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The Publication of the International EPR (ESR) Society

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

Asia-Pacific

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

Europe

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

SECRETARY

Sushil K. Misra
Concordia University,
1455 de Maisonneuve Boulevard West,
Montreal (Quebec), H3G 1M8, Canada
phone: 514-848-2424 ext. 3278, fax: 514-848-2828
e-mail: skmisra@alcor.concordia.ca
web: physics.concordia.ca/faculty/misra.php

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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Institute of Multidisciplinary Research for
Advanced Materials (IMRAM),
Tohoku University,
Katahira-2-1-1,
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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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Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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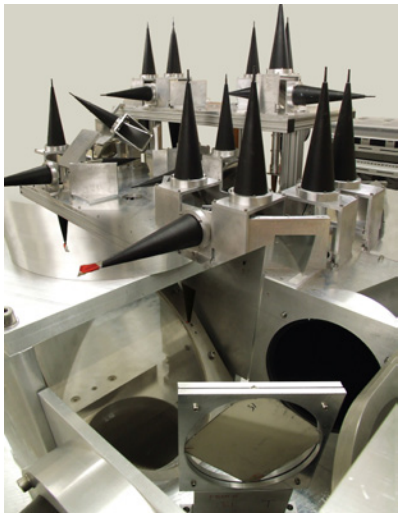

The cover picture illustrates part of the 1 kW W-band pulse EPR spectrometer system, designed by the St Andrews group, headed by Graham M. Smith, recipient of the 2012 IES Silver Medal for Instrumentation.

The strange looking witch's hats are very high quality microwave loads, which help to eliminate standing waves. They are one aspect of a system design that reduces ringdown by up to 12 orders of magnitude, relative to conventional cavity-based spectrometers, in an effort to eliminate system deadtime.

The design mantra "high frequency, high power and high sample volume" has guided the overall design of a spectrometer that has a GHz instantaneous bandwidth and a very high concentration sensitivity. It is estimated that PELDOR sensitivity is currently increased by a factor of more than 30, relative to standard measurements at X-band and that factors of 1000 improvement are possible.

This level of improvement opens up many new opportunities in pulse EPR, and one active area of research seeks to demonstrate that orientation sensitive PELDOR can be a routine and powerful method in biomolecular structure determination.

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ETH
Eidgenössische Technische Hochschule Zürich
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Editorial

Dear colleagues,

I wonder if you might like to start reading in this issue the article by Stephan Zech "Transitions: From EPR to Drug Discovery" in the *IES Young Investigator Award Revisited* column (p. 6). It won't be surprising because it is always interesting to read a success story and to realize once again how diverse life is and that one has to work hard and to have a bit of good luck in order to advance in one's career. Have a look at Stephan in 2003 receiving the IES medal from Shirley Fairhurst, then Secretary of the IES (13/3, p.5), and compare this photo with the present one, featuring Stephan-the-Associate-Director. He is certainly a man in the prime of his creativity and we wish Stephan further success in his work in the pharmaceutical industry. Interestingly, during his doctorate, Stephan worked with Robert Bittl (IES Young Investigator Award 1997). Or you might like to first look at the information in the *Awards* column and join us in congratulating Takeji Takui (Bruker Prize 2013), Yuri Tsvetkov (Zavoisky Award 2013) and Christopher Hartland (JEOL Prize 2013) on their highly deserved prizes. Hopefully Christopher's article (pp. 3–5) serves as a good encouragement for students to present their research at various conferences. Whatever article you start with, you will certainly be attracted by Ilya Kuprov's article in the *Software* column (pp. 9–10) even if you do not specialize in magnetic resonance simulations.

It is my pleasure to introduce to you our new sponsor, Magnettech GmbH, a major supporter. Support of our sponsors is important for the society and we look forward to the long-term collaboration with Magnettech GmbH for our mutual benefit. And if you know any other company that may be interested in collaboration with the IES, please feel free to inform their CEOs about us.

The passing away of Nicholas Turro is a great loss for the magnetic resonance community. The *In Memoriam* article written by Malcolm Forbes and V. Ramamurthy (p. 8) shows a remarkable scientist, a dedicated teacher and mentor. It is filled with warmth and sincere feelings. And this could truly be said to quote Malcolm and Murthy: "All of us who knew Nick consider ourselves lucky to be a part of the Turro family". RIP...

Laila Mosina

IES NEWS

The 2013 Annual General Meeting (AGM) of the IES will be held in conjunction with EUROMAR2013 (June 30 – July 5, 2013) in Hersonissos.

The 2013 Young Investigator and IES Fellow awards will be presented during the ESR Symposium at the 55th Annual Rocky Mountain Conference,which will be held in Denver, CO, USA from July 28 to August 1, 2013.

The Bruker Prize 2013 to Takeji Takui

From left to right: Dr Peter Höfer (Director for EPR at Bruker), Prof Takeji Takui (Osaka City University, 2013 Bruker Prize Lecturer) and Mark Newton (Warwick, Chair RSC ESR Group).

For details, see pp. 12–13.

The JEOL Prize 2013 to Christopher Hartland

Dr Peter Meadows of JEOL (UK) Ltd presents Christopher Hartland (Warwick) with the JEOL Student Lecture Prize.

For details, see pp. 12–13.

Christopher Hartland:
First of all I would like to thank the RSC EPR conference organisers and JEOL for giving me the opportunity to present my work at the 46th Annual RSC EPR Meeting at the University of Warwick.

For the first time three JEOL sessions were included in the programme in order to host the eight students selected to give presentations. The quality of presentations was extremely high and the conference committee had a very difficult time in deciding on the results of the award. In addition to the many excellent presentations, special mention should be given to Johannes McKay for his presentation on 'Accurate orientation PELDOR measurements and analysis using rigid spin labels at high fields' and to Daniel Klose for 'Comparing spin label dynamics and DEER -& FRET distances in experiments versus simulations'. Both Johannes and Daniel received prizes for the quality of their presentations.

My PhD research focuses on the identification and characterisation of point defects in chemical vapour deposition (CVD) grown

diamond using EPR and optical spectroscopy. Diamond is an advanced material which is employed in a wide range of fields such as electronics, bio-sensing, magnetometry and quantum optics. In order to produce high performance technologies for these fields a detailed understanding of the consequences of defect incorporation is required. Professor Jörg Wrachtrup showed an example of this in the first talk of the conference when he demonstrated how a single nitrogen vacancy (NV^-) centre in diamond can be used to sense nuclear spins on a nanometre scale.

The Zavoisky Award 2013 to Yuri D. Tsvetkov

Yuri D. Tsvetkov (Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Novosibirsk, Russian Federation) is awarded in recognition of a lifetime's work in magnetic resonance and, in particular, his contribution to the application of pulse EPR methods to studying structure of disordered systems.

For details, see the forthcoming newsletter

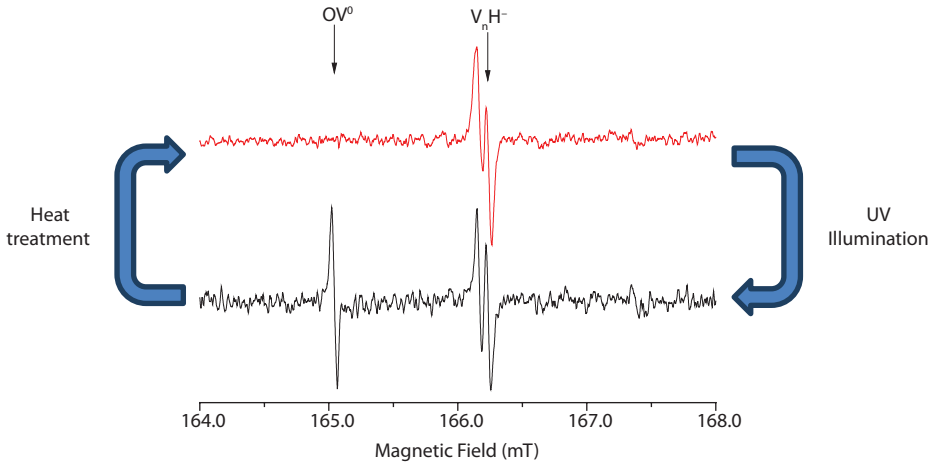

Figure 1. EPR signal observed for the OV^0 defect and the V_nH^- defect after exposure to the two aforementioned charge transfer treatments.

