CO and CN ligands are produced from tyrosine in a radical SAM enzyme, HydG. The initial [4Fe-4S] centered reductive cleavage of SAM (S-adenosylmethionine) produces a 5'-deoxyadenosyl radical which abstracts an H-atom from tyrosine, cleaving the tyrosine and producing an EPR-characterized 4-oxidobenzyl radical [1], along with a dehydroglycine (DHG) which is the ultimate source for the CO and CN ligands of the H-cluster. The CO and CN ligands are bound to Fe at a second Fe-S cluster in an organometallic synthon that is transferred to the H-cluster as shown through ^{57}Fe ENDOR [2]. This second cluster has a fifth Fe, seen as linked via a sulfide bridge in a recent X-ray crystallography study [3], and the coupling to this high spin Fe(II) gives rise to a $S = 5/2$ EPR signal from this cluster. Biochemical assays monitoring this EPR signal as an indicator of the presence of this fifth "dangler Fe" along with ^{13}C ENDOR and ^{57}Fe Mossbauer spectroscopy have led to a new paper from the Britt lab that indicates the dangler Fe is bound as a L-cysteine chelate, with the bridging S now assigned to the cysteine sulfur [4]. The Britt group and collaborators now model the synthon as a $(CO)_2(CN)(cys)Fe(II)$ moiety, raising the interesting possibility that the azadithiolate bridge may be sourced from the cysteine of the synthon.

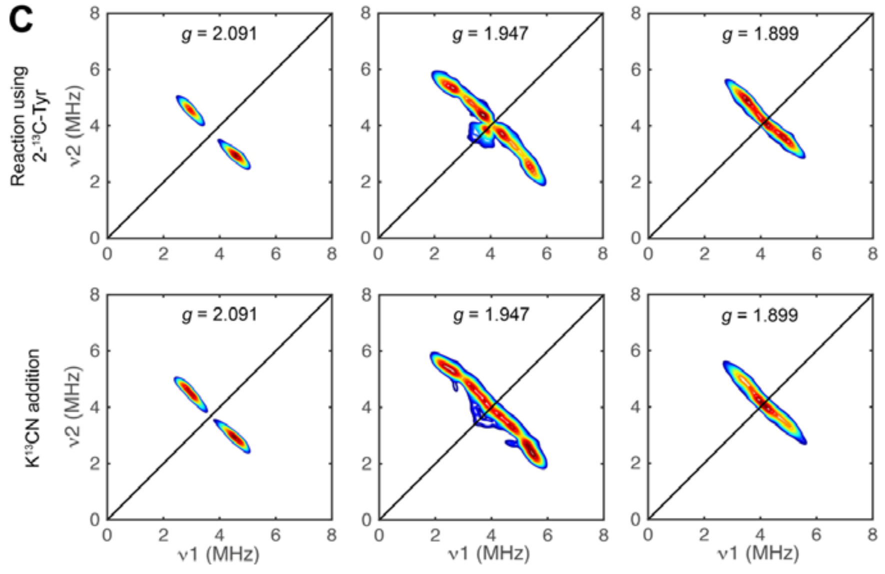

Figure: Comparison of ^{13}C HYSCORE features of HydG treated with ^{13}CN [3] with the spectrum obtained after 20 min reaction time with ^{13}C tyrosine, showing that a CN bound [4Fe-4S] center is created in the HydG reaction, releasing a $(CO)_2(CN)$(l-cysteine)Fe(II) complex as an H-cluster assembly intermediate.

1. Kuchenreuther, J.M., Myers, W.K., Stich, T.A., George, S.J., NajatyJahromy, Y., Swartz, J.R., Britt, R.D. **2013** A Radical intermediate in tyrosine scission to the CO and CN⁻ ligands of FeFe hydrogenase. *Science* 342: 472–475.
2. Kuchenreuther, J.M., Myers, W.K., Suess, D.L.M., Stich, T.A., Pelmentschikov, V., Shiigi, S.A., Cramer, S.P., Swartz, J.R., Britt, R.D., George, S.J. **2014** The HydG enzyme generates an $Fe(CO)_2(CN)$ synthon in assembly of the FeFe hydrogenase H-cluster. *Science* 343: 424–427.
3. Dinis, P., Suess, D.L.M., Fox, S.J., Harmer, J.E., Driesener, R.C., De La Paz, L., Swartz, J.R., Essex, J.W, Britt, R.D., Roach, P.L. **2015** X-ray crystallographic and EPR spectroscopic analysis of HydG, a maturase in [FeFe]-hydrogenase H-cluster assembly. *Proc. Natl. Acad. Sci. U.S.A.* 112: 1362–1367.
4. Suess, D.L.M., Burstel, I., De La Paz, L., Kuchenreuther, J.M., Pham, C., Cramer, S.P., Swartz, J.R., Britt, R.D. **2015** Cysteine as a ligand platform in the biosynthesis of the FeFe hydrogenase H-cluster. *Proc. Natl. Acad. Sci. U.S.A.*, 112: 11455–14460.

Harry Kurreck (1932–2015)

Sadly we have to communicate that on September 6, 2015 Harry Kurreck passed away, after a courageous battle with serious illnesses, at the age of 82. His friends and colleagues of the international science community grieve for him; they have lost an outstanding scientist, an admirable human being, a charming and dedicated friend. With his family we share the mourning for him.

The Kurreck family originates from East Prussia and has Polish roots. In quest of work, Harry's father together with his mother moved west and found a job in Halle (Saale), 175 km south-west of Berlin. In Halle Harry was born as their first son on December 18, 1932. Soon after, the family moved to Berlin and two more brothers of Harry were born. A drastic occurrence was, of course, the beginning of World War II in 1939. Harry's father served as a soldier in the German Army (Wehrmacht), first in Poland and then in Russia, from where he did not return. For five decades Harry was convinced that his father was killed in action during the battle of Stalingrad. Only after the Fall of the Wall, 1989, he learned that his father had died as prisoner of war.

When the Allied aerial attacks of Berlin became terrifying, Harry's mother left Berlin with her sons and moved back to Halle. This refuge turned out to be only of short duration: Harry was expelled from school because of "misconduct", violating Nazi guidelines. Harry's mother decided to return with her sons to Berlin despite the hail of bombs. Harry went to school in Berlin, acquired his high school diploma (Abitur) in 1953 and started to study chemistry, first at the Technical University (TU) and later at the Free University (FU) of Berlin. In 1960, he finished his Diploma in Chemistry, and only two years later, a true record at FU Berlin, he received his doctoral degree (Dr. rer. nat.) with Professor Waldemar Broser at the Institute of Organic Chemistry. He habilitated in Organic Chemistry in 1970 with a topic on paramagnetic cyclopentadienyl compounds, for which to characterize he intensively used EPR spectroscopy. Soon after he became Professor at the Chemistry Department of FU Berlin.

