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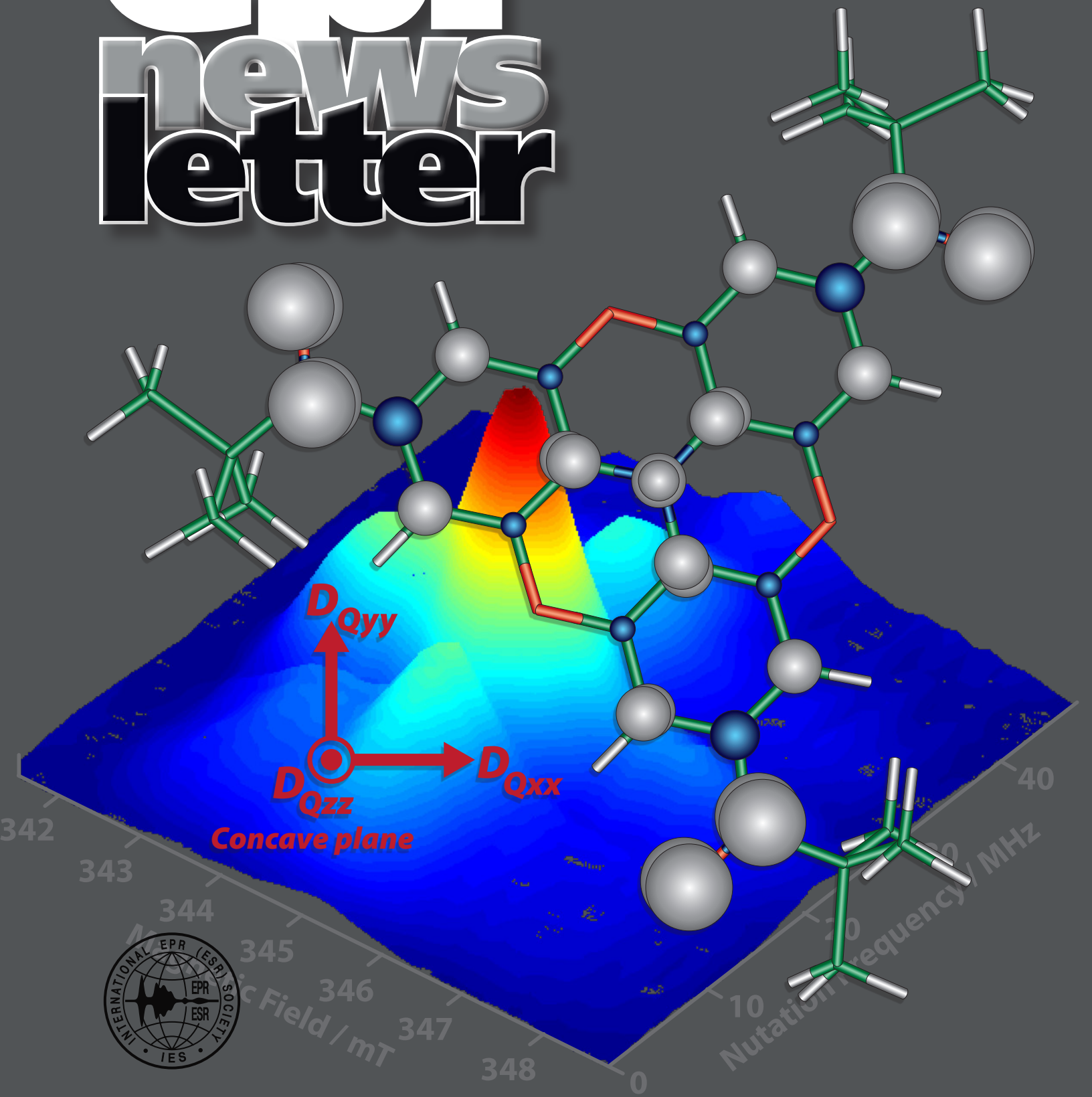

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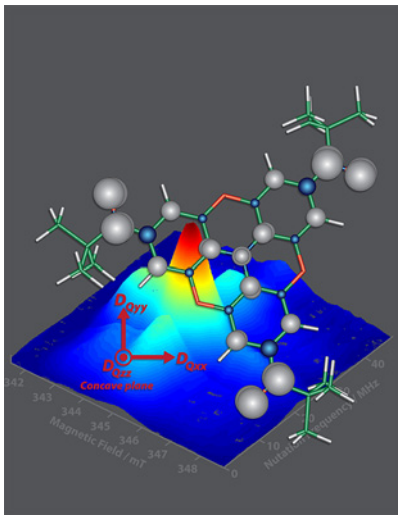

The cover picture illustrates one of the recent achievements carried out by Takeji Takui, the recipient of the Bruker Lectureship Award 2013. A triangular molecule, depicted in front, is a stable and purely organic triradical with the electronic spin-doublet ground state and nearby spin-quartet one. The approximate degeneracy arises from the π-topological symmetry of the electron spin network in the triradical and the local structures of nitroxide radicals at the vertexes, giving rise to weakly exchange-coupled molecular multi-spin systems. The exchange couplings and dipolar interactions between the spins can be controlled by quantum chemistry mediated molecular optimization. The complete characterization of the electronic molecular structures and relevant spin properties/magnetic tensors has been carried out by 2D pulsed electron spin transient nutaion spectroscopy at X-band (see the background behind the picture of the molecule). The molecular optimization and precise identification of multi-spin character for bi- and tri-radicals, and organic multi-spin systems are important in quest for DNP applications of the radicals and molecular spin quantum computers.[1]

[1] K. Ayabe, K. Sato, S. Nakazawa, S. Nishida, K. Sugisaki, T. Ise, Y. Morita, K. Toyota, D. Shiomi, M. Kitagawa, S. Suzuki, K. Okada, T. Takui: "Pulsed electron spin nutation spectroscopy for a weakly exchange-coupled stable triangular triradical: A general theoretical and experimental approach." *Molecular Physics* **111**, no. 18-19, 2767–2787 (2013); http://dx.doi.org/10.1080/00268976.2013.811304

epr newsletter

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Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Editorial

Dear colleagues,

Probably some of you who read my editorial in the previous issue of the *EPR newsletter* 23/3, have made a note about the articles that were announced and are looking for their selected choices in this issue. Yes, as promised, you will find all of them and more. I will not make guesses as to what is the priority list of the majority of you and just comment according to the layout sequence.

In his interview, Takeji Takui-san, Bruker Prize 2013 winner and President of the Asia-Pacific EPR Society 2012–2014, kindly tells us the story of his way in science and shares his experience and ideas, which are undoubtedly beneficial for the young generation of magnetic resonance researchers (pp. 3, 4). The "Awards" column also features his countrymen, Tomoaki Miura, Yoshiaki Uchida, and Keiji Yasukawa, winners of the SEST 2013 Young Investigator Award, with their stories about the relevant research (pp. 4, 5). These awards were given during the 52th Annual Meeting of the Society of Electron Spin Science and Technology of Japan (SEST2013) (please find the report by Kazunori Anzai on pp. 17, 18). It is inspiring that an outstanding scientist and new-generation researchers have the floor on the pages of our newsletter.

In the "Software" column Thomas Baecker, Patrick Carl, and Ralph Weber present the development of Bruker's Xepr software to meet the demand for complete control over external devices and cutting-edge data processing in the EPR experiments (pp. 6, 7). A workshop on rapid-scan EPR was held before the 2013 International EPR Symposium (23/3, p. 17) and in the "Tips and Techniques" column the Eatons et al. describe the rapid-scan EPR techniques (pp. 8, 9). These two instructive articles result from the never ceasing activity of editors, Stephan Stoll and Keith Earle, respectively, whose support is gratefully appreciated.

The "Guest of the Issue" column is presented by its editor, Wolfgang Lubitz, a member of the Lindau Council responsible for chemistry, with a brief overview of the development of the Lindau Nobel Laureates Meetings, an ideal platform to educate, inspire and connect scientific generations (pp. 10–13). Interestingly, Wolfgang's words "it is gratifying to see that in recent years "the two cultures" of NMR and EPR are converging with the parallel development of modern pulse techniques, the transition to higher fields and frequencies and, last but not least, by the possibility to greatly increase the NMR sensitivity via dynamic nuclear polarization (DNP)" find an echo in the report of Jan Henrik Ardenkjær-Larsen about the 4th DNP Symposium (pp. 16, 17).

The "Awards" column also gives us an opportunity to congratulate Yuri Tsvetkov on his Zavoisky Award 2013. The details will be given in the report about the Zavoisky Award ceremony and the International conference, "Modern Development of Magnetic Resonance 2013", in the forthcoming issue of the newsletter.

Laila Mosina

The Zavoisky Award 2013 to Yuri D. Tsvetkov

During the Zavoisky Award 2013 ceremony (from left to right): Yuri D. Tsvetkov, Kev Salikhov, chairman of the Zavoisky Award Committee, and Rimma A. Ratnikova, Deputy Chairman of the State Council of the Republic of Tatarstan.