At the conference I presented 'Electron Paramagnetic Resonance studies on oxygen doped CVD diamond'. This talk focussed on the identification of a previously unreported paramagnetic defect which was found in an as-grown CVD diamond grown in a carbon-hydrogen-oxygen plasma.

It has been shown that the inclusion of oxygen in the growth plasma leads to higher quality single crystal growth [1]. To date no defect structure comprising oxygen has been completely characterised. The reasons for this are: only a very small percentage of oxygen in the growth environment is incorporated into the lattice during growth and the most abundant isotope with non-zero nuclear spin is oxygen-17, with a natural abundance of 0.003%. These factors make the identification of oxygen hyperfine interactions very difficult and therefore the presence of oxygen difficult to confirm.

The defect in question shows a number of very similar properties to those of the negative nitrogen vacancy centre but no impurity hyperfine interaction. Both defects have an electronic spin of 1 and C_{3v} symmetry. While $g_{\|}$,$g_{\perp}$ and D of NV^- are 2.0029(2), 2.0031(2) and 2872(5), respectively, this new defect possesses 2.0029(2), 2.0025(2) and 2887(5), respectively. By analysing the carbon-13 hyperfine satellites we find that both this defect and NV^- have identical sets of equivalent carbon atoms. The majority of the electron localisation for both defects is found to be on three equivalent carbon atoms which implies that they both have an impurity-vacancy structure. The only candidate which is small enough to form an impurity-vacancy structure rather than a split vacancy-impurity complex and which also has a sufficiently dominant natural abundance of $I = 0$ isotopes is oxygen. To be $S = 1$ this defect must therefore be the neutral oxygen vacancy defect, OV^0.

The NV centre in diamond is known to exhibit photo and thermochromism, whereby an electron from a substitutional nitrogen atom, N_s, may be driven to or from a NV centre in order to form the NV^- or NV^0 centre [2]. Since the neutral oxygen vacancy defect is isoelectronic and isostructural with NV^- then one might expect the following process to also be possible:

$$N_s^0 + O_sV^0 \rightleftarrows N_s^+ + O_sV^-.$$

OV^- would be an $S = 1/2$ defect which we expect to be obscured beneath the single substitutional nitrogen which is also $S = 1/2$. N_s^0 is present at concentrations two orders of magnitude greater than OV^0 and so any signal arising from OV^- would be masked by this. Figure 1 shows that the charge transfer process proposed can be achieved and that the process is entirely reversible.

The nitrogen vacancy defect is formed during CVD growth. It can also be generated by irradiation and annealing: this process involves introducing vacancies into the system by irradiation and then annealing the sample which causes those vacancies to migrate to substitutional nitrogen impurities. It is expected that, if there is any substitutional oxygen present in the lattice, OV could also be produced by irradiation and annealing. In order to test for this, irradiation with 4.5 MeV electrons followed by annealing to 800 °C for four hours has been performed twice. The first irradiation produced 0.3(0.05) ppm of vacancies while the second irradiation produced 3.0(0.5) ppm of vacancies: these concentrations are approximately 10% and 100% of the overall N_s^0 concentration present in the sample, respectively. The initial irradiation and anneal did not increase the OV^0 concentration, this is thought to be due to the large ratio of substitutional nitrogen atoms to oxygen thereby making it statistically unlikely to observe a significant increase in OV^0. After the second irradiation and annealing, however, we observed an increase in the OV^0 concentration of around 400% along with a similar percentage increase in NV concentration as shown in Figure 2. This proves that the defect is vacancy related and lends further evidence to its assignment to the OV^0 model. These results also demonstrate the presence of substitutional

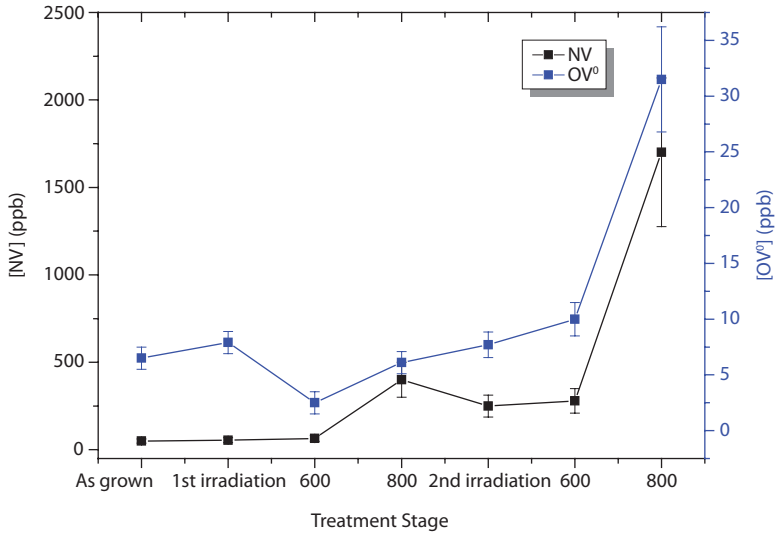

Figure 2. NV and OV^0 concentrations at each treatment stage in the irradiation and annealing study. Anneals at 600 and 800 °C were performed for 4 hours. A significant increase in the concentrations of these defects was observed upon the final annealing stage.

oxygen in the diamond lattice, which has not been reported in the literature.

Finally, I showed that OV^0 does not anneal out until higher temperatures than those observed for the NV^- defect. This is in agreement with predictions made by Goss et al. [3] in which a binding energy of 4.3 eV for NV^- and 4.7 eV for OV^0 was calculated. This was investigated by performing isochronal annealing on a diamond containing OV^0 at 200 °C intervals. The most recent anneal was performed at 1600 °C at which a decrease in the NV^- concentration of approximately 50% was observed while the OV^0 concentration remained constant. Further annealing at temperatures of 1800 °C and beyond is planned for the near future in order to determine at what temperature OV^0 anneals out.

I would like to thank my supervisor, Professor Mark Newton, for all of his advice throughout the course of my PhD so far. I would also like to thank The Diamond Trading Company and the EPSRC for funding. Finally I would like to reiterate my thanks to the conference committee and to JEOL for giving me the chance to present my work.

The opportunity to present research to one's colleagues is invaluable, particularly for those in the early stages of their research career. I encourage all students to take advantage of the opportunity to present their research in the JEOL sessions of next year's conference.

1. P. K. Bachmann, D. Leers, and H. Lydtin: Diamond Relat. Mater. **1**, 1 (1991)
2. R. U. Khan, P. M. Martineau, B. L. Cann, M. E. Newton, D. J. Twitchen: J. Phys.: Condens. Matter **21**, 364214 (2009)
3. J. P. Goss, P. R. Briddon, M. J. Rayson, S. J. Sque, R. Jones: Phys. Rev. B **72**, 035214 (2005)

IES Young Investigator Award Revisited

Transitions: From EPR to Drug Discovery

I'm writing this, returning from a conference in Denver, CO, almost exactly 10 years after I received the honor of the Young-Investigators-Award at a Rocky Mountain Conference here, organized by the Eatons. However, this time the Keystone conference I attended couldn't be further from EPR spectroscopy: "Tumor Metabolism and Cancer Drug Discovery" were the main topics, and I presented our work on developing ligands for novel cancer targets. My research has changed significantly over the past 10 years, but some things remained surprisingly constant. How did I get here?