In the following years Harry cultivated intensive contacts to Polish, Israeli, American, English, Russian and Swiss scientists. In particular, he appreciated Fabian Gerson, a colleague and friend from Basel, who was one of the leading scientists working on EPR spectroscopy of organic radicals. Gerson was a Polish Jew who had lost his parents and sister in the Nazi concentration camp of Treblinka, but he survived in the Buchenwald camp. After his experiences during the Nazi years, he vowed never to step on German soil again. Self-evidently, Harry fully understood this attitude. But, after some years, his friendship with Harry motivated Fabian Gerson to visit Berlin and also some other places in Germany, which he considered now as an accepted member country of Europe. Harry was very happy about this, for him this was in line with his deep conviction that for his generation the trauma of World War II could only be healed when national insularity will be replaced by the idea of a united Europe.

In 1955, as a freshman in his studies, Harry Kurreck organized a chemistry students' ball at FU Berlin. There he met two attractive young ladies, close friends of each other, who would have a great impact on his future life. One of them was Babette, the other Marianne. Babette became his wife, and both enjoyed a happy marriage. In 1969 their only son, Jens, was born. To Harry's and Babette's delight Jens was an excellent student in high school. There he developed, in addition to his love for philosophy, a strong interest in chemistry and biochemistry. He is now Professor for Applied Biochemistry at the TU Berlin. Naturally, Harry was very glad to see that Jens got strongly involved in natural and artificial photosynthesis, the strongholds of his father. Hence, it was a dream for both of them to publish a joint paper on the strategies of structure-function optimization for biological and synthetic photosynthetic cofactors (see J. Kurreck, D. Niethammer, H. Kurreck, *Chemie in unserer Zeit* 1999, **33**, 72). During the last three years, Harry devoted most of his time, as an elixir of life, to assist his son in finishing his book on *Molecular Medicine* (Wiley, to be published December 2015). Until his last days he had read each single chapter, edited it and critically discussed it with his son. Sadly, he did not live long enough to see the book published.

Harry liked to go on long bicycle tours with Babette, even more so after his formal retirement. Both enjoyed the cultural life of Berlin – in particular after its reunification 1989 – which offers so much for connoisseurs of classical music and theater. For many years, Harry owned a sailboat and went out quite regularly with his family, or with friends and colleagues, on Lake Wannsee during the summer months. In good summers, this hobby reduced somewhat his presence at the Institute. Once, some of his co-workers bought him a metal plate saying "... I'd rather be sailing", and nailed it on his door at the Institute. Fortunately, Harry took it in the right spirit – he always loved to hear and tell good jokes – and invited those co-workers to join him on his boat. Such sailing turns, with on-board meals and drinks, were enjoyed also by a number of EPR spectroscopists from all over the world, for example Gus Maki, Hans van Willigen, Chris Winscom, Martin Plato, Burkhard Kirste, Wolfgang Lubitz, Klaus Möbius, just to mention a few (see Fig. 1).

Harry's family fortune lasted for more than 40 years – until Babette's much too early death in 2004. For Harry as a widower a desperate period of loneliness followed – in spite of all the attempts of his son and grandsons to cheer him up. But then, Harry had a reencounter with Marianne in 2005, Babette's dear friend from the 1955 chemistry students' ball, now a widow. Not much later they married and lived happily together in Harry's house in Berlin-Zehlendorf, for the almost 10 years that were still granted to him.

A particularly important role in Harry's life played his two grandsons, Paul (born 1995) and Malte (born 2001). They entered the scene just in time when Harry's professional duties and burdens started to slow down, i.e., when he retired in 1997. The grandsons really made him a different human being. While previously he was always in a rush, focused on his scientific work, suddenly he could watch for hours his grandchildren's sleep, spent hours to play with them or served as a chauffeur to drive them to their sports exercises. As if to make up for the lost time he could not spend with his son Jens because of his professional duties and pleasures. Having said this, one has to mention that Harry always wished for a daughter or a granddaughter. All the more he was happy to learn from Jens, in 2015, that soon a granddaughter will be born. Sadly, he could not live long enough to see her born (little Laura was born on October 8, 2015, one month after Harry's death).

Figure 1: Harry Kurreck sailing on Lake Wannsee with Wolfgang Lubitz among his guests. Photo by Gus Maki.

Harry stayed at the FU Berlin during his whole career, presumably because of strong family ties, his love of the city of Berlin, the very good scientific and cultural environment and the intensive interactions with his friends and colleagues in Berlin – in particular in the Physics Department. Harry's excellent research projects have always been strongly supported by external grants, especially from the Deutsche Forschungsgemeinschaft (DFG) and the Volkswagen (VW)-Stiftung, which made his group largely independent of the notorious budget problems of his Department. For example, his group was an important member of the DFG Collaborative Research Center (Sonderforschungsbereich) "Energy and Charge Transfer in Molecular Aggregates" (1987–1999) and of the VW-Priority Initiative "Intra- and Intermolecular Electron Transfer" (1993–2001).

Organic and bioorganic radicals and triplet states have been Harry's main interest throughout his scientific life. The method of choice to study such systems is EPR spectroscopy. He regularly taught EPR spectroscopy and offered laboratory-training courses and, thus, got many students interested in this field. Harry's lectures have always been a delight to attend; they were vividly and clearly presented and included the latest scientific results. He invested a lot of his time tutoring his students and was, therefore, one of the most popular professors in the Department. No wonder that many students – and often the best in a course – later decided to join his research group.