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

Interview with Takeji Takui on the Occasion of His Bruker Award 2013

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

This is probably the most important and difficult question for me to answer, and it dates me! Like all boys and girls when they start attending school, everything, of course not all, but so many things that I learned from books and nature itself made me interested in science.

The more I learned at school, the more unanswered queries and doubts I had, annoying me increasingly: Why sea water in a shoal looks light blue or greenish, fundamentally why water looks blue or green, why the tides happen and whether the explanation given in text books was true?; why is any effect of the earth's rotation not included in descriptions of tidal motion? From where and how water on the earth came, why the earth precesses and are there any planets without precession? Why the planets of the solar system circulate in almost the same plane, how scientists identify skin colors of dinosaurs in their ages, and isn't the present time still the age of dinosaurs since so many kinds of birds as their descendants are around? These questions are just typical of those that used to be written in my worn-out note pads. I had attempted to find any significant clues to predict the weather everyday in a local area (Osaka) after the observation of the weather conditions at three scheduled times every day for three years, making the weather map and sketching clouds on the horizon and up in the sky with patience. Going to public libraries almost everyday during long holidays didn't help me significantly. I realized that empirical knowledge or science was informative but was just empirical! This experience and all unanswered queries and doubts I had led me to study science at University. In addition, I had also been so interested in mechanisms of human recognition; optical illusions might not be illusions and they might be the results calculated in a sophisticated manner in human brains (recently, this has been partly solved), and among so many puzzles I had, some were ridiculous and some were not. Issues relevant to photosynthesis and related energy conversion processes occurring in biological systems in nature and the behaviour of society and artificial systems interested me considerably. Fortunately, I was allowed to enter the university, Osaka University, in which a brand-new laboratory of the right kind of department had been established. My very first research topics were relevant to the identification of peculiar energy conversions and generalization in relation to their molecular-based design, and I had opportunity to learn brand-new theory from the physics and theoretical side.

Who introduced you into magnetic resonance?

The late Professor Koichi Itoh who was Associate Professor in Professor N. Mataga's Laboratory in the Department of Chemistry, Faculty of Engineering Science, Osaka University, led me into magnetic resonance back in 1967. One year before, when I was an undergraduate student, and before I was engaged in research activity in the Lab., I had attended Prof. Itoh's lecture on the first detection of a high-spin hydrocarbon in its quintet ground state. That lecture destroyed my basic knowledge of chemistry and physics learned from textbooks. Prof. Itoh clearly showed that purely organic hydrocarbons could be ferromagnetic in bulk in spite of the fact that Heisenberg had demonstrated that only d-electrons could be responsible for spontaneous ferromagnetism from a theoretical perspective! This came out of the blue.

What is the driving force for you in your research?

Finding new general ideas or principles derived from experimental results which might lead or contribute to further implementation or progress in electron spin science and spin technology.

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

This is also a very difficult query for me to answer. For myself, the originality at any level is the most important in the course of research. Also, collaborative work makes me happy, simply because I learn unexpected things and knowledge from my collaborators. What I encounter, whether strange or anticipated, and chance discoveries involve serendipity.

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

This query also dates me, thanks to the interviewer, the Editor of the *EPR newsletter*, Dr. Laila Mosina. Probably, factors controlling research are multi-dimensional, but time seems to be one-dimensional. Real life is lived only once, probably, and life is short, but I believe that science will last longer. Indeed, there may be nothing scientific without building on the achievements of those who have gone before, but the forerunners sometimes overlook not only small details but big things too. There will continue to be plenty of room to find something significant, even if one is confined to the field of magnetic resonance.

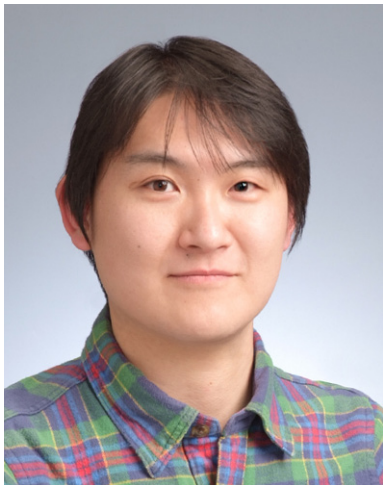
Tomoaki Miura:

I was honored to receive the young scientist award from The Society of Electron Spin Science and Technology (SEST) for "Study on Photo-generated Radical Pairs by Means of Real-Time Measurement of the Spin Dynamics". This study was conducted with many collaborators and I especially thank Prof. Hisao Murai, Prof. Michael R. Wasielewski and Prof. Tadaaki Ikoma. I have been studying the spin dynamics of photo-generated radical pairs by time-domain observation of EPR and optically detected magnetic field effect.

The spin-state mixing of a radical pair in a micelle in low magnetic fields was observed by newly developed transient-absorption detected nanosecond field switching. The observed incoherent process was correlated with diffusional fluctuation of spin-spin interactions by a novel Monte Carlo calculation. This achievement opened up a new horizon for extraction of molecular dynamics of radical pairs in confined media from the low-field spin dynamics.

In fixed-distance donor-acceptor linked systems, detailed mechanisms of long-distance electron transfer were studied by time-resolved EPR and magnetic field effect. From these studies it was demonstrated that the spin dynamics can be a powerful probe as well as an important factor for the electron transfer. Based on this achievement, a molecular spintronic gate was realized by manipulation of the spin dynamics of the charge separated states with a resonance microwave pulse.

Currently, I am studying complex electron transfer mechanisms in biomembrane models, metal containing donor-acceptor systems and organic semiconductor films from the aspect of spin dynamics of the paramagnetic species.



Yoshiaki Uchida:

I was honored to receive the young scientist award from The Society of Electron Spin Science and Technology (SEST) for my studies on magnetic properties of paramagnetic organic radical liquid crystals. This study was

carried out with many collaborators and I especially thank Prof. R. Tamura and Prof. J. Yamauchi at Kyoto University in Japan and group members at Kyoto University. Most of the research was carried out at Kyoto University during 2008 to 2012.

I investigated the magnetic properties of paramagnetic organic radical liquid crystalline (LC) compounds with a radical spin source in the mesogen core. These compounds exhibit nonuniform intermolecular magnetic interactions in the LC phases (magneto-LC effects), which have never been reported in the field of purely organic solid-state molecular magnetism at high temperature. The temperature dependence of magnetic susceptibility obtained by EPR spectroscopy and SQUID magnetization measurement indicates that the magnitude of the nonuniform intermolecular magnetic interactions depends on the type of LC phases; chirality and orientational ordering of the LC phases are factors affecting the magneto-LC effects, and furthermore, the response of paramagnetic LC droplets to the permanent magnet also depends on the kind of LC phases. These studies were published in *Journal of Materials Chemistry*, **18**, 2950 (2008), *Journal of the American Chemical Society*, **132**, 9746 (2010), *Journal of Physical Chemistry B*, **116**, 9791 (2012), and *Journal of Materials Chemistry*, **22**, 6799 (2012). Now I enjoy the research on the magnetic and optical properties of the chiral organic radical LC materials at Osaka University in Japan. I really appreciate the award and encouragement by the members of SEST.

Keiji Yasukawa:

I was honored to receive the SEST 2013 Young Investigator Award for my study on *in vivo* redox monitoring of gastrointestinal disease in mice and rats using magnetic resonance technique. This study was carried out with many collaborators and I especially thank Prof. Hideo Utsumi at Kyushu University.

I investigated the redox status in rats with gastric ulcer induced by stress and non-steroidal anti-inflammatory drugs (NSAIDs) and in mice with colitis by dextran sodium sulfate (DSS) with in vivo ESR/nitroxyl probe technique. However, the visualization of redox status is required to study the relation of the region where redox status changes to the injured tissues. Thus, we focused on redox imaging of both intra- and extra-cellular compartment in several gastrointestinal disease models with Dynamic Nuclear Polarization (DNP)-MRI. We succeeded in visualization of intracellular redox change in gastric epithelium of rats with NSAIDs-induced gastric ulcer. Furthermore, we clarified that intracellular redox change occurs before mucosal injury in the rectum and that the altered redox status expanded to the extracellular compartment of the whole colon as the colitis developed.

I am interested in the mechanism analysis of redox imbalance and its contribution to the gastrointestinal diseases. I hope that such results would additionally provide significant meaning of redox mapping with DNP-MRI and contribute to the drug development research.

Software

The XeprAPI: linking Python with Xepr

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For those of us who have only been doing EPR for the past 20 years, the natural operation of an EPR spectrometer begins in front of a personal computer for spectrometer tuning, experiment definition, data acquisition and finally data processing. In the beginning spectrometer software was focused on the control of the hardware to facilitate spectrum acquisition; however the role of the software has evolved over the years as the user demands have increased to include interfaces to external devices and access to complex data processing routines. No longer is basic control and processing sufficient as even common CW-EPR experiments demand complete control over external devices and cutting-edge data processing.