I studied Chemistry in Berlin in the early 1990s and got introduced to EPR by Wolfgang Lubitz' Physical Chemistry classes. I joined his superbly equipped lab for my diploma thesis, stayed on for my doctorate, and worked with Robert Bittl (IES Young Investigator Award 1997) using time-resolved and pulsed EPR on large membrane proteins. Back then, the measurement of spin-spin distances by EPR was still a fairly novel technology, and we had great success implementing it for light-induced radical pairs in photosynthetic reaction centers.

After obtaining my Ph.D. in 1998, I was looking to explore my options: What to do with the rest of my life? Academia or industry? When I graduated, a swamp of educated people was fighting for the few available positions in industry. After a couple of interviews for rather lame jobs, most of which had no relation to my scientific skills, I decided to wait for better opportunities and stay in academia. I joined Dietmar Stehlik at Freie Universität Berlin for a position on track to become a professor, which, back then, would take about 6-8 years to accomplish. During this time I had the opportunity to work with great people such as Kev Salikhov or John Golbeck. However, the work in Stehlik's lab was fairly similar to what I did in the years before, and I felt that I was destined to repeat my Ph.D. thesis over and over again for the next decades – not an appealing outlook.

Furthermore, if you were hoping for any type of career in Germany, academia or industry, you had to spend a minimum of one year outside the country. After a couple of visits to EPR and NMR labs all over in the US, I decided to join Ann McDermott's group at Columbia University in New York to diversify my skill set and learn solid-state NMR. My initial project, supported by a grant from the Humboldt foundation, was related to my EPR work on light-induced radical pairs, which we planned to investigate by ssNMR. However, getting the equipment in shape turned out to be quite difficult for a newcomer. I made every mistake in the book and, not surprisingly, ended up with 'arching' ssNMR probes, exploding rotors and destroyed protein samples. Chad Rienstra's comment: "I have never seen an NMR probe so severely damaged" somewhat indicated that I might not get much usable data out of this project.

Thankfully, Ann had quite a number of collaborations with academia and industry established, which were able to supply the significant amounts of protein required for ssNMR. So I switched to the hottest topics of the times: "protein structure determination and protein-ligand interactions". In the spring of 2003, the New York Structural Biology Center opened, and Ann's group had access to a 750 MHz ssNMR instrument. Miraculously, within a couple of months, I had enough data to write two JACS papers, one of them became my most cited paper to date.

After two years in NYC I was confronted again with the same decision: academic career path or a switch to industry? However, now the world was much bigger than just Germany. I decided to apply for positions in both the US and Europe, and landed a couple of interviews. My future boss, however, I met through a collaboration of Ann McDermott's group with a small company in Cambridge, MA. EPIX Pharmaceuticals was developing protein targeted contrast agents for MRI applications. Since those agents are usually highly paramagnetic (Gd^{3+}: $S = 7/2$), the job entailed a little bit of everything: MRI, EPR, NMR structural studies of peptides and small molecules, as well as protein-ligand interactions. I joined Peter Caravan's group in January of 2004 as my first position in industry. Surprisingly, pulsed EPR and ENDOR studies on high spin transition metal ions were pretty rare. Our collaborators, Arnold Raitsimring and Andrei Astashkin at U Arizona, had to develop a lot of methodology to drive the understanding of the water coordination of contrast agents, which resulted in quite a number of papers published.

Obviously, companies do not survive on basic research and investors' money alone, they eventually have to sell products. Unfortunately, when the FDA rejected the application for EPIX' first targeted MRI agent, things went downhill quite rapidly, and I was back on the job market. A definitive advantage of being in the Boston area is the huge number of companies in Biotech and Pharma looking for qualified people. It didn't take long to land another job, at ARIAD Pharmaceuticals, located about 10 minute walk from my old job, right next to MIT.

At ARIAD, my work has been expanding from NMR structure determination of natural products, over NMR screening of small molecule libraries to solid-state characterization of pharmaceuticals by ssNMR, and in some cases even EPR spectroscopy. Although EPR is rarely integrated in pharmaceutical research (an obvious reason being that the majority of molecules we make is diamagnetic), it is not that difficult to find niche applications, if one knows what EPR can bring to the table. In the past, we encountered problems with unexpectedly rapid degradation of drugs and large batch-to-batch variations. Only EPR was able to show quickly, that organic free radicals, which gave a nice $g = 2$ EPR signal, were responsible for the degradation. Addition of tiny amounts of a radical trapper not only changed the EPR spectrum, but also solved the degradation issue.

Working in the pharmaceutical industry is much more interdisciplinary and goal driven rather than technology centered, the goal being to develop new therapies. Having a diversified skill set comprising several technologies (in my case: NMR, EPR, and other biophysical techniques), and knowing which one to use effectively to solve a problem, is certainly an advantage. Luckily, we achieved our goal of getting approval of our first leukemia drug at the end of 2012, and are now providing 'Iclusig' to patients with difficult-to-treat cancers.

Stephan G. Zech
Associate Director, Spectroscopy
ARIAD Pharmaceuticals, Inc.
Cambridge, MA
Stephan.Zech@gmail.com

Nicholas J. Turro (1938–2012)

On November 24, 2012, the world lost a remarkable scientist in Nicholas J. Turro, who was renowned as a photochemist and spin chemist. Nick was an exceptional teacher who always filled the room with excitement, energy, and enthusiasm that immediately rubbed off on his students and coworkers. He was elected to the National Academy of Sciences and the American Academy of Arts and Sciences, at the age of 43(!). He also won many awards from the American Chemical Society, the Inter-American Photochemical Society, the European Photochemical Society and the Japanese Photochemical Society.

Nick Turro earned his B.A. in chemistry at Wesleyan University in Middletown, CT, followed by graduate research under George Hammond at Caltech and short postdoc at Harvard with Paul D. Bartlett. His interest in reactive intermediates (excited states and radicals, which are the cornerstones of spin chemistry) was accelerated through his training with these pioneers from 1960 to 1964.

Nick's textbook on photochemistry, the *magnum opus* "Molecular Photochemistry" was already underway at this time, and was published in 1965, only a year after he became an Instructor at Columbia. His beautiful (then-unkown) synthesis of cyclopropanone earned him tenure and promotion to Full Professor only four years later. In the early years of his research program, Nick strove to deeply understand the excited state chemistry of carbonyl compounds, but also targeted other topics such as chemiluminescence, dioxetanes, benzene valence isomers and other strained molecules.

Nick had an exceptional ability to multitask. In an important collaboration with William Dauben and Lionel Salem, Turro developed the use of correlation diagrams for organic photochemical reactions, published in *Acc. Chem. Res.* His second book, published in 1978, was "Modern Molecular Photochemistry", which became the definitive text in the field. Nick was masterful at presenting complicated chemistry concepts with physical pictures that still find use in the community. The latest version of the book, co-authored with V. Ramamurthy and J. C. Scaiano, entitled "Modern Molecular Photochemistry of Organic Molecules", was published in 2009.