In the early 1970s, Harry got fascinated by the exciting, then new, liquid-state ENDOR technique, which was pioneered by Jim Hyde and Gus Maki in USA. Excellent ENDOR-in-solution instrumentation had been built up during the seventies and further developed (e.g., to electron-nuclear-nuclear TRIPLE resonance) in the group of Klaus Möbius in the Physics Department of FU Berlin, together with his doctoral students Peter Dinse and Reinhard Biehl, and his senior co-worker Martin Plato. These methods allowed resolution of the hyperfine couplings – including their signs – even of very complicated and asymmetric radicals. Harry rapidly recognized the power of this method for the large molecular complexes he was synthesizing to overcome the serious limitations of single-resonance EPR. He managed to acquire grants for the advanced instrumentation necessary for doing ENDOR/TRIPLE in solution. This heralded very fruitful decades of cooperation between the Kurreck and the Möbius groups during which many different types of radicals were studied under high resolution conditions using ENDOR/TRIPLE not only for proton nuclei, but extending it to carbon-13 and a variety of other magnetic non-proton nuclei. During this period, Harry's highly original work on sterically crowded radicals, on organic multi-spin systems, on radicals in anisotropic media like liquid crystals and micelles, on flavin radicals *in vitro* and in enzymatic systems as well as on porphyrin and chlorophyll complexes, were milestones in the field. Most of this work was included in the highly cited monograph *Electron Nuclear Double Resonance Spectroscopy of Radicals in Solution. Application to Organic and Biological Chemistry* by H. Kurreck, B. Kirste, W. Lubitz (Wiley, 1988). This book is now considered a standard text in the field.

Prompted by the crystallization of the photosynthetic reaction center in the early 1980s and the enhanced research activity in the field of natural and artificial photosynthesis, Harry became interested in biomimetic model systems for

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Figure 2: First Joint Symposium Novosibirsk-Berlin, September 1989. First row from left to right: Elena Kluchevskaya, Elena Bagryanskaya, Renad Sagdeev, Klaus Möbius, Yuri Molin; second row: Sergei Dikanov, Yuri Grishin, Wolfgang Lubitz, Jenny Schlüpmann, Alexandra Yurkowskaya, Hans-Martin Vieth, Andrei Koptyug, Olaf Burghaus; third row: Anatoly Obynochny, Petr Purtov, Valery Tarasov, Yuri Tsentalovich, Martin Plato, Igor Koptyug, Petr Borbat, Petra Jaegermann, Nikolay Lavrik. Photo by Harry Kurreck.

Figure 3: Stopover in Kazan with Klaus Möbius, Harry Kurreck, Dietmar Stehlik among Kev Salikhov's EPR guests. Photo by Wolfgang Lubitz.

light-induced electron transfer. He embarked on the investigation of the multistep electron-transfer routes in covalently linked porphyrin-quinone dyads, triads and tetrads, which mimic the photosynthetic chromophore chains. His ambitious goal was to develop strategies for synthesizing porphyrin-quinone donor-acceptor model complexes with high quantum yield of light-driven charge separation. In order to mimic membrane properties of the native systems, spectroscopic measurements were not only performed in isotropic solutions, but also in liquid crystals, reversed micelles, and Langmuir-Blodgett films. His group systematically synthesized a large number of novel porphyrin-spacer-quinone donor-acceptor systems with various spacer groups. In this field, the X-band cw-EPR and -ENDOR techniques available in his laboratory turned out to be very helpful. However, other spectroscopic studies, in particular time-resolved EPR at various Zeeman fields (e.g., W-band EPR at high magnetic field (95 GHz, 3 T) and fast pulsed-laser spectroscopy, were required to fully characterize the compounds and elucidate the light-induced electron-transfer pathways. The spectra of the spin-polarized transient radical pairs and triplet states generated in the pulsed light-driven reactions turned out to be most informative in this respect. This work, which was carried out together with several collaborating groups inside and outside Germany, was thoroughly reviewed in a widely-cited article Harry had written together with Martina Huber (H. Kurreck, M. Huber, *Angew. Chem. Int. Ed. Engl*. 1995, **34**, 849). It is certainly fair to say that in the 1990s Harry's group was at the forefront of research in this field worldwide. On the occasion of his 65th birthday a special issue of *Applied Magnetic Resonance* (vol. 13, 1997) was published with many contributions of his scientific colleagues and friends. His achievements were adequately recognized by the International EPR (ESR) Society by honoring Harry Kurreck to become Fellow of the Society in 2003.

Harry Kurreck has co-authored over 120 publications in scientific journals. And the list of his invited lectures is exceedingly long. Many of Harry's frequently cited articles paved the way for other groups working in the field. It gave him great pleasure when, in 2015, he co-authored his last publication in cooperation with colleagues from the Hebrew University of Jerusalem. The paper describes time-resolved EPR spectroscopy on photoinduced electron transfer in Pd porphyrin–quinone and Zn porphyrin–quinone dyads with a cyclohexylene spacer (M. Perchanova, H. Kurreck, A. Berg, *J. Phys. Chem. A* 2015, **11**, 8117). The publication appeared in July 2015, two months before his death.

During his scientific career Harry has worked together with many groups around the world. His collaborations with Hans van Willigen from Boston, Haim Levanon from Jerusalem, Jack Fajer from Brookhaven and Les Sutcliffe from Liverpool had a large impact on his work and social life. The longest and most fruitful collaboration, however, was that with Klaus Möbius and his co-workers from the Physics Department of FU Berlin, especially Martin Plato. It was based on a long-standing personal friendship between Harry and Klaus. Both have shared several students who profited from the interdisciplinary work early in their careers. Here, in particular Wolfgang Lubitz and Martina Huber have to be mentioned. Harry Kurreck's open-minded approach to collaborations with many other groups from physical and inorganic chemistry, biochemistry, physics and biology is indicative for his truly interdisciplinary approach to solve complex scientific problems. This philosophy has affected and inspired many of his students and collaborators.

Harry loved to participate in international conferences and symposia dedicated to magnetic resonance spectroscopy on radicals and triplet states in (bio)organic chemistry. To such conferences he was often invited as a plenary speaker, for example at Gordon Conferences on Free Radicals or at Conferences on Photochemistry and Solar Energy Conversion. He took great delight in meeting many of his co-workers and cooperation partners there – where he could find the time and leisure to discuss with them in detail. In this respect, the meetings were peaked by the "10th International Conference on Photochemical Conversion and Storage of Solar Energy" in Interlaken (Switzerland), July 24–29, 1994 (see H. Kurreck, S. Aguirre, S.N. Batchelor, H. Dieks, J. v. Gersdorff, C.W.M. Kay, H. Mößler, H. Newman, D. Niethammer, J. Schlüpmann, J. Sobek, M. Speck, T. Stabingis, L. Sun, P. Tian, A. Wiehe, K. Möbius, *Solar Energy Materials and Solar Cells* 1995, **38**, 91). The Interlaken Conference was organized by Gion Calzaferri, and he had invited H. Kurreck and K. Möbius to chair one of the four workshops ("Electron transfer in photosynthesis and biomimetic model compounds, magnetic resonance studies").