Since its introduction in 1996, the development of Bruker's Xepr software has focused on meeting the EPR community's need for a platform that provides flexibility in experiment design, control, and execution including the relevant data processing routines. Flexible experiment design in Xepr is reflected in the numerous combinations possible for X and Y abscissa in both CW and Pulse EPR experiments. This allows experiments such as field sweep vs. modulation frequency vs. signal intensity to be easily created and executed within Xepr. Control and integration of spectrometer accessories, such as goniometer and variable temperature systems, is similarly included in Xepr to provide easy automated access to temperature studies and crystal rotation patterns. Finally, Xepr provides a wealth of processing algorithms, such as linear prediction, lineshape fitting, filtering, and various transforms, as well as processing tools to selectively apply processing on regions of the data. A great deal of effort has been directed at providing users with the most common techniques and processing routines via the GUI (graphical user interface) present in Xepr.

To support experimental requirements beyond the common set of techniques for acquisition and processing, the ProDeL (procedure description language) environment was developed. ProDeL is a programming language and environment within Xepr designed for direct access to all of the hardware parameters and to the experimental data. Access to the hardware parameters allows the creation of atypical experiments such as collecting ESEEM data as a function of the stepped microwave frequency and magnetic field, or collection of data with a logarithmic X abscissa. The ProDeL environment also supports data processing through built-in mathematical routines as well as access to all of the processing routines available through the Xepr GUI. While ProDeL has long provided users with a solution for the design of experiments outside of the norm, the rapid growth in the EPR field has demanded a more flexible approach to experiment design and data processing than what has currently been available with ProDeL.

The XeprAPI provides this bridge between the rapid developments in data processing, the requirement for complex EPR data acquisition, and the control of a wide array of instrument accessories (see Fig. 1). The XeprAPI is an interface to Python (www.python.org) which is a robust, open-source programming language with many programming packages for advanced data processing and for communication to external devices via GPIB, Ethernet, USB, etc. Python interfaces nicely to other programming languages such as FORTRAN, C, and C++, so analysis/simulation routines previously developed can be directly used in a Python script. In the simplest sense, the XeprAPI is a set of Python classes and methods for the direct control and operation of Xepr. The four Python classes of the API are: **Xepr**, **Dataset**, **Experiment** and **Parameter**.

The **Xepr class** is the main class used for the interaction with Xepr and encapsulates the other classes for spectrometer control and manipulation. With this class the connection between the Python interpreter and Xepr is established. Further direct access to the native commands available in Xepr is possible. For example the Xepr command for the FFT processing of complex data in Xepr is prFFTcplx. Using the Xepr class, the command Xepr.XeprCmds.prFFTcplx() would transform the data currently in the Xepr window. Methods in the Xepr class allow direct access to the experiments defined in Xepr via the Experiment class and to the data present in Xepr via the Dataset class.

The **Dataset class** provides access to the information available in datasets stored/saved by Xepr. Each Dataset object contains array objects for the X and Y axes as well as the ordinate values. These array objects are supplied by the NumPy module (www.numpy.org) contained in the SciPy (www.scipy.org) package. The SciPy package provides a wide variety of processing opportunities as well as the data structures for advanced processing development. In general use, the Dataset class is used to take data from Xepr, manipulate the data, and then place the data back into Xepr however data can be generated from any simulation routine and this data can be placed into Xepr via the Dataset class. The combination of SciPy and the Dataset class offers users the ability to apply advanced processing techniques directly to data that has been acquired with Xepr as a post processing step. The SciPy package also provides several modules for importing and exporting the data to various file formats including ASCII text, Matlab, and Excel.

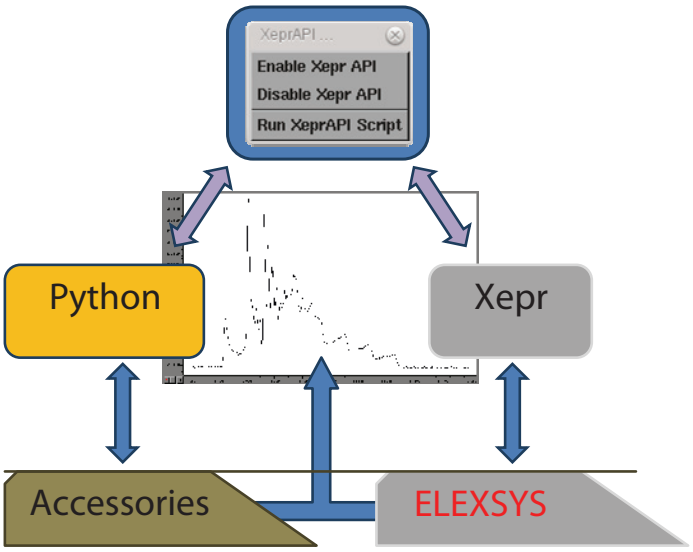

Fig. 1: The XeprAPI bridges Python and Xepr for extended data analysis and instrument control.

The **Experiment** and **Parameter classes** are where experimental creativity is realized. Using the Experiment class, an already existing Xepr experiment may be accessed or a new experiment may be created. Using the Experiment class, data acquisition can be controlled in the same manner as in Xepr with commands to start, stop, abort, and pause an experiment. The current state of an experiment can also be queried to determine if acquisition is running or paused. Unlike in the ProDeL environment, the XeprAPI commands do not block interaction with Xepr. So if an experiment is started from a Python script, the user can still switch to Xepr and perform any normal operations while the Python script is being executed.

Once an Experiment object is created, full access to all spectrometer parameters is available via the Parameter class. The values for parameters can be directly read and set, such as the center field, field sweep range, or MW attenuation. For parameters that include GUI tools for changing the parameter, for example MW frequency or MW phase, the parameter can be incremented as if the mouse was used to click the GUI tool. Parameter control and monitoring also extends to devices that can be directly controlled via Xepr such as goniometer, teslameter, and imaging gradients. For devices not interfaced with Xepr, Python modules for communication (GPIB, Ethernet, etc.) must be used.

Activation of the XeprAPI is done from within Xepr under the Processing menu. As a security measure to prevent unwanted Python access to Xepr, the API can be activated or deactivated from within Xepr (Fig. 1). This mode allows interactive control via iPython (www.ipython.org) or manual script execution from Python. Once a script is debugged and satisfies the user's requirements, the Python script can be directly executed from Xepr via the XeprAPI sub-menu. The XeprAPI is a standard feature of Xepr as of version 2.6b.86 and is independent of the hardware configuration (both LinAcq and OS9 acquisition servers are compatible).

An example of a simple Python script for calculating the signal to noise of a spectrum is shown in Fig. 2. This script can be used for determining the signal-to-noise ratio of a CW EPR spectrum where qualified regions of the data are used to select signal and noise regions. The script first connects to Xepr (1), then reads the data from Xepr (2). If any qualified regions are present, their definition is read from Xepr as sets of begin and end points (3). The data within the qualified regions is then searched for maximum and minimum values to determine which regions to use as noise (4). Finally the signal amplitude is calculated (5) and the root-mean-square noise is determined and reported in a dialog within Xepr (6).

An example of a Python script utilizing a GUI is presented in Figs. 3 and 4. This script is for a CW EPR experiment where first the data is collected with the field sweep in the up direction (1), second the data is collected with the field sweep in the down direction (2), and finally the goniometer angle is incremented (3). The structure of the script has setting of the angle prior to data collection, however if the angle is already set to that as in the GUI, no stepping is done. The script manages the collection of each field sweep direction as well as the goniometer angle and finally assembles the data into a 2D data with the field sweep as the X abscissa, and the Y abscissa is the goniometer angle (every other goniometer angle corresponds to the same sweep direction).

```
#1)
import XeprAPI
Xepr=XeprAPI.Xepr()
import numpy
#2)
data = Xepr.XeprDataset()   # get primary data from Xepr
(X,S) = (data.X, data.O.real)   # short form for abscissa/ordinate data
#3)
qualifier = Xepr.XeprDataset(xeprset="qualifier")   # get the qualifiers
ranges = qualifier.X.reshape(qualifier.X.size/2, 2)   # determine the ranges
ranges.sort(axis=1)
sections = [S[(x1 <= X) & (x2 >= X)] for x1,x2 in ranges]   # extract the data
#4)
maxMinDiffs = [(max(sect) – min(sect)) for sect in sections]   # get signal strengths
# consider everything but the strongest signal to be noise
sections.pop(numpy.argmax(maxMinDiffs))   # remove the signal data, keep noise
#5)
signal = maxMinDiffs[numpy.argmax(maxMinDiffs)]
#6)
# combine noise sections and calculate RMS
noise = numpy.concatenate(sections)
rmsNoise = numpy.sqrt(numpy.mean(noise**2, axis=None))
signalToNoise = signal/rmsNoise
Xepr.printLn("Signal to rms Noise = ", signalToNoise)
```

Fig. 2: Calculating signal to noise for a spectrum with qualified regions in Xepr.