In 1978, Nick moved his research program toward supramolecular photochemistry. Very little was known about the photochemistry of molecules in micelles or other organized assemblies at the time. His work on the photochemistry of dibenzylketone in micelles led to the spectacular discovery these reactions in micelles were subject to unprecedentedly large magnetic field effects. To this end, Nick developed a pulsed laser 'nanosecond systems laboratory' capable of studying transients using a wide range of spectroscopic methods, including UV/VIS absorption and emission, resonance Raman, IR, NMR (chemically induced dynamic nuclear polarization) and ESR (chemically induced dynamic electron polarization). He made systematic investigations of photochemical reactions at the molecular and supramolecular level, studying the interactions of guest organic molecules in hosts such as micelles, porous silica and zeolites. His research on radical pairs in micelles and zeolites demonstrated how the interplay of electron exchange and magnetic effects (spin chemistry) can control the rate and selectivity of one of the most fundamental of all organic reactions, carbon–carbon bond formation.

Nick's versatility positioned him well to tackle complicated problems in 21st Century science that represent a mix of chemistry, biology and materials science. In his last years, his research applied the principles of physical organic chemistry to enantioselective reactions of molecular singlet oxygen and the use of fluorescent molecular beacons for tracking RNA in cells. He also worked on the two allotropes of the hydrogen molecule (ortho-H_2 and para-H_2) incarcerated inside a fullerene, showing that they cannot be interconverted using the principles of spin chemistry.

Nick was a dedicated teacher and mentor. He trained over 180 postdoctoral associates, 80 graduate students and 100 undergraduate students, and had over 950 publications. On top of this, Nick was also an extraordinary classroom teacher who enjoyed teaching General Chemistry, a task many of us try to avoid. His teaching accomplishments were recognized by selection as a Distinguished Teacher Scholar by the National Science Foundation in 2002, and by receipt of the American Chemical Society's Pimentel Award in Chemical Education in 2004.

Nick had a deeply happy personal life that he cherished. He married Sandy in 1960, had two daughters and five grandchildren. Together with Sandy, he treated all those who passed through the 7th floor of Chandler as members of their extended chemical family. They showed extraordinary warmth towards any one whom they knew. All of us who knew Nick consider ourselves lucky to be a part of the Turro family.

It is sad to lose such a giant in the field, but we must be grateful to Nick for tirelessly leading us down a path of excitement and discovery. 'Be prepared for change' was the theme of his research, which was characterized by an astounding breadth, encompassing synthetic organic chemistry, colloidal and interface chemistry, chemical physics, magnetic resonance theory and its applications, mechanistic aspects of molecular and supramolecular organic and inorganic chemistry and sophisticated experimental techniques.

Malcolm D. E. Forbes
Chapel Hill, North Carolina
V. Ramamurthy
Miami, Florida

The EPR community has available to it a list server. The address is epr-list@xenon.che.ilstu.edu.
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That sends a message to Reef Morse who will then manually place you on the list. This honors only legitimate requests to join the list. Reef also moderates the list which keeps it spam-free.

Spinach A Fast and General Spin Dynamics Simulation Library

Ilya Kuprov
Department of Chemistry,
University of Southampton

At the energies commonly encountered in chemical systems, the currently established models of reality (Dirac-Schrodinger, Quantum Field and General Relativity equations) are essentially exact and their general solutions are known. Given enough computing power, it is possible to predict, with absolute accuracy, any property of any chemical system. This situation is perhaps the greatest intellectual triumph of human kind, but for one important qualifier – the computing power required is exponential with the size of the system... "absolute accuracy", while achievable, is realistically limited to about five atoms; in the case of Magnetic Resonance spectroscopy – to about ten spins.

Progress can be made by using approximations – a simulation that is run with a finite time step, for a finite time and in the presence of decoherence can often be performed cheaper and faster than the implacably cruel $O(2^N)$ upper bound would suggest. It was that thought that started our work on *Spinach* – the intention was not to write another simulation package (there are plenty of excellent software tools around), but to test a particular hypothesis that we had about levels of spin correlation in magnetic resonance systems. Another idea was to build a Magnetic Resonance theory lab – to be just like an experimental lab, where all equipment is in the right place, things work as they should and exciting research is done into things unknown. A good lab cannot be bought, borrowed or inherited, it can only be built. And so it began.

The hypothesis quickly turned out to be true – practically encountered levels of spin correlation in liquid state Magnetic Resonance were remarkably low (Figure 1). It took a while to convince Peter Hore and Nicola Wagner-Rundell (who came to the opposite conclusion for their radical pair systems) that this was not a one-off coincidence, and eventually we published a paper together [1], noting in the abstract that "*it actually appears that a majority of states in large spin systems are not essential in magnetic resonance simulations and can safely be dropped from the state space*". This had the potential to accelerate all Magnetic Resonance simulations – the complexity scaling became polynomial rather than exponential with the size of the spin system. A few of our subsequent papers demonstrated that huge systems could be simulated on a laptop with the algorithms proposed [2–4], but the burning question was about the physical reasons for that impressive performance. Intriguingly, there were cases (reported by Jean-Nicolas Dumez, Paul Butler, Meghan Halse and Lyndon Emsley) where reduced state space simulations produced correct answers against all expectations to the contrary [5–7]. We did offer some qualitative justifications in the papers, and so did the Emsley group, but it wasn't until Alexander Karabanov came to Oxford for a three-month visit from Walter Köckenberger's group in Nottingham that quantitative accuracy conditions were established [8]. Meanwhile, the IK group (reinforced by Andreas Biternas, Gareth Charnock, Luke Edwards, Hannah Hogben, Matthew Krzystyniak, Dima Savostyanov and Zenawi Welderufael) kept publishing paper after paper with an order of magnitude or so acceleration reported in each. There were some systems where little acceleration was found to be possible (notably in Spin Chemistry and some solid state NMR/ESR systems), but there were also cases (most liquid state systems) where protein-sized molecules could be done in a matter of minutes, in time domain, in Liouville space and with full Redfield relaxation superoperators, including all cross-relaxation and cross-correlation terms [4]. That was big news and it earned us the front page of the *Journal of Magnetic Resonance* in February 2011 [9].

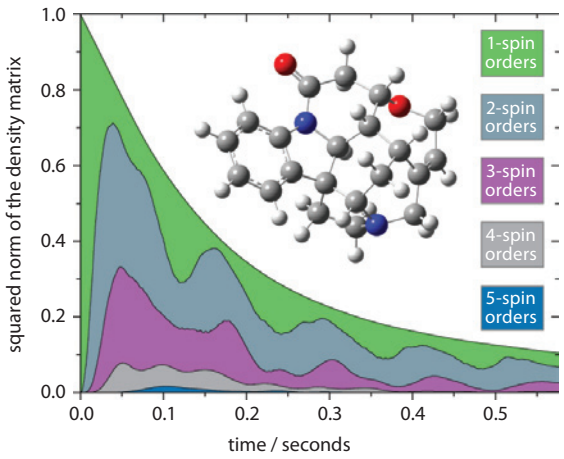

Figure 1. Numerical simulation of the density matrix norm dynamics during the evolution and detection period of a pulse-acquire NMR experiment on the 22-spin system of strychnine. All distances and magnetic parameters imported from a GIAO DFT B3LYP/EPR-II calculation. Bloch-Redfield-Wangsness relaxation superoperator (including DD, CSA and cross-correlation terms) was used with isotropic rotational diffusion correlation time of 200 ps.

We found two words in the Oxford English Dictionary that started with "spin": *spinach* and *spindle*. The latter was neutral, but the former carried with it the image of Popeye the Sailor cracking open a tin and becoming very powerful. The project was dubbed *Spinach* and we went on with the coding – complete SVN repository logs, detailing the code development history with individual authors, comments and dates listed, may be found on our web site (http://spindynamics.org).