Among the many meetings Harry liked so much was also the "First Novosibirsk-Berlin Joint EPR Symposium on Applications of Magnetic Resonance in Physics and Chemistry" that took place in Akademgorodok (Novosibirsk) in early September 1989 (see Fig. 2). We had organized the Symposium together with Renad Sagdeev, Yuri Molin and Kev Salikhov from the Siberian Branch of the USSR Academy of Sciences with whom the EPR groups at the FU Berlin had a long-standing co-operation and friendship. When Kev Salikhov left Akademgorodok to become Director of the Zavoisky Physical-Technical Institute in Kazan, our cooperation smoothly expanded to a menage a trois. Still at the time of the Cold War, amidst all these frictions and hurdles piled up by the ideologists and bureaucrats, we frequently arranged mutual laboratory visits. This is still continuing until today. On September 1, 1989, a number of senior and graduate student members of the Berlin groups embarked on trains and planes to travel to Siberia, with extended stopovers in Moscow, Novosibirsk, Kazan and Leningrad, where the "Berliners" were always kindly tutored by the local EPR colleagues, thereby providing a platform for many Perestroika inspired discussions (see Fig 3).

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Remember that September 1, 1989, was the 50th anniversary of Nazi Germany's invasion of Poland marking the beginning of World War II. While crossing the borders from the German Democratic Republic to the People's Republic of Poland, and from there to the Soviet Union, we shared with our fellow train travelers – Poles, Russians, East Germans – our feelings how lucky we were that currently – in spite of (or because of) the existing Iron Curtain – no war was sweeping Europe, and how much we hoped that the Cold War would never turn into a hot one. Nobody was able to foresee that only two months later the Berlin Wall would peacefully fall, and with it the Iron Curtain. For Harry – as for many of us living in Berlin – this was a great event in our lives. It also opened vast opportunities not only for scientific exchange and cooperation between East and West, but also to foster existing and to open new personal friendships. We felt that the concept of a common European home got a chance for a new beginning.

Despite the disappointing political developments during the last few years, which discredited the idea of a European home so brutally, Harry did not lose his conviction that, in the long run, there is no meaningful alternative to the idea of a united Europe. He liked to quote Jean-Claude Juncker, President of the European Commission: "Those who question Europe or despair about Europe should visit military cemeteries." How much poorer the international science community became without such an outspoken colleague like Harry Kurreck!

Klaus Möbius,
Wolfgang Lubitz

Katharina Pirker (1977–2015)

In mourning we have to announce that our colleague and friend Dr. Katharina Pirker passed away on September 28, 2015 at the age of 37 years. Despite of her young age Kathi was already well known and integrated in the EPR community within Europe. She studied Technical Chemistry at the Vienna University of Technology with focus on analytical and physical chemistry (1997–2002). During her master thesis she spent 3 months at the Scottish Crop Research Institute in Dundee, Scotland, and learned the basics of cw-EPR in combination with spin trapping under the supervision of Bernard Goodman. Already in her PhD thesis (2003–2005) EPR was the central method for answering mechanistic questions about free radical formation during oxidation of some plant and fungal tissues and naturally-occurring phenols.

After her PhD, Kathi started a post-doctoral position at the Austrian Institute of Technology (AIT) and very soon succeeded in getting her first stand-alone project funded by the Austrian Science Fund (FWF): "Free radical chemistry of phenolic compounds investigated by electron paramagnetic resonance (EPR) and related spectroscopic techniques". The main topic of the FWF project was the investigation of oxidation mechanisms in green tea polyphenols (GTP). This included alkaline autoxidation, oxidation by superoxide anion radicals and hydroxyl radicals, *in-situ* electrochemical oxidation as well as the reaction with metal ions, i.e. Cu(II), and DFT calculations of GTPs. Finally, from November 2009 until August 2011, she spent a post-doctoral period in the group of Dr. Christopher Kay (Institute of Structural and Molecular Biology, UCL, London, UK), funded by an Erwin Schrödinger fellowship from FWF. Here she learned the technique of site-directed spin labelling in combination with cw and pulsed EPR spectroscopy for the structural elucidation of proteins. In addition Kathi participated in the organisation of four EPR workshops (including lecturing) with the focus on spin labelling and spin trapping in combination with cw and pulsed EPR spectroscopy. At UCL Kathi was also involved in the reorganisation of a new EPR lab. Back in Austria she joined the group of Christian Obinger at the Department of Chemistry at BOKU – University of Natural Resources and Life Sciences in 2013 and installed the first cw EPR machine at this university. Very soon she was granted with a Hertha Firnberg fellowship by FWF ("Pulsed EPR of the dynamics of catalytic amino acids in heme proteins") and in addition succeeded in getting financed the first Q-band pulsed EPR machine in Austria. This opened an incredible prospect to her and she was very enthusiastic and full of novel ideas and concepts for future projects. At this time she was already well integrated in the EPR community (co)author of 35 SCI publications.

Last August 2014 during a meeting in Zürich she was happy and proud of announcing to await her first baby and already started to think about compatibility of profession and family. A few months later Kathi got the diagnosis of cancer. In order to allow medical treatment she had to give birth to her baby prematurely. Despite of her strength and optimism she lost the fight against her disease and died on September, 28 in Vienna. We have lost an endearing colleague and friend as well as an excellent scientist. We commiserate with her nine months old daughter and her husband.

Christian Obinger

When the news of Katharina Pirker's passing away reached my lab, we were devastated. In the framework of her Hertha Firnberg fellowship, Katharina (Kathi) had started collaborating with us on EPR of chlorite dismutase and had visited my lab at different occasions. Not surprisingly, we all felt very bad, when Kathi received in 2014 the terrible news that she had cancer. However, Kathi remained very positive about the future, and even helped in writing a new grant application on our mutual work. She was also extremely happy that the premature birth of her little daughter, Mylène, went fine and that the baby was doing so well. Every e-mail of Kathi contained a new sparkle of hope. All her positive updates had made us believe and hope that she would pull through and beat the cancer. Sadly, it was not to happen. We will miss Kathi a lot and will remember her as a positive, optimistic and kind woman and a hard working and good scientist. And who knows, perhaps one day, Mylène will become a scientist too and will even be able to read and understand her mother's scientific papers.