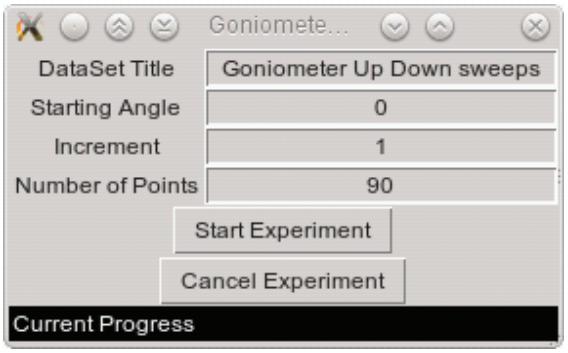

Fig. 3: Python generated GUI for an Xepr experiment with up/down field sweeps and stepping of goniometer.

```
import XeprAPI
Xepr=XeprAPI.Xepr()
import numpy
import Tkinter
import tkMessageBox
from threading import Thread
+
+
+
            currentExperiment = Xepr.XeprExperiment() # get current experiment
…
3)          currentExperiment["Angle"].value=startAngle
            # loop for the goniometer angles to be used
            for n in range(numberGoniometerSteps):
…
                        # setting of field sweep direction
                        # 0 = up, 1 = down, 2 = auto
1)                      currentExperiment["SweepDirection"].value=0
                        # acquire data
                        currentExperiment.aqExpRunAndWait()
                        tempData = Xepr.XeprDataset()
…
                        # change sweep direction to down.
2)                      currentExperiment["SweepDirection"].value=1
                        # acquire data
                        currentExperiment.aqExpRunAndWait()
```

Fig. 4: Excerpts of python script for Xepr control of CW experiment for up/down field sweeps and stepping of goniometer angle. The definitions of the GUI and the arrangement of final data are not shown.

Tips & Techniques

Rapid-Scan EPR

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Magnetic-field modulation and lock-in detection at the modulation frequency has been the mainstay of CW EPR for decades. It is a very effective method of finding the signal amongst the noise. However, it is well-known that EPR line shapes are distorted by the frequency and amplitude of the magnetic field modulation. Guidance on how to acquire CW spectra with minimum distortion is given in "Quantitative EPR" [1]. It is possible to remove the distortion by proper post-acquisition mathematical treatment of the spectra [2], especially if an adequate number of harmonics are recorded [3]. Since most CW spectrometers are designed to acquire only one harmonic, spectral distortions are inherent. The amplitude of the magnetic field modulation can be calibrated by measuring the separation of the peaks of an over-modulated, lock-in-detected, CW spectrum. What happens if you modulate the magnetic field with amplitudes that are large relative to the EPR line width, but use direct detection of the EPR signal instead of using a lock-in amplifier tuned to the modulation frequency? This method is the experimental basis for the new type of EPR that we call rapid-scan EPR. Weger [4] and others have given special meaning to rapid, fast, etc., and our initial papers defined rapid-scan relative to T_2 [5, 6]. However, as the technique becomes more generally applied we propose to use rapid-scan to describe the detection method rather than a particular scan rate regime. For many spin systems, there will be a relaxation-rate dependent response that is achievable by selection of scan rate and microwave power. It is important that the post-processing described for rapid scans [6, 7] can be applied regardless of the rate of passage through resonance.

How, then, does one create rapid magnetic field scans that are large relative to the line width, and directly record the spectrum? The signal detection path for rapid-scan is more like that in a pulse or transient bridge than in a CW bridge. After appropriate low-noise amplification, the microwave signal is detected by a quadrature mixer and digitized. The deconvolution of the transient response yields the absorption and dispersion spectra rather than the traditional first-derivative spectra [6, 7]. The absorption signal is especially advantageous for EPR imaging [6]. The first derivative display facilitates visual observation of hyperfine splittings, but has no real advantage in information content. Once the spectrum is in digital form, many types of filters can be applied to emphasize one or another aspect of the information content of the spectrum.

There was a hint in the preceding discussion that rapid scan is related to pulsed EPR experimentally. It is also related conceptually in that the signal is on resonance for very short periods as the field (or frequency) is swept, similar to pulsed EPR where the microwave power is turned on and off while the field and frequency are kept constant. The FID after the rapid field scan through resonance does not have a constant oscillation frequency, because the field is changing, but otherwise there is considerable similarity between pulse and rapid scan. The fact that the signal is on resonance for a short time means that the turning angle is smaller for a given incident power than for CW and spins relax less during their excitation, hence higher incident powers can be used and larger signals can be obtained before saturating [5, 8, 9].

Rapid-scan EPR requires uniform magnetic field for the scanning field, just as for the main (Zeeman) field. Normal CW spectrometers often have magnetic-field modulation amplitude capabilities up to ca. 40 G, but such values are rarely used because of microphonic noise and heating of the resonator. The nature of phase-sensitive (lock-in) detection with modulation amplitudes that are small relative to line widths, as is used for CW EPR, does not require uniform modulation fields over the sample. If one performs rapid-scan EPR using the modulation coils in standard commercial resonator systems, the sample has to be rather small to have uniform magnetic field over the sample. Thus, a major part of the engineering of a rapid-scan spectrometer is driving a current through magnetic field scan coils that are large enough to create a field that is uniform over the sample. For example, we use ca. 75 mm diameter coils constructed with Litz wire to create uniform fields that can be driven at high scan rates by the sinusoidal drivers of the type described in [10]. The background problems inherent in EPR are mitigated by lock-in detection at the modulation frequency in CW (long ago, it was called base-line stabilization). The main limitation of rapid-scan EPR is that some of the background problems look like EPR signals – that is, they are magnetic-field-dependent. Major engineering effort is required to design and build resonators to minimize background signals. Mechanical vibrations caused by eddy currents are decreased by minimizing the amount of metal exposed to the scanning magnetic field. It has been found effective to use cross-loop resonators constructed with thin wire (Fig. 1), and to use dielectric resonators [11]. Even with improvements in hardware, the background signal is significant, especially for weak signals. Methods have been devel-

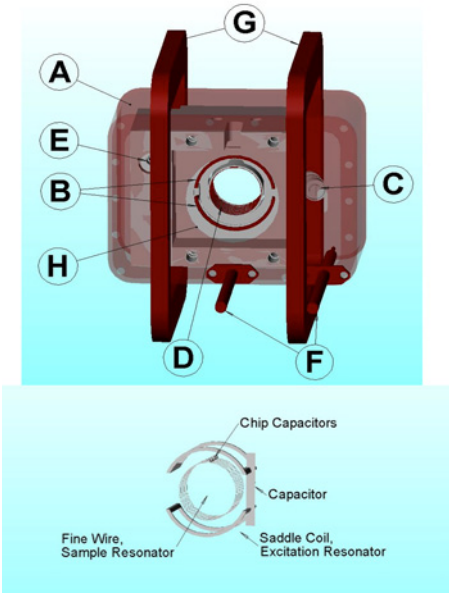

Fig. 1. Example of a cross-loop resonator for 250 MHz. Top – complete assembly with scan coils: A – Wire wound RF shield; B – 25 mm saddle coil excitation resonator; C – frequency adjustment for excitation resonator; D – 16 mm fine-wire sample resonator; E – isolation adjustment; F – input and output coaxial cables; G – 89 mm square Helmholtz scan coils; H – 30 mm sample access hole in RF shield. Bottom – sketch of the resonator coils, without the shield and support structure.

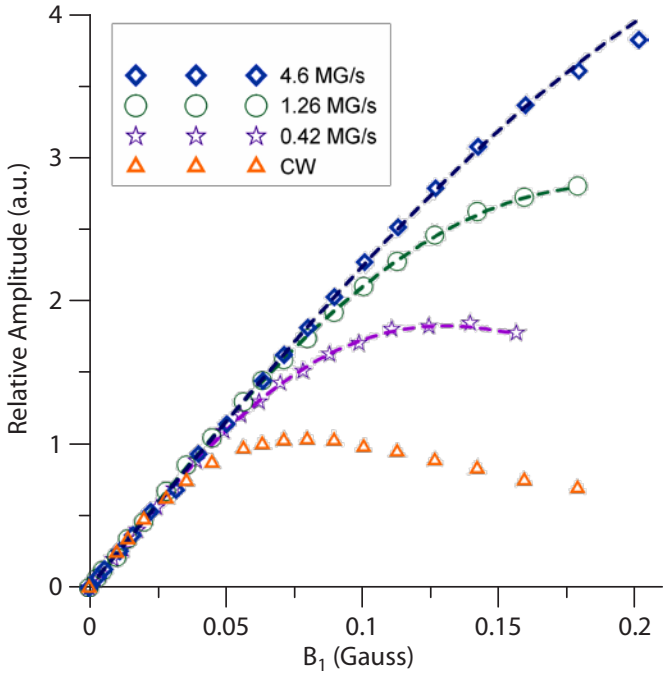

Fig. 2. Amplitude of CW and rapid scan spectra of the low-field nitrogen hyperfine line for 0.2 mM ^{15}N-PDT solution as a function of microwave B_1. The rapid scan frequency was ~30 kHz and the scan width was varied. The y-axis scale is the same for all of the rapid scans. The dashed lines represent the calculated power saturation curves, which were simulated by solving the Bloch equations. The amplitude of the CW spectra is scaled to match that obtained for the rapid scans at low B_1. As the scan rate is increased, higher B_1 can be used without power saturation or power broadening of the spectrum [8].

oped to remove the background signal and correct for non-orthogonality of the detection channels [12].