At the time of writing, *Spinach* is unique in that it supports all forms of magnetic resonance spectroscopy under one roof (Figure 2): NMR, ESR, DNP, Spin Chemistry, Optimal Control, *etc*. To maintain this level of generality, the package is split into two major sections – the "kernel", which is a general algebraic abstraction containing core functions that are used in any simulation of a finite-state quantum system, and the "user-land", which is a collection of case-specific assumptions, experiment settings and examples. The user-land acts as a translation layer that interprets a specific simulation context, passes it to the kernel for processing and then interprets the answer. In this way, the clean generality of the kernel is safeguarded from the huge swarm of special cases that comprise the practical reality of Magnetic Resonance – all special cases are kept in the user-land.

The following features are, either entirely or at that level of generality, currently unique to *Spinach*:

1. Automatic detection of long-lived spin states (*e.g.* singlets). *Spinach* implements a very general case of Bloch-Redfield-Wangsness relaxation

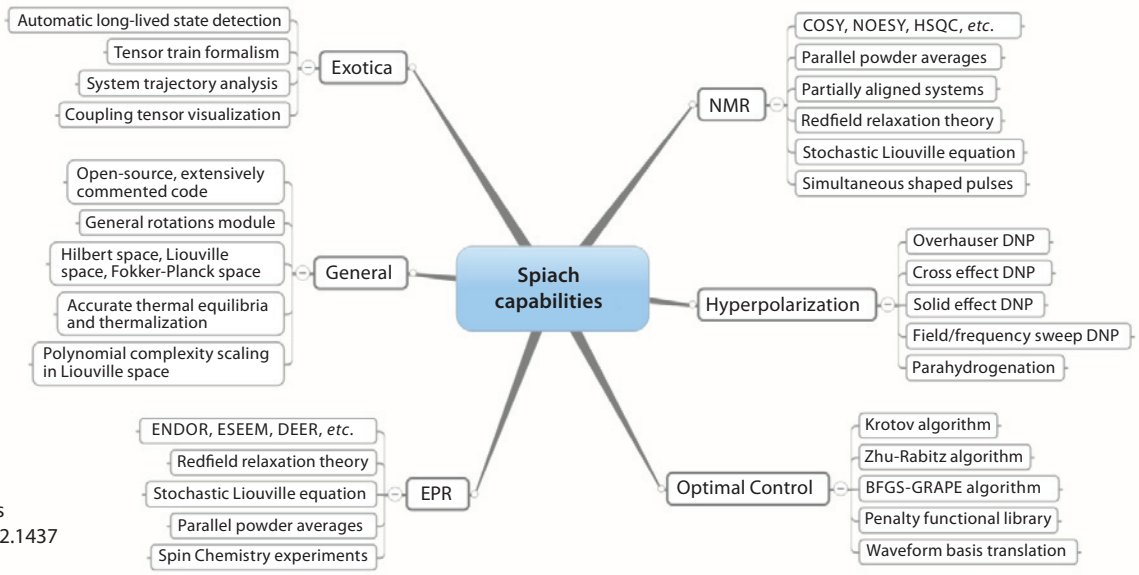

Figure 2. Summary of features available in *Spinach* version 1.2.1437 at the time of writing.

theory that includes all dipolar, quadrupolar, Zeeman and hyperfine mechanisms as well as all cross-correlations thereof. The null space of the relaxation superoperator (which is often sizable) contains the states that are immune to relaxation [10].

2. Optimal control theory module for both NMR and ESR. *Spinach* implements Krotov, Zhu-Rabitz, GRAPE and BFGS-GRAPE algorithms. The implementation of the GRAPE family in particular is very general and supports several propagator derivative calculation algorithms and several types of penalty functionals [11].
3. Trajectory visualization and analysis module. High-dimensional spin system trajectories are often hard to visualize and *Spinach* supports trajectory partitioning into various physically meaningful subspaces. It was the analysis module that generated Figure 1 [12].
4. Fokker-Planck module, supporting any type of spatial dynamics (diffusion, rotation, *etc.*) for NMR, EPR or any other type of spin dynamics in general.
5. Reduced state space infrastructure – *Spinach* was designed from the beginning to support low correlation order basis sets, to automatically detect and take advantage of hidden conservation laws and to aggressively reduce matrix dimensions at all simulation stages. At the time of writing, a 2D NOESY simulation of strychnine (22 protons) in Liouville space with full Redfield superoperator takes about a minute [9].
6. Simulation of all types of DNP spectroscopy. This is a result of a very fruitful collaboration with Walter Köckenberger and Alexander Karabanov at Nottingham University [13]. Restricted state spaces are supported. Waugh and Krylov-Bogolyubov average Hamiltonian theories are also available. Relaxation superoperator options include Redfield theory, Lindblad theory and a relaxation theory that Walter and Alexander specifically designed for DNP [14].

Spinach code is open, extensively commented and uses Matlab as the programming environment. It was our intention to make it easy to modify and re-use parts of the code, if necessary, outside *Spinach*. A collection of example simulations is intended to simplify the initial adoption – it is often easier to modify a generic example than to write a new simulation script from scratch. We continue growing the example set based on the practical simulation requests and queries that we are getting from the users.

An interesting by-product of creating *Spinach* is our Spin Dynamics lecture course (http://spindynamics.org/support.php) – programming something at a high level of efficiency and generality requires deep understanding of the topic, and we distilled that understanding into an online lecture course. That course supplements the manual. According to YouTube, it has scored over 14,000 views and over 120 regular subscribers in the last academic year.

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46th Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry

The 46th Annual International Meeting of the ESR Spectroscopy group of the RSC was held at the University of Warwick 7–11th April 2013. The conference was attended by 94 delegates, and was hosted by Mark Newton, Gavin Morley and Yasmin Kosar. The latter was primarily responsible for the smooth running of the meeting and was ably assisted by the Warwick EPR Group PhD students.

The scientific highlight was the 2013 Bruker Prize Lecture given by Prof. Takeji Takui of Osaka City University. His lecture on "*Recent trends in organic high-spin/open-shell chemistry: electron spin technology*" covered an enormous range of science, from early development of high spin organic molecules through to potential applications in areas as diverse as batteries and quantum information processing. Prof. Takui is the 28th Winner of the Bruker Prize and joins an esteemed list of previous winners from all over the globe.

The conference opened with a keynote lecture from Prof. Jörg Wrachtrup (Stuttgart) on "*Sensing nuclear spins at the nanoscale*", and further keynotes were given by Dr. Graham Smith (St Andrews) on "*Very high sensitivity pulsed EPR for PELDOR applications*", Prof. Marina Bennati (Max Planck Institute for Biophysical Chemistry, Göttingen) on "*Double resonance techniques (EPR/NMR): from sensitivity enhancement to applications in biological science*", Prof Daniella Goldfarb (Weizman Institute of Science) on "*Using ESEEM and DEER to obtain the topology of peptides in model membranes*", and Prof. Peter Saddler (Warwick) on "*Precious metal anticancer complexes with radical mechanisms of action*".

Invited lectures were given by Dr. John Morton (UCL, "*Using nuclear spins to fight electron spin decoherence*"), Dr. Stefan Stoll (Washington, "*Some advances in computational EPR*"), Dr. Johan van Tol (NHMFL, Florida State, "*Electron spin-lattice and spin-spin relaxation in high magnetic field*"), Prof. Joris van Slageren (Stuttgart, "*Crystal field splittings in lanthanide complexes*"), Dr. Enrica Bordignon (ETH Zurich, "*An EPR overview of apoptotic cell death*"), and Prof. David Norman (Dundee, "*Studies in the applicability of the Rx spin label to orientationally selective PELDOR and structure calculation*").