Sabine Van Doorslaer


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Krakow, Poland, October 2–6, 2016

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If you are planning to attend, please email jthelane@mcw.edu
More information coming soon!

The 49th Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry
University of Essex, Colchester, UK, April 3–7, 2016
www.esr-group.org/conferences/2016-conference-essex

Together with the Bruker Corporation, we are also pleased to announce the 2nd Bruker ESR Thesis Prize, set up to recognize outstanding work by PhD students in the field of ESR Spectroscopy. The winner will give a prize lecture at the above conference. All expenses will be covered.
Contact: svist@essex.ac.uk

Asia-Pacific EPR//ESR Symposium 2016
Irkutsk, Russia, August 28 – September 2, 2016
www.apes2016.org

Asia-Pacific EPR/ESR Symposium aims at covering all subareas of EPR/ESR. Contributions dealing with any aspects of recent developments and applications in the theory, applications, methodology, instrumentation and experimental techniques are invited (CW EPR/ESR, pulsed EPR, high frequency and high field EPR, ENDOR, PEDLOR/DEER, time resolved EPR, FMR, MRI, CIDEP, ODMR). Scientific program of the Symposium will include plenary lectures, invited and contributed talks and poster sessions.
Abstract submission will be open February 1, 2016. Please find the Abstract preparation guidelines on the website of the conference
Contact
Dr. Dmitriy Polovyanenko – Secretary
e-mail: apes2016@nioch.nsc.ru
tel: +7 (383) 330-96-61

Xth EFEPR 2016 Conference
Torino, Italy, September 4–8, 2016
www.efepr2016.unito.it

Topics
– EPR of organic and inorganic systems
– Advanced materials
– Biophysical, biochemical and biomedical applications
– DNP and emerging applications of EPR
– Emerging techniques and methodologies
– EPR Imaging and Microscopy
– Spin Trapping and Spin Labeling Chemistry
– Theoretical Chemistry and EPR
Preliminary Information
The Conference will consist of 7 plenary lectures, 10 keynotes, 30 oral communications and 2 poster sessions.
Instruction for abstract submission and information concerning the conference will be available soon on the official website.
Important dates
– March 1, 2016: Second circular
– April 1, 2016: opening of Abstract submission
Contact: efepr2016@unito.it

A Celebration of the Life and Scientific Contributions of Harden M. McConnell

Harden McConnell sadly passed away on October 8, 2014 after many seminal contributions to chemical physics, biochemistry, immunology with particular applications of theory and experiments using magnetic resonance. A symposium to celebrate his life was held on April 18th at Stanford University's Department of Chemistry. The symposium which is described below was informal and was designed more for past students, post doctorates, visiting faculty and colleagues to be able to socialize and reminisce. The talks highlighted key people from his Caltech days, then Stanford and then his later commercial ventures in Palo Alto, ending with the last graduate student who studied with him.

The program was organized by Stanford colleague Steven Boxer, also a collaborator, and Keith hodgson, department chair, both of whom cherished Harden as a colleague and mentor. Two early students/post doctorates from the early days at Caltech, Alvin Kwiram (emeritus, University of Washington) and Hayes Griffith (emeritus, University of Oregon) covered his scientific biography and some of his early contributions that both were involved in, which covered chemical physics and ESR/EPR. A key aspect that they and all of the following speakers emphasized was McConnell's approach to important scientific problems and some seminal work and predictions that have stood the test of time and were many times proven experimentally many decades later. Every speaker related personal anecdotes that 'rang true' and brought back fond memories to all of us who worked for him.

Brian Hoffman, northwestern university, covered the Caltech group that moved to stanford and the subsequent transition from chemical physics to biology. Wayne Hubbell, UCLA, and Nobel laureate Roger Kornberg, Stanford, covered the research in the membrane area and new avenues of their own research that was inspired by their education from McConnell.

A colleague/collaborator, Mark Davis (Stanford) discussed work in the areas where he copublished papers with McConnell. Sarah Keller, University of Washington, described her postdoctoral experience at stanford and how that impacted her current work. Gillian Humphries started as a transfer student from San Jose State University, where she commented about Harden's sensitivity and intuition in taking her on as a student, then a postdoc, then a research associate and then helping McConnell to start Molecular Devices with three other postdocs. The talk was impressive, amusing and a reconfirmation of his McConnell's unique abilities and insights. Lastly, Arun Radhakrishnan (UT Southwestern) discussed his experiences as one of McConnell's graduate students in the late 1990s after which McConnell retired from Stanford. McConnell nonetheless continued to be productive writing several insightful papers until his last days in his Atherton home. His lifetime publication output averaged 9 papers per year, all of which were seminal, some only two pages long.

The attendance was impressive, with over 100 friends, students and colleagues. From his Caltech days, J. D. Roberts and Sunney Chan, were amongst some of the people attending. Seiji Ogawa, Stanford PhD, came all the way from Tokyo to spend this day with us.

For the author of this report, who had the unique honor of being one of McConnell's first two graduate students in the 1960s, it was fantastic to meet with several past students and postdocs who I hadn't seen in many decades. The group proposed a McConnell lecture at Stanford which they fully funded in less than 2 months from officially launching it, which is a record for Stanford and reflects the great respect and dynamics of the McConnell group.

The most rewarding experience was meeting his wife, Sophia, and their three children at the meeting. The day ended with a reception and subsequent optional dinner at a local restaurant. The next day a handful of us met for brunch to discuss future plans and objectives to celebrate our fantastic leader. As Brian Hoffman astutely reminded us, we have possibly to 2 to 3 lives in our existence on this Earth: our own birth that we had no control about; if we marry a family that we might create; and sometimes, albeit more rare, a professional life and family from a unique mentor, namely Harden M. McConnell, who we were fortunate enough to have experienced part of our lives with and who still inspires us,

Larry Berliner
PhD, 1967, Stanford University
Immediate Past President, IES

The 3rd Awaji Island International Workshop on Electron Spin Science & Technology: Biological and Materials Science Oriented Applications (AWEST2015)

Awaji Island, Hyogo, Japan, June 14–17, 2015

The 3rd Awaji Island International Workshop on Electron Spin Science & Technology: Biological and Materials Science Oriented Applications, AWEST2015, was held on June 14–17th, 2015 at Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan.