The applications of rapid-scan EPR that have been published so far demonstrate very large signal-to-noise (S/N) advantages for rapid-scan over CW EPR for a variety of organic radicals and defects in solids [9, 13]. The widest scans that we have achieved so far are 166 G, which is adequate for rigid-lattice spectra of organic radicals such as nitroxides and many defects in solids. For transition metal spectra, the Hyde lab has performed scans of wider spectra by piece-wise acquisition of ca. 5 G scans [14].

The reasons for improved S/N in rapid scan include (a) the entire signal is detected by rapid scan, whereas only a small fraction of the signal is detected in CW when the modulation is small relative to line width; (b) in the regime where larger B_1 can be used (Fig. 2), a larger signal can be created; (c) noise is reduced by averaging the signal thousands of times a second; (d) averaging of a periodic signal is equivalent to a comb filter in the frequency domain [15]. The width of the comb is inversely proportional to the number of scans averaged, which makes it a much narrower filter bandwidth than is used in CW experiments. Coherent averaging of the periodic rapid-scan signal offsets the signal in the frequency domain to the region of the noise spectrum where the noise spectrum is approximately frequency independent. This principle was demonstrated by Klein and Barton in 1963 [16].

A Workshop on rapid-scan EPR was held before the 2013 International EPR Symposium. The illustrations used in that Workshop are available at http://epr-center.du.edu/rapid-scan.html. A listing of our rapid scan papers also is available on that web site.

We are working with Bruker BioSpin to make rapid scan spectroscopy widely available.

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Guest of the issue

The Lindau Nobel Laureate Meetings

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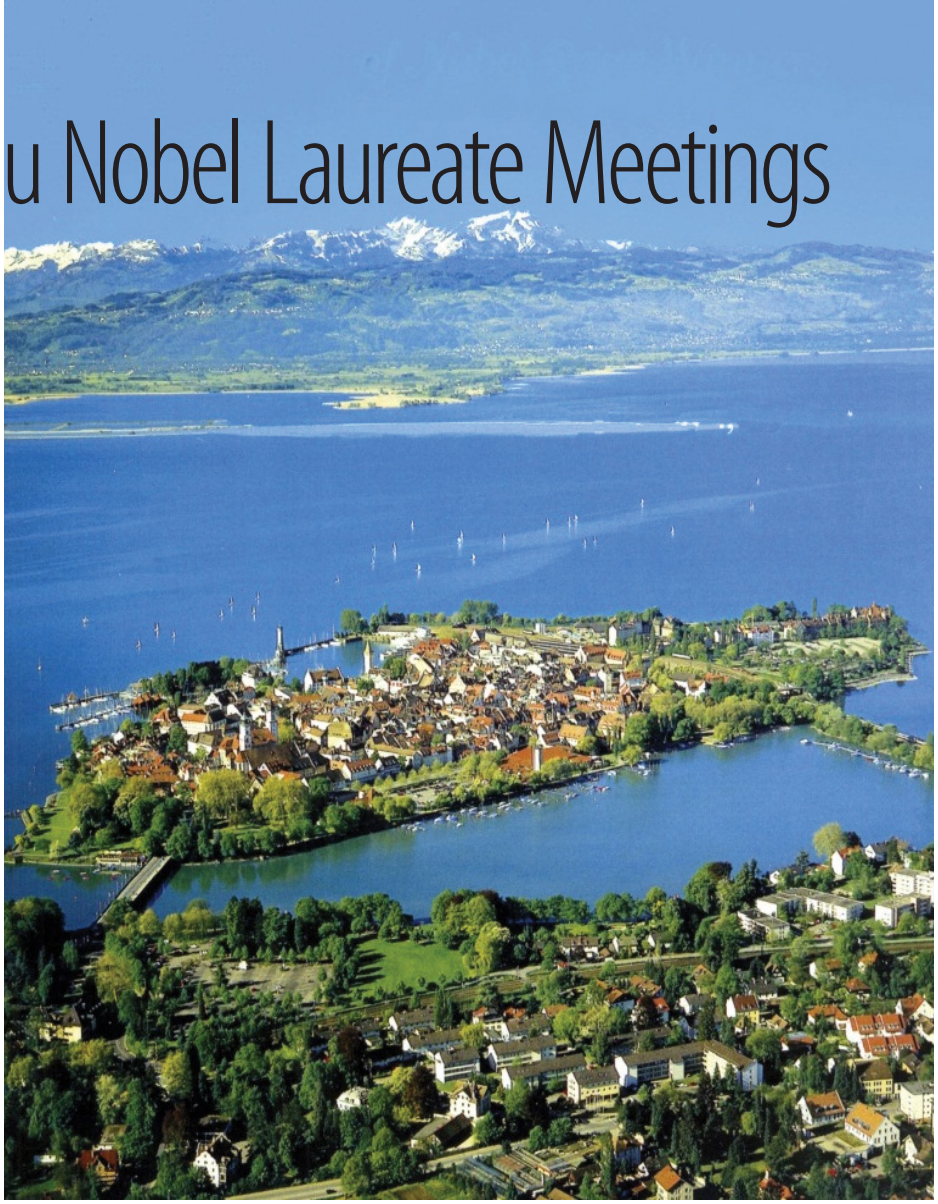


More than 60 years ago a remarkable conference series was initiated in Lindau, a small medieval town at Lake Constance in Germany. In 1949 two physicians, Franz Karl Hein and Gustav Parade, approached Count Lennart Bernadotte, the grandson of Gustav V, King of Sweden who lived on the Isle of Mainau, with the idea to invite Nobel Laureates to Lindau for an annual discussion meeting. The first meeting took place in June 1951 with seven laureates from five different countries and about 400 physicians attending – mostly from Germany and neighboring countries, at a time where Germany was still isolated politically and economically after World War II. This laid the cornerstone for a series of annual meetings that were soon extended to all three disciplines, Chemistry, Physics and Medicine & Physiology, for which the Nobel Prize is given in the sciences.

Count Lennart recognized early on that the meeting provides an ideal platform to *educate*, *inspire* and *connect* scientific generations, which has become the central motto of the Lindau meetings. In subsequent years an increasing number of students, first mainly from Germany and then also from other countries, was invited to participate in the meetings, which alternated between the three different scientific disciplines. The Council for the Lindau Nobel Laureate Meetings was founded in 1954 with Count Lennart Bernadotte (1909–2004) as its first president. After 33 years his wife Countess Sonja (1944–2008) took over the presidency. The council is now led by their eldest daughter Countess Bettina.

Countess Bettina Bernadotte, President of the Council, speaking at the 2013 Lindau Nobel Laureate Meeting on Chemistry

The council evolved over the years; it now includes Swedish and German scientist representing the disciplines chemistry, physics and medicine, a representative of the Nobel Laureates along with economists and experts from other foundations, the press and public relations.

The council organizes the annual meetings in Lindau. It is also given the responsibility of adapting and expanding the meetings to address the challenges of a constantly changing social and political world, specifically with regard to scientific education, research and development. In 2000 the "Foundation Lindau Nobel Prize Winners Meetings at Lake Constance" was established upon the initiative of 50 laureates, the council and the Bernadotte family. The Founders Assembly has now expanded to 264 Nobel Laureates. The Board of Directors is chaired by Wolfgang Schürer (St. Gallen).