The 2013 JEOL Student Prize Lecture competition was won by Christopher Hartland (Warwick) with an excellent presentation on "*EPR studies on oxygen doped CVD diamond*." The runners up were Johannes McKay (St Andrews, "*Accurate orientation PELDOR measurements and analysis using rigid spin labels at high fields*") and Daniel Klose (Osnabrück, "*Comparing spin label dynamics and DEER- & FRET distances in experiments versus simulations*"). The other five entrants for 2013 JEOL Student Prize Lecture competition, who all gave excellent presentations, included, Gary Wolfowicz (UCL, "*Atomic clock transitions in bismuth donors in silicon*"), Junjie Liu (NHMFL, "*High-field EPR studies of anisotropic molecular magnets*"), Benesh Joseph (ETH Zurich, "*Mechanism of vitamin B12 transport by the E coli ABC importer BtuCD-F revealed by pulsed EPR spectroscopy*"), Dennis Kurzbach (Max Planck Institute for Polymer Research, Mainz, "*Applications of DEER in complex systems*") and Morgan Bye (East Anglia, "*Complex docking models – elucidating protein-protein interactions with EPR*").

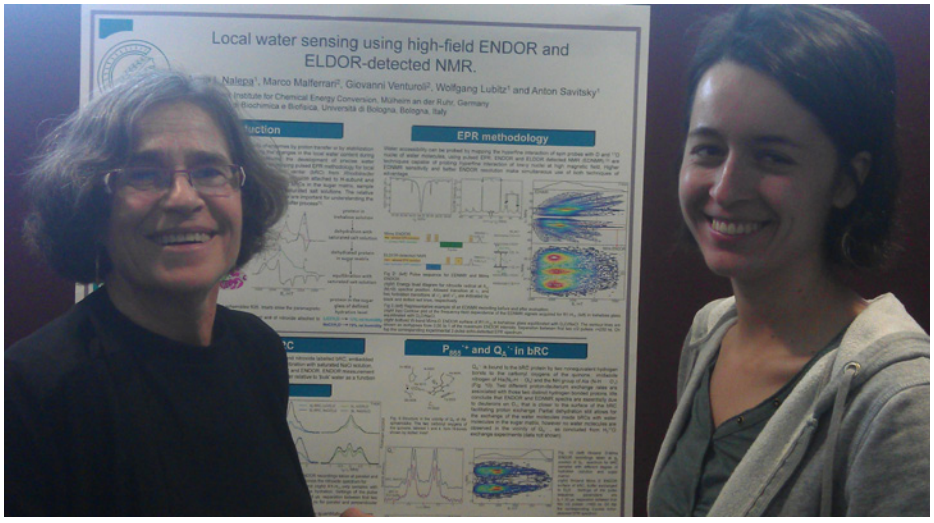
Dr. Peter Meadows JEOL (UK) Ltd with the runners up for the JEOL Student Lecture Prize, left, Johannes McKay (St Andrews) and centre Daniel Klose (Osnabrück).

The delegates of the 46th Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry.

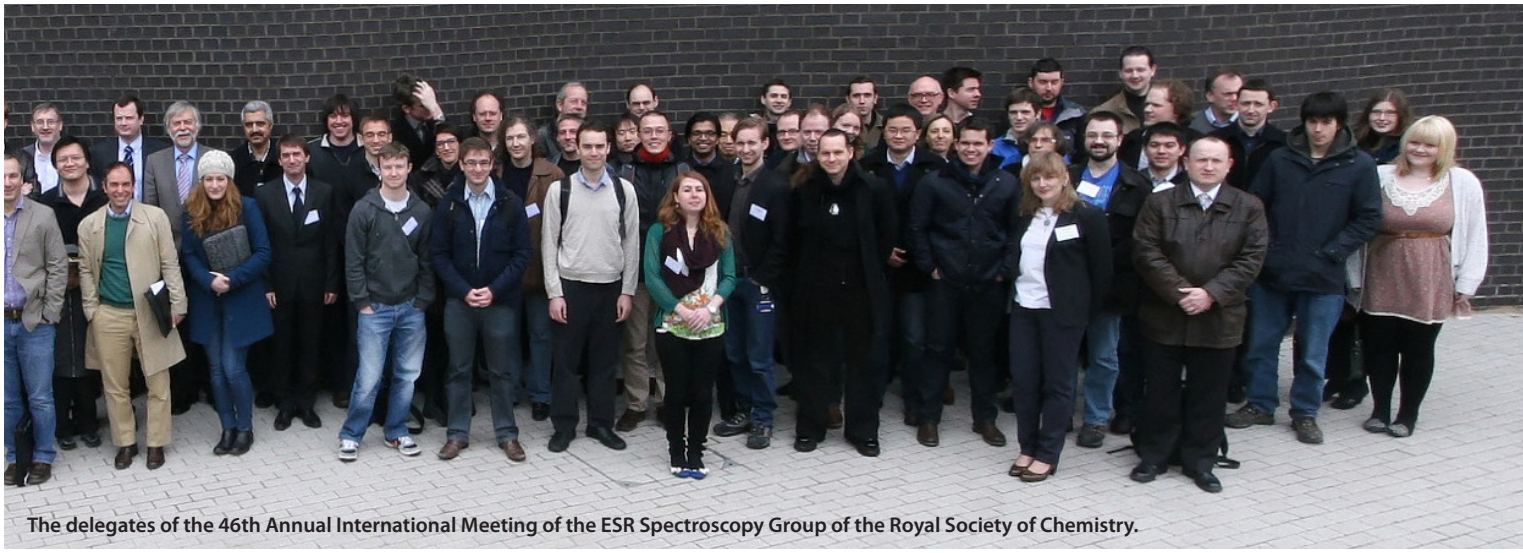
The prize for the best poster was won by Anna I. Nalepa of the Max-Planck-Institut für Chemische Energiekonversion, Mülheim for her poster "*Local water sensing using high-field ENDOR and ELDOR detected NMR*". As has been the case in recent years the overall quality of the posters was excellent and the RSC ESR Group Committee considers the Poster Sessions to be an important part of the meeting.

On the free afternoon the delegates were free to enjoy the local sites of interest including Shakespeare's birthplace and the imposing Warwick Castle. The conference was a great success and the RSC ESR Group Committee would like to thank Bruker and JEOL for their continued sponsorship and support of this meeting. The committee would also like to acknowledge the support of Adani, Cryogenic and Oxford Instruments, who all exhibited at the meeting. At the RSC ESR Group AGM, Dr. Graham Smith (St Andrews) was elected as incoming Chair of the group. Drs. Arzhang Ardavan (Oxford), Chris Kay (UCL) and Ilya Kuprov were elected as Ordinary Members; the latter returns as Web Master. Drs. Helen Williams (Astra Zeneca) and Dima Svistunenko (Essex) retired from the committee in 2013, and were thanked for all their hard work on behalf of the RSC ESR group. The 47th International Meeting of the RSC ESR Group will be held at the University of Dundee 6–10th April 2014 (local organisers David Norman and David Keeble). Information about the 2013 and 2014 meetings can be found at the website esr-group.org.

Prof. E. J. L. McInnes
Secretary to the RSC ESR group
Prof. M. E. Newton
Outgoing-Chair of the RSC ESR group



Prof. Daniella Goldfarb (Weizmann Institute of Science) with Anna Nalepa (Mülheim), winner of the Poster Prize.



The delegates of the 46th Annual International Meeting of the ESR Spectroscopy Group of the Royal Society of Chemistry.