The AWEST has been organized in mid-June every year at the same venue, Awaji Island since 2013. The aim of the AWEST is to provide an international/global forum for discussions of interdisciplinary issues on electron spin science/technology relevant to open shell systems/compounds and electron-mediated phenomena to biologists, chemists, materials scientists, physicists and other scientists with both academic and industrial backgrounds. Particularly, the AWEST fo-

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cuses on methodological developments of molecular electron spin science as well as biological/materials science oriented applications of electron spin science/technology. The AWEST also places emphasis on syntheses of novel open shell compounds with exotic applications and quests for novel functionalities of open-shell systems as diverse as possible; structural biology/biological science, materials and polymer science/engineering, organic/inorganic chemistry and physics.

A style of the AWEST is quite an intensive and short-term meeting. In the AWEST, graduate students are strongly encouraged to present their research work. Particularly, the 3rd AWEST invited graduate students from India and Taiwan.

The 3rd AWEST started with 2-min. flash talks by all the poster presenters. The session was co-chaired by overseas invited speakers, Dr. Maxie Roessler and Prof. Juergen Schnack. The first opening talk was given by the current IES President, Prof. Hitoshi Ohta. The President introduced some activities of the IES as well as his research topics on high-frequency/field THz-ESR spectroscopy. In the following two days, various topics were presented: dynamic nuclear polarization, photochemistry of the Photosystem-II and photo-excited organic compounds, magnetic field effects, molecular magnetic materials, molecular spin quantum computing, biological compounds such as protein, enzyme, hydrogenase/dehydrogenase and the others. The AWEST covered widely spread scientific fields with a variety of measurements such as cw/pulse ESR/ELDOR spectroscopy, time-resolved ESR spectroscopy, neutron scattering and Raman spectroscopy in their highly advanced scheme. The total number of the participants was 92 from 10 countries, including 33 overseas participants.

The AWEST places emphasis on giving International Awards to young researchers for their excellent poster presentations. In addition to Springer Award, this year the IES kindly prepared IES Poster Awards. The president Ohta delivered the IES Poster Awards by hand at the ceremony. The AWEST International Poster Awards went to Ms. Mizue Asada (Nagoya Univ.) for Springer Award, and Mr. Tsubasa Okamoto (Kobe Univ.) and Mr. Takeshi Yamane (Osaka City Univ.) for the IES Awards under the review by Award Committee whose members were the 24 overseas invited speakers.

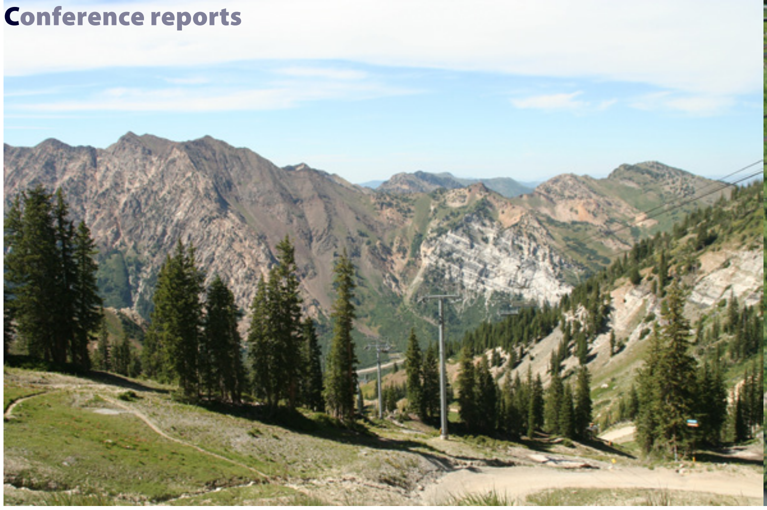
On June 17, there was a conference excursion to 1993 ENESCO World Heritage site, Himeji Castle, Himeji, Hyogo. The Himeji Castle is nicknamed "Shira-sagi (White Heron)" castle built in 1609. The Himeji Castle has been just reopened after major renovations.

In next mid-June (June 19–22, 2016), we organize the 4th Awaji Island Conference (AWEST2016) at the same venue. We look forward to welcoming you from many countries and giving us your recent results relevant to electron spin science/technology. Awaji Island in the Gulf of Osaka is located near Kobe-Osaka, and it is convenient for overseas participants to access the venue from Kansai International Airport.

Kazunobu Sato
Executive Secretary, AWEST Secretariat
Professor
Department of Chemistry and Molecular Materials Science
Graduate School of Science
Osaka City University

Website: http://www.qcqis.sci.osaka-cu.ac.jp/awest/2015/

From left to right: Prof. Juergen Schnack (Universität Bielefeld, Germany), Dr. Maxie Roessler (Queen Mary University of London, UK), Mr. Takeshi Yamane (Osaka City Univ.), Ms. Mizue Asada (Nagoya Univ.), Mr. Tsubasa Okamoto (Kobe Univ.), Prof. Takeji Takui (Osaka City Univ.), Prof. Hitoshi Ohta (IES president & Kobe Univ.)



Panorama of the Wasatch Range in Utah, from above Snowbird Resort.

The Snowbird Tram takes riders to the peak at 11,000 ft (3,353 m).

57th Rocky Mountain Conference: 38th EPR Symposium

Snowbirth, Utah, USA, July 26–31, 2015

The EPR Symposium of the 57th Rocky Mountain Conference (RMC) was held outside of Colorado, for the first time, in 2015. We ventured down-range to the Snowbird Resort and Conference Center, in Snowbird, Utah. Ready travel access to the conference was enabled by the SLC Airport, outside of nearby Salt Lake City. The dioxygen content of the air at base (7760 ft , 3350 m) assured a relatively comfortable experience for all ages. Those who hiked or took the cable-car towards the summit were treated to spectacular views of the Little Cottonwood Canyon, which earned a reputation in the mid-19th century from silver mining, and the surrounding Wasatch Mountains.

The EPR Symposium ran "solo" at the 2015 RMC. This continued the trend of solo-EPR and conjoined EPR-NMR gatherings in alternate years, that started with the 2011 meeting. The number of registered attendees was 134, which was comparable to the solo cohort for the 2013 meeting, which took place in the traditional Denver setting. Thus, EPR spectroscopy and associated fields show promise for sustained presence, and growth.