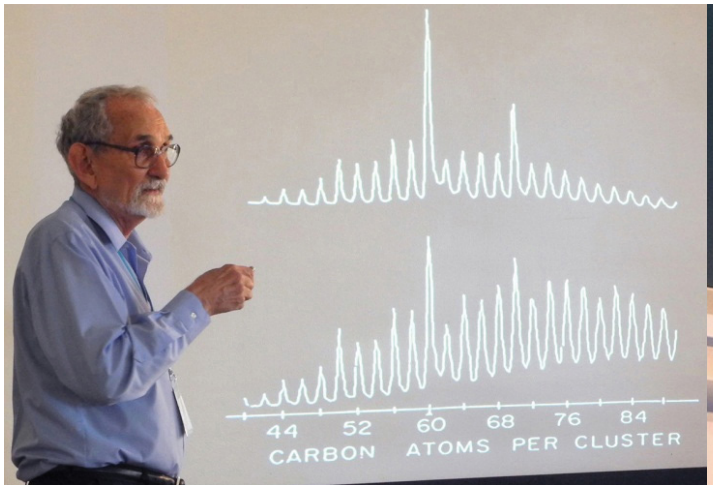
Ten years ago, in 2004 and 50 years after its establishment, I was elected as member of the Council responsible for chemistry together with Astrid Gräslund, Secretary of the Nobel Committee for Chemistry (Stockholm). During this last decade the format of the meetings has significantly changed, for example larger interdisciplinary meetings were included every five years, and a separate biannual meeting on Economic Sciences was established. The most important administrative challenge of the last years was the introduction of a new data base for applications of young researchers. This, together with a stringent selection process by the scientific council members, has resulted in an remarkable increase of the

Panel discussion on "Why Communicate" with laureates Ada Yonath (Israel), Brian Kobilka (USA) and Harold Kroto (UK)

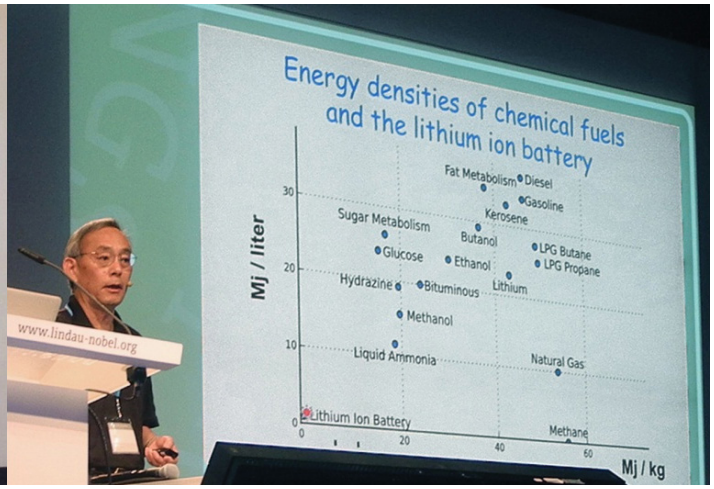
quality of the meetings, which now bring together the best young talents worldwide with the Nobel Laureates. This results in a fantastic scientific and personal atmosphere during the meetings, making the small island in Lake Constance for one week each year the *scientific center of the world*.

The Lindau Nobel Laureate Meetings have evolved over the course of its 63 year lifespan and witnessed remarkable events of historical importance; a brief overview of this development is listed below.

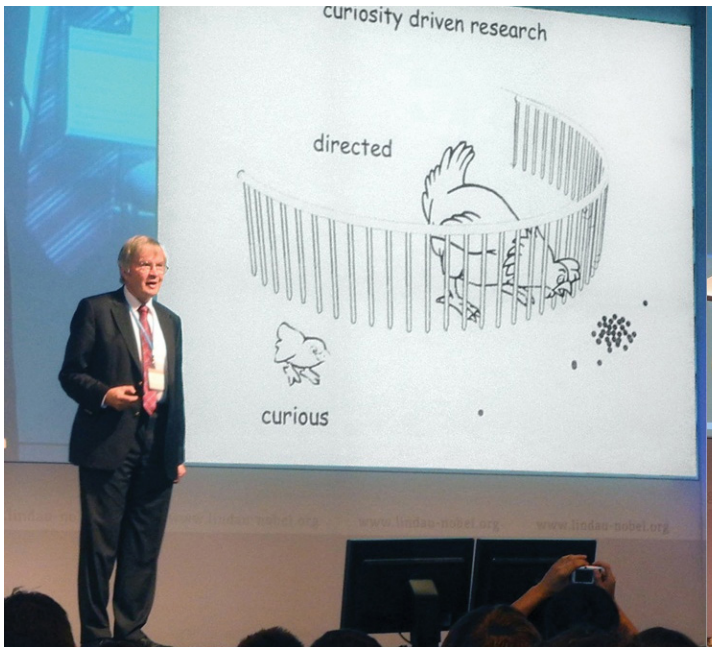
- In 1955 fifteen laureates signed the "Mainau Manifest against Nuclear Weapons", which was co-signed by another 34 laureates by the end of the year. Important discussions during the early meetings supported the foundation of the European Center for Nuclear Research CERN in Geneva.
- In 1961 Count Bernadotte introduced the topic of sustainability and environmental protection with his "Green Charta of Mainau".
- The student revolution in the late sixties led to a new culture of discussions between students and laureates that was already felt at the meeting in 1967.
- In his speech in Lindau in 1968 Cardinal König, Archbishop of Vienna, announced a revision of the trial against Galileo Galilei that finally led to his rehabilitation in 1992 by Pope John Paul II.
- After the establishment of the Prize in Economic Sciences in Memory of Alfred Nobel by the Swedish National Bank in 1969 the first laureate participated in the Lindau meeting in 1971 – but it took until 2004 before regular meetings on the Economic Sciences started in Lindau.
- The German Chancellor Willy Brandt participated in the Lindau meeting in 1972, a year after receiving the Peace Noble Prize, and gave a remarkable speech on "The environment as an international mission". This was the second visit of a peace laureate at the meetings after Albert Schweitzer in 1954.
- The physics laureate Dennis Gabor, founding member of the Club of Rome (1968), addressed the problem of the world's limited energy supplies in his Lindau speech in 1973, shortly before the first oil crisis.
- In 1993 Nobel 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 1995 Roman Herzog was the first President of the Federal Republic of Germany to attend the Lindau meetings; he later became Honorary President of the "Foundation Lindau Nobel Prize Winners Meetings at Lake Constance" established in 2000.
- Commemorating the 100th birthday of Count Lennart Bernadotte the Council and Foundation decided to organize exhibitions on the Isle of Mainau, which represented over a period of three years urgent topics ranging from "water" (2009) over "energy" (2010) to "health" (2011). Panel discussions related to these themes were held for the first time in 2009 and regularly each year on the island with the laureates and young researchers.



Robert Curl Jr. (USA) on carbon chemistry



Steven Chu (USA) on energy and climate change



Theodor Hänsch (Germany) on lasers, frequencies and curiosity driven research

Richard Ernst (Switzerland) on rat races, competitive science, human values and other passions

– During the physics meeting in 2012 the discussion on the discovery of the Higgs boson at CERN was transmitted live to Lindau on July 4th, giving the laureates the chance to participate in the discussion.

The last event in June 2013 marked the 20th Meeting of the Nobel Laureates devoted to Chemistry. It brought together 625 young researchers from 78 countries with 34 Nobel Laureates – mostly from Chemistry but also from other disciplines. These impressive numbers show a growing interest both on the side of the young researchers and the laureates to attend this meeting. The scientific program, which comprised lectures by the laureates, two panel discussions on "Chemical Energy Conversion and Storage" and on "Why Communicate?", scientific master classes as well as discussion sessions, in which the laureates and young researchers met in a relaxed personal atmosphere for extensive discussions [1].

During the meeting many social events took place, for example "Scientific Breakfasts" organized by representatives of Mars and BASF and other organizations, a "Get-Together Party", "Academic Dinners" at various locations in Lindau sponsored by academic partners, and a "Bavarian Evening" in the Inselhalle. On the last day of the meeting a boat trip and visit of the Isle of Mainau has been organized and sponsored by the State of Baden-Wurttemberg. All these events gave ample opportunity to get further scientific and personal information, to meet and connect.

The lectures given by the Laureates demonstrated the enormous breadth of scientific research spanning the medical and biochemical and chemical sciences. They included topics such as drug design, protein interactions, synthesis and chemical reactions, catalysis, adaptive chemistry, smart materials and new (bio)physical techniques.

Laureates also presented selected topics from physics such as the impending energy problem, super conductivity, the application of lasers and quantum effects. Furthermore lectures on Science & Society were also presented. "Green Chemistry" has been a focal

Richard Ernst and Kurt Wüthrich (both Switzerland) with the meeting chairs Astrid Gräslund (Sweden) and Wolfgang Lubitz (Germany)

Gerhard Ertl (Germany) with young researchers from the Max Planck Society

point on the meeting's agenda as well as the generation, conversion and storage of energy.

For the young researchers it was not only interesting to learn about the research achievements of the laureates but also about the practical applications and the impact of their scientific work on society. Further points of discussion included: how to find a mentor and choose the right topic to work on, how to plan and conduct the right experiments, write papers, communicate results, and handle public relation issues. In particular for young women the combination of a scientific career with family planning was addressed. The discussion and personal contact in the afternoons has been much appreciated by both the laureates and the young researchers and is considered a unique feature and probably the most important part of the Lindau meetings.

The three science master classes were chaired by different laureates, in which young researchers presented their work followed by a discussion. This feature was introduced to the Lindau meeting only a few years ago but has rapidly become an important part [2] since it allows young researchers to present their results and get feedback from the laureates and other participants of the meeting.

In the context of this article, written for the *EPR Newsletter*, the class conducted by Kurt Wüthrich and seconded by Richard Ernst on "Magnetic Resonance in Chemistry, Structural Biology and Medical Diagnosis" was of special interest. More than 100 participants, among them several laureates, attended and discussed the lectures given by a number of young researchers from different countries.