4th International DNP Symposium
Copenhagen, Denmark
28–31 August, 2013
www.dnpsymposium.org/index.php/DNP/4thDNP

The 4th International Meeting on Dynamic Nuclear Polarization will be held August 28-31, 2013, in Copenhagen, Denmark, following the highly successful meetings in Nottingham (2007), Koenigstein (2009) and Lausanne (2011). Current issues and new trends in DNP will be presented, including the developments in Overhauser effect, dissolution DNP, instrumentation, radical chemistry, and hyperpolarized imaging. The symposium is supported by EU COST action TD1103 European Network for Hyperpolarization Physics and Methodology in NMR and MRI. An ESMRMB summer school entitled Acquisition Strategies for Hyperpolarised Spin Systems will be held in connection with the symposium. The school is organized in the context of ESMRMB Lectures on MR. The Suraj Manrao Student Travel Fund has kindly made a donation that will used as prizes for the three best oral and poster presentations by presenting authors at the postdoctoral level or earlier.

Registration has been extended to August 1.

International Conference Modern Development of Magnetic Resonance-2013
Kazan, Russian Federation
24–28 September, 2013
www.kfti.knc.ru/magnetic_resonance2013

The Zavoisky Physical-Technical Institute of the Russian Academy of Sciences organizes the Zavoisky Week from 24 till 28 September 2013 including the Annual International Conference "Modern Development of Magnetic Resonance-2013" and Zavoisky Award 2013 ceremony (www.kfti.knc.ru/eng/zavoisky).

The conference is organized under the auspices of the Groupement AMPERE.

The scope of the conference covers the following topics: Theory of magnetic resonance · Low-dimensional systems and nano-systems · Electron spin based methods for electronic and spatial structure determination in physics, chemistry and biology · Molecular magnets and liquid crystals · Spin-based information processing · Strongly correlated electron systems · Chemical and biological systems · Medical physics · Magnetic resonance imaging · Other applications of magnetic resonance · Modern methods of magnetic resonance · Magnetic resonance instrumentation · Related phenomena

Chairman Kev M. Salikhov, Full Member of the Russian Academy of Sciences
e-mail: salikhov@kfti.knc.ru
Scientific Secretary Violeta K. Voronkova, Dr. Sci., e-mail: vio@kfti.knc.ru
phone: 7 (843)2319086,
fax: 7 (843)2725075

IXth International Workshop on EPR in Biology and Medicine
Krakow, Poland, 7–10 October, 2013
www.eprworkshop.mol.uj.edu.pl

The Workshop will review progress in EPR instrumentation and methodology and cover selected topics of biomedical applications of advanced EPR spectroscopy, such as metals in biology, distance measurements by site-directed spin labeling, synthesis and use of new spin labels and spin traps in biological research, reactive oxygen and nitrogen species and oxidative damage, EPR imaging, oximetry, free radicals and excited state in photobiology.

Preliminary program:

- Recent advances in EPR instrumentation and methodology – organized by W. Froncisz
- Metals in Biology – organized by W. Lubitz
- Distance measurements by site-directed spin labeling – organized by G. Jeschke
- New spin traps, spin probes and fluorescent probes for detecting reactive oxygen species – organized by A. Sikora
- Spin trapping studies: an update – co-organized by M. Davies and R. Mason
- Hyperpolarized MRI and Metabolomics – co-organized by C. M. Krishna and B. Kalyanaraman
- Advances in lipids and membrane biophysics – organized by W. K. Subczynski
- In vivo EPR imaging and EPR oximetry – co-organized by H. J. Halpern and P. Kuppusamy
- Oxidative stress –modification of proteins and other biomolecules – organized by G. Bartosz
- Free radicals and excited states in photobiology and photomedicine – co-organized by T. Sarna and L. Weiner
- Detection of Reactive Oxygen and Nitrogen Species – organized and chaired by E. Ruuge

The meeting should provide great opportunities for exchanging new ideas and research experience and facilitate participation of students and post-doctoral fellows in this important scientific event. We look forward to meeting you in Krakow in October!

Conference Co-Chairs:

Prof. Balaraman Kalyanaraman
Medical College of Wisconsin
Milwaukee, WI, USA
Prof. Wolfgang Lubitz
Max Planck Institute for
Chemical Energy Conversion
Mulheim, Germany
Prof. Tadeusz Sarna
JagiellonianUniversity
Krakow, Poland

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

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

POSITIONS

Ohio State University – EPR Center Molecular Imaging Program

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

Strong background in synthetic chemistry, compound purification and characterization required. Knowledge of radical chemistry and EPR spectroscopy desirable.

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

Ohio State University – EPR Center

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

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

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

Post-doctoral position in structural studies of kinesins

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

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

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

Associate Director
Electron Paramagnetic Resonance Center (EPR Center), Department of Radiology
Geisel School of Medicine at Dartmouth College

Location: Hanover, New Hampshire.

Position Description: We are seeking an Associate Director for our highly successful EPR Center. This individual will work closely with the director, Harold Swartz, to continue and expand the activities of the Center. He/she will be expected to play an active role in the development of the clinical and preclinical activities of the Center, including development of new funding sources.

Qualifications: The ideal candidate must have a Ph.D. and direct and extensive experience with in vivo EPR and active funded research that can be transferred to the Geisel School of Medicine. Extensive experience in the administration of complex high quality research programs is strongly desired.

Compensation, etc.: This will be a tenure track position with a competitive salary.

The individual will receive an appropriate academic appointment as a member of the faculty of the Geisel School of Medicine.

Application Process: Qualified applicants should send their contact information, CV with research interests and current funding, letter describing their qualifications, and the names and addresses of five references to:

E-mail: Traci.Rosenbaum@Dartmouth.edu

Mail: Traci Rosenbaum, Administrative Director, EPR Center, Geisel School of Medicine at Dartmouth College,
Vail Building 705, Hanover, NH 03755

The Geisel School of Medicine/Dartmouth College is an Equal Opportunity and Affirmative Action Employer. We welcome applications from & will extend equal opportunity to all individuals without regard for gender, race, religion, color, national origin, sexual orientation, age, disability, handicap or veteran status.

EPR Specialist Position at Johns Hopkins

Postdoctoral or specialist (staff) position is available immediately to study membrane proteins at the Johns Hopkins University School of Medicine in Baltimore, Maryland, USA. We study conserved membrane enzymes with implications for human health (see Nature Chem Biol 8:759, eLife 1:e00173, and Nature Rev Micro 7:411), and are generously funded by the National Institutes of Health (NIH) and the Howard Hughes Medical Institute (HHMI). The project uses site-directed spin labeling (SDSL) with nitroxide probes to study the dynamics, distance measurements, and saturation kinetics with CW-EPR methods. The applicant must have at least 3 years of prior experience in SDSL, EPR, spectrum

simulations, and distance measurements as evidenced by publications. Experience with membrane proteins is preferred but not essential. Position will come with generous salary and benefits, depending on experience and record of achievement. Interested applicants please send detailed CV and contact information for 3 references to rosanna@jhmi.edu.

Research Positions – Advanced EPR of Biochemical and Chemical Systems

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

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

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

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

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

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

Post doctoral/Ph.D positions available

Two post doctoral (or Ph.D) positions are available in the laboratory of Prof. Daniella Goldfarb at the department of Chemical Physics, Weizmann Institute, Rehovot, Israel.

The research focus is development of pulse EPR methodology, including distance measurements using standard and new spin labels, and applications of pulse EPR to biological systems.

The positions require background in Magnetic Resonance, and/or Biochemistry/Structural Biology.