The scientific program for 2015 demonstrated the vast scope of EPR spectroscopic and research-related applications, and was built around the following general topic areas, as organized by the session chairs: Biological EPR/Spin Labeling (Fraser MacMillan), Biological Macromolecules (John McCracken), In Vivo EPR and EPR imaging (Boris Epel), Materials (Christoph Boehme), Methods (including DNP) (Susumu Takahashi) and Spin Devices (Ania Bleszynski-Jayich). The program rolled-out over the Monday-Thursday, 3.5 day run-time, packed with a total of 63 speakers, of which 15 were invited. Attendees returned after dinner to view and discuss the 47 posters in spirited, high-decibel evening Poster Sessions. The seemingly disparate meeting topics – stretching from, for example, biological mechanism to spin devices – are united by the central role of the spectroscopy and physics of electron and coupled nuclear spins, and their chemical and materials manifestations, which provides for a fundamental language that ignites the interest of all members of the "EPR community."

Awards studded the proceedings. A special session was devoted to awards from the International EPR/ESR Society (IES), and was chaired by Steve Hill, IES Vice-President of the Americas. Eric McInnes received the Silver Medal in Chemistry, and presented a glowing talk, "Electronic structure of novel paramagnetic actinide complexes." Ilia Kaminker received the Young Investigator Award, and delivered an address, "CW and pulsed EPR study of complex coacervation of the mussel

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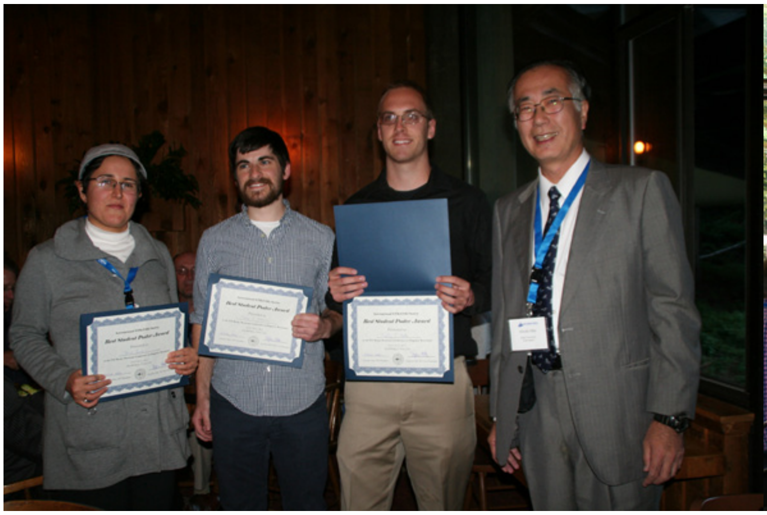
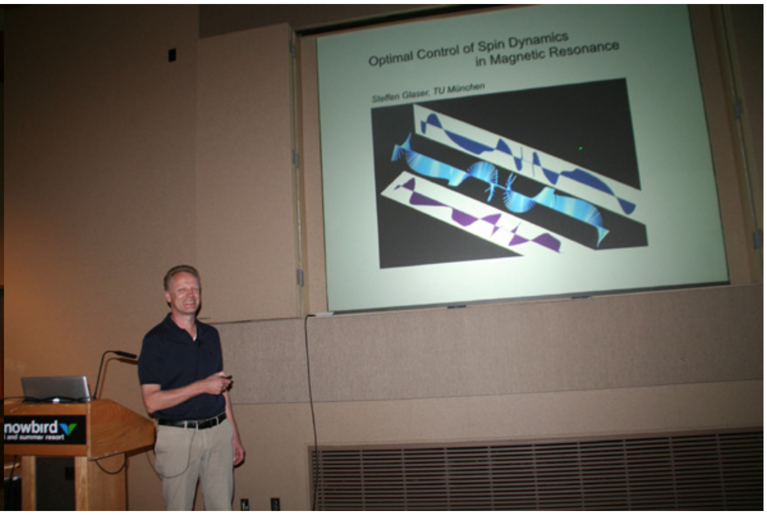


EPR Symposium Poster Award winners, following presentation by Professor Hitoshi Ohta, President of the IES. Left-to-right: Shirlin Jamali, Thomas Edwards, Timothy Keller, Professor Ohta.

EPR Symposium attendees enjoy a break for lunch at the Snowbird Resort.

Professor Tadeusz Sarna delivers the Piette Lecture.



Professor Steffen Glaser in control of the spin dynamics presentation.

foot protein inspired adhesives," that had attendees glued to the screen. The Lawrence Piette Lecture Award was introduced and presented by Sandra Eaton. Tadeusz Sarna delivered an illuminating Piette Lecture: "Melanin – An important biological pigment with unique physico-chemical properties." Vice Chair John Morton presided over the Poster Awards, which were sponsored jointly by the IES and RMC. Poster Award winners and categories were as follows: Thomas Edwards (EPR Methods; Stoll group), Shirin Jamali (Applications: Physics; Boehme group), and Timothy Keller (Applications: Biochemistry/Chemistry; Han group). In addition, seven graduate students and postdocs received Travel Stipend Awards toward attendance of the meeting (Hannah DeBerg, Joanna Guse, Bouchra Hajjaj, Ellen Hayes, Tom Keevers, Arthur Sikora and Umar Twahir).

Premium support of the EPR Symposium continued from Bruker Biospin and the National High Magnetic Field Laboratory (NHMFL). Art Heiss and the Bruker Biospin development group kicked-off the meeting activities on Sunday evening with the Bruker EPR User's Meeting, and the follow-up mixer and dinner. Other supporters included Avanti, Cambridge Isotope Laboratories, Medinox (Piette Lecture Award), National Science Foundation (NSF) and Wilmad/LabGlass. Exhibitors also included Active Spectrum, ADANI, Elsevier, and Millitech.

The RMC was followed by the inaugural Grand Challenge Workshop (GCW), chaired by Gary Gerfen. This one-day event was supported by the recently-funded, NSF collaborative research grant, "SHARED EPR Research – Supporting, Highlighting, and Advancing Recent Developments in EPR Research" (PI, Gary Gerfen). The GCW is an integral component of the SHARED EPR Research project. The EPR Symposium and GCW were tangibly tied together by overlap of invited speakers, and a large number of co-attendees. The chosen topic of the 2015 GCW was "EPR on a Chip." The seven research presentations, from leaders in the field of miniaturizing the magnetic resonance/spin detection experiment, focused on microchip design and fabrication, detection sensitivity, and spectral and spatial resolution.

The 2016 EPR Symposium will be chaired by John Morton, and co-chaired by John McCracken (rising chair for the 2017 EPR-solo meeting, which will be held in Denver). The 2016 EPR Symposium of the 58th Rocky Mountain Conference will be held on July 17–22, in concert with the solid-state NMR community. The venue will be the Beaver Run Resort and Conference Center, in Breckenridge, back in Colorado. See you there!