It is interesting to note that the Nobel Prize has been given several times for the development and application of magnetic resonance (see *EPR Newsletter* 14/1-2, 2004). The laureates were Otto Stern (physics, 1943), Isidor Rabi (physics, 1944), Felix Bloch and Edward M. Purcell (physics, 1952), Richard Ernst (chemistry, 1991), Kurt Wüthrich (chemistry, 2002) and Paul C. Lauterbur and Peter Mansfield (physiology or medicine, 2003). This list beautifully illustrates the evolution of magnetic resonance from its early beginning in the field of physics, and its subsequent methodological development towards applications, in particular in (bio)chemistry and medicine. All prizes thus far have been awarded for nuclear magnetic resonance (NMR); a Prize has not yet been bestowed on any of the pioneers of the sister method electron paramagnetic resonance (EPR). This certainly mirrors the broader scope and the enormous number of applications and related publications of NMR that is not matched by EPR. Nevertheless, the EPR method has very important applications in many fields of physics, chemistry, biology and even medicine, where paramagnetic species are present or can be introduced as spin probes. The range of modern EPR developments and applications are nicely demonstrated in a recently published special issue of *Molecular Physics* [3]. It is gratifying to see that in recent years "the two cultures" [4] of NMR and EPR are converging with the parallel development of modern pulse techniques, the transition to higher fields and frequencies and, last but not least, by the possibility to greatly increase the NMR sensitivity via dynamic nuclear polarization (DNP) [5].

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All photos by Gisela and Wolfgang Lubitz (Mülheim/Ruhr, Germany)

4th International DNP Symposium
Elsinore, Denmark, August 28–31, 2013

The 4th International Symposium on Dynamic Nuclear Polarization was held August 2013, in Elsinore, Denmark, following the highly successful meetings in Nottingham (2007), Koenigstein (2009) and Lausanne (2011). Current issues and new trends in DNP were presented, including the developments in Overhauser effect, solid state and dissolution DNP; as well as instrumentation, radical chemistry, and hyperpolarized imaging. The full program and abstracts can be found on the symposium webpage: www.DNPsymposium.org.

We had a total of 192 participants at the meeting and 124 abstracts were received. The scientific review board consisted of past organizers and key figures in the field and a blinded review process was used to build the most balanced program and to maintain a high scientific level. 64 of the abstracts were presented in oral sessions and the remainder in the poster session. Short talks were favored to allow the maximum amount of research to be presented in the most coherent manner. The venue for this meeting was chosen as a compromise between travel convenience and providing an environment that would stimulate discussion during breaks and over meals in a relaxing atmosphere. Meals and catering in general were a particular highlight, and the food seemed to be enjoyed by most people. Elsinore is just north of Copenhagen with a one hour direct train connection from the airport. The Friday evening cultural event was a visit to Kronborg Castle, the castle of Hamlet.

The oral sessions consisted of multiple sessions on In Vivo DNP and DNP-NMR as well as sessions covering Theory, Instrumentation, Overhauser DNP and EPR. Each session commenced with a plenary talk presented by the session chair, which typically detailed several significant accomplishments and provided necessary background information for the session.

In DNP-NMR, plenary talks were given by Prof. Geoffrey Bodenhausen who detailed DNP in spinning samples, Prof. Bob Griffin who described developments in high frequency DNP, Prof. Lyndon Emsley who presented updates on the use of DNP for surface enhanced NMR, and Dr. Rob Tycko who described Biomolecular DNP-NMR at temperatures less than 30 K. There were also talks presented on key areas of interest such as cross polarization, new polarizing agents, the role of glassing agents, new measurement schemes, and the polarization of more exotic agents such as nanodiamonds and silicon nanoparticles. Numerous advances in DNP instrumentation were detailed as gyrotrons and DNP-NMR probes are now available for 400, 600 and 800 MHz systems. Advances in the field of DNP-NMR have enabled a variety of applications from protein structure to porous materials.

In the other major area of interest, In vivo DNP enhanced techniques, there were also a number of plenary talks. Prof. Klaes Golman provided an overview and the history of hyperpolarization using DNP, Prof. Kevin Brindle described advances in the assessment of tumor microenvironment and response to treatment using hyperpolarized ^{13}C substrates, Prof. Dan Vigneron described the recently published results of a successful clinical study on prostate cancer patients, Prof. Rahim Rizi offered an overview of the use of hyperpolarized ^{13}C for monitoring of pulmonary disorders and Dr. Mathilde Lerche described advances in the use of DNP-NMR for studying in-cell biochemistry. Additional talks were presented on metabolism and how it is altered by injury and disease, new hyperpolarized agents and formulations, as well as new types of experiments to best harness the hyperpolarized signal. Especially notable were several talks on long-lived singlet states. This most exciting idea was introduced by the Levitt group in

2004 and opens up the possibility of extending the application of hyperpolarization to much longer time scales. Prof. Warren Warren presented encouraging results on new symmetric molecular structures with impressive singlet-state life times and new pulse sequences to read in and out of these states.

The session on the theory of DNP was chaired by Prof Shimon Vega who described the theory behind solid state DNP. Additional talks were given on the theory of DNP mechanisms. Two talks described the use of photo-excited triplet states at 100 K and room temperature. Much progress is seen on trying to bridge the gap between experiment and theory and develop quantum mechanical descriptions of DNP in the solid state. This is a computationally demanding problem and algorithms to accelerate the simulations by making appropriate assumptions were presented. Some of these developments are implemented in Spinach and a sunrise lecture was given by Prof. Ilya Kuprov demonstrating the capability of Spinach to simulate DNP. The classical spin temperature based models are also being refined to obtain better agreement with experimental observations.

In the Overhauser DNP and EPR session, the plenary talk was delivered by Dr. Vasyl Denysenkov who described liquid state DNP of water at 9.2 T. Talks were also presented on the use of MD simulations, the use of protein surface hydration water dynamics for membrane protein structure studies, progress on DNP in a microfluidic context, and updates on sample shuttling Overhauser DNP.

The crucial role of instrumentation in DNP was discussed by Prof. Arnaud Comment in his plenary talk in the instrumentation session. Additional talks discussed advances in array coils for imaging experiments, a rapid melt DNP-NMR probe for temperature jump experiments, and development of microwave transparent RF coils.

Together these sessions as well as the poster session provided excellent insight into the state of the art in DNP and allowed for excellent scientific discussions which cannot always occur at larger meetings. The 5th International DNP Symposium will be organized in 2015 by the Dutch groups in Nijmegen and Utrecht.

The symposium was supported by EU COST action TD1103 European Network for Hyperpolarization Physics and Methodology in NMR and MRI. This network embraces 24 European countries.

Jan Henrik Ardenkjær-Larsen

The 52th Annual Meeting of the Society of Electron Spin Science and Technology of Japan (SEST2013)

Saitama, Japan, October 24–26, 2013

The 52th Annual Meeting of the Society of Electro Spin Science and Technology (SEST2013) was held at Omiya Sonic City Building in Saitama city, Japan, during October 24 to 26 in 2013. The meeting covered all aspects of the research fields in the electron spin science and technology including its advanced detection and theory and areas such as material sciences, chemical reactions, life sciences and environmental concerns. It was organized by the Society of Electron Spin Science and Technology of Japan (SEST), and was cosponsored by the Chemical Society of Japan, the Physical Society of Japan, the Japanese Society of Analytical Chemistry, the Pharmaceutical Society of Japan, and Society for Free Radical Research Japan. It attracted 194 participants (including 65 students). Two plenary lectures, three award lectures, nine invited talks, 55 oral talks and 50 posters were presented in the meeting. The presenters of the plenary lectures were Profs. H. Utsumi and S. Fukuzumi, both the recipient of the Medal of Honor with Purple Ribbon in 2012. Two memorial mini symposiums were dedicated to the late Prof. S. Yamauchi and Prof. H. Yokoyama, both passed away in 2012.

Following the opening talk by the chairperson, seven talks were given by nominees for the Award for Excellent Work and Presentation by Young Investigator. In the evening of the first day, two parallel oral sessions were held.

The second day started with the first memorial mini symposium for Prof. Hidekatsu Yokoyama on "The development of in vivo ESR technique and its applications to medical fields" organized by Prof. A. Hirayama (Tsukuba Tech. Univ.) and Prof. M. Lee (Kanagawa Dental Univ.). There were four excellent presentations including "In vivo ESR studies carried out by Professor Hidekatsu Yokoyama" by Profs. T. Ogata (Yamagata Univ.) and M. Tada (Tohoku Inst. Tech.), "In vivo imaging of mouse models of brain disease using three-dimensional EPR imaging system" by Prof. H. Fujii (Sapporo Med. Univ.), "In vivo extracellular pH monitoring using EPR spectroscopy" by Prof. H. Hirata, and "Redox imaging of biological function in small animals" by K. Ichikawa (Kyushu Univ.). In the afternoon, the first plenary lecture entitled "Redox molecular imaging" was given by Prof. H. Utsumi (Kyushu Univ.). After the plenary lecture, the general meeting of SEST was held. Following researchers were elected as the SEST Council Members for 2014–2015 during the meeting.