Information about the groups and the Weizmann Institute can be found at www.weizmann.ac.il/chemphys/EPR_group and www.weizmann.ac.il.

Interested candidates should contact Daniella Goldfarb (daniella.goldfarb@weizmann.ac.il) for further information.

For serious suitable candidates the possibility of a funded visit to the lab will be offered prior to final decisions.

Bruker BioSpin Corp

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

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

EQUIPMENT

For sale

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

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

For sale

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

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

Design and construction of EPR electronics

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

For sale: Varian and ESR equipment

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

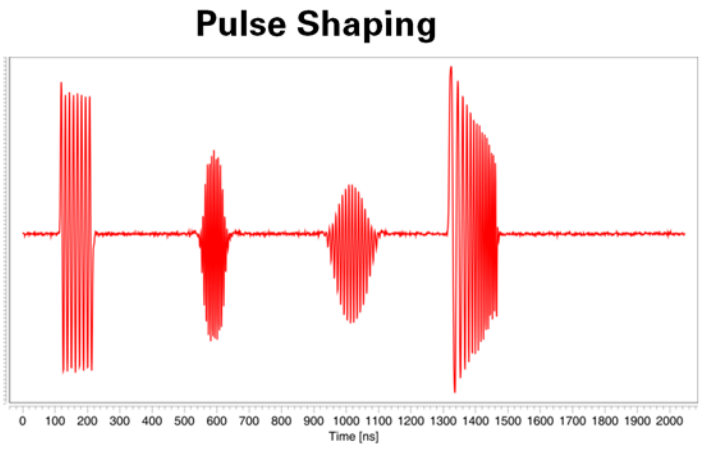
Please contact: Clarence Arnow, President, e-mail: 8400sales@resonanceinstruments.com, phone: 1-847-583-1000, fax: 1-847-583-1021.

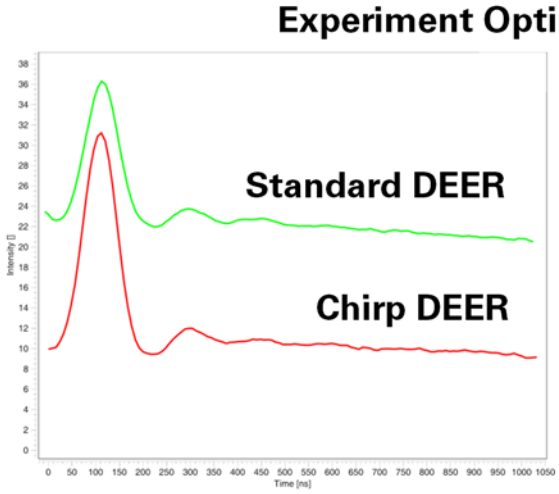
Available: Used Varian EPR equipment

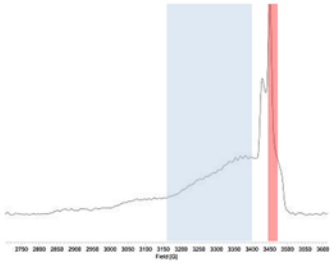
(1) Varian E-104 EPR spectrometer with vertical style bridge and e-line fieldial. (2) Varian E-9 EPR spectrometer. Both available with warranty and continued service support. (3) Varian TM cavity with flat cell holders and flat cells. (4) Varian E-257 variable temperature controller with heater sensor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

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

The Next Step in EPR







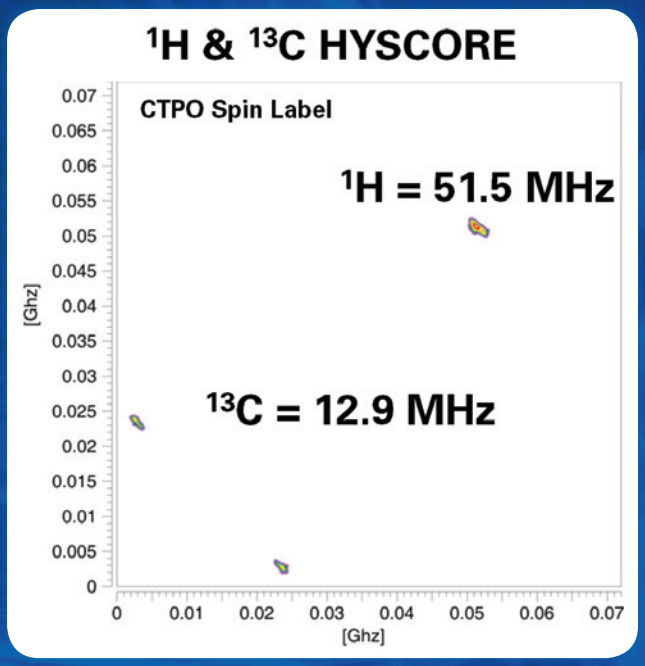
Cu-NO sample courtesy T. Prisner

Arbitrary Waveform Generation

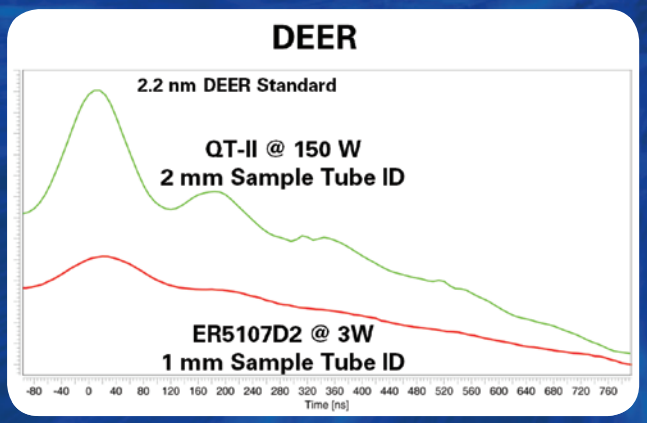
The AWG makes a wide array of exciting opportunities available in the field of pulse-EPR.
Available for each pulse is a combination Amplitude, Phase, Shape, Frequency and Frequency Profile.
The AWG is an addition to all pulse systems offering:

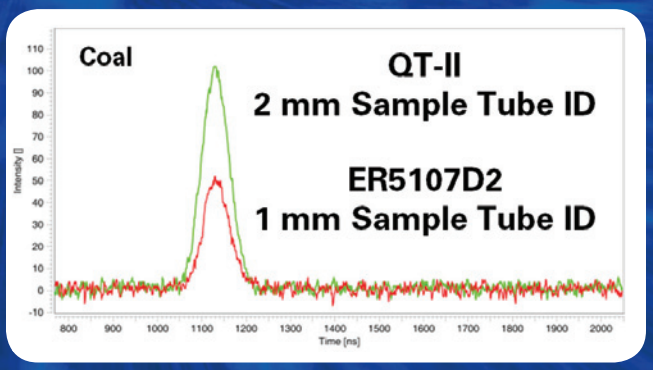
- Complete Xepr control
- Optimum control pulse input
- Integrated Bruker IF compatibility (263 GHz, W, Q, S, L-band operation)

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



With Great Power Comes Great Sensitivity





www.bruker.com/epr

Pulse Q-band with the QT-II and the 150 W TWT

The new large volume pulse resonator (QT-II) in combination with the 150 W TWT offers increased concentration and effect sensitivity as demonstrated in the DEER and the HYSCORE experiments.

DEER:
- t_{ELDOR} = 12 ns @ 150 W
- Factor 4 modulation depth enhancement vs 3 W
- Factor 2 echo amplitude increase vs ER5107D2

HYSCORE:
- More than enough B_1 for ^{1}H excitation at 50 MHz
- More than 150 MHz Bandwidth for detection