Kurt Warncke,
Chair, 2015 EPR Symposium
Scientific Committee

EPR Symposium participants engaged in an evening Poster Session.

Professor Gary Gerfen, chair of the Grand Challenge Workshop, introduces the SHARED EPR Network.

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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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Market place

POSITIONS

Cryogenic EPR Postdoctoral Position

A postdoctoral position is available immediately for a collaborative project between Professor Cory's lab at The Institute for Quantum Computing (IQC) and a local startup. The project uses superconducting resonators and Optimal Control Theory (OCT) to increase the sensitivity of pulsed electron spin resonance at cryogenic temperatures. The goal of the project is to also demonstrate applications to molecularly thin samples. This program is expected to reveal new and interesting results of EPR of biochemical processes.

The successful applicant should have an advanced degree (PhD) in chemistry, biochemistry or physics with significant experience in EPR of biomolecules.

The appointment will be for two years with the possibility of renewal. The salary is competitive and commensurate with experience, ranging from $55,000 to $70,000. Women and minorities are encouraged to apply.

Apply to grum.teklemariam@highqlp.com.

Postdoctoral Position Microresonators for EPR Technische Universit?t Dortmund

A postdoctoral position is available at the Technical University of Dortmund for a motivated and qualified scientist who is interested to continue the development of miniaturized resonators for EPR. These microresonators are optimized for detecting small samples (down to the nanometer range) with high sensitivity. Candidates should have a firm background and proven track record in the field of magnetic resonance and an interest in numerical simulations of the resonators.

The development of these resonator is a central project in the priority program 1601 of the DFG "New Frontiers in Sensitivity for EPR Spectroscopy: From Biological Cells to Nano Materials" (http://spp1601.de): the resonators are developed in Dortmund and shared with other members of the SPP for a range of different applications.

Additional information on the project is available at http://e3.physik.uni-dortmund.de/~suter/research/EPR_Microresonators.pdf

Applications and requests for additional information should be sent to Dieter.Suter@tu-dortmund.de

Research Scientist (Postdoctoral associate)

The Institute of Macromolecular Chemistry AS CR, v.v.i. seeks a postdoctoral associate / research scientist to join the Laboratory of electron paramagnetic resonance of polymer systems (EPR)

Requirements: University degree and PhD in the field of chemistry, physical chemistry or physics / Practical experience with the method of electron paramagnetic resonance (EPR) / Knowledge of and working experience with polymers and EPR imaging will be an advantage / Stays abroad will be an advantage / Good knowledge of English language / Good publication activity / Independence, reliability. Details about research work can be obtained from RNDr. Petr Štěpánek, DrSc., stepanek@imc.cas.cz

Candidates should submit a structured CV emphasizing experience relevant to the advertised position, a motivation letter and a list of publications and other results to e-mail: fencl@umch.cz HR department tel. (420) 296 809 385.

Available: Used EPR Spectroscopist

Old, but well maintained EPR Spectroscopist, with wide application experience, seeks opportunity to support active research group. EPR- based publications over 5 decades, most recently 2011, mass spectrometry publications to 2014. Experience in the study of transient organic and organometallic free-radicals; transition metal complexes; spin-trapping; spin probe; radical ions; matrix isolation and γ-radiolysis techniques; photocatalysis; polymer degradation and stabilisation etc. Has Bruker, Varian and JEOL operating experience, plus track record in NMR and mass spectrometry techniques. Would prefer to work in biochem/biological area, but would consider anything interesting. Opportunity arises due to restructure of Research Department in Australian steel company after 26 years faithful service. Excellent grant writing skills, 100% success rate. Speaks English, German and some French.

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

Postdoctoral Associateships in Magnetics at NIST

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

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.

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

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Wanted: Badly needed certain parts of, or even a complete Bruker X-Band microwave unit from the mid-seventies, the one which came with the Bruker B-ER 420 system. Particularly, the klystron heating and protection board, B-E-Z 10. Please contact Prof. Dr. Wolfgang E. Trommer, Department of Chemistry, TU Kaiserslautern, P.O.Box 3049, D-67653 Kaiserslautern, Germany. E-mail: trommer@chemie.uni-kl.de.

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

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

Design and construction of EPR electronics

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 kHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field-control units to 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

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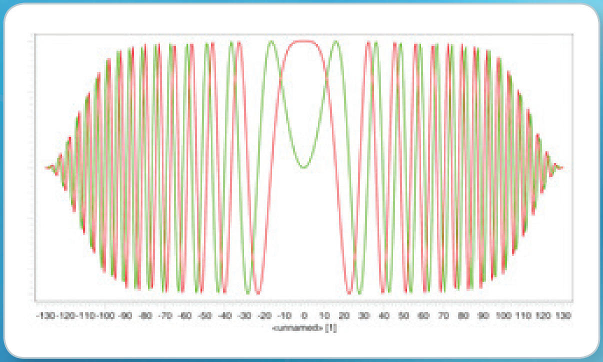

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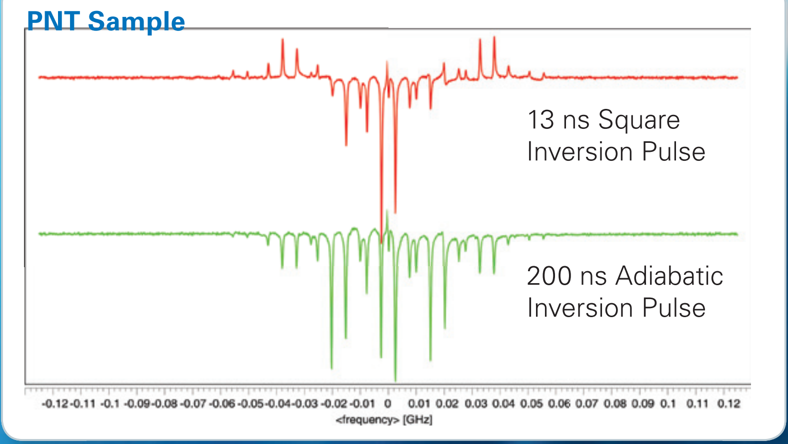

Angew. Chem. , P. E. Spindler, S. J. Glaser, T. E. Skinner, T. F. Prisner, v52, p3425, 2013

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