President: *Keizo Takeshita* (Sojo Univ.)
Vice-President: *Toshikazu Nakamura* (Inst. Mol. Sci.)
Secretary: *Yasuhiro Kobori* (Kobe Univ.)
Treasurer: *Kazunobu Sato* (Osaka City Univ.)
Publication and academic activities: *Hiroshi Hirata* (Hokkaido Univ.)

Chief editor: *Ken-ichi Yamada* (Kyushu Univ.)
Support for young scientists: *Hitoshi Ohta* (Kobe Univ.)
Other members: *Motoko Asano* (Tokyo Metropolitan Univ.), *Kazunori Anzai* (Nihon Pharmaceutical Univ.), *Yasunori Ohba* (Tohoku Univ.), *Masahiro Kohno* (Tokyo Inst. Tech.), *Hiroyuki Mino* (Nagoya Univ.), *Masaichi Lee* (Kanagawa Dent. Univ.)
Auditors: *Toshihiko Ozawa* (Yokohama College of Pharmacy), *Jun Yamauchi* (Kyoto Univ.)

Then, Young Investigator Awards were given to Drs. Y. Uchida (Osaka Univ.), T. Miura (Niigata Univ.), and K. Yasukawa (Kyushu Univ.). There was no prize winner of SEST Award in this year. Followed by the three award lectures, the poster session took place. After the poster presentation, a banquet was held with about 120 participants.

The final day started with the second memorial mini symposium for Prof. Seigo Yamauchi on "Development of EPR spectroscopy for short-lived paramagnetic species" organized by Profs. A. Kawai (Tokyo Inst. Tech.) and M. Kobori (Kobe Univ.). There were five excellent presentations including "Pulsed EPR for time-resolved measurements of transient paramagnetic species" by Y. Ohba (Tohoku Univ.), "Toward triplet harvest from magnetic spectroscopy of triplet molecules" by T. Ikoma (Niigata Univ.), "Time-resolved EPR studies on radical ion pairs and excited triplet state" by T. Yago (Saitama Univ.), "The excited multiplet states – Observations and applications" by K. Ishii (Tokyo Univ.), "Prolonged lifetime of short-lived paramagnetic species due to reservior mechanism" by M. S. Asano, and "Development of a time-resolved ESR method and detection of the excited triplet spin state" by H. Murai. After the symposium, the second plenary lecture entitled "Current status and perspective of artificial photosynthesis" was presented by Prof. S. Fukuzumi (Osaka Univ.). In the afternoon, two parallel sessions were held until the end of the meeting.

It was announced that the next SEST2014 Annual Meeting will be held in Nara organized by Prof. A. Kajiwara (Nara University of Education) during November 12–16, 2014 jointed with APES and IES meeting.

Kazunori Anzai
Chair of SEST2013

notices of Meetings

Joint Conference of APES (9th), IES (1st) and SEST (53rd) (APES-IES-SEST2014)

Nara, Japan, November 12–16, 2014
http://apes-ies-sest.org

Joint Conference of Asia-Pacific EPR/ESR Symposium (APES 9th), International EPR(ESR) Symposium (IES 1st) and the annual meeting of Society of Electron Spin Science and Technology (SEST 53rd) (APES-IES-SEST2014) will be held at the Todaiji Cultural Center, Nara, Japan during November 12–16, 2014. We would like to remind you that each member of the society will get large reductions of the registration fee this time. Nara is the oldest capital in Japan, and the conference site is situated in the heart of Nara Park, which is the main tourist's attraction in Nara. The transportation is also very convenient because there is a direct limousine bus from Kansai airport to Nara. The conference will cover the wide range of EPR/ESR applications in physics, chemistry, biology and medicine. Following the tradition of APES and SEST, many distinguished scientists from overseas will give tutorial and plenary lectures, and invited talks at the conference. Participants from all over the world are welcome. We also encourage young scientists to apply for the APES Young Scientist Awarad.

For further information, please see the web site or contact: Hitoshi Ohta (APES & IES Chairperson), Atsushi Kajiwara (SEST Chairperson), Susumu Okubo (Secretary General), Organizing Committee, e-mail: apes@kobe-u.ac.jp

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

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

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

The scope of the conference

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

Chairman: Albert Aganov,
Scientific Secretary: Alex Dooglav
e-mail: Alexander.Dooglav@kpfu.ru

First Adriatic Symposium on Biophysical Approaches in Biomedical Studies

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

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

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

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

POSITIONS

Postdoctoral Associateships in Magnetics at NIST

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

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

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

Ohio State University – EPR Center Molecular Imaging Program

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

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

Ohio State University – EPR Center

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

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

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

Post-doctoral position in structural studies of kinesins

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

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

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

EPR Specialist Position at Johns Hopkins

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

Research Positions – Advanced EPR of Biochemical and Chemical Systems

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

In-house projects:

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

Collaborative projects:

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

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

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

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

Bruker BioSpin Corp

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

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

EQUIPMENT

EPR parts, electronics and hardware

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

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

For sale

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

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

For sale

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

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

Design and construction of EPR electronics

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

For sale: Varian and ESR equipment

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

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

Available: Used Varian EPR equipment

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

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

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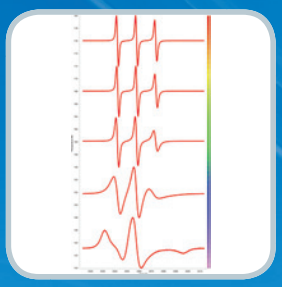
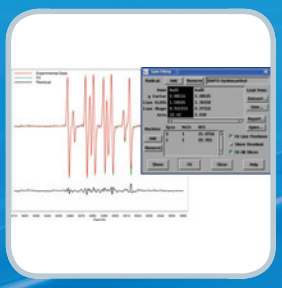


Nitrogen VT system for 100–600K

PremiumX optional microwave units for weak-pitch S/N of 2000:1



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- Extensive range of accessories
- Weak-pitch signal-to-noise of 1200:1

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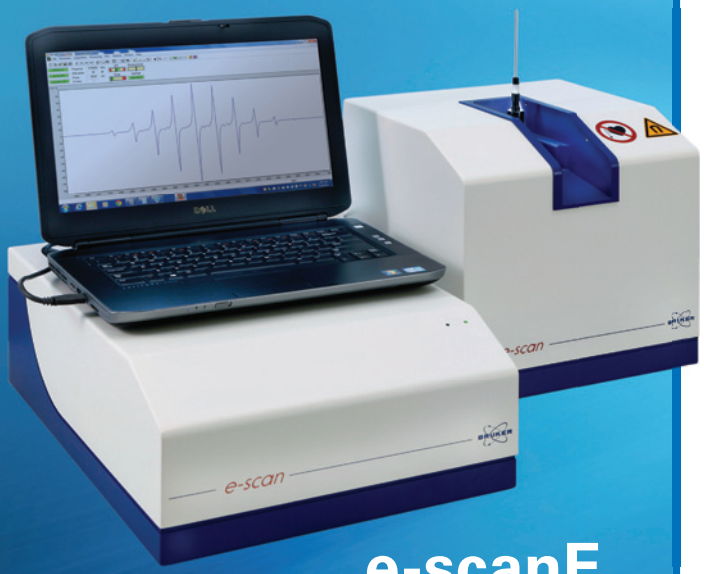
www.bruker.com/epr

EPR Educational Package



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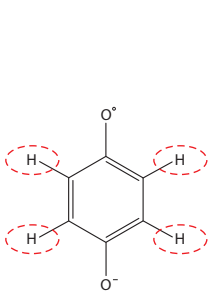
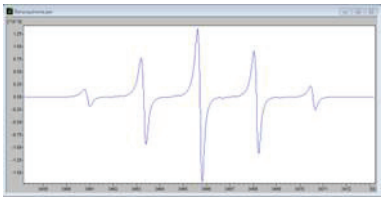
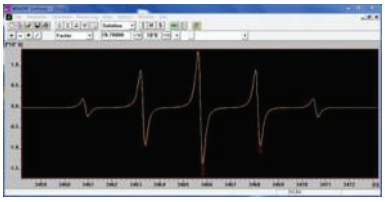
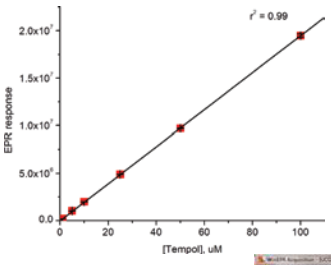


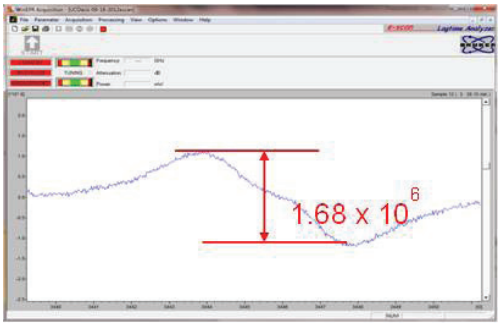


Experiment



Simulation





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